



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:24 PM BST

PDB ID : 4V78  
EMDB ID: : EMD-2475  
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post3a)  
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 : 20.00 Å(reported)  
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

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

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

A user guide is available at

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

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

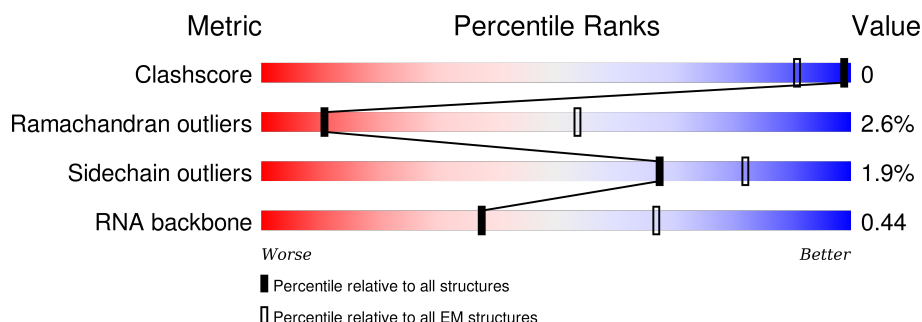
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 20.00 Å.

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















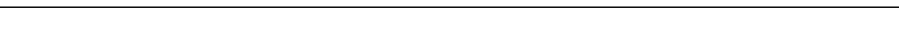

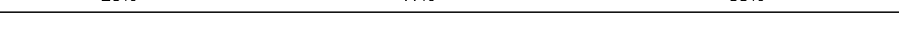

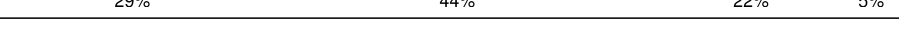





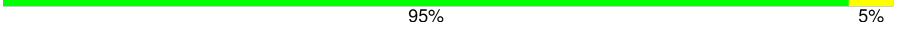
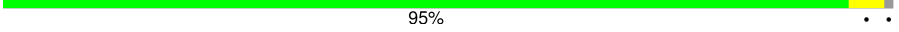

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	AB	220	94% 5% .
2	AC	208	87% 13%
3	AD	206	86% 12% .
4	AE	152	94% 6%
5	AF	101	87% 13%
6	AG	152	88% 11% .
7	AH	130	92% 8% .
8	AI	128	84% 16%

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Mol	Chain	Length	Quality of chain
9	AJ	100	 86% 13% .
10	AK	118	 92% 7% .
11	AL	124	 85% 15% .
12	AM	115	 90% 10% .
13	AN	101	 87% 10% ..
14	AO	89	 88% 11% .
15	AP	81	 78% 22%
16	AQ	82	 90% 9% .
17	AR	57	 84% 16%
18	AS	81	 90% 9% .
19	AT	86	 86% 13% .
20	AU	53	 75% 25%
21	AA	1533	 23% 50% 22% .
22	A1	76	 26% 41% 33%
23	A2	15	 60% 27% 13%
24	A3	77	 29% 44% 22% 5%
25	BC	273	 89% 9% .
26	BD	209	 90% 9%
27	BE	201	 89% 10%
28	BF	179	 89% 10% ..
29	BG	177	 89% 10% .
30	BH	149	 95% 5%
31	BI	142	 95% . .
32	BJ	142	 90% 10%
33	BK	123	 89% 11%

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Mol	Chain	Length	Quality of chain
34	BL	144	86% 13% ..
35	BM	136	90% 9% .
36	BN	121	88% 11% .
37	BO	117	87% 11% ..
38	BP	115	84% 15% .
39	BQ	118	85% 14% ..
40	BR	103	92% 8%
41	BS	110	92% 7% .
42	BT	94	91% 7% .
43	BU	104	88% 12% .
44	BV	94	95% 5%
45	BW	80	89% 10% .
46	BX	79	86% 11% .
47	BY	63	92% 8%
48	BZ	59	85% 12% ..
49	B0	57	77% 21% .
50	B1	52	87% 13%
51	B2	46	78% 22%
52	B3	65	85% 14% .
53	B4	38	87% 13%
54	BA	2903	22% 52% 22% .
55	BB	118	17% 59% 19% ..
56	B5	234	88% 7% 5%

## 2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

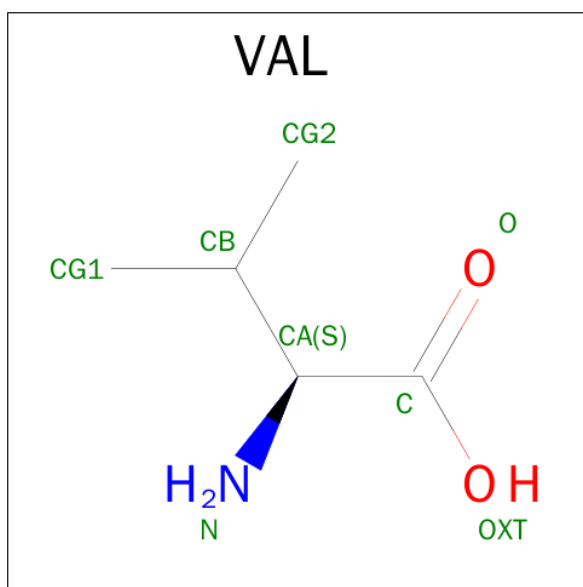
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

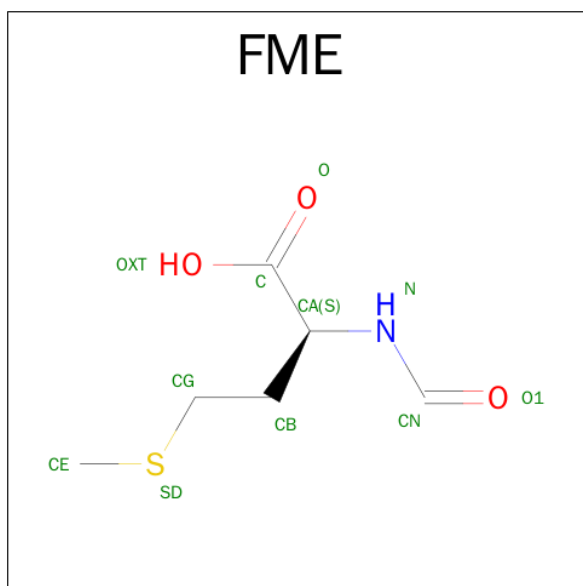
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



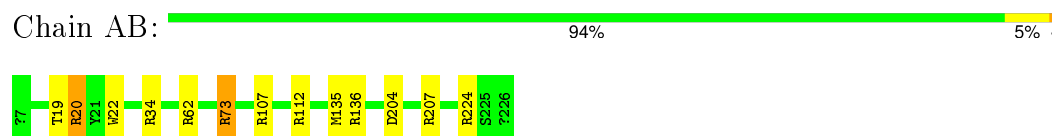
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



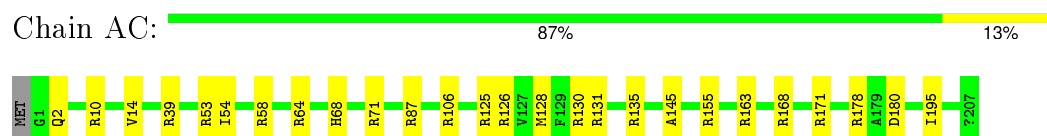
### 3 Residue-property plots

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

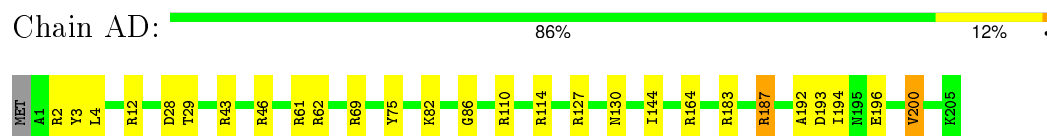
- Molecule 1: 30S ribosomal protein S2



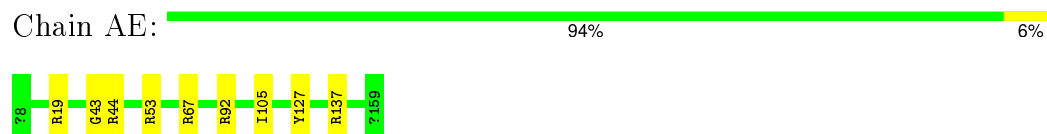
- Molecule 2: 30S ribosomal protein S3



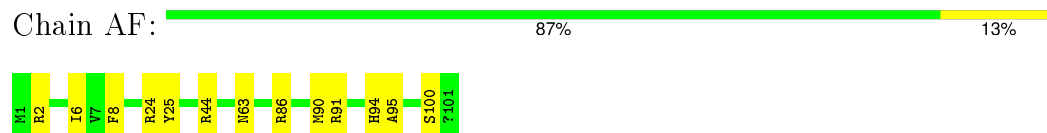
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 84% 16%



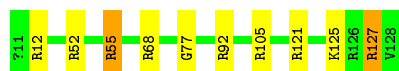
- Molecule 9: 30S ribosomal protein S10

Chain AJ: 86% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 92% 7%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 85% 15%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 90% 10%

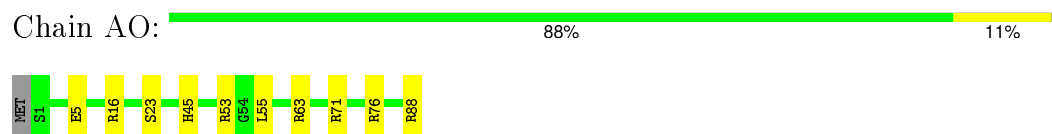


- Molecule 13: 30S ribosomal protein S14

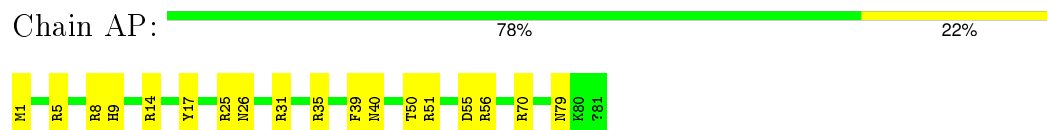
Chain AN: 87% 10%



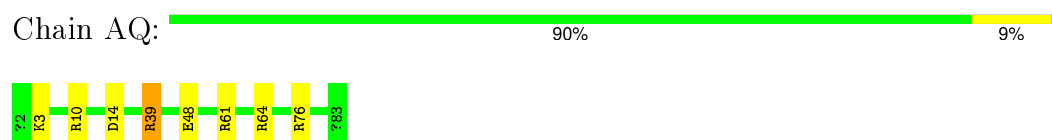
- Molecule 14: 30S ribosomal protein S15



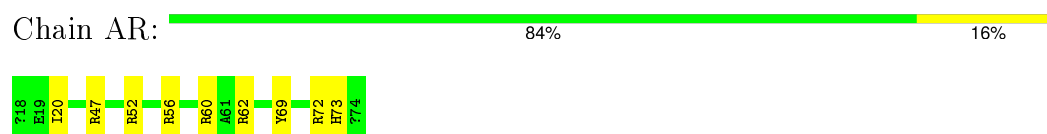
- Molecule 15: 30S ribosomal protein S16



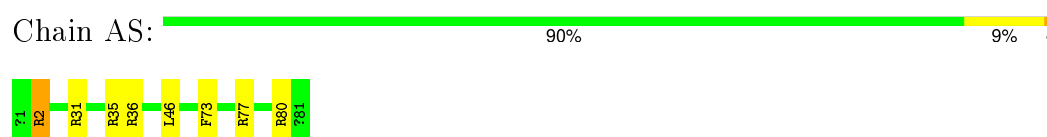
- Molecule 16: 30S ribosomal protein S17



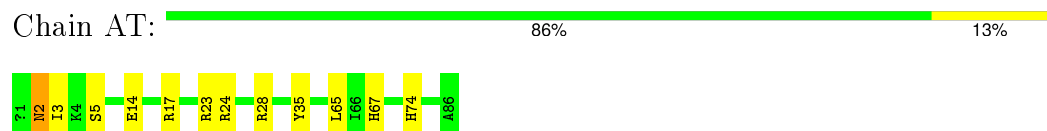
- Molecule 17: 30S ribosomal protein S18



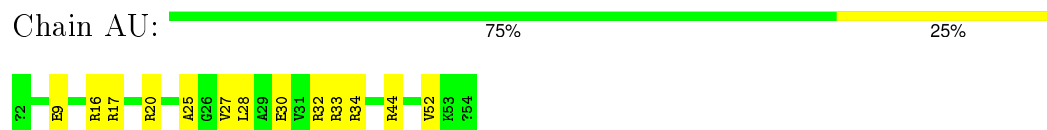
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



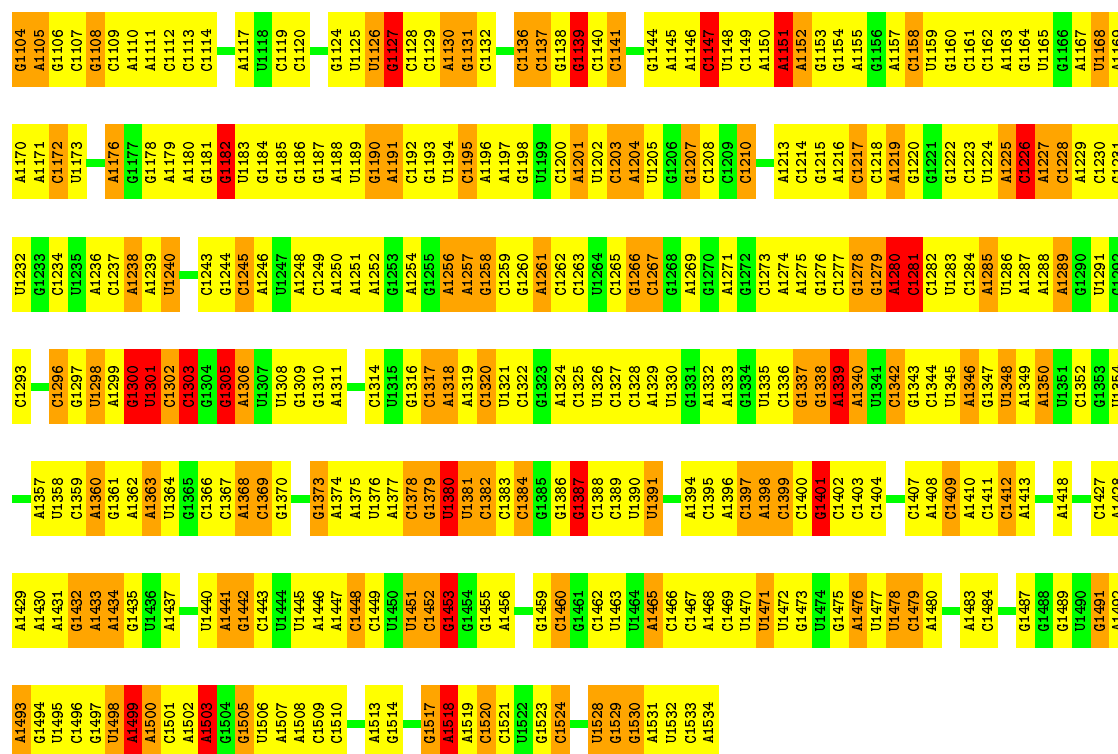
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA



A	A	U	U5	G6	A7	G9	A10	G11	U12	U13	U14	A16	A17	G18	A19	U20	U21	G22	C23	U24	C25	A26	G27	A28	U29	U30	G31	A32	G33	G34	G35	C36	U37	G38	C40	G41	C43	A44		C47	C48	U49	A50	A51	C52	A53	C54	G55		C58	A59	A60	G61	U62	C63						
G64	A65	A66	C67	G68	G69	U70	A71	C72	A74		A77	G78	A80	U81	A81	G82	C83	U84	U85	G86	C87	U88	U89	C90	U91	U92	U93	G94	C95	U96	G97	A98	C99	G100	A101	G102	C106	G107	G108	A109		C110	G111	G112		G115	A116	C119	A120	U121		C124	U125	G128	A129	U130	A132				
A131	C132		G135	C136	U137	G138	A139	U140	G141	G142	A143	G148	A149	C143	U150	A151	C152	C153	U154	A155	C156	U157	U158	G159	A160	A161	U162	C163		U166	G167	G168	C169	G100	A171	U172	A173	C175	G176	G178	A179	U180	G181	A182	C183	U185	A189	U190	G191	G192	U193	A195									
A195	G259	C222	U223	G224	A263	G265	C266	C267	U268	A205	C206	U207	U208	C210	G211	G212	C214	C215	U216	C217		C221	C222	U224	C225	G226	C227	A228	C229	U230	G231	U232	C233	C234	C235	A236	G240	C241	G242	A243	U244	U245	A181	A182	G246	C248	U249	A250	U252	C253	G255	C256	A259								
A389	C399	C322	U323	G324	A325	G326	A327	C328	C329	C330		U333	C334	C335	A336	G337	A338	C339	U340	C341	C342	U343	A344	C345	G346	G347	C348	C349	G350	C351	C352	C353	U354	G355	C356	U357	U358		G362	A363	A364	U365	A366	U367	U368	G369	C370	C371	C372	A373	C374	C379	G380	C381	A382	C383	U384	G385	C386	A448	G449
G450	A451	A452	A453	G454	G455	A456	A459	A460	A461	A462	U463	U464	A465	A466	U467	A468	C469	C470	U471	U472	U473	G474	C475	U476	C477	A478	U479	A482	C483	A484	U485	U486	A487	C488	C489	C490	A491	C492	A493	A494	A495	A496	A497	A498	A499	G500	C501	A502	A503	C504	G505	G506	C507	U508	A509	A510	C511				
U512	C513	C514	G515	U516	G517	C518	C519	A520	G521	A522	A523	C524	C525	C526	C527	C528	G529	C530	U531	A532	A533	U534	C535	C536	G537	C538	A539	G542	U543	C544	C545	A546	A547	G548	C549	A553	A554	U555	C556	G557	A558	A559	A560	U561	U562	A563	C564	U565	G566	C567	C568	G569	C570	U571	A572	A573	A574				
G575	A640	U641	A642	C643	G646	C647	A648	A649	C651	A655	G656	U657	C658	U659	C660	G661	U662	A663	A664	A665	U666	C667	G668	G669	G670	A673	G674	A675	A676	A677	U678	C679	C680	A681	A687	A688	C689	U692	G693	A694	A695	A696	A697	U698	C699	U700	U701	C702	G703	A704	G705	A706	U707	C708							
U709	G710	G711	A712	G713	C714	A715	A716	U717	A718	C719	G720	G721	G722	U723	G724	C725	G726	G727	A728	U729	C730	G731	G732	C733	C734	C735	C736	C737	C738	C739	U740	G741	G742	A743	C744	G745	A746	A747	C748	A749	C750	U751	G752	A753	C754	G755	C756			A759	G760	C761	C764	A765	U766	A767	U768	G769	C770		
G776	A777	G778	A779	C780	A781	A782	C783	A784	C785	G786	A787	A790	G791	C792	A793	G794	C795	C796	C797	G800	U801	A802	C805	C806	C807	C808	C809	C810	C811	G812	U813	A814	A815	A816	A681	A687	A688	C689	U692	G693	A694	A695	A696	A697	U698	C699	U700	U701	C702	G703	A704	G705	A706	U707	C708						
G844	A845	A846	G847	C848	C849	U850	G851	G852	C853	C856	C857	G858	G859	A860	G861	C862	U863	A864	A865	C866	U867	C868	G869	U870	U871	A872	A873	U874	C875	C876	A877	A878	C879	C880	C881	C882	C883	U884	C885	C886	A888	G889	U891	A892	C893	C896	C897	C898	C899	A900	A901	G902	G903	A906	A907						
A908	A909	C910	U911	C912	A913	A914	A915	A918	A919	A920	U921	G922	A923	C924	G925	G926	G927	G928	G929	C930	C931	C932	C933	C934	A935	A936	A937	A938	G939	C940	G941	G942	G945	A946	G947	C948	A949	U950	G951	G954	A958	A959	U960	U961	C962	G963	A964	U965	U966	A967	A968	A969	C970	C971	C972						
G973	A974	A975	A976	A977	A978	C979	C980	U981	U982	A983	C984	C985	G988	U989	C990	G991	U992	G993	U994	C995	U996	C997	C998	C999	A1000	C1001	A1004	C1006	A1007	G1008	U1009	C1010	G1011	A1012	U1013	A1014	G1015	A1016		A1019	U1020	A1021	U1022	U1023	G1024	U1025	G1026	C1027	U1028	C1029	U1030	C1031	G1032	A1035	A1102	C1103					
C1037	C1038	G1039	U1040	C1041	A1042	G1043	A1044	C1045	A1046	G1047	U1048	U1049	C1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	G1058	C1059	U1060	G1061	U1062	C1063	G1064	U1065	C1066	A1067	G1068	C1069	U1070	C1071	G1072		G1077	U1078	A1079	A1080	A1081	A1082	U1083	G1084	U1085	U1086		A1092	A1093	G1094	U1095	C1096	C1097	C1098	G1099	C1100	A1101	C1102	A1103	A1104	





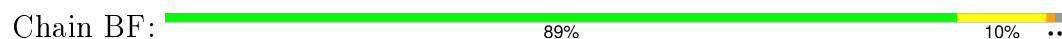
- Molecule 26: 50S ribosomal protein L3



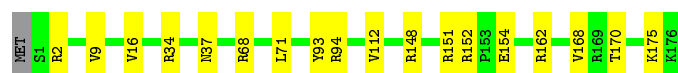
- Molecule 27: 50S ribosomal protein L4



- Molecule 28: 50S ribosomal protein L5



- Molecule 29: 50S ribosomal protein L6



- Molecule 30: 50S ribosomal protein L9



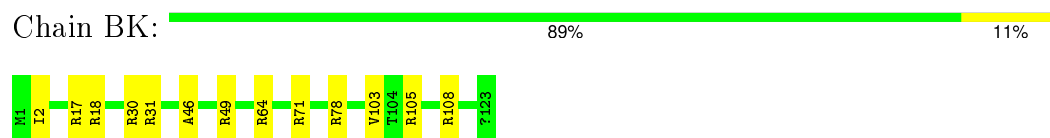
- Molecule 31: 50S ribosomal protein L11



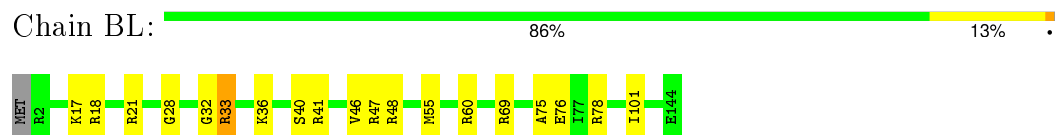
- Molecule 32: 50S ribosomal protein L13



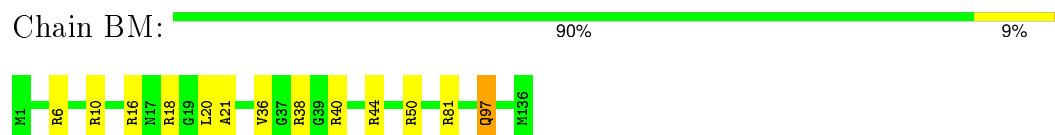
- Molecule 33: 50S ribosomal protein L14



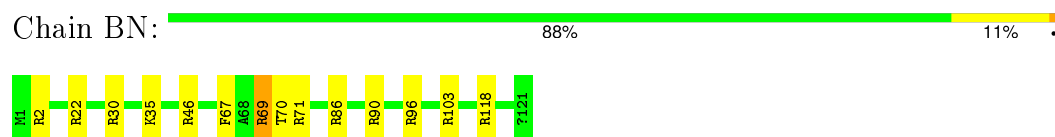
- Molecule 34: 50S ribosomal protein L15



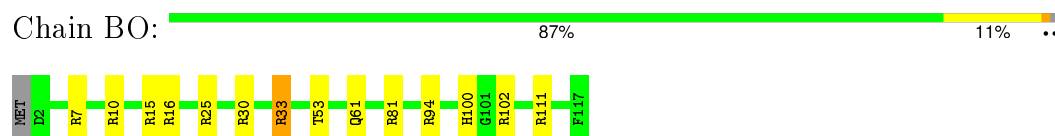
- Molecule 35: 50S ribosomal protein L16



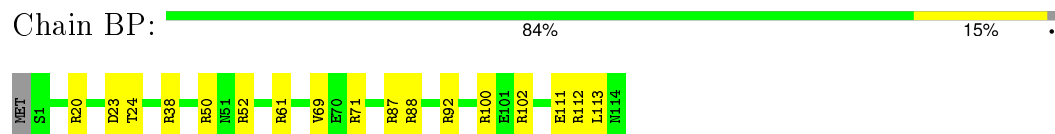
- Molecule 36: 50S ribosomal protein L17



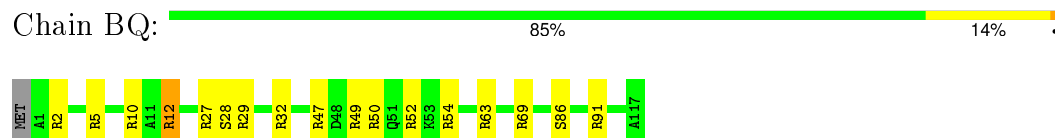
- Molecule 37: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L20



- Molecule 40: 50S ribosomal protein L21

Chain BR:  92% 8%



- Molecule 41: 50S ribosomal protein L22

Chain BS:  92% 7%




- Molecule 42: 50S ribosomal protein L23

Chain BT:  91% 7%



- Molecule 43: 50S ribosomal protein L24

Chain BU:  88% 12%



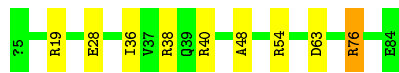
- Molecule 44: 50S ribosomal protein L25

Chain BV:  95% 5%




- Molecule 45: 50S ribosomal protein L27

Chain BW:  89% 10%



- Molecule 46: 50S ribosomal protein L28

Chain BX:  86% 11%



- Molecule 47: 50S ribosomal protein L29

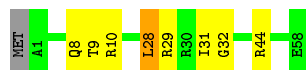
Chain BY:  92% 8%





- Molecule 48: 50S ribosomal protein L30

Chain BZ: 85% 12% . .



- Molecule 49: 50S ribosomal protein L32

Chain B0: 77% 21% .



- Molecule 50: 50S ribosomal protein L33

Chain B1: 87% 13%



- Molecule 51: 50S ribosomal protein L34

Chain B2: 78% 22%



- Molecule 52: 50S ribosomal protein L35

Chain B3: 85% 14% .



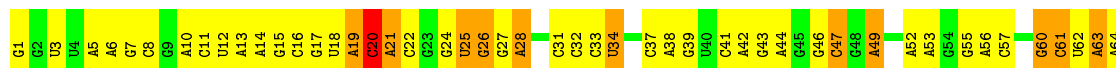
- Molecule 53: 50S ribosomal protein L36

Chain B4: 87% 13%



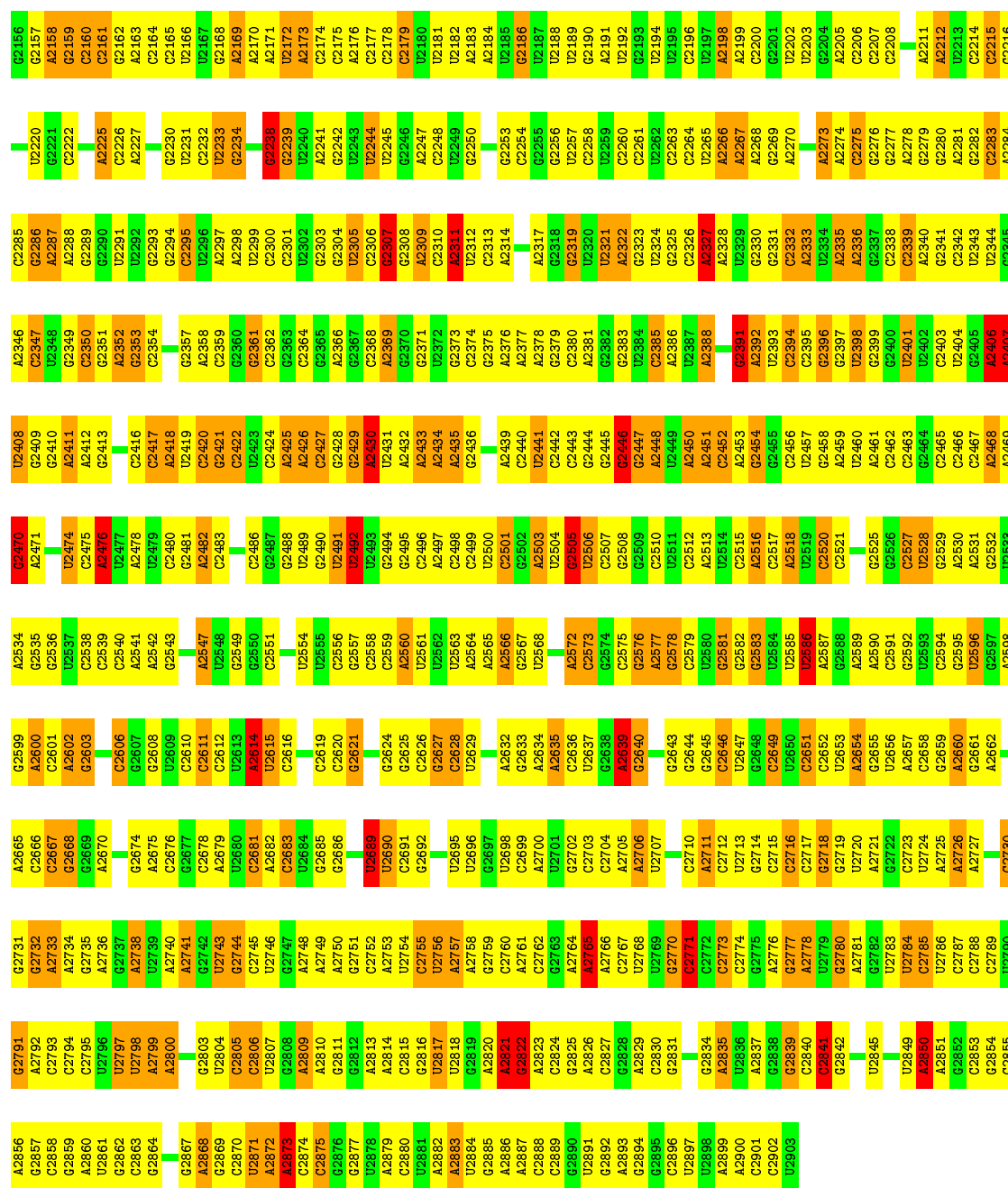
- Molecule 54: 23S ribosomal RNA

Chain BA: 22% 52% 22% .



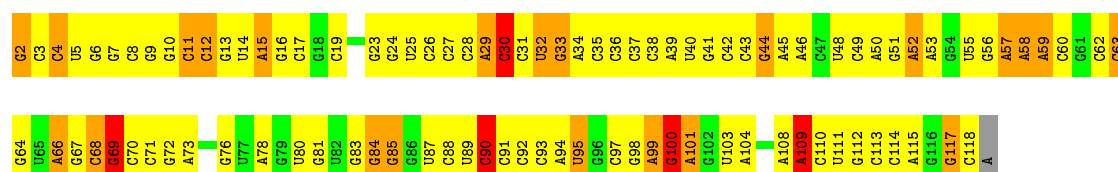
U1081	U1018	C957	U766	U703	C640	C578	G512	C444	G379	G317	A256	A196	C128	U65
U1082	U1019	C958	U767	G704	U641	G579	A513	C445	C382	C318	C257	A197	C129	C66
U1083	U1083	U958	G768	A705	U642	U580	A514	G446	C383	G319	G258	C198	C130	U67
A1084	A1021	C959		A706	A643	C581	A515	A447	C384	A320	G259	A199	A131	G68
A1085	G1022	C960	C772	U709	A644	A582	C516	U448	C385	U321	G260	U200	G132	C69
A1086	U1023	C961	U773	U709	C645	G583	C517	U449	C385	A322	G261	C201	U133	G70
G1087	G1024	C938	U774	U710	U646	C584	G518	G450	G386	C323	A262	U202	G134	A71
A1088	G1025	C901	G775	G711	U647	G585		U451	U387	A324	G263	A203	U135	U72
A1089	G1026	C965	G776		G648	A586	A522	G452	G388	G325	C264	A204	A73	A73
A1090	A1027	G966	G777	U714	C649	C587	C523	A453	G389	G326	A265	G205	U138	A74
G1091	A1028	U967		A715	C650	U588	G524	A454	U390	G327	G266	U206	U139	G75
C1092	A1029	C968	G780	C717	U650	U589	U525	C455	A391		C267	A207	C140	C76
A1095	U1030	U906	A781	A716	A654	U590	A526	C456	U392	A330	C268	C208	G141	G77
A1096	G1031	U970	A782	C718	A655	A590	C527	A457	C393	C331	C269	C209	A142	U78
U1097	A1032	C971	A783	C719	U656	A592	A528	G458	C394	A332	A270	C210	C143	C79
U1098	U1033	A972	G784	U720	U657	C595	A529	U459		G333	G271	C211	A144	G80
G1034	G1034	A973	G785	A721	U658	U596	G530	A460	U397	C334	A272	G212	C145	G81
U1035	U1035	G974	G786	A722	C659	U596	C531	C461	C398	C335	G273	A213	A146	U82
C1100		A975	C787	C723	C660	U598	A532	C462	U399	C336	C274	G214	C147	A83
U1101	A1039		A788	U724	A661	U598	G535	G463	G400	C337	C275	G215	U148	A84
C1102	A1040		A789	G725	C662	A599	G536	U464	A401	G338	U276	A216	A149	G85
A1103		A979	U790	G726	G663	G600	G536	G465	A402	U339	G277	A217	U150	G86
U1104	C1043	A980	G791	G727	U664	C601	G537	A466	U403	A340	A278	A218	C151	U87
C1105	C1044	C981	A792	G728	U665	A602	A538		A404	C341	A279	A219	A152	G88
U1106	C1045	C982	G793	G729	A666	A603	G539	A470		C342	U280	G220	A155	A89
G1107	A1046	A983	A794	A730	U667	G604	C540	A471	G408	C343	C281	A221	A156	U90
U1108	G1047	G859	G795	C731	A668	G605	A541	A472	G409	C344	A282	A222	A157	A91
A1109	A1048	U860	C796	G732	C669	U606	C542	G473	G410	A345	G283	A223	C157	
G1110	C1049	C986		G733	A670	U607	G543		G411	A346	U284	U224	U158	A94
A1111	A1050	C987	A800	A734	C671	A608	C544	A477	A412	A347	G285	C225	G159	A95
C1112	G1051	A988	G801	C735	C672	A609	U545	A478	C413	A348	U286	A226	A160	C96
U1113	C1052	G989	A802	C736	C673	C610	U546	A479	C414	U349		A227	A161	C97
C1114	C1053	C990	U803	C737	U674	C611	A547	A480	A415	G350	G289	C228	U162	G98
G1115	A1054	A926	A804	G738	A675	G612	G548	G481	U416	C351	U290	C229	C163	U99
C1116	G1055	C992	G805	A739	A676	A613	G549	A482	C417	A352	G291	C230	C164	U100
G1117	U1056	G993	C806	C740	A677	A614	C550	A483	C418	C353	U292	A231	A165	A101
C1118	A1057	C994	U807	U741	C678	U615	G551	C484	U419	A354	U293	G232	U166	U102
	U1058	C995	U807	C741	C679	A616	U552	C485	C420	U355	A294	U234	A167	A103
C1121	G1059	A996	U809	A742	C680	G617	G553	C486	C421	G356	G295	U234	A104	A104
G1122	U1060	C997	U810	U744	G681			C487	A422	C357	U296	U235	C105	C105
C1123	U1061	C998	U811	U744	G682	G620	A556	G488	A423	U360	G297	C236	U171	C106
G1124	G1062	U999	C812	U747	U683	A621	C557	C489		U361	G298	C237	A172	
A1125	C1063	A1000	U813	G748	U684	G622	U558	C490	C426	G361	A299	C238	A173	C109
U1126	G1064	A1001	C814	A749	A685	C623	C559	C491	U427	A362	A300	C239	U174	G110
A1127	U1065	G1002	C815	A750	U686	C624	C560	A492	A428	G363	G301	C240	G175	A111
G1128	C1066	G1003	C816	A751	C687	G625		G493	A429	C364	C302	A241	A176	U112
U1129	A1067	A941	C817	A752	U688	A626	A563		A430	U365	G303	G242	G177	U113
A1130	G1068	C1005	U818	A753	A689	A627	C564	U497	U431	C366	U304	U243	G178	U114
G1131	U1069	C1006	G819	U754	C690	G628	C565		A432	G367	C305	A244	C179	C115
U1132	C1070	A1007	A820	U755	C691	G629	U566	A501	C433	A368	U306	G245	G180	C116
A1133	G1071	U884	A821	A756	C692	G630		A502	U434	U369	G307	C246	A181	G117
C1134	C1072	A1009	G822	G757	A693	A631	U569	A503	C435	G370	G308	G247	A182	A118
G1135	A1073	A1010	C823	C758	U694	A632	G570	A504	C436	A371	A309	G248	C183	A119
C1136	G1074	C948	U824	G759	C695	A633	U571	A505	U437	G372	A310	C249	C184	U120
U1137	C1075	U1012	A825	G760		C634	A572	G506	G438	U373	A311	G250	G121	G121
G1138	C1076	C1013	U826	A761	C698	C635	U573	A507	C439	A374	A312	A251	A190	G122
U1139	A1077	U889	U827	G762	A699	G636	A574	A508	C440	G375	G314	G252	A191	
C1140	U1078	U1015	U828	G763	G700	A637	A575	C509	U441	G376	G314	C192	C192	A125
U1141	C1079	G952	U829	A764	U701	G638	U576	C510	G442	C377	G315	G254	A126	A126
A1142	A1080	C1016	A830	G765	C702	U639	C577	U511	A442	C378	C316	G254	A127	A127






• Molecule 55: 5S ribosomal RNA

Chain BB: 17% 59% 19%



• Molecule 56: 50S ribosomal protein L1

Chain B5:  88% 7% 5%



## 4 Experimental information

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	AB	0.67	0/1736	1.06	12/2340 (0.5%)
10	AK	0.73	0/894	1.10	8/1207 (0.7%)
11	AL	0.73	0/969	1.29	17/1300 (1.3%)
12	AM	0.72	0/884	1.36	14/1181 (1.2%)
13	AN	0.75	0/817	1.18	10/1088 (0.9%)
14	AO	0.70	0/722	1.18	7/964 (0.7%)
15	AP	0.74	0/648	1.27	11/870 (1.3%)
16	AQ	0.66	0/658	1.17	7/883 (0.8%)
17	AR	0.76	0/463	1.17	6/623 (1.0%)
18	AS	0.72	0/653	1.19	7/879 (0.8%)
19	AT	0.67	0/672	1.13	6/890 (0.7%)
2	AC	0.70	0/1651	1.18	18/2225 (0.8%)
20	AU	0.83	0/431	1.48	7/572 (1.2%)
21	AA	1.61	27/36759 (0.1%)	2.23	2065/57346 (3.6%)
22	A1	1.63	0/1668	2.16	80/2595 (3.1%)
23	A2	1.49	0/343	2.31	18/531 (3.4%)
24	A3	1.64	0/1722	2.26	102/2685 (3.8%)
25	BC	0.73	0/2121	1.28	21/2852 (0.7%)
26	BD	0.65	0/1586	1.19	14/2134 (0.7%)
27	BE	0.66	0/1571	1.22	14/2113 (0.7%)
28	BF	0.72	0/1444	1.18	12/1937 (0.6%)
29	BG	0.65	0/1343	1.14	9/1816 (0.5%)
3	AD	0.74	0/1665	1.20	17/2227 (0.8%)
30	BH	0.62	0/1122	1.08	5/1515 (0.3%)
31	BI	0.63	0/1046	1.03	4/1410 (0.3%)
32	BJ	0.71	0/1152	1.22	10/1551 (0.6%)
33	BK	0.70	0/947	1.23	10/1268 (0.8%)
34	BL	0.72	0/1054	1.29	10/1403 (0.7%)
35	BM	0.71	0/1093	1.19	9/1460 (0.6%)
36	BN	0.75	0/973	1.34	12/1301 (0.9%)
37	BO	0.71	0/902	1.27	13/1209 (1.1%)
38	BP	0.70	0/929	1.22	11/1242 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.76	0/960	1.30	16/1278 (1.3%)
4	AE	0.66	0/1119	1.03	7/1506 (0.5%)
40	BR	0.68	0/829	1.18	8/1107 (0.7%)
41	BS	0.63	0/864	1.22	10/1156 (0.9%)
42	BT	0.62	0/744	1.19	7/994 (0.7%)
43	BU	0.65	0/787	1.21	6/1051 (0.6%)
44	BV	0.66	0/766	1.06	4/1025 (0.4%)
45	BW	0.71	0/604	1.26	7/799 (0.9%)
46	BX	0.72	0/635	1.28	7/848 (0.8%)
47	BY	0.65	0/510	1.24	5/677 (0.7%)
48	BZ	0.67	0/453	1.23	5/605 (0.8%)
49	B0	0.72	0/450	1.30	7/599 (1.2%)
5	AF	0.71	0/835	1.12	7/1128 (0.6%)
50	B1	0.68	0/417	1.10	2/556 (0.4%)
51	B2	0.79	0/380	1.49	9/498 (1.8%)
52	B3	0.70	0/513	1.23	6/676 (0.9%)
53	B4	0.69	0/303	1.35	5/397 (1.3%)
54	BA	1.48	61/69796 (0.1%)	2.23	4183/108888 (3.8%)
55	BB	1.48	1/2800 (0.0%)	2.19	150/4367 (3.4%)
56	B5	0.62	0/1673	1.09	11/2255 (0.5%)
6	AG	0.72	0/1188	1.27	17/1593 (1.1%)
7	AH	0.69	0/989	1.07	8/1326 (0.6%)
8	AI	0.77	0/1035	1.21	13/1377 (0.9%)
9	AJ	0.71	0/797	1.16	9/1079 (0.8%)
All	All	1.34	89/160085 (0.1%)	2.01	7075/239402 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	AK	0	1
21	AA	0	374
22	A1	0	20
23	A2	0	5
24	A3	0	13
25	BC	0	1
26	BD	0	1
3	AD	0	1
31	BI	0	1
35	BM	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	BN	0	1
54	BA	0	623
55	BB	0	30
All	All	0	1072

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2507	C	C4-N4	-5.63	1.28	1.33
21	AA	742	G	C2-N2	-5.58	1.28	1.34
21	AA	756	C	C4-N4	-5.57	1.28	1.33
54	BA	2164	C	C4-N4	-5.44	1.29	1.33
21	AA	984	C	C4-N4	-5.43	1.29	1.33
21	AA	1317	C	C4-N4	-5.41	1.29	1.33
54	BA	1507	C	C4-N4	-5.36	1.29	1.33
54	BA	635	C	C4-N4	-5.34	1.29	1.33
54	BA	1814	G	C2-N2	-5.33	1.29	1.34
54	BA	2481	G	C2-N2	-5.33	1.29	1.34
54	BA	858	G	C2-N2	-5.32	1.29	1.34
21	AA	879	C	C4-N4	-5.31	1.29	1.33
21	AA	339	C	C4-N4	-5.30	1.29	1.33
54	BA	673	C	C4-N4	-5.30	1.29	1.33
54	BA	1297	C	C4-N4	-5.30	1.29	1.33
21	AA	1096	C	C4-N4	-5.29	1.29	1.33
54	BA	1838	C	C4-N4	-5.28	1.29	1.33
54	BA	787	C	C4-N4	-5.28	1.29	1.33
21	AA	36	C	C4-N4	-5.27	1.29	1.33
54	BA	2902	C	C4-N4	-5.25	1.29	1.33
54	BA	394	C	C4-N4	-5.24	1.29	1.33
54	BA	1843	C	C4-N4	-5.23	1.29	1.33
21	AA	582	C	C4-N4	-5.22	1.29	1.33
21	AA	1266	G	C2-N2	-5.22	1.29	1.34
54	BA	298	G	C2-N2	-5.22	1.29	1.34
54	BA	1311	G	C2-N2	-5.22	1.29	1.34
54	BA	1158	C	C4-N4	-5.21	1.29	1.33
21	AA	615	G	C2-N2	-5.21	1.29	1.34
54	BA	726	G	C2-N2	-5.20	1.29	1.34
54	BA	935	C	C4-N4	-5.20	1.29	1.33
54	BA	650	C	C4-N4	-5.20	1.29	1.33
54	BA	157	C	C4-N4	-5.20	1.29	1.33
21	AA	1214	C	C4-N4	-5.20	1.29	1.33
21	AA	755	G	C2-N2	-5.19	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1934	C	C4-N4	-5.19	1.29	1.33
54	BA	840	C	C4-N4	-5.19	1.29	1.33
54	BA	2805	C	C4-N4	-5.19	1.29	1.33
54	BA	66	C	C4-N4	-5.18	1.29	1.33
54	BA	1136	G	C2-N2	-5.17	1.29	1.34
54	BA	2463	C	C4-N4	-5.17	1.29	1.33
55	BB	28	C	C4-N4	-5.17	1.29	1.33
21	AA	1278	G	C2-N2	-5.16	1.29	1.34
21	AA	556	C	C4-N4	-5.16	1.29	1.33
54	BA	485	C	C4-N4	-5.14	1.29	1.33
21	AA	188	C	C4-N4	-5.13	1.29	1.33
54	BA	1052	C	C4-N4	-5.12	1.29	1.33
54	BA	1104	C	C4-N4	-5.12	1.29	1.33
21	AA	719	C	C4-N4	-5.12	1.29	1.33
54	BA	630	G	N1-C2	-5.12	1.33	1.37
21	AA	857	C	C4-N4	-5.12	1.29	1.33
54	BA	2610	C	C4-N4	-5.12	1.29	1.33
21	AA	599	C	C4-N4	-5.12	1.29	1.33
54	BA	456	C	C4-N4	-5.11	1.29	1.33
54	BA	1533	C	C4-N4	-5.11	1.29	1.33
54	BA	2133	G	C2-N2	-5.11	1.29	1.34
54	BA	1737	G	C2-N2	-5.11	1.29	1.34
54	BA	1962	C	C4-N4	-5.10	1.29	1.33
54	BA	318	C	C4-N4	-5.09	1.29	1.33
54	BA	660	C	C4-N4	-5.09	1.29	1.33
21	AA	326	G	C2-N2	-5.08	1.29	1.34
21	AA	1361	G	C2-N2	-5.08	1.29	1.34
54	BA	1153	C	C4-N4	-5.08	1.29	1.33
54	BA	1699	G	C2-N2	-5.08	1.29	1.34
54	BA	1837	C	C4-N4	-5.07	1.29	1.33
54	BA	1107	G	C2-N2	-5.07	1.29	1.34
21	AA	856	C	C4-N4	-5.07	1.29	1.33
54	BA	672	C	C4-N4	-5.07	1.29	1.33
54	BA	1895	C	C4-N4	-5.07	1.29	1.33
54	BA	2175	C	C4-N4	-5.06	1.29	1.33
54	BA	2527	C	C4-N4	-5.06	1.29	1.33
54	BA	1298	C	C4-N4	-5.05	1.29	1.33
54	BA	2858	C	C4-N4	-5.05	1.29	1.33
54	BA	1530	G	C2-N2	-5.04	1.29	1.34
54	BA	484	C	C4-N4	-5.04	1.29	1.33
21	AA	862	C	C4-N4	-5.03	1.29	1.33
54	BA	1585	C	C4-N4	-5.03	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	810	C	C4-N4	-5.02	1.29	1.33
54	BA	1697	G	C2-N2	-5.02	1.29	1.34
54	BA	1179	G	C2-N2	-5.02	1.29	1.34
54	BA	1531	C	C4-N4	-5.02	1.29	1.33
54	BA	2444	G	C2-N2	-5.02	1.29	1.34
21	AA	637	C	C4-N4	-5.01	1.29	1.33
21	AA	1218	C	C4-N4	-5.01	1.29	1.33
54	BA	2072	C	C4-N4	-5.01	1.29	1.33
54	BA	420	C	C4-N4	-5.01	1.29	1.33
54	BA	1007	C	C4-N4	-5.00	1.29	1.33
54	BA	1990	C	C4-N4	-5.00	1.29	1.33
54	BA	2718	G	C2-N2	-5.00	1.29	1.34
21	AA	616	G	C2-N2	-5.00	1.29	1.34

All (7075) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1617	C	N3-C2-O2	-16.02	110.69	121.90
54	BA	640	C	N3-C2-O2	-15.80	110.84	121.90
24	A3	73	A	N1-C6-N6	-13.57	110.46	118.60
54	BA	1847	A	N1-C6-N6	-13.18	110.69	118.60
54	BA	323	C	O4'-C1'-N1	12.86	118.49	108.20
21	AA	665	A	N1-C6-N6	-12.61	111.03	118.60
54	BA	2453	A	N1-C6-N6	-12.48	111.11	118.60
21	AA	977	A	N1-C6-N6	-12.36	111.19	118.60
54	BA	1668	A	N1-C6-N6	-12.18	111.30	118.60
21	AA	1319	A	N1-C6-N6	-12.16	111.30	118.60
54	BA	1352	U	O4'-C1'-N1	12.13	117.90	108.20
55	BB	99	A	N1-C6-N6	-12.12	111.33	118.60
54	BA	1854	A	N1-C6-N6	-12.11	111.33	118.60
21	AA	1288	A	N1-C6-N6	-12.07	111.36	118.60
54	BA	1434	A	N1-C6-N6	-11.81	111.51	118.60
21	AA	499	A	N1-C6-N6	-11.81	111.51	118.60
54	BA	1237	A	N1-C6-N6	-11.77	111.54	118.60
12	AM	97	ARG	NE-CZ-NH1	11.73	126.17	120.30
21	AA	573	A	N1-C6-N6	-11.70	111.58	118.60
21	AA	814	A	N1-C6-N6	-11.67	111.60	118.60
54	BA	1569	A	N1-C6-N6	-11.64	111.61	118.60
54	BA	1916	A	N1-C6-N6	-11.63	111.62	118.60
54	BA	1307	A	N1-C6-N6	-11.62	111.62	118.60
24	A3	36	A	N1-C6-N6	-11.60	111.64	118.60
54	BA	38	A	N1-C6-N6	-11.60	111.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	130	A	N1-C6-N6	-11.60	111.64	118.60
54	BA	1635	A	N1-C6-N6	-11.58	111.65	118.60
54	BA	1077	A	N1-C6-N6	-11.57	111.66	118.60
21	AA	1101	A	N1-C6-N6	-11.57	111.66	118.60
34	BL	48	ARG	NE-CZ-NH1	11.55	126.08	120.30
21	AA	1287	A	N1-C6-N6	-11.52	111.69	118.60
54	BA	2378	A	N1-C6-N6	-11.48	111.71	118.60
54	BA	1610	A	O4'-C1'-N9	11.43	117.34	108.20
21	AA	1251	A	N1-C6-N6	-11.42	111.75	118.60
21	AA	223	A	N1-C6-N6	-11.41	111.76	118.60
54	BA	346	A	N1-C6-N6	-11.40	111.76	118.60
54	BA	196	A	N1-C6-N6	-11.38	111.78	118.60
21	AA	767	A	N1-C6-N6	-11.24	111.85	118.60
21	AA	143	A	N1-C6-N6	-11.24	111.86	118.60
54	BA	2060	A	N1-C6-N6	-11.22	111.87	118.60
21	AA	673	A	N1-C6-N6	-11.22	111.87	118.60
54	BA	422	A	N1-C6-N6	-11.21	111.87	118.60
55	BB	73	A	N1-C6-N6	-11.20	111.88	118.60
54	BA	1609	A	N1-C6-N6	-11.18	111.89	118.60
54	BA	1617	C	N1-C2-O2	11.18	125.61	118.90
54	BA	2726	A	N1-C6-N6	-11.16	111.90	118.60
54	BA	1758	U	O4'-C1'-N1	11.15	117.12	108.20
54	BA	1890	A	N1-C6-N6	-11.14	111.92	118.60
54	BA	1876	A	N1-C6-N6	-11.10	111.94	118.60
54	BA	2781	A	N1-C6-N6	-11.08	111.95	118.60
54	BA	2425	A	N1-C6-N6	-11.08	111.95	118.60
21	AA	389	A	N1-C6-N6	-11.07	111.96	118.60
21	AA	1289	A	N1-C6-N6	-11.05	111.97	118.60
54	BA	886	A	N1-C6-N6	-11.05	111.97	118.60
54	BA	528	A	N1-C6-N6	-11.02	111.99	118.60
54	BA	800	A	N1-C6-N6	-11.01	111.99	118.60
54	BA	1069	A	N1-C6-N6	-11.01	111.99	118.60
21	AA	554	A	N1-C6-N6	-10.98	112.01	118.60
21	AA	1519	A	N1-C6-N6	-10.98	112.01	118.60
54	BA	1783	A	N1-C6-N6	-10.96	112.02	118.60
54	BA	501	A	N1-C6-N6	-10.95	112.03	118.60
21	AA	563	A	N1-C6-N6	-10.94	112.04	118.60
21	AA	1396	A	N1-C6-N6	-10.93	112.04	118.60
24	A3	59	A	N1-C6-N6	-10.93	112.04	118.60
54	BA	2009	A	N1-C6-N6	-10.92	112.05	118.60
21	AA	872	A	C1'-O4'-C4'	-10.91	101.17	109.90
54	BA	2750	A	N1-C6-N6	-10.91	112.05	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2547	A	N1-C6-N6	-10.91	112.05	118.60
54	BA	219	A	N1-C6-N6	-10.91	112.06	118.60
21	AA	913	A	N1-C6-N6	-10.89	112.07	118.60
54	BA	415	A	N1-C6-N6	-10.89	112.07	118.60
54	BA	207	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	2586	U	O4'-C1'-N1	10.85	116.88	108.20
54	BA	213	A	N1-C6-N6	-10.84	112.10	118.60
21	AA	609	A	N1-C6-N6	-10.84	112.10	118.60
54	BA	1126	A	N1-C6-N6	-10.83	112.10	118.60
21	AA	197	A	N1-C6-N6	-10.83	112.10	118.60
21	AA	199	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	931	U	O4'-C1'-N1	10.78	116.82	108.20
54	BA	1977	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	1808	A	N1-C6-N6	-10.77	112.14	118.60
54	BA	126	A	N1-C6-N6	-10.75	112.15	118.60
54	BA	2274	A	N1-C6-N6	-10.72	112.17	118.60
54	BA	2051	A	N1-C6-N6	-10.70	112.18	118.60
54	BA	2516	A	N1-C6-N6	-10.70	112.18	118.60
54	BA	2418	A	N1-C6-N6	-10.69	112.19	118.60
54	BA	2899	A	N1-C6-N6	-10.67	112.20	118.60
54	BA	1808	A	O4'-C1'-N9	10.66	116.72	108.20
5	AF	2	ARG	NE-CZ-NH1	10.65	125.63	120.30
54	BA	1858	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1952	A	N1-C6-N6	-10.63	112.22	118.60
23	A2	82	A	N1-C6-N6	-10.63	112.22	118.60
21	AA	1246	A	N1-C6-N6	-10.62	112.23	118.60
54	BA	2015	A	N1-C6-N6	-10.61	112.23	118.60
21	AA	60	A	N1-C6-N6	-10.59	112.25	118.60
21	AA	510	A	N1-C6-N6	-10.57	112.26	118.60
21	AA	1216	A	N1-C6-N6	-10.55	112.27	118.60
54	BA	1998	A	N1-C6-N6	-10.52	112.29	118.60
55	BB	41	G	O4'-C1'-N9	10.51	116.61	108.20
21	AA	937	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	2135	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	2572	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	2147	A	N1-C6-N6	-10.49	112.30	118.60
54	BA	1759	A	N1-C6-N6	-10.49	112.31	118.60
21	AA	172	A	N1-C6-N6	-10.47	112.32	118.60
25	BC	235	GLU	OE1-CD-OE2	-10.45	110.76	123.30
24	A3	60	A	N1-C6-N6	-10.45	112.33	118.60
21	AA	607	A	N1-C6-N6	-10.44	112.34	118.60
55	BB	87	U	O4'-C1'-N1	10.43	116.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	766	A	N1-C6-N6	-10.42	112.35	118.60
54	BA	1755	A	N1-C6-N6	-10.42	112.35	118.60
21	AA	303	A	N1-C6-N6	-10.42	112.35	118.60
54	BA	2328	A	N1-C6-N6	-10.40	112.36	118.60
21	AA	560	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	2809	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	119	A	N1-C6-N6	-10.39	112.36	118.60
54	BA	718	A	N1-C6-N6	-10.38	112.37	118.60
54	BA	2407	A	N1-C6-N6	-10.38	112.37	118.60
54	BA	2339	C	O4'-C1'-N1	10.38	116.50	108.20
55	BB	94	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	1919	A	N1-C6-N6	-10.36	112.39	118.60
21	AA	306	A	N1-C6-N6	-10.35	112.39	118.60
55	BB	46	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	2266	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	1133	A	N1-C6-N6	-10.34	112.39	118.60
54	BA	1784	A	N1-C6-N6	-10.34	112.40	118.60
54	BA	2386	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	1046	A	O4'-C1'-N9	10.31	116.45	108.20
38	BP	61	ARG	NE-CZ-NH1	10.30	125.45	120.30
54	BA	1142	A	N1-C6-N6	-10.29	112.43	118.60
54	BA	626	A	N1-C6-N6	-10.28	112.43	118.60
21	AA	559	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	515	A	N1-C6-N6	-10.27	112.44	118.60
21	AA	968	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	981	A	N1-C6-N6	-10.24	112.46	118.60
54	BA	1591	A	N1-C6-N6	-10.23	112.46	118.60
55	BB	50	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1197	A	N1-C6-N6	-10.21	112.48	118.60
54	BA	941	A	N1-C6-N6	-10.21	112.48	118.60
16	AQ	48	GLU	OE1-CD-OE2	-10.20	111.06	123.30
54	BA	218	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	959	A	N1-C6-N6	-10.19	112.48	118.60
54	BA	270	A	N1-C6-N6	-10.18	112.49	118.60
21	AA	1229	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	849	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	1265	A	N1-C6-N6	-10.17	112.50	118.60
54	BA	2814	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	1496	A	N1-C6-N6	-10.15	112.51	118.60
54	BA	1070	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	152	A	N1-C6-N6	-10.14	112.52	118.60
12	AM	56	ARG	NE-CZ-NH1	10.13	125.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	441	A	N1-C6-N6	-10.13	112.52	118.60
21	AA	1311	A	N1-C6-N6	-10.12	112.53	118.60
54	BA	1495	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	2654	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	1717	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	371	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	2736	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	844	A	N1-C6-N6	-10.07	112.56	118.60
21	AA	448	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	655	A	O4'-C1'-N9	10.06	116.25	108.20
21	AA	313	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	1586	A	N1-C6-N6	-10.03	112.58	118.60
23	A2	90	U	C1'-O4'-C4'	-10.03	101.88	109.90
54	BA	282	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	2634	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	1384	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	2058	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	2679	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	696	A	N1-C6-N6	-9.99	112.61	118.60
21	AA	1022	A	N1-C6-N6	-9.97	112.61	118.60
21	AA	1333	A	N1-C6-N6	-9.97	112.62	118.60
24	A3	38	A	N1-C6-N6	-9.97	112.62	118.60
21	AA	338	A	N1-C6-N6	-9.96	112.62	118.60
54	BA	2433	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	1304	A	N1-C6-N6	-9.96	112.62	118.60
54	BA	2163	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	1377	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	1004	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	1000	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	982	C	N3-C2-O2	-9.93	114.95	121.90
54	BA	1679	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	608	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	947	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	1301	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	633	A	N1-C6-N6	-9.89	112.67	118.60
54	BA	722	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	2900	A	N1-C6-N6	-9.86	112.68	118.60
21	AA	482	A	N1-C6-N6	-9.86	112.68	118.60
54	BA	1169	A	N1-C6-N6	-9.86	112.68	118.60
21	AA	253	A	N1-C6-N6	-9.86	112.69	118.60
54	BA	592	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	1885	A	N1-C6-N6	-9.84	112.70	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AC	53	ARG	NE-CZ-NH1	9.83	125.22	120.30
21	AA	363	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	2879	A	N1-C6-N6	-9.83	112.70	118.60
21	AA	190	A	N1-C6-N6	-9.82	112.71	118.60
21	AA	1204	A	N1-C6-N6	-9.82	112.71	118.60
21	AA	1363	A	N1-C6-N6	-9.82	112.71	118.60
3	AD	61	ARG	NE-CZ-NH1	9.81	125.21	120.30
25	BC	261	ARG	NE-CZ-NH1	9.81	125.21	120.30
54	BA	1272	A	N1-C6-N6	-9.81	112.71	118.60
40	BR	84	ARG	NE-CZ-NH1	9.81	125.20	120.30
21	AA	974	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	1156	A	N1-C6-N6	-9.81	112.72	118.60
54	BA	1260	A	N1-C6-N6	-9.80	112.72	118.60
36	BN	96	ARG	NE-CZ-NH1	9.80	125.20	120.30
54	BA	311	A	N1-C6-N6	-9.79	112.73	118.60
54	BA	146	A	N1-C6-N6	-9.79	112.73	118.60
21	AA	53	A	N1-C6-N6	-9.78	112.73	118.60
21	AA	1431	A	N1-C6-N6	-9.77	112.73	118.60
54	BA	1275	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	298	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	228	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	336	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	632	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	752	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	2430	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	1413	A	N1-C6-N6	-9.75	112.75	118.60
25	BC	68	ARG	NE-CZ-NH1	9.75	125.18	120.30
21	AA	807	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	1672	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	900	A	N1-C6-N6	-9.74	112.76	118.60
21	AA	195	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	1785	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2352	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	103	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1080	A	N1-C6-N6	-9.73	112.76	118.60
21	AA	179	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1515	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1937	A	N1-C6-N6	-9.73	112.76	118.60
21	AA	246	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	2176	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	1805	A	N1-C6-N6	-9.72	112.77	118.60
21	AA	777	A	N1-C6-N6	-9.72	112.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	960	A	N1-C6-N6	-9.72	112.77	118.60
53	B4	24	ARG	NE-CZ-NH1	9.71	125.16	120.30
21	AA	171	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	1913	A	N1-C6-N6	-9.71	112.78	118.60
21	AA	825	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1522	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1095	A	N1-C6-N6	-9.69	112.78	118.60
54	BA	2020	A	N1-C6-N6	-9.69	112.78	118.60
54	BA	1749	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	101	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	734	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	1067	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	2665	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	982	C	O4'-C1'-N1	9.65	115.92	108.20
55	BB	109	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	1429	A	N1-C6-N6	-9.65	112.81	118.60
22	A1	35	A	N1-C6-N6	-9.64	112.82	118.60
54	BA	1774	C	N3-C2-O2	-9.64	115.16	121.90
54	BA	2070	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2564	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	99	U	O4'-C1'-N1	9.62	115.90	108.20
27	BE	102	ARG	NE-CZ-NH1	9.62	125.11	120.30
54	BA	861	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1978	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	1227	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1353	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	2013	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	282	A	N1-C6-N6	-9.61	112.84	118.60
21	AA	675	A	N1-C6-N6	-9.61	112.84	118.60
54	BA	125	A	N1-C6-N6	-9.61	112.84	118.60
39	BQ	91	ARG	NE-CZ-NH1	9.60	125.10	120.30
54	BA	1583	A	N1-C6-N6	-9.60	112.84	118.60
21	AA	749	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	2281	A	N1-C6-N6	-9.60	112.84	118.60
24	A3	77	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	1552	A	O4'-C1'-N9	9.59	115.87	108.20
54	BA	2887	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	1544	A	N1-C6-N6	-9.59	112.85	118.60
21	AA	1130	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1701	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	2610	C	N3-C2-O2	-9.57	115.20	121.90
55	BB	34	A	N1-C6-N6	-9.57	112.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	227	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	63	A	N1-C6-N6	-9.56	112.87	118.60
54	BA	943	A	N1-C6-N6	-9.56	112.87	118.60
54	BA	2518	A	N1-C6-N6	-9.56	112.86	118.60
21	AA	831	A	N1-C6-N6	-9.55	112.87	118.60
3	AD	12	ARG	NE-CZ-NH1	9.55	125.07	120.30
54	BA	637	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	751	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	2497	A	N1-C6-N6	-9.54	112.87	118.60
21	AA	74	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	199	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	2307	G	O4'-C1'-N9	9.54	115.83	108.20
51	B2	21	ARG	NE-CZ-NH1	9.54	125.07	120.30
54	BA	2287	A	N1-C6-N6	-9.53	112.88	118.60
14	AO	16	ARG	NE-CZ-NH1	9.53	125.06	120.30
54	BA	1213	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2171	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2435	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	1014	A	N1-C6-N6	-9.53	112.89	118.60
54	BA	1652	A	N1-C6-N6	-9.53	112.89	118.60
54	BA	750	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2142	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2635	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	1508	A	N1-C6-N6	-9.51	112.89	118.60
55	BB	39	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	1434	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	1145	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	241	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	280	U	O4'-C1'-N1	9.50	115.80	108.20
54	BA	1532	A	N1-C6-N6	-9.50	112.90	118.60
24	A3	22	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	2126	A	N1-C6-N6	-9.49	112.90	118.60
54	BA	2879	A	C5-C6-N1	9.49	122.45	117.70
54	BA	1084	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	181	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	397	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	493	A	N1-C6-N6	-9.49	112.91	118.60
16	AQ	39	ARG	NE-CZ-NH1	9.48	125.04	120.30
54	BA	654	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	1936	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	1889	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	1014	A	N1-C6-N6	-9.47	112.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	26	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1871	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1943	U	O4'-C1'-N1	9.46	115.77	108.20
54	BA	2590	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	482	A	N1-C6-N6	-9.46	112.92	118.60
21	AA	1368	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1744	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	262	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	1143	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	1637	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	784	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	1256	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	454	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	142	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	279	A	N1-C6-N6	-9.43	112.94	118.60
12	AM	28	ARG	NE-CZ-NH1	9.43	125.01	120.30
21	AA	1225	A	N1-C6-N6	-9.42	112.95	118.60
26	BD	77	ARG	NE-CZ-NH1	9.42	125.01	120.30
54	BA	1420	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1722	A	N1-C6-N6	-9.42	112.95	118.60
22	A1	21	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1009	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1151	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	192	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	1068	G	O4'-C1'-N9	9.41	115.73	108.20
54	BA	1819	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	1250	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	919	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	2587	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	782	A	N1-C6-N6	-9.39	112.96	118.60
54	BA	983	A	N1-C6-N6	-9.39	112.96	118.60
9	AJ	5	ARG	NE-CZ-NH1	9.39	124.99	120.30
54	BA	479	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	2108	A	N1-C6-N6	-9.39	112.97	118.60
4	AE	53	ARG	NE-CZ-NH1	9.38	124.99	120.30
21	AA	98	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	1610	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	1082	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	1046	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	443	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	1302	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1593	A	N1-C6-N6	-9.37	112.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	466	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	503	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1932	A	N1-C6-N6	-9.37	112.98	118.60
23	A2	79	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	412	A	N1-C6-N6	-9.36	112.98	118.60
21	AA	792	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	203	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	1789	A	N1-C6-N6	-9.36	112.99	118.60
54	BA	909	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	2602	A	O4'-C1'-N9	9.34	115.67	108.20
37	BO	102	ARG	NE-CZ-NH1	9.34	124.97	120.30
54	BA	160	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1525	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1010	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	802	A	N1-C6-N6	-9.32	113.00	118.60
54	BA	1535	A	N1-C6-N6	-9.32	113.01	118.60
55	BB	66	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	2376	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	2478	A	N1-C6-N6	-9.32	113.01	118.60
22	A1	9	A	N1-C6-N6	-9.31	113.01	118.60
46	BX	44	ARG	NE-CZ-NH1	9.31	124.96	120.30
54	BA	979	A	O4'-C1'-N9	9.31	115.65	108.20
54	BA	2820	A	N1-C6-N6	-9.31	113.02	118.60
21	AA	743	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	2581	G	O4'-C1'-N9	9.30	115.64	108.20
21	AA	1394	A	N1-C6-N6	-9.30	113.02	118.60
15	AP	25	ARG	NE-CZ-NH1	9.29	124.95	120.30
54	BA	2725	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	933	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	1320	C	O4'-C1'-N1	9.29	115.64	108.20
54	BA	2792	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	635	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	1408	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	408	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	1468	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	2037	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	896	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	344	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2711	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	1239	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2835	A	N1-C6-N6	-9.28	113.03	118.60
24	A3	11	A	N1-C6-N6	-9.27	113.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	547	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	2560	A	N1-C6-N6	-9.27	113.04	118.60
3	AD	127	ARG	NE-CZ-NH1	9.27	124.93	120.30
21	AA	1433	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	676	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	2381	A	N1-C6-N6	-9.26	113.04	118.60
21	AA	572	A	N1-C6-N6	-9.26	113.05	118.60
21	AA	1430	A	N1-C6-N6	-9.26	113.05	118.60
26	BD	59	ARG	NE-CZ-NH1	9.26	124.93	120.30
54	BA	322	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	1428	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	155	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	932	U	O4'-C1'-N1	9.24	115.59	108.20
54	BA	2706	A	N1-C6-N6	-9.24	113.06	118.60
21	AA	702	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	2101	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	111	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	265	A	N1-C6-N6	-9.23	113.06	118.60
1	AB	34	ARG	NE-CZ-NH1	9.23	124.91	120.30
27	BE	162	ARG	NE-CZ-NH1	9.23	124.91	120.30
54	BA	1027	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	131	A	N1-C6-N6	-9.22	113.06	118.60
54	BA	344	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1815	A	N1-C6-N6	-9.22	113.06	118.60
14	AO	53	ARG	NE-CZ-NH1	9.22	124.91	120.30
21	AA	465	A	N1-C6-N6	-9.21	113.07	118.60
21	AA	780	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	2614	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	804	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	195	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	1340	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	753	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	2541	A	N1-C6-N6	-9.19	113.08	118.60
21	AA	718	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	176	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	2825	G	O4'-C1'-N9	9.18	115.55	108.20
54	BA	1067	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	348	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1791	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	522	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	468	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	1398	A	N1-C6-N6	-9.17	113.10	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	864	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	676	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	309	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	2542	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	1274	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	1395	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	1194	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	456	C	N3-C2-O2	-9.15	115.49	121.90
54	BA	572	A	C5-C6-N1	9.15	122.28	117.70
54	BA	1147	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	196	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	1005	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1274	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2030	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2268	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	915	A	N1-C6-N6	-9.14	113.11	118.60
54	BA	458	G	O4'-C1'-N9	9.14	115.51	108.20
54	BA	644	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	787	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	608	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	2675	A	N1-C6-N6	-9.14	113.12	118.60
55	BB	52	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	748	G	O4'-C1'-N9	9.14	115.51	108.20
21	AA	1021	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	975	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	250	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	1213	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	637	A	C5-C6-N1	9.12	122.26	117.70
54	BA	2212	A	O4'-C1'-N9	9.12	115.50	108.20
21	AA	996	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2868	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	72	A	C5-C6-N1	9.12	122.26	117.70
54	BA	352	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2469	A	N1-C6-N6	-9.11	113.13	118.60
25	BC	237	ARG	NE-CZ-NH1	9.11	124.86	120.30
54	BA	127	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	1580	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	1509	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	2273	A	N1-C6-N6	-9.11	113.14	118.60
37	BO	94	ARG	NE-CZ-NH1	9.10	124.85	120.30
21	AA	1339	A	C5-C6-N1	9.10	122.25	117.70
54	BA	1419	A	N1-C6-N6	-9.10	113.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1953	A	N1-C6-N6	-9.10	113.14	118.60
7	AH	79	ARG	NE-CZ-NH1	9.09	124.85	120.30
2	AC	58	ARG	NE-CZ-NH1	9.09	124.84	120.30
54	BA	655	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	1029	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	2670	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	1630	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	1853	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	1654	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	151	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1155	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1342	C	P-O3'-C3'	9.07	130.59	119.70
54	BA	1439	A	O4'-C1'-N9	9.07	115.46	108.20
54	BA	1566	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	2335	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	523	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1329	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	825	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	2657	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	471	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	243	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	1380	U	N3-C2-O2	-9.06	115.86	122.20
54	BA	191	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	196	A	C5-C6-N1	9.06	122.23	117.70
21	AA	649	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	783	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	1382	G	O4'-C1'-N9	9.05	115.44	108.20
54	BA	661	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1308	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	1367	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	2850	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	460	A	N1-C6-N6	-9.04	113.17	118.60
21	AA	983	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2531	A	N1-C6-N6	-9.04	113.18	118.60
21	AA	553	A	N1-C6-N6	-9.03	113.18	118.60
24	A3	39	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1739	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	643	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1608	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	1042	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	181	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	262	A	N1-C6-N6	-9.01	113.19	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1238	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	1054	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	95	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1301	A	C5-C6-N1	9.00	122.20	117.70
21	AA	279	A	C5-C6-N1	9.00	122.20	117.70
54	BA	1453	A	N1-C6-N6	-9.00	113.20	118.60
32	BJ	116	ARG	NE-CZ-NH1	9.00	124.80	120.30
54	BA	1960	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	342	A	N1-C6-N6	-8.99	113.20	118.60
21	AA	19	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	231	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	497	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	1046	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	2314	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	1700	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	914	A	N1-C6-N6	-8.98	113.21	118.60
26	BD	46	ARG	NE-CZ-NH1	8.98	124.79	120.30
54	BA	1618	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	1480	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	300	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	80	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1268	A	N1-C6-N6	-8.96	113.22	118.60
27	BE	114	ARG	NE-CZ-NH1	8.95	124.78	120.30
54	BA	508	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	925	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	2450	A	N1-C6-N6	-8.95	113.23	118.60
10	AK	92	ARG	NE-CZ-NH1	8.95	124.77	120.30
54	BA	1549	A	N1-C6-N6	-8.95	113.23	118.60
38	BP	38	ARG	NE-CZ-NH1	8.95	124.77	120.30
21	AA	152	A	C5-C6-N1	8.94	122.17	117.70
21	AA	729	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1048	A	N1-C6-N6	-8.93	113.24	118.60
3	AD	62	ARG	NE-CZ-NH1	8.93	124.77	120.30
54	BA	2632	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	2628	C	N3-C2-O2	-8.93	115.65	121.90
21	AA	167	A	N1-C6-N6	-8.92	113.25	118.60
6	AG	108	ARG	NE-CZ-NH1	8.92	124.76	120.30
21	AA	461	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	53	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	716	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	892	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	2327	A	N1-C6-N6	-8.91	113.25	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1616	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1129	A	N1-C6-N6	-8.91	113.26	118.60
54	BA	432	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1606	C	N3-C2-O2	-8.90	115.67	121.90
54	BA	905	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	622	A	N1-C6-N6	-8.90	113.26	118.60
33	BK	17	ARG	NE-CZ-NH1	8.90	124.75	120.30
21	AA	1179	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	1476	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	689	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1966	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2660	A	N1-C6-N6	-8.90	113.26	118.60
47	BY	47	ARG	NE-CZ-NH1	8.89	124.75	120.30
54	BA	613	A	N1-C6-N6	-8.89	113.27	118.60
54	BA	1241	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	602	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	996	A	C1'-O4'-C4'	-8.89	102.79	109.90
21	AA	1188	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	277	G	O4'-C1'-N9	8.88	115.31	108.20
54	BA	449	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	706	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	670	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	330	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1773	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	2821	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1322	A	N1-C6-N6	-8.87	113.28	118.60
55	BB	103	U	O4'-C1'-N1	8.87	115.30	108.20
21	AA	579	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	1163	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	2406	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	1377	A	C5-C6-N1	8.86	122.13	117.70
21	AA	197	A	C5-C6-N1	8.85	122.13	117.70
54	BA	1276	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	2426	A	N1-C6-N6	-8.84	113.29	118.60
21	AA	913	A	C5-C6-N1	8.84	122.12	117.70
22	A1	59	U	O4'-C1'-N1	8.84	115.27	108.20
21	AA	205	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	1392	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	144	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	687	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	1456	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	547	A	N1-C6-N6	-8.82	113.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AM	89	ARG	NE-CZ-NH1	8.82	124.71	120.30
22	A1	23	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1089	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	648	A	N1-C6-N6	-8.79	113.32	118.60
24	A3	76	C	N3-C2-O2	-8.79	115.74	121.90
54	BA	161	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1570	A	N1-C6-N6	-8.79	113.33	118.60
24	A3	45	A	N1-C6-N6	-8.78	113.33	118.60
42	BT	12	ARG	NE-CZ-NH1	8.79	124.69	120.30
54	BA	2727	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1848	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2094	A	N1-C6-N6	-8.78	113.33	118.60
20	AU	44	ARG	NE-CZ-NH1	8.78	124.69	120.30
54	BA	2033	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1134	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2059	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2598	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	311	A	C5-C6-N1	8.76	122.08	117.70
54	BA	1069	A	C5-C6-N1	8.76	122.08	117.70
54	BA	1320	C	N3-C2-O2	-8.75	115.77	121.90
54	BA	2534	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	451	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	44	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	255	A	N1-C6-N6	-8.74	113.35	118.60
54	BA	749	A	N1-C6-N6	-8.74	113.35	118.60
54	BA	945	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	988	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1597	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1877	A	N1-C6-N6	-8.74	113.36	118.60
21	AA	958	A	N1-C6-N6	-8.74	113.36	118.60
23	A2	91	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	817	C	N3-C2-O2	-8.73	115.79	121.90
21	AA	900	A	N1-C6-N6	-8.73	113.36	118.60
27	BE	170	ARG	NE-CZ-NH1	8.73	124.66	120.30
12	AM	69	ARG	NE-CZ-NH1	8.72	124.66	120.30
21	AA	495	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	621	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	2090	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	2893	A	N1-C6-N6	-8.72	113.37	118.60
55	BB	15	A	N1-C6-N6	-8.72	113.37	118.60
41	BS	18	ARG	NE-CZ-NH1	8.72	124.66	120.30
21	AA	1271	A	N1-C6-N6	-8.71	113.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1073	A	O4'-C1'-N9	8.71	115.17	108.20
21	AA	236	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	1534	U	O4'-C1'-N1	8.71	115.16	108.20
54	BA	2071	A	N1-C6-N6	-8.71	113.38	118.60
21	AA	1152	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	1731	G	O4'-C1'-N9	8.70	115.16	108.20
2	AC	178	ARG	NE-CZ-NH1	8.70	124.65	120.30
21	AA	889	A	N1-C6-N6	-8.69	113.38	118.60
54	BA	56	A	N1-C6-N6	-8.69	113.38	118.60
54	BA	362	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	228	C	N3-C2-O2	-8.68	115.82	121.90
54	BA	28	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	788	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1885	A	C5-C6-N1	8.68	122.04	117.70
54	BA	927	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	274	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	1446	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	118	A	C5-C6-N1	8.68	122.04	117.70
21	AA	969	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1365	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	665	A	C5-C6-N1	8.67	122.03	117.70
54	BA	275	C	N3-C2-O2	-8.66	115.84	121.90
54	BA	2725	A	C5-C6-N1	8.66	122.03	117.70
21	AA	1503	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	346	A	C5-C6-N1	8.66	122.03	117.70
54	BA	1641	A	N1-C6-N6	-8.66	113.41	118.60
54	BA	2071	A	C5-C6-N1	8.66	122.03	117.70
54	BA	483	A	N1-C6-N6	-8.66	113.41	118.60
21	AA	1219	A	N1-C6-N6	-8.66	113.41	118.60
6	AG	77	ARG	NE-CZ-NH1	8.65	124.63	120.30
54	BA	2459	A	C5-C6-N1	8.65	122.03	117.70
21	AA	498	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	1092	A	N1-C6-N6	-8.65	113.41	118.60
49	B0	9	ARG	NE-CZ-NH1	8.65	124.62	120.30
54	BA	86	G	O4'-C1'-N9	8.65	115.12	108.20
54	BA	320	A	N1-C6-N6	-8.65	113.41	118.60
22	A1	41	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	371	A	C5-C6-N1	8.64	122.02	117.70
54	BA	2077	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	535	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	648	A	C5-C6-N1	8.63	122.02	117.70
54	BA	844	A	C5-C6-N1	8.63	122.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2173	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	371	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	51	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	1044	C	N3-C2-O2	-8.62	115.87	121.90
54	BA	466	A	N1-C6-N6	-8.62	113.43	118.60
30	BH	68	ARG	NE-CZ-NH1	8.61	124.61	120.30
54	BA	526	A	C5-C6-N1	8.61	122.01	117.70
54	BA	2565	A	N1-C6-N6	-8.61	113.43	118.60
21	AA	1381	U	C5'-C4'-O4'	8.61	119.43	109.10
54	BA	507	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	1981	A	O4'-C1'-N9	8.61	115.09	108.20
54	BA	2388	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	819	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	2377	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	401	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1096	A	N1-C6-N6	-8.59	113.44	118.60
21	AA	1280	A	N1-C6-N6	-8.59	113.44	118.60
21	AA	65	A	N1-C6-N6	-8.59	113.45	118.60
40	BR	13	ARG	NE-CZ-NH1	8.59	124.60	120.30
54	BA	84	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	6	G	O4'-C1'-N9	8.59	115.07	108.20
54	BA	706	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	1360	A	C5-C6-N1	8.57	121.99	117.70
54	BA	1890	A	C5-C6-N1	8.57	121.99	117.70
54	BA	2005	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	1269	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	490	C	N3-C2-O2	-8.57	115.90	121.90
54	BA	2171	A	C5-C6-N1	8.57	121.98	117.70
54	BA	789	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2689	U	O4'-C1'-N1	8.57	115.05	108.20
54	BA	2461	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	694	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	91	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	1127	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	1226	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	2705	A	N1-C6-N6	-8.56	113.47	118.60
54	BA	2482	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	161	A	N1-C6-N6	-8.55	113.47	118.60
55	BB	78	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	13	A	N1-C6-N6	-8.55	113.47	118.60
45	BW	38	ARG	NE-CZ-NH1	8.54	124.57	120.30
54	BA	226	A	N1-C6-N6	-8.54	113.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1981	A	C5-C6-N1	8.54	121.97	117.70
21	AA	353	A	C5-C6-N1	8.54	121.97	117.70
21	AA	994	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	820	A	C5-C6-N1	8.54	121.97	117.70
54	BA	1262	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	814	A	C5-C6-N1	8.53	121.97	117.70
21	AA	353	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	2080	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	865	A	N1-C6-N6	-8.52	113.48	118.60
21	AA	907	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	1189	A	N1-C6-N6	-8.52	113.49	118.60
19	AT	23	ARG	NE-CZ-NH1	8.52	124.56	120.30
54	BA	819	A	C5-C6-N1	8.52	121.96	117.70
21	AA	1045	C	N3-C2-O2	-8.51	115.94	121.90
54	BA	1085	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1552	A	C5-C6-N1	8.51	121.96	117.70
21	AA	432	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	428	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	2799	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	794	A	N1-C6-N6	-8.51	113.50	118.60
25	BC	12	ARG	NE-CZ-NH1	8.51	124.55	120.30
54	BA	345	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1336	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1494	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1738	G	O4'-C1'-N9	8.51	115.01	108.20
54	BA	1755	A	C5-C6-N1	8.51	121.95	117.70
54	BA	2117	A	C5-C6-N1	8.51	121.95	117.70
54	BA	2340	A	C5-C6-N1	8.50	121.95	117.70
54	BA	391	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	845	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1000	A	C5-C6-N1	8.50	121.95	117.70
21	AA	655	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	590	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	980	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	1665	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	2721	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	33	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	1086	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	1252	A	C5-C6-N1	8.49	121.94	117.70
21	AA	767	A	C5-C6-N1	8.48	121.94	117.70
54	BA	1403	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	918	A	N1-C6-N6	-8.48	113.51	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	716	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	1318	A	N1-C6-N6	-8.48	113.51	118.60
47	BY	48	ARG	NE-CZ-NH1	8.48	124.54	120.30
54	BA	49	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	780	A	C5-C6-N1	8.48	121.94	117.70
54	BA	2211	A	C5-C6-N1	8.47	121.94	117.70
21	AA	456	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	1439	A	N1-C6-N6	-8.47	113.52	118.60
21	AA	1465	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	804	A	C5-C6-N1	8.47	121.93	117.70
21	AA	574	A	N1-C6-N6	-8.46	113.52	118.60
24	A3	73	A	C4-C5-C6	-8.46	112.77	117.00
21	AA	675	A	C5-C6-N1	8.46	121.93	117.70
21	AA	1117	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	42	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	332	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	572	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1253	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	2468	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	10	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	300	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	1794	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	845	A	N1-C6-N6	-8.45	113.53	118.60
49	B0	15	ARG	NE-CZ-NH2	8.45	124.53	120.30
21	AA	959	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	1158	C	N3-C2-O2	-8.45	115.98	121.90
54	BA	504	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	1350	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	1214	C	N3-C2-O2	-8.45	115.99	121.90
54	BA	204	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2753	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	1248	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	272	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	347	A	N1-C6-N6	-8.44	113.53	118.60
7	AH	76	ARG	NE-CZ-NH1	8.44	124.52	120.30
54	BA	125	A	C5-C6-N1	8.44	121.92	117.70
54	BA	650	C	N3-C2-O2	-8.43	116.00	121.90
54	BA	1098	A	N1-C6-N6	-8.43	113.54	118.60
18	AS	36	ARG	NE-CZ-NH1	8.43	124.51	120.30
21	AA	411	A	C5-C6-N1	8.43	121.91	117.70
21	AA	1322	C	N3-C2-O2	-8.43	116.00	121.90
22	A1	66	A	N1-C6-N6	-8.43	113.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	278	A	N1-C6-N6	-8.43	113.55	118.60
54	BA	526	A	N1-C6-N6	-8.43	113.55	118.60
21	AA	1093	A	N1-C6-N6	-8.42	113.55	118.60
7	AH	12	ARG	NE-CZ-NH1	8.42	124.51	120.30
54	BA	793	A	C5-C6-N1	8.42	121.91	117.70
54	BA	2005	A	C5-C6-N1	8.42	121.91	117.70
21	AA	1362	A	N1-C6-N6	-8.42	113.55	118.60
39	BQ	52	ARG	NE-CZ-NH1	8.42	124.51	120.30
54	BA	721	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2800	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	173	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	1786	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	273	G	O4'-C1'-N9	8.41	114.93	108.20
54	BA	513	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	2596	U	O4'-C1'-N1	8.41	114.93	108.20
54	BA	1142	A	C5-C6-N1	8.41	121.90	117.70
21	AA	1035	A	N1-C6-N6	-8.40	113.56	118.60
37	BO	111	ARG	NE-CZ-NH1	8.40	124.50	120.30
54	BA	693	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	1640	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2750	A	C5-C6-N1	8.40	121.90	117.70
54	BA	73	A	C5-C6-N1	8.40	121.90	117.70
21	AA	162	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	972	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2666	C	N3-C2-O2	-8.40	116.02	121.90
27	BE	40	ARG	NE-CZ-NH1	8.40	124.50	120.30
54	BA	1433	A	C5-C6-N1	8.39	121.90	117.70
54	BA	1590	A	N1-C6-N6	-8.39	113.56	118.60
24	A3	3	C	N3-C2-O2	-8.39	116.03	121.90
54	BA	1300	G	O4'-C1'-N9	8.39	114.92	108.20
54	BA	2340	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	222	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2755	C	O4'-C1'-N1	8.39	114.91	108.20
21	AA	975	A	N1-C6-N6	-8.39	113.57	118.60
35	BM	6	ARG	NE-CZ-NH1	8.39	124.49	120.30
54	BA	1780	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	2542	A	C5-C6-N1	8.39	121.89	117.70
21	AA	1081	A	N1-C6-N6	-8.38	113.57	118.60
33	BK	108	ARG	NE-CZ-NH1	8.38	124.49	120.30
54	BA	2333	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	182	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	2064	C	N3-C2-O2	-8.38	116.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BO	16	ARG	NE-CZ-NH1	8.37	124.49	120.30
21	AA	873	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1230	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1668	A	C5-C6-N1	8.37	121.89	117.70
54	BA	1866	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1079	C	N3-C2-O2	-8.37	116.04	121.90
21	AA	681	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	1610	A	C5-C6-N1	8.36	121.88	117.70
54	BA	156	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	933	A	C5-C6-N1	8.36	121.88	117.70
54	BA	2317	A	N1-C6-N6	-8.36	113.59	118.60
11	AL	30	ARG	NE-CZ-NH1	8.35	124.48	120.30
21	AA	1257	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	149	A	N1-C6-N6	-8.35	113.59	118.60
32	BJ	34	ARG	NE-CZ-NH1	8.35	124.47	120.30
54	BA	1626	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	182	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	802	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1100	C	N3-C2-O2	-8.35	116.06	121.90
24	A3	39	A	C5-C6-N1	8.35	121.87	117.70
54	BA	2336	A	C5-C6-N1	8.35	121.87	117.70
21	AA	452	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	886	A	C5-C6-N1	8.34	121.87	117.70
36	BN	22	ARG	NE-CZ-NH1	8.34	124.47	120.30
54	BA	1502	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	1213	A	C5-C6-N1	8.34	121.87	117.70
54	BA	1021	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	2577	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	945	A	C5-C6-N1	8.33	121.87	117.70
54	BA	460	A	C5-C6-N1	8.33	121.86	117.70
54	BA	1962	C	N3-C2-O2	-8.33	116.07	121.90
46	BX	71	ARG	NE-CZ-NH1	8.33	124.46	120.30
54	BA	743	A	N1-C6-N6	-8.33	113.61	118.60
21	AA	845	A	O4'-C1'-N9	8.32	114.86	108.20
54	BA	456	C	N1-C2-O2	8.32	123.89	118.90
54	BA	1490	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	2306	C	O4'-C1'-N1	8.32	114.86	108.20
24	A3	73	A	C5-C6-N1	8.32	121.86	117.70
54	BA	1901	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	1340	U	O4'-C1'-N1	8.31	114.85	108.20
54	BA	2042	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	77	A	N1-C6-N6	-8.31	113.61	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1180	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	509	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2114	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	1872	A	N1-C6-N6	-8.31	113.62	118.60
54	BA	1928	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	21	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	2114	A	C5-C6-N1	8.30	121.85	117.70
48	BZ	44	ARG	NE-CZ-NH1	8.29	124.45	120.30
54	BA	404	A	N1-C6-N6	-8.29	113.62	118.60
21	AA	532	A	N1-C6-N6	-8.29	113.62	118.60
21	AA	1299	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	1328	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1566	A	C5-C6-N1	8.29	121.85	117.70
54	BA	2528	U	O4'-C1'-N1	8.29	114.83	108.20
32	BJ	37	ARG	NE-CZ-NH1	8.29	124.44	120.30
21	AA	50	A	N1-C6-N6	-8.29	113.63	118.60
21	AA	71	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	793	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1918	A	N1-C6-N6	-8.28	113.63	118.60
1	AB	107	ARG	NE-CZ-NH1	8.28	124.44	120.30
21	AA	819	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	781	A	C5-C6-N1	8.28	121.84	117.70
54	BA	2792	A	C5-C6-N1	8.28	121.84	117.70
21	AA	715	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	643	A	O4'-C1'-N9	8.28	114.82	108.20
54	BA	1607	C	N3-C2-O2	-8.28	116.11	121.90
54	BA	1603	A	C5-C6-N1	8.27	121.84	117.70
54	BA	2158	A	C5-C6-N1	8.27	121.84	117.70
21	AA	1014	A	C5-C6-N1	8.27	121.83	117.70
54	BA	761	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	1808	A	C5-C6-N1	8.27	121.83	117.70
54	BA	1395	A	C5-C6-N1	8.27	121.83	117.70
18	AS	35	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	889	C	N3-C2-O2	-8.26	116.12	121.90
54	BA	481	G	O4'-C1'-N9	8.26	114.81	108.20
21	AA	397	A	C5-C6-N1	8.26	121.83	117.70
54	BA	149	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	1086	A	C5-C6-N1	8.25	121.83	117.70
55	BB	53	A	C5-C6-N1	8.25	121.82	117.70
43	BU	5	ARG	NE-CZ-NH1	8.25	124.42	120.30
21	AA	539	A	N1-C6-N6	-8.24	113.65	118.60
21	AA	1036	A	N1-C6-N6	-8.24	113.65	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1167	A	C5-C6-N1	8.24	121.82	117.70
54	BA	515	A	C5-C6-N1	8.24	121.82	117.70
54	BA	896	A	C5-C6-N1	8.24	121.82	117.70
55	BB	59	A	N1-C6-N6	-8.24	113.65	118.60
56	B5	122	ARG	NE-CZ-NH2	8.24	124.42	120.30
2	AC	131	ARG	NE-CZ-NH1	8.24	124.42	120.30
21	AA	459	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1016	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1289	A	C5-C6-N1	8.24	121.82	117.70
21	AA	1502	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	1669	A	C5-C6-N1	8.24	121.82	117.70
54	BA	2682	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1493	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	627	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2501	C	N3-C2-O2	-8.23	116.14	121.90
28	BF	149	ARG	NE-CZ-NH1	8.23	124.42	120.30
54	BA	2434	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	487	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	1264	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2134	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2147	A	C5-C6-N1	8.23	121.81	117.70
54	BA	528	A	C5-C6-N1	8.22	121.81	117.70
54	BA	2886	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	996	A	C5-C6-N1	8.21	121.81	117.70
54	BA	1919	A	C5-C6-N1	8.21	121.81	117.70
21	AA	412	A	N1-C6-N6	-8.21	113.67	118.60
37	BO	25	ARG	NE-CZ-NH1	8.21	124.41	120.30
54	BA	199	A	C5-C6-N1	8.21	121.81	117.70
54	BA	2169	A	O4'-C1'-N9	8.21	114.77	108.20
54	BA	1393	A	C5-C6-N1	8.21	121.81	117.70
21	AA	152	A	C4-C5-C6	-8.21	112.90	117.00
21	AA	676	A	C5-C6-N1	8.21	121.80	117.70
24	A3	11	A	C5-C6-N1	8.21	121.80	117.70
54	BA	2191	A	N1-C6-N6	-8.21	113.68	118.60
25	BC	257	ARG	NE-CZ-NH1	8.21	124.40	120.30
54	BA	1717	A	C5-C6-N1	8.21	121.80	117.70
54	BA	1626	A	C5-C6-N1	8.20	121.80	117.70
54	BA	2711	A	C5-C6-N1	8.20	121.80	117.70
54	BA	586	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	2117	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	2564	A	C5-C6-N1	8.20	121.80	117.70
54	BA	901	C	N3-C2-O2	-8.19	116.17	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2418	A	C5-C6-N1	8.19	121.80	117.70
21	AA	1399	C	N3-C2-O2	-8.19	116.17	121.90
21	AA	1533	C	N3-C2-O2	-8.19	116.17	121.90
54	BA	1815	A	C5-C6-N1	8.19	121.80	117.70
54	BA	541	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2199	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	1360	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2170	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	984	A	N1-C6-N6	-8.18	113.69	118.60
32	BJ	35	ARG	NE-CZ-NH1	8.18	124.39	120.30
54	BA	64	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	2476	A	C5-C6-N1	8.18	121.79	117.70
54	BA	2448	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	2458	G	O4'-C1'-N9	8.18	114.74	108.20
54	BA	91	A	O4'-C1'-N9	8.17	114.74	108.20
54	BA	833	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2826	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	14	A	C5-C6-N1	8.17	121.78	117.70
8	AI	10	ARG	NE-CZ-NH1	8.17	124.38	120.30
24	A3	58	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	1040	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	429	A	N1-C6-N6	-8.17	113.70	118.60
6	AG	3	ARG	NE-CZ-NH2	8.16	124.38	120.30
21	AA	435	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1027	A	C5-C6-N1	8.16	121.78	117.70
54	BA	1914	C	N3-C2-O2	-8.16	116.19	121.90
19	AT	24	ARG	NE-CZ-NH1	8.16	124.38	120.30
54	BA	279	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1007	C	N3-C2-O2	-8.16	116.19	121.90
54	BA	2851	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	2492	U	N3-C2-O2	-8.16	116.49	122.20
21	AA	1157	A	C5-C6-N1	8.16	121.78	117.70
27	BE	69	ARG	NE-CZ-NH1	8.16	124.38	120.30
54	BA	2212	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1147	A	C5-C6-N1	8.16	121.78	117.70
54	BA	2468	A	C5-C6-N1	8.16	121.78	117.70
54	BA	1745	A	C5-C6-N1	8.15	121.78	117.70
54	BA	1008	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1246	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	1012	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1451	C	N3-C2-O2	-8.15	116.19	121.90
54	BA	1439	A	C5-C6-N1	8.15	121.77	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AF	86	ARG	NE-CZ-NH1	8.15	124.37	120.30
54	BA	1772	A	N1-C6-N6	-8.14	113.71	118.60
24	A3	44	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	1640	A	C5-C6-N1	8.14	121.77	117.70
54	BA	631	A	C5-C6-N1	8.13	121.77	117.70
54	BA	1678	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	2412	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	781	A	C5-C6-N1	8.13	121.77	117.70
54	BA	251	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	2054	A	N1-C6-N6	-8.13	113.72	118.60
9	AJ	9	ARG	NE-CZ-NH1	8.13	124.36	120.30
54	BA	478	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1096	A	C5-C6-N1	8.13	121.76	117.70
21	AA	167	A	C5-C6-N1	8.12	121.76	117.70
54	BA	2322	A	N1-C6-N6	-8.12	113.72	118.60
54	BA	556	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	1067	A	C4-C5-C6	-8.12	112.94	117.00
21	AA	964	A	C5-C6-N1	8.12	121.76	117.70
21	AA	1269	A	C5-C6-N1	8.12	121.76	117.70
54	BA	38	A	C4-C5-C6	-8.12	112.94	117.00
54	BA	640	C	N1-C2-O2	8.12	123.77	118.90
54	BA	928	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	1346	A	C5-C6-N1	8.11	121.76	117.70
21	AA	1452	C	N3-C2-O2	-8.11	116.22	121.90
54	BA	1175	A	C5-C6-N1	8.11	121.75	117.70
11	AL	82	ARG	NE-CZ-NH1	8.11	124.36	120.30
54	BA	219	A	C5-C6-N1	8.11	121.75	117.70
54	BA	699	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2430	A	C5-C6-N1	8.11	121.75	117.70
21	AA	101	A	N1-C6-N6	-8.11	113.74	118.60
21	AA	747	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	538	A	N1-C6-N6	-8.11	113.74	118.60
21	AA	913	A	C4-C5-C6	-8.11	112.95	117.00
21	AA	1274	A	C5-C6-N1	8.11	121.75	117.70
21	AA	1150	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	1012	A	C5-C6-N1	8.10	121.75	117.70
21	AA	983	A	C5-C6-N1	8.10	121.75	117.70
55	BB	108	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	499	A	C5-C6-N1	8.09	121.75	117.70
41	BS	88	ARG	NE-CZ-NH1	8.09	124.35	120.30
25	BC	181	ARG	NE-CZ-NH1	8.09	124.35	120.30
54	BA	928	A	C5-C6-N1	8.09	121.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1385	A	N1-C6-N6	-8.09	113.74	118.60
54	BA	2749	A	N1-C6-N6	-8.09	113.74	118.60
20	AU	17	ARG	NE-CZ-NH1	8.09	124.35	120.30
54	BA	1809	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2284	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	1713	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2682	A	C5-C6-N1	8.08	121.74	117.70
21	AA	183	C	N3-C2-O2	-8.08	116.24	121.90
21	AA	915	A	C5-C6-N1	8.08	121.74	117.70
54	BA	2298	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	1110	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	83	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	723	C	N3-C2-O2	-8.08	116.25	121.90
21	AA	1285	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	1534	A	C5-C6-N1	8.07	121.74	117.70
54	BA	74	A	N1-C6-N6	-8.07	113.76	118.60
1	AB	136	ARG	NE-CZ-NH1	8.07	124.34	120.30
37	BO	7	ARG	NE-CZ-NH1	8.07	124.34	120.30
21	AA	66	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	1000	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	1130	A	C5-C6-N1	8.07	121.73	117.70
54	BA	472	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2520	C	N3-C2-O2	-8.07	116.25	121.90
21	AA	665	A	C4-C5-C6	-8.06	112.97	117.00
47	BY	52	ARG	NE-CZ-NH1	8.06	124.33	120.30
54	BA	118	A	N1-C6-N6	-8.06	113.76	118.60
25	BC	220	ARG	NE-CZ-NH1	8.06	124.33	120.30
54	BA	866	A	C5-C6-N1	8.06	121.73	117.70
54	BA	877	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	1393	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	1503	A	C5-C6-N1	8.05	121.73	117.70
54	BA	504	A	C5-C6-N1	8.05	121.73	117.70
55	BB	108	A	C5-C6-N1	8.05	121.73	117.70
21	AA	1004	A	C5-C6-N1	8.05	121.72	117.70
21	AA	1261	A	N1-C6-N6	-8.04	113.77	118.60
54	BA	981	A	C5-C6-N1	8.04	121.72	117.70
21	AA	109	A	C5-C6-N1	8.04	121.72	117.70
21	AA	1111	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	1508	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	514	A	C5-C6-N1	8.04	121.72	117.70
54	BA	2732	G	O4'-C1'-N9	8.04	114.63	108.20
21	AA	1332	A	C5-C6-N1	8.04	121.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AN	81	ARG	NE-CZ-NH1	8.04	124.32	120.30
54	BA	996	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	1020	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	1871	A	C5-C6-N1	8.04	121.72	117.70
21	AA	270	A	C5-C6-N1	8.04	121.72	117.70
21	AA	430	A	N1-C6-N6	-8.04	113.78	118.60
45	BW	76	ARG	NE-CZ-NH1	8.03	124.32	120.30
54	BA	190	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	1987	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	878	A	C5-C6-N1	8.03	121.72	117.70
21	AA	1357	A	N1-C6-N6	-8.03	113.78	118.60
55	BB	34	A	C4-C5-C6	-8.03	112.98	117.00
54	BA	735	A	C5-C6-N1	8.03	121.71	117.70
21	AA	1446	A	C5-C6-N1	8.03	121.71	117.70
54	BA	1614	A	C5-C6-N1	8.03	121.71	117.70
21	AA	969	A	C5-C6-N1	8.02	121.71	117.70
54	BA	1579	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	1754	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	1952	A	C5-C6-N1	8.02	121.71	117.70
21	AA	864	A	C5-C6-N1	8.02	121.71	117.70
54	BA	1029	A	C5-C6-N1	8.02	121.71	117.70
54	BA	1147	A	C4-C5-C6	-8.02	112.99	117.00
22	A1	73	A	N1-C6-N6	-8.01	113.79	118.60
21	AA	288	A	N1-C6-N6	-8.01	113.79	118.60
21	AA	1196	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	742	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	789	A	C5-C6-N1	8.01	121.70	117.70
54	BA	2051	A	C5-C6-N1	8.01	121.70	117.70
54	BA	644	A	C5-C6-N1	8.01	121.70	117.70
54	BA	1603	A	N1-C6-N6	-8.01	113.80	118.60
3	AD	114	ARG	NE-CZ-NH1	8.00	124.30	120.30
39	BQ	12	ARG	NE-CZ-NH2	8.00	124.30	120.30
54	BA	256	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	59	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	918	A	N1-C6-N6	-8.00	113.80	118.60
35	BM	81	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	961	C	N3-C2-O2	-8.00	116.30	121.90
21	AA	1022	A	C5-C6-N1	7.99	121.70	117.70
21	AA	1519	A	C5-C6-N1	7.99	121.70	117.70
54	BA	523	C	N3-C2-O2	-7.99	116.31	121.90
54	BA	1133	A	C5-C6-N1	7.99	121.69	117.70
54	BA	2589	A	N1-C6-N6	-7.99	113.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1434	A	C5-C6-N1	7.98	121.69	117.70
11	AL	113	ARG	NE-CZ-NH1	7.98	124.29	120.30
21	AA	693	G	O4'-C1'-N9	7.98	114.58	108.20
54	BA	1247	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	344	A	C5-C6-N1	7.98	121.69	117.70
54	BA	603	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	1544	A	C5-C6-N1	7.98	121.69	117.70
21	AA	1410	A	N1-C6-N6	-7.97	113.81	118.60
21	AA	1411	C	N3-C2-O2	-7.97	116.32	121.90
21	AA	60	A	C5-C6-N1	7.96	121.68	117.70
54	BA	2346	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	2799	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1698	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1713	A	C4-C5-C6	-7.96	113.02	117.00
43	BU	93	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	2503	A	N1-C6-N6	-7.96	113.82	118.60
21	AA	130	A	C4-C5-C6	-7.96	113.02	117.00
54	BA	371	A	C4-C5-C6	-7.96	113.02	117.00
54	BA	621	A	N1-C6-N6	-7.96	113.83	118.60
54	BA	2009	A	C5-C6-N1	7.96	121.68	117.70
54	BA	505	A	N1-C6-N6	-7.96	113.83	118.60
54	BA	1583	A	C5-C6-N1	7.96	121.68	117.70
21	AA	55	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	381	C	N3-C2-O2	-7.95	116.33	121.90
54	BA	119	A	C5-C6-N1	7.95	121.67	117.70
54	BA	1669	A	N1-C6-N6	-7.95	113.83	118.60
29	BG	152	ARG	NE-CZ-NH1	7.95	124.27	120.30
21	AA	321	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1677	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1080	A	C5-C6-N1	7.94	121.67	117.70
54	BA	1129	A	O4'-C1'-N9	7.94	114.55	108.20
54	BA	1505	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	2274	A	C5-C6-N1	7.94	121.67	117.70
54	BA	2394	C	N3-C2-O2	-7.94	116.34	121.90
21	AA	640	A	C5-C6-N1	7.93	121.67	117.70
24	A3	58	A	C5-C6-N1	7.93	121.67	117.70
54	BA	2471	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1265	A	C5-C6-N1	7.93	121.66	117.70
21	AA	738	C	N3-C2-O2	-7.93	116.35	121.90
21	AA	1346	A	N1-C6-N6	-7.93	113.84	118.60
51	B2	35	ARG	NE-CZ-NH1	7.93	124.26	120.30
54	BA	1899	A	C5-C6-N1	7.93	121.66	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	729	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1876	A	C5-C6-N1	7.92	121.66	117.70
54	BA	2417	C	N3-C2-O2	-7.92	116.35	121.90
55	BB	11	C	N3-C2-O2	-7.92	116.35	121.90
54	BA	240	C	N3-C2-O2	-7.92	116.35	121.90
54	BA	415	A	C4-C5-C6	-7.92	113.04	117.00
14	AO	88	ARG	NE-CZ-NH1	7.92	124.26	120.30
21	AA	329	A	C5-C6-N1	7.92	121.66	117.70
54	BA	689	A	C5-C6-N1	7.92	121.66	117.70
54	BA	508	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1103	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	2119	A	C5-C6-N1	7.92	121.66	117.70
54	BA	2765	A	N1-C6-N6	-7.92	113.85	118.60
55	BB	45	A	N1-C6-N6	-7.91	113.85	118.60
21	AA	72	A	N1-C6-N6	-7.91	113.85	118.60
21	AA	1499	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	2815	C	N3-C2-O2	-7.91	116.36	121.90
21	AA	28	A	N1-C6-N6	-7.91	113.86	118.60
21	AA	931	C	N3-C2-O2	-7.91	116.36	121.90
21	AA	1151	A	N1-C6-N6	-7.91	113.86	118.60
39	BQ	63	ARG	NE-CZ-NH1	7.91	124.25	120.30
54	BA	453	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	402	A	C5-C6-N1	7.91	121.65	117.70
54	BA	2734	A	N1-C6-N6	-7.91	113.86	118.60
22	A1	6	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	614	A	C5-C6-N1	7.90	121.65	117.70
43	BU	6	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	1384	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2142	A	C4-C5-C6	-7.90	113.05	117.00
21	AA	320	A	N1-C6-N6	-7.90	113.86	118.60
51	B2	39	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	614	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	322	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2873	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	366	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1394	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2740	A	C5-C6-N1	7.90	121.65	117.70
54	BA	262	A	C5-C6-N1	7.89	121.65	117.70
22	A1	66	A	C5-C6-N1	7.89	121.65	117.70
55	BB	88	C	N3-C2-O2	-7.89	116.38	121.90
21	AA	949	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	982	C	N1-C2-O2	7.89	123.63	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	191	A	C5-C6-N1	7.89	121.64	117.70
54	BA	910	A	C5-C6-N1	7.89	121.64	117.70
54	BA	2309	A	N1-C6-N6	-7.89	113.87	118.60
1	AB	207	ARG	NE-CZ-NH1	7.88	124.24	120.30
12	AM	91	ARG	NE-CZ-NH1	7.88	124.24	120.30
21	AA	65	A	O4'-C1'-N9	7.88	114.50	108.20
21	AA	1105	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	2047	C	N3-C2-O2	-7.88	116.38	121.90
54	BA	582	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	2675	A	C5-C6-N1	7.88	121.64	117.70
54	BA	384	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	706	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1040	A	C5-C6-N1	7.88	121.64	117.70
54	BA	2425	A	C4-C5-C6	-7.88	113.06	117.00
54	BA	221	A	C5-C6-N1	7.88	121.64	117.70
54	BA	152	A	C5-C6-N1	7.87	121.64	117.70
54	BA	705	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	1648	U	O4'-C1'-N1	7.87	114.50	108.20
21	AA	1214	C	N1-C2-O2	7.87	123.62	118.90
54	BA	782	A	N1-C6-N6	-7.87	113.88	118.60
13	AN	75	ARG	NE-CZ-NH1	7.87	124.23	120.30
22	A1	69	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	502	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	1453	A	C5-C6-N1	7.87	121.63	117.70
21	AA	309	A	C5-C6-N1	7.87	121.63	117.70
54	BA	655	A	C5-C6-N1	7.87	121.63	117.70
54	BA	1288	G	O4'-C1'-N9	7.87	114.49	108.20
21	AA	393	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	615	U	O4'-C1'-N1	7.86	114.49	108.20
21	AA	1283	U	O4'-C1'-N1	7.86	114.49	108.20
21	AA	1437	A	C5-C6-N1	7.86	121.63	117.70
54	BA	715	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	2019	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	2602	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	2758	A	C5-C6-N1	7.86	121.63	117.70
21	AA	1170	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1508	A	C5-C6-N1	7.86	121.63	117.70
54	BA	207	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2062	A	C5-C6-N1	7.85	121.63	117.70
21	AA	160	A	C5-C6-N1	7.85	121.63	117.70
21	AA	563	A	C5-C6-N1	7.85	121.62	117.70
54	BA	975	A	C5-C6-N1	7.85	121.62	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1677	A	C5-C6-N1	7.84	121.62	117.70
21	AA	1157	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	1678	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2288	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	1028	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	1608	A	C5-C6-N1	7.84	121.62	117.70
54	BA	28	A	C5-C6-N1	7.84	121.62	117.70
54	BA	1953	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2601	C	N3-C2-O2	-7.84	116.41	121.90
54	BA	1676	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	2606	C	N3-C2-O2	-7.83	116.42	121.90
21	AA	466	A	C5-C6-N1	7.83	121.62	117.70
54	BA	752	A	C5-C6-N1	7.83	121.62	117.70
54	BA	1965	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	172	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	324	A	C5-C6-N1	7.83	121.62	117.70
54	BA	2765	A	C5-C6-N1	7.83	121.62	117.70
21	AA	1044	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1032	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	1288	A	C5-C6-N1	7.83	121.61	117.70
2	AC	130	ARG	NE-CZ-NH2	7.83	124.21	120.30
47	BY	29	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	1522	A	C5-C6-N1	7.82	121.61	117.70
21	AA	306	A	C4-C5-C6	-7.82	113.09	117.00
21	AA	1111	A	C5-C6-N1	7.82	121.61	117.70
54	BA	241	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1155	A	N1-C6-N6	-7.82	113.91	118.60
21	AA	1176	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	877	A	C5-C6-N1	7.81	121.61	117.70
21	AA	1246	A	C4-C5-C6	-7.81	113.09	117.00
54	BA	1938	A	C5-C6-N1	7.81	121.61	117.70
54	BA	2725	A	C4-C5-C6	-7.81	113.09	117.00
54	BA	2781	A	C5-C6-N1	7.81	121.61	117.70
54	BA	1559	U	O4'-C1'-N1	7.81	114.45	108.20
54	BA	2309	A	C5-C6-N1	7.81	121.60	117.70
54	BA	1616	A	C5-C6-N1	7.81	121.60	117.70
21	AA	596	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	777	A	C5-C6-N1	7.80	121.60	117.70
21	AA	374	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	1067	A	C5-C6-N1	7.80	121.60	117.70
54	BA	786	C	N3-C2-O2	-7.80	116.44	121.90
21	AA	77	A	C5-C6-N1	7.80	121.60	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	899	C	N3-C2-O2	-7.80	116.44	121.90
22	A1	74	C	N1-C2-O2	7.80	123.58	118.90
20	AU	32	ARG	NE-CZ-NH2	7.80	124.20	120.30
21	AA	1257	A	C5-C6-N1	7.80	121.60	117.70
24	A3	35	C	N3-C2-O2	-7.80	116.44	121.90
54	BA	1070	A	C5-C6-N1	7.79	121.60	117.70
54	BA	1565	C	N3-C2-O2	-7.79	116.44	121.90
21	AA	262	A	C4-C5-C6	-7.79	113.11	117.00
54	BA	44	A	C5-C6-N1	7.79	121.60	117.70
54	BA	2015	A	C5-C6-N1	7.79	121.60	117.70
54	BA	1598	A	N1-C6-N6	-7.79	113.93	118.60
55	BB	118	C	N3-C2-O2	-7.79	116.45	121.90
21	AA	129	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	2264	C	O4'-C1'-N1	7.79	114.43	108.20
21	AA	1283	U	N3-C2-O2	-7.79	116.75	122.20
54	BA	699	A	C5-C6-N1	7.79	121.59	117.70
54	BA	896	A	C4-C5-C6	-7.79	113.11	117.00
54	BA	1007	C	N1-C2-O2	7.78	123.57	118.90
54	BA	1169	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1447	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	97	C	O4'-C1'-N1	7.78	114.43	108.20
54	BA	2776	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	264	C	N3-C2-O2	-7.78	116.45	121.90
54	BA	219	A	C4-C5-C6	-7.78	113.11	117.00
54	BA	792	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	1320	C	N1-C2-O2	7.78	123.57	118.90
54	BA	1746	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	2551	C	N3-C2-O2	-7.78	116.45	121.90
54	BA	2712	C	N3-C2-O2	-7.78	116.45	121.90
54	BA	344	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1236	A	C5-C6-N1	7.78	121.59	117.70
54	BA	532	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	920	A	N1-C6-N6	-7.78	113.94	118.60
54	BA	1354	A	N1-C6-N6	-7.78	113.93	118.60
24	A3	60	A	C5-C6-N1	7.77	121.59	117.70
54	BA	196	A	C5-C6-N1	7.77	121.59	117.70
54	BA	1175	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	630	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	160	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1244	A	N1-C6-N6	-7.77	113.94	118.60
1	AB	62	ARG	NE-CZ-NH1	7.77	124.18	120.30
54	BA	1353	A	C5-C6-N1	7.77	121.58	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1496	A	C5-C6-N1	7.77	121.58	117.70
55	BB	39	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1705	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	197	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1572	A	C5-C6-N1	7.76	121.58	117.70
55	BB	52	A	C5-C6-N1	7.76	121.58	117.70
21	AA	306	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2740	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	78	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1676	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2314	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2565	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1829	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2154	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1672	A	C5-C6-N1	7.75	121.58	117.70
54	BA	323	C	N3-C2-O2	-7.75	116.47	121.90
54	BA	2755	C	N3-C2-O2	-7.75	116.47	121.90
36	BN	86	ARG	NE-CZ-NH1	7.75	124.18	120.30
36	BN	96	ARG	NE-CZ-NH2	-7.75	116.42	120.30
21	AA	382	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	974	A	C5-C6-N1	7.75	121.57	117.70
54	BA	666	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1359	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1786	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2530	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1383	A	C5-C6-N1	7.75	121.57	117.70
54	BA	1076	C	N3-C2-O2	-7.74	116.48	121.90
54	BA	1077	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1241	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2492	U	O4'-C1'-N1	7.74	114.40	108.20
21	AA	393	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1042	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2758	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	1701	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2267	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	1048	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1912	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1965	C	O4'-C1'-N1	7.74	114.39	108.20
54	BA	144	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2860	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	815	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	1299	A	C5-C6-N1	7.73	121.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1126	A	C5-C6-N1	7.73	121.57	117.70
54	BA	1762	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	60	A	C4-C5-C6	-7.73	113.14	117.00
54	BA	176	A	C5-C6-N1	7.73	121.56	117.70
54	BA	574	A	C5-C6-N1	7.73	121.56	117.70
54	BA	685	A	C5-C6-N1	7.73	121.56	117.70
21	AA	1146	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	2052	A	C5-C6-N1	7.73	121.56	117.70
21	AA	66	A	C5-C6-N1	7.72	121.56	117.70
21	AA	909	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1580	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1650	A	N1-C6-N6	-7.72	113.97	118.60
11	AL	109	ARG	NE-CZ-NH1	7.72	124.16	120.30
21	AA	436	C	N3-C2-O2	-7.72	116.50	121.90
54	BA	6	A	C5-C6-N1	7.72	121.56	117.70
21	AA	787	A	C5-C6-N1	7.71	121.56	117.70
54	BA	640	C	C2-N3-C4	-7.71	116.05	119.90
21	AA	183	C	O4'-C1'-N1	7.71	114.37	108.20
54	BA	1755	A	C4-C5-C6	-7.71	113.14	117.00
21	AA	728	A	C5-C6-N1	7.71	121.55	117.70
54	BA	394	C	N3-C2-O2	-7.71	116.50	121.90
54	BA	1757	A	C5-C6-N1	7.71	121.55	117.70
21	AA	695	A	N1-C6-N6	-7.71	113.98	118.60
21	AA	1158	C	N1-C2-O2	7.71	123.52	118.90
2	AC	135	ARG	NE-CZ-NH1	7.71	124.15	120.30
54	BA	2088	A	N1-C6-N6	-7.71	113.98	118.60
21	AA	131	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2176	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2541	A	C5-C6-N1	7.70	121.55	117.70
21	AA	768	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	1102	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	906	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1570	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	706	A	C5-C6-N1	7.69	121.55	117.70
21	AA	732	C	N3-C2-O2	-7.69	116.52	121.90
54	BA	2060	A	C5-C6-N1	7.69	121.55	117.70
54	BA	2610	C	N1-C2-O2	7.69	123.52	118.90
27	BE	21	ARG	NE-CZ-NH1	7.69	124.14	120.30
21	AA	493	A	C5-C6-N1	7.69	121.54	117.70
21	AA	747	A	C5-C6-N1	7.68	121.54	117.70
21	AA	1246	A	C5-C6-N1	7.68	121.54	117.70
21	AA	1531	A	C5-C6-N1	7.68	121.54	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1927	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2858	C	N3-C2-O2	-7.68	116.52	121.90
21	AA	819	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1650	A	C5-C6-N1	7.68	121.54	117.70
21	AA	573	A	C5-C6-N1	7.68	121.54	117.70
54	BA	941	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1829	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	792	A	C5-C6-N1	7.68	121.54	117.70
21	AA	1096	C	N3-C2-O2	-7.68	116.52	121.90
21	AA	1167	A	N1-C6-N6	-7.68	113.99	118.60
33	BK	64	ARG	NE-CZ-NH1	7.68	124.14	120.30
21	AA	1082	A	C5-C6-N1	7.67	121.54	117.70
54	BA	718	A	O4'-C1'-N9	7.67	114.34	108.20
54	BA	2247	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	196	A	C4-C5-C6	-7.67	113.17	117.00
22	A1	74	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	668	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	1625	C	N3-C2-O2	-7.67	116.53	121.90
21	AA	1191	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1398	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1204	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	303	A	C4-C5-C6	-7.67	113.17	117.00
54	BA	19	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1349	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1548	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	621	A	C5-C6-N1	7.66	121.53	117.70
54	BA	513	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2611	C	N3-C2-O2	-7.66	116.54	121.90
21	AA	520	A	N1-C6-N6	-7.66	114.00	118.60
54	BA	582	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2700	A	N1-C6-N6	-7.66	114.00	118.60
31	BI	64	ARG	NE-CZ-NH1	7.66	124.13	120.30
54	BA	2425	A	C5-C6-N1	7.66	121.53	117.70
21	AA	907	A	C5-C6-N1	7.66	121.53	117.70
21	AA	1306	A	C5-C6-N1	7.66	121.53	117.70
21	AA	1433	A	C5-C6-N1	7.66	121.53	117.70
54	BA	911	A	N1-C6-N6	-7.66	114.00	118.60
54	BA	1169	A	C4-C5-C6	-7.65	113.17	117.00
54	BA	1937	A	C5-C6-N1	7.65	121.53	117.70
54	BA	2274	A	C4-C5-C6	-7.65	113.17	117.00
21	AA	174	A	C4-C5-C6	-7.65	113.17	117.00
22	A1	41	A	C5-C6-N1	7.65	121.53	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	990	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	1321	A	N1-C6-N6	-7.65	114.01	118.60
17	AR	62	ARG	NE-CZ-NH1	7.65	124.12	120.30
21	AA	73	C	N3-C2-O2	-7.65	116.55	121.90
21	AA	329	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	1545	A	N1-C6-N6	-7.65	114.01	118.60
55	BB	73	A	C5-C6-N1	7.65	121.53	117.70
21	AA	327	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	2417	C	O4'-C1'-N1	7.65	114.32	108.20
21	AA	1163	A	C5-C6-N1	7.64	121.52	117.70
24	A3	59	A	C5-C6-N1	7.64	121.52	117.70
21	AA	364	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	705	A	C5-C6-N1	7.64	121.52	117.70
2	AC	10	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	AD	187	ARG	NE-CZ-NH1	7.64	124.12	120.30
21	AA	576	C	C1'-O4'-C4'	-7.64	103.79	109.90
54	BA	800	A	C5-C6-N1	7.64	121.52	117.70
54	BA	878	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	2422	C	O4'-C1'-N1	7.64	114.31	108.20
54	BA	845	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2169	A	C5-C6-N1	7.64	121.52	117.70
3	AD	183	ARG	NE-CZ-NH1	7.63	124.12	120.30
54	BA	1347	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	2311	A	C5-C6-N1	7.63	121.52	117.70
54	BA	1603	A	C4-C5-C6	-7.63	113.18	117.00
21	AA	98	A	C5-C6-N1	7.63	121.52	117.70
21	AA	363	A	C5-C6-N1	7.63	121.52	117.70
21	AA	583	A	C5-C6-N1	7.63	121.52	117.70
21	AA	767	A	C4-C5-C6	-7.63	113.18	117.00
21	AA	787	A	C4-C5-C6	-7.63	113.18	117.00
54	BA	936	A	C4-C5-C6	-7.63	113.19	117.00
54	BA	470	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	1304	A	C4-C5-C6	-7.63	113.19	117.00
21	AA	50	A	C5-C6-N1	7.63	121.51	117.70
54	BA	753	A	C5-C6-N1	7.63	121.51	117.70
54	BA	1936	A	C5-C6-N1	7.63	121.51	117.70
54	BA	979	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	673	A	C4-C5-C6	-7.62	113.19	117.00
21	AA	1223	C	N3-C2-O2	-7.62	116.56	121.90
24	A3	22	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	89	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	531	C	N3-C2-O2	-7.62	116.56	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1156	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1536	C	N3-C2-O2	-7.62	116.56	121.90
54	BA	1635	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1670	C	N3-C2-O2	-7.62	116.56	121.90
54	BA	2792	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	1211	C	N3-C2-O2	-7.62	116.57	121.90
21	AA	1019	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	863	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1009	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2359	C	N3-C2-O2	-7.62	116.57	121.90
21	AA	197	A	C4-C5-C6	-7.62	113.19	117.00
21	AA	1518	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1780	A	C5-C6-N1	7.62	121.51	117.70
54	BA	466	A	C5-C6-N1	7.62	121.51	117.70
54	BA	751	A	C5-C6-N1	7.62	121.51	117.70
54	BA	223	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	2377	A	C5-C6-N1	7.61	121.51	117.70
54	BA	2432	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	947	A	C4-C5-C6	-7.61	113.19	117.00
21	AA	363	A	C4-C5-C6	-7.61	113.19	117.00
21	AA	1229	A	C5-C6-N1	7.61	121.50	117.70
54	BA	310	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	892	A	N1-C6-N6	-7.61	114.04	118.60
21	AA	1171	A	N1-C6-N6	-7.61	114.04	118.60
54	BA	2306	C	N3-C2-O2	-7.61	116.58	121.90
54	BA	1001	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	356	A	C5-C6-N1	7.60	121.50	117.70
54	BA	104	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	932	C	N3-C2-O2	-7.60	116.58	121.90
21	AA	214	C	N3-C2-O2	-7.60	116.58	121.90
21	AA	1403	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	382	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	1067	A	C5-C6-N1	7.60	121.50	117.70
21	AA	54	C	O4'-C1'-N1	7.60	114.28	108.20
54	BA	637	A	C4-C5-C6	-7.59	113.20	117.00
54	BA	2097	A	N1-C6-N6	-7.59	114.04	118.60
21	AA	977	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1885	A	C4-C5-C6	-7.59	113.20	117.00
54	BA	2241	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	127	A	C5-C6-N1	7.59	121.50	117.70
54	BA	2518	A	O4'-C1'-N9	7.59	114.27	108.20
21	AA	499	A	C4-C5-C6	-7.59	113.21	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	889	A	C5-C6-N1	7.59	121.49	117.70
54	BA	2600	A	N1-C6-N6	-7.59	114.05	118.60
15	AP	14	ARG	NE-CZ-NH1	7.58	124.09	120.30
54	BA	936	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	1023	U	O4'-C1'-N1	7.58	114.27	108.20
54	BA	1962	C	P-O3'-C3'	7.58	128.80	119.70
21	AA	238	A	C5-C6-N1	7.58	121.49	117.70
21	AA	487	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1285	A	C5-C6-N1	7.58	121.49	117.70
8	AI	112	ARG	NE-CZ-NH1	7.58	124.09	120.30
23	A2	82	A	C5-C6-N1	7.58	121.49	117.70
52	B3	44	ARG	NE-CZ-NH1	7.58	124.09	120.30
54	BA	602	A	N1-C6-N6	-7.58	114.06	118.60
54	BA	2628	C	N1-C2-O2	7.58	123.44	118.90
21	AA	1080	A	C5-C6-N1	7.57	121.49	117.70
54	BA	877	A	C4-C5-C6	-7.57	113.21	117.00
55	BB	73	A	C4-C5-C6	-7.57	113.21	117.00
45	BW	40	ARG	NE-CZ-NH1	7.57	124.09	120.30
6	AG	95	ARG	NE-CZ-NH1	7.57	124.08	120.30
54	BA	1713	A	C5-C6-N1	7.57	121.48	117.70
21	AA	996	A	C4-C5-C6	-7.57	113.22	117.00
21	AA	1105	A	C5-C6-N1	7.57	121.48	117.70
21	AA	8	A	C5-C6-N1	7.57	121.48	117.70
24	A3	40	C	N3-C2-O2	-7.57	116.60	121.90
54	BA	1746	A	C5-C6-N1	7.57	121.48	117.70
21	AA	431	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	362	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1757	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	435	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	627	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2778	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	1609	A	C5-C6-N1	7.56	121.48	117.70
54	BA	502	A	N1-C6-N6	-7.56	114.07	118.60
54	BA	2273	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2534	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2706	A	C5-C6-N1	7.55	121.48	117.70
54	BA	217	A	C5-C6-N1	7.55	121.48	117.70
21	AA	946	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	465	A	C5-C6-N1	7.55	121.47	117.70
21	AA	640	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1784	A	C4-C5-C6	-7.55	113.23	117.00
2	AC	64	ARG	NE-CZ-NH1	7.55	124.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	114	ARG	NE-CZ-NH2	-7.55	116.53	120.30
21	AA	1510	C	N3-C2-O2	-7.54	116.62	121.90
54	BA	1080	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	640	C	N1-C2-N3	7.54	124.48	119.20
21	AA	270	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	728	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	908	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	1349	A	N1-C6-N6	-7.54	114.08	118.60
43	BU	81	ARG	NE-CZ-NH1	7.54	124.07	120.30
54	BA	1328	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1664	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	599	A	N1-C6-N6	-7.54	114.08	118.60
2	AC	163	ARG	NE-CZ-NH1	7.54	124.07	120.30
21	AA	746	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	1531	A	N1-C6-N6	-7.54	114.08	118.60
55	BB	58	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	675	A	C5-C6-N1	7.53	121.47	117.70
54	BA	1489	C	N3-C2-O2	-7.53	116.63	121.90
22	A1	76	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	1637	A	C5-C6-N1	7.53	121.47	117.70
54	BA	1133	A	C4-C5-C6	-7.53	113.23	117.00
21	AA	1169	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	791	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	2422	C	N3-C2-O2	-7.53	116.63	121.90
55	BB	27	C	N3-C2-O2	-7.53	116.63	121.90
21	AA	26	A	C5-C6-N1	7.53	121.46	117.70
21	AA	704	A	C5-C6-N1	7.53	121.46	117.70
21	AA	1333	A	C5-C6-N1	7.53	121.46	117.70
21	AA	994	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1483	A	N1-C6-N6	-7.52	114.09	118.60
24	A3	3	C	N1-C2-O2	7.52	123.41	118.90
54	BA	497	A	C5-C6-N1	7.52	121.46	117.70
54	BA	886	A	C4-C5-C6	-7.52	113.24	117.00
54	BA	1580	A	C4-C5-C6	-7.52	113.24	117.00
25	BC	268	ARG	NE-CZ-NH1	7.52	124.06	120.30
54	BA	2450	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1431	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2872	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	10	A	C5-C6-N1	7.52	121.46	117.70
21	AA	718	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1046	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1260	A	C4-C5-C6	-7.52	113.24	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2095	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2835	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1201	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	526	A	C4-C5-C6	-7.51	113.24	117.00
54	BA	213	A	C5-C6-N1	7.51	121.46	117.70
54	BA	599	A	C5-C6-N1	7.51	121.46	117.70
21	AA	1513	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	1947	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	1918	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2476	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	1493	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	1899	A	N1-C6-N6	-7.51	114.10	118.60
54	BA	2483	C	N3-C2-O2	-7.51	116.64	121.90
21	AA	300	A	C5-C6-N1	7.50	121.45	117.70
54	BA	544	C	N3-C2-O2	-7.50	116.65	121.90
54	BA	2614	A	C5-C6-N1	7.50	121.45	117.70
54	BA	920	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1419	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1548	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	1854	A	C5-C6-N1	7.50	121.45	117.70
21	AA	482	A	C5-C6-N1	7.50	121.45	117.70
21	AA	938	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	541	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	800	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	1392	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2288	A	C5-C6-N1	7.50	121.45	117.70
21	AA	968	A	C5-C6-N1	7.50	121.45	117.70
54	BA	784	G	O4'-C1'-N9	7.50	114.20	108.20
29	BG	162	ARG	NE-CZ-NH1	7.50	124.05	120.30
40	BR	68	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	203	A	C5-C6-N1	7.50	121.45	117.70
54	BA	608	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2406	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1188	A	C5-C6-N1	7.49	121.45	117.70
42	BT	69	ARG	NE-CZ-NH1	7.49	124.05	120.30
54	BA	1783	A	C5-C6-N1	7.49	121.45	117.70
39	BQ	69	ARG	NE-CZ-NH1	7.49	124.05	120.30
54	BA	1451	C	O4'-C1'-N1	7.49	114.19	108.20
54	BA	1551	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	2439	A	N1-C6-N6	-7.49	114.11	118.60
21	AA	120	A	C5-C6-N1	7.49	121.44	117.70
21	AA	383	A	N1-C6-N6	-7.49	114.11	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1340	A	C4-C5-C6	-7.49	113.26	117.00
36	BN	46	ARG	NE-CZ-NH1	7.49	124.04	120.30
6	AG	69	ARG	NE-CZ-NH1	7.49	124.04	120.30
21	AA	687	A	C4-C5-C6	-7.49	113.26	117.00
54	BA	2411	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	1953	A	C4-C5-C6	-7.49	113.26	117.00
54	BA	2031	A	N1-C6-N6	-7.49	114.11	118.60
55	BB	99	A	C5-C6-N1	7.49	121.44	117.70
21	AA	906	A	N1-C6-N6	-7.48	114.11	118.60
21	AA	1429	A	C4-C5-C6	-7.48	113.26	117.00
24	A3	77	A	C5-C6-N1	7.48	121.44	117.70
35	BM	40	ARG	NE-CZ-NH1	7.48	124.04	120.30
56	B5	164	ARG	NE-CZ-NH1	7.48	124.04	120.30
7	AH	14	ARG	NE-CZ-NH1	7.48	124.04	120.30
54	BA	1140	C	O4'-C1'-N1	7.48	114.19	108.20
54	BA	603	A	O4'-C1'-N9	7.48	114.18	108.20
21	AA	282	A	C5-C6-N1	7.48	121.44	117.70
21	AA	845	A	C5-C6-N1	7.47	121.44	117.70
54	BA	477	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	1048	A	C4-C5-C6	-7.47	113.26	117.00
54	BA	2082	A	N1-C6-N6	-7.47	114.12	118.60
21	AA	461	A	C5-C6-N1	7.47	121.44	117.70
21	AA	576	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	1698	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	218	A	C5-C6-N1	7.47	121.43	117.70
54	BA	821	A	C5-C6-N1	7.47	121.43	117.70
54	BA	1810	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	2733	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	37	C	N3-C2-O2	-7.46	116.67	121.90
54	BA	890	C	N3-C2-O2	-7.46	116.67	121.90
54	BA	2388	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1847	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1180	A	C5-C6-N1	7.46	121.43	117.70
40	BR	90	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	1069	A	O4'-C1'-N9	7.46	114.17	108.20
21	AA	642	A	C5-C6-N1	7.46	121.43	117.70
26	BD	124	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	163	C	N3-C2-O2	-7.46	116.68	121.90
55	BB	36	C	N3-C2-O2	-7.46	116.68	121.90
54	BA	505	A	C5-C6-N1	7.46	121.43	117.70
26	BD	128	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	1706	C	N3-C2-O2	-7.46	116.68	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	299	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	1227	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1268	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1503	A	N1-C6-N6	-7.45	114.13	118.60
49	B0	16	ARG	NE-CZ-NH2	7.45	124.02	120.30
54	BA	2070	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1095	A	C5-C6-N1	7.45	121.42	117.70
19	AT	28	ARG	NE-CZ-NH1	7.45	124.02	120.30
21	AA	109	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	321	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1848	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2883	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	1977	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	1332	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	2632	A	C5-C6-N1	7.44	121.42	117.70
8	AI	84	ARG	NE-CZ-NH1	7.44	124.02	120.30
21	AA	131	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	696	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	935	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	131	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1254	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	1646	C	N3-C2-O2	-7.44	116.69	121.90
11	AL	11	ARG	NE-CZ-NH1	7.44	124.02	120.30
54	BA	1431	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1579	A	C5-C6-N1	7.44	121.42	117.70
21	AA	389	A	C5-C6-N1	7.43	121.42	117.70
54	BA	990	A	C5-C6-N1	7.43	121.42	117.70
21	AA	547	A	C5-C6-N1	7.43	121.42	117.70
21	AA	65	A	C5-C6-N1	7.43	121.41	117.70
21	AA	78	A	C5-C6-N1	7.43	121.42	117.70
21	AA	84	U	O4'-C1'-N1	7.43	114.14	108.20
21	AA	36	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	816	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	94	A	N1-C6-N6	-7.42	114.14	118.60
21	AA	1399	C	N1-C2-O2	7.42	123.35	118.90
21	AA	80	A	C5-C6-N1	7.42	121.41	117.70
54	BA	631	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	523	A	C5-C6-N1	7.42	121.41	117.70
54	BA	401	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1730	C	N3-C2-O2	-7.42	116.71	121.90
54	BA	2824	C	N3-C2-O2	-7.42	116.71	121.90
22	A1	69	A	C5-C6-N1	7.42	121.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	616	A	C5-C6-N1	7.42	121.41	117.70
54	BA	980	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1552	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	278	A	C5-C6-N1	7.42	121.41	117.70
54	BA	730	A	N1-C6-N6	-7.42	114.15	118.60
24	A3	76	C	P-O3'-C3'	7.42	128.60	119.70
54	BA	223	A	C5-C6-N1	7.41	121.41	117.70
21	AA	1339	A	N1-C6-N6	-7.41	114.15	118.60
21	AA	54	C	N3-C4-N4	-7.41	112.81	118.00
21	AA	608	A	C5-C6-N1	7.41	121.40	117.70
54	BA	1091	G	O4'-C1'-N9	7.41	114.13	108.20
54	BA	1286	A	C5-C6-N1	7.41	121.40	117.70
54	BA	1618	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2478	A	C5-C6-N1	7.41	121.40	117.70
54	BA	722	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2311	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	1298	U	O4'-C1'-N1	7.40	114.12	108.20
54	BA	1084	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2798	U	O4'-C1'-N1	7.40	114.12	108.20
6	AG	2	ARG	NE-CZ-NH1	7.40	124.00	120.30
54	BA	5	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	345	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1532	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	1548	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2275	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	1229	A	C4-C5-C6	-7.40	113.30	117.00
21	AA	366	A	C5-C6-N1	7.40	121.40	117.70
21	AA	912	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	1597	A	O4'-C1'-N9	7.40	114.12	108.20
54	BA	2225	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	2670	A	C5-C6-N1	7.40	121.40	117.70
21	AA	964	A	N1-C6-N6	-7.39	114.16	118.60
29	BG	68	ARG	NE-CZ-NH1	7.39	124.00	120.30
54	BA	1536	C	O4'-C1'-N1	7.39	114.11	108.20
21	AA	908	A	C5-C6-N1	7.39	121.40	117.70
3	AD	46	ARG	NE-CZ-NH1	7.39	124.00	120.30
21	AA	1476	A	C5-C6-N1	7.39	121.39	117.70
54	BA	528	A	C4-C5-C6	-7.39	113.31	117.00
35	BM	18	ARG	NE-CZ-NH1	7.39	123.99	120.30
54	BA	2147	A	C4-C5-C6	-7.39	113.31	117.00
21	AA	81	A	N1-C6-N6	-7.39	114.17	118.60
21	AA	909	A	N1-C6-N6	-7.39	114.17	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	788	A	C5-C6-N1	7.39	121.39	117.70
54	BA	2598	A	C5-C6-N1	7.39	121.39	117.70
54	BA	613	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	2278	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	2448	A	C5-C6-N1	7.38	121.39	117.70
21	AA	1093	A	C5-C6-N1	7.38	121.39	117.70
54	BA	79	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	2268	A	C5-C6-N1	7.38	121.39	117.70
21	AA	320	A	C5-C6-N1	7.38	121.39	117.70
54	BA	267	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	229	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	2738	A	N1-C6-N6	-7.38	114.17	118.60
6	AG	52	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	67	C	N3-C2-O2	-7.38	116.73	121.90
21	AA	629	A	C5-C6-N1	7.38	121.39	117.70
21	AA	915	A	C4-C5-C6	-7.38	113.31	117.00
21	AA	1465	A	C5-C6-N1	7.38	121.39	117.70
21	AA	412	A	C5-C6-N1	7.38	121.39	117.70
54	BA	661	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	1304	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1615	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	151	A	C5-C6-N1	7.37	121.39	117.70
21	AA	759	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	13	A	C5-C6-N1	7.37	121.39	117.70
54	BA	71	A	C5-C6-N1	7.37	121.39	117.70
54	BA	101	A	O4'-C1'-N9	7.37	114.10	108.20
54	BA	2126	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2665	A	C5-C6-N1	7.37	121.39	117.70
54	BA	53	A	C5-C6-N1	7.37	121.38	117.70
54	BA	1451	C	N1-C2-O2	7.37	123.32	118.90
54	BA	2899	A	C5-C6-N1	7.37	121.38	117.70
21	AA	889	A	C4-C5-C6	-7.37	113.32	117.00
21	AA	1418	A	C5-C6-N1	7.37	121.38	117.70
54	BA	1050	A	C5-C6-N1	7.37	121.38	117.70
54	BA	2741	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	781	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	1342	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2703	C	N3-C2-O2	-7.36	116.75	121.90
6	AG	110	ARG	NE-CZ-NH1	7.36	123.98	120.30
39	BQ	47	ARG	NE-CZ-NH1	7.36	123.98	120.30
21	AA	349	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	176	A	C4-C5-C6	-7.36	113.32	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	947	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2711	A	C4-C5-C6	-7.36	113.32	117.00
21	AA	189	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	821	A	C4-C5-C6	-7.36	113.32	117.00
54	BA	1088	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2062	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	103	A	C5-C6-N1	7.36	121.38	117.70
54	BA	715	A	C5-C6-N1	7.36	121.38	117.70
54	BA	677	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	746	A	C5-C6-N1	7.35	121.38	117.70
54	BA	892	A	C4-C5-C6	-7.35	113.33	117.00
54	BA	1787	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	1055	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	1155	A	C5-C6-N1	7.35	121.37	117.70
21	AA	1287	A	C5-C6-N1	7.35	121.37	117.70
54	BA	1469	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1735	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	2547	A	C5-C6-N1	7.35	121.37	117.70
21	AA	238	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	2392	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1008	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2077	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	2660	A	O4'-C1'-N9	7.34	114.08	108.20
21	AA	1369	C	N3-C2-O2	-7.34	116.76	121.90
21	AA	1378	C	N3-C2-O2	-7.34	116.76	121.90
21	AA	16	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	2868	A	C5-C6-N1	7.34	121.37	117.70
21	AA	817	C	N3-C2-O2	-7.34	116.76	121.90
28	BF	132	ARG	NE-CZ-NH1	7.34	123.97	120.30
4	AE	92	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	1913	A	C5-C6-N1	7.33	121.37	117.70
21	AA	163	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	447	A	C5-C6-N1	7.33	121.36	117.70
54	BA	718	A	C5-C6-N1	7.33	121.37	117.70
21	AA	535	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2287	A	O4'-C1'-N9	7.33	114.06	108.20
54	BA	449	A	C5-C6-N1	7.33	121.36	117.70
54	BA	634	C	N3-C2-O2	-7.33	116.77	121.90
21	AA	313	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2757	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	325	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2634	A	C4-C5-C6	-7.32	113.34	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	352	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2063	C	N3-C2-O2	-7.32	116.77	121.90
21	AA	1278	G	P-O3'-C3'	7.32	128.48	119.70
54	BA	152	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	812	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	1285	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	2184	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	2893	A	C5-C6-N1	7.32	121.36	117.70
21	AA	574	A	C5-C6-N1	7.32	121.36	117.70
54	BA	103	A	C4-C5-C6	-7.32	113.34	117.00
21	AA	496	A	C5-C6-N1	7.32	121.36	117.70
21	AA	975	A	O4'-C1'-N9	7.32	114.05	108.20
54	BA	126	A	C5-C6-N1	7.32	121.36	117.70
54	BA	829	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2517	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	1784	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2856	A	N1-C6-N6	-7.31	114.21	118.60
21	AA	53	A	C4-C5-C6	-7.31	113.34	117.00
54	BA	1502	A	C4-C5-C6	-7.31	113.34	117.00
14	AO	71	ARG	NE-CZ-NH1	7.31	123.95	120.30
21	AA	1413	A	C4-C5-C6	-7.31	113.35	117.00
24	A3	59	A	C4-C5-C6	-7.31	113.35	117.00
54	BA	74	A	C5-C6-N1	7.31	121.35	117.70
54	BA	472	A	C5-C6-N1	7.31	121.35	117.70
54	BA	671	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	2800	A	C5-C6-N1	7.31	121.35	117.70
21	AA	781	A	N1-C6-N6	-7.31	114.22	118.60
21	AA	177	G	O4'-C1'-N9	7.30	114.04	108.20
54	BA	2266	A	C5-C6-N1	7.30	121.35	117.70
21	AA	969	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	1634	A	N1-C6-N6	-7.30	114.22	118.60
22	A1	35	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2169	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	399	U	O4'-C1'-N1	7.30	114.04	108.20
54	BA	899	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2376	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1109	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	1593	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	575	A	C5-C6-N1	7.29	121.35	117.70
54	BA	820	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	765	G	O4'-C1'-N9	7.29	114.03	108.20
54	BA	973	A	N1-C6-N6	-7.29	114.22	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1803	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	630	A	C5-C6-N1	7.29	121.35	117.70
23	A2	79	A	C5-C6-N1	7.29	121.35	117.70
54	BA	38	A	C5-C6-N1	7.29	121.35	117.70
54	BA	2450	A	C4-C5-C6	-7.29	113.36	117.00
21	AA	371	A	C5-C6-N1	7.29	121.34	117.70
21	AA	749	A	C4-C5-C6	-7.29	113.36	117.00
54	BA	1630	A	C4-C5-C6	-7.29	113.36	117.00
24	A3	75	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	439	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	1378	A	C5-C6-N1	7.29	121.34	117.70
54	BA	1938	A	N1-C6-N6	-7.29	114.23	118.60
21	AA	949	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1566	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	560	A	C5-C6-N1	7.28	121.34	117.70
54	BA	382	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1420	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1490	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1806	C	N3-C2-O2	-7.28	116.80	121.90
54	BA	2513	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	1293	C	N3-C2-O2	-7.28	116.81	121.90
21	AA	1377	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	574	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	1395	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	1507	A	C5-C6-N1	7.28	121.34	117.70
54	BA	532	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1165	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1433	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	1655	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	1899	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	2757	A	C5-C6-N1	7.28	121.34	117.70
21	AA	373	A	N1-C6-N6	-7.27	114.24	118.60
21	AA	860	A	N1-C6-N6	-7.27	114.24	118.60
54	BA	2191	A	C5-C6-N1	7.27	121.34	117.70
54	BA	2565	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	768	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1264	A	C5-C6-N1	7.27	121.34	117.70
54	BA	2059	A	C5-C6-N1	7.27	121.34	117.70
21	AA	808	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	2346	A	C5-C6-N1	7.27	121.33	117.70
54	BA	613	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1144	A	N1-C6-N6	-7.27	114.24	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	988	A	C5-C6-N1	7.27	121.33	117.70
21	AA	136	C	N3-C2-O2	-7.26	116.82	121.90
21	AA	554	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1308	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2646	C	N3-C2-O2	-7.26	116.81	121.90
24	A3	1	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	1062	G	O4'-C1'-N9	7.26	114.01	108.20
54	BA	959	A	O4'-C1'-N9	7.26	114.01	108.20
54	BA	1469	A	C5-C6-N1	7.26	121.33	117.70
21	AA	74	A	C5-C6-N1	7.26	121.33	117.70
21	AA	566	G	P-O3'-C3'	7.26	128.41	119.70
54	BA	603	A	C5-C6-N1	7.26	121.33	117.70
54	BA	995	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	1668	A	C4-C5-C6	-7.26	113.37	117.00
21	AA	1374	A	N1-C6-N6	-7.26	114.25	118.60
55	BB	29	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1785	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1427	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	1794	A	C5-C6-N1	7.25	121.33	117.70
2	AC	39	ARG	NE-CZ-NH1	7.25	123.93	120.30
21	AA	250	A	C5-C6-N1	7.25	121.33	117.70
54	BA	449	A	C4-C5-C6	-7.25	113.37	117.00
54	BA	507	A	C5-C6-N1	7.25	121.33	117.70
21	AA	186	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	280	C	N3-C2-O2	-7.25	116.83	121.90
54	BA	1759	A	C4-C5-C6	-7.25	113.38	117.00
55	BB	94	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1649	G	O4'-C1'-N9	7.25	114.00	108.20
54	BA	2297	A	N1-C6-N6	-7.25	114.25	118.60
22	A1	26	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2278	A	C5-C6-N1	7.24	121.32	117.70
21	AA	1352	C	N3-C2-O2	-7.24	116.83	121.90
21	AA	1395	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	556	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2164	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	2198	A	C5-C6-N1	7.24	121.32	117.70
55	BB	15	A	C5-C6-N1	7.24	121.32	117.70
21	AA	205	A	C5-C6-N1	7.24	121.32	117.70
21	AA	288	A	C4-C5-C6	-7.24	113.38	117.00
21	AA	199	A	C5-C6-N1	7.24	121.32	117.70
21	AA	1508	A	C5-C6-N1	7.24	121.32	117.70
41	BS	25	ARG	NE-CZ-NH1	7.24	123.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2761	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	480	A	C5-C6-N1	7.23	121.32	117.70
54	BA	1644	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	2434	A	C5-C6-N1	7.23	121.32	117.70
21	AA	192	A	C4-C5-C6	-7.23	113.38	117.00
54	BA	1759	A	C5-C6-N1	7.23	121.32	117.70
12	AM	112	ARG	NE-CZ-NH1	7.23	123.92	120.30
21	AA	414	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	2820	A	C5-C6-N1	7.23	121.31	117.70
55	BB	97	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	336	A	C4-C5-C6	-7.23	113.39	117.00
54	BA	547	A	C5-C6-N1	7.23	121.31	117.70
54	BA	626	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2386	A	C4-C5-C6	-7.23	113.39	117.00
21	AA	631	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	2094	A	C5-C6-N1	7.23	121.31	117.70
21	AA	949	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	2327	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2666	C	N1-C2-O2	7.22	123.23	118.90
54	BA	2721	A	C5-C6-N1	7.22	121.31	117.70
55	BB	99	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	265	A	C5-C6-N1	7.22	121.31	117.70
54	BA	347	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2515	C	N3-C2-O2	-7.22	116.84	121.90
54	BA	2749	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2886	A	C5-C6-N1	7.22	121.31	117.70
21	AA	328	C	P-O3'-C3'	7.22	128.37	119.70
28	BF	114	ARG	NE-CZ-NH1	7.22	123.91	120.30
54	BA	1650	A	C4-C5-C6	-7.22	113.39	117.00
21	AA	607	A	C5-C6-N1	7.22	121.31	117.70
54	BA	33	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	1553	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2163	A	C5-C6-N1	7.22	121.31	117.70
21	AA	274	A	C5-C6-N1	7.22	121.31	117.70
21	AA	807	A	C5-C6-N1	7.22	121.31	117.70
54	BA	94	A	C5-C6-N1	7.22	121.31	117.70
54	BA	514	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	787	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	1821	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	2183	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2322	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2227	A	N1-C6-N6	-7.21	114.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	622	A	C5-C6-N1	7.21	121.31	117.70
21	AA	44	A	N1-C6-N6	-7.21	114.27	118.60
53	B4	19	ARG	NE-CZ-NH1	7.21	123.91	120.30
54	BA	352	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	1942	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	2635	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	2761	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1569	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2435	A	C4-C5-C6	-7.21	113.39	117.00
21	AA	371	A	C4-C5-C6	-7.21	113.39	117.00
21	AA	509	A	C5-C6-N1	7.21	121.30	117.70
21	AA	1325	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	1978	A	C5-C6-N1	7.21	121.30	117.70
21	AA	1239	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2748	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	1378	A	N1-C6-N6	-7.20	114.28	118.60
39	BQ	29	ARG	NE-CZ-NH2	7.20	123.90	120.30
54	BA	323	C	N1-C2-O2	7.20	123.22	118.90
54	BA	761	A	C5-C6-N1	7.20	121.30	117.70
54	BA	632	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1287	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	2882	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	223	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	2385	C	O4'-C1'-N1	7.20	113.96	108.20
54	BA	2586	U	N3-C2-O2	-7.20	117.16	122.20
54	BA	2587	A	C5-C6-N1	7.20	121.30	117.70
55	BB	115	A	N1-C6-N6	-7.19	114.28	118.60
21	AA	856	C	N3-C2-O2	-7.19	116.86	121.90
54	BA	944	C	O4'-C1'-N1	7.19	113.95	108.20
54	BA	2628	C	O4'-C1'-N1	7.19	113.95	108.20
54	BA	1278	C	O4'-C1'-N1	7.19	113.95	108.20
14	AO	76	ARG	NE-CZ-NH1	7.19	123.89	120.30
54	BA	2101	A	C5-C6-N1	7.19	121.30	117.70
21	AA	726	C	N3-C2-O2	-7.19	116.87	121.90
54	BA	226	A	C5-C6-N1	7.19	121.29	117.70
54	BA	1046	A	C5-C6-N1	7.19	121.29	117.70
21	AA	572	A	C5-C6-N1	7.19	121.29	117.70
54	BA	340	A	C5-C6-N1	7.19	121.29	117.70
21	AA	171	A	C5-C6-N1	7.18	121.29	117.70
54	BA	182	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1322	A	C5-C6-N1	7.18	121.29	117.70
16	AQ	61	ARG	NE-CZ-NH1	7.18	123.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1470	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1591	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2033	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2534	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	372	C	C1'-O4'-C4'	-7.17	104.16	109.90
21	AA	502	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1499	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1970	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2103	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	642	A	N1-C6-N6	-7.17	114.30	118.60
24	A3	22	A	C5-C6-N1	7.17	121.29	117.70
25	BC	79	ARG	NE-CZ-NH1	7.17	123.89	120.30
54	BA	1655	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1912	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2281	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	2426	A	C4-C5-C6	-7.17	113.41	117.00
21	AA	110	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	313	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	1073	A	N1-C6-N6	-7.17	114.30	118.60
46	BX	56	ARG	NE-CZ-NH1	7.17	123.88	120.30
54	BA	414	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	1802	A	N1-C6-N6	-7.17	114.30	118.60
55	BB	24	G	O4'-C1'-N9	7.17	113.93	108.20
21	AA	796	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	391	A	C5-C6-N1	7.16	121.28	117.70
54	BA	586	A	C5-C6-N1	7.16	121.28	117.70
11	AL	30	ARG	NE-CZ-NH2	-7.16	116.72	120.30
21	AA	129	A	C5-C6-N1	7.16	121.28	117.70
21	AA	919	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	1311	A	C5-C6-N1	7.16	121.28	117.70
51	B2	34	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	216	A	N1-C6-N6	-7.16	114.30	118.60
21	AA	498	A	C5-C6-N1	7.16	121.28	117.70
22	A1	66	A	C4-C5-C6	-7.16	113.42	117.00
54	BA	621	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2374	C	N3-C2-O2	-7.16	116.89	121.90
22	A1	76	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2082	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2823	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	227	A	O4'-C1'-N9	7.15	113.92	108.20
54	BA	2426	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1253	A	C5-C6-N1	7.15	121.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	205	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	849	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1029	A	C4-C5-C6	-7.15	113.42	117.00
22	A1	48	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	1414	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	2020	A	C5-C6-N1	7.15	121.27	117.70
21	AA	195	A	C5-C6-N1	7.15	121.27	117.70
21	AA	356	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	309	A	C4-C5-C6	-7.15	113.43	117.00
21	AA	182	A	C5-C6-N1	7.14	121.27	117.70
21	AA	415	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1284	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	1780	A	O4'-C1'-N9	7.14	113.92	108.20
21	AA	559	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1112	C	N3-C2-O2	-7.14	116.90	121.90
24	A3	36	A	C5-C6-N1	7.14	121.27	117.70
54	BA	482	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1571	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	1802	A	C5-C6-N1	7.14	121.27	117.70
21	AA	546	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1360	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	923	A	C5-C6-N1	7.14	121.27	117.70
54	BA	829	A	N1-C6-N6	-7.14	114.32	118.60
54	BA	1006	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1569	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	2468	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	872	A	N1-C6-N6	-7.14	114.32	118.60
21	AA	1319	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1000	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	893	C	N3-C2-O2	-7.14	116.91	121.90
2	AC	171	ARG	NE-CZ-NH2	7.13	123.87	120.30
54	BA	167	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	77	A	C4-C5-C6	-7.13	113.43	117.00
21	AA	1333	A	C4-C5-C6	-7.13	113.43	117.00
31	BI	133	ARG	NE-CZ-NH1	7.13	123.87	120.30
54	BA	845	A	C4-C5-C6	-7.13	113.43	117.00
21	AA	1350	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1551	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2248	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	936	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1085	A	C5-C6-N1	7.13	121.27	117.70
21	AA	564	C	N3-C2-O2	-7.13	116.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1275	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	1467	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	404	A	C5-C6-N1	7.13	121.26	117.70
54	BA	2077	A	C5-C6-N1	7.13	121.26	117.70
21	AA	143	A	C5-C6-N1	7.12	121.26	117.70
21	AA	298	A	C5-C6-N1	7.12	121.26	117.70
21	AA	934	C	N3-C2-O2	-7.12	116.91	121.90
21	AA	1063	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	1090	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2840	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	331	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	841	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	328	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	1252	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2657	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1031	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	22	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	2572	A	C5-C6-N1	7.12	121.26	117.70
56	B5	9	ARG	NE-CZ-NH1	7.12	123.86	120.30
11	AL	98	ARG	NE-CZ-NH1	7.11	123.86	120.30
21	AA	1136	C	N3-C2-O2	-7.11	116.92	121.90
32	BJ	13	ARG	NE-CZ-NH1	7.11	123.86	120.30
21	AA	959	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2377	A	C4-C5-C6	-7.11	113.44	117.00
21	AA	139	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	609	A	C5-C6-N1	7.11	121.25	117.70
54	BA	173	A	C5-C6-N1	7.11	121.25	117.70
21	AA	549	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	994	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	2146	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	2358	A	C5-C6-N1	7.11	121.25	117.70
21	AA	98	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	1226	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2339	C	N3-C2-O2	-7.11	116.93	121.90
21	AA	1019	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1550	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	2145	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	411	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	1549	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1449	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	844	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	1028	A	C5-C6-N1	7.10	121.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2872	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1493	A	C5-C6-N1	7.09	121.25	117.70
22	A1	58	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1327	A	N1-C6-N6	-7.09	114.34	118.60
54	BA	2170	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2883	A	C5-C6-N1	7.09	121.25	117.70
21	AA	478	A	N1-C6-N6	-7.09	114.34	118.60
54	BA	2726	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2823	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2850	A	C5-C6-N1	7.09	121.25	117.70
54	BA	878	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1454	C	O4'-C1'-N1	7.09	113.87	108.20
21	AA	1363	A	C5-C6-N1	7.09	121.24	117.70
21	AA	217	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	338	A	C5-C6-N1	7.09	121.24	117.70
54	BA	1359	A	C5-C6-N1	7.09	121.24	117.70
55	BB	109	A	C4-C5-C6	-7.09	113.46	117.00
21	AA	1176	A	C5-C6-N1	7.08	121.24	117.70
21	AA	1196	A	C5-C6-N1	7.08	121.24	117.70
54	BA	385	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	1020	A	C5-C6-N1	7.08	121.24	117.70
21	AA	984	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	1314	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	2211	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	1365	A	C5-C6-N1	7.08	121.24	117.70
54	BA	233	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1598	A	C5-C6-N1	7.08	121.24	117.70
22	A1	16	C	N3-C2-O2	-7.08	116.95	121.90
42	BT	3	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	222	A	C5-C6-N1	7.08	121.24	117.70
54	BA	670	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2212	A	C5-C6-N1	7.08	121.24	117.70
11	AL	8	ARG	NE-CZ-NH1	7.07	123.84	120.30
21	AA	1200	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	899	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	1901	A	C5-C6-N1	7.07	121.24	117.70
54	BA	2378	A	C4-C5-C6	-7.07	113.46	117.00
21	AA	63	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	192	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1532	A	C5-C6-N1	7.07	121.24	117.70
21	AA	1092	A	C5-C6-N1	7.07	121.23	117.70
54	BA	457	A	N1-C6-N6	-7.07	114.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	960	A	C5-C6-N1	7.07	121.23	117.70
21	AA	124	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1073	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2503	A	C5-C6-N1	7.07	121.23	117.70
1	AB	224	ARG	NE-CZ-NH1	7.07	123.83	120.30
21	AA	794	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	2829	A	C4-C5-C6	-7.07	113.47	117.00
21	AA	339	C	N3-C2-O2	-7.06	116.95	121.90
21	AA	520	A	C5-C6-N1	7.06	121.23	117.70
55	BB	35	C	N3-C2-O2	-7.06	116.95	121.90
21	AA	189	A	C5-C6-N1	7.06	121.23	117.70
21	AA	441	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	10	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	483	A	C5-C6-N1	7.06	121.23	117.70
54	BA	730	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2433	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2752	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	2058	A	C5-C6-N1	7.06	121.23	117.70
22	A1	6	A	C5-C6-N1	7.06	121.23	117.70
54	BA	503	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2850	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2336	A	N1-C6-N6	-7.06	114.37	118.60
6	AG	137	ARG	NE-CZ-NH1	7.05	123.83	120.30
54	BA	197	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1415	U	O4'-C1'-N1	7.05	113.84	108.20
54	BA	2009	A	C4-C5-C6	-7.05	113.47	117.00
8	AI	48	ARG	NE-CZ-NH1	7.05	123.83	120.30
29	BG	148	ARG	NE-CZ-NH1	7.05	123.83	120.30
54	BA	357	C	N3-C2-O2	-7.05	116.97	121.90
21	AA	74	A	C4-C5-C6	-7.05	113.48	117.00
21	AA	620	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	430	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	901	C	O4'-C1'-N1	7.05	113.84	108.20
54	BA	927	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1541	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	1728	C	N3-C2-O2	-7.05	116.97	121.90
55	BB	101	A	N1-C6-N6	-7.04	114.37	118.60
21	AA	702	A	C5-C6-N1	7.04	121.22	117.70
54	BA	42	A	C5-C6-N1	7.04	121.22	117.70
54	BA	764	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1044	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	265	A	O4'-C1'-N9	7.04	113.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	515	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	685	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	2439	A	C5-C6-N1	7.04	121.22	117.70
21	AA	32	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	900	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1388	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	1161	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	2733	A	C5-C6-N1	7.04	121.22	117.70
21	AA	938	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1050	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	1089	A	C5-C6-N1	7.04	121.22	117.70
54	BA	182	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2518	A	C5-C6-N1	7.03	121.22	117.70
21	AA	262	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2682	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	147	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1010	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1167	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	2856	A	C5-C6-N1	7.03	121.22	117.70
48	BZ	10	ARG	NE-CZ-NH1	7.03	123.81	120.30
54	BA	1347	A	C5-C6-N1	7.03	121.21	117.70
55	BB	46	A	C5-C6-N1	7.03	121.22	117.70
21	AA	336	A	C5-C6-N1	7.03	121.21	117.70
21	AA	526	C	N3-C2-O2	-7.03	116.98	121.90
21	AA	704	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	428	A	C5-C6-N1	7.03	121.21	117.70
54	BA	2465	C	O4'-C1'-N1	7.03	113.82	108.20
21	AA	1434	A	C5-C6-N1	7.03	121.21	117.70
54	BA	668	A	C5-C6-N1	7.03	121.21	117.70
54	BA	1937	A	C4-C5-C6	-7.03	113.49	117.00
55	BB	99	A	O4'-C1'-N9	7.03	113.82	108.20
21	AA	303	A	C5-C6-N1	7.02	121.21	117.70
21	AA	937	A	C4-C5-C6	-7.02	113.49	117.00
48	BZ	29	ARG	NE-CZ-NH1	7.02	123.81	120.30
54	BA	1151	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1101	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1021	A	C5-C6-N1	7.02	121.21	117.70
54	BA	151	C	N3-C2-O2	-7.02	116.99	121.90
54	BA	1096	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	654	A	C5-C6-N1	7.02	121.21	117.70
54	BA	925	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1791	A	C5-C6-N1	7.02	121.21	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	45	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1571	A	C5-C6-N1	7.02	121.21	117.70
21	AA	595	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	1146	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	2738	A	C5-C6-N1	7.01	121.21	117.70
55	BB	115	A	C5-C6-N1	7.01	121.21	117.70
55	BB	39	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	1468	A	C5-C6-N1	7.01	121.20	117.70
54	BA	91	A	C5-C6-N1	7.01	121.20	117.70
54	BA	609	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	641	U	O4'-C1'-N1	7.01	113.81	108.20
54	BA	1291	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	647	C	N3-C2-O2	-7.01	117.00	121.90
21	AA	1278	G	N3-C2-N2	-7.01	115.00	119.90
21	AA	1469	C	N3-C2-O2	-7.01	117.00	121.90
54	BA	52	A	N1-C6-N6	-7.01	114.40	118.60
54	BA	1039	A	C5-C6-N1	7.01	121.20	117.70
21	AA	325	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	901	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1635	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1076	C	N1-C2-O2	7.00	123.10	118.90
54	BA	1504	A	C5-C6-N1	7.00	121.20	117.70
21	AA	496	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	1441	A	N1-C6-N6	-7.00	114.40	118.60
55	BB	57	A	C5-C6-N1	7.00	121.20	117.70
21	AA	547	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	2507	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	223	A	C5-C6-N1	7.00	121.20	117.70
24	A3	74	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2432	A	C5-C6-N1	7.00	121.20	117.70
21	AA	522	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	1066	U	O4'-C1'-N1	7.00	113.80	108.20
54	BA	1088	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	1495	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1688	U	O4'-C1'-N1	7.00	113.80	108.20
54	BA	1936	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	1100	C	N1-C2-O2	6.99	123.10	118.90
35	BM	10	ARG	NE-CZ-NH1	6.99	123.80	120.30
54	BA	1434	A	O4'-C1'-N9	6.99	113.80	108.20
54	BA	221	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	1387	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	2358	A	N1-C6-N6	-6.99	114.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	448	A	C5-C6-N1	6.99	121.19	117.70
21	AA	695	A	C4-C5-C6	-6.99	113.50	117.00
21	AA	1055	A	C5-C6-N1	6.99	121.20	117.70
54	BA	213	A	C4-C5-C6	-6.99	113.50	117.00
21	AA	389	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	1939	U	O4'-C1'-N1	6.99	113.79	108.20
54	BA	2270	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2298	A	C5-C6-N1	6.99	121.19	117.70
54	BA	384	A	C5-C6-N1	6.99	121.19	117.70
21	AA	19	A	C5-C6-N1	6.98	121.19	117.70
21	AA	207	C	N3-C2-O2	-6.98	117.01	121.90
22	A1	38	A	C5-C6-N1	6.98	121.19	117.70
54	BA	155	A	C5-C6-N1	6.98	121.19	117.70
54	BA	179	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	480	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	2378	A	C5-C6-N1	6.98	121.19	117.70
21	AA	696	A	C5-C6-N1	6.98	121.19	117.70
54	BA	204	A	C5-C6-N1	6.98	121.19	117.70
54	BA	249	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	1596	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2482	A	C5-C6-N1	6.98	121.19	117.70
44	BV	19	ARG	NE-CZ-NH1	6.98	123.79	120.30
54	BA	2814	A	C5-C6-N1	6.98	121.19	117.70
21	AA	501	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	216	A	C5-C6-N1	6.98	121.19	117.70
54	BA	279	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1086	A	O4'-C1'-N9	6.98	113.78	108.20
21	AA	546	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	1141	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	130	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1609	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	1827	U	O4'-C1'-N1	6.97	113.78	108.20
21	AA	1400	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2129	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2547	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	2900	A	C5-C6-N1	6.97	121.19	117.70
21	AA	174	A	C5-C6-N1	6.97	121.18	117.70
21	AA	179	A	C4-C5-C6	-6.97	113.52	117.00
21	AA	1306	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	961	C	N1-C2-O2	6.97	123.08	118.90
54	BA	1117	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	1352	U	N3-C2-O2	-6.97	117.32	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1999	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2726	A	C5-C6-N1	6.97	121.18	117.70
24	A3	39	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	1027	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	1596	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	1705	A	C5-C6-N1	6.97	121.18	117.70
24	A3	42	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	426	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	2042	A	C5-C6-N1	6.96	121.18	117.70
24	A3	16	C	N1-C2-O2	6.96	123.08	118.90
54	BA	479	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1204	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1502	A	C5-C6-N1	6.96	121.18	117.70
28	BF	147	ARG	NE-CZ-NH1	6.96	123.78	120.30
21	AA	194	C	N3-C2-O2	-6.96	117.03	121.90
22	A1	26	A	C4-C5-C6	-6.96	113.52	117.00
24	A3	69	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	959	A	C5-C6-N1	6.96	121.18	117.70
54	BA	227	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1606	C	N1-C2-O2	6.96	123.07	118.90
54	BA	1815	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	2366	A	N1-C6-N6	-6.96	114.43	118.60
21	AA	1507	A	N1-C6-N6	-6.96	114.43	118.60
22	A1	71	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	627	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	643	A	C5-C6-N1	6.96	121.18	117.70
54	BA	756	A	C5-C6-N1	6.96	121.18	117.70
21	AA	865	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	1213	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	1247	A	C5-C6-N1	6.95	121.18	117.70
54	BA	2561	U	O4'-C1'-N1	6.95	113.76	108.20
55	BB	108	A	C4-C5-C6	-6.95	113.52	117.00
21	AA	161	A	C5-C6-N1	6.95	121.18	117.70
54	BA	635	C	N3-C2-O2	-6.95	117.03	121.90
21	AA	206	C	N3-C2-O2	-6.95	117.03	121.90
50	B1	27	ARG	NE-CZ-NH1	6.95	123.78	120.30
54	BA	119	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	348	A	C5-C6-N1	6.95	121.17	117.70
54	BA	529	A	C5-C6-N1	6.95	121.18	117.70
54	BA	743	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2352	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	825	A	C4-C5-C6	-6.95	113.53	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	992	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	1496	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	2030	A	C5-C6-N1	6.95	121.17	117.70
21	AA	155	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	286	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	1155	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	1544	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	1739	A	C5-C6-N1	6.95	121.17	117.70
21	AA	431	A	C5-C6-N1	6.94	121.17	117.70
21	AA	478	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1801	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1957	C	O4'-C1'-N1	6.94	113.76	108.20
54	BA	2813	A	C5-C6-N1	6.94	121.17	117.70
21	AA	1130	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	550	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	1145	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	2600	A	C5-C6-N1	6.94	121.17	117.70
54	BA	143	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	1632	A	N1-C6-N6	-6.94	114.44	118.60
21	AA	695	A	C5-C6-N1	6.94	121.17	117.70
17	AR	60	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	2639	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	295	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	658	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	984	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1847	A	C4-C5-C6	-6.93	113.53	117.00
55	BB	52	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	432	A	C5-C6-N1	6.93	121.17	117.70
54	BA	460	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	602	A	C5-C6-N1	6.93	121.16	117.70
21	AA	780	A	C4-C5-C6	-6.93	113.54	117.00
21	AA	937	A	C5-C6-N1	6.93	121.16	117.70
21	AA	1413	A	C5-C6-N1	6.93	121.16	117.70
54	BA	666	A	C5-C6-N1	6.93	121.16	117.70
21	AA	73	C	N1-C2-O2	6.92	123.05	118.90
21	AA	716	A	C5-C6-N1	6.92	121.16	117.70
21	AA	878	A	N1-C6-N6	-6.92	114.44	118.60
21	AA	1245	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	829	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1833	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	2902	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	1585	C	N3-C2-O2	-6.92	117.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	188	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	228	A	C5-C6-N1	6.92	121.16	117.70
21	AA	970	C	N3-C2-O2	-6.92	117.05	121.90
11	AL	55	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	422	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1275	A	C4-C5-C6	-6.92	113.54	117.00
19	AT	17	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	677	A	C5-C6-N1	6.92	121.16	117.70
54	BA	6	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	149	A	C5-C6-N1	6.92	121.16	117.70
54	BA	740	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	474	G	N3-C2-N2	-6.92	115.06	119.90
54	BA	346	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	233	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	675	A	C4-C5-C6	-6.91	113.54	117.00
54	BA	1354	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1507	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	1762	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1908	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	911	A	C5-C6-N1	6.91	121.16	117.70
54	BA	972	A	C5-C6-N1	6.91	121.16	117.70
21	AA	364	A	C5-C6-N1	6.91	121.16	117.70
21	AA	872	A	C5-C6-N1	6.91	121.16	117.70
54	BA	146	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1111	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1205	A	N1-C6-N6	-6.91	114.45	118.60
21	AA	1203	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	1238	A	C5-C6-N1	6.91	121.15	117.70
54	BA	1919	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2706	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2873	A	C5-C6-N1	6.91	121.15	117.70
21	AA	341	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	1150	A	C5-C6-N1	6.91	121.15	117.70
54	BA	332	A	O4'-C1'-N9	6.91	113.72	108.20
54	BA	492	A	C5-C6-N1	6.91	121.15	117.70
54	BA	2827	C	N3-C2-O2	-6.91	117.07	121.90
55	BB	34	A	C5-C6-N1	6.91	121.15	117.70
54	BA	2003	A	N1-C6-N6	-6.90	114.46	118.60
21	AA	794	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1500	A	N1-C6-N6	-6.90	114.46	118.60
35	BM	50	ARG	NE-CZ-NH1	6.90	123.75	120.30
21	AA	190	A	C5-C6-N1	6.90	121.15	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	734	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2463	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	414	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1502	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1143	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2734	A	C5-C6-N1	6.90	121.15	117.70
55	BB	53	A	C4-C5-C6	-6.90	113.55	117.00
12	AM	2	ARG	NE-CZ-NH2	6.90	123.75	120.30
21	AA	54	C	C1'-O4'-C4'	-6.90	104.38	109.90
21	AA	1329	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	1336	A	C5-C6-N1	6.90	121.15	117.70
55	BB	60	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	1205	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1796	U	O4'-C1'-N1	6.89	113.72	108.20
12	AM	92	ARG	NE-CZ-NH2	-6.89	116.85	120.30
21	AA	1483	A	C5-C6-N1	6.89	121.15	117.70
54	BA	354	A	N1-C6-N6	-6.89	114.47	118.60
54	BA	912	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	583	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	330	A	C4-C5-C6	-6.89	113.55	117.00
21	AA	1251	A	C5-C6-N1	6.89	121.14	117.70
54	BA	873	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	2261	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	1396	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	603	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	1104	C	N3-C2-O2	-6.89	117.08	121.90
56	B5	74	ARG	NE-CZ-NH1	6.89	123.74	120.30
21	AA	689	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	282	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	455	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	457	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2516	A	C5-C6-N1	6.88	121.14	117.70
54	BA	722	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1597	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1746	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2411	A	C5-C6-N1	6.88	121.14	117.70
54	BA	183	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	228	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2381	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1055	A	C4-C5-C6	-6.88	113.56	117.00
26	BD	141	ARG	NE-CZ-NH2	6.88	123.74	120.30
54	BA	2268	A	C4-C5-C6	-6.88	113.56	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1321	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1615	C	O4'-C1'-N1	6.87	113.70	108.20
54	BA	2134	A	C5-C6-N1	6.87	121.14	117.70
21	AA	183	C	N1-C2-O2	6.87	123.02	118.90
21	AA	468	A	C5-C6-N1	6.87	121.14	117.70
21	AA	600	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	1332	G	O4'-C1'-N9	6.87	113.70	108.20
54	BA	2527	C	N3-C2-O2	-6.87	117.09	121.90
24	A3	14	A	N1-C6-N6	-6.87	114.48	118.60
21	AA	737	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	1230	C	N3-C2-O2	-6.87	117.09	121.90
24	A3	11	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	1129	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1722	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1735	A	C5-C6-N1	6.87	121.13	117.70
54	BA	2809	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1383	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	2705	A	C5-C6-N1	6.86	121.13	117.70
54	BA	330	A	C5-C6-N1	6.86	121.13	117.70
54	BA	803	U	O4'-C1'-N1	6.86	113.69	108.20
54	BA	2826	A	C5-C6-N1	6.86	121.13	117.70
54	BA	324	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	1504	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	443	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2014	A	N1-C6-N6	-6.86	114.49	118.60
54	BA	195	A	C5-C6-N1	6.86	121.13	117.70
34	BL	21	ARG	NE-CZ-NH1	6.85	123.73	120.30
54	BA	477	A	C5-C6-N1	6.85	121.13	117.70
54	BA	825	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	998	C	O4'-C1'-N1	6.85	113.68	108.20
54	BA	1978	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	2416	C	N3-C2-O2	-6.85	117.10	121.90
54	BA	177	G	O4'-C1'-N9	6.85	113.68	108.20
54	BA	2412	A	C5-C6-N1	6.85	121.12	117.70
54	BA	608	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	167	A	C5-C6-N1	6.85	121.12	117.70
54	BA	804	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1403	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1590	A	C5-C6-N1	6.84	121.12	117.70
54	BA	351	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	732	C	O4'-C1'-N1	6.84	113.67	108.20
38	BP	52	ARG	NE-CZ-NH1	6.84	123.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2335	A	C5-C6-N1	6.84	121.12	117.70
21	AA	16	A	C5-C6-N1	6.84	121.12	117.70
21	AA	290	C	N3-C2-O2	-6.84	117.11	121.90
34	BL	69	ARG	NE-CZ-NH1	6.84	123.72	120.30
54	BA	1638	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1789	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2566	A	N1-C6-N6	-6.84	114.50	118.60
55	BB	42	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	974	A	C4-C5-C6	-6.84	113.58	117.00
24	A3	60	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1675	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	576	C	N1-C2-O2	6.84	123.00	118.90
54	BA	316	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1866	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2013	A	C5-C6-N1	6.84	121.12	117.70
54	BA	892	A	C5-C6-N1	6.83	121.12	117.70
21	AA	470	C	N3-C2-O2	-6.83	117.12	121.90
22	A1	25	C	N3-C2-O2	-6.83	117.12	121.90
34	BL	41	ARG	NE-CZ-NH1	6.83	123.72	120.30
54	BA	164	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	1254	A	C5-C6-N1	6.83	121.12	117.70
54	BA	1366	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	1816	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	101	A	C5-C6-N1	6.83	121.12	117.70
54	BA	1966	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2015	A	C4-C5-C6	-6.83	113.58	117.00
21	AA	694	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1059	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1346	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	1342	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	2196	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	119	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	715	A	C5-C6-N1	6.83	121.11	117.70
22	A1	26	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	1143	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	1289	C	N3-C2-O2	-6.83	117.12	121.90
23	A2	91	A	C5-C6-N1	6.82	121.11	117.70
54	BA	125	A	O4'-C1'-N9	6.82	113.66	108.20
54	BA	1494	A	C5-C6-N1	6.82	121.11	117.70
21	AA	744	C	N3-C2-O2	-6.82	117.12	121.90
44	BV	93	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	1314	C	O4'-C1'-N1	6.82	113.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2418	A	C4-C5-C6	-6.82	113.59	117.00
36	BN	103	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	2748	A	C5-C6-N1	6.82	121.11	117.70
21	AA	338	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	2328	A	C4-C5-C6	-6.82	113.59	117.00
32	BJ	96	ARG	NE-CZ-NH1	6.82	123.71	120.30
35	BM	44	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	1204	A	O4'-C1'-N9	6.82	113.65	108.20
54	BA	1398	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	1969	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2154	A	C5-C6-N1	6.82	121.11	117.70
54	BA	165	A	N1-C6-N6	-6.81	114.51	118.60
54	BA	1592	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	243	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	294	A	C5-C6-N1	6.81	121.11	117.70
54	BA	347	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	2516	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	2612	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	693	A	C5-C6-N1	6.81	121.11	117.70
54	BA	749	A	C5-C6-N1	6.81	121.11	117.70
54	BA	501	A	C5-C6-N1	6.81	121.11	117.70
54	BA	1269	A	N1-C6-N6	-6.81	114.52	118.60
21	AA	253	A	C4-C5-C6	-6.81	113.60	117.00
54	BA	1632	A	C5-C6-N1	6.81	121.10	117.70
21	AA	400	C	N3-C2-O2	-6.81	117.14	121.90
21	AA	452	A	O4'-C1'-N9	6.81	113.64	108.20
54	BA	2333	A	C5-C6-N1	6.81	121.10	117.70
55	BB	94	A	C4-C5-C6	-6.81	113.60	117.00
21	AA	528	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	1409	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	1207	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	1276	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	2681	C	N3-C2-O2	-6.80	117.14	121.90
55	BB	78	A	C5-C6-N1	6.80	121.10	117.70
22	A1	73	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1985	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	251	G	P-O3'-C3'	6.80	127.86	119.70
21	AA	1110	A	C5-C6-N1	6.80	121.10	117.70
54	BA	192	C	O4'-C1'-N1	6.80	113.64	108.20
54	BA	582	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	1616	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	1793	C	N3-C2-O2	-6.80	117.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1327	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	673	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1111	A	C4-C5-C6	-6.80	113.60	117.00
24	A3	73	A	C6-C5-N7	6.80	137.06	132.30
54	BA	412	A	C5-C6-N1	6.80	121.10	117.70
54	BA	453	A	C5-C6-N1	6.80	121.10	117.70
54	BA	170	U	O4'-C1'-N1	6.79	113.64	108.20
54	BA	920	A	C4-C5-C6	-6.79	113.60	117.00
21	AA	288	A	C5-C6-N1	6.79	121.10	117.70
21	AA	327	A	C5-C6-N1	6.79	121.10	117.70
21	AA	876	C	P-O3'-C3'	6.79	127.85	119.70
21	AA	1216	A	C5-C6-N1	6.79	121.10	117.70
54	BA	1574	C	N3-C2-O2	-6.79	117.14	121.90
21	AA	1216	A	C4-C5-C6	-6.79	113.61	117.00
24	A3	72	C	N3-C2-O2	-6.79	117.14	121.90
27	BE	40	ARG	NE-CZ-NH2	-6.79	116.90	120.30
54	BA	236	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	2158	A	N1-C6-N6	-6.79	114.53	118.60
21	AA	935	A	C5-C6-N1	6.79	121.09	117.70
21	AA	1281	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	1443	C	N3-C2-O2	-6.79	117.15	121.90
52	B3	41	ARG	NE-CZ-NH1	6.79	123.69	120.30
21	AA	1110	A	C4-C5-C6	-6.79	113.61	117.00
39	BQ	32	ARG	NE-CZ-NH1	6.79	123.69	120.30
54	BA	217	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	676	A	C5-C6-N1	6.79	121.09	117.70
55	BB	46	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	1380	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	569	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	748	G	C1'-O4'-C4'	-6.79	104.47	109.90
54	BA	1325	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	2352	A	C5-C6-N1	6.79	121.09	117.70
21	AA	172	A	C5-C6-N1	6.78	121.09	117.70
22	A1	21	A	C5-C6-N1	6.78	121.09	117.70
49	B0	51	ARG	NE-CZ-NH1	6.78	123.69	120.30
54	BA	522	A	C5-C6-N1	6.78	121.09	117.70
54	BA	968	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	739	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	1427	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	1940	U	O4'-C1'-N1	6.78	113.62	108.20
21	AA	985	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	1456	A	C5-C6-N1	6.78	121.09	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	951	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	1237	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1272	A	C5-C6-N1	6.78	121.09	117.70
44	BV	21	ARG	NE-CZ-NH1	6.78	123.69	120.30
54	BA	2448	A	C4-C5-C6	-6.78	113.61	117.00
55	BB	68	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	795	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	505	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	1057	A	N1-C6-N6	-6.77	114.53	118.60
21	AA	120	A	N1-C6-N6	-6.77	114.54	118.60
21	AA	554	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	239	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	1366	A	C5-C6-N1	6.77	121.09	117.70
54	BA	1916	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2369	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2670	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	162	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2328	A	C5-C6-N1	6.77	121.08	117.70
55	BB	3	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	1431	A	C5-C6-N1	6.77	121.08	117.70
54	BA	812	C	O4'-C1'-N1	6.77	113.62	108.20
54	BA	861	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1100	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	1302	A	C5-C6-N1	6.77	121.08	117.70
21	AA	282	A	C4-C5-C6	-6.77	113.62	117.00
54	BA	1591	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	414	A	C4-C5-C6	-6.76	113.62	117.00
53	B4	4	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	1656	C	N3-C2-O2	-6.76	117.16	121.90
54	BA	492	A	N1-C6-N6	-6.76	114.54	118.60
21	AA	430	A	C5-C6-N1	6.76	121.08	117.70
21	AA	924	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	575	A	N1-C6-N6	-6.76	114.54	118.60
54	BA	1480	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2129	C	O4'-C1'-N1	6.76	113.61	108.20
54	BA	2160	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2453	A	C5-C6-N1	6.76	121.08	117.70
54	BA	2675	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	66	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	729	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1045	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1152	C	N3-C2-O2	-6.76	117.17	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2590	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	142	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1230	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1275	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1998	A	C5-C6-N1	6.76	121.08	117.70
21	AA	174	A	N1-C6-N6	-6.75	114.55	118.60
21	AA	451	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1328	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	321	U	O4'-C1'-N1	6.75	113.60	108.20
54	BA	2094	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	1428	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	1430	A	C5-C6-N1	6.75	121.08	117.70
22	A1	36	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	1858	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1213	A	C5-C6-N1	6.75	121.08	117.70
54	BA	861	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	1533	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	2386	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1077	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	1889	A	C5-C6-N1	6.75	121.08	117.70
54	BA	2366	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1170	A	N1-C6-N6	-6.75	114.55	118.60
21	AA	1274	A	C4-C5-C6	-6.75	113.63	117.00
28	BF	177	ARG	NE-CZ-NH1	6.75	123.67	120.30
54	BA	207	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	654	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	672	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	2014	A	C5-C6-N1	6.75	121.07	117.70
54	BA	2442	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	1081	A	C5-C6-N1	6.74	121.07	117.70
38	BP	88	ARG	NE-CZ-NH1	6.74	123.67	120.30
51	B2	3	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	2829	A	N1-C6-N6	-6.74	114.55	118.60
21	AA	1534	A	N1-C6-N6	-6.74	114.56	118.60
39	BQ	49	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	1214	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1287	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2198	A	N1-C6-N6	-6.74	114.56	118.60
21	AA	768	A	C4-C5-C6	-6.74	113.63	117.00
41	BS	92	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	909	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	965	C	N3-C2-O2	-6.74	117.18	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1049	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	272	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1357	A	C5-C6-N1	6.74	121.07	117.70
54	BA	244	A	N1-C6-N6	-6.74	114.56	118.60
54	BA	311	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	854	C	N3-C2-O2	-6.74	117.19	121.90
54	BA	930	G	O4'-C1'-N9	6.74	113.59	108.20
21	AA	624	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2741	A	C5-C6-N1	6.73	121.07	117.70
21	AA	511	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	648	A	C4-C5-C6	-6.73	113.63	117.00
21	AA	978	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	1732	C	N3-C2-O2	-6.73	117.19	121.90
20	AU	16	ARG	NE-CZ-NH1	6.73	123.67	120.30
21	AA	345	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	857	G	N3-C2-N2	-6.73	115.19	119.90
54	BA	2434	A	C4-C5-C6	-6.73	113.64	117.00
21	AA	108	G	O4'-C1'-N9	6.73	113.58	108.20
21	AA	1056	U	O4'-C1'-N1	6.73	113.58	108.20
54	BA	611	C	N3-C2-O2	-6.73	117.19	121.90
1	AB	73	ARG	NE-CZ-NH1	6.73	123.66	120.30
54	BA	454	A	C5-C6-N1	6.73	121.06	117.70
54	BA	1039	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	1557	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1799	G	P-O3'-C3'	6.73	127.77	119.70
1	AB	112	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	274	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	2283	C	O4'-C1'-N1	6.72	113.58	108.20
51	B2	41	ARG	NE-CZ-NH2	6.72	123.66	120.30
54	BA	2054	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2759	G	O4'-C1'-N9	6.72	113.58	108.20
21	AA	649	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	1451	U	P-O3'-C3'	6.72	127.77	119.70
54	BA	461	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	675	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	1535	A	C5-C6-N1	6.72	121.06	117.70
21	AA	1069	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	1699	G	O4'-C1'-N9	6.72	113.58	108.20
21	AA	143	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	1362	A	C5-C6-N1	6.72	121.06	117.70
21	AA	1492	A	C5-C6-N1	6.72	121.06	117.70
6	AG	101	ARG	NE-CZ-NH1	6.71	123.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	622	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	601	C	N3-C2-O2	-6.71	117.20	121.90
55	BB	104	A	C5-C6-N1	6.71	121.06	117.70
21	AA	487	A	C4-C5-C6	-6.71	113.64	117.00
43	BU	21	ARG	NE-CZ-NH1	6.71	123.66	120.30
54	BA	217	A	N1-C6-N6	-6.71	114.57	118.60
54	BA	1370	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	495	A	C5-C6-N1	6.71	121.06	117.70
21	AA	1501	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	106	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1515	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1170	C	O4'-C1'-N1	6.71	113.56	108.20
54	BA	2660	A	C5-C6-N1	6.71	121.05	117.70
55	BB	28	C	N3-C2-O2	-6.71	117.20	121.90
55	BB	59	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1769	U	O4'-C1'-N1	6.71	113.56	108.20
55	BB	88	C	N1-C2-O2	6.71	122.92	118.90
54	BA	31	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	599	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	717	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1165	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2407	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2462	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2634	A	C5-C6-N1	6.70	121.05	117.70
54	BA	173	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	199	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	501	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1127	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1689	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1970	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2117	A	O4'-C1'-N9	6.70	113.56	108.20
54	BA	2461	A	C5-C6-N1	6.70	121.05	117.70
24	A3	26	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1298	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	546	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	958	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1669	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2175	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	452	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2861	U	O4'-C1'-N1	6.70	113.56	108.20
21	AA	452	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1565	C	O4'-C1'-N1	6.69	113.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1678	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	1363	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	1275	A	C5-C6-N1	6.69	121.05	117.70
54	BA	471	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1634	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1952	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	2868	A	C4-C5-C6	-6.69	113.66	117.00
9	AJ	72	ARG	NE-CZ-NH1	6.69	123.64	120.30
21	AA	879	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	1145	A	C5-C6-N1	6.69	121.04	117.70
21	AA	1146	A	C5-C6-N1	6.69	121.04	117.70
54	BA	838	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	1496	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	119	A	C5-C6-N1	6.68	121.04	117.70
21	AA	663	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	794	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1176	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	14	A	C4-C5-C6	-6.68	113.66	117.00
55	BB	114	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	523	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	423	A	C5-C6-N1	6.68	121.04	117.70
54	BA	888	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1297	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1905	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	1524	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	990	C	N3-C2-O2	-6.68	117.23	121.90
54	BA	43	G	O4'-C1'-N9	6.68	113.54	108.20
54	BA	251	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1260	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2764	A	N1-C6-N6	-6.68	114.59	118.60
21	AA	1480	A	C5-C6-N1	6.67	121.04	117.70
42	BT	73	ARG	NE-CZ-NH1	6.67	123.64	120.30
54	BA	61	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1096	A	O4'-C1'-N9	6.67	113.54	108.20
54	BA	1285	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1735	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	2050	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2391	G	O4'-C1'-N9	6.67	113.54	108.20
54	BA	165	A	C5-C6-N1	6.67	121.04	117.70
21	AA	373	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1737	G	O4'-C1'-N9	6.67	113.54	108.20
54	BA	1760	C	N3-C2-O2	-6.67	117.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2059	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	1961	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2090	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2566	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2889	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	608	A	C4-C5-C6	-6.67	113.67	117.00
50	B1	5	ARG	NE-CZ-NH1	6.67	123.63	120.30
54	BA	63	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2285	C	N3-C2-O2	-6.67	117.23	121.90
3	AD	2	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	1019	A	C4-C5-C6	-6.66	113.67	117.00
25	BC	270	ARG	NE-CZ-NH1	6.66	123.63	120.30
54	BA	231	A	C4-C5-C6	-6.66	113.67	117.00
13	AN	85	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	649	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1419	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1708	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	10	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	1168	U	O4'-C1'-N1	6.66	113.53	108.20
54	BA	294	A	N1-C6-N6	-6.66	114.60	118.60
21	AA	1389	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	385	C	O4'-C1'-N1	6.66	113.53	108.20
54	BA	590	A	C5-C6-N1	6.66	121.03	117.70
54	BA	590	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	602	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2727	A	C5-C6-N1	6.66	121.03	117.70
54	BA	309	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2635	A	C5-C6-N1	6.66	121.03	117.70
21	AA	436	C	O4'-C1'-N1	6.65	113.52	108.20
54	BA	863	A	C5-C6-N1	6.65	121.03	117.70
21	AA	16	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	663	A	C5-C6-N1	6.65	121.03	117.70
39	BQ	27	ARG	NE-CZ-NH1	6.65	123.63	120.30
54	BA	632	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	902	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	1262	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	629	A	N1-C6-N6	-6.65	114.61	118.60
54	BA	20	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1134	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	1502	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	563	A	N1-C6-N6	-6.65	114.61	118.60
21	AA	892	A	C5-C6-N1	6.64	121.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	975	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1686	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	816	A	C1'-O4'-C4'	-6.64	104.59	109.90
21	AA	1016	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2639	A	C5-C6-N1	6.64	121.02	117.70
38	BP	71	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	957	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1690	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1072	C	O4'-C1'-N1	6.64	113.51	108.20
54	BA	1155	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1717	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2019	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2088	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2336	A	O4'-C1'-N9	6.64	113.51	108.20
54	BA	5	A	C5-C6-N1	6.64	121.02	117.70
54	BA	820	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	909	A	C5-C6-N1	6.64	121.02	117.70
11	AL	120	ARG	NE-CZ-NH1	6.64	123.62	120.30
21	AA	936	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	482	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	975	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1315	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2214	C	N3-C2-O2	-6.64	117.25	121.90
55	BB	109	A	C5-C6-N1	6.64	121.02	117.70
21	AA	580	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	906	A	C4-C5-C6	-6.63	113.68	117.00
54	BA	231	A	C5-C6-N1	6.63	121.02	117.70
54	BA	393	C	O4'-C1'-N1	6.63	113.51	108.20
54	BA	1134	A	C5-C6-N1	6.63	121.02	117.70
25	BC	269	ARG	NE-CZ-NH1	6.63	123.62	120.30
54	BA	157	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	310	A	C5-C6-N1	6.63	121.02	117.70
21	AA	1381	U	C1'-O4'-C4'	-6.63	104.60	109.90
54	BA	510	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	739	A	C5-C6-N1	6.63	121.01	117.70
54	BA	1092	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1395	A	C1'-O4'-C4'	-6.63	104.60	109.90
54	BA	2632	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	635	A	C5-C6-N1	6.63	121.01	117.70
21	AA	825	A	C5-C6-N1	6.63	121.01	117.70
22	A1	14	A	N1-C6-N6	-6.63	114.62	118.60
22	A1	21	A	C4-C5-C6	-6.63	113.69	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	16	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	502	A	C5-C6-N1	6.63	121.01	117.70
54	BA	1040	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	285	G	O4'-C1'-N9	6.62	113.50	108.20
54	BA	1477	A	N1-C6-N6	-6.62	114.62	118.60
54	BA	2538	C	N3-C2-O2	-6.62	117.26	121.90
10	AK	121	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	155	A	C5-C6-N1	6.62	121.01	117.70
21	AA	1155	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	172	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1630	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2720	U	O4'-C1'-N1	6.62	113.50	108.20
54	BA	2723	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	81	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	712	A	N1-C6-N6	-6.62	114.63	118.60
21	AA	797	C	N3-C2-O2	-6.62	117.27	121.90
32	BJ	27	ARG	NE-CZ-NH1	6.62	123.61	120.30
52	B3	12	ARG	NE-CZ-NH1	6.62	123.61	120.30
54	BA	1821	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	489	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	239	C	O4'-C1'-N1	6.62	113.49	108.20
54	BA	2715	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	99	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	1303	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1069	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1508	A	O4'-C1'-N9	6.62	113.49	108.20
21	AA	215	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	578	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	84	A	C5-C6-N1	6.61	121.01	117.70
54	BA	2284	A	C5-C6-N1	6.61	121.01	117.70
21	AA	1149	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	1280	A	C5-C6-N1	6.61	121.01	117.70
54	BA	1757	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	344	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	462	C	O4'-C1'-N1	6.61	113.49	108.20
21	AA	1230	C	N1-C2-O2	6.61	122.86	118.90
54	BA	281	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1413	A	N1-C6-N6	-6.61	114.64	118.60
55	BB	43	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	354	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1783	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	1795	C	N3-C2-O2	-6.61	117.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1836	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	2761	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	1000	A	C5-C6-N1	6.61	121.00	117.70
54	BA	929	U	O4'-C1'-N1	6.61	113.48	108.20
54	BA	2781	A	C4-C5-C6	-6.60	113.70	117.00
4	AE	19	ARG	NE-CZ-NH1	6.60	123.60	120.30
21	AA	334	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	1096	C	N1-C2-O2	6.60	122.86	118.90
54	BA	181	A	C5-C6-N1	6.60	121.00	117.70
54	BA	572	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	1254	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	983	A	C5-C6-N1	6.60	121.00	117.70
21	AA	1520	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	865	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	932	U	N3-C2-O2	-6.60	117.58	122.20
54	BA	1872	A	C5-C6-N1	6.60	121.00	117.70
21	AA	914	A	C5-C6-N1	6.60	121.00	117.70
21	AA	1368	A	C5-C6-N1	6.60	121.00	117.70
22	A1	38	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	2342	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	815	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1803	A	C5-C6-N1	6.60	121.00	117.70
21	AA	1492	A	N1-C6-N6	-6.59	114.64	118.60
54	BA	1967	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	2135	A	C5-C6-N1	6.59	121.00	117.70
54	BA	2598	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1805	A	C5-C6-N1	6.59	121.00	117.70
54	BA	2158	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	120	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	574	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	919	A	C5-C6-N1	6.59	121.00	117.70
25	BC	62	ARG	NE-CZ-NH1	6.59	123.60	120.30
54	BA	1522	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1773	A	C5-C6-N1	6.59	121.00	117.70
54	BA	1912	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	2736	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	2809	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	979	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	1404	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1221	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	2860	A	C5-C6-N1	6.59	120.99	117.70
12	AM	92	ARG	NE-CZ-NH1	6.59	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AM	108	ARG	NE-CZ-NH1	6.59	123.59	120.30
21	AA	1394	A	C4-C5-C6	-6.59	113.71	117.00
21	AA	1226	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	680	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1608	A	C4-C5-C6	-6.59	113.71	117.00
54	BA	2469	A	C5-C6-N1	6.59	120.99	117.70
54	BA	2829	A	C5-C6-N1	6.59	120.99	117.70
9	AJ	89	ARG	NE-CZ-NH1	6.58	123.59	120.30
21	AA	749	A	C5-C6-N1	6.58	120.99	117.70
24	A3	57	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	1367	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2433	A	C5-C6-N1	6.58	120.99	117.70
54	BA	633	A	C5-C6-N1	6.58	120.99	117.70
54	BA	983	A	C4-C5-C6	-6.58	113.71	117.00
33	BK	49	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	2072	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	2691	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	623	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	415	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	13	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	56	A	C5-C6-N1	6.58	120.99	117.70
54	BA	532	A	O4'-C1'-N9	6.58	113.46	108.20
54	BA	802	A	C5-C6-N1	6.58	120.99	117.70
54	BA	972	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1004	U	O4'-C1'-N1	6.58	113.46	108.20
54	BA	1900	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	2771	C	N3-C2-O2	-6.58	117.30	121.90
21	AA	269	C	N3-C2-O2	-6.58	117.30	121.90
41	BS	110	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	2420	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1340	U	N3-C2-O2	-6.57	117.60	122.20
21	AA	53	A	C5-C6-N1	6.57	120.98	117.70
21	AA	1480	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	69	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	71	A	N1-C6-N6	-6.57	114.66	118.60
54	BA	97	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1272	A	C4-C5-C6	-6.57	113.72	117.00
21	AA	279	A	C4-C5-C6	-6.57	113.72	117.00
21	AA	1103	C	N3-C2-O2	-6.57	117.30	121.90
34	BL	60	ARG	NE-CZ-NH1	6.57	123.58	120.30
54	BA	1105	U	O4'-C1'-N1	6.57	113.45	108.20
21	AA	681	A	C4-C5-C6	-6.57	113.72	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1810	A	C5-C6-N1	6.57	120.98	117.70
24	A3	36	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	368	A	C5-C6-N1	6.57	120.98	117.70
54	BA	422	A	C5-C6-N1	6.57	120.98	117.70
55	BB	57	A	N1-C6-N6	-6.57	114.66	118.60
21	AA	85	U	N3-C2-O2	-6.56	117.61	122.20
54	BA	821	A	N1-C6-N6	-6.56	114.66	118.60
54	BA	1874	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	355	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	366	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	25	U	O4'-C1'-N1	6.56	113.45	108.20
54	BA	257	C	O4'-C1'-N1	6.56	113.45	108.20
54	BA	423	A	N1-C6-N6	-6.56	114.66	118.60
20	AU	20	ARG	NE-CZ-NH1	6.56	123.58	120.30
21	AA	78	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	630	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2101	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2882	A	C5-C6-N1	6.56	120.98	117.70
55	BB	66	A	C5-C6-N1	6.56	120.98	117.70
8	AI	44	ARG	NE-CZ-NH1	6.56	123.58	120.30
21	AA	200	G	N1-C6-O6	-6.56	115.97	119.90
21	AA	679	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	1447	A	C5-C6-N1	6.56	120.98	117.70
22	A1	59	U	N3-C2-O2	-6.56	117.61	122.20
37	BO	7	ARG	NE-CZ-NH2	-6.56	117.02	120.30
54	BA	1118	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2602	A	C5-C6-N1	6.56	120.98	117.70
21	AA	1108	G	N1-C6-O6	-6.56	115.97	119.90
21	AA	1428	A	C5-C6-N1	6.56	120.98	117.70
54	BA	666	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	1114	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1531	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	2589	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	973	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	2776	A	C5-C6-N1	6.55	120.98	117.70
21	AA	171	A	C4-C5-C6	-6.55	113.72	117.00
24	A3	63	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	89	A	C5-C6-N1	6.55	120.98	117.70
54	BA	95	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1092	C	O4'-C1'-N1	6.55	113.44	108.20
54	BA	1373	A	N1-C6-N6	-6.55	114.67	118.60
21	AA	1319	A	C4-C5-C6	-6.55	113.73	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	971	G	N1-C6-O6	-6.55	115.97	119.90
21	AA	1375	A	C5-C6-N1	6.55	120.97	117.70
54	BA	2267	A	C5-C6-N1	6.55	120.97	117.70
21	AA	1204	A	C4-C5-C6	-6.55	113.73	117.00
22	A1	30	C	N3-C2-O2	-6.55	117.32	121.90
24	A3	74	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	454	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	943	A	C5-C6-N1	6.55	120.97	117.70
54	BA	2211	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	2247	A	C5-C6-N1	6.55	120.97	117.70
54	BA	2851	A	C5-C6-N1	6.55	120.97	117.70
21	AA	1097	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	1120	C	N3-C2-O2	-6.54	117.32	121.90
24	A3	38	A	C5-C6-N1	6.54	120.97	117.70
24	A3	49	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	32	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	1169	A	C5-C6-N1	6.54	120.97	117.70
21	AA	1289	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	1476	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2008	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	2173	A	C5-C6-N1	6.54	120.97	117.70
54	BA	2003	A	C5-C6-N1	6.54	120.97	117.70
21	AA	1519	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	660	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	1990	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	2471	A	C4-C5-C6	-6.54	113.73	117.00
4	AE	53	ARG	NE-CZ-NH2	-6.53	117.03	120.30
21	AA	862	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1397	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	233	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	415	A	C5-C6-N1	6.53	120.97	117.70
54	BA	484	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	795	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	853	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	2368	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1128	G	O4'-C1'-N9	6.53	113.42	108.20
21	AA	618	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1162	C	N3-C2-O2	-6.53	117.33	121.90
45	BW	19	ARG	NE-CZ-NH1	6.53	123.56	120.30
54	BA	2573	C	N3-C2-O2	-6.53	117.33	121.90
25	BC	269	ARG	NE-CZ-NH2	-6.53	117.04	120.30
21	AA	316	C	N3-C2-O2	-6.53	117.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1256	A	C5-C6-N1	6.53	120.96	117.70
54	BA	1135	C	N3-C4-C5	6.53	124.51	121.90
54	BA	1469	A	C4-C5-C6	-6.53	113.74	117.00
21	AA	756	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1509	A	C5-C6-N1	6.53	120.96	117.70
54	BA	2058	A	C4-C5-C6	-6.53	113.74	117.00
39	BQ	50	ARG	NE-CZ-NH1	6.52	123.56	120.30
21	AA	868	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	8	C	O4'-C1'-N1	6.52	113.42	108.20
54	BA	275	C	N1-C2-O2	6.52	122.81	118.90
54	BA	749	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2440	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	957	C	O4'-C1'-N1	6.52	113.42	108.20
2	AC	168	ARG	NE-CZ-NH1	6.52	123.56	120.30
21	AA	312	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	1022	A	C4-C5-C6	-6.52	113.74	117.00
28	BF	29	ARG	NE-CZ-NH1	6.52	123.56	120.30
54	BA	1593	A	C5-C6-N1	6.52	120.96	117.70
21	AA	181	A	C5-C6-N1	6.52	120.96	117.70
21	AA	507	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	720	C	N3-C2-O2	-6.52	117.34	121.90
22	A1	75	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	727	A	N1-C6-N6	-6.52	114.69	118.60
54	BA	2542	A	C4-C5-C6	-6.52	113.74	117.00
56	B5	60	ARG	NE-CZ-NH1	6.52	123.56	120.30
21	AA	735	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	1324	A	N1-C6-N6	-6.52	114.69	118.60
21	AA	374	A	C5-C6-N1	6.51	120.96	117.70
21	AA	1251	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	868	U	O4'-C1'-N1	6.51	113.41	108.20
54	BA	1005	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	1434	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	15	G	O4'-C1'-N9	6.51	113.41	108.20
54	BA	973	A	C5-C6-N1	6.51	120.96	117.70
30	BH	50	ARG	NE-CZ-NH1	6.51	123.56	120.30
21	AA	1066	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	7	A	C5-C6-N1	6.51	120.95	117.70
42	BT	6	ARG	NE-CZ-NH2	6.51	123.55	120.30
54	BA	792	A	C5-C6-N1	6.51	120.95	117.70
54	BA	987	C	N3-C2-O2	-6.51	117.35	121.90
54	BA	1809	A	O4'-C1'-N9	6.51	113.41	108.20
54	BA	2177	C	N3-C2-O2	-6.51	117.35	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	54	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	607	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	540	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	26	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	966	G	N3-C4-C5	-6.50	125.35	128.60
54	BA	155	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	2424	C	N3-C2-O2	-6.50	117.35	121.90
17	AR	47	ARG	NE-CZ-NH2	6.50	123.55	120.30
21	AA	156	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	308	C	N3-C2-O2	-6.50	117.35	121.90
22	A1	23	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1928	A	C5-C6-N1	6.50	120.95	117.70
21	AA	411	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	142	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1286	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	1289	C	C3'-C2'-C1'	6.50	106.70	101.50
54	BA	2498	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	270	A	C5-C6-N1	6.50	120.95	117.70
54	BA	524	G	N1-C6-O6	-6.50	116.00	119.90
54	BA	833	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1809	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2153	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	460	A	N1-C6-N6	-6.49	114.70	118.60
54	BA	197	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1276	A	C5-C6-N1	6.49	120.95	117.70
21	AA	7	A	N1-C6-N6	-6.49	114.70	118.60
21	AA	441	A	C5-C6-N1	6.49	120.95	117.70
54	BA	439	A	C5-C6-N1	6.49	120.95	117.70
54	BA	2456	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	210	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	1344	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	146	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1918	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	530	G	N3-C4-C5	-6.49	125.36	128.60
21	AA	321	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	703	U	O4'-C1'-N1	6.49	113.39	108.20
21	AA	782	A	C5-C6-N1	6.49	120.94	117.70
54	BA	432	A	C5-C6-N1	6.49	120.94	117.70
54	BA	490	C	N1-C2-O2	6.48	122.79	118.90
54	BA	716	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1727	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	681	A	C5-C6-N1	6.48	120.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1916	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	583	A	N1-C6-N6	-6.48	114.71	118.60
54	BA	2095	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2657	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2712	C	N1-C2-O2	6.48	122.79	118.90
21	AA	1236	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	569	U	C1'-O4'-C4'	-6.48	104.72	109.90
54	BA	2614	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	139	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1037	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	1201	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1225	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1505	A	C5-C6-N1	6.48	120.94	117.70
24	A3	68	C	N3-C2-O2	-6.48	117.37	121.90
54	BA	2108	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1054	A	C5-C6-N1	6.47	120.94	117.70
21	AA	32	A	C5-C6-N1	6.47	120.94	117.70
54	BA	392	U	O4'-C1'-N1	6.47	113.38	108.20
54	BA	927	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1165	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	1335	C	O4'-C1'-N1	6.47	113.38	108.20
21	AA	634	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	708	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1234	C	N3-C2-O2	-6.47	117.37	121.90
22	A1	58	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	210	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	485	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1175	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1362	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2163	A	C4-C5-C6	-6.47	113.77	117.00
55	BB	8	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	436	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	721	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1610	A	C1'-O4'-C4'	-6.46	104.73	109.90
21	AA	510	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	517	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1246	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1639	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2132	U	O4'-C1'-N1	6.46	113.37	108.20
8	AI	32	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	382	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1296	C	N3-C2-O2	-6.46	117.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	BT	76	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	184	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2590	A	C5-C6-N1	6.46	120.93	117.70
54	BA	789	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1600	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1612	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2654	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2765	A	O4'-C1'-N9	6.46	113.37	108.20
16	AQ	10	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	977	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1014	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1437	A	N1-C6-N6	-6.46	114.73	118.60
54	BA	624	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2254	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2317	A	C5-C6-N1	6.46	120.93	117.70
21	AA	579	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2738	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	190	A	C5-C6-N1	6.45	120.93	117.70
54	BA	772	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	2513	A	C5-C6-N1	6.45	120.93	117.70
21	AA	1132	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	764	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	1101	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	1287	A	C4-C5-C6	-6.45	113.78	117.00
23	A2	90	U	O4'-C1'-N1	6.45	113.36	108.20
54	BA	917	A	C5-C6-N1	6.45	120.93	117.70
54	BA	997	G	N3-C2-N2	-6.45	115.39	119.90
54	BA	2150	C	N3-C2-O2	-6.45	117.39	121.90
8	AI	11	ARG	NE-CZ-NH1	6.45	123.52	120.30
21	AA	816	A	C5-C6-N1	6.45	120.92	117.70
21	AA	900	A	C4-C5-C6	-6.45	113.78	117.00
23	A2	83	U	N3-C2-O2	-6.45	117.69	122.20
35	BM	16	ARG	NE-CZ-NH1	6.45	123.52	120.30
54	BA	2700	A	C5-C6-N1	6.45	120.92	117.70
54	BA	565	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1962	C	N1-C2-O2	6.45	122.77	118.90
21	AA	816	A	N1-C6-N6	-6.45	114.73	118.60
43	BU	21	ARG	NE-CZ-NH2	-6.45	117.08	120.30
54	BA	446	G	O4'-C1'-N9	6.45	113.36	108.20
54	BA	563	A	C5-C6-N1	6.45	120.92	117.70
54	BA	1127	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1853	A	C5-C6-N1	6.44	120.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2313	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2467	C	N3-C2-O2	-6.44	117.39	121.90
3	AD	43	ARG	NE-CZ-NH1	6.44	123.52	120.30
21	AA	235	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	1324	A	C5-C6-N1	6.44	120.92	117.70
54	BA	825	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1503	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	1081	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2340	A	C4-C5-C6	-6.44	113.78	117.00
22	A1	62	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	160	A	N1-C6-N6	-6.44	114.74	118.60
26	BD	33	ARG	NE-CZ-NH1	6.44	123.52	120.30
54	BA	126	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1679	A	C5-C6-N1	6.44	120.92	117.70
21	AA	790	A	N1-C6-N6	-6.44	114.74	118.60
21	AA	1430	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1144	A	C5-C6-N1	6.44	120.92	117.70
54	BA	2407	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	177	G	N3-C4-C5	-6.43	125.38	128.60
21	AA	267	C	N3-C2-O2	-6.43	117.39	121.90
21	AA	621	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	784	A	C5-C6-N1	6.43	120.92	117.70
21	AA	1082	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1030	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1749	A	C5-C6-N1	6.43	120.92	117.70
21	AA	872	A	O4'-C1'-N9	6.43	113.34	108.20
21	AA	1129	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	1163	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1742	U	O4'-C1'-N1	6.43	113.35	108.20
54	BA	1854	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	831	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	28	A	C5-C6-N1	6.43	120.92	117.70
21	AA	860	A	C5-C6-N1	6.43	120.91	117.70
54	BA	866	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	2183	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	1614	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	1819	A	C5-C6-N1	6.43	120.91	117.70
54	BA	616	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	742	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1103	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1402	U	O4'-C1'-N1	6.42	113.34	108.20
54	BA	1508	A	C4-C5-C6	-6.42	113.79	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	845	A	C1'-O4'-C4'	-6.42	104.76	109.90
21	AA	83	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	325	A	C4-C5-C6	-6.42	113.79	117.00
26	BD	124	ARG	NE-CZ-NH2	-6.42	117.09	120.30
54	BA	676	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2721	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	236	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1339	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	368	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	941	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1009	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1774	C	N1-C2-O2	6.42	122.75	118.90
21	AA	754	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	910	C	N3-C2-O2	-6.42	117.41	121.90
29	BG	34	ARG	NE-CZ-NH1	6.42	123.51	120.30
54	BA	739	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	815	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1274	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2805	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1238	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1170	A	C4-C5-C6	-6.41	113.79	117.00
21	AA	1350	A	C4-C5-C6	-6.41	113.79	117.00
36	BN	2	ARG	NE-CZ-NH1	6.41	123.51	120.30
41	BS	99	ARG	NE-CZ-NH1	6.41	123.51	120.30
54	BA	394	C	O4'-C1'-N1	6.41	113.33	108.20
54	BA	2398	U	O4'-C1'-N1	6.41	113.33	108.20
55	BB	62	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	451	A	P-O3'-C3'	6.41	127.39	119.70
54	BA	447	A	N1-C6-N6	-6.41	114.75	118.60
54	BA	1319	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1525	A	C5-C6-N1	6.41	120.91	117.70
21	AA	47	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	364	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	897	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1909	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	2088	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2142	A	C5-C6-N1	6.41	120.91	117.70
15	AP	31	ARG	NE-CZ-NH1	6.41	123.50	120.30
54	BA	1237	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	510	A	C5-C6-N1	6.41	120.90	117.70
21	AA	1219	A	C5-C6-N1	6.41	120.90	117.70
54	BA	49	A	C5-C6-N1	6.41	120.90	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1075	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	1114	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	1288	G	N1-C6-O6	-6.41	116.06	119.90
54	BA	1399	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	1941	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	2019	A	C5-C6-N1	6.41	120.90	117.70
54	BA	2900	A	C4-C5-C6	-6.41	113.80	117.00
55	BB	31	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	607	U	O4'-C1'-N1	6.40	113.32	108.20
9	AJ	62	ARG	NE-CZ-NH1	6.40	123.50	120.30
21	AA	1035	A	C5-C6-N1	6.40	120.90	117.70
23	A2	80	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	11	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	95	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2564	A	C4-C5-C6	-6.40	113.80	117.00
55	BB	50	A	C5-C6-N1	6.40	120.90	117.70
10	AK	105	ARG	NE-CZ-NH1	6.40	123.50	120.30
21	AA	886	G	N1-C6-O6	-6.40	116.06	119.90
54	BA	2232	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2403	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1345	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1490	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	19	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	1210	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	1250	A	C5-C6-N1	6.39	120.90	117.70
54	BA	900	A	C5-C6-N1	6.39	120.90	117.70
54	BA	1694	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	2813	A	C4-C5-C6	-6.39	113.80	117.00
11	AL	35	ARG	NE-CZ-NH1	6.39	123.50	120.30
54	BA	626	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	782	A	C5-C6-N1	6.39	120.90	117.70
54	BA	979	A	C5-C6-N1	6.39	120.90	117.70
21	AA	859	G	N3-C2-N2	-6.39	115.43	119.90
25	BC	213	ARG	NE-CZ-NH1	6.39	123.50	120.30
54	BA	408	G	N1-C6-O6	-6.39	116.07	119.90
54	BA	421	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	945	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1230	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1414	C	O4'-C1'-N1	6.39	113.31	108.20
54	BA	1677	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	2497	A	C5-C6-N1	6.39	120.89	117.70
15	AP	56	ARG	NE-CZ-NH1	6.39	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1392	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1859	U	O4'-C1'-N1	6.39	113.31	108.20
54	BA	2332	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	66	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	952	G	N1-C6-O6	-6.39	116.07	119.90
54	BA	1373	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2025	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2899	A	C4-C5-C6	-6.39	113.81	117.00
21	AA	397	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1938	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	1364	U	N3-C2-O2	-6.38	117.73	122.20
54	BA	788	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1726	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	1441	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1111	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2222	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2314	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2452	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2521	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	791	C	N3-C4-N4	-6.38	113.53	118.00
54	BA	1979	U	O4'-C1'-N1	6.38	113.30	108.20
54	BA	2753	A	C5-C6-N1	6.38	120.89	117.70
54	BA	645	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2837	A	N1-C6-N6	-6.38	114.77	118.60
3	AD	164	ARG	NE-CZ-NH1	6.38	123.49	120.30
21	AA	32	A	C4-C5-C6	-6.38	113.81	117.00
24	A3	45	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1088	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2241	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2753	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2813	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	1353	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2260	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	918	A	C5-C6-N1	6.37	120.89	117.70
54	BA	2054	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2324	U	O4'-C1'-N1	6.37	113.30	108.20
54	BA	1977	A	C5-C6-N1	6.37	120.89	117.70
54	BA	2064	C	N1-C2-O2	6.37	122.72	118.90
15	AP	8	ARG	NE-CZ-NH1	6.37	123.48	120.30
54	BA	1307	A	C5-C6-N1	6.37	120.88	117.70
54	BA	1387	A	C5-C6-N1	6.37	120.89	117.70
54	BA	1637	A	C4-C5-C6	-6.37	113.82	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2764	A	C5-C6-N1	6.37	120.88	117.70
54	BA	430	A	C5-C6-N1	6.37	120.88	117.70
21	AA	221	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	365	U	O4'-C1'-N1	6.37	113.29	108.20
33	BK	31	ARG	NE-CZ-NH1	6.37	123.48	120.30
54	BA	885	C	O4'-C1'-N1	6.37	113.29	108.20
54	BA	2707	U	O4'-C1'-N1	6.37	113.29	108.20
2	AC	106	ARG	NE-CZ-NH1	6.36	123.48	120.30
11	AL	53	ARG	NE-CZ-NH1	6.36	123.48	120.30
13	AN	65	ARG	NE-CZ-NH1	6.36	123.48	120.30
21	AA	1318	A	C5-C6-N1	6.36	120.88	117.70
22	A1	76	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1262	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1614	A	C4-C5-C6	-6.36	113.82	117.00
55	BB	104	A	N1-C6-N6	-6.36	114.78	118.60
22	A1	9	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1233	C	O4'-C1'-N1	6.36	113.29	108.20
54	BA	302	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2037	A	C5-C6-N1	6.36	120.88	117.70
21	AA	680	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	1396	A	C5-C6-N1	6.36	120.88	117.70
54	BA	57	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	298	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	794	A	N1-C6-N6	-6.36	114.78	118.60
54	BA	1268	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1567	G	O4'-C1'-N9	6.36	113.29	108.20
21	AA	1239	A	C4-C5-C6	-6.36	113.82	117.00
55	BB	45	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1564	C	N3-C2-O2	-6.35	117.45	121.90
2	AC	155	ARG	NE-CZ-NH1	6.35	123.48	120.30
21	AA	802	A	C4-C5-C6	-6.35	113.82	117.00
22	A1	56	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	497	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	1993	U	O4'-C1'-N1	6.35	113.28	108.20
54	BA	2206	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	2870	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	59	A	C5-C6-N1	6.35	120.88	117.70
21	AA	563	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	1045	C	N1-C2-O2	6.35	122.71	118.90
21	AA	436	C	N1-C2-O2	6.35	122.71	118.90
54	BA	1032	A	C5-C6-N1	6.35	120.88	117.70
54	BA	1287	A	C4-C5-C6	-6.35	113.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2651	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	2766	A	C5-C6-N1	6.35	120.88	117.70
21	AA	401	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	393	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	966	G	N1-C6-O6	-6.35	116.09	119.90
54	BA	1494	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	2225	A	C5-C6-N1	6.35	120.87	117.70
54	BA	2326	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2451	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	1507	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	1699	G	O4'-C1'-C2'	-6.35	99.45	105.80
21	AA	55	A	C5-C6-N1	6.34	120.87	117.70
21	AA	72	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	167	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	544	C	N1-C2-O2	6.34	122.71	118.90
54	BA	1084	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	1151	A	C5-C6-N1	6.34	120.87	117.70
54	BA	2362	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	167	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1528	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1934	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	368	U	C1'-O4'-C4'	-6.34	104.83	109.90
21	AA	179	A	C5-C6-N1	6.34	120.87	117.70
21	AA	826	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1563	U	O4'-C1'-N1	6.34	113.27	108.20
21	AA	443	C	N3-C2-O2	-6.33	117.47	121.90
25	BC	176	ARG	NE-CZ-NH1	6.33	123.47	120.30
26	BD	13	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	238	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	362	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	2392	A	C5-C6-N1	6.33	120.87	117.70
21	AA	408	A	C4-C5-C6	-6.33	113.83	117.00
21	AA	807	A	C4-C5-C6	-6.33	113.83	117.00
34	BL	78	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	271	G	O4'-C1'-N9	6.33	113.27	108.20
54	BA	673	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1477	A	C5-C6-N1	6.33	120.87	117.70
54	BA	2531	A	C5-C6-N1	6.33	120.87	117.70
54	BA	2745	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	753	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	23	C	N3-C2-O2	-6.33	117.47	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1172	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1282	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1079	C	N1-C2-O2	6.33	122.70	118.90
21	AA	815	A	C5-C6-N1	6.33	120.86	117.70
54	BA	183	C	O4'-C1'-N1	6.33	113.26	108.20
54	BA	885	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1738	G	N3-C4-C5	-6.33	125.44	128.60
54	BA	2889	C	O4'-C1'-N1	6.33	113.26	108.20
21	AA	643	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1679	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	1706	C	N1-C2-O2	6.33	122.69	118.90
54	BA	1768	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	564	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	1222	U	O4'-C1'-N1	6.32	113.26	108.20
54	BA	2164	C	N1-C2-O2	6.32	122.69	118.90
54	BA	2658	C	N3-C2-O2	-6.32	117.47	121.90
21	AA	276	G	N3-C2-N2	-6.32	115.47	119.90
54	BA	1890	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	1491	G	N1-C6-O6	-6.32	116.11	119.90
54	BA	20	C	O4'-C1'-N1	6.32	113.25	108.20
54	BA	2589	A	C5-C6-N1	6.32	120.86	117.70
21	AA	488	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	609	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1088	A	O4'-C1'-N9	6.32	113.25	108.20
54	BA	1570	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1597	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	2875	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	1219	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	814	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2778	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2887	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	299	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	981	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	2146	C	N1-C2-O2	6.31	122.69	118.90
21	AA	431	A	C4-C5-C6	-6.31	113.84	117.00
38	BP	87	ARG	NE-CZ-NH1	6.31	123.45	120.30
54	BA	299	A	C5-C6-N1	6.31	120.86	117.70
54	BA	1665	A	C5-C6-N1	6.31	120.86	117.70
55	BB	4	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	466	A	C4-C5-C6	-6.31	113.85	117.00
24	A3	66	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	750	C	N3-C2-O2	-6.31	117.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	581	C	N3-C2-O2	-6.31	117.49	121.90
54	BA	1794	A	C4-C5-C6	-6.31	113.85	117.00
21	AA	25	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	81	A	C5-C6-N1	6.30	120.85	117.70
21	AA	483	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1997	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2699	C	N3-C2-O2	-6.30	117.49	121.90
55	BB	111	U	O4'-C1'-N1	6.30	113.24	108.20
21	AA	1117	A	C5-C6-N1	6.30	120.85	117.70
21	AA	1263	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1347	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2887	A	C5-C6-N1	6.30	120.85	117.70
21	AA	946	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	1105	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	750	A	C5-C6-N1	6.30	120.85	117.70
54	BA	2021	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	311	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1279	G	O4'-C1'-N9	6.30	113.24	108.20
54	BA	203	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1553	A	N1-C6-N6	-6.30	114.82	118.60
54	BA	2679	A	C5-C6-N1	6.30	120.85	117.70
55	BB	38	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	346	A	O4'-C1'-N9	6.29	113.24	108.20
21	AA	482	A	C4-C5-C6	-6.29	113.85	117.00
8	AI	48	ARG	NE-CZ-NH2	-6.29	117.15	120.30
21	AA	71	A	C5-C6-N1	6.29	120.85	117.70
21	AA	236	A	C5-C6-N1	6.29	120.85	117.70
21	AA	1012	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	379	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	256	A	C5-C6-N1	6.29	120.84	117.70
54	BA	1121	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1431	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1773	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	596	A	C5-C6-N1	6.29	120.84	117.70
21	AA	1005	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	893	C	N3-C2-O2	-6.29	117.50	121.90
3	AD	3	TYR	CB-CG-CD2	-6.28	117.23	121.00
5	AF	91	ARG	NE-CZ-NH1	6.28	123.44	120.30
21	AA	18	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	200	G	O4'-C1'-N9	6.28	113.23	108.20
54	BA	264	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2750	A	C4-C5-C6	-6.28	113.86	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	132	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	631	C	C1'-O4'-C4'	-6.28	104.87	109.90
21	AA	1446	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1879	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2284	A	C4-C5-C6	-6.28	113.86	117.00
18	AS	77	ARG	NE-CZ-NH2	6.28	123.44	120.30
54	BA	479	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	762	U	P-O3'-C3'	6.28	127.23	119.70
54	BA	1809	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	33	A	C5-C6-N1	6.28	120.84	117.70
21	AA	1092	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	538	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1413	A	C5-C6-N1	6.28	120.84	117.70
14	AO	53	ARG	NE-CZ-NH2	-6.28	117.16	120.30
54	BA	650	C	N1-C2-O2	6.28	122.67	118.90
54	BA	1393	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1764	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	2022	U	O4'-C1'-N1	6.28	113.22	108.20
21	AA	48	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1408	A	C5-C6-N1	6.27	120.84	117.70
54	BA	693	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	865	A	C5-C6-N1	6.27	120.84	117.70
21	AA	1000	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	1196	A	O4'-C1'-N9	6.27	113.22	108.20
21	AA	1340	A	C5-C6-N1	6.27	120.84	117.70
6	AG	78	ARG	NE-CZ-NH1	6.27	123.44	120.30
54	BA	1126	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	1876	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	1004	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	10	A	C5-C6-N1	6.27	120.83	117.70
54	BA	234	U	O4'-C1'-N1	6.27	113.22	108.20
54	BA	1685	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1715	G	O4'-C1'-N9	6.27	113.22	108.20
54	BA	1754	A	C5-C6-N1	6.27	120.83	117.70
54	BA	1960	A	C5-C6-N1	6.27	120.83	117.70
21	AA	1465	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	2858	C	N1-C2-O2	6.27	122.66	118.90
54	BA	332	A	C5-C6-N1	6.27	120.83	117.70
54	BA	796	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2347	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	329	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	978	A	C5-C6-N1	6.26	120.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BK	78	ARG	NE-CZ-NH1	6.26	123.43	120.30
38	BP	20	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	196	A	O4'-C1'-N9	6.26	113.21	108.20
54	BA	1974	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2710	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	507	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	823	C	O4'-C1'-N1	6.26	113.21	108.20
21	AA	1374	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2281	A	C5-C6-N1	6.26	120.83	117.70
54	BA	900	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2703	C	N1-C2-O2	6.26	122.66	118.90
8	AI	121	ARG	NE-CZ-NH1	6.26	123.43	120.30
21	AA	1201	A	P-O3'-C3'	6.26	127.21	119.70
37	BO	81	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	2047	C	O4'-C1'-N1	6.26	113.21	108.20
54	BA	26	G	O4'-C1'-N9	6.25	113.20	108.20
54	BA	497	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	1556	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	2287	A	C5-C6-N1	6.25	120.83	117.70
54	BA	130	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	560	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	1901	A	C4-C5-C6	-6.25	113.87	117.00
22	A1	68	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	2196	C	O4'-C1'-N1	6.25	113.20	108.20
21	AA	323	U	O4'-C1'-N1	6.25	113.20	108.20
21	AA	1180	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	19	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	160	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	840	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1327	A	C5-C6-N1	6.25	120.82	117.70
54	BA	2060	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2886	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	1987	A	C5-C6-N1	6.25	120.82	117.70
54	BA	2369	A	C4-C5-C6	-6.25	113.88	117.00
2	AC	125	ARG	NE-CZ-NH1	6.24	123.42	120.30
54	BA	817	C	N1-C2-O2	6.24	122.65	118.90
54	BA	1089	A	C4-C5-C6	-6.24	113.88	117.00
22	A1	38	A	N1-C6-N6	-6.24	114.86	118.60
54	BA	127	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	865	C	O4'-C1'-N1	6.24	113.19	108.20
54	BA	2364	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	676	A	C4-C5-C6	-6.24	113.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	60	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	111	A	C5-C6-N1	6.24	120.82	117.70
54	BA	698	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1583	A	C4-C5-C6	-6.24	113.88	117.00
24	A3	58	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	823	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1433	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2451	A	C5-C6-N1	6.24	120.82	117.70
21	AA	1250	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1513	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1465	G	N1-C6-O6	-6.24	116.16	119.90
54	BA	2073	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2736	A	C5-C6-N1	6.24	120.82	117.70
21	AA	238	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1402	C	N3-C2-O2	-6.24	117.53	121.90
22	A1	73	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	44	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	758	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2166	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	2600	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1418	A	N1-C6-N6	-6.23	114.86	118.60
54	BA	1064	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1745	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2810	A	C5-C6-N1	6.23	120.82	117.70
21	AA	611	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1320	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1513	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	332	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	1772	A	C5-C6-N1	6.23	120.82	117.70
54	BA	2020	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2785	C	N3-C2-O2	-6.23	117.54	121.90
15	AP	51	ARG	NE-CZ-NH1	6.23	123.42	120.30
21	AA	612	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	369	U	O4'-C1'-N1	6.23	113.18	108.20
54	BA	2385	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	392	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1582	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2821	A	C5-C6-N1	6.23	120.81	117.70
54	BA	2457	U	O4'-C1'-N1	6.23	113.18	108.20
54	BA	440	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	775	G	O4'-C1'-N9	6.23	113.18	108.20
54	BA	2568	U	O4'-C1'-N1	6.23	113.18	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2760	C	O4'-C1'-N1	6.23	113.18	108.20
21	AA	87	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	517	C	O4'-C1'-N1	6.22	113.18	108.20
54	BA	2411	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	532	A	C5-C6-N1	6.22	120.81	117.70
21	AA	873	A	C5-C6-N1	6.22	120.81	117.70
21	AA	883	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	249	C	N1-C2-O2	6.22	122.63	118.90
54	BA	1166	G	N1-C6-O6	-6.22	116.17	119.90
54	BA	2577	A	C5-C6-N1	6.22	120.81	117.70
54	BA	910	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	2451	A	N1-C6-N6	-6.22	114.87	118.60
21	AA	178	C	N3-C2-O2	-6.22	117.55	121.90
55	BB	118	C	N1-C2-O2	6.22	122.63	118.90
21	AA	901	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	756	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	781	A	C4-C5-C6	-6.22	113.89	117.00
25	BC	155	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	1229	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2690	U	O4'-C1'-N1	6.22	113.17	108.20
54	BA	2826	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	33	A	C4-C5-C6	-6.21	113.89	117.00
53	B4	24	ARG	NE-CZ-NH2	-6.21	117.19	120.30
21	AA	753	A	C5-C6-N1	6.21	120.81	117.70
21	AA	827	U	O4'-C1'-N1	6.21	113.17	108.20
54	BA	756	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	828	U	N3-C2-O2	-6.21	117.85	122.20
54	BA	1730	C	N1-C2-O2	6.21	122.63	118.90
21	AA	1429	A	C5-C6-N1	6.21	120.81	117.70
54	BA	2095	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1644	C	O4'-C1'-N1	6.21	113.17	108.20
54	BA	1998	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2416	C	O4'-C1'-N1	6.21	113.17	108.20
54	BA	2453	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	315	A	C5-C6-N1	6.21	120.80	117.70
22	A1	14	A	C5-C6-N1	6.21	120.80	117.70
46	BX	73	ARG	NE-CZ-NH1	6.21	123.40	120.30
54	BA	38	A	C6-C5-N7	6.21	136.65	132.30
54	BA	1610	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1900	A	C5-C6-N1	6.21	120.80	117.70
55	BB	95	U	O4'-C1'-N1	6.21	113.17	108.20
54	BA	125	A	C4-C5-C6	-6.21	113.90	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2183	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	545	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	725	G	N1-C6-O6	-6.20	116.18	119.90
54	BA	2800	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	151	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1410	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2231	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1551	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2901	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	153	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	419	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	770	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1049	U	C1'-O4'-C4'	-6.20	104.94	109.90
54	BA	140	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2265	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1097	U	O4'-C1'-N1	6.20	113.16	108.20
40	BR	78	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	AA	800	G	N1-C6-O6	-6.19	116.18	119.90
21	AA	403	C	N3-C2-O2	-6.19	117.56	121.90
21	AA	864	A	C4-C5-C6	-6.19	113.90	117.00
21	AA	1011	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	670	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	692	C	N3-C2-O2	-6.19	117.56	121.90
54	BA	1887	C	N3-C2-O2	-6.19	117.56	121.90
55	BB	66	A	C4-C5-C6	-6.19	113.90	117.00
21	AA	264	C	N1-C2-O2	6.19	122.61	118.90
21	AA	386	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	237	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	55	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	1021	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	2754	U	O4'-C1'-N1	6.19	113.15	108.20
55	BB	85	G	O4'-C1'-N9	6.19	113.15	108.20
21	AA	866	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1288	G	C3'-C2'-C1'	6.19	106.45	101.50
54	BA	2031	A	C5-C6-N1	6.19	120.79	117.70
21	AA	1311	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	1462	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	661	A	C5-C6-N1	6.18	120.79	117.70
54	BA	908	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	994	C	O4'-C1'-N1	6.18	113.15	108.20
54	BA	1894	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	802	A	C5-C6-N1	6.18	120.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	897	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	909	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	980	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	1188	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	905	A	C5-C6-N1	6.18	120.79	117.70
54	BA	1018	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	2585	U	O4'-C1'-N1	6.18	113.15	108.20
21	AA	1431	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	115	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1208	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1545	A	C5-C6-N1	6.18	120.79	117.70
54	BA	1818	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2317	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	244	A	C5-C6-N1	6.18	120.79	117.70
54	BA	1258	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	1947	C	N1-C2-O2	6.18	122.61	118.90
21	AA	271	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	857	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	1364	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2214	C	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2587	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	1342	C	O4'-C1'-N1	6.17	113.14	108.20
54	BA	2572	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	2896	C	N3-C2-O2	-6.17	117.58	121.90
55	BB	101	A	C5-C6-N1	6.17	120.79	117.70
21	AA	1051	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1665	A	C4-C5-C6	-6.17	113.91	117.00
18	AS	2	ARG	NE-CZ-NH2	6.17	123.39	120.30
21	AA	502	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	268	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	412	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	2122	U	O4'-C1'-N1	6.17	113.14	108.20
54	BA	2560	A	C5-C6-N1	6.17	120.78	117.70
21	AA	582	C	N3-C2-O2	-6.17	117.58	121.90
24	A3	17	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1284	A	C5-C6-N1	6.17	120.78	117.70
54	BA	1385	A	C5-C6-N1	6.17	120.78	117.70
54	BA	2030	A	O4'-C1'-N9	6.17	113.13	108.20
21	AA	477	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	993	G	N3-C4-C5	-6.16	125.52	128.60
54	BA	83	A	C5-C6-N1	6.16	120.78	117.70
54	BA	228	C	N1-C2-O2	6.16	122.60	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2198	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	250	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1153	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2452	C	O4'-C1'-N1	6.16	113.13	108.20
21	AA	1248	A	C4-C5-C6	-6.16	113.92	117.00
22	A1	70	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	453	A	C5'-C4'-O4'	6.16	116.49	109.10
54	BA	1008	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1641	A	C4-C5-C6	-6.16	113.92	117.00
55	BB	12	C	N3-C2-O2	-6.16	117.59	121.90
55	BB	58	A	C5-C6-N1	6.16	120.78	117.70
55	BB	73	A	O4'-C1'-N9	6.16	113.13	108.20
21	AA	370	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	525	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	983	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	716	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1929	G	N3-C2-N2	-6.16	115.59	119.90
21	AA	518	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	614	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	56	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	398	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1654	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1843	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	589	U	O4'-C1'-N1	6.15	113.12	108.20
21	AA	1259	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	595	A	C5-C6-N1	6.15	120.78	117.70
21	AA	805	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	918	A	C5-C6-N1	6.15	120.78	117.70
21	AA	1049	U	P-O3'-C3'	6.15	127.08	119.70
21	AA	1285	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	201	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1164	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2225	A	O4'-C1'-N9	6.15	113.12	108.20
21	AA	1254	A	N1-C6-N6	-6.15	114.91	118.60
54	BA	281	C	O4'-C1'-N1	6.15	113.12	108.20
54	BA	1858	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	2179	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	320	A	C4-C5-C6	-6.15	113.92	117.00
22	A1	20	G	N3-C4-C5	-6.15	125.53	128.60
54	BA	404	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	2205	A	C5-C6-N1	6.15	120.78	117.70
2	AC	126	ARG	NE-CZ-NH1	6.15	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1461	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	1779	U	O4'-C1'-N1	6.15	113.12	108.20
54	BA	2746	U	O4'-C1'-N1	6.15	113.12	108.20
40	BR	21	ARG	NE-CZ-NH1	6.15	123.37	120.30
54	BA	2636	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	2837	A	C4-C5-C6	-6.15	113.93	117.00
6	AG	142	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	152	A	N1-C6-N6	-6.14	114.91	118.60
54	BA	1509	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1338	G	N3-C2-N2	-6.14	115.60	119.90
54	BA	1503	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1654	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1877	A	C5-C6-N1	6.14	120.77	117.70
21	AA	192	A	C5-C6-N1	6.14	120.77	117.70
27	BE	88	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	1267	U	O4'-C1'-N1	6.14	113.11	108.20
54	BA	247	G	N1-C6-O6	-6.14	116.22	119.90
21	AA	1277	C	N3-C2-O2	-6.14	117.61	121.90
24	A3	67	C	N3-C2-O2	-6.14	117.60	121.90
52	B3	7	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	767	U	O4'-C1'-N1	6.14	113.11	108.20
54	BA	1868	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2435	A	C5-C6-N1	6.14	120.77	117.70
54	BA	2789	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	1521	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	218	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	1561	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2530	A	C5-C6-N1	6.13	120.77	117.70
21	AA	52	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2104	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	182	A	O4'-C1'-N9	6.13	113.11	108.20
21	AA	635	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	1705	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	2161	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1832	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2013	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2652	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	1314	C	N3-C2-O2	-6.13	117.61	121.90
22	A1	20	G	O4'-C1'-N9	6.13	113.10	108.20
44	BV	79	ARG	NE-CZ-NH1	6.13	123.36	120.30
51	B2	12	ARG	NE-CZ-NH2	6.13	123.36	120.30
53	B4	12	ARG	NE-CZ-NH1	6.13	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	64	A	C5-C6-N1	6.13	120.76	117.70
54	BA	835	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	60	G	N3-C2-N2	-6.13	115.61	119.90
54	BA	2432	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2823	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	1005	A	C5-C6-N1	6.12	120.76	117.70
54	BA	144	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	211	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	776	G	O4'-C1'-N9	6.12	113.10	108.20
21	AA	623	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	704	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	878	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1328	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1332	G	N3-C4-C5	-6.12	125.54	128.60
54	BA	1837	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	2301	C	N3-C2-O2	-6.12	117.61	121.90
24	A3	52	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1420	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1698	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2476	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2837	A	C5-C6-N1	6.12	120.76	117.70
54	BA	946	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1378	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2717	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2835	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1689	A	N1-C6-N6	-6.12	114.93	118.60
21	AA	324	G	N1-C6-O6	-6.12	116.23	119.90
21	AA	456	A	C5-C6-N1	6.12	120.76	117.70
21	AA	646	G	N1-C6-O6	-6.12	116.23	119.90
21	AA	792	A	O4'-C1'-N9	6.12	113.09	108.20
21	AA	1433	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	52	A	C5-C6-N1	6.12	120.76	117.70
54	BA	314	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1780	A	C4-C5-C6	-6.11	113.94	117.00
6	AG	91	ARG	NE-CZ-NH1	6.11	123.36	120.30
21	AA	1113	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1515	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	541	A	C5-C6-N1	6.11	120.75	117.70
54	BA	1744	A	C5-C6-N1	6.11	120.75	117.70
54	BA	2176	A	C4-C5-C6	-6.11	113.94	117.00
55	BB	29	A	N1-C6-N6	-6.11	114.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	51	A	C5-C6-N1	6.11	120.75	117.70
21	AA	1533	C	N1-C2-O2	6.11	122.56	118.90
22	A1	72	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	526	A	C1'-O4'-C4'	-6.11	105.01	109.90
54	BA	1437	C	O4'-C1'-N1	6.11	113.09	108.20
54	BA	2108	A	C4-C5-C6	-6.11	113.95	117.00
21	AA	40	C	N3-C2-O2	-6.11	117.63	121.90
21	AA	1157	A	C4-C5-C6	-6.11	113.95	117.00
31	BI	102	ARG	NE-CZ-NH1	6.11	123.35	120.30
54	BA	787	C	N1-C2-O2	6.11	122.56	118.90
54	BA	2035	G	O4'-C1'-N9	6.11	113.08	108.20
54	BA	2084	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	1739	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	314	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	759	A	C5-C6-N1	6.10	120.75	117.70
54	BA	161	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	706	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1313	U	N3-C2-O2	-6.10	117.93	122.20
54	BA	1417	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1866	A	C4-C5-C6	-6.10	113.95	117.00
55	BB	92	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	777	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	823	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1411	C	N1-C2-O2	6.10	122.56	118.90
54	BA	592	A	C5-C6-N1	6.10	120.75	117.70
21	AA	663	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	1252	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	15	G	N3-C2-N2	-6.10	115.63	119.90
54	BA	1512	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1933	G	O4'-C1'-N9	6.10	113.08	108.20
54	BA	2381	A	C5-C6-N1	6.10	120.75	117.70
21	AA	1317	C	N3-C2-O2	-6.10	117.63	121.90
24	A3	41	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	432	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	849	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1528	A	N1-C6-N6	-6.10	114.94	118.60
54	BA	731	C	N3-C2-O2	-6.09	117.63	121.90
54	BA	764	A	N1-C6-N6	-6.09	114.94	118.60
54	BA	1351	C	N3-C2-O2	-6.09	117.63	121.90
55	BB	113	C	N3-C2-O2	-6.09	117.63	121.90
21	AA	349	A	C5-C6-N1	6.09	120.75	117.70
21	AA	382	A	C4-C5-C6	-6.09	113.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	553	A	C5-C6-N1	6.09	120.75	117.70
54	BA	1741	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2154	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	2520	C	O4'-C1'-N1	6.09	113.07	108.20
21	AA	251	G	O4'-C1'-N9	6.09	113.07	108.20
21	AA	1236	A	N1-C6-N6	-6.09	114.95	118.60
51	B2	19	ARG	NE-CZ-NH1	6.09	123.34	120.30
54	BA	16	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2767	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	948	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2700	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	106	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	406	G	C5'-C4'-C3'	-6.09	106.26	116.00
54	BA	810	U	O4'-C1'-N1	6.09	113.07	108.20
21	AA	80	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1870	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	130	A	C6-C5-N7	6.08	136.56	132.30
21	AA	831	A	C5-C6-N1	6.08	120.74	117.70
21	AA	914	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	1217	C	N3-C2-O2	-6.08	117.64	121.90
41	BS	95	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	1196	C	O4'-C1'-N1	6.08	113.07	108.20
54	BA	2591	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2794	C	N3-C2-O2	-6.08	117.64	121.90
41	BS	11	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	442	G	N1-C6-O6	-6.08	116.25	119.90
54	BA	2376	A	C4-C5-C6	-6.08	113.96	117.00
55	BB	50	A	C4-C5-C6	-6.08	113.96	117.00
56	B5	53	ARG	NE-CZ-NH1	6.08	123.34	120.30
21	AA	493	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	322	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	984	A	O4'-C1'-N9	6.08	113.06	108.20
54	BA	2565	A	O4'-C1'-N9	6.08	113.06	108.20
5	AF	25	TYR	CB-CG-CD2	-6.08	117.35	121.00
54	BA	819	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	1117	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	1336	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	1308	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2858	C	O4'-C1'-N1	6.08	113.06	108.20
21	AA	36	C	N1-C2-O2	6.08	122.55	118.90
54	BA	602	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1404	C	N3-C2-O2	-6.08	117.65	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	222	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	433	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	101	A	C5-C6-N1	6.07	120.74	117.70
54	BA	1424	G	O4'-C1'-N9	6.07	113.06	108.20
54	BA	1640	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	2332	C	O4'-C1'-N1	6.07	113.06	108.20
54	BA	1944	U	O4'-C1'-N1	6.07	113.06	108.20
22	A1	32	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2241	A	C4-C5-C6	-6.07	113.97	117.00
7	AH	1	SER	C-N-CA	6.07	136.87	121.70
21	AA	231	U	O4'-C1'-N1	6.07	113.05	108.20
21	AA	784	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	255	A	C5-C6-N1	6.07	120.73	117.70
54	BA	630	G	N1-C6-O6	-6.07	116.26	119.90
54	BA	1178	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1302	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	1700	A	C5-C6-N1	6.07	120.73	117.70
54	BA	2051	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	2080	A	C5-C6-N1	6.07	120.73	117.70
54	BA	2853	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	179	C	O4'-C1'-N1	6.06	113.05	108.20
9	AJ	48	ARG	NE-CZ-NH2	6.06	123.33	120.30
21	AA	116	A	C5-C6-N1	6.06	120.73	117.70
21	AA	243	A	C5-C6-N1	6.06	120.73	117.70
54	BA	246	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1243	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2052	A	C4-C5-C6	-6.06	113.97	117.00
35	BM	38	ARG	NE-CZ-NH1	6.06	123.33	120.30
54	BA	320	A	C5-C6-N1	6.06	120.73	117.70
54	BA	1123	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	58	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	1112	C	N1-C2-O2	6.06	122.54	118.90
54	BA	10	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1273	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	1819	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	600	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1014	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1053	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2751	G	O4'-C1'-N9	6.06	113.05	108.20
21	AA	460	A	C5-C6-N1	6.05	120.73	117.70
54	BA	338	G	O4'-C1'-N9	6.05	113.04	108.20
54	BA	1212	G	N3-C2-N2	-6.05	115.66	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	687	A	C5-C6-N1	6.05	120.73	117.70
19	AT	2	ASN	C-N-CA	6.05	136.83	121.70
21	AA	8	A	N1-C6-N6	-6.05	114.97	118.60
21	AA	234	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	747	A	C4-C5-C6	-6.05	113.98	117.00
22	A1	69	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1189	A	C5-C6-N1	6.05	120.72	117.70
54	BA	1611	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	523	C	N1-C2-O2	6.05	122.53	118.90
54	BA	2704	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	41	G	N1-C6-O6	-6.05	116.27	119.90
21	AA	533	A	C5-C6-N1	6.05	120.72	117.70
21	AA	1273	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1307	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1571	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	262	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1413	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2480	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	509	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1288	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	300	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	318	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	657	U	O4'-C1'-N1	6.04	113.03	108.20
54	BA	1857	G	O4'-C1'-N9	6.04	113.03	108.20
54	BA	2270	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2338	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	105	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	330	A	O4'-C1'-N9	6.04	113.03	108.20
54	BA	1700	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	241	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1920	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2814	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	274	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1969	A	N1-C6-N6	-6.04	114.98	118.60
54	BA	2616	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	958	A	C5-C6-N1	6.04	120.72	117.70
12	AM	89	ARG	NE-CZ-NH2	-6.04	117.28	120.30
54	BA	374	A	N1-C6-N6	-6.04	114.98	118.60
54	BA	1314	C	C3'-C2'-C1'	6.04	106.33	101.50
54	BA	1462	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2184	A	C5-C6-N1	6.04	120.72	117.70
21	AA	160	A	C4-C5-C6	-6.03	113.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	714	G	N3-C2-N2	-6.03	115.68	119.90
21	AA	876	C	C5'-C4'-O4'	6.03	116.34	109.10
54	BA	12	U	O4'-C1'-N1	6.03	113.03	108.20
54	BA	161	A	C5-C6-N1	6.03	120.72	117.70
54	BA	527	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1039	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2540	C	N3-C2-O2	-6.03	117.68	121.90
55	BB	42	C	N1-C2-O2	6.03	122.52	118.90
21	AA	535	A	C4-C5-C6	-6.03	113.98	117.00
25	BC	211	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	592	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	415	A	O4'-C1'-N9	6.03	113.02	108.20
21	AA	539	A	C5-C6-N1	6.03	120.71	117.70
21	AA	1167	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	1479	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	1508	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	513	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	730	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	1960	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	309	A	N1-C6-N6	-6.03	114.98	118.60
21	AA	712	A	C4-C5-C6	-6.03	113.99	117.00
29	BG	94	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	1801	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	2045	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	41	C	N3-C2-O2	-6.02	117.68	121.90
21	AA	135	C	N3-C2-O2	-6.02	117.68	121.90
21	AA	998	C	N3-C2-O2	-6.02	117.68	121.90
54	BA	911	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1626	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2406	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2818	U	O4'-C1'-N1	6.02	113.02	108.20
54	BA	318	C	O4'-C1'-N1	6.02	113.02	108.20
3	AD	69	ARG	NE-CZ-NH1	6.02	123.31	120.30
21	AA	137	U	O4'-C1'-N1	6.02	113.02	108.20
21	AA	459	A	C5-C6-N1	6.02	120.71	117.70
21	AA	553	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	575	G	P-O3'-C3'	6.02	126.92	119.70
24	A3	73	A	P-O3'-C3'	6.02	126.92	119.70
54	BA	1672	A	C4-C5-C6	-6.02	113.99	117.00
55	BB	29	A	C4-C5-C6	-6.02	113.99	117.00
14	AO	63	ARG	NE-CZ-NH1	6.02	123.31	120.30
21	AA	718	A	C4-C5-C6	-6.02	113.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1086	U	O4'-C1'-N1	6.02	113.02	108.20
21	AA	1131	G	N3-C2-N2	-6.02	115.69	119.90
54	BA	509	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	851	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1676	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	806	C	N3-C2-O2	-6.02	117.69	121.90
22	A1	51	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	182	A	O4'-C1'-N9	6.02	113.01	108.20
54	BA	233	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	44	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	999	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	1271	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	104	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	678	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2266	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	335	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	432	A	C4-C5-C6	-6.01	113.99	117.00
24	A3	76	C	N1-C2-O2	6.01	122.51	118.90
54	BA	1526	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1805	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2447	G	O4'-C1'-N9	6.01	113.01	108.20
21	AA	408	A	C5-C6-N1	6.01	120.70	117.70
54	BA	269	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	453	A	O4'-C1'-N9	6.01	113.01	108.20
55	BB	117	G	O4'-C1'-N9	6.01	113.01	108.20
54	BA	2062	A	C4-C5-C6	-6.01	114.00	117.00
17	AR	56	ARG	NE-CZ-NH1	6.01	123.30	120.30
54	BA	94	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2263	C	N3-C2-O2	-6.00	117.70	121.90
36	BN	30	ARG	NE-CZ-NH1	6.00	123.30	120.30
39	BQ	2	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	83	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	118	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2579	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1119	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	478	A	C5-C6-N1	6.00	120.70	117.70
54	BA	752	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2468	A	C3'-C2'-C1'	6.00	106.30	101.50
21	AA	448	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	456	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	876	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	73	A	N1-C6-N6	-6.00	115.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	149	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	675	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1836	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	2043	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2134	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2542	A	O4'-C1'-N9	6.00	113.00	108.20
21	AA	1036	A	C5-C6-N1	6.00	120.70	117.70
55	BB	32	U	O4'-C1'-N1	6.00	113.00	108.20
21	AA	285	C	N3-C2-O2	-5.99	117.70	121.90
21	AA	1137	C	N3-C2-O2	-5.99	117.70	121.90
21	AA	1161	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	1294	U	O4'-C1'-N1	5.99	113.00	108.20
54	BA	2005	A	C4-C5-C6	-5.99	114.00	117.00
55	BB	26	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	694	U	O4'-C1'-N1	5.99	112.99	108.20
21	AA	1208	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	1500	A	C5-C6-N1	5.99	120.69	117.70
54	BA	660	C	N1-C2-O2	5.99	122.49	118.90
54	BA	2716	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	422	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1231	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	2612	C	N1-C2-O2	5.99	122.49	118.90
21	AA	129	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	1509	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	504	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1499	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2643	G	N1-C6-O6	-5.99	116.31	119.90
21	AA	1456	A	C4-C5-C6	-5.98	114.01	117.00
52	B3	39	ARG	NE-CZ-NH1	5.98	123.29	120.30
54	BA	1032	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2705	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1150	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1213	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1284	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	436	C	O4'-C1'-N1	5.98	112.98	108.20
54	BA	1098	A	C5-C6-N1	5.98	120.69	117.70
11	AL	49	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	315	A	N1-C6-N6	-5.98	115.01	118.60
54	BA	1590	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1617	C	C6-N1-C2	-5.98	117.91	120.30
54	BA	2270	A	N1-C6-N6	-5.98	115.01	118.60
21	AA	655	A	C5-C6-N1	5.98	120.69	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1305	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	2140	G	O4'-C1'-N9	5.98	112.98	108.20
21	AA	504	C	N3-C2-O2	-5.98	117.72	121.90
23	A2	93	U	N3-C2-O2	-5.98	118.02	122.20
54	BA	402	A	N1-C6-N6	-5.98	115.01	118.60
54	BA	1749	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2732	G	N3-C4-C5	-5.98	125.61	128.60
21	AA	573	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	679	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1194	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	2247	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	28	A	C4-C5-C6	-5.97	114.01	117.00
24	A3	74	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	8	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1170	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1241	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	1168	U	N3-C2-O2	-5.97	118.02	122.20
54	BA	685	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	952	G	C5-C6-N1	5.97	114.48	111.50
54	BA	1768	C	O4'-C1'-N1	5.97	112.98	108.20
54	BA	2841	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2856	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	396	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	172	A	C4-C5-C6	-5.97	114.02	117.00
32	BJ	95	ARG	NE-CZ-NH1	5.97	123.28	120.30
54	BA	444	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2165	C	N3-C2-O2	-5.97	117.72	121.90
55	BB	115	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	1460	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	2359	C	N1-C2-O2	5.96	122.48	118.90
54	BA	2430	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1306	C	O4'-C1'-N1	5.96	112.97	108.20
21	AA	43	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	613	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	1044	A	C5-C6-N1	5.96	120.68	117.70
21	AA	1195	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	821	A	O4'-C1'-N9	5.96	112.97	108.20
21	AA	560	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	1107	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1533	C	N1-C2-O2	5.96	122.48	118.90
54	BA	1618	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2208	C	N3-C2-O2	-5.96	117.73	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2730	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	882	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	866	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1150	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	435	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	63	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1135	C	C2-N3-C4	-5.96	116.92	119.90
54	BA	1428	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2000	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2139	U	O4'-C1'-N1	5.96	112.96	108.20
21	AA	738	C	N1-C2-O2	5.95	122.47	118.90
21	AA	742	G	N1-C6-O6	-5.95	116.33	119.90
21	AA	766	A	C5-C6-N1	5.95	120.68	117.70
54	BA	2459	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	328	C	N1-C2-O2	5.95	122.47	118.90
21	AA	496	A	O4'-C1'-N9	5.95	112.96	108.20
21	AA	814	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	1038	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	1136	C	N1-C2-O2	5.95	122.47	118.90
54	BA	19	A	C5-C6-N1	5.95	120.67	117.70
21	AA	161	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	74	A	O4'-C1'-N9	5.95	112.96	108.20
54	BA	512	G	N1-C6-O6	-5.95	116.33	119.90
54	BA	2199	A	C5-C6-N1	5.95	120.67	117.70
54	BA	227	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	640	C	C6-N1-C2	-5.95	117.92	120.30
54	BA	1711	A	C5-C6-N1	5.95	120.67	117.70
36	BN	69	ARG	NE-CZ-NH1	5.95	123.27	120.30
54	BA	948	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	2879	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	801	G	N1-C6-O6	-5.94	116.33	119.90
21	AA	1347	G	N1-C6-O6	-5.94	116.33	119.90
54	BA	47	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	557	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1284	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1967	C	O4'-C1'-N1	5.94	112.95	108.20
21	AA	1035	A	O4'-C1'-N9	5.94	112.95	108.20
54	BA	791	C	O4'-C1'-N1	5.94	112.95	108.20
54	BA	889	C	N1-C2-O2	5.94	122.46	118.90
54	BA	216	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	959	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	810	C	N3-C2-O2	-5.94	117.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2070	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1472	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	879	C	N1-C2-O2	5.93	122.46	118.90
48	BZ	10	ARG	NE-CZ-NH2	5.93	123.27	120.30
54	BA	21	A	C5-C6-N1	5.93	120.67	117.70
54	BA	1331	G	N1-C6-O6	-5.93	116.34	119.90
54	BA	1403	A	O4'-C1'-N9	5.93	112.94	108.20
21	AA	263	A	C5-C6-N1	5.93	120.67	117.70
21	AA	637	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1228	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	104	A	C5-C6-N1	5.93	120.67	117.70
54	BA	1798	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	2459	A	N1-C6-N6	-5.93	115.04	118.60
55	BB	51	G	C5-C6-N1	5.93	114.47	111.50
54	BA	895	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	1013	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	1111	A	C4-C5-C6	-5.93	114.04	117.00
54	BA	1801	A	N1-C6-N6	-5.93	115.04	118.60
21	AA	469	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	556	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1098	C	N3-C2-O2	-5.93	117.75	121.90
23	A2	91	A	C4-C5-C6	-5.93	114.04	117.00
54	BA	2003	A	C4-C5-C6	-5.93	114.04	117.00
21	AA	765	G	N3-C4-C5	-5.92	125.64	128.60
21	AA	967	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	1152	A	C5-C6-N1	5.92	120.66	117.70
54	BA	156	A	C5-C6-N1	5.92	120.66	117.70
54	BA	782	A	O4'-C1'-N9	5.92	112.94	108.20
54	BA	1447	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1586	A	C5-C6-N1	5.92	120.66	117.70
55	BB	59	A	C4-C5-C6	-5.92	114.04	117.00
55	BB	70	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	1382	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	1194	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	1628	G	C5'-C4'-O4'	5.92	116.21	109.10
54	BA	1916	A	O4'-C1'-N9	5.92	112.94	108.20
54	BA	1348	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	1446	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	418	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	712	A	C5-C6-N1	5.92	120.66	117.70
24	A3	76	C	C2'-C3'-O3'	5.92	123.17	113.70
54	BA	382	A	C4-C5-C6	-5.92	114.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	661	A	P-O3'-C3'	5.92	126.80	119.70
54	BA	994	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	1653	G	O4'-C1'-N9	5.92	112.94	108.20
54	BA	2727	A	C4-C5-C6	-5.92	114.04	117.00
55	BB	78	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2175	C	O4'-C1'-N1	5.92	112.93	108.20
21	AA	465	A	C4-C5-C6	-5.92	114.04	117.00
30	BH	116	ARG	NE-CZ-NH1	5.92	123.26	120.30
55	BB	91	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	33	C	N1-C2-O2	5.91	122.45	118.90
54	BA	1888	G	O4'-C1'-N9	5.91	112.93	108.20
21	AA	756	C	N3-C4-C5	5.91	124.27	121.90
54	BA	609	A	C5-C6-N1	5.91	120.66	117.70
54	BA	1386	C	N3-C2-O2	-5.91	117.76	121.90
29	BG	93	TYR	CB-CG-CD2	-5.91	117.45	121.00
48	BZ	10	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
54	BA	1142	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	1257	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2339	C	C1'-O4'-C4'	-5.91	105.17	109.90
21	AA	307	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1012	U	O4'-C1'-N1	5.91	112.93	108.20
25	BC	237	ARG	NE-CZ-NH2	-5.91	117.35	120.30
21	AA	1093	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	2787	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1104	G	N1-C6-O6	-5.90	116.36	119.90
21	AA	1171	A	C5-C6-N1	5.90	120.65	117.70
24	A3	29	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1288	G	N3-C4-C5	-5.90	125.65	128.60
21	AA	946	A	C5-C6-N1	5.90	120.65	117.70
54	BA	466	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	393	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	1145	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1711	A	N1-C6-N6	-5.90	115.06	118.60
21	AA	665	A	C6-C5-N7	5.90	136.43	132.30
24	A3	38	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1489	C	N1-C2-O2	5.90	122.44	118.90
54	BA	2841	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	418	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1032	G	O4'-C1'-N9	5.89	112.92	108.20
54	BA	196	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	750	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	905	A	C4-C5-C6	-5.89	114.05	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1384	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	1821	A	C5-C6-N1	5.89	120.65	117.70
15	AP	70	ARG	NE-CZ-NH1	5.89	123.25	120.30
54	BA	209	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1945	G	N1-C6-O6	-5.89	116.36	119.90
54	BA	2137	U	N3-C2-O2	-5.89	118.08	122.20
54	BA	2874	C	N3-C2-O2	-5.89	117.78	121.90
55	BB	63	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	128	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	383	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1046	A	C4-C5-C6	-5.89	114.05	117.00
21	AA	326	G	N1-C6-O6	-5.89	116.37	119.90
54	BA	931	U	N3-C2-O2	-5.89	118.08	122.20
21	AA	309	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	1067	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	2311	A	C4-C5-C6	-5.89	114.06	117.00
3	AD	110	ARG	NE-CZ-NH1	5.88	123.24	120.30
21	AA	610	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	2001	C	N3-C2-O2	-5.88	117.78	121.90
28	BF	124	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	403	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	1385	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1785	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1952	A	O4'-C1'-N9	5.88	112.91	108.20
54	BA	1121	C	O4'-C1'-N1	5.88	112.90	108.20
21	AA	67	C	N1-C2-O2	5.88	122.43	118.90
21	AA	723	U	O4'-C1'-N1	5.88	112.90	108.20
21	AA	1517	G	N1-C6-O6	-5.88	116.37	119.90
21	AA	495	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1787	A	C5-C6-N1	5.88	120.64	117.70
54	BA	2454	G	N1-C6-O6	-5.88	116.37	119.90
55	BB	19	C	N3-C2-O2	-5.88	117.79	121.90
21	AA	345	C	C1'-O4'-C4'	-5.88	105.20	109.90
21	AA	1254	A	C5-C6-N1	5.88	120.64	117.70
21	AA	817	C	O4'-C1'-N1	5.87	112.90	108.20
54	BA	978	G	N1-C6-O6	-5.87	116.38	119.90
54	BA	1495	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	1080	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	1595	C	O4'-C1'-N1	5.87	112.90	108.20
54	BA	2065	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2178	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2869	G	N3-C2-N2	-5.87	115.79	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	270	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	99	U	N3-C2-O2	-5.87	118.09	122.20
21	AA	1518	A	C5-C6-N1	5.87	120.63	117.70
54	BA	255	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	1470	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	44	A	C5-C6-N1	5.87	120.63	117.70
21	AA	756	C	N1-C2-O2	5.87	122.42	118.90
21	AA	960	U	N3-C2-O2	-5.87	118.09	122.20
54	BA	439	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	1638	C	N1-C2-O2	5.87	122.42	118.90
21	AA	492	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	890	G	O4'-C1'-N9	5.86	112.89	108.20
54	BA	2678	C	N3-C2-O2	-5.86	117.80	121.90
55	BB	15	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1652	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1732	C	N1-C2-O2	5.86	122.42	118.90
54	BA	1987	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	328	C	O4'-C1'-N1	5.86	112.89	108.20
54	BA	1057	A	C5-C6-N1	5.86	120.63	117.70
54	BA	2052	A	N1-C6-N6	-5.86	115.08	118.60
21	AA	263	A	N1-C6-N6	-5.86	115.09	118.60
21	AA	381	C	N1-C2-O2	5.86	122.41	118.90
54	BA	2354	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2556	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	356	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	1016	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	337	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	894	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2558	C	N3-C2-O2	-5.85	117.80	121.90
21	AA	624	C	O4'-C1'-N1	5.85	112.88	108.20
21	AA	1534	A	C4-C5-C6	-5.85	114.07	117.00
23	A2	79	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	2507	C	N1-C2-O2	5.85	122.41	118.90
21	AA	1197	A	C5-C6-N1	5.85	120.63	117.70
54	BA	348	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	1531	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1354	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1781	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2425	A	O4'-C1'-N9	5.85	112.88	108.20
54	BA	2870	C	O4'-C1'-N1	5.85	112.88	108.20
55	BB	30	C	N3-C2-O2	-5.85	117.81	121.90
29	BG	2	ARG	NE-CZ-NH1	5.85	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1244	A	C5-C6-N1	5.85	120.62	117.70
54	BA	2036	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	2458	G	N3-C4-C5	-5.85	125.68	128.60
54	BA	2527	C	N1-C2-O2	5.85	122.41	118.90
22	A1	11	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	253	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	998	C	N3-C2-O2	-5.85	117.81	121.90
55	BB	56	G	O4'-C1'-N9	5.85	112.88	108.20
21	AA	175	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2007	U	O4'-C1'-N1	5.84	112.88	108.20
55	BB	31	C	O4'-C1'-N1	5.84	112.88	108.20
21	AA	1261	A	C5-C6-N1	5.84	120.62	117.70
54	BA	353	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	853	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	1761	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2874	C	N1-C2-O2	5.84	122.41	118.90
54	BA	470	A	C5-C6-N1	5.84	120.62	117.70
21	AA	272	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	503	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	498	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	2207	C	N3-C2-O2	-5.84	117.81	121.90
12	AM	86	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	AA	811	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	111	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1054	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1877	A	C4-C5-C6	-5.84	114.08	117.00
55	BB	17	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	1248	A	C5-C6-N1	5.83	120.62	117.70
54	BA	222	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	181	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	1407	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1624	U	O4'-C1'-N1	5.83	112.87	108.20
54	BA	2422	C	N1-C2-O2	5.83	122.40	118.90
54	BA	2582	G	N3-C4-C5	-5.83	125.68	128.60
54	BA	2667	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	374	A	C5-C6-N1	5.83	120.62	117.70
54	BA	2090	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	2893	A	C4-C5-C6	-5.83	114.08	117.00
15	AP	51	ARG	NE-CZ-NH2	-5.83	117.39	120.30
21	AA	610	U	N3-C2-O2	-5.83	118.12	122.20
54	BA	172	A	C5-C6-N1	5.83	120.61	117.70
54	BA	2784	U	O4'-C1'-N1	5.83	112.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BD	58	ASN	C-N-CA	5.83	136.27	121.70
54	BA	2820	A	C4-C5-C6	-5.83	114.09	117.00
38	BP	88	ARG	NE-CZ-NH2	-5.83	117.39	120.30
54	BA	898	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1001	A	C5-C6-N1	5.83	120.61	117.70
54	BA	1001	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	975	A	C1'-O4'-C4'	-5.82	105.24	109.90
54	BA	1311	G	N3-C4-C5	-5.82	125.69	128.60
54	BA	2330	G	C4'-C3'-C2'	-5.82	96.78	102.60
55	BB	87	U	N3-C2-O2	-5.82	118.12	122.20
21	AA	385	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1145	A	C3'-C2'-C1'	5.82	106.16	101.50
21	AA	1374	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1399	C	O4'-C1'-N1	5.82	112.86	108.20
3	AD	61	ARG	NE-CZ-NH2	-5.82	117.39	120.30
21	AA	629	A	C4-C5-C6	-5.82	114.09	117.00
23	A2	82	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1172	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1857	G	N1-C6-O6	-5.82	116.41	119.90
54	BA	2399	G	N1-C6-O6	-5.82	116.41	119.90
21	AA	631	C	O4'-C1'-N1	5.82	112.86	108.20
54	BA	119	A	O4'-C1'-N9	5.82	112.86	108.20
54	BA	1312	U	P-O3'-C3'	5.82	126.68	119.70
54	BA	1565	C	N1-C2-O2	5.82	122.39	118.90
21	AA	586	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1452	C	N1-C2-O2	5.82	122.39	118.90
54	BA	2258	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1171	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2330	G	O4'-C1'-N9	5.82	112.85	108.20
54	BA	2733	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	1237	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1994	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2468	A	O4'-C4'-C3'	5.81	110.75	106.10
54	BA	1052	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1916	A	C6-C5-N7	5.81	136.37	132.30
54	BA	324	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2194	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	2500	U	N3-C2-O2	-5.81	118.13	122.20
8	AI	98	ARG	NE-CZ-NH1	5.81	123.20	120.30
54	BA	2091	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2135	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2458	G	N1-C6-O6	-5.81	116.41	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1265	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	270	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	1652	A	C5-C6-N1	5.81	120.60	117.70
54	BA	2264	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2888	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	198	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2031	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	2478	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	694	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1191	A	C5-C6-N1	5.80	120.60	117.70
54	BA	1156	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1278	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1990	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2175	C	N3-C4-C5	5.80	124.22	121.90
21	AA	101	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1499	A	C4-C5-C6	-5.80	114.10	117.00
24	A3	44	A	C5-C6-N1	5.80	120.60	117.70
54	BA	415	A	C6-C5-N7	5.80	136.36	132.30
54	BA	960	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2807	U	O4'-C1'-N1	5.80	112.84	108.20
21	AA	1095	U	C5-C6-N1	-5.80	119.80	122.70
54	BA	485	C	N1-C2-O2	5.80	122.38	118.90
54	BA	1363	C	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2117	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	209	U	C3'-C2'-C1'	5.80	106.14	101.50
21	AA	880	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	903	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1424	G	N1-C6-O6	-5.80	116.42	119.90
56	B5	7	ARG	NE-CZ-NH1	5.80	123.20	120.30
16	AQ	61	ARG	NE-CZ-NH2	-5.80	117.40	120.30
21	AA	1035	A	C4-C5-C6	-5.80	114.10	117.00
25	BC	86	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	79	C	N1-C2-O2	5.80	122.38	118.90
54	BA	226	A	O4'-C1'-N9	5.80	112.84	108.20
54	BA	487	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	635	C	N1-C2-O2	5.80	122.38	118.90
54	BA	764	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1290	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	2305	U	C5'-C4'-C3'	-5.79	106.73	116.00
20	AU	33	ARG	NE-CZ-NH2	5.79	123.20	120.30
21	AA	1301	U	N3-C2-O2	-5.79	118.14	122.20
54	BA	413	C	N3-C2-O2	-5.79	117.84	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	683	U	C5'-C4'-O4'	5.79	116.05	109.10
54	BA	2041	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2806	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	740	C	N1-C2-O2	5.79	122.37	118.90
54	BA	1893	C	O4'-C1'-N1	5.79	112.83	108.20
21	AA	1080	A	N1-C6-N6	-5.79	115.13	118.60
21	AA	1318	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	1339	A	C5'-C4'-O4'	5.79	116.05	109.10
27	BE	61	ARG	NE-CZ-NH1	5.79	123.19	120.30
54	BA	876	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	991	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1147	A	O4'-C1'-N9	5.79	112.83	108.20
54	BA	1383	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2119	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2520	C	N1-C2-O2	5.79	122.37	118.90
54	BA	2849	U	N3-C2-O2	-5.79	118.15	122.20
55	BB	11	C	N1-C2-O2	5.79	122.37	118.90
21	AA	853	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1233	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1246	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2513	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2766	A	N1-C6-N6	-5.79	115.13	118.60
21	AA	176	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	520	A	C4-C5-C6	-5.79	114.11	117.00
28	BF	91	ARG	NE-CZ-NH1	5.79	123.19	120.30
54	BA	1605	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2364	C	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2583	G	N1-C6-O6	-5.78	116.43	119.90
22	A1	6	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1299	G	N7-C8-N9	5.78	115.99	113.10
15	AP	5	ARG	NE-CZ-NH1	5.78	123.19	120.30
32	BJ	37	ARG	NE-CZ-NH2	-5.78	117.41	120.30
54	BA	158	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	335	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	702	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	793	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1938	A	O4'-C1'-N9	5.78	112.82	108.20
54	BA	1990	C	O4'-C1'-N1	5.78	112.82	108.20
54	BA	2184	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	935	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	178	G	N1-C6-O6	-5.78	116.43	119.90
54	BA	1357	C	N3-C2-O2	-5.78	117.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1711	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	993	G	C5-C6-N1	5.78	114.39	111.50
21	AA	1244	G	N1-C6-O6	-5.78	116.43	119.90
21	AA	1342	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	394	C	N1-C2-O2	5.78	122.37	118.90
54	BA	1266	G	N1-C6-O6	-5.78	116.43	119.90
54	BA	1326	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	1367	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	322	C	N3-C2-O2	-5.78	117.86	121.90
21	AA	860	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1336	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2205	A	N1-C6-N6	-5.78	115.13	118.60
54	BA	2765	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1043	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1232	G	C5-C6-N1	5.77	114.39	111.50
54	BA	2503	A	O4'-C1'-N9	5.77	112.82	108.20
22	A1	18	G	O4'-C1'-N9	5.77	112.82	108.20
24	A3	42	C	N1-C2-O2	5.77	122.36	118.90
54	BA	109	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	2309	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	2788	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1095	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	2603	G	O4'-C1'-N9	5.77	112.82	108.20
54	BA	2830	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	2880	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	166	U	O4'-C1'-N1	5.77	112.81	108.20
54	BA	257	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1378	A	C1'-O4'-C4'	-5.77	105.28	109.90
21	AA	876	C	O4'-C4'-C3'	-5.77	98.23	104.00
54	BA	1536	C	N1-C2-O2	5.77	122.36	118.90
54	BA	1550	C	N1-C2-O2	5.77	122.36	118.90
54	BA	2226	C	O4'-C1'-N1	5.77	112.81	108.20
21	AA	658	C	N1-C2-O2	5.77	122.36	118.90
21	AA	99	C	N1-C2-O2	5.76	122.36	118.90
21	AA	119	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	209	U	O4'-C1'-N1	5.76	112.81	108.20
21	AA	503	C	N3-C2-O2	-5.76	117.86	121.90
22	A1	48	C	N1-C2-O2	5.76	122.36	118.90
54	BA	634	C	N1-C2-O2	5.76	122.36	118.90
54	BA	1595	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	1797	G	N7-C8-N9	5.76	115.98	113.10
21	AA	631	C	N1-C2-O2	5.76	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1549	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	1145	A	O4'-C1'-N9	5.76	112.81	108.20
21	AA	1408	A	C4-C5-C6	-5.76	114.12	117.00
36	BN	71	ARG	NE-CZ-NH1	5.76	123.18	120.30
37	BO	33	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	226	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1518	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	1690	A	N1-C6-N6	-5.76	115.14	118.60
54	BA	2528	U	C5-C6-N1	-5.76	119.82	122.70
55	BB	49	C	C3'-C2'-C1'	5.76	106.11	101.50
21	AA	722	G	N1-C6-O6	-5.76	116.44	119.90
21	AA	1375	A	N1-C6-N6	-5.76	115.14	118.60
21	AA	1403	C	N1-C2-O2	5.76	122.36	118.90
21	AA	1503	A	C4-C5-C6	-5.76	114.12	117.00
24	A3	14	A	C5-C6-N1	5.76	120.58	117.70
28	BF	101	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	928	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1085	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1090	A	C5-C6-N1	5.76	120.58	117.70
54	BA	1168	G	N1-C6-O6	-5.76	116.44	119.90
54	BA	1575	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2114	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2404	U	O4'-C1'-N1	5.76	112.81	108.20
10	AK	55	ARG	NE-CZ-NH1	5.76	123.18	120.30
21	AA	808	C	N1-C2-O2	5.76	122.36	118.90
21	AA	1354	U	N3-C2-O2	-5.76	118.17	122.20
54	BA	947	A	C6-C5-N7	5.76	136.33	132.30
54	BA	1914	C	N1-C2-O2	5.76	122.36	118.90
54	BA	1986	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	923	A	C4-C5-C6	-5.76	114.12	117.00
39	BQ	5	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	786	C	N1-C2-O2	5.76	122.35	118.90
54	BA	1259	G	O4'-C1'-N9	5.76	112.81	108.20
54	BA	2050	C	N1-C2-O2	5.76	122.35	118.90
54	BA	2698	U	O4'-C1'-N1	5.76	112.81	108.20
4	AE	44	ARG	NE-CZ-NH1	5.75	123.18	120.30
21	AA	743	A	C5-C6-N1	5.75	120.58	117.70
21	AA	1203	C	O4'-C1'-N1	5.75	112.80	108.20
24	A3	24	C	N3-C2-O2	-5.75	117.87	121.90
24	A3	69	C	N1-C2-O2	5.75	122.35	118.90
54	BA	2486	C	N3-C2-O2	-5.75	117.87	121.90
7	AH	113	ARG	NE-CZ-NH1	5.75	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	373	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	1226	C	N1-C2-O2	5.75	122.35	118.90
54	BA	42	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2559	C	N3-C2-O2	-5.75	117.87	121.90
55	BB	110	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	926	G	C8-N9-C4	-5.75	104.10	106.40
21	AA	1518	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2491	U	O4'-C1'-N1	5.75	112.80	108.20
21	AA	207	C	N1-C2-O2	5.75	122.35	118.90
34	BL	18	ARG	NE-CZ-NH1	5.75	123.17	120.30
54	BA	342	A	C5-C6-N1	5.75	120.57	117.70
21	AA	421	U	O4'-C1'-N1	5.75	112.80	108.20
21	AA	600	A	C5-C6-N1	5.75	120.57	117.70
32	BJ	35	ARG	NH1-CZ-NH2	-5.75	113.08	119.40
54	BA	1539	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2460	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2611	C	N1-C2-O2	5.75	122.35	118.90
54	BA	2715	C	O4'-C1'-N1	5.75	112.80	108.20
18	AS	80	ARG	NE-CZ-NH2	-5.75	117.43	120.30
54	BA	1393	A	O4'-C4'-C3'	5.75	110.70	106.10
21	AA	190	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	350	G	C1'-O4'-C4'	-5.74	105.31	109.90
54	BA	225	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	107	G	N1-C6-O6	-5.74	116.45	119.90
21	AA	211	G	N3-C4-C5	-5.74	125.73	128.60
21	AA	571	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1254	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1664	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2055	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	2443	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	818	G	O4'-C1'-N9	5.74	112.79	108.20
54	BA	2741	A	C4-C5-C6	-5.74	114.13	117.00
24	A3	59	A	C6-C5-N7	5.73	136.31	132.30
34	BL	47	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	1927	A	C5-C6-N1	5.73	120.57	117.70
21	AA	95	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	486	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	753	A	C4-C5-C6	-5.73	114.13	117.00
54	BA	1752	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1755	A	C6-C5-N7	5.73	136.31	132.30
13	AN	90	ARG	NE-CZ-NH2	5.73	123.17	120.30
21	AA	689	C	O4'-C1'-N1	5.73	112.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	715	A	C4-C5-C6	-5.73	114.14	117.00
33	BK	105	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	2295	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2679	A	C4-C5-C6	-5.73	114.14	117.00
41	BS	84	ARG	NE-CZ-NH1	5.73	123.17	120.30
21	AA	78	A	C1'-O4'-C4'	-5.73	105.32	109.90
21	AA	1383	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	301	G	O4'-C1'-N9	5.73	112.78	108.20
54	BA	471	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	2396	G	N1-C6-O6	-5.73	116.46	119.90
54	BA	964	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1301	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	82	U	O4'-C1'-N1	5.72	112.78	108.20
54	BA	672	C	N1-C2-O2	5.72	122.33	118.90
54	BA	2277	G	N1-C6-O6	-5.72	116.47	119.90
21	AA	1026	G	N3-C2-N2	-5.72	115.89	119.90
54	BA	1264	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2361	G	O4'-C1'-N9	5.72	112.78	108.20
54	BA	2557	G	C5-C6-N1	5.72	114.36	111.50
55	BB	35	C	N1-C2-O2	5.72	122.33	118.90
21	AA	471	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	599	C	N3-C2-O2	-5.72	117.89	121.90
21	AA	1192	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	2023	C	N3-C2-O2	-5.72	117.89	121.90
21	AA	1140	C	N3-C2-O2	-5.72	117.90	121.90
49	B0	49	ARG	NE-CZ-NH1	5.72	123.16	120.30
54	BA	857	G	O4'-C1'-N9	5.72	112.78	108.20
54	BA	1772	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	303	G	C3'-C2'-C1'	5.72	106.07	101.50
21	AA	112	G	N1-C6-O6	-5.72	116.47	119.90
54	BA	644	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2273	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2465	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	519	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1271	A	C5-C6-N1	5.71	120.56	117.70
54	BA	253	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	734	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1979	U	C4'-C3'-C2'	-5.71	96.89	102.60
54	BA	2755	C	N1-C2-O2	5.71	122.33	118.90
55	BB	71	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	2133	G	C8-N9-C4	-5.71	104.11	106.40
54	BA	112	U	O4'-C1'-N1	5.71	112.77	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	334	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	606	U	O4'-C1'-N1	5.71	112.77	108.20
54	BA	649	G	C3'-C2'-C1'	5.71	106.07	101.50
54	BA	1534	U	N3-C2-O2	-5.71	118.20	122.20
55	BB	46	A	C6-C5-N7	5.71	136.30	132.30
54	BA	2030	A	C4-C5-C6	-5.71	114.14	117.00
21	AA	530	G	O4'-C1'-N9	5.71	112.77	108.20
21	AA	1396	A	C6-C5-N7	5.71	136.30	132.30
54	BA	26	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	2774	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	2350	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	1104	C	N1-C2-O2	5.70	122.32	118.90
54	BA	1218	G	C5-C6-N1	5.70	114.35	111.50
54	BA	2096	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	761	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	985	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	1547	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	2181	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	943	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1848	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2225	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2227	A	C5-C6-N1	5.70	120.55	117.70
21	AA	749	A	C6-C5-N7	5.69	136.28	132.30
21	AA	1404	C	N3-C4-N4	-5.69	114.01	118.00
21	AA	1483	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	195	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2649	C	N3-C2-O2	-5.69	117.91	121.90
21	AA	743	A	C4-C5-C6	-5.69	114.15	117.00
39	BQ	10	ARG	NE-CZ-NH1	5.69	123.15	120.30
54	BA	1141	U	N3-C2-O2	-5.69	118.22	122.20
54	BA	2369	A	N1-C6-N6	-5.69	115.19	118.60
54	BA	2430	A	C2-N3-C4	5.69	113.45	110.60
21	AA	1257	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1159	U	O4'-C1'-N1	5.69	112.75	108.20
54	BA	2460	U	C4'-C3'-C2'	-5.69	96.91	102.60
54	BA	705	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1890	A	O4'-C1'-N9	5.69	112.75	108.20
21	AA	1102	A	C5-C6-N1	5.69	120.54	117.70
21	AA	1251	A	C6-C5-N7	5.69	136.28	132.30
21	AA	1310	G	N1-C6-O6	-5.69	116.49	119.90
54	BA	873	C	N1-C2-O2	5.69	122.31	118.90
54	BA	1475	G	N1-C6-O6	-5.69	116.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1269	A	C5-C6-N1	5.69	120.54	117.70
54	BA	1902	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	2297	A	C5-C6-N1	5.69	120.54	117.70
21	AA	364	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	706	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	670	A	P-O3'-C3'	5.68	126.52	119.70
54	BA	974	G	N3-C2-N2	-5.68	115.92	119.90
54	BA	1365	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	1330	U	N1-C2-N3	5.68	118.31	114.90
54	BA	1576	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1701	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1765	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1808	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	2480	C	O4'-C1'-N1	5.68	112.75	108.20
6	AG	94	ARG	NE-CZ-NH1	5.68	123.14	120.30
16	AQ	64	ARG	NE-CZ-NH1	5.68	123.14	120.30
18	AS	31	ARG	NE-CZ-NH1	5.68	123.14	120.30
21	AA	163	C	N1-C2-O2	5.68	122.31	118.90
54	BA	429	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	1477	U	O4'-C1'-N1	5.68	112.74	108.20
21	AA	489	C	O4'-C1'-N1	5.68	112.74	108.20
21	AA	984	C	N1-C2-O2	5.68	122.31	118.90
54	BA	242	G	O4'-C1'-N9	5.68	112.74	108.20
54	BA	2330	G	N9-C4-C5	5.68	107.67	105.40
21	AA	422	C	N3-C4-C5	5.67	124.17	121.90
21	AA	839	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	1190	G	P-O3'-C3'	5.67	126.51	119.70
54	BA	2374	C	N1-C2-O2	5.67	122.31	118.90
54	BA	2507	C	N3-C4-C5	5.67	124.17	121.90
21	AA	248	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	615	U	C1'-O4'-C4'	-5.67	105.36	109.90
54	BA	1771	C	N3-C2-O2	-5.67	117.93	121.90
17	AR	72	ARG	NE-CZ-NH1	5.67	123.14	120.30
24	A3	44	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	1115	G	N1-C6-O6	-5.67	116.50	119.90
54	BA	1795	C	N1-C2-O2	5.67	122.30	118.90
54	BA	1843	C	N1-C2-O2	5.67	122.30	118.90
54	BA	2071	A	C4-C5-C6	-5.67	114.17	117.00
16	AQ	76	ARG	NE-CZ-NH1	5.67	123.14	120.30
21	AA	1200	C	N3-C4-C5	5.67	124.17	121.90
45	BW	54	ARG	NE-CZ-NH2	5.67	123.14	120.30
54	BA	208	C	N3-C2-O2	-5.67	117.93	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	870	U	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2447	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	870	U	N3-C2-O2	-5.67	118.23	122.20
21	AA	912	C	N1-C2-O2	5.67	122.30	118.90
54	BA	338	G	N3-C4-C5	-5.67	125.77	128.60
54	BA	574	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	890	C	N1-C2-O2	5.67	122.30	118.90
54	BA	2510	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	746	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	320	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	1789	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2353	G	O4'-C1'-N9	5.66	112.73	108.20
21	AA	345	C	N1-C2-O2	5.66	122.30	118.90
21	AA	1028	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1126	U	C3'-C2'-C1'	5.66	106.03	101.50
21	AA	1404	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	638	G	N3-C4-C5	-5.66	125.77	128.60
21	AA	1027	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1223	C	N1-C2-O2	5.66	122.29	118.90
54	BA	191	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	267	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	2289	G	C5-C6-N1	5.66	114.33	111.50
18	AS	80	ARG	NE-CZ-NH1	5.66	123.13	120.30
21	AA	533	A	N1-C6-N6	-5.66	115.21	118.60
21	AA	1322	C	N1-C2-O2	5.66	122.29	118.90
54	BA	884	U	O4'-C1'-N1	5.66	112.72	108.20
54	BA	1262	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2321	U	N3-C2-O2	-5.66	118.24	122.20
54	BA	2793	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1410	A	C4-C5-C6	-5.65	114.17	117.00
22	A1	27	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	305	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	291	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	671	C	N1-C2-O2	5.65	122.29	118.90
54	BA	2286	G	C5-C6-N1	5.65	114.33	111.50
55	BB	49	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	532	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	938	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	518	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	664	G	N1-C6-O6	-5.65	116.51	119.90
21	AA	253	A	C5-C6-N1	5.65	120.52	117.70
54	BA	157	C	O4'-C1'-N1	5.65	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1913	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	2128	G	O4'-C1'-N9	5.65	112.72	108.20
54	BA	2428	G	N1-C6-O6	-5.65	116.51	119.90
21	AA	559	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	721	G	N3-C4-C5	-5.64	125.78	128.60
22	A1	31	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	116	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	529	A	N1-C6-N6	-5.64	115.21	118.60
54	BA	1089	A	O4'-C1'-N9	5.64	112.72	108.20
54	BA	1109	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1140	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2097	A	C5-C6-N1	5.64	120.52	117.70
21	AA	233	C	N1-C2-O2	5.64	122.29	118.90
21	AA	536	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	648	A	C1'-O4'-C4'	-5.64	105.39	109.90
31	BI	126	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	814	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	915	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1157	G	N1-C6-O6	-5.64	116.51	119.90
54	BA	2388	A	C4-C5-C6	-5.64	114.18	117.00
2	AC	87	ARG	NE-CZ-NH1	5.64	123.12	120.30
21	AA	567	G	C5-C6-N1	5.64	114.32	111.50
54	BA	28	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	163	C	N1-C2-O2	5.64	122.28	118.90
54	BA	1737	G	N1-C6-O6	-5.64	116.52	119.90
54	BA	1891	G	O4'-C1'-N9	5.64	112.71	108.20
54	BA	2310	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	1367	C	N3-C2-O2	-5.64	117.95	121.90
34	BL	33	ARG	NE-CZ-NH1	5.64	123.12	120.30
21	AA	582	C	N3-C4-C5	5.64	124.16	121.90
21	AA	1362	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	417	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	870	U	C5-C6-N1	-5.64	119.88	122.70
54	BA	2335	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	422	A	C6-C5-N7	5.63	136.24	132.30
55	BB	55	U	O4'-C1'-N1	5.63	112.71	108.20
11	AL	8	ARG	NE-CZ-NH2	-5.63	117.48	120.30
21	AA	227	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	1152	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	272	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	584	C	O4'-C1'-N1	5.63	112.71	108.20
54	BA	2205	A	C4-C5-C6	-5.63	114.18	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	514	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	1497	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	389	G	N3-C2-N2	-5.63	115.96	119.90
54	BA	1427	A	P-O3'-C3'	5.63	126.46	119.70
54	BA	1211	C	N1-C2-O2	5.63	122.28	118.90
54	BA	1892	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	2037	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	36	C	N3-C4-N4	-5.63	114.06	118.00
54	BA	1015	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	1991	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	2171	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	2202	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	2322	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	719	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	1699	G	N3-C2-N2	-5.63	115.96	119.90
54	BA	2044	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	277	C	N3-C2-O2	-5.62	117.96	121.90
21	AA	779	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	1151	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1226	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	511	C	O4'-C1'-N1	5.62	112.70	108.20
21	AA	576	C	O4'-C1'-N1	5.62	112.70	108.20
21	AA	728	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1288	A	C6-C5-N7	5.62	136.24	132.30
54	BA	417	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	735	A	N1-C6-N6	-5.62	115.23	118.60
54	BA	737	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	783	A	C5-C6-N1	5.62	120.51	117.70
54	BA	980	A	P-O3'-C3'	5.62	126.45	119.70
54	BA	1194	A	C5-C6-N1	5.62	120.51	117.70
54	BA	2291	U	O4'-C1'-N1	5.62	112.70	108.20
54	BA	2777	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	47	C	N1-C2-O2	5.62	122.27	118.90
54	BA	129	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1366	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1823	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	1774	C	O4'-C1'-N1	5.62	112.70	108.20
1	AB	20	ARG	NE-CZ-NH2	-5.62	117.49	120.30
54	BA	860	U	O4'-C1'-N1	5.62	112.69	108.20
54	BA	1118	C	N1-C2-O2	5.62	122.27	118.90
54	BA	1505	A	C5'-C4'-O4'	5.62	115.84	109.10
21	AA	1223	C	N3-C4-N4	-5.62	114.07	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1412	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	315	G	O4'-C1'-N9	5.62	112.69	108.20
24	A3	40	C	N1-C2-O2	5.62	122.27	118.90
54	BA	354	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	758	C	O4'-C1'-N1	5.62	112.69	108.20
54	BA	910	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1014	A	C5-C6-N1	5.62	120.51	117.70
54	BA	1204	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2087	G	C5-C6-N1	5.62	114.31	111.50
54	BA	2151	U	O4'-C1'-N1	5.62	112.69	108.20
21	AA	513	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	884	U	C1'-O4'-C4'	-5.61	105.41	109.90
54	BA	2475	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	206	C	N1-C2-O2	5.61	122.27	118.90
54	BA	629	G	P-O3'-C3'	5.61	126.43	119.70
54	BA	959	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	2592	G	O4'-C1'-N9	5.61	112.69	108.20
54	BA	1376	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1847	A	O4'-C1'-N9	5.61	112.69	108.20
54	BA	1934	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2886	A	C4-C5-C6	-5.61	114.19	117.00
21	AA	848	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	105	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1617	C	N1-C2-N3	5.61	123.13	119.20
54	BA	1865	U	C5-C6-N1	-5.61	119.90	122.70
54	BA	2466	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	2731	G	N1-C6-O6	-5.61	116.53	119.90
55	BB	58	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	344	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	554	A	C6-C5-N7	5.61	136.22	132.30
54	BA	282	A	C5-C6-N1	5.61	120.50	117.70
54	BA	815	C	P-O3'-C3'	5.61	126.43	119.70
54	BA	1875	G	N1-C6-O6	-5.61	116.54	119.90
54	BA	1981	A	N1-C6-N6	-5.61	115.24	118.60
54	BA	2386	A	C6-C5-N7	5.61	136.22	132.30
54	BA	2686	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	556	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1016	G	O4'-C1'-N9	5.60	112.68	108.20
54	BA	1023	U	C3'-C2'-C1'	5.60	105.98	101.50
54	BA	1437	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1872	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	2676	C	N3-C2-O2	-5.60	117.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2842	G	O4'-C1'-N9	5.60	112.68	108.20
54	BA	2510	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2620	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	2655	G	C3'-C2'-C1'	-5.60	97.02	101.50
55	BB	51	G	N1-C6-O6	-5.60	116.54	119.90
20	AU	34	ARG	NE-CZ-NH1	5.60	123.10	120.30
21	AA	1466	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	610	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1102	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1704	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	2280	G	N1-C6-O6	-5.60	116.54	119.90
21	AA	533	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	816	A	C4-C5-C6	-5.59	114.20	117.00
26	BD	179	ARG	NE-CZ-NH1	5.59	123.10	120.30
54	BA	1822	C	N3-C2-O2	-5.59	117.98	121.90
54	BA	2749	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	912	C	N3-C4-N4	-5.59	114.08	118.00
22	A1	65	C	N3-C2-O2	-5.59	117.99	121.90
24	A3	47	G	C3'-C2'-C1'	5.59	105.97	101.50
54	BA	996	A	C5-C6-N1	5.59	120.50	117.70
55	BB	110	C	O4'-C1'-N1	5.59	112.67	108.20
21	AA	819	A	C4-C5-C6	-5.59	114.20	117.00
24	A3	77	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	18	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	633	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	1825	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	2175	C	N1-C2-O2	5.59	122.25	118.90
11	AL	85	ARG	NE-CZ-NH1	5.59	123.09	120.30
21	AA	194	C	N1-C2-O2	5.59	122.25	118.90
54	BA	300	A	C5-C6-N1	5.59	120.49	117.70
54	BA	2373	G	N3-C2-N2	-5.59	115.99	119.90
54	BA	918	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	2396	G	O4'-C1'-N9	5.59	112.67	108.20
54	BA	2578	G	C5-C6-N1	5.59	114.29	111.50
54	BA	2821	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	1258	G	N3-C4-C5	-5.58	125.81	128.60
54	BA	429	A	C5-C6-N1	5.58	120.49	117.70
54	BA	1244	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2283	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	193	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	86	G	C1'-O4'-C4'	-5.58	105.43	109.90
54	BA	336	C	N3-C2-O2	-5.58	117.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	472	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2516	A	C6-C5-N7	5.58	136.21	132.30
21	AA	187	G	N3-C2-N2	-5.58	115.99	119.90
21	AA	441	A	C6-C5-N7	5.58	136.21	132.30
21	AA	1328	C	N1-C2-O2	5.58	122.25	118.90
55	BB	53	A	N1-C6-N6	-5.58	115.25	118.60
21	AA	417	G	C5-C6-N1	5.58	114.29	111.50
54	BA	1786	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2637	U	O4'-C1'-N1	5.58	112.66	108.20
21	AA	470	C	N1-C2-O2	5.58	122.25	118.90
54	BA	718	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1020	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1691	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	2144	G	N1-C6-O6	-5.58	116.56	119.90
12	AM	108	ARG	NE-CZ-NH2	-5.57	117.51	120.30
54	BA	343	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1019	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	2149	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	2621	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	2715	C	N1-C2-O2	5.57	122.24	118.90
54	BA	2758	A	C4-C5-C6	-5.57	114.21	117.00
54	BA	531	C	N1-C2-O2	5.57	122.24	118.90
54	BA	1075	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	456	C	N3-C4-C5	5.57	124.13	121.90
21	AA	781	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	265	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	340	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	1221	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	1802	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	254	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	479	A	C6-C5-N7	5.57	136.20	132.30
54	BA	1135	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1924	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	922	C	N3-C2-O2	-5.56	118.00	121.90
54	BA	2505	G	C5-C6-N1	5.56	114.28	111.50
21	AA	243	A	P-O3'-C3'	5.56	126.38	119.70
22	A1	23	A	C4-C5-C6	-5.56	114.22	117.00
37	BO	30	ARG	NE-CZ-NH1	5.56	123.08	120.30
54	BA	739	A	N1-C6-N6	-5.56	115.26	118.60
54	BA	2170	A	C4-C5-C6	-5.56	114.22	117.00
5	AF	86	ARG	NE-CZ-NH2	-5.56	117.52	120.30
21	AA	154	U	O4'-C1'-N1	5.56	112.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BN	118	ARG	NE-CZ-NH2	-5.56	117.52	120.30
54	BA	79	C	C3'-C2'-C1'	5.56	105.95	101.50
2	AC	71	ARG	NE-CZ-NH1	5.56	123.08	120.30
21	AA	569	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1129	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1147	A	C6-C5-N7	5.56	136.19	132.30
21	AA	53	A	C6-C5-N7	5.56	136.19	132.30
21	AA	223	A	C6-C5-N7	5.56	136.19	132.30
21	AA	934	C	N3-C4-N4	-5.56	114.11	118.00
21	AA	1243	C	N3-C2-O2	-5.56	118.01	121.90
21	AA	1401	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	238	C	N1-C2-O2	5.56	122.23	118.90
54	BA	341	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	668	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1646	C	N1-C2-O2	5.56	122.23	118.90
54	BA	578	G	N1-C6-O6	-5.56	116.57	119.90
54	BA	686	U	O4'-C1'-N1	5.56	112.64	108.20
54	BA	1525	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	344	A	O4'-C1'-N9	5.55	112.64	108.20
21	AA	829	G	O4'-C1'-N9	5.55	112.64	108.20
22	A1	9	A	C4-C5-C6	-5.55	114.22	117.00
22	A1	33	U	N3-C2-O2	-5.55	118.31	122.20
54	BA	1128	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	1728	C	N1-C2-O2	5.55	122.23	118.90
54	BA	1729	U	N3-C2-O2	-5.55	118.31	122.20
54	BA	2174	C	N3-C2-O2	-5.55	118.01	121.90
21	AA	1203	C	P-O3'-C3'	5.55	126.36	119.70
46	BX	27	ARG	NE-CZ-NH1	5.55	123.08	120.30
54	BA	131	A	N1-C6-N6	-5.55	115.27	118.60
54	BA	441	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	840	C	N1-C2-O2	5.55	122.23	118.90
54	BA	1625	C	N1-C2-O2	5.55	122.23	118.90
54	BA	1747	U	O4'-C1'-N1	5.55	112.64	108.20
21	AA	195	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1784	A	C6-C5-N7	5.55	136.19	132.30
54	BA	2575	C	N3-C4-C5	5.55	124.12	121.90
21	AA	246	A	C5-C6-N1	5.55	120.47	117.70
21	AA	597	G	N3-C4-C5	-5.55	125.83	128.60
21	AA	889	A	C6-C5-N7	5.55	136.18	132.30
21	AA	1448	C	N3-C2-O2	-5.55	118.02	121.90
21	AA	873	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	341	C	O4'-C1'-N1	5.54	112.64	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1110	G	O4'-C1'-N9	5.54	112.64	108.20
54	BA	2091	C	O4'-C1'-N1	5.54	112.64	108.20
21	AA	1061	G	N3-C2-N2	-5.54	116.02	119.90
22	A1	36	C	N1-C2-O2	5.54	122.23	118.90
54	BA	89	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1298	C	N1-C2-O2	5.54	122.23	118.90
54	BA	1322	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2743	U	O4'-C1'-N1	5.54	112.64	108.20
17	AR	52	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	719	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	1151	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2456	C	O4'-C1'-N1	5.54	112.63	108.20
21	AA	990	C	N1-C2-O2	5.54	122.22	118.90
54	BA	76	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2425	A	P-O3'-C3'	5.54	126.35	119.70
21	AA	186	C	N1-C2-O2	5.54	122.22	118.90
21	AA	1059	C	N1-C2-O2	5.54	122.22	118.90
21	AA	1179	A	C5-C6-N1	5.54	120.47	117.70
54	BA	899	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2755	C	C3'-C2'-C1'	5.54	105.93	101.50
22	A1	18	G	N1-C6-O6	-5.54	116.58	119.90
54	BA	863	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2206	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	2860	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	152	A	C6-C5-N7	5.54	136.18	132.30
54	BA	806	C	N3-C2-O2	-5.54	118.03	121.90
54	BA	1868	C	O4'-C1'-N1	5.54	112.63	108.20
21	AA	1437	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	1468	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	876	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2633	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	37	C	C5'-C4'-O4'	5.53	115.74	109.10
54	BA	1528	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1853	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	730	G	N1-C6-O6	-5.53	116.58	119.90
21	AA	1296	C	N1-C2-O2	5.53	122.22	118.90
21	AA	1359	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	477	A	C4-C5-C6	-5.53	114.24	117.00
21	AA	81	A	C1'-O4'-C4'	-5.53	105.48	109.90
21	AA	465	A	O4'-C1'-N9	5.53	112.62	108.20
21	AA	1128	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	37	C	O4'-C1'-N1	5.53	112.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	692	C	N1-C2-O2	5.53	122.22	118.90
54	BA	1962	C	N3-C4-C5	5.53	124.11	121.90
54	BA	2015	A	C6-C5-N7	5.53	136.17	132.30
54	BA	2073	C	C4'-C3'-C2'	-5.53	97.07	102.60
54	BA	2342	C	N1-C2-O2	5.53	122.22	118.90
27	BE	79	ARG	NE-CZ-NH1	5.52	123.06	120.30
54	BA	37	C	N1-C2-O2	5.52	122.22	118.90
54	BA	1567	G	N3-C2-N2	-5.52	116.03	119.90
54	BA	1981	A	C6-N1-C2	-5.52	115.29	118.60
21	AA	423	G	N3-C4-C5	-5.52	125.84	128.60
38	BP	92	ARG	NE-CZ-NH1	5.52	123.06	120.30
54	BA	698	C	N1-C2-O2	5.52	122.21	118.90
54	BA	1403	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	876	C	C3'-C2'-C1'	-5.52	97.08	101.50
21	AA	1011	C	N1-C2-O2	5.52	122.21	118.90
54	BA	310	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2471	A	C5-C6-N1	5.52	120.46	117.70
54	BA	2853	C	O4'-C1'-N1	5.52	112.62	108.20
21	AA	579	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	673	A	C6-C5-N7	5.52	136.16	132.30
54	BA	690	G	N1-C6-O6	-5.52	116.59	119.90
21	AA	919	A	O4'-C1'-N9	5.52	112.61	108.20
21	AA	1169	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1710	G	O4'-C1'-N9	5.52	112.61	108.20
54	BA	1791	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1958	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	2349	G	O4'-C1'-N9	5.52	112.61	108.20
54	BA	2654	A	C4-C5-C6	-5.52	114.24	117.00
55	BB	80	U	O4'-C1'-N1	5.52	112.61	108.20
21	AA	1267	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	412	A	O4'-C1'-N9	5.51	112.61	108.20
54	BA	1439	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	1858	A	O4'-C1'-N9	5.51	112.61	108.20
21	AA	87	C	N1-C2-O2	5.51	122.21	118.90
21	AA	248	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	430	A	C4-C5-C6	-5.51	114.24	117.00
21	AA	790	A	C5-C6-N1	5.51	120.46	117.70
21	AA	1266	G	N1-C6-O6	-5.51	116.59	119.90
21	AA	1402	C	N1-C2-O2	5.51	122.21	118.90
54	BA	689	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	1828	G	O4'-C1'-N9	5.51	112.61	108.20
21	AA	300	A	C4-C5-C6	-5.51	114.25	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	429	U	C5-C6-N1	-5.51	119.94	122.70
21	AA	660	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	615	U	N3-C2-O2	-5.51	118.34	122.20
54	BA	1463	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	2200	C	N3-C2-O2	-5.51	118.04	121.90
27	BE	69	ARG	NH1-CZ-NH2	-5.51	113.34	119.40
54	BA	14	A	N1-C6-N6	-5.51	115.30	118.60
54	BA	2427	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	383	A	C4-C5-C6	-5.51	114.25	117.00
21	AA	1357	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	351	C	N1-C2-O2	5.51	122.20	118.90
54	BA	1977	A	C6-C5-N7	5.51	136.16	132.30
55	BB	99	A	C6-C5-N7	5.51	136.16	132.30
54	BA	929	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	1668	A	C6-C5-N7	5.50	136.15	132.30
54	BA	1824	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	435	A	C5-C6-N1	5.50	120.45	117.70
54	BA	611	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	823	C	N1-C2-O2	5.50	122.20	118.90
54	BA	991	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1240	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1594	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1745	A	N1-C6-N6	-5.50	115.30	118.60
54	BA	2575	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	452	A	C6-C5-N7	5.50	136.15	132.30
54	BA	714	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	2506	U	N3-C2-O2	-5.50	118.35	122.20
54	BA	2740	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	51	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	352	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	972	C	N3-C2-O2	-5.50	118.05	121.90
22	A1	50	G	N1-C6-O6	-5.50	116.60	119.90
5	AF	44	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	AA	580	C	O4'-C1'-N1	5.50	112.60	108.20
27	BE	44	ARG	NE-CZ-NH1	5.50	123.05	120.30
54	BA	378	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1577	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1976	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	2463	C	N1-C2-O2	5.50	122.20	118.90
54	BA	2809	A	C4'-C3'-C2'	-5.50	97.10	102.60
21	AA	374	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	427	U	N3-C2-O2	-5.50	118.35	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1344	C	N1-C2-O2	5.50	122.20	118.90
54	BA	366	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1453	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1928	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	336	A	C6-C5-N7	5.50	136.15	132.30
54	BA	980	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	11	C	O4'-C1'-N1	5.49	112.59	108.20
54	BA	1829	A	C4-C5-C6	-5.49	114.25	117.00
21	AA	398	U	O4'-C1'-N1	5.49	112.59	108.20
55	BB	93	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	1506	U	O4'-C1'-N1	5.49	112.59	108.20
24	A3	10	G	N1-C6-O6	-5.49	116.61	119.90
54	BA	728	G	C5-C6-N1	5.49	114.25	111.50
54	BA	2469	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	2840	C	N1-C2-O2	5.49	122.19	118.90
54	BA	522	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	2006	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	1641	A	C5-C6-N1	5.48	120.44	117.70
21	AA	490	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	996	A	C6-C5-N7	5.48	136.14	132.30
54	BA	1259	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	1615	C	N1-C2-O2	5.48	122.19	118.90
54	BA	2560	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	510	A	O4'-C1'-N9	5.48	112.58	108.20
21	AA	716	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	726	C	N1-C2-O2	5.48	122.19	118.90
21	AA	1251	A	O4'-C1'-N9	5.48	112.58	108.20
54	BA	421	C	N1-C2-O2	5.48	122.19	118.90
54	BA	1269	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1286	A	O4'-C1'-N9	5.48	112.58	108.20
54	BA	1323	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	732	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	1139	G	N1-C6-O6	-5.48	116.61	119.90
52	B3	29	ARG	NE-CZ-NH1	5.48	123.04	120.30
54	BA	1578	U	N1-C2-N3	5.48	118.19	114.90
54	BA	2551	C	N1-C2-O2	5.48	122.19	118.90
54	BA	2653	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2785	C	O4'-C1'-N1	5.48	112.58	108.20
54	BA	990	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	303	A	C6-C5-N7	5.47	136.13	132.30
21	AA	856	C	N1-C2-O2	5.47	122.18	118.90
54	BA	179	C	N1-C2-O2	5.47	122.18	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	292	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	1830	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	1368	A	C3'-C2'-C1'	5.47	105.88	101.50
54	BA	1295	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	461	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	878	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	1646	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	2662	A	C5-C6-N1	5.47	120.44	117.70
54	BA	2719	G	C5-C6-N1	5.47	114.23	111.50
54	BA	2770	G	C3'-C2'-C1'	5.47	105.88	101.50
8	AI	123	ARG	NE-CZ-NH1	5.47	123.03	120.30
21	AA	251	G	N3-C4-C5	-5.47	125.87	128.60
54	BA	457	A	O4'-C1'-N9	5.47	112.57	108.20
54	BA	1964	G	N3-C4-C5	-5.47	125.87	128.60
21	AA	94	G	N3-C2-N2	-5.47	116.07	119.90
54	BA	464	U	C3'-C2'-C1'	5.47	105.87	101.50
54	BA	723	C	N1-C2-O2	5.47	122.18	118.90
54	BA	727	A	C5-C6-N1	5.47	120.43	117.70
54	BA	766	U	O4'-C1'-N1	5.47	112.57	108.20
54	BA	2734	A	C4-C5-C6	-5.47	114.27	117.00
21	AA	65	A	C1'-O4'-C4'	-5.46	105.53	109.90
21	AA	500	G	O4'-C1'-N9	5.46	112.57	108.20
21	AA	1049	U	N3-C2-O2	-5.46	118.38	122.20
21	AA	1505	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	219	A	C6-C5-N7	5.46	136.13	132.30
21	AA	169	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	1484	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	8	C	N1-C2-O2	5.46	122.18	118.90
54	BA	357	C	N1-C2-O2	5.46	122.18	118.90
54	BA	894	U	N3-C2-O2	-5.46	118.38	122.20
54	BA	2080	A	C4-C5-C6	-5.46	114.27	117.00
11	AL	13	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	1396	U	N3-C2-O2	-5.46	118.38	122.20
54	BA	2191	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2512	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	34	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	136	C	N1-C2-O2	5.46	122.17	118.90
21	AA	1493	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	264	C	N1-C2-O2	5.46	122.18	118.90
55	BB	28	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	795	C	N1-C2-O2	5.46	122.17	118.90
49	B0	12	ARG	NE-CZ-NH2	5.46	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	384	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	720	U	O4'-C1'-N1	5.46	112.56	108.20
54	BA	937	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	2119	A	N1-C6-N6	-5.46	115.33	118.60
54	BA	2539	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	467	U	N3-C2-O2	-5.45	118.38	122.20
21	AA	1046	A	C4-C5-C6	-5.45	114.27	117.00
21	AA	1300	G	N3-C2-N2	-5.45	116.08	119.90
54	BA	1633	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	2275	C	O4'-C1'-N1	5.45	112.56	108.20
54	BA	1973	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	2055	C	N1-C2-O2	5.45	122.17	118.90
21	AA	569	C	N3-C4-C5	5.45	124.08	121.90
54	BA	221	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	2303	G	N1-C6-O6	-5.45	116.63	119.90
21	AA	892	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	1078	U	O4'-C1'-N1	5.45	112.56	108.20
21	AA	1347	G	O4'-C1'-N9	5.45	112.56	108.20
21	AA	1469	C	N1-C2-O2	5.45	122.17	118.90
54	BA	765	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	1340	U	P-O3'-C3'	5.45	126.24	119.70
54	BA	2046	G	O4'-C1'-N9	5.45	112.56	108.20
54	BA	2566	A	C4-C5-C6	-5.45	114.28	117.00
24	A3	70	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	631	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2226	C	N3-C2-O2	-5.45	118.09	121.90
21	AA	810	C	N1-C2-O2	5.45	122.17	118.90
21	AA	962	C	N3-C2-O2	-5.45	118.09	121.90
21	AA	1319	A	C6-C5-N7	5.45	136.11	132.30
30	BH	27	ARG	NE-CZ-NH1	5.45	123.02	120.30
54	BA	660	C	C5'-C4'-O4'	5.45	115.63	109.10
54	BA	2576	G	C3'-C2'-C1'	5.45	105.86	101.50
21	AA	478	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	782	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	648	G	C5-C6-N1	5.44	114.22	111.50
54	BA	1799	G	C8-N9-C4	-5.44	104.22	106.40
21	AA	1230	C	C3'-C2'-C1'	5.44	105.85	101.50
54	BA	610	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	800	A	C6-C5-N7	5.44	136.11	132.30
54	BA	857	G	C8-N9-C4	-5.44	104.22	106.40
54	BA	1554	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	1754	A	O4'-C1'-N9	5.44	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	199	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	1391	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	654	A	C6-C5-N7	5.44	136.11	132.30
54	BA	2070	A	O4'-C1'-N9	5.44	112.55	108.20
54	BA	2619	C	N3-C2-O2	-5.44	118.09	121.90
4	AE	67	ARG	NE-CZ-NH1	5.44	123.02	120.30
54	BA	1681	G	O4'-C1'-N9	5.44	112.55	108.20
21	AA	262	A	C6-C5-N7	5.44	136.11	132.30
21	AA	699	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	192	C	N1-C2-O2	5.44	122.16	118.90
54	BA	240	C	N1-C2-O2	5.44	122.16	118.90
54	BA	570	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	1059	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	1403	A	C4'-C3'-C2'	-5.44	97.16	102.60
54	BA	2274	A	C6-C5-N7	5.44	136.11	132.30
54	BA	2506	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	6	A	O4'-C1'-N9	5.44	112.55	108.20
54	BA	443	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	108	G	N3-C4-C5	-5.43	125.88	128.60
21	AA	475	C	N3-C2-O2	-5.43	118.09	121.90
21	AA	1120	C	N1-C2-O2	5.43	122.16	118.90
54	BA	1125	G	C8-N9-C4	-5.43	104.23	106.40
54	BA	342	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	1265	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	1507	C	N1-C2-O2	5.43	122.16	118.90
54	BA	2087	G	N1-C6-O6	-5.43	116.64	119.90
1	AB	73	ARG	NE-CZ-NH2	-5.43	117.58	120.30
21	AA	139	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	995	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	1160	G	N3-C2-N2	-5.43	116.10	119.90
22	A1	44	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1332	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1788	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	1932	A	C5-C6-N1	5.43	120.42	117.70
54	BA	2417	C	N1-C2-O2	5.43	122.16	118.90
54	BA	2532	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	2885	G	O4'-C1'-N9	5.43	112.54	108.20
54	BA	112	U	C5-C6-N1	-5.43	119.99	122.70
54	BA	542	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	986	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	992	C	O4'-C1'-N1	5.43	112.54	108.20
10	AK	68	ARG	NE-CZ-NH1	5.43	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	196	A	C6-C5-N7	5.43	136.10	132.30
21	AA	727	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	739	C	N1-C2-O2	5.43	122.16	118.90
21	AA	766	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	993	G	N1-C6-O6	-5.43	116.64	119.90
47	BY	23	ARG	NE-CZ-NH1	5.43	123.01	120.30
54	BA	430	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	1022	G	O4'-C1'-N9	5.43	112.54	108.20
54	BA	1050	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	372	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	1117	C	N1-C2-O2	5.42	122.16	118.90
21	AA	436	C	C1'-O4'-C4'	-5.42	105.56	109.90
21	AA	970	C	N1-C2-O2	5.42	122.15	118.90
54	BA	2643	G	O4'-C1'-N9	5.42	112.54	108.20
54	BA	1045	C	N1-C2-O2	5.42	122.15	118.90
54	BA	1907	G	N1-C6-O6	-5.42	116.65	119.90
21	AA	142	G	N1-C6-O6	-5.42	116.65	119.90
21	AA	228	A	C6-C5-N7	5.42	136.09	132.30
21	AA	1390	U	O4'-C1'-N1	5.42	112.54	108.20
54	BA	1261	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	2577	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	462	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	1434	A	C4-C5-C6	-5.42	114.29	117.00
7	AH	116	ARG	NE-CZ-NH1	5.42	123.01	120.30
21	AA	1086	U	C1'-O4'-C4'	-5.42	105.57	109.90
54	BA	238	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	688	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1466	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2169	A	C4-C5-C6	-5.41	114.29	117.00
21	AA	908	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	145	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	833	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	1313	U	C2-N1-C1'	5.41	124.19	117.70
21	AA	969	A	C6-C5-N7	5.41	136.09	132.30
54	BA	621	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1108	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1558	C	N3-C2-O2	-5.41	118.11	121.90
56	B5	12	ARG	NE-CZ-NH1	5.41	123.01	120.30
8	AI	40	ARG	NE-CZ-NH1	5.41	123.00	120.30
13	AN	61	ARG	NE-CZ-NH1	5.41	123.00	120.30
21	AA	1129	C	N1-C2-O2	5.41	122.14	118.90
21	AA	1377	A	C6-C5-N7	5.41	136.09	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1760	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2339	C	N1-C2-O2	5.41	122.15	118.90
54	BA	1176	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1188	U	N3-C2-O2	-5.41	118.42	122.20
21	AA	353	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	396	C	N3-C4-C5	5.40	124.06	121.90
23	A2	83	U	O4'-C1'-N1	5.40	112.52	108.20
45	BW	38	ARG	NE-CZ-NH2	-5.40	117.60	120.30
54	BA	180	G	C5-C6-N1	5.40	114.20	111.50
54	BA	294	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	673	C	N3-C4-C5	5.40	124.06	121.90
21	AA	615	G	O4'-C1'-N9	5.40	112.52	108.20
24	A3	49	C	N3-C4-C5	5.40	124.06	121.90
54	BA	69	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	141	G	N3-C4-C5	-5.40	125.90	128.60
54	BA	721	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	968	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	1647	U	O4'-C1'-N1	5.40	112.52	108.20
21	AA	885	G	N9-C4-C5	5.40	107.56	105.40
51	B2	28	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	1041	G	N1-C6-O6	-5.40	116.66	119.90
21	AA	1246	A	C6-C5-N7	5.40	136.08	132.30
54	BA	244	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1477	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	426	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	858	G	O4'-C1'-N9	5.40	112.52	108.20
54	BA	970	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2606	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	1058	G	N3-C2-N2	-5.39	116.12	119.90
33	BK	17	ARG	NE-CZ-NH2	-5.39	117.60	120.30
54	BA	179	C	C4'-C3'-C2'	-5.39	97.21	102.60
54	BA	1270	C	N3-C2-O2	-5.39	118.12	121.90
54	BA	2535	G	N1-C6-O6	-5.39	116.66	119.90
21	AA	930	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	531	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1010	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	2873	A	O4'-C1'-N9	5.39	112.52	108.20
21	AA	716	A	O4'-C1'-N9	5.39	112.51	108.20
21	AA	783	C	N3-C2-O2	-5.39	118.13	121.90
39	BQ	54	ARG	NE-CZ-NH1	5.39	123.00	120.30
54	BA	1832	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	2792	A	C6-C5-N7	5.39	136.07	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2425	A	C6-C5-N7	5.39	136.07	132.30
54	BA	2470	G	O4'-C1'-N9	5.39	112.51	108.20
54	BA	269	C	N1-C2-O2	5.39	122.13	118.90
54	BA	372	G	C3'-C2'-C1'	-5.39	97.19	101.50
54	BA	49	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	106	C	C5'-C4'-O4'	5.39	115.56	109.10
54	BA	229	C	N1-C2-O2	5.39	122.13	118.90
54	BA	285	G	C3'-C2'-C1'	-5.39	97.19	101.50
3	AD	192	ALA	C-N-CA	5.38	135.16	121.70
54	BA	743	A	O4'-C1'-N9	5.38	112.51	108.20
54	BA	1474	U	C5-C6-N1	-5.38	120.01	122.70
54	BA	2845	U	O4'-C1'-N1	5.38	112.51	108.20
54	BA	340	A	N1-C6-N6	-5.38	115.37	118.60
54	BA	1427	A	C5-C6-N1	5.38	120.39	117.70
21	AA	1147	C	O4'-C1'-N1	5.38	112.50	108.20
26	BD	83	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BA	43	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	419	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	694	U	N3-C2-O2	-5.38	118.43	122.20
54	BA	935	C	N3-C2-O2	-5.38	118.13	121.90
54	BA	1452	G	O4'-C1'-N9	5.38	112.50	108.20
54	BA	1634	A	P-O3'-C3'	5.38	126.16	119.70
54	BA	1699	G	N3-C4-C5	-5.38	125.91	128.60
54	BA	2346	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	271	C	N1-C2-O2	5.38	122.13	118.90
21	AA	526	C	N1-C2-O2	5.38	122.13	118.90
21	AA	829	G	N1-C6-O6	-5.38	116.67	119.90
21	AA	1302	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	1086	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	125	U	O4'-C1'-N1	5.38	112.50	108.20
21	AA	333	U	O4'-C1'-N1	5.38	112.50	108.20
21	AA	767	A	C6-C5-N7	5.38	136.06	132.30
21	AA	1214	C	C1'-O4'-C4'	-5.38	105.60	109.90
54	BA	641	U	N3-C2-O2	-5.38	118.44	122.20
54	BA	699	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	988	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	2089	C	N3-C2-O2	-5.38	118.14	121.90
21	AA	13	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	528	A	O4'-C1'-N9	5.38	112.50	108.20
54	BA	2461	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	412	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	478	A	C4-C5-C6	-5.37	114.31	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1196	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1762	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	2685	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	229	U	N3-C2-O2	-5.37	118.44	122.20
46	BX	17	ARG	NE-CZ-NH2	5.37	122.98	120.30
54	BA	293	U	O4'-C1'-N1	5.37	112.50	108.20
54	BA	1061	U	O4'-C4'-C3'	5.37	110.40	106.10
54	BA	1658	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	2257	U	O4'-C1'-N1	5.37	112.50	108.20
54	BA	2300	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	2824	C	N1-C2-O2	5.37	122.12	118.90
21	AA	396	C	N1-C2-O2	5.37	122.12	118.90
21	AA	726	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	834	G	O4'-C1'-N9	5.37	112.50	108.20
21	AA	1303	C	N1-C2-O2	5.37	122.12	118.90
54	BA	595	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	607	U	C5'-C4'-O4'	5.37	115.54	109.10
54	BA	693	A	C4'-C3'-C2'	-5.37	97.23	102.60
54	BA	1169	A	C6-C5-N7	5.37	136.06	132.30
54	BA	1467	U	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2719	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	169	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	1335	U	N1-C2-N3	5.37	118.12	114.90
54	BA	542	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2215	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	2518	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	755	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	6	A	C4-C5-C6	-5.37	114.32	117.00
54	BA	383	C	P-O3'-C3'	5.37	126.14	119.70
54	BA	796	C	N3-C4-C5	5.37	124.05	121.90
54	BA	2503	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	869	G	N3-C2-N2	-5.36	116.15	119.90
24	A3	23	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	457	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1129	A	C1'-O4'-C4'	-5.36	105.61	109.90
54	BA	1664	A	C5-C6-N1	5.36	120.38	117.70
54	BA	2397	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	2744	G	N1-C6-O6	-5.36	116.68	119.90
54	BA	882	G	N1-C6-O6	-5.36	116.68	119.90
54	BA	1102	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1854	A	C6-C5-N7	5.36	136.05	132.30
21	AA	1164	G	N1-C6-O6	-5.36	116.68	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	442	G	C5-C6-N1	5.36	114.18	111.50
54	BA	1889	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2155	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	1274	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1720	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1880	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1925	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	2576	G	C5-C6-N1	5.36	114.18	111.50
54	BA	2874	C	O4'-C1'-N1	5.36	112.49	108.20
21	AA	98	A	C6-C5-N7	5.36	136.05	132.30
21	AA	1349	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	1532	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	957	C	N3-C4-C5	5.36	124.04	121.90
26	BD	141	ARG	NE-CZ-NH1	-5.36	117.62	120.30
54	BA	355	U	O4'-C1'-N1	5.36	112.48	108.20
54	BA	835	C	O4'-C1'-N1	5.36	112.48	108.20
54	BA	933	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2072	C	N1-C2-O2	5.36	122.11	118.90
54	BA	2902	C	N1-C2-O2	5.36	122.11	118.90
21	AA	851	G	N3-C4-C5	-5.35	125.92	128.60
54	BA	2468	A	O4'-C1'-N9	5.35	112.48	108.20
10	AK	52	ARG	NE-CZ-NH1	5.35	122.98	120.30
21	AA	1198	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	1327	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	2883	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	467	U	O4'-C1'-N1	5.35	112.48	108.20
21	AA	1094	G	C5-C6-N1	5.35	114.17	111.50
21	AA	1100	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	516	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	543	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	691	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	848	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	2652	C	N1-C2-O2	5.35	122.11	118.90
55	BB	90	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	225	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	964	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	1609	A	C6-C5-N7	5.35	136.04	132.30
54	BA	2398	U	C5-C6-N1	-5.35	120.03	122.70
21	AA	1373	G	N3-C2-N2	-5.35	116.16	119.90
54	BA	2795	C	N3-C2-O2	-5.35	118.16	121.90
55	BB	71	C	O4'-C1'-N1	5.35	112.48	108.20
55	BB	73	A	C6-C5-N7	5.35	136.04	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	363	A	C6-C5-N7	5.34	136.04	132.30
21	AA	813	U	N3-C2-O2	-5.34	118.46	122.20
21	AA	1333	A	C6-C5-N7	5.34	136.04	132.30
21	AA	1382	C	N3-C4-C5	5.34	124.04	121.90
46	BX	10	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BA	114	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	235	U	C5'-C4'-O4'	5.34	115.51	109.10
54	BA	2059	A	C6-C5-N7	5.34	136.04	132.30
54	BA	2872	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	312	C	N1-C2-O2	5.34	122.11	118.90
54	BA	2133	G	N9-C4-C5	5.34	107.54	105.40
21	AA	759	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	918	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	1071	C	N3-C2-O2	-5.34	118.16	121.90
21	AA	1453	G	N3-C4-C5	-5.34	125.93	128.60
36	BN	118	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BA	812	C	N1-C2-O2	5.34	122.11	118.90
54	BA	834	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	1606	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2042	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2393	U	O4'-C1'-N1	5.34	112.47	108.20
21	AA	840	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	318	C	N3-C4-C5	5.34	124.03	121.90
54	BA	611	C	N1-C2-O2	5.34	122.10	118.90
54	BA	1021	A	C5-C6-N1	5.34	120.37	117.70
54	BA	415	A	O4'-C1'-N9	5.34	112.47	108.20
54	BA	497	A	C6-C5-N7	5.34	136.04	132.30
54	BA	743	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	1585	C	N1-C2-O2	5.34	122.10	118.90
21	AA	755	G	N3-C2-N2	-5.34	116.17	119.90
54	BA	530	G	N3-C2-N2	-5.34	116.16	119.90
54	BA	589	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	742	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2875	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2825	G	N3-C4-C5	-5.33	125.93	128.60
21	AA	100	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	290	C	N1-C2-O2	5.33	122.10	118.90
21	AA	985	C	N1-C2-O2	5.33	122.10	118.90
24	A3	31	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	867	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	339	C	N1-C2-O2	5.33	122.10	118.90
54	BA	782	A	C4-C5-C6	-5.33	114.33	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	814	C	N1-C2-O2	5.33	122.10	118.90
54	BA	1957	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	2799	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	1110	A	O4'-C1'-N9	5.33	112.46	108.20
54	BA	995	C	N1-C2-O2	5.33	122.10	118.90
21	AA	188	C	N1-C2-O2	5.33	122.10	118.90
21	AA	455	G	C8-N9-C4	-5.33	104.27	106.40
21	AA	890	G	C8-N9-C4	-5.33	104.27	106.40
38	BP	88	ARG	CD-NE-CZ	5.33	131.06	123.60
54	BA	96	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	119	A	C6-C5-N7	5.33	136.03	132.30
54	BA	763	G	C5'-C4'-C3'	-5.33	107.48	116.00
54	BA	859	G	C5-C6-N1	5.33	114.17	111.50
54	BA	1095	A	C3'-C2'-C1'	5.33	105.76	101.50
54	BA	1335	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	657	U	N3-C2-O2	-5.33	118.47	122.20
21	AA	1249	C	N3-C2-O2	-5.33	118.17	121.90
24	A3	13	C	O4'-C1'-N1	5.33	112.46	108.20
54	BA	792	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	2639	A	C4-C5-C6	-5.33	114.34	117.00
24	A3	75	C	N1-C2-O2	5.33	122.10	118.90
54	BA	235	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	584	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	1389	G	N3-C4-C5	-5.33	125.94	128.60
54	BA	1515	A	C6-C5-N7	5.33	136.03	132.30
54	BA	1535	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	1927	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	111	G	N1-C6-O6	-5.32	116.70	119.90
21	AA	1141	C	N1-C2-O2	5.32	122.09	118.90
54	BA	156	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	808	G	N3-C4-C5	-5.32	125.94	128.60
54	BA	1670	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1812	U	O4'-C1'-N1	5.32	112.46	108.20
21	AA	1447	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	337	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	366	C	N3-C2-O2	-5.32	118.17	121.90
13	AN	75	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
21	AA	745	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	1197	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	2045	C	O4'-C1'-N1	5.32	112.46	108.20
21	AA	140	U	O4'-C1'-N1	5.32	112.45	108.20
21	AA	879	C	N3-C4-C5	5.32	124.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1191	G	C5-C6-N1	5.32	114.16	111.50
6	AG	3	ARG	NE-CZ-NH1	-5.32	117.64	120.30
28	BF	111	ARG	NE-CZ-NH1	5.32	122.96	120.30
54	BA	809	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	858	G	C3'-C2'-C1'	5.32	105.75	101.50
54	BA	2126	A	O4'-C1'-N9	5.32	112.45	108.20
21	AA	225	C	N3-C2-O2	-5.32	118.18	121.90
21	AA	1432	G	O4'-C1'-N9	5.32	112.45	108.20
54	BA	871	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	1137	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	2536	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	2662	A	N1-C6-N6	-5.32	115.41	118.60
54	BA	2725	A	O4'-C1'-N9	5.32	112.45	108.20
21	AA	910	C	C5'-C4'-C3'	-5.31	107.50	116.00
54	BA	1985	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	817	C	C1'-O4'-C4'	-5.31	105.65	109.90
54	BA	284	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1022	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	2040	G	O4'-C1'-N9	5.31	112.45	108.20
54	BA	2227	A	O4'-C1'-N9	5.31	112.45	108.20
54	BA	2634	A	C6-C5-N7	5.31	136.02	132.30
21	AA	306	A	C6-C5-N7	5.31	136.02	132.30
21	AA	661	G	N1-C6-O6	-5.31	116.71	119.90
21	AA	1332	A	C4-C5-C6	-5.31	114.34	117.00
24	A3	2	G	C6-C5-N7	5.31	133.59	130.40
54	BA	232	G	C5-C6-N1	5.31	114.16	111.50
54	BA	1181	U	O4'-C1'-N1	5.31	112.45	108.20
21	AA	575	G	O4'-C1'-N9	5.31	112.45	108.20
21	AA	971	G	C1'-O4'-C4'	-5.31	105.65	109.90
22	A1	10	G	N3-C4-C5	-5.31	125.95	128.60
54	BA	737	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	539	A	C4-C5-C6	-5.31	114.35	117.00
22	A1	8	U	N3-C2-O2	-5.31	118.48	122.20
55	BB	83	G	O4'-C1'-N9	5.31	112.44	108.20
21	AA	1232	U	O4'-C1'-N1	5.31	112.44	108.20
54	BA	614	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	1068	G	N3-C4-C5	-5.31	125.95	128.60
54	BA	2814	A	C6-C5-N7	5.31	136.01	132.30
54	BA	2896	C	O4'-C1'-N1	5.31	112.44	108.20
21	AA	349	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	326	G	C4'-C3'-C2'	-5.30	97.30	102.60
54	BA	1099	G	O4'-C1'-N9	5.30	112.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1130	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2096	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2103	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2601	C	N1-C2-O2	5.30	122.08	118.90
21	AA	1234	C	N1-C2-O2	5.30	122.08	118.90
54	BA	1070	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	2188	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	132	C	N1-C2-O2	5.30	122.08	118.90
21	AA	727	G	C5-C6-N1	5.30	114.15	111.50
21	AA	1523	G	O4'-C4'-C3'	5.30	110.34	106.10
54	BA	102	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	587	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	1003	G	N1-C6-O6	-5.30	116.72	119.90
9	AJ	68	ARG	NE-CZ-NH1	5.30	122.95	120.30
21	AA	736	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	2606	C	N1-C2-O2	5.30	122.08	118.90
21	AA	1071	C	O4'-C1'-N1	5.30	112.44	108.20
21	AA	440	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	524	G	O4'-C1'-N9	5.30	112.44	108.20
54	BA	1003	G	N3-C2-N2	-5.30	116.19	119.90
54	BA	1537	G	N3-C4-C5	-5.30	125.95	128.60
54	BA	2404	U	C5-C6-N1	-5.30	120.05	122.70
21	AA	1078	U	N3-C2-O2	-5.29	118.49	122.20
54	BA	2244	U	C5-C6-N1	-5.29	120.05	122.70
21	AA	214	C	N1-C2-O2	5.29	122.08	118.90
21	AA	1165	U	O4'-C1'-N1	5.29	112.44	108.20
54	BA	1242	U	O4'-C1'-N1	5.29	112.44	108.20
54	BA	1596	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	1727	C	C5'-C4'-O4'	5.29	115.45	109.10
54	BA	1929	G	C8-N9-C4	-5.29	104.28	106.40
9	AJ	9	ARG	NE-CZ-NH2	-5.29	117.65	120.30
21	AA	932	C	N1-C2-O2	5.29	122.08	118.90
21	AA	988	G	O4'-C1'-N9	5.29	112.43	108.20
21	AA	1449	C	N1-C2-O2	5.29	122.08	118.90
21	AA	1528	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	428	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	1481	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1518	C	N3-C4-C5	5.29	124.02	121.90
54	BA	1634	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	2528	U	P-O3'-C3'	5.29	126.05	119.70
54	BA	345	A	C4-C5-C6	-5.29	114.36	117.00
21	AA	1173	U	O4'-C1'-N1	5.29	112.43	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	68	C	N1-C2-O2	5.29	122.07	118.90
54	BA	177	G	N3-C4-C5	-5.29	125.96	128.60
54	BA	658	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	731	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2670	A	C4'-C3'-C2'	-5.29	97.31	102.60
21	AA	876	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2066	C	N3-C2-O2	-5.29	118.20	121.90
21	AA	297	G	C5-C6-N1	5.29	114.14	111.50
21	AA	1227	A	O4'-C1'-N9	5.29	112.43	108.20
21	AA	1510	C	N1-C2-O2	5.29	122.07	118.90
30	BH	51	ARG	NE-CZ-NH1	5.29	122.94	120.30
34	BL	32	GLY	C-N-CA	5.29	134.91	121.70
54	BA	317	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	1983	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	2109	U	O4'-C1'-N1	5.29	112.43	108.20
21	AA	742	G	O4'-C1'-N9	5.28	112.43	108.20
21	AA	1463	U	C5-C6-N1	-5.28	120.06	122.70
54	BA	582	A	O4'-C1'-N9	5.28	112.43	108.20
54	BA	897	C	O4'-C1'-N1	5.28	112.43	108.20
54	BA	1066	U	N1-C2-N3	5.28	118.07	114.90
54	BA	1795	C	O4'-C1'-N1	5.28	112.43	108.20
54	BA	2791	G	O4'-C1'-N9	5.28	112.43	108.20
21	AA	792	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1184	U	O4'-C1'-N1	5.28	112.43	108.20
54	BA	2278	A	C4-C5-C6	-5.28	114.36	117.00
4	AE	137	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	AA	1102	A	C4-C5-C6	-5.28	114.36	117.00
24	A3	10	G	C5-C6-N1	5.28	114.14	111.50
54	BA	181	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	254	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	538	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	979	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1279	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	1459	G	N3-C4-C5	-5.28	125.96	128.60
21	AA	54	C	C5'-C4'-O4'	5.28	115.43	109.10
54	BA	273	G	C1'-O4'-C4'	-5.28	105.68	109.90
54	BA	399	U	C5-C6-N1	-5.28	120.06	122.70
54	BA	435	C	N1-C2-O2	5.28	122.07	118.90
54	BA	1200	C	N3-C2-O2	-5.28	118.21	121.90
54	BA	1552	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	549	C	N1-C2-O2	5.28	122.06	118.90
21	AA	641	U	N3-C2-O2	-5.28	118.51	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1042	A	C4-C5-C6	-5.28	114.36	117.00
24	A3	12	G	C5-C6-N1	5.28	114.14	111.50
54	BA	1574	C	N1-C2-O2	5.28	122.06	118.90
54	BA	1727	C	O4'-C1'-N1	5.28	112.42	108.20
21	AA	968	A	C2-N3-C4	5.27	113.24	110.60
21	AA	1532	U	C1'-O4'-C4'	-5.27	105.68	109.90
21	AA	861	G	C5-C6-N1	5.27	114.14	111.50
21	AA	934	C	N1-C2-O2	5.27	122.06	118.90
21	AA	1398	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	724	U	N3-C2-O2	-5.27	118.51	122.20
54	BA	987	C	N1-C2-O2	5.27	122.06	118.90
54	BA	2474	U	C3'-C2'-C1'	5.27	105.72	101.50
21	AA	177	G	N3-C2-N2	-5.27	116.21	119.90
33	BK	30	ARG	NE-CZ-NH1	5.27	122.94	120.30
54	BA	1540	G	O4'-C1'-N9	5.27	112.42	108.20
21	AA	209	U	N1-C2-N3	5.27	118.06	114.90
21	AA	572	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	1327	A	O4'-C1'-N9	5.27	112.42	108.20
54	BA	2336	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	1388	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	1442	U	O4'-C1'-N1	5.27	112.41	108.20
54	BA	1573	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	1810	A	C4-C5-C6	-5.27	114.37	117.00
54	BA	1876	A	C2-N3-C4	5.27	113.23	110.60
54	BA	1996	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	2082	A	O4'-C1'-N9	5.27	112.41	108.20
54	BA	2321	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2462	C	O4'-C1'-N1	5.27	112.41	108.20
56	B5	71	ARG	NE-CZ-NH1	5.27	122.93	120.30
6	AG	6	ILE	CA-C-N	5.27	126.73	116.20
21	AA	264	C	N3-C4-N4	-5.27	114.31	118.00
54	BA	2378	A	C6-C5-N7	5.27	135.99	132.30
54	BA	2773	C	N3-C2-O2	-5.27	118.21	121.90
55	BB	2	G	N3-C2-N2	-5.27	116.21	119.90
24	A3	47	G	N3-C2-N2	-5.26	116.22	119.90
54	BA	259	G	C5'-C4'-O4'	5.26	115.42	109.10
54	BA	623	C	N1-C2-O2	5.26	122.06	118.90
54	BA	1606	C	C3'-C2'-C1'	5.26	105.71	101.50
54	BA	2102	G	N1-C6-O6	-5.26	116.74	119.90
55	BB	37	C	N3-C2-O2	-5.26	118.22	121.90
55	BB	81	G	C5-C6-N1	5.26	114.13	111.50
21	AA	796	C	N1-C2-O2	5.26	122.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1329	A	C5-C6-N1	5.26	120.33	117.70
21	AA	284	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	327	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1273	C	N1-C2-O2	5.26	122.06	118.90
54	BA	545	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	1247	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1297	C	N1-C2-O2	5.26	122.06	118.90
54	BA	1537	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	2554	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	2568	U	C5-C6-N1	-5.26	120.07	122.70
54	BA	2766	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	379	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	98	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	1881	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	565	U	C1'-O4'-C4'	-5.26	105.69	109.90
21	AA	1179	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1194	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	296	U	C5'-C4'-O4'	5.26	115.41	109.10
54	BA	1260	A	C6-C5-N7	5.26	135.98	132.30
54	BA	2674	G	N1-C6-O6	-5.26	116.75	119.90
21	AA	1453	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	510	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2103	C	N1-C2-O2	5.25	122.05	118.90
21	AA	1487	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	629	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	2214	C	N3-C4-C5	5.25	124.00	121.90
54	BA	2647	U	O4'-C1'-N1	5.25	112.40	108.20
55	BB	100	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	102	U	N3-C2-O2	-5.25	118.53	122.20
54	BA	922	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1007	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1303	G	C5-C6-N1	5.25	114.12	111.50
21	AA	313	A	C6-C5-N7	5.25	135.97	132.30
54	BA	163	C	N3-C4-C5	5.25	124.00	121.90
54	BA	1291	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1313	U	N1-C1'-C2'	5.25	120.83	114.00
1	AB	20	ARG	NE-CZ-NH1	5.25	122.92	120.30
21	AA	556	C	N1-C2-O2	5.25	122.05	118.90
21	AA	792	A	C1'-O4'-C4'	-5.25	105.70	109.90
54	BA	1559	U	N3-C2-O2	-5.25	118.53	122.20
54	BA	1844	C	N3-C2-O2	-5.25	118.23	121.90
54	BA	2494	G	N3-C4-C5	-5.25	125.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	989	U	C5-C6-N1	-5.25	120.08	122.70
54	BA	166	U	C4'-C3'-C2'	-5.25	97.35	102.60
54	BA	1895	C	N3-C2-O2	-5.25	118.23	121.90
54	BA	2757	A	C4-C5-C6	-5.25	114.38	117.00
55	BB	97	C	N1-C2-O2	5.25	122.05	118.90
54	BA	440	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	787	C	N3-C4-C5	5.25	124.00	121.90
54	BA	2760	C	N3-C2-O2	-5.25	118.23	121.90
9	AJ	37	ARG	NE-CZ-NH1	5.24	122.92	120.30
21	AA	438	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	640	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	1029	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	141	G	C5-C6-N1	5.24	114.12	111.50
54	BA	633	A	O4'-C1'-N9	5.24	112.39	108.20
54	BA	1653	G	N1-C6-O6	-5.24	116.75	119.90
54	BA	2822	G	N3-C4-C5	-5.24	125.98	128.60
21	AA	149	A	C5-C6-N1	5.24	120.32	117.70
21	AA	754	C	N1-C2-O2	5.24	122.05	118.90
21	AA	1218	C	N3-C2-O2	-5.24	118.23	121.90
54	BA	944	C	N3-C2-O2	-5.24	118.23	121.90
54	BA	1898	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2173	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	2238	G	C5-C6-N1	5.24	114.12	111.50
21	AA	517	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	2319	G	O4'-C1'-N9	5.24	112.39	108.20
54	BA	2385	C	C5'-C4'-O4'	5.24	115.39	109.10
15	AP	31	ARG	NE-CZ-NH2	-5.24	117.68	120.30
21	AA	1052	U	C5-C6-N1	-5.24	120.08	122.70
54	BA	993	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	1073	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1965	C	N1-C2-O2	5.24	122.04	118.90
54	BA	2380	C	N3-C2-O2	-5.24	118.23	121.90
21	AA	280	C	N1-C2-O2	5.24	122.04	118.90
54	BA	1359	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	2433	A	C1'-O4'-C4'	-5.24	105.71	109.90
10	AK	12	ARG	NE-CZ-NH1	5.24	122.92	120.30
21	AA	1336	C	N1-C2-O2	5.24	122.04	118.90
54	BA	370	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	717	C	N1-C2-O2	5.24	122.04	118.90
54	BA	751	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	2000	C	N1-C2-O2	5.24	122.04	118.90
55	BB	12	C	N1-C2-O2	5.24	122.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	341	C	N1-C2-O2	5.23	122.04	118.90
22	A1	20	G	C8-N9-C4	-5.23	104.31	106.40
21	AA	899	C	N1-C2-O2	5.23	122.04	118.90
21	AA	1478	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	85	G	C5-C6-N1	5.23	114.12	111.50
54	BA	1004	U	C5-C6-N1	-5.23	120.08	122.70
54	BA	1044	C	N1-C2-O2	5.23	122.04	118.90
54	BA	2481	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	372	C	N3-C2-O2	-5.23	118.24	121.90
21	AA	655	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	1604	C	C4'-C3'-C2'	-5.23	97.37	102.60
54	BA	2093	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	2245	U	C5-C6-N1	-5.23	120.08	122.70
55	BB	5	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	1936	A	C6-C5-N7	5.23	135.96	132.30
21	AA	29	U	O4'-C1'-N1	5.23	112.38	108.20
21	AA	250	A	O4'-C1'-N9	5.23	112.38	108.20
21	AA	296	U	N3-C2-O2	-5.23	118.54	122.20
21	AA	1498	U	C3'-C2'-C1'	5.23	105.68	101.50
54	BA	226	A	C3'-C2'-C1'	5.23	105.68	101.50
54	BA	1350	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	1512	C	C5'-C4'-O4'	5.23	115.37	109.10
54	BA	1616	A	C3'-C2'-C1'	-5.23	97.32	101.50
21	AA	455	G	N7-C8-N9	5.22	115.71	113.10
54	BA	147	C	N1-C2-O2	5.22	122.03	118.90
21	AA	603	U	C5-C6-N1	-5.22	120.09	122.70
21	AA	1523	G	C3'-C2'-C1'	5.22	105.68	101.50
54	BA	1874	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2873	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	124	C	N1-C2-O2	5.22	122.03	118.90
21	AA	311	C	N1-C2-O2	5.22	122.03	118.90
21	AA	665	A	C2-N3-C4	5.22	113.21	110.60
54	BA	445	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	2239	G	N3-C4-C5	-5.22	125.99	128.60
22	A1	29	U	C5-C6-N1	-5.22	120.09	122.70
54	BA	1871	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	845	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	1069	C	N1-C2-O2	5.22	122.03	118.90
21	AA	1218	C	C1'-O4'-C4'	-5.22	105.73	109.90
54	BA	1045	C	O4'-C1'-N1	5.22	112.37	108.20
54	BA	1675	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2097	A	C4-C5-C6	-5.22	114.39	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2515	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2579	C	O4'-C1'-N1	5.22	112.37	108.20
21	AA	189	A	C4-C5-C6	-5.21	114.39	117.00
21	AA	1470	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	101	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	560	C	N1-C2-O2	5.21	122.03	118.90
54	BA	959	A	C1'-O4'-C4'	-5.21	105.73	109.90
54	BA	1465	G	O4'-C1'-N9	5.21	112.37	108.20
54	BA	2797	U	O4'-C1'-N1	5.21	112.37	108.20
21	AA	979	C	N1-C2-O2	5.21	122.03	118.90
54	BA	177	G	C5-C6-N1	5.21	114.11	111.50
54	BA	1293	C	N3-C2-O2	-5.21	118.25	121.90
55	BB	103	U	N1-C2-N3	5.21	118.03	114.90
22	A1	13	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	1172	C	O4'-C1'-N1	5.21	112.37	108.20
21	AA	1261	A	C4-C5-C6	-5.21	114.40	117.00
24	A3	5	G	C5'-C4'-C3'	-5.21	107.67	116.00
27	BE	49	ARG	NE-CZ-NH1	5.21	122.90	120.30
54	BA	1498	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	624	C	N1-C2-O2	5.21	122.02	118.90
54	BA	687	C	N3-C2-O2	-5.21	118.26	121.90
54	BA	892	A	C6-C5-N7	5.21	135.94	132.30
54	BA	2496	C	O4'-C1'-N1	5.21	112.36	108.20
21	AA	513	C	N1-C2-O2	5.20	122.02	118.90
21	AA	1413	A	C6-C5-N7	5.20	135.94	132.30
21	AA	1521	C	N1-C2-O2	5.20	122.02	118.90
54	BA	838	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1079	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1708	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2254	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	715	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2441	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2699	C	N1-C2-O2	5.20	122.02	118.90
21	AA	542	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	865	C	N1-C2-O2	5.20	122.02	118.90
54	BA	1773	A	C4'-C3'-C2'	-5.20	97.40	102.60
54	BA	1936	A	P-O3'-C3'	5.20	125.94	119.70
54	BA	2092	U	N3-C2-O2	-5.20	118.56	122.20
55	BB	38	C	C4'-C3'-C2'	-5.20	97.40	102.60
21	AA	1467	C	N1-C2-O2	5.20	122.02	118.90
54	BA	34	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	170	U	C5-C6-N1	-5.20	120.10	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	368	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2762	C	N3-C2-O2	-5.20	118.26	121.90
21	AA	281	G	C3'-C2'-C1'	5.20	105.66	101.50
54	BA	280	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	2590	A	C6-C5-N7	5.20	135.94	132.30
23	A2	90	U	P-O3'-C3'	5.20	125.93	119.70
54	BA	2499	C	N3-C2-O2	-5.20	118.26	121.90
21	AA	401	C	O4'-C1'-N1	5.19	112.36	108.20
24	A3	1	C	N1-C2-O2	5.19	122.02	118.90
28	BF	109	ARG	NE-CZ-NH1	5.19	122.90	120.30
54	BA	1886	U	O4'-C1'-N1	5.19	112.36	108.20
54	BA	260	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	921	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	1173	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	691	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	1072	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	2214	C	N1-C2-O2	5.19	122.02	118.90
54	BA	2506	U	N1-C2-N3	5.19	118.02	114.90
54	BA	2656	U	O4'-C1'-N1	5.19	112.35	108.20
21	AA	501	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1423	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	2837	A	C4'-C3'-C2'	-5.19	97.41	102.60
21	AA	437	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	837	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	1506	U	N3-C2-O2	-5.19	118.57	122.20
54	BA	2076	U	O4'-C1'-N1	5.19	112.35	108.20
21	AA	254	G	C1'-O4'-C4'	-5.19	105.75	109.90
21	AA	697	U	O4'-C1'-N1	5.19	112.35	108.20
29	BG	162	ARG	NE-CZ-NH2	-5.19	117.71	120.30
54	BA	2129	C	N1-C2-O2	5.19	122.01	118.90
54	BA	2358	A	C4-C5-C6	-5.19	114.41	117.00
21	AA	26	A	C3'-C2'-C1'	5.18	105.65	101.50
21	AA	1139	G	C5-C6-N1	5.18	114.09	111.50
21	AA	1200	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1384	C	N3-C2-O2	-5.18	118.27	121.90
21	AA	1441	A	C1'-O4'-C4'	-5.18	105.75	109.90
54	BA	374	A	C5'-C4'-O4'	5.18	115.32	109.10
54	BA	1488	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	1905	C	O4'-C1'-N1	5.18	112.35	108.20
24	A3	49	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	1249	U	C5-C6-N1	-5.18	120.11	122.70
21	AA	1119	C	N3-C2-O2	-5.18	118.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	327	G	N3-C2-N2	-5.18	116.27	119.90
54	BA	917	A	N1-C6-N6	-5.18	115.49	118.60
54	BA	2098	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	2186	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	2232	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	2248	C	N1-C2-O2	5.18	122.01	118.90
54	BA	2786	U	O4'-C1'-N1	5.18	112.34	108.20
21	AA	257	G	C5-C6-N1	5.18	114.09	111.50
21	AA	668	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	1497	G	N9-C4-C5	5.18	107.47	105.40
54	BA	723	C	N3-C4-N4	-5.18	114.38	118.00
54	BA	1806	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1401	G	N3-C4-C5	-5.17	126.01	128.60
24	A3	73	A	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	620	G	N3-C4-C5	-5.17	126.01	128.60
54	BA	2075	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	2702	G	N3-C2-N2	-5.17	116.28	119.90
21	AA	1475	G	C5-C6-N1	5.17	114.09	111.50
54	BA	484	C	N1-C2-O2	5.17	122.00	118.90
21	AA	1278	G	N9-C4-C5	5.17	107.47	105.40
21	AA	1308	U	C1'-O4'-C4'	-5.17	105.76	109.90
24	A3	9	G	C1'-O4'-C4'	-5.17	105.76	109.90
19	AT	35	TYR	CB-CG-CD2	-5.17	117.90	121.00
21	AA	611	C	N3-C4-C5	5.17	123.97	121.90
37	BO	10	ARG	NE-CZ-NH1	5.17	122.89	120.30
54	BA	268	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1128	G	C5-C6-N1	5.17	114.08	111.50
54	BA	1541	C	N1-C2-O2	5.17	122.00	118.90
54	BA	2330	G	N1-C6-O6	-5.17	116.80	119.90
13	AN	13	ARG	NE-CZ-NH1	5.17	122.88	120.30
23	A2	83	U	N1-C2-N3	5.17	118.00	114.90
54	BA	237	C	N1-C2-O2	5.17	122.00	118.90
54	BA	242	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	535	G	C5-C6-N1	5.17	114.08	111.50
21	AA	121	U	N3-C2-O2	-5.17	118.58	122.20
24	A3	26	C	N1-C2-O2	5.17	122.00	118.90
40	BR	80	ARG	NE-CZ-NH1	5.17	122.88	120.30
54	BA	679	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1096	A	C6-C5-N7	5.17	135.92	132.30
54	BA	1297	C	N3-C4-C5	5.17	123.97	121.90
54	BA	2361	G	N1-C6-O6	-5.17	116.80	119.90
56	B5	134	ARG	NE-CZ-NH1	5.17	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1291	U	O4'-C1'-N1	5.17	112.33	108.20
54	BA	465	G	N3-C2-N2	-5.17	116.28	119.90
54	BA	1604	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	553	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	1301	A	C1'-O4'-C4'	-5.16	105.77	109.90
54	BA	1894	C	N1-C2-O2	5.16	122.00	118.90
54	BA	1895	C	N1-C2-O2	5.16	122.00	118.90
54	BA	2746	U	C5-C6-N1	-5.16	120.12	122.70
21	AA	22	G	C5-C6-N1	5.16	114.08	111.50
21	AA	559	A	O4'-C1'-N9	5.16	112.33	108.20
21	AA	1269	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	897	C	N1-C2-O2	5.16	122.00	118.90
21	AA	240	G	N1-C6-O6	-5.16	116.80	119.90
21	AA	282	A	C6-C5-N7	5.16	135.91	132.30
54	BA	223	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	817	C	N1-C2-O2	5.16	122.00	118.90
54	BA	12	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	526	A	C6-C5-N7	5.16	135.91	132.30
54	BA	1649	G	C1'-O4'-C4'	-5.16	105.77	109.90
56	B5	49	GLY	C-N-CA	5.16	134.60	121.70
21	AA	1194	U	C1'-O4'-C4'	-5.16	105.78	109.90
54	BA	1552	A	C2-N3-C4	5.16	113.18	110.60
54	BA	1642	G	O4'-C1'-N9	5.16	112.33	108.20
21	AA	572	A	C1'-O4'-C4'	-5.16	105.78	109.90
21	AA	1387	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	247	G	C5-C6-N1	5.16	114.08	111.50
54	BA	2133	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	2462	C	N1-C2-O2	5.16	121.99	118.90
21	AA	734	G	N3-C4-C5	-5.15	126.02	128.60
54	BA	248	G	N3-C2-N2	-5.15	116.29	119.90
54	BA	2594	C	N3-C2-O2	-5.15	118.29	121.90
54	BA	2805	C	N1-C2-O2	5.15	121.99	118.90
21	AA	994	A	C6-C5-N7	5.15	135.91	132.30
21	AA	1530	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1179	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1743	G	C5-C6-N1	5.15	114.08	111.50
54	BA	1790	C	N3-C2-O2	-5.15	118.29	121.90
54	BA	1815	A	O4'-C1'-N9	5.15	112.32	108.20
54	BA	2392	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	2902	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	493	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	682	G	C5-C6-N1	5.15	114.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1436	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1524	G	C8-N9-C4	-5.15	104.34	106.40
54	BA	2155	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2304	G	C5-C6-N1	5.15	114.08	111.50
22	A1	58	A	C4-C5-C6	-5.15	114.43	117.00
24	A3	62	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	55	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	2778	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	602	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	1366	C	N3-C2-O2	-5.15	118.30	121.90
24	A3	61	U	N3-C2-O2	-5.15	118.60	122.20
54	BA	338	G	C8-N9-C4	-5.15	104.34	106.40
54	BA	744	U	N3-C2-O2	-5.15	118.60	122.20
54	BA	1972	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1983	G	N9-C4-C5	5.15	107.46	105.40
54	BA	2735	G	N1-C6-O6	-5.15	116.81	119.90
13	AN	63	ARG	NE-CZ-NH1	5.14	122.87	120.30
21	AA	1106	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	852	U	O4'-C1'-N1	5.14	112.32	108.20
54	BA	1607	C	N1-C2-O2	5.14	121.99	118.90
54	BA	2871	U	O4'-C1'-N1	5.14	112.32	108.20
21	AA	337	G	N1-C6-O6	-5.14	116.81	119.90
21	AA	368	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	416	G	N1-C6-O6	-5.14	116.81	119.90
21	AA	590	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	1108	U	N1-C2-N3	5.14	117.98	114.90
54	BA	1181	U	C5-C6-N1	-5.14	120.13	122.70
54	BA	2407	A	C6-C5-N7	5.14	135.90	132.30
54	BA	2482	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2592	G	N1-C6-O6	-5.14	116.81	119.90
55	BB	9	G	C5-C6-N1	5.14	114.07	111.50
21	AA	823	C	N3-C4-C5	5.14	123.96	121.90
54	BA	566	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2100	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	2267	A	C4-C5-C6	-5.14	114.43	117.00
55	BB	113	C	N1-C2-O2	5.14	121.98	118.90
21	AA	48	C	C3'-C2'-C1'	5.14	105.61	101.50
21	AA	1214	C	N3-C4-C5	5.14	123.96	121.90
21	AA	1368	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	1485	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2024	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	2288	A	C4-C5-C6	-5.14	114.43	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2586	U	C3'-C2'-C1'	5.14	105.61	101.50
21	AA	977	A	C2-N3-C4	5.14	113.17	110.60
54	BA	135	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	515	A	C6-C5-N7	5.14	135.90	132.30
54	BA	917	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2731	G	O4'-C1'-N9	5.14	112.31	108.20
21	AA	723	U	C5-C6-N1	-5.14	120.13	122.70
21	AA	862	C	N1-C2-O2	5.14	121.98	118.90
21	AA	1318	A	O4'-C1'-N9	5.14	112.31	108.20
26	BD	77	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
54	BA	1371	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	1387	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2033	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2087	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	2463	C	N3-C4-C5	5.14	123.95	121.90
54	BA	2707	U	N3-C2-O2	-5.14	118.60	122.20
54	BA	1	G	C5-C6-N1	5.13	114.07	111.50
54	BA	57	C	O4'-C1'-N1	5.13	112.31	108.20
54	BA	459	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	2627	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2827	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2841	C	N1-C2-O2	5.13	121.98	118.90
21	AA	201	G	C5-C6-N1	5.13	114.07	111.50
54	BA	15	G	C8-N9-C4	-5.13	104.35	106.40
54	BA	853	C	N3-C4-N4	-5.13	114.41	118.00
54	BA	1496	A	C6-C5-N7	5.13	135.89	132.30
54	BA	1561	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2394	C	N1-C2-O2	5.13	121.98	118.90
15	AP	35	ARG	NE-CZ-NH1	5.13	122.86	120.30
21	AA	651	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	870	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	1062	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1205	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	2078	C	N3-C2-O2	-5.13	118.31	121.90
21	AA	1193	G	N3-C2-N2	-5.13	116.31	119.90
21	AA	1305	G	O4'-C4'-C3'	5.13	110.20	106.10
54	BA	2504	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	2576	G	N1-C6-O6	-5.13	116.82	119.90
24	A3	31	G	O4'-C1'-N9	5.13	112.30	108.20
21	AA	1145	A	C6-C5-N7	5.13	135.89	132.30
54	BA	209	C	O4'-C1'-N1	5.13	112.30	108.20
54	BA	996	A	C4-C5-C6	-5.13	114.44	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2126	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	2806	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2864	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	562	U	O4'-C1'-N1	5.12	112.30	108.20
21	AA	939	G	N3-C4-C5	-5.12	126.04	128.60
54	BA	2371	G	N3-C2-N2	-5.12	116.31	119.90
55	BB	56	G	C8-N9-C4	-5.12	104.35	106.40
21	AA	718	A	C3'-C2'-C1'	5.12	105.60	101.50
54	BA	1699	G	C1'-O4'-C4'	-5.12	105.80	109.90
54	BA	2547	A	C6-C5-N7	5.12	135.89	132.30
21	AA	383	A	C5-C6-N1	5.12	120.26	117.70
21	AA	1293	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1182	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1229	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1258	U	C5-C6-N1	-5.12	120.14	122.70
54	BA	1844	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	2189	U	O4'-C1'-N1	5.12	112.30	108.20
21	AA	342	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	274	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1112	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1943	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	2295	C	O4'-C1'-N1	5.12	112.30	108.20
21	AA	1031	C	C2-N3-C4	-5.12	117.34	119.90
54	BA	551	G	N7-C8-N9	5.12	115.66	113.10
54	BA	1421	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1570	A	C6-C5-N7	5.12	135.88	132.30
54	BA	2057	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2163	A	O4'-C1'-N9	5.12	112.30	108.20
54	BA	2678	C	C5'-C4'-O4'	5.12	115.24	109.10
54	BA	2831	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	395	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	886	A	C6-C5-N7	5.12	135.88	132.30
54	BA	1434	A	C2-N3-C4	5.12	113.16	110.60
21	AA	162	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	286	C	N1-C2-O2	5.12	121.97	118.90
21	AA	295	C	N1-C2-O2	5.12	121.97	118.90
21	AA	750	C	N1-C2-O2	5.12	121.97	118.90
54	BA	423	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	473	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	842	U	O4'-C1'-N1	5.12	112.29	108.20
54	BA	1081	U	O4'-C1'-N1	5.12	112.29	108.20
54	BA	1382	G	N3-C4-C5	-5.12	126.04	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2561	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	2756	U	P-O3'-C3'	5.12	125.84	119.70
21	AA	65	A	C4-C5-C6	-5.11	114.44	117.00
21	AA	911	U	N1-C2-N3	5.11	117.97	114.90
22	A1	24	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	141	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	311	A	C6-C5-N7	5.11	135.88	132.30
54	BA	360	U	C5-C6-N1	-5.11	120.14	122.70
54	BA	984	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	1152	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	1448	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	1871	A	O4'-C1'-N9	5.11	112.29	108.20
54	BA	2453	A	C6-C5-N7	5.11	135.88	132.30
21	AA	1529	G	O4'-C1'-N9	5.11	112.29	108.20
54	BA	2521	C	O4'-C1'-N1	5.11	112.29	108.20
10	AK	127	ARG	NE-CZ-NH1	5.11	122.86	120.30
21	AA	35	G	N1-C6-O6	-5.11	116.83	119.90
21	AA	1008	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	1517	G	N3-C2-N2	-5.11	116.32	119.90
23	A2	87	U	C5'-C4'-C3'	-5.11	107.82	116.00
54	BA	709	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	2344	U	N3-C2-O2	-5.11	118.62	122.20
54	BA	2696	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	423	G	C5-C6-N1	5.11	114.06	111.50
21	AA	809	G	C5-C6-N1	5.11	114.06	111.50
21	AA	1207	G	N1-C6-O6	-5.11	116.83	119.90
21	AA	1216	A	C6-C5-N7	5.11	135.88	132.30
22	A1	41	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	483	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	1338	G	C5-C6-N1	5.11	114.06	111.50
54	BA	2453	A	C5-C6-N6	5.11	127.79	123.70
21	AA	20	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	494	G	O4'-C1'-N9	5.11	112.29	108.20
21	AA	724	G	N1-C6-O6	-5.11	116.83	119.90
21	AA	977	A	C5'-C4'-C3'	-5.11	107.83	116.00
54	BA	489	G	N3-C2-N2	-5.11	116.32	119.90
54	BA	812	C	C1'-O4'-C4'	-5.11	105.81	109.90
54	BA	1772	A	O4'-C1'-N9	5.11	112.29	108.20
54	BA	1945	G	N3-C4-C5	-5.11	126.05	128.60
54	BA	2086	U	C5-C6-N1	-5.11	120.15	122.70
54	BA	2659	G	N3-C2-N2	-5.11	116.32	119.90
55	BB	57	A	C4-C5-C6	-5.11	114.45	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	63	C	N1-C2-O2	5.11	121.96	118.90
21	AA	901	A	C4-C5-C6	-5.11	114.45	117.00
21	AA	1335	U	N3-C2-O2	-5.11	118.63	122.20
54	BA	164	C	O4'-C1'-N1	5.11	112.28	108.20
54	BA	204	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	252	G	O4'-C1'-N9	5.11	112.28	108.20
54	BA	1164	C	O4'-C1'-N1	5.11	112.28	108.20
54	BA	2366	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	2541	A	C4-C5-C6	-5.11	114.45	117.00
21	AA	84	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	1217	C	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1348	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	242	G	C5-C6-N1	5.10	114.05	111.50
54	BA	2172	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	473	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	723	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	996	A	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1001	C	N3-C2-O2	-5.10	118.33	121.90
21	AA	1301	U	N1-C2-N3	5.10	117.96	114.90
54	BA	587	C	C3'-C2'-C1'	5.10	105.58	101.50
54	BA	616	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2062	A	O4'-C1'-N9	5.10	112.28	108.20
54	BA	2644	G	C5-C6-N1	5.10	114.05	111.50
21	AA	1205	U	N1-C2-N3	5.10	117.96	114.90
54	BA	1661	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	2716	C	N1-C2-O2	5.10	121.96	118.90
21	AA	483	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1418	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	640	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2579	C	N1-C2-O2	5.10	121.96	118.90
5	AF	24	ARG	NE-CZ-NH1	5.10	122.85	120.30
21	AA	406	G	N3-C4-C5	-5.10	126.05	128.60
21	AA	534	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	585	G	N3-C4-C5	-5.10	126.05	128.60
21	AA	1021	A	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1442	G	N3-C2-N2	-5.10	116.33	119.90
40	BR	13	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
54	BA	290	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	1729	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1036	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2810	A	N1-C6-N6	-5.10	115.54	118.60
21	AA	499	A	C6-C5-N7	5.09	135.87	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	591	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	130	C	O4'-C1'-N1	5.09	112.28	108.20
54	BA	887	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1082	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1504	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	1591	A	C6-C5-N7	5.09	135.87	132.30
54	BA	2233	U	C4'-C3'-C2'	-5.09	97.50	102.60
54	BA	74	A	C1'-O4'-C4'	-5.09	105.83	109.90
54	BA	402	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	1040	A	C6-C5-N7	5.09	135.87	132.30
54	BA	1329	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1578	U	C5-C6-N1	-5.09	120.15	122.70
54	BA	1804	C	N3-C2-O2	-5.09	118.33	121.90
21	AA	11	G	N1-C6-O6	-5.09	116.85	119.90
21	AA	623	C	N1-C2-O2	5.09	121.95	118.90
54	BA	1542	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1615	C	O4'-C1'-C2'	-5.09	100.71	105.80
54	BA	1662	U	C5-C6-N1	-5.09	120.15	122.70
54	BA	1731	G	N3-C4-C5	-5.09	126.05	128.60
54	BA	2341	G	C5-C6-N1	5.09	114.05	111.50
54	BA	2494	G	C5-C6-N1	5.09	114.05	111.50
54	BA	2724	U	C5-C6-N1	-5.09	120.15	122.70
55	BB	44	G	N1-C6-O6	-5.09	116.84	119.90
21	AA	266	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	668	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	1107	C	O4'-C1'-N1	5.09	112.27	108.20
24	A3	11	A	C6-C5-N7	5.09	135.86	132.30
54	BA	64	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	507	A	O4'-C1'-N9	5.09	112.27	108.20
54	BA	550	C	N1-C2-O2	5.09	121.95	118.90
54	BA	2147	A	C6-C5-N7	5.09	135.86	132.30
1	AB	19	THR	C-N-CA	5.09	134.42	121.70
54	BA	258	G	C5-C6-N1	5.09	114.04	111.50
54	BA	304	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	772	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2421	G	O4'-C1'-N9	5.09	112.27	108.20
55	BB	41	G	N3-C4-C5	-5.09	126.06	128.60
21	AA	305	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	479	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	978	A	C4-C5-C6	-5.09	114.46	117.00
24	A3	13	C	N3-C2-O2	-5.09	118.34	121.90
54	BA	96	C	O4'-C1'-N1	5.09	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	223	A	O4'-C1'-N9	5.09	112.27	108.20
54	BA	518	G	O4'-C1'-N9	5.09	112.27	108.20
54	BA	1028	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	1189	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	2408	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2787	C	C5'-C4'-O4'	5.09	115.20	109.10
55	BB	104	A	C4-C5-C6	-5.09	114.46	117.00
21	AA	1259	C	N1-C2-O2	5.08	121.95	118.90
54	BA	74	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	318	C	N3-C4-N4	-5.08	114.44	118.00
54	BA	802	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	2691	C	O4'-C1'-N1	5.08	112.27	108.20
21	AA	919	A	C6-C5-N7	5.08	135.86	132.30
21	AA	1124	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	391	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	573	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	1091	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1603	A	C6-C5-N7	5.08	135.86	132.30
54	BA	1793	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2143	C	N3-C2-O2	-5.08	118.34	121.90
54	BA	2215	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2343	U	O4'-C1'-N1	5.08	112.27	108.20
21	AA	246	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	528	C	N1-C2-O2	5.08	121.95	118.90
21	AA	1146	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1569	A	C6-C5-N7	5.08	135.86	132.30
54	BA	2196	C	C5'-C4'-O4'	5.08	115.20	109.10
54	BA	2245	U	N3-C2-O2	-5.08	118.64	122.20
21	AA	702	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	1399	C	N3-C4-C5	5.08	123.93	121.90
24	A3	6	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	669	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	780	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1632	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	968	A	O4'-C1'-N9	5.08	112.26	108.20
54	BA	710	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1149	G	C5'-C4'-O4'	5.08	115.19	109.10
54	BA	1439	A	C2-N3-C4	5.08	113.14	110.60
54	BA	1716	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1933	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2626	C	N3-C2-O2	-5.08	118.34	121.90
21	AA	1386	G	N3-C4-C5	-5.08	126.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	21	TYR	CB-CG-CD2	-5.08	117.95	121.00
25	BC	13	ARG	NE-CZ-NH1	5.08	122.84	120.30
54	BA	1415	U	N1-C2-N3	5.08	117.95	114.90
54	BA	1807	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	1893	C	N3-C2-O2	-5.08	118.35	121.90
54	BA	2435	A	C6-C5-N7	5.08	135.85	132.30
54	BA	1007	C	N3-C4-C5	5.07	123.93	121.90
54	BA	1647	U	C5-C6-N1	-5.07	120.16	122.70
54	BA	1820	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	1931	U	O4'-C1'-N1	5.07	112.26	108.20
24	A3	54	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	133	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	999	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	1304	A	C6-C5-N7	5.07	135.85	132.30
54	BA	1306	C	C4'-C3'-C2'	-5.07	97.53	102.60
54	BA	2115	G	C5-C6-N1	5.07	114.04	111.50
21	AA	674	G	N3-C4-C5	-5.07	126.06	128.60
21	AA	924	C	N1-C2-O2	5.07	121.94	118.90
21	AA	1324	A	C4-C5-C6	-5.07	114.47	117.00
21	AA	1505	G	C5-C6-N1	5.07	114.03	111.50
54	BA	1767	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2353	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2780	G	N3-C2-N2	-5.07	116.35	119.90
21	AA	1376	U	C5-C6-N1	-5.07	120.17	122.70
21	AA	1453	G	C8-N9-C4	-5.07	104.37	106.40
54	BA	277	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	560	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	999	U	C5-C6-N1	-5.07	120.17	122.70
54	BA	1066	U	C4'-C3'-C2'	-5.07	97.53	102.60
54	BA	1129	A	C5'-C4'-O4'	5.07	115.18	109.10
54	BA	2410	G	C5-C6-N1	5.07	114.03	111.50
54	BA	2695	U	O4'-C1'-N1	5.07	112.25	108.20
21	AA	109	A	C4-C5-C6	-5.07	114.47	117.00
21	AA	292	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	619	U	O4'-C1'-N1	5.07	112.25	108.20
21	AA	667	G	N3-C2-N2	-5.07	116.36	119.90
54	BA	106	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1100	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1804	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1847	A	C5-C6-N6	5.07	127.75	123.70
54	BA	2496	C	N3-C2-O2	-5.07	118.35	121.90
21	AA	155	A	C6-C5-N7	5.06	135.84	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	400	C	N1-C2-O2	5.06	121.94	118.90
21	AA	884	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	884	U	C5-C6-N1	-5.06	120.17	122.70
21	AA	926	G	N1-C6-O6	-5.06	116.86	119.90
21	AA	1352	C	N1-C2-O2	5.06	121.94	118.90
21	AA	419	C	N1-C2-O2	5.06	121.94	118.90
21	AA	733	G	C5-C6-N1	5.06	114.03	111.50
21	AA	890	G	N3-C4-C5	-5.06	126.07	128.60
21	AA	1128	C	N1-C2-O2	5.06	121.94	118.90
21	AA	1196	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	1339	A	C1'-O4'-C4'	-5.06	105.85	109.90
24	A3	7	G	N3-C4-C5	-5.06	126.07	128.60
54	BA	441	U	N1-C2-N3	5.06	117.94	114.90
54	BA	2047	C	N1-C2-O2	5.06	121.94	118.90
54	BA	2616	C	O4'-C1'-N1	5.06	112.25	108.20
21	AA	1240	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	1401	G	N7-C8-N9	5.06	115.63	113.10
22	A1	16	C	N1-C2-O2	5.06	121.94	118.90
39	BQ	49	ARG	NE-CZ-NH2	-5.06	117.77	120.30
42	BT	51	PHE	CB-CG-CD2	-5.06	117.26	120.80
45	BW	40	ARG	NE-CZ-NH2	-5.06	117.77	120.30
54	BA	53	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	110	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	1153	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1428	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1787	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	2457	U	C5-C6-N1	-5.06	120.17	122.70
54	BA	2793	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1210	G	O4'-C1'-N9	5.06	112.25	108.20
54	BA	1692	U	N1-C2-N3	5.06	117.93	114.90
54	BA	2330	G	N3-C2-N2	-5.06	116.36	119.90
21	AA	530	G	N3-C4-N9	5.06	129.03	126.00
21	AA	705	G	N1-C6-O6	-5.06	116.87	119.90
21	AA	1500	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	616	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	1054	C	N3-C2-O2	-5.05	118.36	121.90
21	AA	1182	G	P-O3'-C3'	5.05	125.77	119.70
22	A1	61	C	N3-C2-O2	-5.05	118.36	121.90
54	BA	315	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1424	G	P-O3'-C3'	5.05	125.77	119.70
54	BA	1838	C	N3-C4-C5	5.05	123.92	121.90
54	BA	1955	U	O4'-C1'-N1	5.05	112.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2558	C	N1-C2-O2	5.05	121.93	118.90
55	BB	28	C	N1-C2-O2	5.05	121.93	118.90
8	AI	122	ARG	NE-CZ-NH1	5.05	122.83	120.30
21	AA	1127	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	291	G	N3-C2-N2	-5.05	116.36	119.90
54	BA	857	G	N7-C8-N9	5.05	115.63	113.10
54	BA	953	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	143	A	C6-C5-N7	5.05	135.84	132.30
54	BA	1125	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1613	G	C5-C6-N1	5.05	114.03	111.50
54	BA	1999	C	O4'-C1'-N1	5.05	112.24	108.20
6	AG	3	ARG	CD-NE-CZ	5.05	130.67	123.60
54	BA	1100	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	1358	G	N3-C4-C5	-5.05	126.08	128.60
54	BA	2401	U	C5'-C4'-O4'	5.05	115.16	109.10
21	AA	106	C	C5'-C4'-O4'	5.05	115.16	109.10
21	AA	940	C	N3-C2-O2	-5.05	118.37	121.90
54	BA	151	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1827	U	N3-C2-O2	-5.05	118.67	122.20
54	BA	2704	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2815	C	N1-C2-O2	5.05	121.93	118.90
54	BA	16	C	O4'-C1'-N1	5.04	112.24	108.20
54	BA	198	C	C6-N1-C2	-5.04	118.28	120.30
54	BA	774	G	O4'-C1'-N9	5.04	112.24	108.20
54	BA	1243	C	N1-C2-O2	5.04	121.93	118.90
54	BA	1685	C	N3-C4-C5	5.04	123.92	121.90
21	AA	54	C	C5-C4-N4	5.04	123.73	120.20
21	AA	1155	A	C3'-C2'-C1'	5.04	105.53	101.50
54	BA	376	G	C5-C6-N1	5.04	114.02	111.50
54	BA	1409	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	2039	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2442	C	N1-C2-O2	5.04	121.93	118.90
54	BA	90	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	559	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	738	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2099	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	626	G	N1-C6-O6	-5.04	116.88	119.90
21	AA	732	C	N1-C2-O2	5.04	121.92	118.90
21	AA	755	G	C5'-C4'-C3'	-5.04	107.94	116.00
54	BA	1148	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2155	U	N1-C2-N3	5.04	117.92	114.90
54	BA	2543	G	C5-C6-N1	5.04	114.02	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	39	A	C5'-C4'-O4'	5.04	115.15	109.10
21	AA	77	A	C6-C5-N7	5.04	135.83	132.30
21	AA	563	A	C6-C5-N7	5.04	135.83	132.30
21	AA	607	A	C6-C5-N7	5.04	135.83	132.30
21	AA	632	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	1441	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	638	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2200	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2561	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	650	C	N3-C4-C5	5.04	123.92	121.90
54	BA	859	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	1191	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	2182	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2323	G	N3-C4-C5	-5.04	126.08	128.60
21	AA	784	A	C5'-C4'-O4'	5.04	115.14	109.10
21	AA	1093	A	O4'-C1'-N9	5.04	112.23	108.20
54	BA	279	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	1864	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	2855	C	N3-C2-O2	-5.04	118.38	121.90
21	AA	333	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	353	A	O4'-C1'-N9	5.03	112.23	108.20
21	AA	1271	A	O4'-C1'-N9	5.03	112.23	108.20
54	BA	1031	G	O4'-C1'-N9	5.03	112.23	108.20
54	BA	1733	G	C5-C6-N1	5.03	114.02	111.50
54	BA	2901	C	N1-C2-O2	5.03	121.92	118.90
55	BB	76	G	C5-C6-N1	5.03	114.02	111.50
21	AA	256	U	C5-C6-N1	-5.03	120.18	122.70
54	BA	228	C	C6-N1-C2	-5.03	118.29	120.30
7	AH	76	ARG	NE-CZ-NH2	-5.03	117.78	120.30
54	BA	312	G	C5'-C4'-O4'	5.03	115.14	109.10
54	BA	508	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	1273	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	1526	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1527	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	1645	G	P-O3'-C3'	5.03	125.73	119.70
54	BA	1657	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1688	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	1805	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1879	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1946	U	C5-C6-N1	-5.03	120.19	122.70
21	AA	1338	G	N1-C6-O6	-5.03	116.88	119.90
38	BP	100	ARG	NE-CZ-NH1	5.03	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1312	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	2592	G	C5-C6-N1	5.03	114.01	111.50
54	BA	2839	G	C8-N9-C4	-5.03	104.39	106.40
21	AA	628	G	N1-C6-O6	-5.03	116.88	119.90
33	BK	18	ARG	NE-CZ-NH1	5.03	122.81	120.30
49	B0	16	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
54	BA	578	G	C5-C6-N1	5.03	114.01	111.50
54	BA	1289	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2752	C	N1-C2-O2	5.03	121.92	118.90
21	AA	316	C	O4'-C1'-N1	5.03	112.22	108.20
21	AA	896	C	N3-C2-O2	-5.03	118.38	121.90
54	BA	251	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	447	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	635	C	N3-C4-C5	5.03	123.91	121.90
54	BA	979	A	C1'-O4'-C4'	-5.03	105.88	109.90
54	BA	1091	G	C4'-C3'-C2'	-5.03	97.58	102.60
54	BA	2192	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	2285	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2413	G	C5'-C4'-O4'	5.03	115.13	109.10
21	AA	140	U	C5-C6-N1	-5.02	120.19	122.70
21	AA	273	U	N3-C2-O2	-5.02	118.69	122.20
21	AA	411	A	O4'-C1'-N9	5.02	112.22	108.20
21	AA	1289	A	C6-C5-N7	5.02	135.81	132.30
37	BO	94	ARG	CD-NE-CZ	5.02	130.63	123.60
54	BA	361	G	O4'-C1'-N9	5.02	112.22	108.20
54	BA	1961	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2001	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2069	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	984	C	N3-C4-C5	5.02	123.91	121.90
55	BB	8	C	N1-C2-O2	5.02	121.91	118.90
13	AN	53	ARG	NE-CZ-NH1	5.02	122.81	120.30
54	BA	839	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1237	A	O4'-C1'-N9	5.02	112.22	108.20
54	BA	1803	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	2103	C	N3-C4-N4	-5.02	114.49	118.00
55	BB	45	A	C4-C5-C6	-5.02	114.49	117.00
11	AL	55	ARG	NE-CZ-NH2	-5.02	117.79	120.30
21	AA	851	G	C5-C6-N1	5.02	114.01	111.50
54	BA	983	A	O4'-C1'-N9	5.02	112.21	108.20
54	BA	1307	A	C6-C5-N7	5.02	135.81	132.30
54	BA	1909	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	2285	C	C4'-C3'-C2'	-5.02	97.58	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2732	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2835	A	C3'-C2'-C1'	5.02	105.52	101.50
21	AA	964	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	357	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	1890	A	C6-C5-N7	5.02	135.81	132.30
55	BB	69	G	O4'-C1'-N9	5.02	112.21	108.20
21	AA	68	G	C5-C6-N1	5.01	114.01	111.50
21	AA	850	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	1095	U	C4-C5-C6	5.01	122.71	119.70
21	AA	1378	C	N1-C2-O2	5.01	121.91	118.90
54	BA	349	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	371	A	C6-C5-N7	5.01	135.81	132.30
54	BA	795	C	O4'-C1'-N1	5.01	112.21	108.20
54	BA	888	C	N1-C2-O2	5.01	121.91	118.90
54	BA	889	C	C5'-C4'-C3'	-5.01	107.98	116.00
54	BA	1644	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1842	G	N3-C4-C5	-5.01	126.09	128.60
21	AA	256	U	N3-C2-O2	-5.01	118.69	122.20
21	AA	1297	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	1625	C	C3'-C2'-C1'	5.01	105.51	101.50
54	BA	1960	A	C6-C5-N7	5.01	135.81	132.30
21	AA	915	A	C6-C5-N7	5.01	135.81	132.30
21	AA	1326	U	N3-C2-O2	-5.01	118.69	122.20
21	AA	1501	C	N1-C2-O2	5.01	121.91	118.90
37	BO	15	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	364	C	N1-C2-O2	5.01	121.91	118.90
54	BA	470	A	C4-C5-C6	-5.01	114.49	117.00
54	BA	957	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1215	G	N3-C2-N2	-5.01	116.39	119.90
54	BA	1643	G	O4'-C1'-N9	5.01	112.21	108.20
54	BA	1656	C	N1-C2-O2	5.01	121.91	118.90
54	BA	2863	C	N3-C2-O2	-5.01	118.39	121.90
21	AA	432	A	O4'-C1'-N9	5.01	112.21	108.20
21	AA	445	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	461	A	C4-C5-C6	-5.01	114.50	117.00
21	AA	1494	G	O4'-C1'-N9	5.01	112.21	108.20
54	BA	673	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1330	C	N3-C2-O2	-5.01	118.39	121.90
54	BA	1349	C	N3-C2-O2	-5.01	118.39	121.90
21	AA	656	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	454	A	C6-C5-N7	5.01	135.81	132.30
21	AA	343	U	N3-C2-O2	-5.01	118.70	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	344	A	C3'-C2'-C1'	5.01	105.51	101.50
21	AA	1427	C	N1-C2-O2	5.01	121.90	118.90
21	AA	1440	U	N3-C2-O2	-5.01	118.69	122.20
41	BS	110	ARG	NE-CZ-NH2	-5.01	117.80	120.30
54	BA	711	G	C5'-C4'-C3'	-5.01	107.99	116.00
54	BA	821	A	N9-C1'-C2'	-5.01	106.49	112.00
54	BA	1895	C	N3-C4-C5	5.01	123.90	121.90
54	BA	2619	C	N3-C4-C5	5.01	123.90	121.90
55	BB	34	A	C6-C5-N7	5.01	135.80	132.30
21	AA	544	G	O4'-C1'-N9	5.00	112.20	108.20
21	AA	932	C	O4'-C1'-N1	5.00	112.20	108.20
24	A3	2	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	1035	U	N3-C2-O2	-5.00	118.70	122.20
54	BA	1929	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	2446	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	2884	U	N3-C2-O2	-5.00	118.70	122.20
21	AA	319	G	N1-C6-O6	-5.00	116.90	119.90
21	AA	334	C	N1-C2-O2	5.00	121.90	118.90
21	AA	335	C	N1-C2-O2	5.00	121.90	118.90
21	AA	564	C	N1-C2-O2	5.00	121.90	118.90
54	BA	148	U	C5-C6-N1	-5.00	120.20	122.70
54	BA	993	G	C5-C6-N1	5.00	114.00	111.50
54	BA	1190	G	C5-C6-N1	5.00	114.00	111.50
54	BA	1501	G	C5-C6-N1	5.00	114.00	111.50
54	BA	1537	G	O4'-C1'-N9	5.00	112.20	108.20
21	AA	144	G	N3-C2-N2	-5.00	116.40	119.90
21	AA	900	A	C6-C5-N7	5.00	135.80	132.30
21	AA	1053	G	C5-C6-N1	5.00	114.00	111.50
21	AA	1098	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	1279	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	200	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	213	A	C6-C5-N7	5.00	135.80	132.30
54	BA	1015	U	C5-C6-N1	-5.00	120.20	122.70
54	BA	1597	A	C6-C5-N7	5.00	135.80	132.30
54	BA	1898	U	C5-C6-N1	-5.00	120.20	122.70
54	BA	2507	C	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (1072) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	11	C	Sidechain

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Mol	Chain	Res	Type	Group
22	A1	18	G	Sidechain
22	A1	19	G	Sidechain
22	A1	23	A	Sidechain
22	A1	24	G	Sidechain
22	A1	27	C	Sidechain
22	A1	28	C	Sidechain
22	A1	3	G	Sidechain
22	A1	44	G	Sidechain
22	A1	45	G	Sidechain
22	A1	49	G	Sidechain
22	A1	53	G	Sidechain
22	A1	58	A	Sidechain
22	A1	60	C	Sidechain
22	A1	65	C	Sidechain
22	A1	66	A	Sidechain
22	A1	67	U	Sidechain
22	A1	68	C	Sidechain
22	A1	8	U	Sidechain
22	A1	9	A	Sidechain
23	A2	84	G	Sidechain
23	A2	86	U	Sidechain
23	A2	87	U	Sidechain
23	A2	88	U	Sidechain
23	A2	90	U	Sidechain
24	A3	16	C	Sidechain
24	A3	2	G	Sidechain
24	A3	24	C	Sidechain
24	A3	26	C	Sidechain
24	A3	36	A	Sidechain
24	A3	37	U	Sidechain
24	A3	54	G	Sidechain
24	A3	62	C	Sidechain
24	A3	67	C	Sidechain
24	A3	7	G	Sidechain
24	A3	73	A	Sidechain
24	A3	74	A	Sidechain
24	A3	75	C	Sidechain
21	AA	1007	U	Sidechain
21	AA	1008	U	Sidechain
21	AA	1010	U	Sidechain
21	AA	102	G	Sidechain
21	AA	1022	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1023	U	Sidechain
21	AA	1024	G	Sidechain
21	AA	1029	U	Sidechain
21	AA	1030	U	Sidechain
21	AA	1038	C	Sidechain
21	AA	1039	G	Sidechain
21	AA	1040	U	Sidechain
21	AA	1041	G	Sidechain
21	AA	1045	C	Sidechain
21	AA	1048	G	Sidechain
21	AA	1051	C	Sidechain
21	AA	1061	G	Sidechain
21	AA	1065	U	Sidechain
21	AA	1066	C	Sidechain
21	AA	1072	G	Sidechain
21	AA	1077	G	Sidechain
21	AA	1079	G	Sidechain
21	AA	108	G	Sidechain
21	AA	1084	G	Sidechain
21	AA	1093	A	Sidechain
21	AA	1095	U	Sidechain
21	AA	1104	G	Sidechain
21	AA	1105	A	Sidechain
21	AA	1108	G	Sidechain
21	AA	111	G	Sidechain
21	AA	1127	G	Sidechain
21	AA	1131	G	Sidechain
21	AA	1136	C	Sidechain
21	AA	1137	C	Sidechain
21	AA	1139	G	Sidechain
21	AA	1141	C	Sidechain
21	AA	1144	G	Sidechain
21	AA	1147	C	Sidechain
21	AA	115	G	Sidechain
21	AA	1151	A	Sidechain
21	AA	1153	G	Sidechain
21	AA	1154	G	Sidechain
21	AA	1168	U	Sidechain
21	AA	1172	C	Sidechain
21	AA	1176	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1181	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1182	G	Sidechain
21	AA	1185	G	Sidechain
21	AA	1186	G	Sidechain
21	AA	1187	G	Sidechain
21	AA	1195	C	Sidechain
21	AA	1207	G	Sidechain
21	AA	121	U	Sidechain
21	AA	1210	C	Sidechain
21	AA	1215	G	Sidechain
21	AA	1217	C	Sidechain
21	AA	1219	A	Sidechain
21	AA	1220	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1224	U	Sidechain
21	AA	1226	C	Sidechain
21	AA	124	C	Sidechain
21	AA	1240	U	Sidechain
21	AA	1245	C	Sidechain
21	AA	1261	A	Sidechain
21	AA	1266	G	Sidechain
21	AA	1276	G	Sidechain
21	AA	128	G	Sidechain
21	AA	1280	A	Sidechain
21	AA	1281	C	Sidechain
21	AA	1285	A	Sidechain
21	AA	1289	A	Sidechain
21	AA	130	A	Sidechain
21	AA	1300	G	Sidechain
21	AA	1301	U	Sidechain
21	AA	1302	C	Sidechain
21	AA	1303	C	Sidechain
21	AA	1305	G	Sidechain
21	AA	1306	A	Sidechain
21	AA	1309	G	Sidechain
21	AA	1316	G	Sidechain
21	AA	1318	A	Sidechain
21	AA	1337	G	Sidechain
21	AA	1339	A	Sidechain
21	AA	1346	A	Sidechain
21	AA	1348	U	Sidechain
21	AA	1350	A	Sidechain
21	AA	1358	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1360	A	Sidechain
21	AA	1370	G	Sidechain
21	AA	1373	G	Sidechain
21	AA	1379	G	Sidechain
21	AA	1380	U	Sidechain
21	AA	1382	C	Sidechain
21	AA	1387	G	Sidechain
21	AA	1391	U	Sidechain
21	AA	1399	C	Sidechain
21	AA	1401	G	Sidechain
21	AA	1409	C	Sidechain
21	AA	1412	C	Sidechain
21	AA	142	G	Sidechain
21	AA	1432	G	Sidechain
21	AA	1433	A	Sidechain
21	AA	1434	A	Sidechain
21	AA	1435	G	Sidechain
21	AA	1441	A	Sidechain
21	AA	1442	G	Sidechain
21	AA	1448	C	Sidechain
21	AA	1453	G	Sidechain
21	AA	1455	G	Sidechain
21	AA	1459	G	Sidechain
21	AA	1460	C	Sidechain
21	AA	1465	A	Sidechain
21	AA	1471	U	Sidechain
21	AA	1472	U	Sidechain
21	AA	1473	G	Sidechain
21	AA	1476	A	Sidechain
21	AA	1478	U	Sidechain
21	AA	1479	C	Sidechain
21	AA	148	G	Sidechain
21	AA	1489	G	Sidechain
21	AA	1491	G	Sidechain
21	AA	1499	A	Sidechain
21	AA	1500	A	Sidechain
21	AA	1503	A	Sidechain
21	AA	1514	G	Sidechain
21	AA	1518	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1528	U	Sidechain
21	AA	157	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	159	G	Sidechain
21	AA	166	U	Sidechain
21	AA	180	U	Sidechain
21	AA	187	G	Sidechain
21	AA	191	G	Sidechain
21	AA	195	A	Sidechain
21	AA	196	A	Sidechain
21	AA	197	A	Sidechain
21	AA	198	G	Sidechain
21	AA	200	G	Sidechain
21	AA	215	C	Sidechain
21	AA	228	A	Sidechain
21	AA	232	G	Sidechain
21	AA	235	C	Sidechain
21	AA	237	G	Sidechain
21	AA	242	G	Sidechain
21	AA	246	A	Sidechain
21	AA	25	C	Sidechain
21	AA	250	A	Sidechain
21	AA	252	U	Sidechain
21	AA	255	G	Sidechain
21	AA	258	G	Sidechain
21	AA	259	G	Sidechain
21	AA	26	A	Sidechain
21	AA	262	A	Sidechain
21	AA	266	G	Sidechain
21	AA	269	C	Sidechain
21	AA	270	A	Sidechain
21	AA	280	C	Sidechain
21	AA	281	G	Sidechain
21	AA	288	A	Sidechain
21	AA	29	U	Sidechain
21	AA	290	C	Sidechain
21	AA	297	G	Sidechain
21	AA	31	G	Sidechain
21	AA	310	G	Sidechain
21	AA	316	C	Sidechain
21	AA	318	G	Sidechain
21	AA	319	G	Sidechain
21	AA	321	A	Sidechain
21	AA	323	U	Sidechain
21	AA	324	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	325	A	Sidechain
21	AA	327	A	Sidechain
21	AA	328	C	Sidechain
21	AA	330	C	Sidechain
21	AA	333	U	Sidechain
21	AA	334	C	Sidechain
21	AA	337	G	Sidechain
21	AA	342	C	Sidechain
21	AA	349	A	Sidechain
21	AA	35	G	Sidechain
21	AA	353	A	Sidechain
21	AA	355	C	Sidechain
21	AA	36	C	Sidechain
21	AA	362	G	Sidechain
21	AA	365	U	Sidechain
21	AA	37	U	Sidechain
21	AA	371	A	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	383	A	Sidechain
21	AA	384	G	Sidechain
21	AA	385	C	Sidechain
21	AA	39	G	Sidechain
21	AA	391	G	Sidechain
21	AA	394	G	Sidechain
21	AA	395	C	Sidechain
21	AA	401	C	Sidechain
21	AA	405	U	Sidechain
21	AA	408	A	Sidechain
21	AA	409	U	Sidechain
21	AA	412	A	Sidechain
21	AA	416	G	Sidechain
21	AA	429	U	Sidechain
21	AA	432	A	Sidechain
21	AA	433	G	Sidechain
21	AA	435	A	Sidechain
21	AA	439	U	Sidechain
21	AA	448	A	Sidechain
21	AA	449	G	Sidechain
21	AA	455	G	Sidechain
21	AA	461	A	Sidechain
21	AA	464	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	465	A	Sidechain
21	AA	468	A	Sidechain
21	AA	470	C	Sidechain
21	AA	474	G	Sidechain
21	AA	475	C	Sidechain
21	AA	476	U	Sidechain
21	AA	478	A	Sidechain
21	AA	479	U	Sidechain
21	AA	484	G	Sidechain
21	AA	487	A	Sidechain
21	AA	491	G	Sidechain
21	AA	492	C	Sidechain
21	AA	494	G	Sidechain
21	AA	496	A	Sidechain
21	AA	5	U	Sidechain
21	AA	51	A	Sidechain
21	AA	511	C	Sidechain
21	AA	515	G	Sidechain
21	AA	518	C	Sidechain
21	AA	529	G	Sidechain
21	AA	535	A	Sidechain
21	AA	537	G	Sidechain
21	AA	538	G	Sidechain
21	AA	54	C	Sidechain
21	AA	555	U	Sidechain
21	AA	558	G	Sidechain
21	AA	561	U	Sidechain
21	AA	566	G	Sidechain
21	AA	571	U	Sidechain
21	AA	579	A	Sidechain
21	AA	581	G	Sidechain
21	AA	584	G	Sidechain
21	AA	587	G	Sidechain
21	AA	588	G	Sidechain
21	AA	595	A	Sidechain
21	AA	599	C	Sidechain
21	AA	601	G	Sidechain
21	AA	602	A	Sidechain
21	AA	61	G	Sidechain
21	AA	610	U	Sidechain
21	AA	614	C	Sidechain
21	AA	618	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	622	A	Sidechain
21	AA	625	U	Sidechain
21	AA	63	C	Sidechain
21	AA	631	C	Sidechain
21	AA	632	U	Sidechain
21	AA	640	A	Sidechain
21	AA	649	A	Sidechain
21	AA	650	G	Sidechain
21	AA	651	C	Sidechain
21	AA	656	G	Sidechain
21	AA	664	G	Sidechain
21	AA	668	G	Sidechain
21	AA	67	C	Sidechain
21	AA	670	G	Sidechain
21	AA	676	A	Sidechain
21	AA	678	U	Sidechain
21	AA	681	A	Sidechain
21	AA	687	A	Sidechain
21	AA	692	U	Sidechain
21	AA	693	G	Sidechain
21	AA	695	A	Sidechain
21	AA	706	A	Sidechain
21	AA	71	A	Sidechain
21	AA	710	G	Sidechain
21	AA	716	A	Sidechain
21	AA	717	U	Sidechain
21	AA	719	C	Sidechain
21	AA	721	G	Sidechain
21	AA	722	G	Sidechain
21	AA	723	U	Sidechain
21	AA	725	G	Sidechain
21	AA	727	G	Sidechain
21	AA	728	A	Sidechain
21	AA	731	G	Sidechain
21	AA	732	C	Sidechain
21	AA	735	C	Sidechain
21	AA	740	U	Sidechain
21	AA	752	G	Sidechain
21	AA	753	A	Sidechain
21	AA	754	C	Sidechain
21	AA	755	G	Sidechain
21	AA	760	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	761	G	Sidechain
21	AA	766	A	Sidechain
21	AA	768	A	Sidechain
21	AA	776	G	Sidechain
21	AA	780	A	Sidechain
21	AA	781	A	Sidechain
21	AA	785	G	Sidechain
21	AA	79	G	Sidechain
21	AA	790	A	Sidechain
21	AA	801	U	Sidechain
21	AA	807	A	Sidechain
21	AA	808	C	Sidechain
21	AA	816	A	Sidechain
21	AA	819	A	Sidechain
21	AA	82	G	Sidechain
21	AA	821	G	Sidechain
21	AA	824	G	Sidechain
21	AA	840	C	Sidechain
21	AA	842	U	Sidechain
21	AA	843	U	Sidechain
21	AA	844	G	Sidechain
21	AA	859	G	Sidechain
21	AA	86	G	Sidechain
21	AA	863	U	Sidechain
21	AA	866	C	Sidechain
21	AA	869	G	Sidechain
21	AA	871	U	Sidechain
21	AA	873	A	Sidechain
21	AA	874	G	Sidechain
21	AA	875	U	Sidechain
21	AA	876	C	Sidechain
21	AA	880	C	Sidechain
21	AA	883	C	Sidechain
21	AA	884	U	Sidechain
21	AA	896	C	Sidechain
21	AA	898	G	Sidechain
21	AA	90	C	Sidechain
21	AA	900	A	Sidechain
21	AA	901	A	Sidechain
21	AA	903	G	Sidechain
21	AA	91	U	Sidechain
21	AA	918	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	919	A	Sidechain
21	AA	92	U	Sidechain
21	AA	921	U	Sidechain
21	AA	922	G	Sidechain
21	AA	923	A	Sidechain
21	AA	925	G	Sidechain
21	AA	926	G	Sidechain
21	AA	928	G	Sidechain
21	AA	932	C	Sidechain
21	AA	935	A	Sidechain
21	AA	940	C	Sidechain
21	AA	941	G	Sidechain
21	AA	942	G	Sidechain
21	AA	945	G	Sidechain
21	AA	947	G	Sidechain
21	AA	948	C	Sidechain
21	AA	949	A	Sidechain
21	AA	951	G	Sidechain
21	AA	954	G	Sidechain
21	AA	959	A	Sidechain
21	AA	964	A	Sidechain
21	AA	968	A	Sidechain
21	AA	97	G	Sidechain
21	AA	972	C	Sidechain
21	AA	982	U	Sidechain
21	AA	984	C	Sidechain
21	AA	985	C	Sidechain
21	AA	99	C	Sidechain
21	AA	991	U	Sidechain
21	AA	993	G	Sidechain
21	AA	995	C	Sidechain
21	AA	998	C	Sidechain
21	AA	999	C	Sidechain
3	AD	75	TYR	Sidechain
10	AK	127	ARG	Sidechain
54	BA	1003	G	Sidechain
54	BA	1007	C	Sidechain
54	BA	101	A	Sidechain
54	BA	1016	G	Sidechain
54	BA	1023	U	Sidechain
54	BA	1024	G	Sidechain
54	BA	1055	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	106	C	Sidechain
54	BA	1062	G	Sidechain
54	BA	1072	C	Sidechain
54	BA	1076	C	Sidechain
54	BA	1078	U	Sidechain
54	BA	1083	U	Sidechain
54	BA	109	C	Sidechain
54	BA	1106	G	Sidechain
54	BA	1112	G	Sidechain
54	BA	1114	C	Sidechain
54	BA	1118	C	Sidechain
54	BA	1124	G	Sidechain
54	BA	1125	G	Sidechain
54	BA	113	U	Sidechain
54	BA	1133	A	Sidechain
54	BA	1135	C	Sidechain
54	BA	1139	G	Sidechain
54	BA	1140	C	Sidechain
54	BA	1141	U	Sidechain
54	BA	1144	A	Sidechain
54	BA	1150	C	Sidechain
54	BA	1151	A	Sidechain
54	BA	1153	C	Sidechain
54	BA	1158	C	Sidechain
54	BA	1159	U	Sidechain
54	BA	116	C	Sidechain
54	BA	1162	G	Sidechain
54	BA	1167	C	Sidechain
54	BA	1170	C	Sidechain
54	BA	1174	U	Sidechain
54	BA	1178	C	Sidechain
54	BA	1182	G	Sidechain
54	BA	1189	A	Sidechain
54	BA	1200	C	Sidechain
54	BA	1201	U	Sidechain
54	BA	1215	G	Sidechain
54	BA	1220	G	Sidechain
54	BA	1227	G	Sidechain
54	BA	1233	C	Sidechain
54	BA	1234	U	Sidechain
54	BA	1235	G	Sidechain
54	BA	1241	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1242	U	Sidechain
54	BA	1244	A	Sidechain
54	BA	1248	G	Sidechain
54	BA	125	A	Sidechain
54	BA	1250	G	Sidechain
54	BA	1251	C	Sidechain
54	BA	1254	A	Sidechain
54	BA	1263	U	Sidechain
54	BA	1264	A	Sidechain
54	BA	1270	C	Sidechain
54	BA	1275	A	Sidechain
54	BA	1277	G	Sidechain
54	BA	1288	G	Sidechain
54	BA	1289	C	Sidechain
54	BA	1291	C	Sidechain
54	BA	1299	G	Sidechain
54	BA	1303	G	Sidechain
54	BA	1304	A	Sidechain
54	BA	1311	G	Sidechain
54	BA	1315	C	Sidechain
54	BA	1316	U	Sidechain
54	BA	1319	C	Sidechain
54	BA	1320	C	Sidechain
54	BA	1323	C	Sidechain
54	BA	1328	A	Sidechain
54	BA	1330	C	Sidechain
54	BA	1331	G	Sidechain
54	BA	1333	G	Sidechain
54	BA	134	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1341	G	Sidechain
54	BA	1343	G	Sidechain
54	BA	1346	G	Sidechain
54	BA	1347	A	Sidechain
54	BA	1356	G	Sidechain
54	BA	1359	A	Sidechain
54	BA	1371	G	Sidechain
54	BA	1372	U	Sidechain
54	BA	138	U	Sidechain
54	BA	1386	C	Sidechain
54	BA	1387	A	Sidechain
54	BA	1389	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1398	C	Sidechain
54	BA	1399	C	Sidechain
54	BA	1411	U	Sidechain
54	BA	1418	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1428	C	Sidechain
54	BA	1433	A	Sidechain
54	BA	1438	U	Sidechain
54	BA	1443	U	Sidechain
54	BA	1444	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1451	C	Sidechain
54	BA	1454	C	Sidechain
54	BA	1455	G	Sidechain
54	BA	1457	U	Sidechain
54	BA	1460	U	Sidechain
54	BA	1468	U	Sidechain
54	BA	1476	U	Sidechain
54	BA	1478	G	Sidechain
54	BA	1488	C	Sidechain
54	BA	1490	A	Sidechain
54	BA	1492	G	Sidechain
54	BA	1494	A	Sidechain
54	BA	1497	U	Sidechain
54	BA	150	U	Sidechain
54	BA	1513	U	Sidechain
54	BA	1517	G	Sidechain
54	BA	1527	G	Sidechain
54	BA	1529	G	Sidechain
54	BA	1536	C	Sidechain
54	BA	1538	G	Sidechain
54	BA	1539	U	Sidechain
54	BA	1543	G	Sidechain
54	BA	1547	C	Sidechain
54	BA	1549	A	Sidechain
54	BA	1552	A	Sidechain
54	BA	1558	C	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1564	C	Sidechain
54	BA	1565	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1566	A	Sidechain
54	BA	1573	G	Sidechain
54	BA	1581	G	Sidechain
54	BA	159	G	Sidechain
54	BA	1602	U	Sidechain
54	BA	1606	C	Sidechain
54	BA	1610	A	Sidechain
54	BA	1612	C	Sidechain
54	BA	1615	C	Sidechain
54	BA	1617	C	Sidechain
54	BA	1618	A	Sidechain
54	BA	162	U	Sidechain
54	BA	1631	G	Sidechain
54	BA	164	C	Sidechain
54	BA	1642	G	Sidechain
54	BA	1647	U	Sidechain
54	BA	1649	G	Sidechain
54	BA	1653	G	Sidechain
54	BA	1654	A	Sidechain
54	BA	1658	C	Sidechain
54	BA	1676	A	Sidechain
54	BA	1677	A	Sidechain
54	BA	1680	U	Sidechain
54	BA	1682	G	Sidechain
54	BA	1684	G	Sidechain
54	BA	1697	G	Sidechain
54	BA	1699	G	Sidechain
54	BA	17	G	Sidechain
54	BA	1706	C	Sidechain
54	BA	1709	U	Sidechain
54	BA	171	U	Sidechain
54	BA	1710	G	Sidechain
54	BA	1715	G	Sidechain
54	BA	1716	U	Sidechain
54	BA	1722	A	Sidechain
54	BA	1723	G	Sidechain
54	BA	1731	G	Sidechain
54	BA	1734	G	Sidechain
54	BA	174	U	Sidechain
54	BA	1744	A	Sidechain
54	BA	1748	C	Sidechain
54	BA	175	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1750	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1759	A	Sidechain
54	BA	1761	C	Sidechain
54	BA	1762	A	Sidechain
54	BA	1763	G	Sidechain
54	BA	1777	U	Sidechain
54	BA	1780	A	Sidechain
54	BA	1781	U	Sidechain
54	BA	1783	A	Sidechain
54	BA	1786	A	Sidechain
54	BA	1796	U	Sidechain
54	BA	1797	G	Sidechain
54	BA	1799	G	Sidechain
54	BA	1800	C	Sidechain
54	BA	1807	G	Sidechain
54	BA	1817	G	Sidechain
54	BA	1818	U	Sidechain
54	BA	1821	A	Sidechain
54	BA	1825	U	Sidechain
54	BA	1826	G	Sidechain
54	BA	1827	U	Sidechain
54	BA	1830	C	Sidechain
54	BA	1831	G	Sidechain
54	BA	1833	C	Sidechain
54	BA	1840	G	Sidechain
54	BA	1842	G	Sidechain
54	BA	1843	C	Sidechain
54	BA	1845	G	Sidechain
54	BA	1848	A	Sidechain
54	BA	1849	G	Sidechain
54	BA	1851	U	Sidechain
54	BA	1854	A	Sidechain
54	BA	1859	U	Sidechain
54	BA	1861	G	Sidechain
54	BA	1865	U	Sidechain
54	BA	1876	A	Sidechain
54	BA	1881	C	Sidechain
54	BA	1884	G	Sidechain
54	BA	1892	C	Sidechain
54	BA	19	A	Sidechain
54	BA	1903	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1906	G	Sidechain
54	BA	1907	G	Sidechain
54	BA	1917	U	Sidechain
54	BA	1924	C	Sidechain
54	BA	1926	U	Sidechain
54	BA	1929	G	Sidechain
54	BA	1931	U	Sidechain
54	BA	1938	A	Sidechain
54	BA	1945	G	Sidechain
54	BA	1949	G	Sidechain
54	BA	1951	U	Sidechain
54	BA	1954	G	Sidechain
54	BA	1959	G	Sidechain
54	BA	1973	G	Sidechain
54	BA	1981	A	Sidechain
54	BA	1983	G	Sidechain
54	BA	1985	C	Sidechain
54	BA	1993	U	Sidechain
54	BA	1995	U	Sidechain
54	BA	1996	C	Sidechain
54	BA	20	C	Sidechain
54	BA	200	U	Sidechain
54	BA	2001	C	Sidechain
54	BA	2013	A	Sidechain
54	BA	2014	A	Sidechain
54	BA	2017	U	Sidechain
54	BA	2019	A	Sidechain
54	BA	2027	G	Sidechain
54	BA	2028	U	Sidechain
54	BA	2030	A	Sidechain
54	BA	2032	G	Sidechain
54	BA	2036	C	Sidechain
54	BA	2037	A	Sidechain
54	BA	2038	G	Sidechain
54	BA	2039	U	Sidechain
54	BA	2042	A	Sidechain
54	BA	2047	C	Sidechain
54	BA	2048	G	Sidechain
54	BA	206	U	Sidechain
54	BA	2065	C	Sidechain
54	BA	2071	A	Sidechain
54	BA	2075	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2077	A	Sidechain
54	BA	2078	C	Sidechain
54	BA	2079	U	Sidechain
54	BA	2094	A	Sidechain
54	BA	2095	A	Sidechain
54	BA	21	A	Sidechain
54	BA	2100	G	Sidechain
54	BA	2102	G	Sidechain
54	BA	2120	G	Sidechain
54	BA	2121	G	Sidechain
54	BA	2128	G	Sidechain
54	BA	2130	U	Sidechain
54	BA	2132	U	Sidechain
54	BA	2133	G	Sidechain
54	BA	2140	G	Sidechain
54	BA	2141	G	Sidechain
54	BA	2146	C	Sidechain
54	BA	2148	G	Sidechain
54	BA	2159	G	Sidechain
54	BA	2161	C	Sidechain
54	BA	2162	G	Sidechain
54	BA	2168	G	Sidechain
54	BA	2179	C	Sidechain
54	BA	2186	G	Sidechain
54	BA	2190	G	Sidechain
54	BA	221	A	Sidechain
54	BA	2215	C	Sidechain
54	BA	2220	U	Sidechain
54	BA	2230	G	Sidechain
54	BA	2234	G	Sidechain
54	BA	2238	G	Sidechain
54	BA	224	U	Sidechain
54	BA	2242	G	Sidechain
54	BA	2244	U	Sidechain
54	BA	2250	G	Sidechain
54	BA	2253	G	Sidechain
54	BA	2256	G	Sidechain
54	BA	2267	A	Sidechain
54	BA	2269	G	Sidechain
54	BA	227	A	Sidechain
54	BA	2273	A	Sidechain
54	BA	2279	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	228	C	Sidechain
54	BA	2282	G	Sidechain
54	BA	2287	A	Sidechain
54	BA	2293	G	Sidechain
54	BA	2294	G	Sidechain
54	BA	2295	C	Sidechain
54	BA	2299	U	Sidechain
54	BA	2307	G	Sidechain
54	BA	2311	A	Sidechain
54	BA	2319	G	Sidechain
54	BA	232	G	Sidechain
54	BA	2327	A	Sidechain
54	BA	2331	G	Sidechain
54	BA	2332	C	Sidechain
54	BA	2336	A	Sidechain
54	BA	235	U	Sidechain
54	BA	2352	A	Sidechain
54	BA	2357	G	Sidechain
54	BA	2361	G	Sidechain
54	BA	2369	A	Sidechain
54	BA	2375	G	Sidechain
54	BA	238	C	Sidechain
54	BA	2391	G	Sidechain
54	BA	2392	A	Sidechain
54	BA	2394	C	Sidechain
54	BA	2396	G	Sidechain
54	BA	2398	U	Sidechain
54	BA	24	G	Sidechain
54	BA	2401	U	Sidechain
54	BA	2406	A	Sidechain
54	BA	2407	A	Sidechain
54	BA	2411	A	Sidechain
54	BA	2419	U	Sidechain
54	BA	2420	C	Sidechain
54	BA	2421	G	Sidechain
54	BA	2429	G	Sidechain
54	BA	2430	A	Sidechain
54	BA	2436	G	Sidechain
54	BA	244	A	Sidechain
54	BA	2445	G	Sidechain
54	BA	2446	G	Sidechain
54	BA	2450	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2451	A	Sidechain
54	BA	2452	C	Sidechain
54	BA	2454	G	Sidechain
54	BA	2468	A	Sidechain
54	BA	2470	G	Sidechain
54	BA	2476	A	Sidechain
54	BA	2482	A	Sidechain
54	BA	2488	G	Sidechain
54	BA	2489	U	Sidechain
54	BA	2490	G	Sidechain
54	BA	2492	U	Sidechain
54	BA	2495	G	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2505	G	Sidechain
54	BA	2508	G	Sidechain
54	BA	2516	A	Sidechain
54	BA	2518	A	Sidechain
54	BA	252	G	Sidechain
54	BA	2525	G	Sidechain
54	BA	2527	C	Sidechain
54	BA	2528	U	Sidechain
54	BA	2529	G	Sidechain
54	BA	2547	A	Sidechain
54	BA	2549	G	Sidechain
54	BA	2560	A	Sidechain
54	BA	2563	U	Sidechain
54	BA	2576	G	Sidechain
54	BA	2581	G	Sidechain
54	BA	2583	G	Sidechain
54	BA	2586	U	Sidechain
54	BA	2595	G	Sidechain
54	BA	2596	U	Sidechain
54	BA	26	G	Sidechain
54	BA	2600	A	Sidechain
54	BA	2606	C	Sidechain
54	BA	2608	G	Sidechain
54	BA	2614	A	Sidechain
54	BA	2615	U	Sidechain
54	BA	2621	G	Sidechain
54	BA	2624	G	Sidechain
54	BA	2625	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2627	G	Sidechain
54	BA	2628	C	Sidechain
54	BA	2635	A	Sidechain
54	BA	2639	A	Sidechain
54	BA	2640	G	Sidechain
54	BA	2645	G	Sidechain
54	BA	2649	C	Sidechain
54	BA	2651	C	Sidechain
54	BA	2661	G	Sidechain
54	BA	2668	G	Sidechain
54	BA	2683	C	Sidechain
54	BA	2689	U	Sidechain
54	BA	2692	G	Sidechain
54	BA	2711	A	Sidechain
54	BA	2713	U	Sidechain
54	BA	2716	C	Sidechain
54	BA	2718	G	Sidechain
54	BA	272	A	Sidechain
54	BA	273	G	Sidechain
54	BA	2730	C	Sidechain
54	BA	2738	A	Sidechain
54	BA	274	C	Sidechain
54	BA	2741	A	Sidechain
54	BA	2743	U	Sidechain
54	BA	2755	C	Sidechain
54	BA	2765	A	Sidechain
54	BA	2768	U	Sidechain
54	BA	277	G	Sidechain
54	BA	2771	C	Sidechain
54	BA	2773	C	Sidechain
54	BA	2777	G	Sidechain
54	BA	278	A	Sidechain
54	BA	2783	U	Sidechain
54	BA	2784	U	Sidechain
54	BA	2785	C	Sidechain
54	BA	28	A	Sidechain
54	BA	2803	G	Sidechain
54	BA	2804	U	Sidechain
54	BA	2805	C	Sidechain
54	BA	2806	C	Sidechain
54	BA	2811	G	Sidechain
54	BA	2817	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2821	A	Sidechain
54	BA	2822	G	Sidechain
54	BA	283	G	Sidechain
54	BA	2839	G	Sidechain
54	BA	2841	C	Sidechain
54	BA	2850	A	Sidechain
54	BA	2854	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2859	G	Sidechain
54	BA	2862	G	Sidechain
54	BA	2867	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	2871	U	Sidechain
54	BA	2872	A	Sidechain
54	BA	2873	A	Sidechain
54	BA	2877	G	Sidechain
54	BA	2883	A	Sidechain
54	BA	289	G	Sidechain
54	BA	2891	U	Sidechain
54	BA	2892	G	Sidechain
54	BA	2897	U	Sidechain
54	BA	297	G	Sidechain
54	BA	298	G	Sidechain
54	BA	3	U	Sidechain
54	BA	303	G	Sidechain
54	BA	307	G	Sidechain
54	BA	310	A	Sidechain
54	BA	313	G	Sidechain
54	BA	319	G	Sidechain
54	BA	323	C	Sidechain
54	BA	327	G	Sidechain
54	BA	331	C	Sidechain
54	BA	332	A	Sidechain
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	339	U	Sidechain
54	BA	354	A	Sidechain
54	BA	357	C	Sidechain
54	BA	360	U	Sidechain
54	BA	361	G	Sidechain
54	BA	363	G	Sidechain
54	BA	370	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	375	G	Sidechain
54	BA	382	A	Sidechain
54	BA	385	C	Sidechain
54	BA	386	G	Sidechain
54	BA	39	G	Sidechain
54	BA	391	A	Sidechain
54	BA	392	U	Sidechain
54	BA	394	C	Sidechain
54	BA	397	U	Sidechain
54	BA	403	U	Sidechain
54	BA	409	G	Sidechain
54	BA	410	G	Sidechain
54	BA	418	C	Sidechain
54	BA	420	C	Sidechain
54	BA	430	A	Sidechain
54	BA	431	U	Sidechain
54	BA	433	C	Sidechain
54	BA	437	U	Sidechain
54	BA	445	C	Sidechain
54	BA	446	G	Sidechain
54	BA	457	A	Sidechain
54	BA	458	G	Sidechain
54	BA	463	G	Sidechain
54	BA	47	C	Sidechain
54	BA	471	A	Sidechain
54	BA	472	A	Sidechain
54	BA	473	G	Sidechain
54	BA	477	A	Sidechain
54	BA	479	A	Sidechain
54	BA	481	G	Sidechain
54	BA	485	C	Sidechain
54	BA	489	G	Sidechain
54	BA	49	A	Sidechain
54	BA	491	G	Sidechain
54	BA	492	A	Sidechain
54	BA	493	G	Sidechain
54	BA	502	A	Sidechain
54	BA	507	A	Sidechain
54	BA	508	A	Sidechain
54	BA	515	A	Sidechain
54	BA	518	G	Sidechain
54	BA	522	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	527	C	Sidechain
54	BA	537	G	Sidechain
54	BA	551	G	Sidechain
54	BA	559	G	Sidechain
54	BA	560	C	Sidechain
54	BA	569	U	Sidechain
54	BA	575	A	Sidechain
54	BA	578	G	Sidechain
54	BA	580	U	Sidechain
54	BA	587	C	Sidechain
54	BA	589	U	Sidechain
54	BA	595	C	Sidechain
54	BA	597	G	Sidechain
54	BA	601	C	Sidechain
54	BA	603	A	Sidechain
54	BA	606	U	Sidechain
54	BA	607	U	Sidechain
54	BA	611	C	Sidechain
54	BA	617	G	Sidechain
54	BA	629	G	Sidechain
54	BA	630	G	Sidechain
54	BA	631	A	Sidechain
54	BA	640	C	Sidechain
54	BA	641	U	Sidechain
54	BA	647	G	Sidechain
54	BA	648	G	Sidechain
54	BA	65	U	Sidechain
54	BA	650	C	Sidechain
54	BA	662	G	Sidechain
54	BA	669	G	Sidechain
54	BA	671	C	Sidechain
54	BA	674	G	Sidechain
54	BA	68	G	Sidechain
54	BA	692	C	Sidechain
54	BA	695	G	Sidechain
54	BA	7	G	Sidechain
54	BA	700	G	Sidechain
54	BA	715	A	Sidechain
54	BA	718	A	Sidechain
54	BA	72	U	Sidechain
54	BA	724	U	Sidechain
54	BA	726	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	736	C	Sidechain
54	BA	738	G	Sidechain
54	BA	74	A	Sidechain
54	BA	749	A	Sidechain
54	BA	751	A	Sidechain
54	BA	753	A	Sidechain
54	BA	754	U	Sidechain
54	BA	759	G	Sidechain
54	BA	768	G	Sidechain
54	BA	77	G	Sidechain
54	BA	776	G	Sidechain
54	BA	777	G	Sidechain
54	BA	780	G	Sidechain
54	BA	787	C	Sidechain
54	BA	789	A	Sidechain
54	BA	790	U	Sidechain
54	BA	793	A	Sidechain
54	BA	795	C	Sidechain
54	BA	802	A	Sidechain
54	BA	808	G	Sidechain
54	BA	81	G	Sidechain
54	BA	817	C	Sidechain
54	BA	819	A	Sidechain
54	BA	821	A	Sidechain
54	BA	822	G	Sidechain
54	BA	825	A	Sidechain
54	BA	827	U	Sidechain
54	BA	828	U	Sidechain
54	BA	829	A	Sidechain
54	BA	830	G	Sidechain
54	BA	838	C	Sidechain
54	BA	848	C	Sidechain
54	BA	849	A	Sidechain
54	BA	85	G	Sidechain
54	BA	852	U	Sidechain
54	BA	855	G	Sidechain
54	BA	859	G	Sidechain
54	BA	861	A	Sidechain
54	BA	863	A	Sidechain
54	BA	866	A	Sidechain
54	BA	872	U	Sidechain
54	BA	880	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	893	C	Sidechain
54	BA	902	C	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	917	A	Sidechain
54	BA	918	A	Sidechain
54	BA	923	G	Sidechain
54	BA	930	G	Sidechain
54	BA	931	U	Sidechain
54	BA	936	A	Sidechain
54	BA	940	G	Sidechain
54	BA	946	C	Sidechain
54	BA	949	G	Sidechain
54	BA	951	C	Sidechain
54	BA	954	G	Sidechain
54	BA	959	A	Sidechain
54	BA	960	A	Sidechain
54	BA	964	C	Sidechain
54	BA	965	C	Sidechain
54	BA	966	G	Sidechain
54	BA	972	A	Sidechain
54	BA	979	A	Sidechain
54	BA	981	A	Sidechain
54	BA	983	A	Sidechain
54	BA	984	A	Sidechain
54	BA	987	C	Sidechain
54	BA	989	G	Sidechain
54	BA	990	A	Sidechain
55	BB	10	G	Sidechain
55	BB	100	G	Sidechain
55	BB	109	A	Sidechain
55	BB	11	C	Sidechain
55	BB	112	G	Sidechain
55	BB	117	G	Sidechain
55	BB	12	C	Sidechain
55	BB	2	G	Sidechain
55	BB	23	G	Sidechain
55	BB	30	C	Sidechain
55	BB	33	G	Sidechain
55	BB	4	C	Sidechain
55	BB	40	U	Sidechain
55	BB	48	U	Sidechain

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Mol	Chain	Res	Type	Group
55	BB	57	A	Sidechain
55	BB	58	A	Sidechain
55	BB	59	A	Sidechain
55	BB	6	G	Sidechain
55	BB	63	C	Sidechain
55	BB	64	G	Sidechain
55	BB	66	A	Sidechain
55	BB	67	G	Sidechain
55	BB	68	C	Sidechain
55	BB	69	G	Sidechain
55	BB	7	G	Sidechain
55	BB	72	G	Sidechain
55	BB	84	G	Sidechain
55	BB	90	C	Sidechain
55	BB	95	U	Sidechain
55	BB	98	G	Sidechain
25	BC	102	TYR	Sidechain
26	BD	151	THR	Peptide
31	BI	140	GLU	Mainchain
35	BM	97	GLN	Peptide
36	BN	90	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	1	0
3	AD	1643	0	1710	1	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	1	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	1	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16457	2	0
22	A1	1627	0	832	1	0
23	A2	309	0	158	0	0
24	A3	1642	0	839	0	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	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31205	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BB	2504	0	1269	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99454	17	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 (17) 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)
54:BA:1068:G:H1'	54:BA:1069:A:C6	2.45	0.51
54:BA:1131:G:C5	54:BA:2025:C:H4'	2.50	0.46
22:A1:53:G:C8	22:A1:54:5MU:H72	2.50	0.46
18:AS:46:LEU:HD23	18:AS:46:LEU:H	1.81	0.46
3:AD:86:GLY:H	3:AD:200:VAL:HG23	1.81	0.45
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.82	0.45
8:AI:2:ACE:H1	8:AI:22:PRO:HG2	2.00	0.44
21:AA:477:C:H2'	21:AA:478:A:C8	2.53	0.43
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.37	0.43
21:AA:315:A:HO2'	21:AA:316:C:P	2.42	0.42
54:BA:1801:A:H3'	54:BA:1802:A:C5'	2.49	0.42
54:BA:1132:U:H2'	54:BA:1133:A:C8	2.55	0.42
54:BA:2233:U:H2'	54:BA:2234:G:C8	2.55	0.42
54:BA:1891:G:H2'	54:BA:1892:C:C6	2.55	0.41
2:AC:54:ILE:HG22	2:AC:68:HIS:H	1.86	0.41
54:BA:2014:A:H2'	54:BA:2015:A:C8	2.57	0.40
54:BA:2063:C:H2'	54:BA:2064:C:C6	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	200 (92%)	15 (7%)	3 (1%)	14	58
2	AC	205/208 (99%)	188 (92%)	12 (6%)	5 (2%)	7	47
3	AD	203/206 (98%)	190 (94%)	7 (3%)	6 (3%)	5	42
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	9	51
5	AF	99/101 (98%)	83 (84%)	12 (12%)	4 (4%)	4	35
6	AG	150/152 (99%)	133 (89%)	14 (9%)	3 (2%)	9	51
7	AH	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
8	AI	126/128 (98%)	117 (93%)	6 (5%)	3 (2%)	7	47
9	AJ	98/100 (98%)	87 (89%)	6 (6%)	5 (5%)	2	30
10	AK	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	11	55
11	AL	121/124 (98%)	109 (90%)	8 (7%)	4 (3%)	5	40
12	AM	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
13	AN	98/101 (97%)	86 (88%)	9 (9%)	3 (3%)	5	42
14	AO	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	8	48
15	AP	79/81 (98%)	64 (81%)	9 (11%)	6 (8%)	1	20
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	15	60
17	AR	55/57 (96%)	51 (93%)	3 (6%)	1 (2%)	11	53
18	AS	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	15	60
19	AT	84/86 (98%)	75 (89%)	5 (6%)	4 (5%)	3	32
20	AU	51/53 (96%)	34 (67%)	13 (26%)	4 (8%)	1	20
25	BC	270/273 (99%)	241 (89%)	21 (8%)	8 (3%)	5	42
26	BD	207/209 (99%)	181 (87%)	18 (9%)	8 (4%)	4	36
27	BE	199/201 (99%)	172 (86%)	18 (9%)	9 (4%)	3	33
28	BF	176/179 (98%)	151 (86%)	20 (11%)	5 (3%)	6	44
29	BG	174/177 (98%)	151 (87%)	16 (9%)	7 (4%)	4	35
30	BH	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	14	58
31	BI	139/142 (98%)	128 (92%)	10 (7%)	1 (1%)	26	71
32	BJ	140/142 (99%)	123 (88%)	14 (10%)	3 (2%)	9	50
33	BK	121/123 (98%)	104 (86%)	13 (11%)	4 (3%)	5	40
34	BL	141/144 (98%)	110 (78%)	23 (16%)	8 (6%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BM	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	8	49
36	BN	119/121 (98%)	102 (86%)	16 (13%)	1 (1%)	24	69
37	BO	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
38	BP	112/115 (97%)	96 (86%)	12 (11%)	4 (4%)	4	38
39	BQ	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	21	67
40	BR	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
41	BS	108/110 (98%)	95 (88%)	12 (11%)	1 (1%)	21	67
42	BT	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	8	49
43	BU	101/104 (97%)	83 (82%)	13 (13%)	5 (5%)	3	31
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	63 (81%)	11 (14%)	4 (5%)	2	30
46	BX	75/79 (95%)	68 (91%)	5 (7%)	2 (3%)	6	45
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	50 (89%)	3 (5%)	3 (5%)	2	29
49	B0	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	4	38
50	B1	50/52 (96%)	42 (84%)	4 (8%)	4 (8%)	1	19
51	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8	48
52	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	5	41
53	B4	36/38 (95%)	27 (75%)	8 (22%)	1 (3%)	6	44
56	B5	221/234 (94%)	207 (94%)	11 (5%)	3 (1%)	14	58
All	All	5876/6008 (98%)	5232 (89%)	490 (8%)	154 (3%)	11	45

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	73	ARG
2	AC	14	VAL
3	AD	82	LYS
9	AJ	77	VAL
15	AP	79	ASN
19	AT	3	ILE
20	AU	25	ALA
25	BC	141	HIS
32	BJ	48	VAL
32	BJ	81	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	BP	113	LEU
43	BU	45	GLN
43	BU	70	ALA
45	BW	36	ILE
52	B3	3	ILE
56	B5	50	ILE
1	AB	20	ARG
2	AC	180	ASP
3	AD	194	ILE
4	AE	105	ILE
5	AF	6	ILE
5	AF	63	ASN
6	AG	6	ILE
8	AI	55	ASP
9	AJ	57	VAL
9	AJ	58	ASN
11	AL	15	VAL
13	AN	38	ASP
14	AO	45	HIS
18	AS	2	ARG
20	AU	9	GLU
20	AU	27	VAL
25	BC	68	ARG
25	BC	161	VAL
26	BD	60	VAL
26	BD	146	ILE
27	BE	9	GLN
27	BE	69	ARG
28	BF	12	VAL
28	BF	136	ILE
30	BH	9	VAL
30	BH	121	VAL
31	BI	119	ALA
33	BK	103	VAL
34	BL	33	ARG
34	BL	101	ILE
35	BM	21	ALA
43	BU	12	VAL
46	BX	20	ALA
49	B0	5	ASN
2	AC	2	GLN
3	AD	4	LEU

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Mol	Chain	Res	Type
5	AF	8	PHE
5	AF	90	MET
6	AG	115	MET
9	AJ	75	ASP
11	AL	78	VAL
14	AO	23	SER
15	AP	9	HIS
15	AP	26	ASN
15	AP	50	THR
25	BC	89	ASN
25	BC	142	ASN
26	BD	51	THR
26	BD	119	ALA
26	BD	136	ASN
26	BD	151	THR
27	BE	97	ASN
27	BE	123	LYS
29	BG	151	ARG
33	BK	46	ALA
34	BL	17	LYS
35	BM	20	LEU
35	BM	36	VAL
46	BX	33	HIS
48	BZ	9	THR
50	B1	50	GLU
53	B4	2	LYS
56	B5	91	GLY
1	AB	204	ASP
2	AC	195	ILE
3	AD	29	THR
3	AD	193	ASP
4	AE	127	TYR
8	AI	39	GLY
11	AL	33	CYS
13	AN	92	GLU
15	AP	17	TYR
16	AQ	3	LYS
19	AT	2	ASN
20	AU	52	VAL
25	BC	37	SER
26	BD	22	ILE
27	BE	31	VAL

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Mol	Chain	Res	Type
27	BE	49	ARG
28	BF	123	GLY
28	BF	133	GLU
29	BG	154	GLU
29	BG	175	LYS
34	BL	28	GLY
34	BL	46	VAL
36	BN	70	THR
38	BP	24	THR
42	BT	73	ARG
45	BW	76	ARG
52	B3	46	LYS
4	AE	43	GLY
6	AG	9	ARG
10	AK	125	LYS
11	AL	43	LYS
15	AP	40	ASN
19	AT	67	HIS
27	BE	147	LEU
27	BE	188	MET
29	BG	9	VAL
29	BG	16	VAL
33	BK	2	ILE
34	BL	75	ALA
38	BP	112	ARG
39	BQ	86	SER
41	BS	88	ARG
42	BT	35	ALA
43	BU	90	LYS
45	BW	48	ALA
48	BZ	31	ILE
56	B5	42	VAL
2	AC	145	ALA
3	AD	28	ASP
8	AI	12	LYS
13	AN	63	ARG
19	AT	65	LEU
25	BC	191	LEU
28	BF	103	ILE
34	BL	36	LYS
45	BW	63	ASP
49	B0	54	ILE

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Mol	Chain	Res	Type
50	B1	4	ILE
50	B1	37	LYS
51	B2	44	VAL
10	AK	77	GLY
25	BC	230	PRO
34	BL	55	MET
9	AJ	42	LEU
17	AR	20	ILE
29	BG	168	VAL
32	BJ	11	VAL
43	BU	56	GLY
48	BZ	32	GLY
50	B1	46	VAL
26	BD	93	GLY
29	BG	112	VAL
33	BK	71	ARG
27	BE	169	VAL
38	BP	69	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%)	178 (99%)	2 (1%)	80	91
2	AC	170/171 (99%)	169 (99%)	1 (1%)	90	95
3	AD	172/173 (99%)	167 (97%)	5 (3%)	50	78
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	86 (99%)	1 (1%)	80	91
6	AG	123/123 (100%)	121 (98%)	2 (2%)	70	88
7	AH	104/105 (99%)	101 (97%)	3 (3%)	50	78
8	AI	105/105 (100%)	101 (96%)	4 (4%)	40	73
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	58	83
10	AK	90/90 (100%)	89 (99%)	1 (1%)	80	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	81 (98%)	2 (2%)	57	82
14	AO	76/77 (99%)	74 (97%)	2 (3%)	54	80
15	AP	65/65 (100%)	62 (95%)	3 (5%)	33	68
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	52	79
17	AR	48/48 (100%)	46 (96%)	2 (4%)	36	70
18	AS	70/70 (100%)	69 (99%)	1 (1%)	74	89
19	AT	65/65 (100%)	62 (95%)	3 (5%)	33	68
20	AU	44/44 (100%)	42 (96%)	2 (4%)	34	69
25	BC	216/217 (100%)	211 (98%)	5 (2%)	58	83
26	BD	164/164 (100%)	162 (99%)	2 (1%)	78	90
27	BE	165/165 (100%)	160 (97%)	5 (3%)	48	77
28	BF	149/150 (99%)	146 (98%)	3 (2%)	63	85
29	BG	137/138 (99%)	134 (98%)	3 (2%)	60	83
30	BH	114/114 (100%)	113 (99%)	1 (1%)	84	93
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	54	80
33	BK	103/103 (100%)	103 (100%)	0	100	100
34	BL	102/103 (99%)	100 (98%)	2 (2%)	63	85
35	BM	109/109 (100%)	108 (99%)	1 (1%)	84	93
36	BN	100/100 (100%)	97 (97%)	3 (3%)	48	77
37	BO	86/87 (99%)	82 (95%)	4 (5%)	32	68
38	BP	99/100 (99%)	95 (96%)	4 (4%)	38	71
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	60	83
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	92 (99%)	1 (1%)	80	91
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	57	82
44	BV	78/78 (100%)	77 (99%)	1 (1%)	76	89
45	BW	59/59 (100%)	58 (98%)	1 (2%)	68	87

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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%)	46 (96%)	2 (4%)	36	70
49	B0	47/48 (98%)	43 (92%)	4 (8%)	13	48
50	B1	45/45 (100%)	44 (98%)	1 (2%)	60	83
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	50 (98%)	1 (2%)	63	85
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	171 (99%)	2 (1%)	78	90
All	All	4842/4870 (99%)	4750 (98%)	92 (2%)	67	86

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	22	TRP
1	AB	135	MET
2	AC	128	MET
3	AD	130	ASN
3	AD	144	ILE
3	AD	187	ARG
3	AD	196	GLU
3	AD	200	VAL
5	AF	100	SER
6	AG	57	GLU
6	AG	137	ARG
7	AH	2	MET
7	AH	29	SER
7	AH	66	GLN
8	AI	71	ILE
8	AI	80	HIS
8	AI	105	ARG
8	AI	129	ARG
9	AJ	47	GLU
9	AJ	77	VAL
10	AK	55	ARG
13	AN	71	HIS
13	AN	92	GLU
14	AO	5	GLU
14	AO	55	LEU

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Mol	Chain	Res	Type
15	AP	1	MET
15	AP	39	PHE
15	AP	55	ASP
16	AQ	14	ASP
16	AQ	39	ARG
17	AR	69	TYR
17	AR	73	HIS
18	AS	73	PHE
19	AT	5	SER
19	AT	14	GLU
19	AT	74	HIS
20	AU	28	LEU
20	AU	30	GLU
25	BC	62	ARG
25	BC	85	ASN
25	BC	89	ASN
25	BC	190	THR
25	BC	191	LEU
26	BD	148	GLN
26	BD	151	THR
27	BE	55	SER
27	BE	67	ARG
27	BE	69	ARG
27	BE	105	LEU
27	BE	137	LYS
28	BF	111	ARG
28	BF	142	TYR
28	BF	152	ASP
29	BG	37	ASN
29	BG	71	LEU
29	BG	170	THR
30	BH	14	SER
32	BJ	76	HIS
32	BJ	80	HIS
32	BJ	130	HIS
34	BL	40	SER
34	BL	76	GLU
35	BM	97	GLN
36	BN	35	LYS
36	BN	67	PHE
36	BN	69	ARG
37	BO	33	ARG

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Mol	Chain	Res	Type
37	BO	53	THR
37	BO	61	GLN
37	BO	100	HIS
38	BP	23	ASP
38	BP	50	ARG
38	BP	102	ARG
38	BP	111	GLU
39	BQ	12	ARG
39	BQ	28	SER
40	BR	46	GLU
41	BS	88	ARG
43	BU	44	HIS
43	BU	72	PHE
44	BV	44	HIS
45	BW	28	GLU
48	BZ	8	GLN
48	BZ	28	LEU
49	B0	3	GLN
49	B0	32	THR
49	B0	37	HIS
49	B0	41	HIS
50	B1	31	GLU
52	B3	23	HIS
56	B5	24	ASN
56	B5	168	ASN

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

Mol	Chain	Res	Type
2	AC	184	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	254 (16%)	77 (5%)
22	A1	73/76 (96%)	10 (13%)	3 (4%)
23	A2	14/15 (93%)	8 (57%)	5 (35%)
24	A3	76/77 (98%)	15 (19%)	5 (6%)
54	BA	2902/2903 (99%)	474 (16%)	117 (4%)
55	BB	116/118 (98%)	18 (15%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4710/4722 (99%)	779 (16%)	209 (4%)

All (779) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	8	A
21	AA	15	G
21	AA	16	A
21	AA	22	G
21	AA	27	G
21	AA	30	U
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	55	A
21	AA	68	G
21	AA	69	G
21	AA	70	U
21	AA	81	A
21	AA	83	C
21	AA	86	G
21	AA	90	C
21	AA	109	A
21	AA	120	A
21	AA	131	A
21	AA	151	A
21	AA	182	A
21	AA	185	U
21	AA	189	A
21	AA	197	A
21	AA	198	G
21	AA	212	G
21	AA	235	C
21	AA	240	G
21	AA	243	A
21	AA	244	U
21	AA	247	G
21	AA	251	G
21	AA	252	U
21	AA	266	G

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Mol	Chain	Res	Type
21	AA	267	C
21	AA	289	G
21	AA	299	G
21	AA	306	A
21	AA	315	A
21	AA	316	C
21	AA	321	A
21	AA	328	C
21	AA	329	A
21	AA	347	G
21	AA	350	G
21	AA	352	C
21	AA	353	A
21	AA	354	G
21	AA	358	U
21	AA	367	U
21	AA	369	G
21	AA	372	C
21	AA	373	A
21	AA	381	C
21	AA	390	U
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	409	U
21	AA	412	A
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	449	G
21	AA	452	A
21	AA	462	G
21	AA	463	U
21	AA	467	U
21	AA	468	A
21	AA	474	G
21	AA	484	G
21	AA	486	U
21	AA	496	A
21	AA	499	A
21	AA	500	G
21	AA	501	C

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Mol	Chain	Res	Type
21	AA	505	G
21	AA	511	C
21	AA	523	A
21	AA	524	G
21	AA	527	G
21	AA	530	G
21	AA	531	U
21	AA	547	A
21	AA	559	A
21	AA	562	U
21	AA	566	G
21	AA	567	G
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	577	G
21	AA	607	A
21	AA	610	U
21	AA	632	U
21	AA	649	A
21	AA	650	G
21	AA	665	A
21	AA	694	A
21	AA	700	G
21	AA	703	G
21	AA	717	U
21	AA	722	G
21	AA	724	G
21	AA	727	G
21	AA	729	A
21	AA	734	G
21	AA	755	G
21	AA	756	C
21	AA	777	A
21	AA	781	A
21	AA	794	A
21	AA	812	G
21	AA	819	A
21	AA	821	G
21	AA	828	U
21	AA	829	G

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Mol	Chain	Res	Type
21	AA	841	C
21	AA	843	U
21	AA	844	G
21	AA	845	A
21	AA	846	G
21	AA	861	G
21	AA	876	C
21	AA	877	G
21	AA	899	C
21	AA	900	A
21	AA	902	G
21	AA	910	C
21	AA	920	U
21	AA	932	C
21	AA	934	C
21	AA	935	A
21	AA	936	C
21	AA	939	G
21	AA	940	C
21	AA	945	G
21	AA	959	A
21	AA	960	U
21	AA	961	U
21	AA	966	G
21	AA	967	C
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	972	C
21	AA	975	A
21	AA	976	G
21	AA	977	A
21	AA	978	A
21	AA	979	C
21	AA	980	C
21	AA	983	A
21	AA	984	C
21	AA	993	G
21	AA	996	A
21	AA	998	C
21	AA	1004	A
21	AA	1025	U

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Mol	Chain	Res	Type
21	AA	1026	G
21	AA	1031	C
21	AA	1032	G
21	AA	1037	C
21	AA	1045	C
21	AA	1046	A
21	AA	1049	U
21	AA	1050	G
21	AA	1054	C
21	AA	1056	U
21	AA	1064	G
21	AA	1065	U
21	AA	1068	G
21	AA	1086	U
21	AA	1092	A
21	AA	1093	A
21	AA	1094	G
21	AA	1101	A
21	AA	1125	U
21	AA	1126	U
21	AA	1127	G
21	AA	1130	A
21	AA	1138	G
21	AA	1139	G
21	AA	1147	C
21	AA	1148	U
21	AA	1151	A
21	AA	1152	A
21	AA	1159	U
21	AA	1182	G
21	AA	1183	U
21	AA	1184	G
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1202	U
21	AA	1204	A
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1228	C
21	AA	1231	G

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Mol	Chain	Res	Type
21	AA	1238	A
21	AA	1256	A
21	AA	1257	A
21	AA	1258	G
21	AA	1260	G
21	AA	1267	C
21	AA	1279	G
21	AA	1280	A
21	AA	1281	C
21	AA	1286	U
21	AA	1298	U
21	AA	1300	G
21	AA	1301	U
21	AA	1303	C
21	AA	1317	C
21	AA	1320	C
21	AA	1321	U
21	AA	1337	G
21	AA	1338	G
21	AA	1339	A
21	AA	1340	A
21	AA	1342	C
21	AA	1343	G
21	AA	1345	U
21	AA	1363	A
21	AA	1368	A
21	AA	1369	C
21	AA	1378	C
21	AA	1379	G
21	AA	1381	U
21	AA	1384	C
21	AA	1387	G
21	AA	1397	C
21	AA	1398	A
21	AA	1401	G
21	AA	1452	C
21	AA	1453	G
21	AA	1471	U
21	AA	1493	A
21	AA	1495	U
21	AA	1499	A
21	AA	1503	A

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Mol	Chain	Res	Type
21	AA	1505	G
21	AA	1517	G
21	AA	1518	A
21	AA	1520	C
21	AA	1524	C
21	AA	1529	G
21	AA	1530	G
22	A1	16	C
22	A1	17	U
22	A1	20	G
22	A1	21	A
22	A1	33	U
22	A1	48	C
22	A1	49	G
22	A1	59	U
22	A1	74	C
22	A1	76	A
23	A2	81	U
23	A2	82	A
23	A2	84	G
23	A2	85	G
23	A2	87	U
23	A2	90	U
23	A2	91	A
23	A2	93	U
24	A3	2	G
24	A3	9	G
24	A3	10	G
24	A3	18	U
24	A3	21	H2U
24	A3	22	A
24	A3	36	A
24	A3	40	C
24	A3	48	U
24	A3	49	C
24	A3	72	C
24	A3	73	A
24	A3	74	A
24	A3	76	C
24	A3	77	A
54	BA	20	C
54	BA	27	G

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Mol	Chain	Res	Type
54	BA	34	U
54	BA	60	G
54	BA	61	C
54	BA	62	U
54	BA	63	A
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	77	G
54	BA	85	G
54	BA	86	G
54	BA	88	G
54	BA	91	A
54	BA	98	G
54	BA	101	A
54	BA	103	A
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	139	U
54	BA	141	G
54	BA	142	A
54	BA	143	C
54	BA	149	A
54	BA	181	A
54	BA	197	A
54	BA	204	A
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	223	A
54	BA	230	G
54	BA	239	C
54	BA	242	G
54	BA	245	G
54	BA	248	G
54	BA	265	A
54	BA	266	G
54	BA	274	C
54	BA	278	A

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Mol	Chain	Res	Type
54	BA	286	U
54	BA	295	G
54	BA	316	C
54	BA	323	C
54	BA	330	A
54	BA	331	C
54	BA	332	A
54	BA	335	C
54	BA	346	A
54	BA	347	A
54	BA	362	A
54	BA	370	G
54	BA	372	G
54	BA	377	G
54	BA	383	C
54	BA	384	A
54	BA	386	G
54	BA	387	U
54	BA	411	G
54	BA	422	A
54	BA	428	A
54	BA	430	A
54	BA	444	C
54	BA	451	U
54	BA	453	A
54	BA	454	A
54	BA	455	C
54	BA	457	A
54	BA	458	G
54	BA	470	A
54	BA	471	A
54	BA	481	G
54	BA	484	C
54	BA	490	C
54	BA	491	G
54	BA	501	A
54	BA	504	A
54	BA	505	A
54	BA	509	C
54	BA	527	C
54	BA	531	C
54	BA	532	A

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Mol	Chain	Res	Type
54	BA	546	U
54	BA	547	A
54	BA	549	G
54	BA	571	U
54	BA	572	A
54	BA	573	U
54	BA	578	G
54	BA	586	A
54	BA	588	U
54	BA	604	G
54	BA	607	U
54	BA	611	C
54	BA	614	A
54	BA	615	U
54	BA	616	A
54	BA	617	G
54	BA	629	G
54	BA	630	G
54	BA	631	A
54	BA	634	C
54	BA	637	A
54	BA	638	G
54	BA	650	C
54	BA	654	A
54	BA	655	A
54	BA	662	G
54	BA	671	C
54	BA	672	C
54	BA	687	C
54	BA	715	A
54	BA	719	C
54	BA	722	A
54	BA	723	C
54	BA	724	U
54	BA	726	G
54	BA	736	C
54	BA	747	U
54	BA	748	G
54	BA	752	A
54	BA	763	G
54	BA	765	C
54	BA	775	G

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Mol	Chain	Res	Type
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	790	U
54	BA	791	C
54	BA	792	A
54	BA	793	A
54	BA	800	A
54	BA	804	A
54	BA	814	C
54	BA	816	C
54	BA	822	G
54	BA	823	C
54	BA	827	U
54	BA	858	G
54	BA	859	G
54	BA	889	C
54	BA	890	C
54	BA	907	G
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	924	G
54	BA	931	U
54	BA	934	U
54	BA	950	G
54	BA	961	C
54	BA	973	A
54	BA	974	G
54	BA	980	A
54	BA	981	A
54	BA	983	A
54	BA	996	A
54	BA	1012	U
54	BA	1013	C
54	BA	1022	G
54	BA	1023	U
54	BA	1024	G
54	BA	1026	G
54	BA	1033	U
54	BA	1046	A
54	BA	1055	G

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Mol	Chain	Res	Type
54	BA	1056	G
54	BA	1063	G
54	BA	1067	A
54	BA	1068	G
54	BA	1069	A
54	BA	1070	A
54	BA	1073	A
54	BA	1077	A
54	BA	1088	A
54	BA	1089	A
54	BA	1112	G
54	BA	1124	G
54	BA	1127	A
54	BA	1130	U
54	BA	1131	G
54	BA	1132	U
54	BA	1135	C
54	BA	1141	U
54	BA	1142	A
54	BA	1151	A
54	BA	1155	A
54	BA	1175	A
54	BA	1176	U
54	BA	1186	G
54	BA	1192	G
54	BA	1204	A
54	BA	1206	G
54	BA	1211	C
54	BA	1227	G
54	BA	1237	A
54	BA	1241	A
54	BA	1242	U
54	BA	1253	A
54	BA	1254	A
54	BA	1264	A
54	BA	1265	A
54	BA	1270	C
54	BA	1271	G
54	BA	1272	A
54	BA	1273	U
54	BA	1276	A
54	BA	1292	G

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Mol	Chain	Res	Type
54	BA	1300	G
54	BA	1301	A
54	BA	1302	A
54	BA	1313	U
54	BA	1314	C
54	BA	1315	C
54	BA	1325	U
54	BA	1332	G
54	BA	1341	G
54	BA	1350	C
54	BA	1365	A
54	BA	1366	A
54	BA	1368	G
54	BA	1379	U
54	BA	1380	G
54	BA	1383	A
54	BA	1388	G
54	BA	1393	A
54	BA	1416	G
54	BA	1425	G
54	BA	1427	A
54	BA	1428	C
54	BA	1434	A
54	BA	1435	G
54	BA	1452	G
54	BA	1453	A
54	BA	1454	C
54	BA	1459	G
54	BA	1461	C
54	BA	1482	G
54	BA	1491	G
54	BA	1494	A
54	BA	1509	A
54	BA	1510	G
54	BA	1522	A
54	BA	1536	C
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1559	U
54	BA	1566	A
54	BA	1569	A

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Mol	Chain	Res	Type
54	BA	1598	A
54	BA	1607	C
54	BA	1608	A
54	BA	1610	A
54	BA	1611	C
54	BA	1616	A
54	BA	1618	A
54	BA	1626	A
54	BA	1635	A
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1654	A
54	BA	1661	G
54	BA	1674	G
54	BA	1675	C
54	BA	1696	G
54	BA	1711	A
54	BA	1723	G
54	BA	1729	U
54	BA	1730	C
54	BA	1733	G
54	BA	1734	G
54	BA	1758	U
54	BA	1764	C
54	BA	1773	A
54	BA	1776	G
54	BA	1780	A
54	BA	1783	A
54	BA	1784	A
54	BA	1800	C
54	BA	1801	A
54	BA	1808	A
54	BA	1817	G
54	BA	1830	C
54	BA	1833	C
54	BA	1847	A
54	BA	1870	C
54	BA	1871	A
54	BA	1872	A
54	BA	1873	G
54	BA	1876	A

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Mol	Chain	Res	Type
54	BA	1877	A
54	BA	1884	G
54	BA	1900	A
54	BA	1912	A
54	BA	1914	C
54	BA	1930	G
54	BA	1931	U
54	BA	1937	A
54	BA	1939	U
54	BA	1940	U
54	BA	1941	C
54	BA	1951	U
54	BA	1952	A
54	BA	1953	A
54	BA	1955	U
54	BA	1962	C
54	BA	1963	U
54	BA	1965	C
54	BA	1967	C
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1981	A
54	BA	1982	U
54	BA	1986	C
54	BA	1993	U
54	BA	2017	U
54	BA	2020	A
54	BA	2022	U
54	BA	2023	C
54	BA	2030	A
54	BA	2032	G
54	BA	2043	C
54	BA	2052	A
54	BA	2055	C
54	BA	2059	A
54	BA	2061	G
54	BA	2068	U
54	BA	2069	G
54	BA	2076	U
54	BA	2077	A
54	BA	2092	U

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Mol	Chain	Res	Type
54	BA	2113	U
54	BA	2115	G
54	BA	2116	G
54	BA	2117	A
54	BA	2118	U
54	BA	2126	A
54	BA	2127	G
54	BA	2132	U
54	BA	2133	G
54	BA	2148	G
54	BA	2155	U
54	BA	2157	G
54	BA	2158	A
54	BA	2159	G
54	BA	2160	C
54	BA	2169	A
54	BA	2172	U
54	BA	2173	A
54	BA	2198	A
54	BA	2203	U
54	BA	2212	A
54	BA	2216	G
54	BA	2225	A
54	BA	2238	G
54	BA	2239	G
54	BA	2266	A
54	BA	2275	C
54	BA	2276	G
54	BA	2283	C
54	BA	2305	U
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2311	A
54	BA	2312	U
54	BA	2321	U
54	BA	2322	A
54	BA	2325	G
54	BA	2327	A
54	BA	2333	A
54	BA	2335	A
54	BA	2339	C

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Mol	Chain	Res	Type
54	BA	2347	C
54	BA	2350	C
54	BA	2351	G
54	BA	2353	G
54	BA	2379	G
54	BA	2383	G
54	BA	2385	C
54	BA	2388	A
54	BA	2391	G
54	BA	2395	C
54	BA	2406	A
54	BA	2407	A
54	BA	2408	U
54	BA	2409	G
54	BA	2417	C
54	BA	2418	A
54	BA	2422	C
54	BA	2425	A
54	BA	2426	A
54	BA	2427	C
54	BA	2429	G
54	BA	2430	A
54	BA	2431	U
54	BA	2433	A
54	BA	2434	A
54	BA	2435	A
54	BA	2441	U
54	BA	2446	G
54	BA	2447	G
54	BA	2448	A
54	BA	2470	G
54	BA	2474	U
54	BA	2476	A
54	BA	2491	U
54	BA	2492	U
54	BA	2501	C
54	BA	2503	A
54	BA	2505	G
54	BA	2506	U
54	BA	2520	C
54	BA	2566	A
54	BA	2567	G

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Mol	Chain	Res	Type
54	BA	2572	A
54	BA	2573	C
54	BA	2577	A
54	BA	2578	G
54	BA	2586	U
54	BA	2599	G
54	BA	2602	A
54	BA	2603	G
54	BA	2611	C
54	BA	2614	A
54	BA	2615	U
54	BA	2629	U
54	BA	2639	A
54	BA	2640	G
54	BA	2646	C
54	BA	2654	A
54	BA	2660	A
54	BA	2667	C
54	BA	2668	G
54	BA	2681	C
54	BA	2683	C
54	BA	2689	U
54	BA	2690	U
54	BA	2706	A
54	BA	2714	G
54	BA	2726	A
54	BA	2732	G
54	BA	2733	A
54	BA	2744	G
54	BA	2756	U
54	BA	2757	A
54	BA	2765	A
54	BA	2770	G
54	BA	2771	C
54	BA	2778	A
54	BA	2780	G
54	BA	2791	G
54	BA	2797	U
54	BA	2798	U
54	BA	2799	A
54	BA	2800	A
54	BA	2816	G

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Mol	Chain	Res	Type
54	BA	2817	U
54	BA	2821	A
54	BA	2822	G
54	BA	2834	G
54	BA	2835	A
54	BA	2841	C
54	BA	2850	A
54	BA	2873	A
54	BA	2875	C
54	BA	2894	G
55	BB	13	G
55	BB	14	U
55	BB	15	A
55	BB	16	G
55	BB	25	U
55	BB	29	A
55	BB	30	C
55	BB	33	G
55	BB	44	G
55	BB	69	G
55	BB	84	G
55	BB	85	G
55	BB	89	U
55	BB	90	C
55	BB	99	A
55	BB	100	G
55	BB	101	A
55	BB	109	A

All (209) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	15	G
21	AA	26	A
21	AA	31	G
21	AA	51	A
21	AA	65	A
21	AA	69	G
21	AA	80	A
21	AA	86	G
21	AA	88	U
21	AA	243	A

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Mol	Chain	Res	Type
21	AA	251	G
21	AA	298	A
21	AA	315	A
21	AA	327	A
21	AA	328	C
21	AA	353	A
21	AA	357	G
21	AA	372	C
21	AA	381	C
21	AA	448	A
21	AA	451	A
21	AA	453	G
21	AA	465	A
21	AA	496	A
21	AA	499	A
21	AA	500	G
21	AA	505	G
21	AA	523	A
21	AA	530	G
21	AA	562	U
21	AA	566	G
21	AA	575	G
21	AA	641	U
21	AA	718	A
21	AA	728	A
21	AA	734	G
21	AA	818	G
21	AA	844	G
21	AA	845	A
21	AA	860	A
21	AA	876	C
21	AA	899	C
21	AA	938	A
21	AA	959	A
21	AA	960	U
21	AA	966	G
21	AA	975	A
21	AA	977	A
21	AA	979	C
21	AA	992	U
21	AA	1025	U
21	AA	1030	U

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Mol	Chain	Res	Type
21	AA	1092	A
21	AA	1093	A
21	AA	1126	U
21	AA	1158	C
21	AA	1182	G
21	AA	1190	G
21	AA	1201	A
21	AA	1203	C
21	AA	1225	A
21	AA	1257	A
21	AA	1267	C
21	AA	1278	G
21	AA	1279	G
21	AA	1280	A
21	AA	1296	C
21	AA	1298	U
21	AA	1305	G
21	AA	1337	G
21	AA	1342	C
21	AA	1368	A
21	AA	1380	U
21	AA	1445	U
21	AA	1451	U
21	AA	1498	U
21	AA	1517	G
22	A1	19	G
22	A1	32	C
22	A1	47	U
23	A2	84	G
23	A2	87	U
23	A2	89	U
23	A2	90	U
23	A2	92	U
24	A3	9	G
24	A3	47	G
24	A3	48	U
24	A3	72	C
24	A3	76	C
54	BA	46	G
54	BA	60	G
54	BA	74	A
54	BA	121	G

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Mol	Chain	Res	Type
54	BA	125	A
54	BA	199	A
54	BA	215	G
54	BA	278	A
54	BA	346	A
54	BA	376	G
54	BA	383	C
54	BA	454	A
54	BA	464	U
54	BA	470	A
54	BA	547	A
54	BA	569	U
54	BA	571	U
54	BA	577	G
54	BA	587	C
54	BA	603	A
54	BA	615	U
54	BA	620	G
54	BA	629	G
54	BA	649	G
54	BA	661	A
54	BA	670	A
54	BA	686	U
54	BA	762	U
54	BA	790	U
54	BA	804	A
54	BA	815	C
54	BA	858	G
54	BA	979	A
54	BA	980	A
54	BA	983	A
54	BA	1012	U
54	BA	1023	U
54	BA	1055	G
54	BA	1061	U
54	BA	1068	G
54	BA	1076	C
54	BA	1122	G
54	BA	1126	A
54	BA	1128	G
54	BA	1141	U
54	BA	1144	A

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Mol	Chain	Res	Type
54	BA	1157	G
54	BA	1210	G
54	BA	1224	U
54	BA	1253	A
54	BA	1263	U
54	BA	1265	A
54	BA	1270	C
54	BA	1288	G
54	BA	1289	C
54	BA	1301	A
54	BA	1312	U
54	BA	1314	C
54	BA	1340	U
54	BA	1344	U
54	BA	1378	A
54	BA	1379	U
54	BA	1392	A
54	BA	1420	A
54	BA	1424	G
54	BA	1427	A
54	BA	1452	G
54	BA	1453	A
54	BA	1508	A
54	BA	1509	A
54	BA	1567	G
54	BA	1610	A
54	BA	1634	A
54	BA	1645	G
54	BA	1757	A
54	BA	1783	A
54	BA	1784	A
54	BA	1799	G
54	BA	1876	A
54	BA	1900	A
54	BA	1913	A
54	BA	1936	A
54	BA	1940	U
54	BA	1951	U
54	BA	1961	C
54	BA	1962	C
54	BA	1981	A
54	BA	2016	U

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Mol	Chain	Res	Type
54	BA	2033	A
54	BA	2076	U
54	BA	2115	G
54	BA	2157	G
54	BA	2275	C
54	BA	2286	G
54	BA	2307	G
54	BA	2308	G
54	BA	2312	U
54	BA	2350	C
54	BA	2407	A
54	BA	2417	C
54	BA	2425	A
54	BA	2427	C
54	BA	2429	G
54	BA	2430	A
54	BA	2433	A
54	BA	2434	A
54	BA	2474	U
54	BA	2566	A
54	BA	2572	A
54	BA	2602	A
54	BA	2615	U
54	BA	2726	A
54	BA	2732	G
54	BA	2756	U
54	BA	2770	G
54	BA	2797	U
54	BA	2809	A
55	BB	32	U
55	BB	52	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CM0	A1	34	22	15,26,27	1.83	3 (20%)	18,37,40	3.19	3 (16%)
22	6MZ	A1	37	22	17,25,26	1.01	1 (5%)	15,36,39	1.03	1 (6%)
22	7MG	A1	46	22	20,26,27	2.22	3 (15%)	23,39,42	2.13	2 (8%)
22	5MU	A1	54	22	13,22,23	1.07	1 (7%)	16,32,35	4.73	2 (12%)
22	PSU	A1	55	22	15,21,22	1.10	1 (6%)	16,30,33	3.27	4 (25%)
22	4SU	A1	7	22	12,21,22	1.05	1 (8%)	15,30,33	2.16	1 (6%)
24	H2U	A3	21	24	17,21,22	1.36	2 (11%)	23,30,33	1.26	4 (17%)
24	OMC	A3	33	24	15,22,23	1.08	0	20,31,34	0.76	0
24	5MU	A3	55	24	13,22,23	1.09	1 (7%)	16,32,35	4.64	2 (12%)
24	PSU	A3	56	24	15,21,22	1.22	2 (13%)	16,30,33	3.21	4 (25%)
24	4SU	A3	8	24	12,21,22	1.08	0	15,30,33	2.27	2 (13%)

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.64	1.32	1.45
22	A1	34	CM0	O5-C5	-5.49	1.26	1.37
24	A3	21	H2U	C4-N3	-3.47	1.32	1.37
24	A3	21	H2U	C2-N3	-3.31	1.31	1.38
22	A1	46	7MG	C8-N7	-2.72	1.31	1.43
22	A1	37	6MZ	C8-N7	-2.48	1.29	1.34
22	A1	7	4SU	C2'-C1'	-2.18	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	56	PSU	C6-C5	-2.10	1.35	1.38
22	A1	46	7MG	C6-N1	2.18	1.37	1.33
24	A3	56	PSU	C4-N3	2.19	1.37	1.33
22	A1	55	PSU	C4-N3	2.49	1.37	1.33
22	A1	34	CM0	C4-N3	2.54	1.37	1.33
22	A1	54	5MU	C4-N3	2.57	1.37	1.33
22	A1	34	CM0	C4-C5	2.57	1.47	1.40
24	A3	55	5MU	C4-N3	2.68	1.37	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-12.85	114.56	125.35
24	A3	55	5MU	C5-C4-N3	-12.69	114.70	125.35
24	A3	8	4SU	C5-C4-N3	-8.18	114.89	123.56
22	A1	7	4SU	C5-C4-N3	-7.51	115.60	123.56
22	A1	46	7MG	C5-C6-N1	-6.83	113.22	123.39
24	A3	56	PSU	C5-C6-N1	-3.33	119.74	124.38
22	A1	55	PSU	C5-C1'-C2'	-3.27	109.88	115.44
22	A1	55	PSU	C5-C6-N1	-2.83	120.44	124.38
24	A3	56	PSU	C5-C1'-C2'	-2.65	110.93	115.44
24	A3	8	4SU	C4'-O4'-C1'	-2.19	107.32	109.64
24	A3	21	H2U	C4-N3-C2	2.10	127.67	125.77
22	A1	34	CM0	O5-C7-C8	2.26	112.68	108.01
24	A3	21	H2U	C5-C4-N3	2.31	119.06	116.62
24	A3	21	H2U	C5-C6-N1	2.34	113.33	110.76
22	A1	55	PSU	O4'-C1'-C2'	2.92	107.84	104.69
24	A3	21	H2U	N3-C2-N1	3.12	119.53	116.64
22	A1	37	6MZ	C2-N1-C6	3.19	118.77	116.47
22	A1	34	CM0	C7-O5-C5	3.42	124.11	117.83
24	A3	56	PSU	O4'-C1'-C2'	3.61	108.60	104.69
22	A1	46	7MG	C6-N1-C2	6.66	123.69	115.88
24	A3	56	PSU	C4-N3-C2	11.16	124.47	115.16
22	A1	55	PSU	C4-N3-C2	11.71	124.92	115.16
22	A1	34	CM0	C4-N3-C2	12.29	125.41	115.16
24	A3	55	5MU	C4-N3-C2	13.18	126.15	115.16
22	A1	54	5MU	C4-N3-C2	13.40	126.34	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A1	54	5MU	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	VAL	A1	101	58,22	5,6,7	0.49	0	5,7,9	1.79	1 (20%)
58	FME	BA	3001	57	8,9,10	0.62	0	5,9,11	1.28	1 (20%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-3.52	116.07	125.69
58	BA	3001	FME	O-C-CA	-2.06	120.06	125.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.