



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:54 PM BST

PDB ID : 4V72  
EMDB ID: : EMD-1719  
Title : E. coli 70S-fMetVal-tRNAVal-tRNA<sup>f</sup>Met complex in hybrid pre-translocation state (pre4)  
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 : 13.00 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

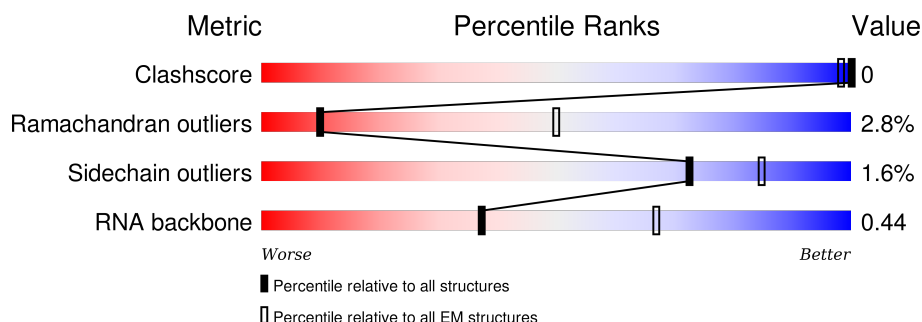
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 13.00 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.












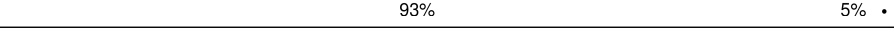

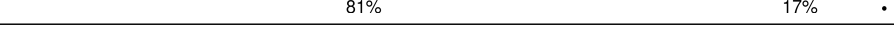
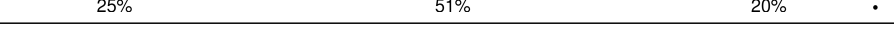


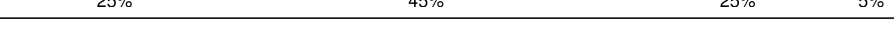



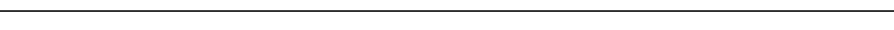

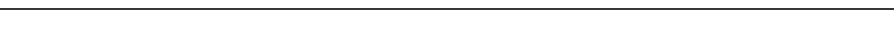
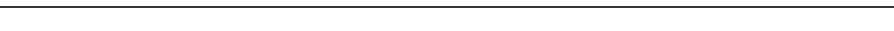


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	92% 8%
2	AC	208	87% 13%
3	AD	206	87% 13%
4	AE	152	90% 10%
5	AF	101	82% 18%
6	AG	152	86% 13% .
7	AH	130	92% 6% ..
8	AI	128	82% 17% .


















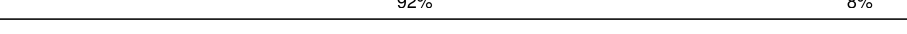



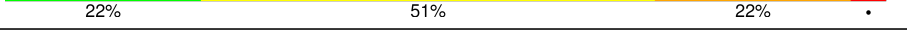
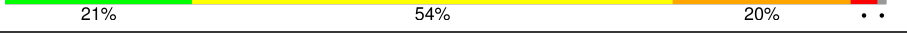
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Mol	Chain	Length	Quality of chain
9	AJ	100	 88% 10% .
10	AK	118	 90% 9% .
11	AL	124	 89% 10% .
12	AM	115	 83% 15% ..
13	AN	101	 88% 10% ..
14	AO	89	 88% 11% .
15	AP	81	 88% 12%
16	AQ	82	 89% 10% .
17	AR	57	 89% 11%
18	AS	81	 93% 5% .
19	AT	86	 91% 9%
20	AU	53	 81% 17% .
21	AA	1533	 25% 51% 20% .
22	A1	76	 33% 47% 16% .
23	A2	15	 27% 27% 33% 13%
24	A3	77	 25% 45% 25% 5%
25	BC	273	 87% 12%
26	BD	209	 91% 8%
27	BE	201	 90% 10%
28	BF	179	 88% 11% ..
29	BG	177	 90% 10% .
30	BH	149	 95% 5%
31	BI	142	 96% . .
32	BJ	142	 90% 9% .
33	BK	123	 85% 13% .

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Mol	Chain	Length	Quality of chain
34	BL	144	 85% 14% ..
35	BM	136	 87% 13% .
36	BN	121	 89% 11%
37	BO	117	 85% 13% ..
38	BP	115	 84% 14% ..
39	BQ	118	 84% 14% ..
40	BR	103	 94% 5% .
41	BS	110	 90% 9% .
42	BT	94	 94% 6%
43	BU	104	 88% 9% ..
44	BV	94	 95% 5%
45	BW	80	 86% 13% .
46	BX	79	 86% 11% .
47	BY	63	 90% 10%
48	BZ	59	 83% 15% .
49	B0	57	 88% 11% .
50	B1	52	 92% 8%
51	B2	46	 78% 20% .
52	B3	65	 83% 14% ..
53	B4	38	 89% 11%
54	BA	2903	 22% 51% 22% .
55	BB	118	 21% 54% 20% ..
56	B5	234	 90% 5% 5%

## 2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

- Molecule 25 is a protein called 50S ribosomal protein 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		

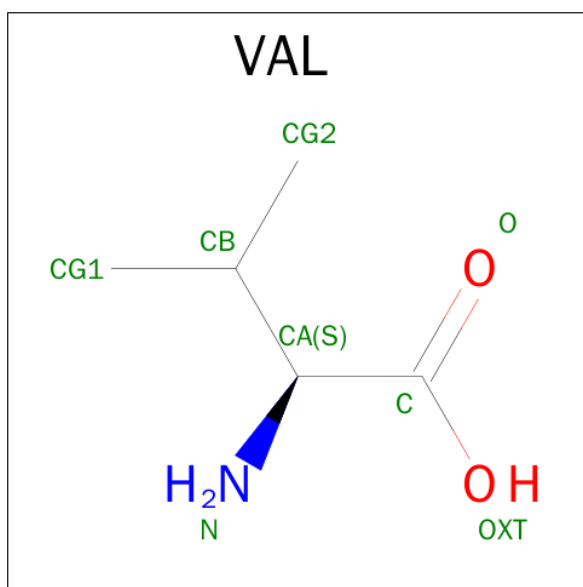
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

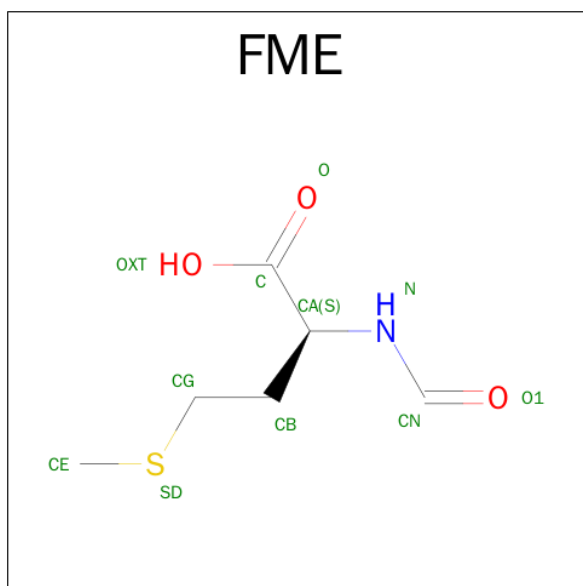
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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:  $C_6H_{11}NO_3S$ ).



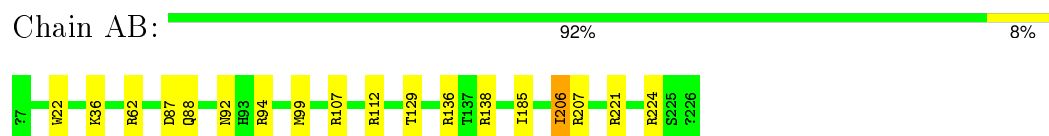
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



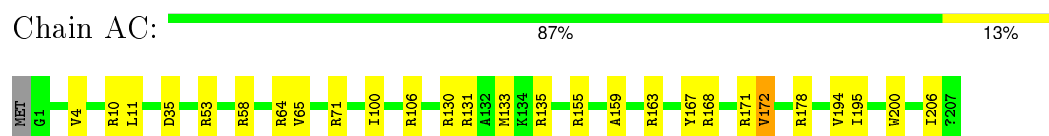
### 3 Residue-property plots

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.

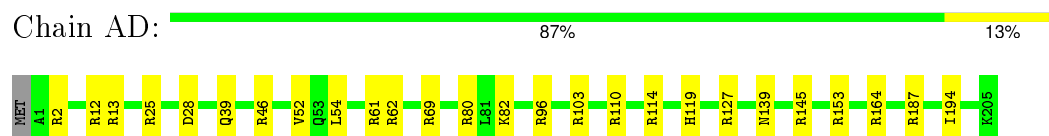
- Molecule 1: 30S ribosomal protein S2



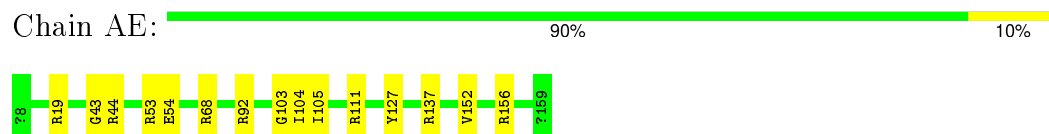
- Molecule 2: 30S ribosomal protein S3



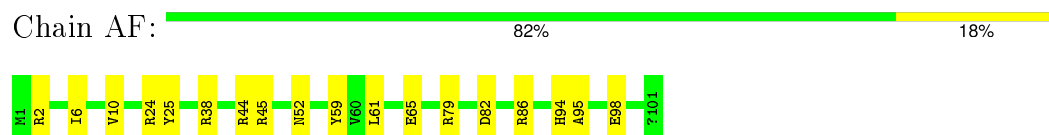
- Molecule 3: 30S ribosomal protein S4



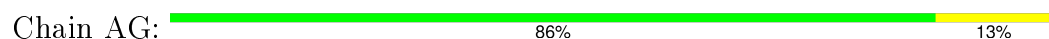
- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 6% ..



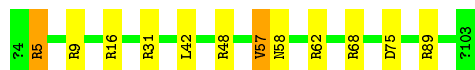
- Molecule 8: 30S ribosomal protein S9

Chain AI: 82% 17% .



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 88% 10% .



- Molecule 10: 30S ribosomal protein S11

Chain AK: 90% 9% .



- Molecule 11: 30S ribosomal protein S12

Chain AL: 89% 10% .



- Molecule 12: 30S ribosomal protein S13

Chain AM: 83% 15% ..




- Molecule 13: 30S ribosomal protein S14

Chain AN: 88% 10% ..



- Molecule 14: 30S ribosomal protein S15

Chain AO:  88% 11%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  88% 12%



- Molecule 16: 30S ribosomal protein S17

Chain AQ:  89% 10%



- Molecule 17: 30S ribosomal protein S18

Chain AR:  89% 11%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  93% 5%




- Molecule 19: 30S ribosomal protein S20

Chain AT:  91% 9%



- Molecule 20: 30S ribosomal protein S21

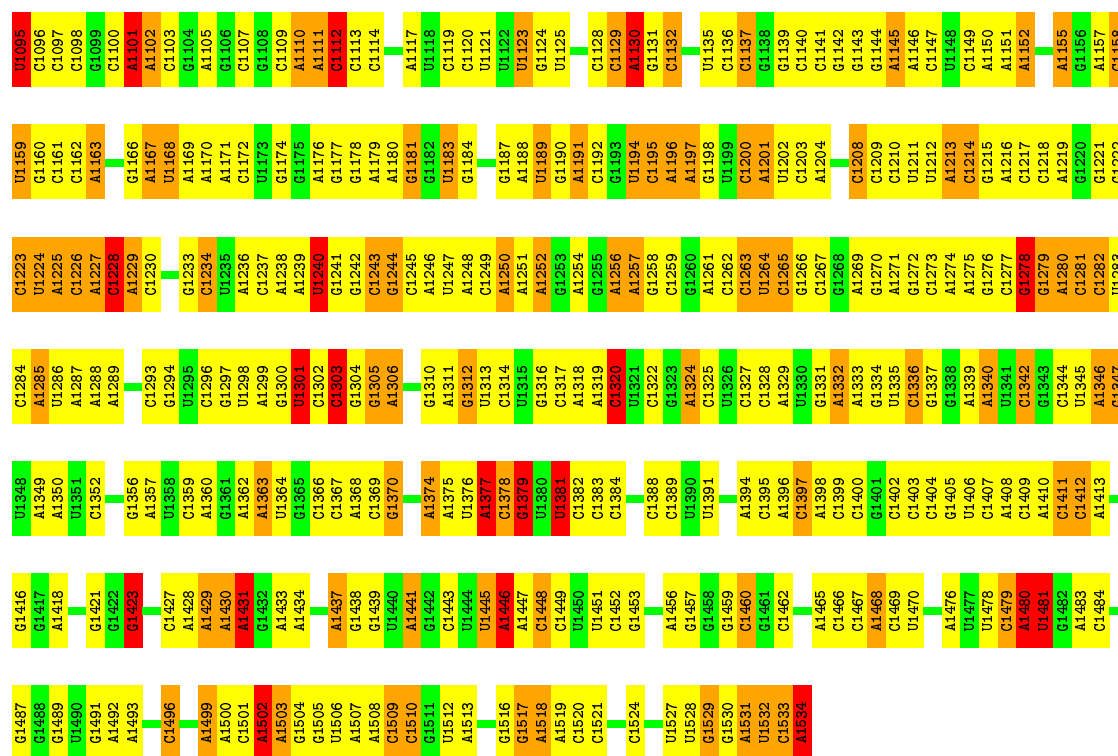
Chain AU:  81% 17%



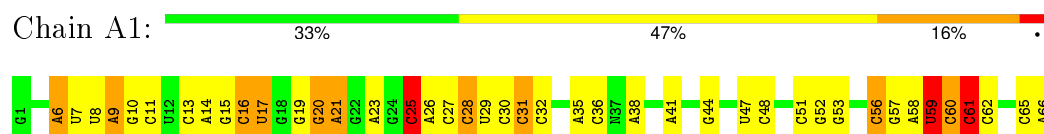
- Molecule 21: 16S ribosomal RNA

Chain AA:  25% 51% 20%

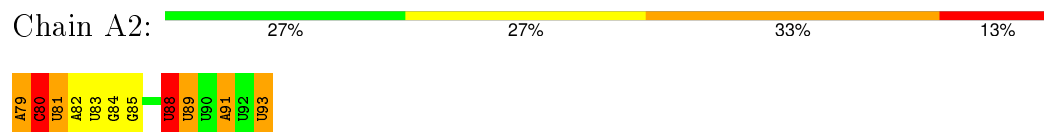
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U1030	A968	A908	C844	C779	A715	C948	A579		A452	C386	A321	A131	A65	U
C1031	A969	A909	A845	A780	A716	A648	C580	G517		U387	C322	C132	A66	U5
G1032	C970	C910	C846	A781	U717	A649	G581	C519	A456	G388	U323	C135	C67	G6
G1033	G971	U911	G847	A782	A718	G650	C582	C519		A389	G324	G136	G68	A7
G1034	C972	C912	C848	C783	C719	C851	A583	A520		U390	A325	C137	A69	A8
A1035	G973	A913	G849	G785	G720	U852	G584	G521	A459	C392	A327	U137	U70	G9
A1036	A974	A914		G786	G721	A653	C586		A460	G393	C328	A139	A71	A10
C1037	G975	A915	C852	G787	U723	A655		G524	A461	G394	A329	G142	A72	C73
G1038	G976	U916	C853		G724	G656	U589	C525	A462	C395	G330	G143	A74	U14
G1039	A977	G917	U854	A790	G725	U857	U590	G526	U464	C396	C331	G144	A75	G15
U1040	A978	A918	C856	G791	G726	C858	U591	G527	A465	A397		G145	A77	U17
G1041	C979	A919		A792	G727	U859	G592	C528	U466	U398	C334		A78	C18
A1042	U920	U920	C857	U793	A728	C660		G529	A467	G399	C335		A79	U20
G1043	U921	U921	U858	U794	A729		A595	U531	A468	C401	A336	G148	A80	A19
A1044	A983	A923	C859	C795		A663	A596	U531	C469	G402	A338	A149	A81	C21
C1045	C984	C924	C861	C796	G732	G665	G597	A532	C470	C403	U340	U150	G82	G22
A1046	C985	G925	C862	C797	G733	A666	U588	A533		G404	C339	A151	G83	C23
G1047	U986	U798	U863	U799	G734	G666	C599	U534	U473	U405	U341	C152	U24	C25
U1049	G987	G927	A864	G799	C735	A670	A600	A535	G474	G406	C342	U154	G86	C26
G1050	G988	G928	A865	G800	C736	G670	G601	C536	G475	G407	U343	C155	G87	A26
C1051	U989	G929	C866	U801	G737		A602		U476	U408	U344	C156		G27
U1052	C990	C930	G867	A802	C738	A873		A539	C477	U409	C345	U157		A28
G1053	U991	C931	C868		G739	G874	U605	G540	A478	U409	G346		C90	A29
C1054	U992	G932		C805	U740	A875	G606	G541	U479	G410	G347	G159	U91	U30
A1055	G993	G933	U871	C806	G741	A876	A607	G542	U480	A411	U283			
U1056	A994	C934	A872	A807	G742	A608	C481	U543	G481	A412	G348	G94	G94	G31
	C995	A935	A873	C808	A743	C679	A609	G544	A482	G413	C285	A161	C95	A32
C1059	A996	C936		G809	G744	C680	U610	C545	C483	A414	C286	A162	U96	A33
U1060	U997	A937	C876	C810	G745	A881	C611	A546	G484	A415	U287	C163	G97	C34
G1061	C998	A938	G877	C811	G746		C612	A547	U485	G416	A288	G164	A98	C35
U1062	C999	G939	A878	G812	A747	G685	C613	G548	U486	G417	G289	G165	C99	C36
C1063	A1000	C940	C879	U813	G748	U686	C614	C549	A487	C418	C355	U166	G100	U37
G1064	C1001	G941	C880	A814	A749	A887	C488	G550	G488	C419	A167	A167	G38	G38
U1065	G1002	G942	G881	A815	C750	G688	C489	U551	C489	U420	A356	G168	A101	C39
C1066	G1003	U943	C882	A816	U751	C689	C490	U552	C490	U421	G359	C169	C40	C40
A1067	A1004	G944	C883	C817	G752	G690	G491	A553	G491	C422		U170	G105	G41
G1068	U1005	G945	U884	G818	A753	G691	C492	A554	C492	G423	G362	A171	C106	G42
C1069	G1006	A946	C885	A819	C754	U692	A493	U555	A493	G424	A363	A172	G107	C43
U1070	U1007	G947	C886	U820	G755	G693	G500	C556	G494		A364	U173	G108	A44
C1071	U1008	C948	G887	G821	C756	A694	C623		A495		U365	A174	A109	G45
	U1009	A949	C888	U822	U757	A695	C624	A559	A496	U429	U367	C175	C110	G46
U1075	C1010	U950	A889	C823	C758	A696	U625	A560	G497	A450	U368	C176	G111	C47
	C1011	G951	C890	G824	A759	U697	G626	U561	A498	A431	U369	G177	G112	C48
U1078	A1012	U952	U891	A825	G760	G698		U562	A499	A432	G369	C178	G113	U49
G1079	G1013	G953	C892	C826	G761	C699	A629	A563	G500	G433	C370	A179	U114	A50
A1080	A1014	G954	C893	U827	U762	G700	A630	C564	C501	U434	A371	U180	G115	A51
A1081	G1015	U955	C894	U828	G763	U701	C631	U565	A502	A435	C372	U181	G116	C52
A1082	A1016	U956	G895	G829	C764	A702	U632	G566	C503	C436	A373	A182	G117	A53
		U957	C896	G830	G765	G703	G633		C504	U437	A374	C183	U118	C54
U1083		U958	C897	A831	A766	A704	C634	C569	G505	U438		C184	U119	A55
G1084	G1020	A959	C898	G832	A767	G705	A635	G506	U506	U439	G377	U185	A120	U56
A1021	A1021	U960	C899		A768	U706	U636	U571	C507	C440	C378	C186	U121	G57
A1022	A1022	U961	U900	U837	G769	U707	C637	A572	U508	A441	C379	G187	G122	C58
		C862	A901	G838	C708			A573	A509	G442	G380	C188	U123	A59
U1091	U1025	G963	G902	C839		G711	U641	A574	A510	C443	C381	A189	C124	A60
A1092	G1026	A964	G903	C840	G775	A712		C576	U512	A448	A382	A190	G61	C61
G1094	C1027			C841	G776		A642				A383	G191	U62	U62



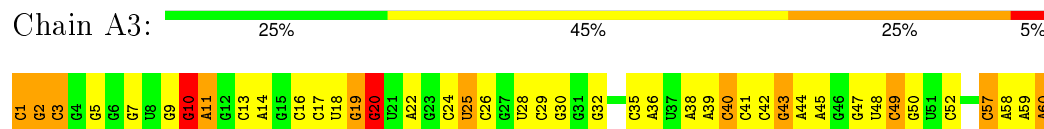
• Molecule 22: fMet-Val-tRNA-Val



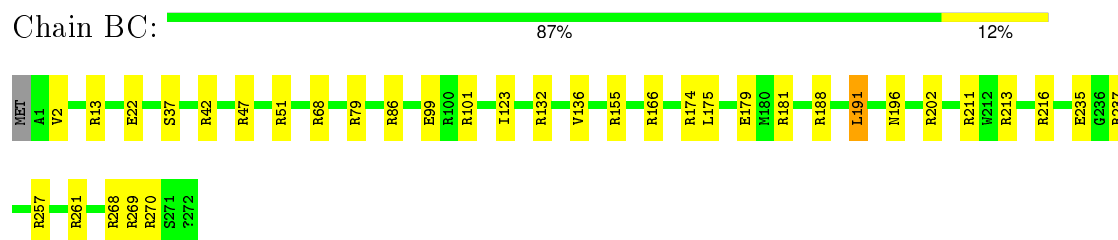
• Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'



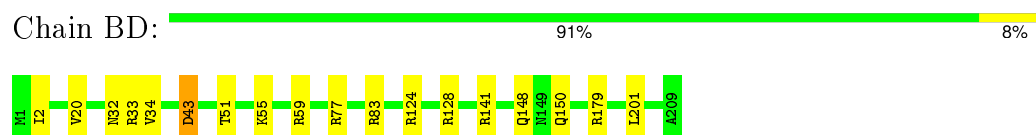
• Molecule 24: tRNA-fMet



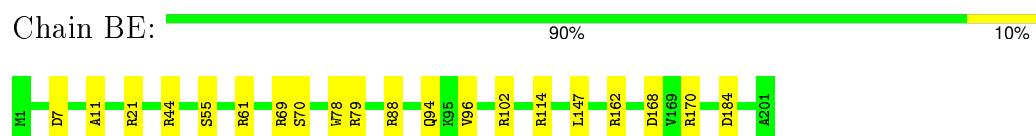
• Molecule 25: 50S ribosomal protein L2



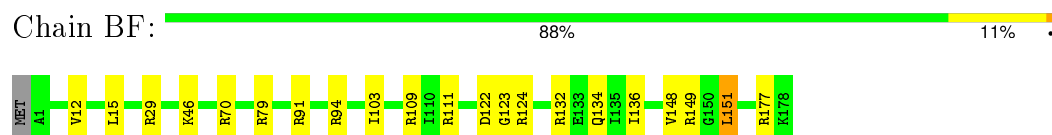
- Molecule 26: 50S ribosomal protein L3



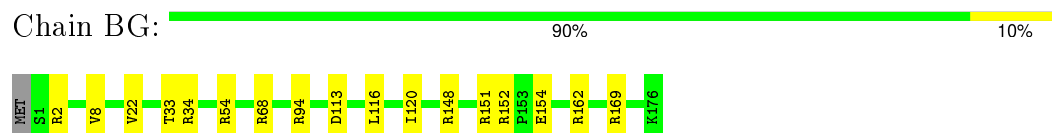
- Molecule 27: 50S ribosomal protein L4



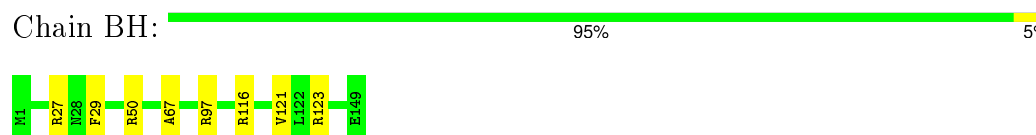
- Molecule 28: 50S ribosomal protein L5



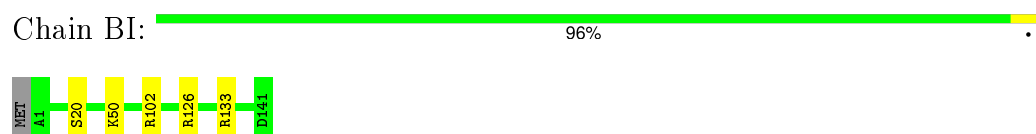
- Molecule 29: 50S ribosomal protein L6



- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L11




- Molecule 32: 50S ribosomal protein L13

Chain BJ:  90% 9% .




- Molecule 33: 50S ribosomal protein L14

Chain BK:  85% 13% .




- Molecule 34: 50S ribosomal protein L15

Chain BL:  85% 14% ..



- Molecule 35: 50S ribosomal protein L16

Chain BM:  87% 13% .




- Molecule 36: 50S ribosomal protein L17

Chain BN:  89% 11%




- Molecule 37: 50S ribosomal protein L18

Chain BO:  85% 13% ..




- Molecule 38: 50S ribosomal protein L19

Chain BP:  84% 14% ..



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  84% 14% ..



- Molecule 40: 50S ribosomal protein L21

Chain BR: 94% 5% .



- Molecule 41: 50S ribosomal protein L22

Chain BS: 90% 9% .



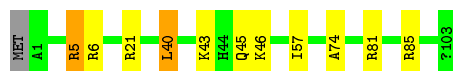
- Molecule 42: 50S ribosomal protein L23

Chain BT: 94% 6%



- Molecule 43: 50S ribosomal protein L24

Chain BU: 88% 9% ..



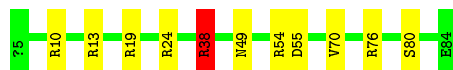
- Molecule 44: 50S ribosomal protein L25

Chain BV: 95% 5%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 86% 13% .



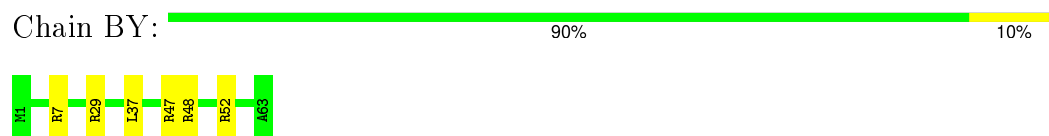
- Molecule 46: 50S ribosomal protein L28

Chain BX: 86% 11% .

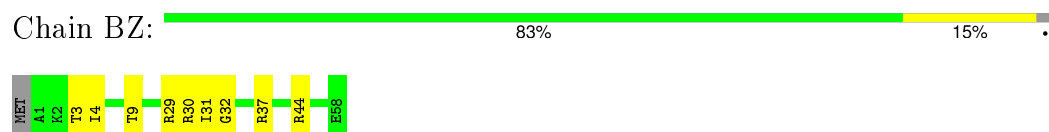




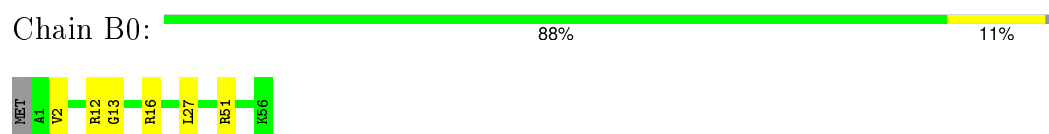
- Molecule 47: 50S ribosomal protein L29



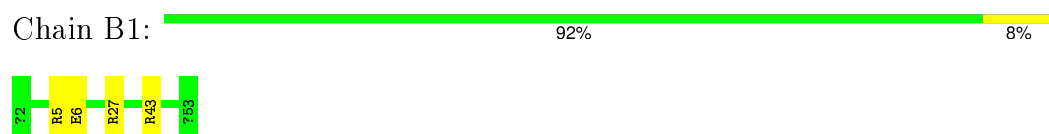
- Molecule 48: 50S ribosomal protein L30



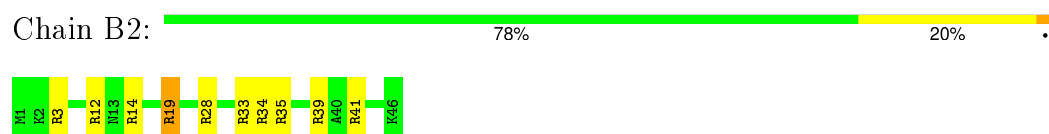
- Molecule 49: 50S ribosomal protein L32



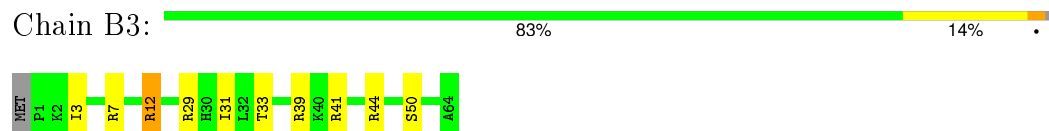
- Molecule 50: 50S ribosomal protein L33



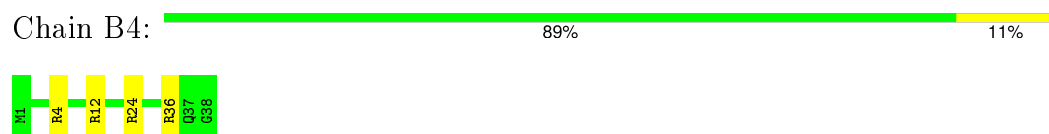
- Molecule 51: 50S ribosomal protein L34



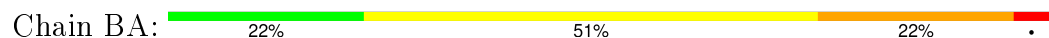
- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36

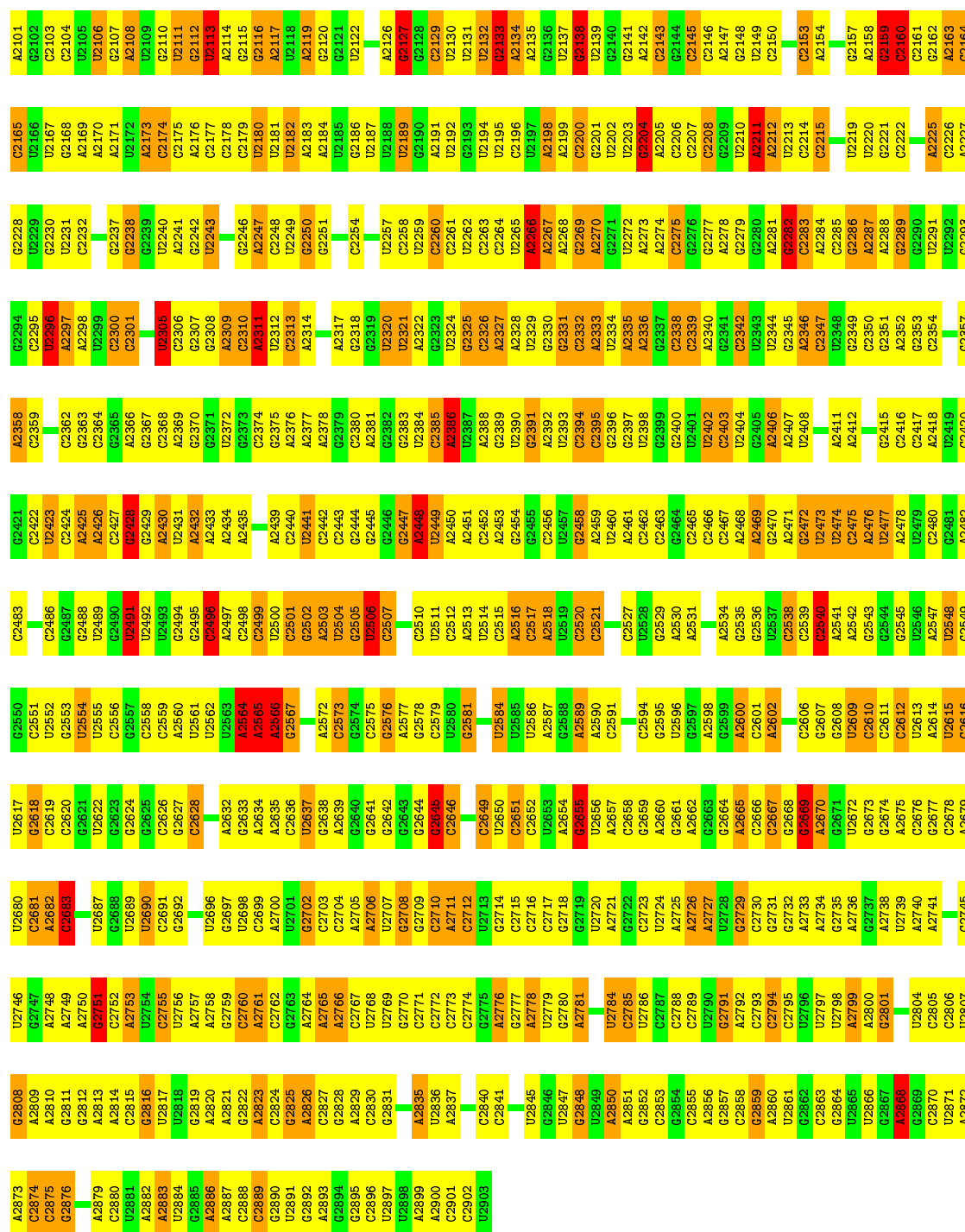


- Molecule 54: 23S ribosomal RNA

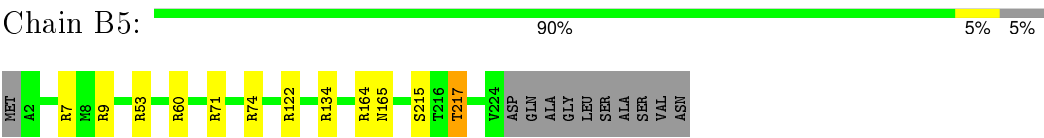


G1025	G1026	G1027	A1028	A1029	C1030	G1031	A1032	A1033	G1034	G1037	G1038	A1039	A1040	G1041	G1042	C1043	C1044	C1045	A1046	G1047	A1048	C1049	C1050	G1051	C1052	C1053	A1054	G1055	C1056	A1057	A1058	G1059	U1060	G1063	C1064	U1065	A1066	G1068	A1069	A1070	G1071	C1072	A1073	G1074	C1075	G1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1086			
G962	G963	C964	C965	G968	G969	U970	G971	A972	A973	G974	A975	G976	G977	A978	A979	A980	A981	C982	A983	A984	C985	C986	C987	A988	G989	G990	A991	C992	A993	C994	G995	A996	G997	C998	G999	A1000	A1001	C1005	C1006	A1007	A1008	A1009	A1010	G1011	U1012	U1013	C1014	U1015	U1016	U1017	U1018	U1019	A1020	A1021	U1022	U1023	C1024		
A889	A900	C901	C902	C903	G904	A905	U906	C907	C908	A909	A910	A911	C912	U913	G914	C915	G916	A917	A918	C919	A920	C921	C922	G923	A924	G925	A926	A927	A928	C929	G930	U931	U932	A933	U934	C935	A936	C937	A941	G942	A943	A944	A945	A946	A947	C948	G949	G950	C951	G954	U955	C956	A957	C958	U959	A960	C961		
G836	C837	C838	U839	C840	G841	U842	G843	A844	A845	U846	U847	C848	A849	U850	C851	U852	C853	C854	C855	U856	C857	C858	C859	U860	A861	G862	A863	A864	C865	A866	C867	U868	C869	U870	U871	U872	C873	G874	C875	C876	A877	A878	G881	U884	C885	A886	U887	C888	C889	C890	C891	A892	C893	U896	A897	C898			
G794	A705	A706	G707	U710	U714	A715	A716	A717	C717	A718	C719	U720	A721	A722	C723	A724	G725	G726	A727	G728	A729	C730	A731	C732	G733	A734	A735	C736	C737	G738	A739	C740	U741	A742	A743	U744	G745	U746	U747	G748	C749	C750	A751	A752	A753	U756	C757	C758	C759	U760	A761	U764	C765	U766	U767	U703			
C772	U773	G774	G775	G776	G777	G778	U779	A780	A781	A782	A783	U784	U785	C786	C787	A788	A789	U790	C791	A792	A793	A794	C795	C796	A800	A801	A802	U803	A804	C805	C806	U809	U810	U811	C812	U813	C814	C815	C816	C817	G818	A819	A820	A821	C822	C823	U824	A825	U826	U827	U828	A829	A833	U834	C835				
G636	A637	G638	U639	C640	U641	U642	A643	A644	U645	U646	G647	C650	U653	A654	A655	G656	C660	A661	G662	U663	A664	U665	A666	U667	A668	G669	A670	C671	C672	C673	A674	A675	A676	A677	C678	C679	C680	G681	A682	U683	U684	A685	U686	C687	C688	A689	A690	A691	A692	A693	C698	A699	G700	U701	U702	U703			
A508	C509	C510	A513	A514	A515	C516	C517	U518	U519	U520	U521	A522	C523	U524	U525	A526	C527	A528	A529	C530	C531	A532	U533	A534	C537	A538	A539	A540	A541	A542	A543	A544	U545	U546	A547	C548	C549	C550	C551	U552	A556	C557	U558	C559	C560	U561	U562	A563	C564	C565	U566	A567	A568	U569	A570	U571			
A447	U448	A449	G450	U451	A452	A453	A454	U455	U456	A457	U458	A459	A460	C461	C462	A463	U464	A465	A466	U467	A468	U469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	C485	C486	A487	U488	A489	C490	U491	A492	A493	A494	C495	U496	A497	U500	A501	A502	A503	A443	A444	A505	A506	A507
C383	A384	C385	G386	U387	G388	C389	U390	A391	U392	C393	C394	U395	G396	U397	C398	U399	A400	A401	A402	U403	A404	U405	G406	G411	A412	C413	A414	A415	A416	C417	C418	U419	C420	C421	C422	A423	G424	C425	C426	U427	A428	A429	A430	U431	A432	C433	U434	C435	C436	A439	U441	U442	A443	A444	A445	G446			
G317	C318	G319	A320	U321	A322	C323	A324	G325	G326	A330	C331	A332	C333	C334	C335	C336	C337	A340	A341	A342	A343	C344	A345	A346	A347	A348	C351	A352	C353	A354	U355	G356	C357	U360	A361	A362	C363	C364	U365	C366	G367	A368	U369	U370	A371	C372	U373	A374	G377	C378	G379	G380	C381	A382					
G254	A255	A256	A257	G258	G259	A262	G263	C264	A265	G266	C267	C268	C269	A270	G271	A272	G273	C274	C275	U276	G277	A278	A279	U280	C281	A282	G285	U288	G289	U290	G291	C292	U293	A294	C295	U296	G297	C298	A299	A300	G301	C302	C303	U304	C305	U306	G307	G308	A309	A310	G311	A312	C313	G314	C315	C316			
C192	U193	G194	A195	A196	A197	C198	A199	U200	G201	U202	A203	A204	G205	U206	C207	C208	C209	C210	C211	G212	A213	A216	A217	A218	A219	G220	A221	A222	A223	C224	C225	A226	A227	C228	U229	C230	A231	G232	A233	C236	C237	C238	C239	C240	A241	G242	U243	A244	G245	C246	A247	C183	C249	G250	A251	G252	C253		
U62	A63	A64	U65	C66	C69	G70	A71	U72	A73	A74	A75	C76	G77	C79	U82	A83	A84	G85	G86	U87	G88	A89	U90	A91	U92	A93	A94	A95	C96	C97	A98	U99	U100	A101	U102	A103	A104	C105	C106	G107	G108	C109	G110	A111	U112	U113	U114	C115	C116	G117	A118	A119	U120	G121	G122	G123			

G1087	U1148	G1219	U1344	G1478	A1544	C1606	A1668	G1731	C1793	U1855	A1918	A1978	G2038
A1088	G1149	G1220	C1345	G1479	A1545	C1607	A1669	C1732	A1794	U1856	A1919	U1979	U2039
A1089	C1150	G1221	G1346	U1480	G1546	A1608	G1670	G1733	C1795	G1857	G1920	G1980	A2042
A1090	A1151	U1282	A1347	U1481	C1547	A1609	U1671	G1734	U1796	A1858	G1921	A1981	C2043
C1091	C1152	G1283	C1348	U1415	A1548	A1610	A1672	A1735	G1797	G1859	G1922	G1982	C2044
C1092	G1153	G1223	C1349	G1416	A1549	C1611	G1673	G1736	U1798	G1860	G1923	G1983	G2045
C1093	G1154	U1224	C1350	G1417	C1550	C1612	G1674	G1738	G1799	G1861	C1924	G1984	C2046
U1094	A1155	G1225	C1351	A1418	A1551	G1613	C1675	A1739	C1800	G1862	G1925	C1985	G2047
A1095	A1156	A1226	U1352	U1419	A1552	A1614	U1676	G1740	A1801	G1863	U1926	C1986	C2048
A1096	G1157	G1227	A1353	A1420	A1553	C1615	A1677	C1741	A1802	U1864	A1927	A1987	C2049
U1097	C1158	G1228	A1354	U1490	U1554	A1616	A1678	U1742	A1803	U1865	A1928	G1988	C2050
A1098	U1159	C1229	G1355	G1492	G1555	C1617	A1679	G1743	C1804	A1866	G1929	G1989	A2051
G1099	G1160	A1230	C1356	C1493	C1556	A1618	U1680	A1744	A1805	G1867	G1930	C1990	A2052
C1100	C1161	G1231	C1357	G1425	C1557	G1619	G1681	A1745	C1806	C1868	U1931	U1991	G2053
U1101	G1164	U1233	G1358	A1427	C1558	G1620	U1682	U1746	G1807	G1869	U1932	G1992	A2054
C1102	A1165	A1234	A1359	A1496	U1559	U1621	G1683	U1747	A1808	C1870	C1933	U1993	C2055
A1103	G1166	G1235	G1360	U1497	G1560	G1622	G1684	C1748	A1809	A1871	C1934	C1994	C2056
C1104	G1167	G1236	G1361	U1498	C1561	G1623	G1685	A1749	A1810	A1872	G1935	U1995	C2057
U1105	C1167	A1237	C1362	C1499	U1562	U1624	C1686	G1750	G1813	G1873	G1936	C1996	A2058
G1106	G1168	G1238	C1363	A1502	U1563	G1625	A1689	U1751	G1814	C1874	C1937	C1997	A2059
U1107	A1169	G1239	C1364	A1503	C1564	A1626	G1695	C1752	G1815	G1875	A1938	A1998	A2060
U1108	C1170	U1240	A1365	A1504	C1565	G1627	A1690	G1753	A1816	A1876	U1939	C1999	A2061
C1109	G1171	A1241	A1366	A1505	A1566	G1628	C1691	A1754	C1817	A1877	U1940	C2000	C2062
G1110	C1172	U1242	A1367	A1506	G1567	U1629	U1692	A1755	G1818	G1878	C1941	C2001	C2063
A1111	U1173	C1243	G1368	U1507	G1568	A1630	U1693	G1756	U1819	C1879	C1942	C2002	C2064
G1112	U1174	A1244	G1369	C1507	A1569	G1631	C1694	A1757	A1819	U1880	U1943	A2003	C2065
U1113	A1175	G1245	C1370	A1508	C1570	A1632	G1695	U1758	G1820	C1881	G2004	G2004	C2066
C1114	U1176	A1246	G1371	A1509	A1571	G1633	G1696	A1759	A1821	U1882	U1945	A2005	G2067
G1115	G1177	U1247	U1372	G1510	A1572	A1634	U1697	C1760	C1822	U1883	U1946	C2006	C2068
U1116	C1177	A1248	A1373	G1511	G1573	A1635	G1698	C1761	G1823	G1884	C1947	U2007	A2070
C1117	C1178	U1249	G1376	G1512	C1574	U1636	G1699	A1762	G1824	A1885	G1948	C2008	A2071
U1118	U1183	G1250	C1377	A1515	C1575	A1637	A1700	G1763	U1825	U1886	G1949	A2009	C2072
C1119	U1184	C1251	U1377	A1518	U1576	C1638	A1701	C1764	G1826	C1887	G1950	G2010	C2073
G1120	G1185	G1252	A1378	C1519	C1577	C1639	G1702	U1765	U1827	G1888	A1952	U2011	U2074
U1121	G1186	A1253	C1379	U1520	U1578	A1640	G1703	G1768	G1828	A1889	A1953	A2013	U2075
G1122	A1189	A1254	U1255	G1521	A1580	G1642	C1704	U1769	A1829	A1890	G1954	A2014	U2076
G1123	G1256	U1256	G1382	G1522	G1581	G1643	C1705	G1770	C1830	G1891	U1955	A2015	C2078
G1124	C1257	C1257	A1383	U1523	C1582	C1644	G1707	C1771	C1832	C1893	U1956	U2016	C2079
U1125	A1194	U1258	A1384	U1524	A1583	G1645	C1708	A1772	C1833	C1894	C1957	U2017	A2080
G1126	G1195	G1259	A1385	G1524	U1584	C1646	U1709	A1773	U1834	C1895	C1958	A2018	U2081
A1127	C1196	C1260	C1386	A1525	C1585	U1647	G1710	C1774	G1835	G1905	A1966	A2019	A2082
G1128	G1197	C1261	A1387	U1526	A1586	U1648	U1711	U1775	C1836	A1899	C1967	C2020	G2083
U1129	U1198	A1262	G1388	C1527	G1587	G1649	U1712	G1776	C1837	A1900	C1968	C2021	C2084
G1132	U1199	U1263	U1389	G1528	A1590	A1650	A1713	U1777	C1838	A1901	C1969	C2022	U2085
U1133	C1200	U1264	U1390	A1529	A1591	G1651	G1714	U1778	G1839	C1902	U1970	C2023	U2086
A1134	U1201	A1265	C1461	G1530	C1592	A1652	G1715	U1779	G1840	G1905	G1910	G2024	G2087
C1135	A1204	G1266	C1462	C1531	A1593	G1653	U1716	A1780	U1841	C1906	C1912	C2025	A2088
G1136	A1205	U1267	C1463	A1532	U1594	A1654	A1717	U1781	G1842	G1907	A1913	U2026	C2089
U1137	G1206	A1268	A1395	C1533	C1595	A1655	G1718	U1782	C1843	C1908	A1914	G2027	A2090
G1138	C1207	A1269	U1396	U1534	A1596	C1656	U1719	A1783	C1844	C1909	C1914	U2028	C2091
C1139	C1208	G1270	U1397	A1535	A1597	U1657	U1720	A1784	G1847	G1909	G1910	G2029	U2092
U1140	U1209	G1271	C1398	C1536	U1598	C1658	G1721	A1785	A1848	C1910	C1911	G2030	G2093
U1141	C1210	A1272	C1399	G1537	U1599	G1659	A1722	U1786	U1849	U1911	G1912	A2031	A2094
U1142	G1211	U1273	A1400	G1538	G1601	U1662	C1726	C1788	G1850	A1913	G1913	G2032	A2095
A1143	C1212	A1274	G1401	U1539	A1602	G1663	U1727	A1789	U1851	C1914	C1914	G2033	C2096
U1144	A1213	A1275	U1402	G1471	U1602	A1664	C1727	A1789	U1852	U1915	C1915	U2034	A2097
A1145	C1214	G1276	A1403	C1472	A1603	A1665	U1728	A1789	U1853	U1916	G1916	C2035	U2098
C1146	G1215	A1277	A1404	U1542	A1604	G1666	U1729	A1791	A1853	A1916	U1917	G2036	C2099
U1147	G1216	C1278	U1405	G1543	C1605	G1667	C1730	G1792	A1854	U1917	A1977	A2037	G2100



- Molecule 56: 50S ribosomal protein L1



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	8375	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	161000	Depositor
Image detector	4k CCD camera (TVIPS)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	AB	0.72	0/1736	1.06	11/2340 (0.5%)
10	AK	0.75	0/894	1.17	11/1207 (0.9%)
11	AL	0.78	0/969	1.24	13/1300 (1.0%)
12	AM	0.75	0/884	1.29	13/1181 (1.1%)
13	AN	0.78	0/817	1.22	10/1088 (0.9%)
14	AO	0.73	0/722	1.14	9/964 (0.9%)
15	AP	0.78	0/648	1.21	7/870 (0.8%)
16	AQ	0.69	0/658	1.21	11/883 (1.2%)
17	AR	0.83	0/463	1.23	7/623 (1.1%)
18	AS	0.76	0/653	1.17	7/879 (0.8%)
19	AT	0.70	0/672	1.11	7/890 (0.8%)
2	AC	0.75	0/1651	1.13	14/2225 (0.6%)
20	AU	0.83	0/431	1.39	7/572 (1.2%)
21	AA	1.52	2/36759 (0.0%)	2.22	1945/57346 (3.4%)
22	A1	1.52	0/1668	2.16	80/2595 (3.1%)
23	A2	1.51	0/343	2.27	22/531 (4.1%)
24	A3	1.54	0/1722	2.21	92/2685 (3.4%)
25	BC	0.76	0/2121	1.32	27/2852 (0.9%)
26	BD	0.69	0/1586	1.14	10/2134 (0.5%)
27	BE	0.68	0/1571	1.18	13/2113 (0.6%)
28	BF	0.76	0/1444	1.15	11/1937 (0.6%)
29	BG	0.69	0/1343	1.16	9/1816 (0.5%)
3	AD	0.78	0/1665	1.20	20/2227 (0.9%)
30	BH	0.67	0/1122	1.14	6/1515 (0.4%)
31	BI	0.67	0/1046	1.04	3/1410 (0.2%)
32	BJ	0.75	0/1152	1.20	9/1551 (0.6%)
33	BK	0.72	0/947	1.25	11/1268 (0.9%)
34	BL	0.75	0/1054	1.38	15/1403 (1.1%)
35	BM	0.76	0/1093	1.25	14/1460 (1.0%)
36	BN	0.77	0/973	1.28	13/1301 (1.0%)
37	BO	0.75	0/902	1.25	13/1209 (1.1%)
38	BP	0.74	0/929	1.26	12/1242 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.82	0/960	1.35	17/1278 (1.3%)
4	AE	0.70	0/1119	1.01	8/1506 (0.5%)
40	BR	0.72	0/829	1.14	6/1107 (0.5%)
41	BS	0.66	0/864	1.18	6/1156 (0.5%)
42	BT	0.67	0/744	1.15	4/994 (0.4%)
43	BU	0.69	0/787	1.16	5/1051 (0.5%)
44	BV	0.74	0/766	1.13	4/1025 (0.4%)
45	BW	0.76	0/604	1.33	9/799 (1.1%)
46	BX	0.76	0/635	1.27	9/848 (1.1%)
47	BY	0.69	0/510	1.26	6/677 (0.9%)
48	BZ	0.70	0/453	1.24	5/605 (0.8%)
49	B0	0.74	0/450	1.17	3/599 (0.5%)
5	AF	0.74	0/835	1.16	8/1128 (0.7%)
50	B1	0.72	0/417	1.15	4/556 (0.7%)
51	B2	0.83	0/380	1.65	11/498 (2.2%)
52	B3	0.75	0/513	1.25	5/676 (0.7%)
53	B4	0.71	0/303	1.34	5/397 (1.3%)
54	BA	1.40	0/69796	2.21	4043/108888 (3.7%)
55	BB	1.41	0/2800	2.18	152/4367 (3.5%)
56	B5	0.67	0/1673	1.09	10/2255 (0.4%)
6	AG	0.74	0/1188	1.21	15/1593 (0.9%)
7	AH	0.71	0/989	1.03	6/1326 (0.5%)
8	AI	0.82	0/1035	1.31	19/1377 (1.4%)
9	AJ	0.71	0/797	1.18	8/1079 (0.7%)
All	All	1.28	2/160085 (0.0%)	2.00	6820/239402 (2.8%)

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
2	AC	0	1
21	AA	0	369
22	A1	0	10
23	A2	0	4
24	A3	0	19
37	BO	0	1
52	B3	0	1
54	BA	0	715
55	BB	0	28
6	AG	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	AH	0	1
All	All	0	1150

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1533	C	C4-N4	-5.16	1.29	1.33
21	AA	942	G	C5'-C4'	5.05	1.57	1.51

All (6820) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	704	A	N1-C6-N6	-13.07	110.76	118.60
54	BA	1274	A	N1-C6-N6	-12.32	111.21	118.60
34	BL	41	ARG	NE-CZ-NH1	12.26	126.43	120.30
54	BA	910	A	N1-C6-N6	-12.23	111.26	118.60
21	AA	913	A	N1-C6-N6	-12.01	111.40	118.60
22	A1	35	A	N1-C6-N6	-11.94	111.44	118.60
54	BA	1077	A	N1-C6-N6	-11.88	111.47	118.60
54	BA	783	A	N1-C6-N6	-11.83	111.50	118.60
54	BA	1213	A	N1-C6-N6	-11.82	111.50	118.60
54	BA	670	A	N1-C6-N6	-11.82	111.51	118.60
21	AA	576	C	C1'-O4'-C4'	-11.81	100.45	109.90
54	BA	2112	G	O4'-C1'-N9	11.79	117.63	108.20
51	B2	34	ARG	NE-CZ-NH1	11.75	126.18	120.30
21	AA	1155	A	N1-C6-N6	-11.63	111.62	118.60
54	BA	2872	A	N1-C6-N6	-11.56	111.66	118.60
54	BA	718	A	N1-C6-N6	-11.50	111.70	118.60
21	AA	1446	A	N1-C6-N6	-11.50	111.70	118.60
54	BA	845	A	N1-C6-N6	-11.47	111.72	118.60
21	AA	364	A	N1-C6-N6	-11.46	111.72	118.60
21	AA	622	A	N1-C6-N6	-11.37	111.78	118.60
21	AA	393	A	N1-C6-N6	-11.35	111.79	118.60
54	BA	1916	A	N1-C6-N6	-11.32	111.81	118.60
54	BA	2654	A	N1-C6-N6	-11.29	111.82	118.60
54	BA	1580	A	N1-C6-N6	-11.28	111.83	118.60
25	BC	86	ARG	NE-CZ-NH1	11.26	125.93	120.30
40	BR	80	ARG	NE-CZ-NH1	11.20	125.90	120.30
21	AA	71	A	N1-C6-N6	-11.16	111.90	118.60
54	BA	2030	A	N1-C6-N6	-11.13	111.92	118.60
21	AA	1275	A	N1-C6-N6	-11.10	111.94	118.60
21	AA	1311	A	N1-C6-N6	-11.06	111.96	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	864	A	N1-C6-N6	-11.06	111.97	118.60
21	AA	1468	A	N1-C6-N6	-11.02	111.99	118.60
54	BA	984	A	N1-C6-N6	-10.96	112.02	118.60
54	BA	1439	A	O4'-C1'-N9	10.96	116.97	108.20
54	BA	1630	A	N1-C6-N6	-10.96	112.03	118.60
15	AP	8	ARG	NE-CZ-NH1	10.93	125.77	120.30
54	BA	199	A	N1-C6-N6	-10.92	112.05	118.60
54	BA	1635	A	N1-C6-N6	-10.89	112.07	118.60
54	BA	91	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	49	A	N1-C6-N6	-10.86	112.08	118.60
54	BA	2095	A	N1-C6-N6	-10.85	112.09	118.60
54	BA	119	A	N1-C6-N6	-10.84	112.09	118.60
54	BA	574	A	N1-C6-N6	-10.82	112.11	118.60
54	BA	2660	A	O4'-C1'-N9	10.81	116.85	108.20
54	BA	1084	A	N1-C6-N6	-10.81	112.12	118.60
21	AA	162	A	N1-C6-N6	-10.80	112.12	118.60
21	AA	609	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	1503	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	1780	A	N1-C6-N6	-10.77	112.14	118.60
54	BA	2820	A	N1-C6-N6	-10.77	112.14	118.60
54	BA	1505	A	N1-C6-N6	-10.74	112.15	118.60
21	AA	243	A	N1-C6-N6	-10.74	112.16	118.60
54	BA	1829	A	N1-C6-N6	-10.71	112.17	118.60
54	BA	547	A	O4'-C1'-N9	10.69	116.75	108.20
54	BA	2590	A	N1-C6-N6	-10.68	112.19	118.60
54	BA	2666	C	N3-C2-O2	-10.67	114.43	121.90
21	AA	223	A	N1-C6-N6	-10.67	112.20	118.60
21	AA	782	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1637	A	N1-C6-N6	-10.65	112.21	118.60
21	AA	702	A	N1-C6-N6	-10.63	112.22	118.60
54	BA	2534	A	N1-C6-N6	-10.62	112.23	118.60
21	AA	1333	A	N1-C6-N6	-10.61	112.23	118.60
21	AA	1196	A	N1-C6-N6	-10.61	112.23	118.60
21	AA	716	A	N1-C6-N6	-10.58	112.25	118.60
54	BA	979	A	N1-C6-N6	-10.55	112.27	118.60
54	BA	95	A	N1-C6-N6	-10.55	112.27	118.60
54	BA	1067	A	N1-C6-N6	-10.53	112.28	118.60
21	AA	825	A	N1-C6-N6	-10.52	112.29	118.60
21	AA	1456	A	N1-C6-N6	-10.51	112.30	118.60
54	BA	844	A	N1-C6-N6	-10.51	112.30	118.60
54	BA	1679	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	1932	A	N1-C6-N6	-10.50	112.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2679	A	N1-C6-N6	-10.49	112.30	118.60
54	BA	2450	A	N1-C6-N6	-10.49	112.31	118.60
54	BA	2738	A	N1-C6-N6	-10.49	112.31	118.60
54	BA	2333	A	N1-C6-N6	-10.49	112.31	118.60
54	BA	1260	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	1420	A	N1-C6-N6	-10.47	112.32	118.60
21	AA	23	C	N3-C2-O2	-10.46	114.58	121.90
21	AA	493	A	N1-C6-N6	-10.45	112.33	118.60
54	BA	2163	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	603	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	1858	A	N1-C6-N6	-10.44	112.34	118.60
21	AA	1176	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	1129	A	N1-C6-N6	-10.40	112.36	118.60
21	AA	563	A	N1-C6-N6	-10.40	112.36	118.60
21	AA	665	A	N1-C6-N6	-10.39	112.36	118.60
54	BA	946	C	O4'-C1'-N1	10.38	116.51	108.20
27	BE	21	ARG	NE-CZ-NH1	10.38	125.49	120.30
21	AA	1101	A	N1-C6-N6	-10.38	112.37	118.60
54	BA	479	A	N1-C6-N6	-10.36	112.38	118.60
21	AA	520	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	2581	G	O4'-C1'-N9	10.34	116.47	108.20
54	BA	1301	A	N1-C6-N6	-10.34	112.40	118.60
54	BA	101	A	N1-C6-N6	-10.32	112.41	118.60
54	BA	1086	A	N1-C6-N6	-10.32	112.41	118.60
21	AA	279	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	309	A	N1-C6-N6	-10.31	112.42	118.60
54	BA	1853	A	N1-C6-N6	-10.31	112.42	118.60
54	BA	1392	A	N1-C6-N6	-10.30	112.42	118.60
21	AA	635	A	N1-C6-N6	-10.29	112.42	118.60
21	AA	1254	A	N1-C6-N6	-10.29	112.42	118.60
24	A3	38	A	N1-C6-N6	-10.29	112.42	118.60
54	BA	2423	U	O4'-C1'-N1	10.29	116.43	108.20
21	AA	509	A	N1-C6-N6	-10.29	112.43	118.60
21	AA	1476	A	N1-C6-N6	-10.29	112.43	118.60
54	BA	382	A	N1-C6-N6	-10.28	112.43	118.60
54	BA	1010	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	2108	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	2725	A	N1-C6-N6	-10.27	112.44	118.60
21	AA	648	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	699	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	2741	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	2461	A	N1-C6-N6	-10.25	112.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	780	A	N1-C6-N6	-10.23	112.46	118.60
34	BL	33	ARG	NE-CZ-NH1	10.23	125.42	120.30
54	BA	821	A	N1-C6-N6	-10.23	112.46	118.60
54	BA	1569	A	N1-C6-N6	-10.22	112.47	118.60
54	BA	2879	A	N1-C6-N6	-10.21	112.47	118.60
21	AA	495	A	N1-C6-N6	-10.21	112.48	118.60
54	BA	2614	A	N1-C6-N6	-10.21	112.48	118.60
54	BA	2418	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	504	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	2721	A	N1-C6-N6	-10.20	112.48	118.60
21	AA	994	A	N1-C6-N6	-10.19	112.49	118.60
54	BA	1854	A	N1-C6-N6	-10.18	112.50	118.60
54	BA	1755	A	N1-C6-N6	-10.17	112.50	118.60
21	AA	831	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	2711	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	1690	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	2322	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	171	A	N1-C6-N6	-10.14	112.52	118.60
21	AA	1014	A	N1-C6-N6	-10.13	112.52	118.60
21	AA	109	A	N1-C6-N6	-10.12	112.53	118.60
21	AA	196	A	N1-C6-N6	-10.12	112.53	118.60
21	AA	1239	A	N1-C6-N6	-10.12	112.53	118.60
54	BA	2281	A	N1-C6-N6	-10.12	112.53	118.60
54	BA	2761	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	1494	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	1433	A	N1-C6-N6	-10.10	112.54	118.60
39	BQ	69	ARG	NE-CZ-NH1	10.10	125.35	120.30
54	BA	2705	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	363	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	465	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	278	A	N1-C6-N6	-10.09	112.54	118.60
21	AA	794	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	1713	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	453	A	N1-C6-N6	-10.07	112.56	118.60
21	AA	344	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	1404	C	N3-C2-O2	-10.05	114.86	121.90
13	AN	81	ARG	NE-CZ-NH1	10.05	125.33	120.30
54	BA	716	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	222	A	N1-C6-N6	-10.04	112.57	118.60
54	BA	643	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	2270	A	N1-C6-N6	-10.04	112.58	118.60
21	AA	383	A	N1-C6-N6	-10.04	112.58	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AK	126	ARG	NE-CZ-NH2	10.04	125.32	120.30
54	BA	2135	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	905	A	N1-C6-N6	-10.03	112.58	118.60
21	AA	1531	A	N1-C6-N6	-10.02	112.59	118.60
54	BA	1142	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	845	A	N1-C6-N6	-10.01	112.59	118.60
54	BA	972	A	N1-C6-N6	-10.01	112.59	118.60
54	BA	1127	A	N1-C6-N6	-10.01	112.59	118.60
21	AA	72	A	N1-C6-N6	-10.01	112.60	118.60
44	BV	19	ARG	NE-CZ-NH1	10.01	125.30	120.30
54	BA	2169	A	O4'-C1'-N9	10.00	116.20	108.20
21	AA	747	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	1014	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	964	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	190	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	677	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	2134	A	N1-C6-N6	-9.96	112.63	118.60
54	BA	1021	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	1758	U	O4'-C1'-N1	9.95	116.16	108.20
54	BA	1598	A	N1-C6-N6	-9.95	112.63	118.60
55	BB	34	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	2893	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	2358	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	1211	C	O4'-C1'-N1	9.93	116.15	108.20
21	AA	139	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	26	A	N1-C6-N6	-9.92	112.65	118.60
26	BD	141	ARG	NE-CZ-NH1	9.91	125.26	120.30
21	AA	766	A	N1-C6-N6	-9.91	112.65	118.60
54	BA	2104	C	O4'-C1'-N1	9.91	116.13	108.20
21	AA	1256	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	2700	A	N1-C6-N6	-9.89	112.66	118.60
21	AA	958	A	N1-C6-N6	-9.89	112.67	118.60
21	AA	101	A	N1-C6-N6	-9.89	112.67	118.60
21	AA	629	A	N1-C6-N6	-9.89	112.67	118.60
54	BA	280	U	O4'-C1'-N1	9.88	116.11	108.20
21	AA	872	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	1427	A	N1-C6-N6	-9.87	112.68	118.60
5	AF	2	ARG	NE-CZ-NH1	9.86	125.23	120.30
21	AA	199	A	N1-C6-N6	-9.86	112.69	118.60
55	BB	46	A	N1-C6-N6	-9.86	112.69	118.60
54	BA	1805	A	N1-C6-N6	-9.85	112.69	118.60
21	AA	441	A	N1-C6-N6	-9.84	112.70	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2632	A	N1-C6-N6	-9.84	112.70	118.60
21	AA	1349	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	1347	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	2666	C	N1-C2-O2	9.83	124.80	118.90
54	BA	2448	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	2733	A	N1-C6-N6	-9.83	112.70	118.60
21	AA	116	A	N1-C6-N6	-9.83	112.70	118.60
21	AA	183	C	N3-C2-O2	-9.83	115.02	121.90
21	AA	389	A	N1-C6-N6	-9.83	112.70	118.60
8	AI	122	ARG	NE-CZ-NH1	9.82	125.21	120.30
54	BA	2060	A	N1-C6-N6	-9.82	112.70	118.60
21	AA	1267	C	N3-C2-O2	-9.82	115.03	121.90
54	BA	207	A	N1-C6-N6	-9.82	112.71	118.60
54	BA	1912	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	422	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	626	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	2154	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	1785	A	N1-C6-N6	-9.81	112.72	118.60
21	AA	7	A	N1-C6-N6	-9.81	112.72	118.60
24	A3	22	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	2386	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	1264	A	N1-C6-N6	-9.80	112.72	118.60
21	AA	1319	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	483	A	N1-C6-N6	-9.79	112.72	118.60
24	A3	44	A	N1-C6-N6	-9.79	112.73	118.60
54	BA	2042	A	N1-C6-N6	-9.79	112.73	118.60
21	AA	655	A	N1-C6-N6	-9.78	112.73	118.60
21	AA	1213	A	N1-C6-N6	-9.78	112.73	118.60
21	AA	59	A	N1-C6-N6	-9.76	112.75	118.60
21	AA	415	A	N1-C6-N6	-9.76	112.74	118.60
54	BA	1885	A	N1-C6-N6	-9.76	112.75	118.60
54	BA	99	U	O4'-C1'-N1	9.75	116.00	108.20
21	AA	595	A	N1-C6-N6	-9.75	112.75	118.60
21	AA	728	A	N1-C6-N6	-9.75	112.75	118.60
21	AA	1055	A	N1-C6-N6	-9.75	112.75	118.60
55	BB	78	A	N1-C6-N6	-9.74	112.75	118.60
54	BA	1678	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	2825	G	O4'-C1'-N9	9.73	115.98	108.20
54	BA	2169	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	793	A	N1-C6-N6	-9.72	112.77	118.60
21	AA	1447	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	2873	A	N1-C6-N6	-9.71	112.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	8	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	572	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	165	A	N1-C6-N6	-9.71	112.78	118.60
54	BA	2753	A	N1-C6-N6	-9.71	112.78	118.60
47	BY	7	ARG	NE-CZ-NH1	9.70	125.15	120.30
54	BA	886	A	N1-C6-N6	-9.69	112.78	118.60
54	BA	734	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	2675	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	492	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	505	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	1889	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	328	C	N3-C2-O2	-9.68	115.12	121.90
21	AA	1250	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	320	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	1495	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	1276	A	N1-C6-N6	-9.66	112.80	118.60
51	B2	33	ARG	NE-CZ-NH1	9.66	125.13	120.30
54	BA	2565	A	N1-C6-N6	-9.66	112.81	118.60
21	AA	608	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	142	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	861	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	936	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	1287	A	N1-C6-N6	-9.65	112.81	118.60
1	AB	107	ARG	NE-CZ-NH1	9.64	125.12	120.30
54	BA	900	A	N1-C6-N6	-9.63	112.82	118.60
21	AA	1251	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	1809	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	1942	C	N3-C2-O2	-9.62	115.16	121.90
54	BA	362	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1451	C	N3-C2-O2	-9.62	115.17	121.90
54	BA	1156	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	996	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	1918	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	130	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	1701	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	13	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	28	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	330	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	1307	A	N1-C6-N6	-9.60	112.84	118.60
55	BB	15	A	O4'-C1'-N9	9.60	115.88	108.20
54	BA	482	A	N1-C6-N6	-9.60	112.84	118.60
21	AA	968	A	N1-C6-N6	-9.59	112.85	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	730	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	896	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	2335	A	N1-C6-N6	-9.59	112.85	118.60
3	AD	12	ARG	NE-CZ-NH1	9.59	125.09	120.30
21	AA	313	A	N1-C6-N6	-9.59	112.85	118.60
21	AA	1434	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	2809	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1050	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1650	A	N1-C6-N6	-9.57	112.86	118.60
22	A1	41	A	N1-C6-N6	-9.56	112.86	118.60
55	BB	57	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	590	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	466	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	2670	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	1067	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	1046	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	1377	A	N1-C6-N6	-9.55	112.87	118.60
24	A3	73	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	2170	A	N1-C6-N6	-9.54	112.87	118.60
55	BB	109	A	N1-C6-N6	-9.54	112.88	118.60
21	AA	435	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	348	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	1677	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	532	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	1408	A	N1-C6-N6	-9.52	112.89	118.60
41	BS	25	ARG	NE-CZ-NH1	9.52	125.06	120.30
54	BA	502	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	192	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	892	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	1054	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	197	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	1275	A	N1-C6-N6	-9.50	112.90	118.60
3	AD	114	ARG	NE-CZ-NH1	9.50	125.05	120.30
54	BA	2147	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	627	A	N1-C6-N6	-9.49	112.90	118.60
54	BA	2381	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	1205	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	279	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	2434	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	126	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	300	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	718	A	O4'-C1'-N9	9.48	115.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AC	58	ARG	NE-CZ-NH1	9.48	125.04	120.30
21	AA	1502	A	N1-C6-N6	-9.48	112.91	118.60
34	BL	48	ARG	NE-CZ-NH1	9.47	125.04	120.30
55	BB	52	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	1418	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	743	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	1534	U	O4'-C1'-N1	9.46	115.77	108.20
21	AA	288	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	1201	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	1151	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1970	A	N1-C6-N6	-9.44	112.93	118.60
21	AA	172	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	2328	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	1508	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	1238	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	980	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	1398	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	1262	A	N1-C6-N6	-9.43	112.94	118.60
6	AG	108	ARG	NE-CZ-NH1	9.43	125.01	120.30
54	BA	1808	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	575	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	1194	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	2406	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	127	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	194	C	N3-C2-O2	-9.42	115.31	121.90
54	BA	1890	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1762	A	N1-C6-N6	-9.41	112.95	118.60
22	A1	69	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	1711	A	N1-C6-N6	-9.41	112.96	118.60
54	BA	2031	A	N1-C6-N6	-9.41	112.96	118.60
21	AA	532	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	1288	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	784	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	2851	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	181	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	969	A	N1-C6-N6	-9.40	112.96	118.60
22	A1	58	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	644	A	N1-C6-N6	-9.39	112.96	118.60
54	BA	56	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	1126	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	1586	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	1928	A	N1-C6-N6	-9.39	112.97	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1535	A	O4'-C1'-N9	9.38	115.71	108.20
21	AA	642	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	1787	A	N1-C6-N6	-9.38	112.97	118.60
34	BL	60	ARG	NE-CZ-NH1	9.38	124.99	120.30
54	BA	1308	A	N1-C6-N6	-9.37	112.97	118.60
54	BA	1352	U	O4'-C1'-N1	9.37	115.70	108.20
54	BA	1509	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	901	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	783	A	C5-C6-N1	9.37	122.38	117.70
54	BA	1096	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	1214	C	N3-C2-O2	-9.36	115.35	121.90
54	BA	227	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	2076	U	O4'-C1'-N1	9.36	115.69	108.20
54	BA	2547	A	N1-C6-N6	-9.36	112.99	118.60
54	BA	1937	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	599	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	439	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	1241	A	N1-C6-N6	-9.34	112.99	118.60
54	BA	2666	C	O4'-C1'-N1	9.34	115.67	108.20
54	BA	2094	A	N1-C6-N6	-9.34	113.00	118.60
55	BB	15	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	654	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	547	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	613	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	2199	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	315	A	N1-C6-N6	-9.32	113.01	118.60
35	BM	55	ARG	NE-CZ-NH2	9.32	124.96	120.30
21	AA	1082	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	151	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	909	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	1191	A	N1-C6-N6	-9.31	113.01	118.60
34	BL	78	ARG	NE-CZ-NH1	9.31	124.95	120.30
54	BA	1459	G	O4'-C1'-N9	9.31	115.65	108.20
21	AA	179	A	N1-C6-N6	-9.31	113.02	118.60
54	BA	299	A	N1-C6-N6	-9.30	113.02	118.60
21	AA	205	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	988	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1204	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	2887	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	2284	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	10	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	523	A	N1-C6-N6	-9.29	113.03	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BE	114	ARG	NE-CZ-NH1	9.28	124.94	120.30
54	BA	428	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	743	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	5	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	423	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	2433	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	1021	A	N1-C6-N6	-9.26	113.04	118.60
21	AA	576	C	O4'-C1'-N1	9.26	115.61	108.20
21	AA	1289	A	N1-C6-N6	-9.26	113.04	118.60
54	BA	1739	A	N1-C6-N6	-9.26	113.05	118.60
54	BA	2377	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	1054	C	N3-C2-O2	-9.25	115.43	121.90
54	BA	478	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	2478	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	1669	A	N1-C6-N6	-9.24	113.06	118.60
21	AA	19	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	1359	A	N1-C6-N6	-9.24	113.06	118.60
21	AA	602	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	1877	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	16	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	371	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	1441	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	311	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1821	A	N1-C6-N6	-9.22	113.07	118.60
21	AA	461	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	1960	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	1772	A	N1-C6-N6	-9.21	113.07	118.60
21	AA	250	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	397	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	819	A	N1-C6-N6	-9.21	113.08	118.60
54	BA	347	A	N1-C6-N6	-9.21	113.08	118.60
54	BA	1919	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	1340	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	1265	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	1133	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	38	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	1470	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	1871	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	865	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	2080	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	1269	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	750	A	N1-C6-N6	-9.19	113.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AM	78	ARG	NE-CZ-NH1	9.18	124.89	120.30
54	BA	354	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	2792	A	N1-C6-N6	-9.18	113.09	118.60
21	AA	23	C	N1-C2-O2	9.17	124.40	118.90
54	BA	371	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	800	A	N1-C6-N6	-9.17	113.10	118.60
29	BG	94	ARG	NE-CZ-NH1	9.17	124.88	120.30
53	B4	36	ARG	NE-CZ-NH1	9.16	124.88	120.30
54	BA	1286	A	N1-C6-N6	-9.16	113.10	118.60
30	BH	123	ARG	NE-CZ-NH1	9.16	124.88	120.30
52	B3	7	ARG	NE-CZ-NH1	9.16	124.88	120.30
54	BA	1009	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2309	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	889	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	262	A	N1-C6-N6	-9.14	113.11	118.60
54	BA	2119	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	749	A	N1-C6-N6	-9.14	113.12	118.60
22	A1	76	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	1731	G	O4'-C1'-N9	9.14	115.51	108.20
54	BA	2726	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	1430	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	1248	A	N1-C6-N6	-9.12	113.13	118.60
24	A3	11	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1929	G	O4'-C1'-N9	9.12	115.49	108.20
21	AA	328	C	N1-C2-O2	9.12	124.37	118.90
54	BA	2273	A	N1-C6-N6	-9.12	113.13	118.60
23	A2	79	A	N1-C6-N6	-9.11	113.13	118.60
24	A3	60	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	933	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	631	A	N1-C6-N6	-9.11	113.14	118.60
38	BP	88	ARG	NE-CZ-NH2	-9.10	115.75	120.30
54	BA	1246	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2211	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2241	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	941	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	947	A	N1-C6-N6	-9.10	113.14	118.60
3	AD	153	ARG	NE-CZ-NH1	9.09	124.84	120.30
54	BA	1384	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	937	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	1597	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	1518	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	1171	A	N1-C6-N6	-9.07	113.16	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1584	U	O4'-C1'-N1	9.07	115.46	108.20
54	BA	454	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	675	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	256	A	N1-C6-N6	-9.06	113.16	118.60
37	BO	16	ARG	NE-CZ-NH1	9.06	124.83	120.30
54	BA	689	A	N1-C6-N6	-9.06	113.17	118.60
45	BW	19	ARG	NE-CZ-NH1	9.05	124.82	120.30
54	BA	675	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1268	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	2542	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	2587	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	2706	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1745	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	2051	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	2432	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	1070	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	1508	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	582	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2727	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	1197	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	866	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1321	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	2734	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	527	C	N3-C2-O2	-9.02	115.58	121.90
54	BA	2369	A	N1-C6-N6	-9.02	113.19	118.60
22	A1	73	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	306	A	N1-C6-N6	-9.01	113.19	118.60
22	A1	66	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	2058	A	N1-C6-N6	-9.01	113.19	118.60
21	AA	1329	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	346	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1532	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	125	A	N1-C6-N6	-8.99	113.20	118.60
54	BA	1419	A	N1-C6-N6	-8.99	113.20	118.60
21	AA	197	A	C5-C6-N1	8.99	122.20	117.70
21	AA	298	A	N1-C6-N6	-8.99	113.20	118.60
21	AA	456	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	1610	A	N1-C6-N6	-8.99	113.20	118.60
54	BA	1672	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	2835	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	2212	A	N1-C6-N6	-8.98	113.21	118.60
3	AD	110	ARG	NE-CZ-NH1	8.98	124.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1480	A	P-O3'-C3'	8.98	130.48	119.70
54	BA	782	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2317	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	1350	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	959	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1404	C	O4'-C1'-N1	8.96	115.37	108.20
54	BA	101	A	O4'-C1'-N9	8.96	115.37	108.20
54	BA	1801	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	265	A	N1-C6-N6	-8.96	113.23	118.60
21	AA	914	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	219	A	N1-C6-N6	-8.95	113.23	118.60
21	AA	270	A	N1-C6-N6	-8.94	113.24	118.60
51	B2	34	ARG	NE-CZ-NH2	-8.94	115.83	120.30
54	BA	155	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	94	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1247	A	N1-C6-N6	-8.93	113.24	118.60
17	AR	72	ARG	NE-CZ-NH1	8.93	124.77	120.30
31	BI	133	ARG	NE-CZ-NH1	8.93	124.77	120.30
54	BA	802	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	182	A	N1-C6-N6	-8.93	113.25	118.60
54	BA	633	A	N1-C6-N6	-8.93	113.25	118.60
54	BA	794	A	N1-C6-N6	-8.93	113.25	118.60
54	BA	928	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	1784	A	N1-C6-N6	-8.92	113.25	118.60
21	AA	1519	A	N1-C6-N6	-8.92	113.25	118.60
8	AI	17	ARG	NE-CZ-NH1	8.92	124.76	120.30
54	BA	1943	U	O4'-C1'-N1	8.92	115.33	108.20
54	BA	961	C	N3-C2-O2	-8.92	115.66	121.90
21	AA	768	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	2740	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	752	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1938	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1552	A	N1-C6-N6	-8.91	113.25	118.60
21	AA	718	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1759	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	547	A	C5-C6-N1	8.90	122.15	117.70
21	AA	411	A	N1-C6-N6	-8.89	113.26	118.60
54	BA	160	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	197	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	1093	A	N1-C6-N6	-8.89	113.27	118.60
54	BA	2132	U	O4'-C1'-N1	8.88	115.31	108.20
21	AA	81	A	N1-C6-N6	-8.88	113.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	246	A	N1-C6-N6	-8.88	113.27	118.60
29	BG	152	ARG	NE-CZ-NH1	8.88	124.74	120.30
54	BA	1320	C	N3-C2-O2	-8.88	115.68	121.90
56	B5	122	ARG	NE-CZ-NH1	8.88	124.74	120.30
54	BA	1214	A	N1-C6-N6	-8.88	113.28	118.60
54	BA	2298	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	183	C	O4'-C1'-N1	8.86	115.29	108.20
45	BW	76	ARG	NE-CZ-NH1	8.86	124.73	120.30
54	BA	1998	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	2516	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	789	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	1008	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	1429	A	N1-C6-N6	-8.84	113.29	118.60
54	BA	1439	A	N1-C6-N6	-8.84	113.29	118.60
54	BA	1393	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	1545	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	449	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	1088	A	N1-C6-N6	-8.83	113.30	118.60
21	AA	1318	A	N1-C6-N6	-8.83	113.31	118.60
11	AL	113	ARG	NE-CZ-NH1	8.82	124.71	120.30
33	BK	105	ARG	NE-CZ-NH1	8.82	124.71	120.30
54	BA	2482	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	1783	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	2858	C	O4'-C1'-N1	8.81	115.25	108.20
54	BA	2868	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	152	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1722	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	414	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	1394	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	2013	A	N1-C6-N6	-8.81	113.32	118.60
54	BA	982	C	O4'-C1'-N1	8.80	115.24	108.20
54	BA	2158	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	282	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	1404	C	N1-C2-O2	8.80	124.18	118.90
21	AA	338	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	2376	A	N1-C6-N6	-8.80	113.32	118.60
51	B2	14	ARG	NE-CZ-NH1	8.79	124.70	120.30
54	BA	877	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	1179	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	2288	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1048	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	696	A	N1-C6-N6	-8.79	113.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1876	A	N1-C6-N6	-8.78	113.33	118.60
23	A2	91	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	1067	A	C5-C6-N1	8.78	122.09	117.70
54	BA	2560	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	415	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1342	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1535	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1609	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	1145	A	C5-C6-N1	8.76	122.08	117.70
11	AL	93	ARG	NE-CZ-NH1	8.76	124.68	120.30
21	AA	906	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	681	A	N1-C6-N6	-8.76	113.35	118.60
54	BA	1027	A	N1-C6-N6	-8.76	113.35	118.60
54	BA	1981	A	N1-C6-N6	-8.76	113.35	118.60
55	BB	50	A	N1-C6-N6	-8.76	113.35	118.60
21	AA	1446	A	C5-C6-N1	8.75	122.08	117.70
5	AF	24	ARG	NE-CZ-NH1	8.75	124.67	120.30
54	BA	820	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	1966	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	1987	A	N1-C6-N6	-8.74	113.35	118.60
54	BA	2682	A	N1-C6-N6	-8.74	113.35	118.60
54	BA	1553	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1847	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	368	A	N1-C6-N6	-8.73	113.36	118.60
19	AT	73	ARG	NE-CZ-NH1	8.73	124.67	120.30
21	AA	263	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	487	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1515	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	608	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	22	C	N3-C2-O2	-8.72	115.79	121.90
54	BA	2539	C	O4'-C1'-N1	8.72	115.18	108.20
21	AA	345	C	N3-C2-O2	-8.72	115.80	121.90
54	BA	111	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	1363	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	412	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	1054	C	O4'-C1'-N1	8.72	115.17	108.20
21	AA	553	A	N1-C6-N6	-8.71	113.38	118.60
9	AJ	68	ARG	NE-CZ-NH1	8.71	124.65	120.30
54	BA	42	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	144	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	2639	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	2099	U	O4'-C1'-N1	8.70	115.16	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2227	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	1525	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	2104	C	N3-C2-O2	-8.69	115.82	121.90
54	BA	2412	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	1042	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	320	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	507	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1900	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	1170	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	119	A	C5-C6-N1	8.68	122.04	117.70
54	BA	819	A	C5-C6-N1	8.68	122.04	117.70
55	BB	45	A	C5-C6-N1	8.68	122.04	117.70
21	AA	274	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1434	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	753	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	2378	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	1092	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	2451	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	1544	A	N1-C6-N6	-8.66	113.41	118.60
54	BA	372	G	O4'-C1'-N9	8.65	115.12	108.20
54	BA	721	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	1413	A	N1-C6-N6	-8.65	113.41	118.60
55	BB	58	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	2766	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	189	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	1794	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	2439	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	514	A	N1-C6-N6	-8.63	113.42	118.60
55	BB	94	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	765	G	O4'-C1'-N9	8.63	115.11	108.20
54	BA	204	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	1169	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	804	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	356	A	N1-C6-N6	-8.62	113.43	118.60
27	BE	102	ARG	NE-CZ-NH1	8.62	124.61	120.30
2	AC	155	ARG	NE-CZ-NH1	8.61	124.61	120.30
21	AA	640	A	N1-C6-N6	-8.61	113.44	118.60
21	AA	50	A	N1-C6-N6	-8.61	113.44	118.60
21	AA	1012	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	44	A	N1-C6-N6	-8.60	113.44	118.60
2	AC	10	ARG	NE-CZ-NH1	8.60	124.60	120.30
54	BA	432	A	N1-C6-N6	-8.60	113.44	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	547	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1165	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	60	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	1229	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	2503	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	2070	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	432	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	1383	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	1253	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	161	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	2518	A	C5-C6-N1	8.58	121.99	117.70
54	BA	89	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	1754	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	1870	C	N3-C2-O2	-8.58	115.89	121.90
21	AA	607	A	N1-C6-N6	-8.58	113.45	118.60
42	BT	6	ARG	NE-CZ-NH1	8.58	124.59	120.30
54	BA	666	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	2336	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	573	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	706	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	802	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2426	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	2311	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	65	A	N1-C6-N6	-8.56	113.47	118.60
54	BA	2758	A	C5-C6-N1	8.56	121.98	117.70
54	BA	352	A	N1-C6-N6	-8.56	113.47	118.60
55	BB	59	A	N1-C6-N6	-8.56	113.47	118.60
54	BA	1040	A	C5-C6-N1	8.55	121.98	117.70
54	BA	2104	C	N1-C2-O2	8.55	124.03	118.90
54	BA	2184	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2411	A	C5-C6-N1	8.55	121.97	117.70
54	BA	1169	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	1090	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	429	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	2088	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	1095	A	O4'-C1'-N9	8.54	115.03	108.20
54	BA	1679	A	C5-C6-N1	8.54	121.97	117.70
21	AA	712	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	1616	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	241	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	896	A	C5-C6-N1	8.53	121.97	117.70
54	BA	1640	A	N1-C6-N6	-8.53	113.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2019	A	N1-C6-N6	-8.53	113.48	118.60
47	BY	29	ARG	NE-CZ-NH1	8.52	124.56	120.30
21	AA	349	A	N1-C6-N6	-8.51	113.50	118.60
24	A3	45	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1847	A	C5-C6-N1	8.51	121.95	117.70
21	AA	344	A	C5-C6-N1	8.51	121.95	117.70
54	BA	2173	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	2424	C	N3-C2-O2	-8.51	115.94	121.90
54	BA	2602	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	2198	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	238	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1175	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1269	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1689	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	282	A	C5-C6-N1	8.49	121.95	117.70
24	A3	58	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	430	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	1073	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	2327	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	1267	C	N1-C2-O2	8.48	123.99	118.90
54	BA	756	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	2476	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	600	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	2829	A	C5-C6-N1	8.48	121.94	117.70
25	BC	269	ARG	NE-CZ-NH2	8.48	124.54	120.30
54	BA	1717	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	2900	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	2799	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	2750	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	147	C	O4'-C1'-N1	8.46	114.97	108.20
55	BB	39	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	510	A	C5-C6-N1	8.46	121.93	117.70
21	AA	1201	A	C5-C6-N1	8.46	121.93	117.70
21	AA	1437	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1502	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	1428	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	592	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	53	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	780	A	C5-C6-N1	8.45	121.93	117.70
54	BA	1815	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	443	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	104	A	N1-C6-N6	-8.45	113.53	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	621	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2453	A	C5-C6-N1	8.45	121.92	117.70
6	AG	95	ARG	NE-CZ-NH1	8.44	124.52	120.30
54	BA	346	A	C5-C6-N1	8.44	121.92	117.70
54	BA	981	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	1219	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	899	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	1507	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	204	A	C5-C6-N1	8.44	121.92	117.70
21	AA	50	A	C5-C6-N1	8.43	121.91	117.70
54	BA	602	A	N1-C6-N6	-8.43	113.55	118.60
54	BA	2662	A	N1-C6-N6	-8.42	113.55	118.60
25	BC	68	ARG	NE-CZ-NH1	8.42	124.51	120.30
54	BA	1548	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2435	A	N1-C6-N6	-8.42	113.55	118.60
1	AB	138	ARG	NE-CZ-NH1	8.41	124.51	120.30
21	AA	1493	A	C5-C6-N1	8.41	121.90	117.70
54	BA	1392	A	C5-C6-N1	8.41	121.90	117.70
54	BA	2748	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	1044	A	N1-C6-N6	-8.40	113.56	118.60
23	A2	82	A	N1-C6-N6	-8.39	113.56	118.60
55	BB	15	A	C5-C6-N1	8.39	121.90	117.70
21	AA	315	A	C5-C6-N1	8.39	121.90	117.70
54	BA	2278	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2503	A	O4'-C1'-N9	8.39	114.91	108.20
21	AA	845	A	C5-C6-N1	8.38	121.89	117.70
54	BA	1786	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	1927	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	103	A	N1-C6-N6	-8.38	113.57	118.60
7	AH	83	ARG	NE-CZ-NH1	8.38	124.49	120.30
21	AA	373	A	N1-C6-N6	-8.38	113.58	118.60
21	AA	819	A	C5-C6-N1	8.37	121.89	117.70
21	AA	502	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	2274	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	452	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	1528	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	2287	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	1158	C	N3-C2-O2	-8.36	116.05	121.90
54	BA	1549	A	N1-C6-N6	-8.36	113.58	118.60
21	AA	325	A	N1-C6-N6	-8.36	113.59	118.60
54	BA	621	A	N1-C6-N6	-8.36	113.59	118.60
54	BA	2191	A	N1-C6-N6	-8.35	113.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2451	A	C5-C6-N1	8.35	121.88	117.70
21	AA	459	A	N1-C6-N6	-8.35	113.59	118.60
32	BJ	27	ARG	NE-CZ-NH1	8.35	124.47	120.30
54	BA	265	A	C5-C6-N1	8.35	121.87	117.70
54	BA	1069	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	2856	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	949	A	C5-C6-N1	8.34	121.87	117.70
54	BA	233	A	N1-C6-N6	-8.34	113.60	118.60
11	AL	35	ARG	NE-CZ-NH1	8.34	124.47	120.30
21	AA	754	C	N3-C2-O2	-8.34	116.07	121.90
54	BA	384	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	637	A	N1-C6-N6	-8.34	113.60	118.60
30	BH	50	ARG	NE-CZ-NH1	8.33	124.47	120.30
54	BA	1451	C	N1-C2-O2	8.33	123.90	118.90
21	AA	596	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	1375	A	N1-C6-N6	-8.33	113.60	118.60
51	B2	3	ARG	NE-CZ-NH2	8.33	124.46	120.30
54	BA	173	A	N1-C6-N6	-8.33	113.61	118.60
54	BA	2307	G	O4'-C1'-N9	8.33	114.86	108.20
54	BA	1057	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	1350	C	N3-C2-O2	-8.32	116.07	121.90
54	BA	1496	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	1373	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	2541	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	352	C	N3-C2-O2	-8.32	116.08	121.90
54	BA	2657	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	974	G	O4'-C1'-N9	8.31	114.85	108.20
54	BA	1367	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2406	A	C5-C6-N1	8.31	121.86	117.70
54	BA	2503	A	C5-C6-N1	8.31	121.86	117.70
12	AM	89	ARG	NE-CZ-NH1	8.31	124.45	120.30
54	BA	1080	A	N1-C6-N6	-8.31	113.62	118.60
37	BO	33	ARG	NE-CZ-NH1	8.31	124.45	120.30
54	BA	1913	A	N1-C6-N6	-8.30	113.62	118.60
21	AA	959	A	N1-C6-N6	-8.30	113.62	118.60
24	A3	74	A	C5-C6-N1	8.30	121.85	117.70
54	BA	222	A	C5-C6-N1	8.30	121.85	117.70
54	BA	1570	A	N1-C6-N6	-8.30	113.62	118.60
21	AA	1102	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	1469	A	N1-C6-N6	-8.30	113.62	118.60
21	AA	889	A	C5-C6-N1	8.30	121.85	117.70
54	BA	1977	A	N1-C6-N6	-8.30	113.62	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	472	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	1654	A	N1-C6-N6	-8.30	113.62	118.60
21	AA	792	A	N1-C6-N6	-8.29	113.62	118.60
21	AA	977	A	N1-C6-N6	-8.29	113.62	118.60
21	AA	807	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	2826	A	N1-C6-N6	-8.29	113.63	118.60
21	AA	687	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	2062	A	C5-C6-N1	8.28	121.84	117.70
21	AA	1430	A	C5-C6-N1	8.28	121.84	117.70
39	BQ	27	ARG	NE-CZ-NH1	8.28	124.44	120.30
54	BA	892	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	1431	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	1722	A	C5-C6-N1	8.27	121.84	117.70
54	BA	2614	A	C5-C6-N1	8.27	121.84	117.70
21	AA	746	A	N1-C6-N6	-8.27	113.64	118.60
55	BB	73	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	1016	A	N1-C6-N6	-8.26	113.64	118.60
21	AA	1503	A	C5-C6-N1	8.26	121.83	117.70
54	BA	483	A	C5-C6-N1	8.26	121.83	117.70
54	BA	131	A	N1-C6-N6	-8.26	113.65	118.60
54	BA	2497	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2530	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	1735	A	N1-C6-N6	-8.25	113.65	118.60
21	AA	32	A	C5-C6-N1	8.24	121.82	117.70
54	BA	322	A	N1-C6-N6	-8.24	113.65	118.60
55	BB	104	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1346	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	2117	A	C5-C6-N1	8.24	121.82	117.70
54	BA	2665	A	N1-C6-N6	-8.24	113.66	118.60
38	BP	20	ARG	NE-CZ-NH1	8.23	124.42	120.30
21	AA	574	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	768	A	C5-C6-N1	8.23	121.82	117.70
54	BA	1760	C	N3-C2-O2	-8.23	116.14	121.90
54	BA	2173	A	C5-C6-N1	8.23	121.81	117.70
7	AH	87	ARG	NE-CZ-NH2	8.22	124.41	120.30
21	AA	1306	A	N1-C6-N6	-8.22	113.67	118.60
19	AT	17	ARG	NE-CZ-NH1	8.22	124.41	120.30
21	AA	262	A	C5-C6-N1	8.22	121.81	117.70
21	AA	1513	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	353	A	O4'-C1'-N9	8.21	114.77	108.20
54	BA	2634	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	2860	A	N1-C6-N6	-8.21	113.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	728	A	C5-C6-N1	8.21	121.80	117.70
54	BA	1264	A	C5-C6-N1	8.21	121.80	117.70
21	AA	938	A	C5-C6-N1	8.20	121.80	117.70
54	BA	161	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	466	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1393	A	C5-C6-N1	8.20	121.80	117.70
54	BA	2054	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	1280	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	676	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	872	A	C1'-O4'-C4'	-8.19	103.35	109.90
54	BA	73	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	983	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2114	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	600	A	C5-C6-N1	8.19	121.79	117.70
37	BO	7	ARG	NE-CZ-NH1	8.18	124.39	120.30
18	AS	2	ARG	NE-CZ-NH1	8.18	124.39	120.30
54	BA	332	A	C5-C6-N1	8.18	121.79	117.70
54	BA	890	C	N3-C2-O2	-8.18	116.17	121.90
54	BA	1103	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	74	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	935	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	371	A	C5-C6-N1	8.18	121.79	117.70
54	BA	2297	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	673	A	N1-C6-N6	-8.17	113.70	118.60
21	AA	729	A	N1-C6-N6	-8.17	113.70	118.60
21	AA	1360	A	N1-C6-N6	-8.17	113.70	118.60
21	AA	1437	A	C5-C6-N1	8.17	121.78	117.70
54	BA	2584	U	O4'-C1'-N1	8.17	114.74	108.20
8	AI	79	ARG	NE-CZ-NH1	8.17	124.38	120.30
25	BC	188	ARG	NE-CZ-NH1	8.16	124.38	120.30
54	BA	829	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	909	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	1022	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	33	A	N1-C6-N6	-8.16	113.70	118.60
36	BN	96	ARG	NE-CZ-NH1	8.16	124.38	120.30
54	BA	1304	A	N1-C6-N6	-8.16	113.71	118.60
7	AH	113	ARG	NE-CZ-NH1	8.15	124.38	120.30
54	BA	2266	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1590	A	C5-C6-N1	8.14	121.77	117.70
54	BA	2198	A	O4'-C1'-N9	8.14	114.72	108.20
21	AA	1157	A	N1-C6-N6	-8.14	113.71	118.60
54	BA	911	A	N1-C6-N6	-8.14	113.71	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2163	A	C5-C6-N1	8.14	121.77	117.70
54	BA	2752	C	N3-C2-O2	-8.14	116.20	121.90
21	AA	51	A	N1-C6-N6	-8.14	113.72	118.60
21	AA	460	A	N1-C6-N6	-8.14	113.72	118.60
21	AA	663	A	C5-C6-N1	8.14	121.77	117.70
29	BG	148	ARG	NE-CZ-NH1	8.14	124.37	120.30
54	BA	146	A	C5-C6-N1	8.14	121.77	117.70
54	BA	661	A	N1-C6-N6	-8.14	113.72	118.60
21	AA	753	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	6	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	1952	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	2453	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1284	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1385	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1761	C	N3-C2-O2	-8.13	116.21	121.90
21	AA	393	A	C4-C5-C6	-8.13	112.94	117.00
21	AA	468	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	1150	A	N1-C6-N6	-8.12	113.72	118.60
48	BZ	29	ARG	NE-CZ-NH1	8.12	124.36	120.30
21	AA	98	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	2092	U	O4'-C1'-N1	8.12	114.70	108.20
21	AA	919	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	162	U	O4'-C1'-N1	8.12	114.69	108.20
54	BA	1354	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	706	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	1104	C	N3-C2-O2	-8.12	116.22	121.90
21	AA	78	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	1271	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2020	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	878	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	1254	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	1848	A	C5-C6-N1	8.11	121.75	117.70
21	AA	356	A	C5-C6-N1	8.10	121.75	117.70
54	BA	1366	A	C5-C6-N1	8.10	121.75	117.70
54	BA	2589	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	1396	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	2800	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	1132	C	N3-C2-O2	-8.10	116.23	121.90
12	AM	70	ARG	NE-CZ-NH1	8.10	124.35	120.30
21	AA	1299	A	N1-C6-N6	-8.10	113.74	118.60
34	BL	69	ARG	NE-CZ-NH1	8.10	124.35	120.30
54	BA	655	A	C5-C6-N1	8.10	121.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1652	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1746	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	815	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	742	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	982	C	N3-C2-O2	-8.09	116.24	121.90
54	BA	203	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	497	A	N1-C6-N6	-8.09	113.75	118.60
14	AO	87	ARG	NE-CZ-NH1	8.08	124.34	120.30
21	AA	152	A	C5-C6-N1	8.08	121.74	117.70
54	BA	1453	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	2101	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	49	A	C5-C6-N1	8.08	121.74	117.70
54	BA	592	A	C5-C6-N1	8.08	121.74	117.70
54	BA	1133	A	C5-C6-N1	8.08	121.74	117.70
54	BA	213	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	1936	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	788	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	1978	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	143	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	1901	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	21	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	152	A	N1-C6-N6	-8.06	113.76	118.60
35	BM	66	ARG	NE-CZ-NH1	8.06	124.33	120.30
43	BU	5	ARG	NE-CZ-NH1	8.06	124.33	120.30
18	AS	2	ARG	NE-CZ-NH2	-8.05	116.28	120.30
21	AA	327	A	N1-C6-N6	-8.05	113.77	118.60
22	A1	14	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	1314	C	N3-C2-O2	-8.05	116.27	121.90
21	AA	431	A	N1-C6-N6	-8.04	113.77	118.60
54	BA	1230	A	N1-C6-N6	-8.04	113.78	118.60
55	BB	99	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	412	A	C5-C6-N1	8.04	121.72	117.70
21	AA	1197	A	C5-C6-N1	8.04	121.72	117.70
21	AA	1257	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	2781	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	8	A	C5-C6-N1	8.03	121.72	117.70
44	BV	21	ARG	NE-CZ-NH1	8.03	124.32	120.30
21	AA	814	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	1872	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2736	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	533	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	1429	A	C5-C6-N1	8.03	121.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	58	A	C5-C6-N1	8.03	121.71	117.70
24	A3	74	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	108	G	O4'-C1'-N9	8.02	114.62	108.20
21	AA	183	C	N1-C2-O2	8.02	123.71	118.90
54	BA	1603	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	430	A	N1-C6-N6	-8.02	113.79	118.60
34	BL	123	ARG	NE-CZ-NH1	8.02	124.31	120.30
17	AR	56	ARG	NE-CZ-NH1	8.02	124.31	120.30
21	AA	1468	A	C5-C6-N1	8.02	121.71	117.70
54	BA	340	A	N1-C6-N6	-8.02	113.79	118.60
25	BC	216	ARG	NE-CZ-NH1	8.02	124.31	120.30
54	BA	668	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	1403	A	C5-C6-N1	8.01	121.71	117.70
54	BA	1134	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	1866	A	C5-C6-N1	8.01	121.70	117.70
21	AA	196	A	C5-C6-N1	8.01	121.70	117.70
21	AA	55	A	N1-C6-N6	-8.01	113.80	118.60
21	AA	523	A	C5-C6-N1	8.01	121.70	117.70
21	AA	946	A	N1-C6-N6	-8.01	113.80	118.60
25	BC	202	ARG	NE-CZ-NH1	8.01	124.30	120.30
54	BA	627	A	C5-C6-N1	8.01	121.70	117.70
54	BA	793	A	C5-C6-N1	8.01	121.70	117.70
54	BA	1028	A	C5-C6-N1	8.01	121.70	117.70
54	BA	1086	A	C5-C6-N1	8.01	121.70	117.70
54	BA	1302	A	C5-C6-N1	8.01	121.70	117.70
21	AA	759	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	321	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	621	A	C5-C6-N1	8.00	121.70	117.70
54	BA	1606	C	N3-C2-O2	-8.00	116.30	121.90
54	BA	2411	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1070	A	C5-C6-N1	7.99	121.70	117.70
54	BA	613	A	C5-C6-N1	7.99	121.69	117.70
54	BA	2476	A	C5-C6-N1	7.99	121.69	117.70
23	A2	79	A	C5-C6-N1	7.99	121.69	117.70
54	BA	2879	A	C5-C6-N1	7.99	121.69	117.70
54	BA	477	A	C5-C6-N1	7.99	121.69	117.70
54	BA	2430	A	C5-C6-N1	7.99	121.69	117.70
54	BA	2758	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	499	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	1269	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1046	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	2311	A	C5-C6-N1	7.98	121.69	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2682	A	C5-C6-N1	7.98	121.69	117.70
27	BE	170	ARG	NE-CZ-NH1	7.98	124.29	120.30
54	BA	196	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	546	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	101	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1286	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1641	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	1785	A	C5-C6-N1	7.98	121.69	117.70
21	AA	1196	A	C5-C6-N1	7.98	121.69	117.70
54	BA	761	A	N1-C6-N6	-7.98	113.81	118.60
47	BY	52	ARG	NE-CZ-NH1	7.97	124.29	120.30
54	BA	176	A	N1-C6-N6	-7.97	113.81	118.60
54	BA	345	A	N1-C6-N6	-7.97	113.81	118.60
54	BA	1551	A	C5-C6-N1	7.97	121.69	117.70
54	BA	311	A	C5-C6-N1	7.97	121.69	117.70
54	BA	1413	A	C5-C6-N1	7.97	121.69	117.70
54	BA	1111	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	583	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	146	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	2823	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	1403	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	2097	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	2158	A	C5-C6-N1	7.97	121.68	117.70
54	BA	2176	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	118	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	979	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1816	C	N3-C2-O2	-7.96	116.32	121.90
54	BA	2129	C	N3-C2-O2	-7.96	116.32	121.90
54	BA	2573	C	N3-C2-O2	-7.96	116.33	121.90
21	AA	978	A	N1-C6-N6	-7.96	113.83	118.60
54	BA	278	A	C5-C6-N1	7.96	121.68	117.70
54	BA	2776	A	P-O3'-C3'	7.96	129.25	119.70
21	AA	1413	A	N1-C6-N6	-7.95	113.83	118.60
35	BM	50	ARG	NE-CZ-NH1	7.95	124.28	120.30
21	AA	1117	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	1277	C	N3-C2-O2	-7.95	116.34	121.90
21	AA	228	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	878	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	1004	A	N1-C6-N6	-7.94	113.83	118.60
21	AA	1167	A	C5-C6-N1	7.94	121.67	117.70
21	AA	1257	A	C5-C6-N1	7.94	121.67	117.70
54	BA	457	A	N1-C6-N6	-7.94	113.83	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2635	A	N1-C6-N6	-7.94	113.83	118.60
21	AA	1054	C	N1-C2-O2	7.94	123.66	118.90
21	AA	253	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	1307	A	C5-C6-N1	7.94	121.67	117.70
54	BA	2062	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	2126	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	2154	A	C5-C6-N1	7.94	121.67	117.70
22	A1	6	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	71	A	C4-C5-C6	-7.93	113.03	117.00
34	BL	2	ARG	NE-CZ-NH1	7.93	124.26	120.30
21	AA	1339	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	2126	A	O4'-C1'-N9	7.93	114.54	108.20
28	BF	109	ARG	NE-CZ-NH1	7.92	124.26	120.30
54	BA	781	A	N1-C6-N6	-7.92	113.84	118.60
54	BA	2602	A	C5-C6-N1	7.92	121.66	117.70
54	BA	910	A	C5-C6-N1	7.92	121.66	117.70
54	BA	401	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1274	A	C5-C6-N1	7.91	121.66	117.70
54	BA	1705	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	2829	A	N1-C6-N6	-7.91	113.85	118.60
21	AA	408	A	N1-C6-N6	-7.91	113.85	118.60
21	AA	974	A	N1-C6-N6	-7.91	113.86	118.60
21	AA	1346	A	C5-C6-N1	7.91	121.65	117.70
54	BA	973	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	1353	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	1614	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	2378	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2856	A	C5-C6-N1	7.90	121.65	117.70
54	BA	172	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	2566	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1036	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	758	C	N3-C2-O2	-7.90	116.37	121.90
22	A1	76	A	C5-C6-N1	7.89	121.65	117.70
54	BA	241	A	C5-C6-N1	7.89	121.65	117.70
54	BA	1791	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	2469	A	N1-C6-N6	-7.89	113.86	118.60
21	AA	1031	C	N3-C2-O2	-7.89	116.38	121.90
21	AA	1251	A	C5-C6-N1	7.89	121.65	117.70
21	AA	968	A	C5-C6-N1	7.89	121.64	117.70
54	BA	497	A	C5-C6-N1	7.89	121.64	117.70
54	BA	2850	A	N1-C6-N6	-7.89	113.87	118.60
21	AA	1519	A	C5-C6-N1	7.88	121.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1634	A	N1-C6-N6	-7.88	113.87	118.60
21	AA	364	A	C5-C6-N1	7.88	121.64	117.70
54	BA	506	G	O4'-C1'-N9	7.88	114.50	108.20
54	BA	2598	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	1890	A	C5-C6-N1	7.88	121.64	117.70
54	BA	71	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1211	C	N3-C2-O2	-7.88	116.39	121.90
54	BA	739	A	N1-C6-N6	-7.88	113.88	118.60
54	BA	800	A	C4-C5-C6	-7.88	113.06	117.00
54	BA	1126	A	C5-C6-N1	7.88	121.64	117.70
54	BA	2340	A	C5-C6-N1	7.88	121.64	117.70
2	AC	178	ARG	NE-CZ-NH1	7.87	124.24	120.30
3	AD	80	ARG	NE-CZ-NH1	7.87	124.24	120.30
54	BA	1155	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	1275	A	C5-C6-N1	7.87	121.64	117.70
16	AQ	5	ARG	NE-CZ-NH1	7.87	124.23	120.30
54	BA	1618	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	1534	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	1383	A	C5-C6-N1	7.87	121.63	117.70
21	AA	171	A	C5-C6-N1	7.87	121.63	117.70
21	AA	704	A	C4-C5-C6	-7.87	113.07	117.00
52	B3	29	ARG	NE-CZ-NH1	7.87	124.23	120.30
54	BA	1008	A	C5-C6-N1	7.87	121.63	117.70
54	BA	2266	A	C5-C6-N1	7.87	121.63	117.70
54	BA	2572	A	C5-C6-N1	7.87	121.63	117.70
54	BA	1953	A	C5-C6-N1	7.86	121.63	117.70
4	AE	68	ARG	NE-CZ-NH1	7.86	124.23	120.30
21	AA	914	A	C5-C6-N1	7.86	121.63	117.70
54	BA	19	A	N1-C6-N6	-7.86	113.88	118.60
21	AA	831	A	C4-C5-C6	-7.86	113.07	117.00
54	BA	156	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	199	A	C5-C6-N1	7.86	121.63	117.70
54	BA	556	A	N1-C6-N6	-7.86	113.88	118.60
21	AA	120	A	C5-C6-N1	7.86	121.63	117.70
44	BV	93	ARG	NE-CZ-NH1	7.86	124.23	120.30
54	BA	984	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1698	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	1952	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2837	A	N1-C6-N6	-7.86	113.89	118.60
34	BL	59	ARG	NE-CZ-NH1	7.85	124.23	120.30
54	BA	1029	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	1522	A	N1-C6-N6	-7.85	113.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	115	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2501	C	N3-C2-O2	-7.85	116.41	121.90
54	BA	2590	A	C4-C5-C6	-7.85	113.08	117.00
54	BA	1433	A	C5-C6-N1	7.85	121.62	117.70
54	BA	1912	A	C5-C6-N1	7.85	121.62	117.70
21	AA	539	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2564	A	N1-C6-N6	-7.84	113.89	118.60
55	BB	109	A	C5-C6-N1	7.84	121.62	117.70
21	AA	1483	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	927	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	1089	A	C5-C6-N1	7.84	121.62	117.70
21	AA	306	A	C5-C6-N1	7.84	121.62	117.70
21	AA	510	A	N1-C6-N6	-7.84	113.90	118.60
21	AA	781	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	2660	A	N1-C6-N6	-7.84	113.90	118.60
37	BO	9	ARG	NE-CZ-NH1	7.84	124.22	120.30
54	BA	275	C	N3-C2-O2	-7.84	116.41	121.90
54	BA	722	A	N1-C6-N6	-7.84	113.90	118.60
21	AA	1493	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	435	A	C5-C6-N1	7.83	121.62	117.70
21	AA	573	A	C5-C6-N1	7.83	121.62	117.70
54	BA	270	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	1105	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1469	A	C5-C6-N1	7.83	121.61	117.70
54	BA	2126	A	C5-C6-N1	7.83	121.61	117.70
55	BB	57	A	C5-C6-N1	7.83	121.61	117.70
38	BP	38	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	221	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	983	A	C5-C6-N1	7.82	121.61	117.70
54	BA	2145	C	N3-C2-O2	-7.82	116.43	121.90
54	BA	739	A	C5-C6-N1	7.82	121.61	117.70
39	BQ	54	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	2459	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	2712	C	N3-C2-O2	-7.82	116.43	121.90
24	A3	17	C	N3-C2-O2	-7.81	116.43	121.90
24	A3	40	C	N3-C2-O2	-7.81	116.43	121.90
21	AA	189	A	C5-C6-N1	7.81	121.61	117.70
54	BA	344	A	N1-C6-N6	-7.81	113.92	118.60
54	BA	1214	A	C5-C6-N1	7.81	121.60	117.70
54	BA	1829	A	C5-C6-N1	7.81	121.60	117.70
33	BK	49	ARG	NE-CZ-NH1	7.81	124.20	120.30
54	BA	1040	A	N1-C6-N6	-7.81	113.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2868	A	C5-C6-N1	7.81	121.60	117.70
54	BA	563	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	1328	A	C5-C6-N1	7.80	121.60	117.70
21	AA	549	C	N3-C2-O2	-7.80	116.44	121.90
46	BX	71	ARG	NE-CZ-NH1	7.80	124.20	120.30
21	AA	149	A	C5-C6-N1	7.80	121.60	117.70
21	AA	465	A	C5-C6-N1	7.80	121.60	117.70
54	BA	1302	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	2482	A	C5-C6-N1	7.80	121.60	117.70
54	BA	2531	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	715	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	1189	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	622	A	C5-C6-N1	7.80	121.60	117.70
54	BA	73	A	C5-C6-N1	7.79	121.60	117.70
21	AA	1237	C	N3-C2-O2	-7.79	116.44	121.90
24	A3	77	A	C5-C6-N1	7.79	121.60	117.70
9	AJ	16	ARG	NE-CZ-NH1	7.79	124.19	120.30
21	AA	1030	U	O4'-C1'-N1	7.79	114.43	108.20
54	BA	715	A	C5-C6-N1	7.79	121.59	117.70
54	BA	829	A	C5-C6-N1	7.79	121.59	117.70
54	BA	1634	A	C5-C6-N1	7.79	121.59	117.70
22	A1	21	A	N1-C6-N6	-7.79	113.93	118.60
22	A1	23	A	C5-C6-N1	7.79	121.59	117.70
54	BA	980	A	C5-C6-N1	7.79	121.59	117.70
54	BA	2281	A	C5-C6-N1	7.79	121.59	117.70
21	AA	493	A	C5-C6-N1	7.78	121.59	117.70
21	AA	676	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	1256	A	C5-C6-N1	7.78	121.59	117.70
54	BA	931	U	O4'-C1'-N1	7.78	114.42	108.20
54	BA	1009	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1357	A	N1-C6-N6	-7.78	113.93	118.60
22	A1	36	C	N3-C2-O2	-7.78	116.45	121.90
39	BQ	10	ARG	NE-CZ-NH1	7.78	124.19	120.30
54	BA	270	A	C5-C6-N1	7.78	121.59	117.70
54	BA	466	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2369	A	C5-C6-N1	7.78	121.59	117.70
21	AA	59	A	C5-C6-N1	7.78	121.59	117.70
21	AA	554	A	N1-C6-N6	-7.78	113.93	118.60
33	BK	18	ARG	NE-CZ-NH1	7.78	124.19	120.30
54	BA	752	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2872	A	C5-C6-N1	7.77	121.59	117.70
21	AA	1333	A	C5-C6-N1	7.77	121.58	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1513	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2082	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	397	A	C5-C6-N1	7.76	121.58	117.70
21	AA	1374	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	2309	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2042	A	C5-C6-N1	7.76	121.58	117.70
21	AA	101	A	C5-C6-N1	7.76	121.58	117.70
21	AA	267	C	N3-C2-O2	-7.76	116.47	121.90
54	BA	228	C	N3-C2-O2	-7.76	116.47	121.90
54	BA	1244	A	C5-C6-N1	7.76	121.58	117.70
55	BB	12	C	N3-C2-O2	-7.76	116.47	121.90
13	AN	85	ARG	NE-CZ-NH1	7.76	124.18	120.30
21	AA	51	A	C5-C6-N1	7.76	121.58	117.70
21	AA	119	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	83	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1365	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2850	A	C5-C6-N1	7.76	121.58	117.70
21	AA	1005	A	N1-C6-N6	-7.76	113.95	118.60
21	AA	1183	U	O4'-C1'-N1	7.76	114.41	108.20
21	AA	574	A	C5-C6-N1	7.75	121.58	117.70
54	BA	1332	G	O4'-C1'-N9	7.75	114.40	108.20
54	BA	1536	C	N3-C2-O2	-7.75	116.47	121.90
54	BA	2036	C	N3-C2-O2	-7.75	116.47	121.90
54	BA	2820	A	C5-C6-N1	7.75	121.58	117.70
21	AA	499	A	C5-C6-N1	7.75	121.57	117.70
22	A1	58	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1368	A	C5-C6-N1	7.75	121.57	117.70
32	BJ	120	ARG	NE-CZ-NH1	7.75	124.17	120.30
54	BA	1803	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	2813	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1050	A	C5-C6-N1	7.75	121.57	117.70
8	AI	129	ARG	NE-CZ-NH1	7.74	124.17	120.30
54	BA	324	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	1029	A	C5-C6-N1	7.74	121.57	117.70
21	AA	461	A	C5-C6-N1	7.74	121.57	117.70
54	BA	945	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	1020	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	1089	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	2459	A	C5-C6-N1	7.74	121.57	117.70
54	BA	111	A	C5-C6-N1	7.74	121.57	117.70
54	BA	282	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	2726	A	C5-C6-N1	7.74	121.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	59	A	N1-C6-N6	-7.73	113.96	118.60
10	AK	55	ARG	NE-CZ-NH1	7.73	124.17	120.30
54	BA	223	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	323	C	N3-C2-O2	-7.73	116.49	121.90
54	BA	2346	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	83	A	C5-C6-N1	7.72	121.56	117.70
54	BA	2013	A	C5-C6-N1	7.72	121.56	117.70
54	BA	2590	A	C5-C6-N1	7.72	121.56	117.70
21	AA	977	A	C5-C6-N1	7.72	121.56	117.70
21	AA	412	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	687	A	C5-C6-N1	7.72	121.56	117.70
21	AA	1216	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2297	A	C5-C6-N1	7.72	121.56	117.70
54	BA	71	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	1134	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1151	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	1571	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	1593	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2610	C	N3-C2-O2	-7.72	116.50	121.90
21	AA	353	A	C5-C6-N1	7.71	121.56	117.70
21	AA	363	A	C5-C6-N1	7.71	121.56	117.70
54	BA	1549	A	C5-C6-N1	7.71	121.56	117.70
54	BA	1615	C	N3-C2-O2	-7.71	116.50	121.90
54	BA	2478	A	C5-C6-N1	7.71	121.56	117.70
54	BA	849	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	383	A	C5-C6-N1	7.71	121.56	117.70
54	BA	472	A	C5-C6-N1	7.71	121.56	117.70
21	AA	579	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	629	A	C5-C6-N1	7.71	121.56	117.70
54	BA	1762	A	C5-C6-N1	7.71	121.56	117.70
21	AA	1318	A	C5-C6-N1	7.71	121.55	117.70
41	BS	92	ARG	NE-CZ-NH1	7.71	124.15	120.30
54	BA	1069	A	C5-C6-N1	7.71	121.55	117.70
54	BA	2516	A	C4-C5-C6	-7.71	113.14	117.00
21	AA	274	A	C5-C6-N1	7.71	121.55	117.70
21	AA	609	A	C5-C6-N1	7.71	121.55	117.70
25	BC	270	ARG	NE-CZ-NH1	7.71	124.15	120.30
54	BA	84	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	2513	A	C5-C6-N1	7.71	121.55	117.70
21	AA	279	A	C5-C6-N1	7.70	121.55	117.70
21	AA	915	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	609	A	N1-C6-N6	-7.70	113.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2422	C	N3-C2-O2	-7.70	116.51	121.90
27	BE	61	ARG	NE-CZ-NH1	7.70	124.15	120.30
54	BA	727	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	845	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1938	A	C5-C6-N1	7.70	121.55	117.70
54	BA	226	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1032	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1321	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2776	A	N1-C6-N6	-7.70	113.98	118.60
16	AQ	26	ARG	NE-CZ-NH1	7.70	124.15	120.30
21	AA	906	A	C5-C6-N1	7.70	121.55	117.70
21	AA	915	A	C5-C6-N1	7.70	121.55	117.70
21	AA	161	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2883	A	C5-C6-N1	7.70	121.55	117.70
54	BA	620	G	N3-C2-N2	-7.69	114.52	119.90
54	BA	1871	A	C5-C6-N1	7.69	121.55	117.70
21	AA	1000	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	2170	A	C5-C6-N1	7.69	121.55	117.70
21	AA	190	A	C5-C6-N1	7.69	121.54	117.70
21	AA	767	A	N1-C6-N6	-7.69	113.99	118.60
36	BN	118	ARG	NE-CZ-NH1	7.69	124.14	120.30
54	BA	332	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	979	A	C4-C5-C6	-7.69	113.16	117.00
54	BA	1378	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	2614	A	C4-C5-C6	-7.69	113.16	117.00
54	BA	1630	A	C4-C5-C6	-7.68	113.16	117.00
21	AA	900	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	1252	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1265	A	C5-C6-N1	7.68	121.54	117.70
54	BA	2556	C	N3-C2-O2	-7.68	116.52	121.90
21	AA	282	A	C4-C5-C6	-7.68	113.16	117.00
54	BA	2746	U	O4'-C1'-N1	7.68	114.34	108.20
15	AP	5	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	943	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1941	C	N3-C2-O2	-7.68	116.53	121.90
54	BA	2037	A	N1-C6-N6	-7.68	113.99	118.60
22	A1	66	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1327	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	949	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	1095	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2654	A	C5-C6-N1	7.68	121.54	117.70
55	BB	29	A	C5-C6-N1	7.67	121.54	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	195	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	675	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1477	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2117	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	118	A	C5-C6-N1	7.67	121.53	117.70
54	BA	515	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	702	A	C5-C6-N1	7.67	121.53	117.70
54	BA	63	A	N1-C6-N6	-7.66	114.00	118.60
54	BA	429	A	C5-C6-N1	7.66	121.53	117.70
54	BA	753	A	C5-C6-N1	7.66	121.53	117.70
21	AA	1155	A	C4-C5-C6	-7.66	113.17	117.00
21	AA	131	A	N1-C6-N6	-7.66	114.01	118.60
21	AA	900	A	C5-C6-N1	7.65	121.53	117.70
54	BA	693	A	C5-C6-N1	7.65	121.53	117.70
55	BB	109	A	O4'-C1'-N9	7.65	114.32	108.20
54	BA	693	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	2227	A	C5-C6-N1	7.65	121.53	117.70
21	AA	182	A	C5-C6-N1	7.65	121.53	117.70
24	A3	45	A	C5-C6-N1	7.65	121.53	117.70
21	AA	572	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	899	A	C5-C6-N1	7.65	121.52	117.70
8	AI	48	ARG	NE-CZ-NH1	7.65	124.12	120.30
54	BA	574	A	C5-C6-N1	7.64	121.52	117.70
21	AA	1167	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	328	C	O4'-C1'-N1	7.64	114.31	108.20
21	AA	60	A	C5-C6-N1	7.64	121.52	117.70
25	BC	174	ARG	NE-CZ-NH1	7.64	124.12	120.30
54	BA	614	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	761	A	C5-C6-N1	7.64	121.52	117.70
21	AA	967	C	N3-C2-O2	-7.64	116.55	121.90
54	BA	635	C	O4'-C1'-N1	7.64	114.31	108.20
54	BA	1287	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	2565	A	C5-C6-N1	7.64	121.52	117.70
21	AA	1225	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	1384	A	C5-C6-N1	7.63	121.52	117.70
54	BA	2090	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	2183	A	C5-C6-N1	7.63	121.52	117.70
21	AA	983	A	C5-C6-N1	7.63	121.52	117.70
54	BA	990	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	1287	A	C5-C6-N1	7.63	121.52	117.70
54	BA	1085	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	1749	A	N1-C6-N6	-7.63	114.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	802	A	C5-C6-N1	7.63	121.51	117.70
54	BA	1010	A	C5-C6-N1	7.63	121.52	117.70
21	AA	327	A	C5-C6-N1	7.63	121.51	117.70
21	AA	535	A	N1-C6-N6	-7.63	114.02	118.60
22	A1	38	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1966	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2171	A	O4'-C1'-N9	7.62	114.30	108.20
20	AU	32	ARG	NE-CZ-NH1	7.62	124.11	120.30
54	BA	603	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2576	G	O4'-C1'-N9	7.62	114.30	108.20
32	BJ	37	ARG	NE-CZ-NH1	7.62	124.11	120.30
54	BA	279	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1470	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1877	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2051	A	C5-C6-N1	7.62	121.51	117.70
21	AA	28	A	C5-C6-N1	7.61	121.51	117.70
54	BA	1376	C	O4'-C1'-N1	7.61	114.29	108.20
54	BA	294	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	249	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	262	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	309	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	923	A	C5-C6-N1	7.61	121.50	117.70
25	BC	261	ARG	NE-CZ-NH1	7.61	124.10	120.30
24	A3	16	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	1789	A	C5-C6-N1	7.61	121.50	117.70
21	AA	33	A	C5-C6-N1	7.61	121.50	117.70
21	AA	648	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1270	C	N3-C2-O2	-7.61	116.58	121.90
54	BA	1608	A	N1-C6-N6	-7.61	114.04	118.60
54	BA	2288	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1773	A	C5-C6-N1	7.60	121.50	117.70
21	AA	313	A	C5-C6-N1	7.60	121.50	117.70
53	B4	4	ARG	NE-CZ-NH1	7.60	124.10	120.30
54	BA	1789	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	1936	A	C5-C6-N1	7.60	121.50	117.70
21	AA	120	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	1465	A	N1-C6-N6	-7.60	114.04	118.60
33	BK	78	ARG	NE-CZ-NH1	7.60	124.10	120.30
21	AA	695	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	1281	C	N3-C2-O2	-7.59	116.58	121.90
54	BA	1650	A	C5-C6-N1	7.59	121.50	117.70
24	A3	36	A	C5-C6-N1	7.59	121.50	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2764	A	C5-C6-N1	7.59	121.50	117.70
21	AA	501	C	N3-C2-O2	-7.59	116.58	121.90
21	AA	1507	A	C5-C6-N1	7.59	121.50	117.70
54	BA	2171	A	N1-C6-N6	-7.59	114.05	118.60
21	AA	451	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	1354	A	C5-C6-N1	7.59	121.49	117.70
21	AA	1434	A	C5-C6-N1	7.59	121.49	117.70
54	BA	1284	A	C5-C6-N1	7.59	121.49	117.70
54	BA	2764	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	2766	A	C5-C6-N1	7.59	121.49	117.70
21	AA	1287	A	C5-C6-N1	7.58	121.49	117.70
22	A1	60	C	N3-C2-O2	-7.58	116.59	121.90
54	BA	217	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	342	A	C5-C6-N1	7.58	121.49	117.70
54	BA	541	A	N1-C6-N6	-7.58	114.05	118.60
21	AA	321	A	C5-C6-N1	7.58	121.49	117.70
21	AA	792	A	C5-C6-N1	7.58	121.49	117.70
21	AA	975	A	N1-C6-N6	-7.58	114.05	118.60
35	BM	6	ARG	NE-CZ-NH1	7.58	124.09	120.30
53	B4	12	ARG	NE-CZ-NH2	7.58	124.09	120.30
54	BA	2721	A	C5-C6-N1	7.58	121.49	117.70
21	AA	300	A	N1-C6-N6	-7.58	114.06	118.60
21	AA	495	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1394	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1585	C	N3-C2-O2	-7.58	116.60	121.90
54	BA	2381	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2665	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2750	A	C5-C6-N1	7.58	121.49	117.70
54	BA	910	A	C4-C5-C6	-7.57	113.21	117.00
54	BA	2055	C	N3-C2-O2	-7.57	116.60	121.90
12	AM	100	ARG	NE-CZ-NH1	7.57	124.09	120.30
21	AA	1502	A	C5-C6-N1	7.57	121.49	117.70
54	BA	10	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	1336	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	2468	A	C5-C6-N1	7.57	121.49	117.70
54	BA	2882	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	2263	C	O4'-C1'-N1	7.57	114.25	108.20
21	AA	777	A	N1-C6-N6	-7.57	114.06	118.60
6	AG	69	ARG	NE-CZ-NH1	7.56	124.08	120.30
21	AA	336	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	1304	A	C5-C6-N1	7.56	121.48	117.70
21	AA	924	C	N3-C2-O2	-7.56	116.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AN	41	ARG	NE-CZ-NH1	7.56	124.08	120.30
21	AA	1332	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	1095	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1342	A	C5-C6-N1	7.56	121.48	117.70
54	BA	119	A	C4-C5-C6	-7.56	113.22	117.00
21	AA	1280	A	C5-C6-N1	7.56	121.48	117.70
54	BA	764	A	N1-C6-N6	-7.56	114.07	118.60
54	BA	1598	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2781	A	C5-C6-N1	7.56	121.48	117.70
54	BA	943	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	880	C	N3-C2-O2	-7.55	116.61	121.90
54	BA	126	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2352	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	2430	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	649	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	1362	A	C5-C6-N1	7.55	121.47	117.70
51	B2	41	ARG	NE-CZ-NH1	7.55	124.07	120.30
54	BA	2433	A	C5-C6-N1	7.55	121.47	117.70
55	BB	97	C	O4'-C1'-N1	7.55	114.24	108.20
54	BA	522	A	N1-C6-N6	-7.54	114.07	118.60
21	AA	451	A	C5-C6-N1	7.54	121.47	117.70
24	A3	38	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1144	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1147	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1632	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	428	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1652	A	C5-C6-N1	7.54	121.47	117.70
54	BA	2366	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	563	A	C5-C6-N1	7.54	121.47	117.70
26	BD	59	ARG	NE-CZ-NH1	7.54	124.07	120.30
54	BA	63	A	C5-C6-N1	7.54	121.47	117.70
54	BA	2095	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	2711	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	207	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1096	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1698	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1794	A	C5-C6-N1	7.54	121.47	117.70
21	AA	101	A	C4-C5-C6	-7.53	113.23	117.00
21	AA	307	C	N3-C2-O2	-7.53	116.63	121.90
21	AA	704	A	C5-C6-N1	7.53	121.47	117.70
21	AA	1216	A	C5-C6-N1	7.53	121.47	117.70
32	BJ	35	ARG	NE-CZ-NH1	7.53	124.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BL	18	ARG	NE-CZ-NH1	7.53	124.07	120.30
21	AA	109	A	C5-C6-N1	7.53	121.47	117.70
21	AA	1262	C	N3-C2-O2	-7.53	116.63	121.90
21	AA	1499	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	1144	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	2058	A	C5-C6-N1	7.53	121.47	117.70
21	AA	194	C	N1-C2-O2	7.53	123.42	118.90
54	BA	866	A	C5-C6-N1	7.53	121.46	117.70
54	BA	2765	A	N1-C6-N6	-7.53	114.08	118.60
17	AR	42	ARG	NE-CZ-NH2	7.53	124.06	120.30
54	BA	255	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1382	G	O4'-C1'-N9	7.52	114.22	108.20
54	BA	1557	C	N3-C2-O2	-7.52	116.63	121.90
54	BA	2541	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1163	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	1225	A	C5-C6-N1	7.52	121.46	117.70
54	BA	294	A	C5-C6-N1	7.52	121.46	117.70
21	AA	119	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1151	A	C4-C5-C6	-7.52	113.24	117.00
46	BX	36	ARG	NE-CZ-NH1	7.52	124.06	120.30
54	BA	1508	A	C5-C6-N1	7.52	121.46	117.70
54	BA	2254	C	N3-C2-O2	-7.52	116.64	121.90
21	AA	1214	C	N1-C2-O2	7.51	123.41	118.90
54	BA	918	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2205	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2809	A	C5-C6-N1	7.51	121.46	117.70
24	A3	36	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	509	A	C5-C6-N1	7.51	121.45	117.70
54	BA	743	A	C4-C5-C6	-7.51	113.24	117.00
54	BA	1505	A	C4-C5-C6	-7.51	113.24	117.00
54	BA	74	A	C5-C6-N1	7.51	121.45	117.70
54	BA	1579	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2198	A	C5-C6-N1	7.51	121.45	117.70
21	AA	77	A	C5-C6-N1	7.51	121.45	117.70
21	AA	143	A	C5-C6-N1	7.51	121.45	117.70
21	AA	171	A	C4-C5-C6	-7.51	113.25	117.00
21	AA	1274	A	N1-C6-N6	-7.51	114.10	118.60
21	AA	1433	A	C5-C6-N1	7.51	121.45	117.70
39	BQ	49	ARG	NE-CZ-NH1	7.51	124.05	120.30
54	BA	689	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2471	A	N1-C6-N6	-7.51	114.10	118.60
21	AA	65	A	C5-C6-N1	7.50	121.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1136	C	N3-C2-O2	-7.50	116.65	121.90
54	BA	2009	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	2247	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	1637	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	1876	A	C5-C6-N1	7.50	121.45	117.70
54	BA	546	U	O4'-C1'-N1	7.50	114.20	108.20
54	BA	1885	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1311	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	251	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1586	A	C5-C6-N1	7.50	121.45	117.70
21	AA	130	A	C4-C5-C6	-7.49	113.25	117.00
54	BA	1899	A	C5-C6-N1	7.49	121.45	117.70
54	BA	1801	A	C5-C6-N1	7.49	121.45	117.70
10	AK	92	ARG	NE-CZ-NH1	7.49	124.05	120.30
21	AA	1288	A	C5-C6-N1	7.49	121.44	117.70
54	BA	819	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	988	A	C5-C6-N1	7.49	121.44	117.70
54	BA	1237	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	2377	A	C4-C5-C6	-7.49	113.25	117.00
54	BA	2418	A	C4-C5-C6	-7.49	113.25	117.00
21	AA	1377	A	C5-C6-N1	7.49	121.44	117.70
54	BA	532	A	C5-C6-N1	7.49	121.44	117.70
54	BA	2517	C	N3-C2-O2	-7.49	116.66	121.90
54	BA	147	C	C1'-O4'-C4'	-7.49	103.91	109.90
54	BA	404	A	C5-C6-N1	7.49	121.44	117.70
54	BA	1819	A	C5-C6-N1	7.49	121.44	117.70
54	BA	1665	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	2340	A	N1-C6-N6	-7.48	114.11	118.60
15	AP	28	ARG	NE-CZ-NH1	7.48	124.04	120.30
54	BA	1269	A	C5-C6-N1	7.48	121.44	117.70
21	AA	1329	A	C5-C6-N1	7.48	121.44	117.70
54	BA	586	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	838	C	N3-C2-O2	-7.48	116.66	121.90
54	BA	2033	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	2900	A	C5-C6-N1	7.48	121.44	117.70
28	BF	91	ARG	NE-CZ-NH1	7.48	124.04	120.30
32	BJ	69	ARG	NE-CZ-NH1	7.48	124.04	120.30
54	BA	631	A	C5-C6-N1	7.48	121.44	117.70
54	BA	1655	A	N1-C6-N6	-7.48	114.11	118.60
24	A3	11	A	C5-C6-N1	7.48	121.44	117.70
54	BA	781	A	C5-C6-N1	7.47	121.44	117.70
54	BA	922	C	N3-C2-O2	-7.47	116.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2598	A	C5-C6-N1	7.47	121.44	117.70
54	BA	342	A	N1-C6-N6	-7.47	114.12	118.60
21	AA	174	A	C5-C6-N1	7.47	121.44	117.70
54	BA	975	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1268	A	C5-C6-N1	7.47	121.44	117.70
21	AA	498	A	C5-C6-N1	7.47	121.44	117.70
35	BM	81	ARG	NE-CZ-NH1	7.47	124.03	120.30
54	BA	1618	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2860	A	C5-C6-N1	7.47	121.43	117.70
21	AA	373	A	C5-C6-N1	7.47	121.43	117.70
21	AA	1413	A	C5-C6-N1	7.47	121.43	117.70
21	AA	160	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	787	C	N3-C2-O2	-7.46	116.67	121.90
54	BA	2765	A	C5-C6-N1	7.46	121.43	117.70
21	AA	308	C	N3-C2-O2	-7.46	116.68	121.90
54	BA	61	C	N3-C2-O2	-7.46	116.68	121.90
54	BA	161	A	C5-C6-N1	7.46	121.43	117.70
21	AA	78	A	C5-C6-N1	7.46	121.43	117.70
25	BC	47	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	447	A	C5-C6-N1	7.46	121.43	117.70
54	BA	944	C	N3-C2-O2	-7.46	116.68	121.90
54	BA	1272	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	2314	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1227	A	N1-C6-N6	-7.46	114.13	118.60
21	AA	1238	A	C4-C5-C6	-7.46	113.27	117.00
1	AB	136	ARG	NE-CZ-NH1	7.46	124.03	120.30
21	AA	815	A	C5-C6-N1	7.46	121.43	117.70
21	AA	116	A	C5-C6-N1	7.45	121.43	117.70
54	BA	1213	A	C4-C5-C6	-7.45	113.27	117.00
54	BA	2468	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	2030	A	C5-C6-N1	7.45	121.42	117.70
21	AA	1518	A	C5-C6-N1	7.45	121.42	117.70
38	BP	102	ARG	NE-CZ-NH1	7.45	124.02	120.30
39	BQ	52	ARG	NE-CZ-NH1	7.45	124.02	120.30
55	BB	45	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	130	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2077	A	C5-C6-N1	7.45	121.42	117.70
21	AA	1492	A	N1-C6-N6	-7.44	114.13	118.60
21	AA	649	A	C5-C6-N1	7.44	121.42	117.70
24	A3	58	A	C5-C6-N1	7.44	121.42	117.70
54	BA	886	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2823	A	C5-C6-N1	7.44	121.42	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AO	57	ARG	NE-CZ-NH1	7.44	124.02	120.30
21	AA	448	A	C5-C6-N1	7.44	121.42	117.70
21	AA	1332	A	C5-C6-N1	7.44	121.42	117.70
21	AA	1403	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	2461	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2725	A	C5-C6-N1	7.44	121.42	117.70
24	A3	60	A	C5-C6-N1	7.44	121.42	117.70
21	AA	32	A	N1-C6-N6	-7.44	114.14	118.60
21	AA	975	A	C5-C6-N1	7.44	121.42	117.70
54	BA	231	A	C5-C6-N1	7.44	121.42	117.70
21	AA	214	C	N3-C2-O2	-7.43	116.70	121.90
21	AA	756	C	N3-C2-O2	-7.43	116.69	121.90
21	AA	1324	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	1085	A	C5-C6-N1	7.43	121.42	117.70
54	BA	1913	A	C5-C6-N1	7.43	121.42	117.70
54	BA	1347	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2893	A	C5-C6-N1	7.43	121.41	117.70
21	AA	790	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	1472	C	O4'-C1'-N1	7.43	114.14	108.20
54	BA	2899	A	C5-C6-N1	7.43	121.41	117.70
17	AR	47	ARG	NE-CZ-NH1	7.42	124.01	120.30
21	AA	974	A	C5-C6-N1	7.42	121.41	117.70
32	BJ	13	ARG	NE-CZ-NH1	7.42	124.01	120.30
54	BA	510	C	N3-C2-O2	-7.42	116.70	121.90
54	BA	1241	A	C5-C6-N1	7.42	121.41	117.70
54	BA	547	A	C5-C6-N1	7.42	121.41	117.70
21	AA	98	A	C5-C6-N1	7.42	121.41	117.70
54	BA	811	U	O4'-C1'-N1	7.42	114.14	108.20
54	BA	1272	A	C5-C6-N1	7.42	121.41	117.70
21	AA	188	C	N3-C2-O2	-7.42	116.71	121.90
54	BA	2388	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	2425	A	C5-C6-N1	7.42	121.41	117.70
21	AA	182	A	N1-C6-N6	-7.41	114.15	118.60
54	BA	1953	A	N1-C6-N6	-7.41	114.15	118.60
54	BA	1960	A	C5-C6-N1	7.41	121.41	117.70
54	BA	368	A	C5-C6-N1	7.41	121.41	117.70
54	BA	391	A	C5-C6-N1	7.41	121.41	117.70
54	BA	1420	A	C5-C6-N1	7.41	121.41	117.70
21	AA	382	A	N1-C6-N6	-7.41	114.15	118.60
21	AA	498	A	N1-C6-N6	-7.41	114.15	118.60
54	BA	1774	C	N3-C2-O2	-7.41	116.71	121.90
54	BA	2705	A	C5-C6-N1	7.41	121.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	57	A	C4-C5-C6	-7.41	113.30	117.00
19	AT	73	ARG	NE-CZ-NH2	-7.40	116.60	120.30
21	AA	918	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	99	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	546	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1188	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	508	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1701	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1938	A	O4'-C1'-N9	7.40	114.12	108.20
54	BA	38	A	C5-C6-N1	7.40	121.40	117.70
54	BA	460	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	783	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	927	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1470	A	C4-C5-C6	-7.40	113.30	117.00
21	AA	1418	A	C5-C6-N1	7.40	121.40	117.70
54	BA	503	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1119	U	O4'-C1'-N1	7.40	114.12	108.20
54	BA	1365	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	527	C	N1-C2-O2	7.40	123.34	118.90
54	BA	1503	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	1156	A	C5-C6-N1	7.39	121.40	117.70
21	AA	325	A	C5-C6-N1	7.39	121.40	117.70
54	BA	471	A	N1-C6-N6	-7.39	114.16	118.60
54	BA	1243	C	N3-C2-O2	-7.39	116.72	121.90
21	AA	1218	C	N3-C2-O2	-7.39	116.73	121.90
54	BA	2506	U	N3-C2-O2	-7.39	117.03	122.20
54	BA	2513	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	2837	A	C5-C6-N1	7.39	121.40	117.70
54	BA	947	A	C4-C5-C6	-7.39	113.31	117.00
54	BA	2135	A	C5-C6-N1	7.39	121.39	117.70
54	BA	2632	A	C4-C5-C6	-7.39	113.31	117.00
21	AA	71	A	C5-C6-N1	7.39	121.39	117.70
54	BA	255	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	2003	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	2738	A	C4-C5-C6	-7.39	113.31	117.00
21	AA	80	A	C5-C6-N1	7.38	121.39	117.70
54	BA	825	A	C5-C6-N1	7.38	121.39	117.70
24	A3	39	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	572	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1509	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1808	A	O4'-C1'-N9	7.38	114.11	108.20
21	AA	336	A	C5-C6-N1	7.38	121.39	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1239	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2060	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2681	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	2717	C	N3-C2-O2	-7.38	116.73	121.90
55	BB	34	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1596	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	2129	C	O4'-C1'-N1	7.38	114.10	108.20
21	AA	459	A	C5-C6-N1	7.38	121.39	117.70
54	BA	661	A	C5-C6-N1	7.37	121.39	117.70
54	BA	861	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1088	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1614	A	C5-C6-N1	7.37	121.39	117.70
41	BS	18	ARG	NE-CZ-NH1	7.37	123.98	120.30
54	BA	460	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2184	A	C5-C6-N1	7.37	121.39	117.70
54	BA	634	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	794	A	C4-C5-C6	-7.37	113.32	117.00
54	BA	800	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1438	U	N3-C2-O2	-7.37	117.04	122.20
21	AA	1374	A	C5-C6-N1	7.37	121.38	117.70
26	BD	124	ARG	NE-CZ-NH1	7.37	123.98	120.30
54	BA	219	A	C5-C6-N1	7.37	121.38	117.70
54	BA	430	A	C5-C6-N1	7.37	121.38	117.70
54	BA	915	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	920	A	C5-C6-N1	7.37	121.38	117.70
54	BA	925	A	C5-C6-N1	7.37	121.38	117.70
54	BA	2639	A	C5-C6-N1	7.37	121.38	117.70
6	AG	9	ARG	NE-CZ-NH1	7.36	123.98	120.30
54	BA	918	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2667	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	2851	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2886	A	C5-C6-N1	7.36	121.38	117.70
21	AA	747	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1515	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1755	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1916	A	C4-C5-C6	-7.36	113.32	117.00
21	AA	1238	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1274	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1285	A	N1-C6-N6	-7.36	114.18	118.60
55	BB	53	A	C5-C6-N1	7.36	121.38	117.70
44	BV	9	ARG	NE-CZ-NH1	7.36	123.98	120.30
19	AT	24	ARG	NE-CZ-NH1	7.36	123.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	160	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1571	A	C5-C6-N1	7.36	121.38	117.70
21	AA	937	A	C5-C6-N1	7.35	121.38	117.70
54	BA	423	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2154	A	C4-C5-C6	-7.35	113.32	117.00
21	AA	597	G	N3-C2-N2	-7.35	114.75	119.90
21	AA	844	G	N1-C6-O6	-7.35	115.49	119.90
54	BA	973	A	C5-C6-N1	7.35	121.38	117.70
55	BB	41	G	O4'-C1'-N9	7.35	114.08	108.20
21	AA	1081	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	1117	A	C5-C6-N1	7.35	121.38	117.70
22	A1	69	A	C4-C5-C6	-7.35	113.33	117.00
54	BA	959	A	C4-C5-C6	-7.35	113.33	117.00
21	AA	303	A	C5-C6-N1	7.35	121.37	117.70
54	BA	52	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	2547	A	C5-C6-N1	7.35	121.37	117.70
54	BA	2810	A	C5-C6-N1	7.35	121.37	117.70
21	AA	288	A	C5-C6-N1	7.35	121.37	117.70
21	AA	431	A	C5-C6-N1	7.35	121.37	117.70
2	AC	64	ARG	NE-CZ-NH1	7.34	123.97	120.30
16	AQ	63	CYS	C-N-CA	7.34	140.06	121.70
54	BA	877	A	C5-C6-N1	7.34	121.37	117.70
21	AA	1014	A	C5-C6-N1	7.34	121.37	117.70
54	BA	508	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2231	U	O4'-C1'-N1	7.34	114.07	108.20
54	BA	2814	A	N1-C6-N6	-7.34	114.19	118.60
21	AA	279	A	C4-C5-C6	-7.34	113.33	117.00
21	AA	412	A	O4'-C1'-N9	7.34	114.07	108.20
21	AA	793	U	C1'-O4'-C4'	-7.34	104.03	109.90
54	BA	2169	A	C5-C6-N1	7.34	121.37	117.70
39	BQ	63	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	384	A	C5-C6-N1	7.34	121.37	117.70
35	BM	38	ARG	NE-CZ-NH1	7.34	123.97	120.30
21	AA	1531	A	C5-C6-N1	7.33	121.37	117.70
54	BA	812	C	N3-C2-O2	-7.33	116.77	121.90
21	AA	172	A	C5-C6-N1	7.33	121.37	117.70
21	AA	1217	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	2327	A	C5-C6-N1	7.33	121.37	117.70
54	BA	2757	A	N1-C6-N6	-7.33	114.20	118.60
3	AD	103	ARG	NE-CZ-NH1	7.33	123.96	120.30
54	BA	1583	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	1626	A	N1-C6-N6	-7.33	114.20	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BN	63	ARG	NE-CZ-NH1	7.33	123.96	120.30
54	BA	2281	A	C4-C5-C6	-7.33	113.34	117.00
1	AB	206	ILE	C-N-CA	7.33	140.01	121.70
21	AA	942	G	C5'-C4'-O4'	7.33	117.89	109.10
21	AA	1093	A	C5-C6-N1	7.33	121.36	117.70
54	BA	1226	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	2600	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	1377	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	1048	A	C5-C6-N1	7.32	121.36	117.70
54	BA	470	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	1591	A	C5-C6-N1	7.32	121.36	117.70
21	AA	181	A	C5-C6-N1	7.32	121.36	117.70
54	BA	239	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	1211	C	N1-C2-O2	7.32	123.29	118.90
21	AA	263	A	C5-C6-N1	7.32	121.36	117.70
54	BA	582	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2821	A	C5-C6-N1	7.31	121.36	117.70
21	AA	1150	A	C5-C6-N1	7.31	121.36	117.70
54	BA	402	A	N1-C6-N6	-7.31	114.21	118.60
54	BA	825	A	N1-C6-N6	-7.31	114.21	118.60
54	BA	1000	A	N1-C6-N6	-7.31	114.21	118.60
54	BA	1772	A	C5-C6-N1	7.31	121.36	117.70
54	BA	1204	A	C5-C6-N1	7.31	121.36	117.70
54	BA	1301	A	C5-C6-N1	7.31	121.36	117.70
21	AA	892	A	C5-C6-N1	7.31	121.36	117.70
21	AA	1146	A	C5-C6-N1	7.31	121.36	117.70
54	BA	155	A	C4-C5-C6	-7.31	113.34	117.00
54	BA	945	A	C5-C6-N1	7.31	121.35	117.70
54	BA	1367	A	C5-C6-N1	7.31	121.35	117.70
54	BA	2273	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2813	A	C5-C6-N1	7.31	121.35	117.70
21	AA	665	A	C4-C5-C6	-7.31	113.35	117.00
21	AA	908	A	N1-C6-N6	-7.31	114.22	118.60
54	BA	1143	A	N1-C6-N6	-7.31	114.22	118.60
54	BA	1535	A	C5-C6-N1	7.31	121.35	117.70
54	BA	2655	G	O4'-C1'-N9	7.31	114.05	108.20
21	AA	1004	A	C5-C6-N1	7.31	121.35	117.70
54	BA	1431	A	C5-C6-N1	7.31	121.35	117.70
54	BA	487	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	972	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1241	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	2385	C	N3-C2-O2	-7.30	116.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	751	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1672	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2778	A	N1-C6-N6	-7.30	114.22	118.60
21	AA	164	G	C1'-O4'-C4'	-7.30	104.06	109.90
54	BA	2483	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	2566	A	C5-C6-N1	7.30	121.35	117.70
21	AA	959	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1534	A	C5-C6-N1	7.30	121.35	117.70
54	BA	959	A	O4'-C1'-N9	7.30	114.04	108.20
54	BA	716	A	C5-C6-N1	7.30	121.35	117.70
24	A3	69	C	N3-C2-O2	-7.29	116.79	121.90
10	AK	36	ARG	NE-CZ-NH1	7.29	123.95	120.30
29	BG	54	ARG	NE-CZ-NH1	7.29	123.95	120.30
21	AA	393	A	C5-C6-N1	7.29	121.35	117.70
21	AA	1152	A	C5-C6-N1	7.29	121.35	117.70
54	BA	655	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	759	A	C5-C6-N1	7.29	121.34	117.70
54	BA	1650	A	C4-C5-C6	-7.29	113.36	117.00
54	BA	1713	A	C5-C6-N1	7.29	121.34	117.70
54	BA	2453	A	C4-C5-C6	-7.29	113.36	117.00
54	BA	2887	A	C5-C6-N1	7.29	121.34	117.70
21	AA	768	A	C4-C5-C6	-7.29	113.36	117.00
21	AA	478	A	C5-C6-N1	7.28	121.34	117.70
21	AA	502	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1246	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1413	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	1230	A	C5-C6-N1	7.28	121.34	117.70
46	BX	56	ARG	NE-CZ-NH1	7.28	123.94	120.30
54	BA	1711	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2287	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1219	A	C5-C6-N1	7.28	121.34	117.70
50	B1	43	ARG	NE-CZ-NH1	7.28	123.94	120.30
21	AA	1155	A	C5-C6-N1	7.28	121.34	117.70
54	BA	94	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1640	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2418	A	C5-C6-N1	7.28	121.34	117.70
6	AG	77	ARG	NE-CZ-NH1	7.28	123.94	120.30
21	AA	179	A	C5-C6-N1	7.28	121.34	117.70
21	AA	309	A	C5-C6-N1	7.28	121.34	117.70
54	BA	677	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2309	A	O4'-C1'-N9	7.28	114.02	108.20
55	BB	62	C	N3-C2-O2	-7.28	116.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	309	A	C5-C6-N1	7.27	121.34	117.70
54	BA	1045	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	1610	A	O4'-C1'-N9	7.27	114.02	108.20
54	BA	2727	A	C5-C6-N1	7.27	121.34	117.70
21	AA	819	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	478	A	N1-C6-N6	-7.27	114.24	118.60
37	BO	15	ARG	NE-CZ-NH1	7.27	123.94	120.30
54	BA	1490	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1679	A	C4-C5-C6	-7.27	113.37	117.00
9	AJ	31	ARG	NE-CZ-NH1	7.27	123.93	120.30
21	AA	162	A	C5-C6-N1	7.27	121.33	117.70
54	BA	330	A	C1'-O4'-C4'	-7.27	104.09	109.90
54	BA	1678	A	C5-C6-N1	7.27	121.33	117.70
54	BA	2019	A	C5-C6-N1	7.27	121.33	117.70
8	AI	118	ARG	NE-CZ-NH1	7.26	123.93	120.30
21	AA	329	A	N1-C6-N6	-7.26	114.24	118.60
21	AA	873	A	C5-C6-N1	7.26	121.33	117.70
28	BF	149	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	1378	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1728	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	2530	A	C5-C6-N1	7.26	121.33	117.70
21	AA	7	A	C5-C6-N1	7.26	121.33	117.70
21	AA	149	A	N1-C6-N6	-7.26	114.24	118.60
22	A1	26	A	N1-C6-N6	-7.26	114.24	118.60
54	BA	1128	G	C1'-O4'-C4'	-7.26	104.09	109.90
54	BA	1755	A	C4-C5-C6	-7.26	113.37	117.00
21	AA	167	A	N1-C6-N6	-7.26	114.24	118.60
22	A1	73	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	1226	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2724	U	O4'-C1'-N1	7.26	114.01	108.20
21	AA	878	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1496	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1253	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2326	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	996	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1020	A	C5-C6-N1	7.25	121.33	117.70
54	BA	2873	A	C5-C6-N1	7.25	121.33	117.70
54	BA	668	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1151	A	C5-C6-N1	7.25	121.33	117.70
21	AA	1299	A	C5-C6-N1	7.25	121.33	117.70
10	AK	127	ARG	NE-CZ-NH1	7.25	123.92	120.30
21	AA	1236	A	C5-C6-N1	7.25	121.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	155	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1077	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1552	A	C5-C6-N1	7.25	121.32	117.70
21	AA	243	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	357	C	N3-C2-O2	-7.25	116.83	121.90
54	BA	743	A	C5-C6-N1	7.25	121.32	117.70
54	BA	796	C	N3-C2-O2	-7.25	116.83	121.90
54	BA	640	C	N3-C2-O2	-7.25	116.83	121.90
54	BA	2427	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	363	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	1532	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1664	A	C5-C6-N1	7.24	121.32	117.70
54	BA	644	A	O4'-C1'-N9	7.24	113.99	108.20
54	BA	2171	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2211	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	1489	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	1544	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1098	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	1103	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1987	A	C4-C5-C6	-7.24	113.38	117.00
21	AA	718	A	C5-C6-N1	7.23	121.32	117.70
54	BA	2721	A	C4-C5-C6	-7.23	113.38	117.00
21	AA	518	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	1158	C	N1-C2-O2	7.23	123.24	118.90
54	BA	353	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	990	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	1080	A	C5-C6-N1	7.23	121.31	117.70
22	A1	35	A	C4-C5-C6	-7.23	113.39	117.00
52	B3	39	ARG	NE-CZ-NH1	7.23	123.91	120.30
54	BA	513	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1540	G	O4'-C1'-N9	7.23	113.98	108.20
21	AA	766	A	C5-C6-N1	7.23	121.31	117.70
54	BA	804	A	C5-C6-N1	7.23	121.31	117.70
21	AA	435	A	C4-C5-C6	-7.22	113.39	117.00
21	AA	482	A	C5-C6-N1	7.22	121.31	117.70
21	AA	345	C	N1-C2-O2	7.22	123.23	118.90
21	AA	441	A	C5-C6-N1	7.22	121.31	117.70
21	AA	1180	A	C5-C6-N1	7.22	121.31	117.70
24	A3	77	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	91	A	C5-C6-N1	7.22	121.31	117.70
54	BA	484	C	N3-C2-O2	-7.22	116.84	121.90
54	BA	507	A	C5-C6-N1	7.22	121.31	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1977	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2893	A	C4-C5-C6	-7.22	113.39	117.00
21	AA	315	A	C4-C5-C6	-7.22	113.39	117.00
21	AA	364	A	C4-C5-C6	-7.22	113.39	117.00
21	AA	1398	A	C5-C6-N1	7.22	121.31	117.70
22	A1	26	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1213	A	C5-C6-N1	7.22	121.31	117.70
21	AA	907	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	959	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1000	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1118	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	560	A	C5-C6-N1	7.22	121.31	117.70
38	BP	61	ARG	NE-CZ-NH1	7.22	123.91	120.30
42	BT	76	ARG	NE-CZ-NH1	7.22	123.91	120.30
54	BA	528	A	C5-C6-N1	7.22	121.31	117.70
21	AA	831	A	C5-C6-N1	7.21	121.31	117.70
36	BN	8	ARG	NE-CZ-NH1	7.21	123.91	120.30
54	BA	676	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1970	A	C5-C6-N1	7.21	121.31	117.70
21	AA	66	A	N1-C6-N6	-7.21	114.27	118.60
21	AA	696	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1191	A	C5-C6-N1	7.21	121.31	117.70
54	BA	197	A	C5-C6-N1	7.21	121.31	117.70
54	BA	231	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	574	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	2322	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2450	A	C5-C6-N1	7.21	121.31	117.70
24	A3	39	A	C5-C6-N1	7.21	121.30	117.70
54	BA	1833	C	O4'-C1'-N1	7.21	113.97	108.20
21	AA	716	A	C4-C5-C6	-7.21	113.40	117.00
21	AA	1500	A	N1-C6-N6	-7.21	114.28	118.60
54	BA	14	A	N1-C6-N6	-7.21	114.28	118.60
54	BA	526	A	C5-C6-N1	7.21	121.30	117.70
54	BA	601	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	1616	A	C5-C6-N1	7.21	121.30	117.70
54	BA	2005	A	C5-C6-N1	7.21	121.30	117.70
54	BA	2052	A	C5-C6-N1	7.21	121.30	117.70
54	BA	2176	A	C5-C6-N1	7.21	121.30	117.70
30	BH	97	ARG	NE-CZ-NH1	7.21	123.90	120.30
21	AA	1021	A	C4-C5-C6	-7.20	113.40	117.00
21	AA	1359	C	N3-C2-O2	-7.20	116.86	121.90
28	BF	29	ARG	NE-CZ-NH1	7.20	123.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BG	169	ARG	NE-CZ-NH1	7.20	123.90	120.30
41	BS	11	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	1205	A	C5-C6-N1	7.20	121.30	117.70
54	BA	6	A	C5-C6-N1	7.20	121.30	117.70
54	BA	324	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2534	A	C5-C6-N1	7.20	121.30	117.70
21	AA	338	A	C5-C6-N1	7.20	121.30	117.70
16	AQ	61	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	2577	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	298	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1518	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	1757	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	334	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	1165	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1580	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1783	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2328	A	C4-C5-C6	-7.20	113.40	117.00
21	AA	1059	C	N3-C2-O2	-7.19	116.87	121.90
30	BH	123	ARG	NE-CZ-NH2	-7.19	116.70	120.30
54	BA	844	A	C4-C5-C6	-7.19	113.40	117.00
55	BB	29	A	N1-C6-N6	-7.19	114.28	118.60
54	BA	632	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	1175	A	O4'-C1'-N9	7.19	113.95	108.20
54	BA	2761	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2853	C	N3-C2-O2	-7.19	116.87	121.90
21	AA	640	A	C5-C6-N1	7.19	121.29	117.70
54	BA	1889	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2733	A	C5-C6-N1	7.19	121.30	117.70
21	AA	1228	C	N3-C2-O2	-7.19	116.87	121.90
54	BA	2014	A	N1-C6-N6	-7.19	114.29	118.60
21	AA	1437	A	C4-C5-C6	-7.19	113.41	117.00
54	BA	2025	C	N3-C2-O2	-7.19	116.87	121.90
21	AA	1016	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1322	A	N1-C6-N6	-7.18	114.29	118.60
21	AA	996	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	227	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	2725	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	81	A	C5-C6-N1	7.18	121.29	117.70
21	AA	665	A	C5-C6-N1	7.18	121.29	117.70
54	BA	633	A	C5-C6-N1	7.18	121.29	117.70
54	BA	125	A	C5-C6-N1	7.18	121.29	117.70
54	BA	331	C	N3-C2-O2	-7.18	116.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2378	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	2882	A	C5-C6-N1	7.18	121.29	117.70
54	BA	14	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1802	A	N1-C6-N6	-7.18	114.29	118.60
21	AA	533	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1151	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1538	G	O4'-C1'-N9	7.17	113.94	108.20
54	BA	218	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1999	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	2440	C	N3-C2-O2	-7.17	116.88	121.90
55	BB	46	A	C5-C6-N1	7.17	121.29	117.70
21	AA	532	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1022	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1505	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2542	A	C5-C6-N1	7.17	121.28	117.70
54	BA	705	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	1604	C	O4'-C1'-N1	7.17	113.94	108.20
21	AA	169	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	1113	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	2030	A	O4'-C1'-N9	7.17	113.93	108.20
55	BB	78	A	C5-C6-N1	7.17	121.28	117.70
21	AA	466	A	C5-C6-N1	7.16	121.28	117.70
21	AA	1254	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	1469	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	1596	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2170	A	C4-C5-C6	-7.16	113.42	117.00
9	AJ	5	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	1548	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2679	A	C5-C6-N1	7.16	121.28	117.70
21	AA	1468	A	C4-C5-C6	-7.16	113.42	117.00
19	AT	59	ARG	NE-CZ-NH1	7.16	123.88	120.30
21	AA	205	A	C5-C6-N1	7.16	121.28	117.70
21	AA	1322	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	1129	A	C5-C6-N1	7.16	121.28	117.70
21	AA	1038	C	N3-C2-O2	-7.15	116.89	121.90
21	AA	1105	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1533	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	2393	U	O4'-C1'-N1	7.15	113.92	108.20
21	AA	465	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	256	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	503	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2799	A	C5-C6-N1	7.15	121.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2883	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	629	A	C4-C5-C6	-7.15	113.43	117.00
54	BA	1427	A	C5-C6-N1	7.15	121.27	117.70
54	BA	2851	A	C4-C5-C6	-7.15	113.43	117.00
55	BB	101	A	C5-C6-N1	7.15	121.27	117.70
21	AA	1456	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	1200	C	N3-C2-O2	-7.14	116.90	121.90
24	A3	59	A	C5-C6-N1	7.14	121.27	117.70
25	BC	211	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	269	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1833	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1244	A	N1-C6-N6	-7.14	114.32	118.60
54	BA	10	A	C5-C6-N1	7.14	121.27	117.70
54	BA	190	A	C5-C6-N1	7.14	121.27	117.70
54	BA	685	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1566	A	N1-C6-N6	-7.14	114.32	118.60
54	BA	2003	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2333	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1147	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	2200	C	O4'-C1'-N1	7.13	113.91	108.20
55	BB	26	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	1493	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	2591	C	N3-C2-O2	-7.13	116.91	121.90
6	AG	3	ARG	NE-CZ-NH1	7.13	123.86	120.30
21	AA	1333	A	C4-C5-C6	-7.13	113.44	117.00
21	AA	1483	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1084	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2538	C	O4'-C1'-N1	7.13	113.90	108.20
22	A1	9	A	C5-C6-N1	7.13	121.27	117.70
54	BA	845	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	645	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	2071	A	N1-C6-N6	-7.13	114.32	118.60
33	BK	31	ARG	NE-CZ-NH1	7.13	123.86	120.30
54	BA	28	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	1566	A	C5-C6-N1	7.13	121.26	117.70
54	BA	1677	A	C5-C6-N1	7.13	121.26	117.70
21	AA	469	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	181	A	N1-C6-N6	-7.12	114.33	118.60
55	BB	101	A	N1-C6-N6	-7.12	114.33	118.60
21	AA	923	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2407	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	522	A	C5-C6-N1	7.12	121.26	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1275	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	1551	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	1853	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	889	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	1887	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	2866	U	O4'-C1'-N1	7.12	113.89	108.20
21	AA	383	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	622	A	C4-C5-C6	-7.12	113.44	117.00
51	B2	12	ARG	NE-CZ-NH1	7.12	123.86	120.30
54	BA	131	A	C5-C6-N1	7.12	121.26	117.70
54	BA	504	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1027	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1413	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	2134	A	C5-C6-N1	7.12	121.26	117.70
54	BA	279	A	C4-C5-C6	-7.11	113.44	117.00
54	BA	1730	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	1349	A	C5-C6-N1	7.11	121.26	117.70
54	BA	362	A	C5-C6-N1	7.11	121.26	117.70
54	BA	1419	A	C5-C6-N1	7.11	121.26	117.70
54	BA	182	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2711	A	C5-C6-N1	7.11	121.26	117.70
21	AA	937	A	C4-C5-C6	-7.11	113.44	117.00
21	AA	1531	A	C4-C5-C6	-7.11	113.44	117.00
24	A3	14	A	C5-C6-N1	7.11	121.25	117.70
54	BA	1322	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2021	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	509	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	1780	A	C5-C6-N1	7.11	121.25	117.70
21	AA	607	A	C5-C6-N1	7.11	121.25	117.70
21	AA	1395	C	N3-C2-O2	-7.11	116.93	121.90
21	AA	1447	A	C5-C6-N1	7.11	121.25	117.70
21	AA	1452	C	N3-C2-O2	-7.11	116.93	121.90
46	BX	2	ARG	NE-CZ-NH1	7.11	123.85	120.30
54	BA	1802	A	C5-C6-N1	7.11	121.25	117.70
54	BA	1806	C	N3-C2-O2	-7.11	116.93	121.90
54	BA	1858	A	C5-C6-N1	7.11	121.25	117.70
54	BA	575	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2212	A	C5-C6-N1	7.10	121.25	117.70
54	BA	347	A	C5-C6-N1	7.10	121.25	117.70
55	BB	109	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	538	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	1689	A	C5-C6-N1	7.10	121.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2723	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	44	A	C5-C6-N1	7.10	121.25	117.70
54	BA	213	A	C5-C6-N1	7.10	121.25	117.70
54	BA	227	A	C5-C6-N1	7.10	121.25	117.70
54	BA	480	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	721	A	C5-C6-N1	7.10	121.25	117.70
54	BA	892	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1494	A	C5-C6-N1	7.10	121.25	117.70
39	BQ	29	ARG	NE-CZ-NH1	7.10	123.85	120.30
54	BA	272	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	1128	C	N3-C2-O2	-7.09	116.93	121.90
54	BA	1504	A	N1-C6-N6	-7.09	114.34	118.60
21	AA	1340	A	C5-C6-N1	7.09	121.25	117.70
21	AA	609	A	C4-C5-C6	-7.09	113.45	117.00
52	B3	41	ARG	NE-CZ-NH1	7.09	123.84	120.30
54	BA	878	A	C5-C6-N1	7.09	121.25	117.70
54	BA	996	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2142	A	N1-C6-N6	-7.09	114.34	118.60
54	BA	2358	A	C5-C6-N1	7.09	121.25	117.70
16	AQ	39	ARG	NE-CZ-NH1	7.09	123.84	120.30
21	AA	482	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	144	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1784	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1739	A	C5-C6-N1	7.09	121.24	117.70
21	AA	1259	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	225	C	O4'-C1'-N1	7.09	113.87	108.20
54	BA	911	A	C5-C6-N1	7.09	121.24	117.70
54	BA	992	C	N3-C2-O2	-7.09	116.94	121.90
37	BO	81	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	1079	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	2369	A	C4-C5-C6	-7.08	113.46	117.00
56	B5	74	ARG	NE-CZ-NH1	7.08	123.84	120.30
21	AA	1480	A	C5-C6-N1	7.08	121.24	117.70
22	A1	21	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2510	C	N3-C2-O2	-7.08	116.94	121.90
13	AN	61	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	637	A	C5-C6-N1	7.08	121.24	117.70
54	BA	644	A	C5-C6-N1	7.08	121.24	117.70
2	AC	106	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	221	A	C5-C6-N1	7.08	121.24	117.70
54	BA	223	A	C5-C6-N1	7.08	121.24	117.70
54	BA	233	A	C5-C6-N1	7.08	121.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	925	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	2847	U	O4'-C1'-N1	7.08	113.86	108.20
54	BA	127	A	C5-C6-N1	7.07	121.24	117.70
54	BA	2425	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	676	A	C5-C6-N1	7.07	121.24	117.70
25	BC	268	ARG	NE-CZ-NH1	7.07	123.84	120.30
54	BA	677	A	C4-C5-C6	-7.07	113.46	117.00
21	AA	595	A	C5-C6-N1	7.07	121.24	117.70
54	BA	337	C	O4'-C1'-N1	7.07	113.86	108.20
54	BA	2386	A	C5-C6-N1	7.07	121.23	117.70
54	BA	19	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1111	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2191	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2434	A	C5-C6-N1	7.07	121.23	117.70
21	AA	1035	A	C5-C6-N1	7.07	121.23	117.70
54	BA	794	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1572	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	1757	A	C5-C6-N1	7.07	121.23	117.70
21	AA	1320	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	1362	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	2270	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1969	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	2572	A	N1-C6-N6	-7.06	114.36	118.60
21	AA	370	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	415	A	O4'-C1'-N9	7.06	113.85	108.20
21	AA	1500	A	C5-C6-N1	7.06	121.23	117.70
25	BC	13	ARG	NE-CZ-NH1	7.06	123.83	120.30
54	BA	788	A	C5-C6-N1	7.06	121.23	117.70
54	BA	300	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2005	A	N1-C6-N6	-7.06	114.36	118.60
21	AA	642	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1233	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	1981	A	C5-C6-N1	7.06	121.23	117.70
21	AA	1446	A	C4-C5-C6	-7.06	113.47	117.00
22	A1	69	A	C5-C6-N1	7.06	121.23	117.70
36	BN	46	ARG	NE-CZ-NH1	7.06	123.83	120.30
54	BA	149	A	C5-C6-N1	7.06	121.23	117.70
54	BA	614	A	C5-C6-N1	7.06	121.23	117.70
21	AA	648	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	262	A	C4-C5-C6	-7.05	113.47	117.00
21	AA	295	C	N3-C2-O2	-7.05	116.96	121.90
24	A3	35	C	N3-C2-O2	-7.05	116.96	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	892	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	1871	A	O4'-C1'-N9	7.05	113.84	108.20
21	AA	559	A	C5-C6-N1	7.05	121.22	117.70
21	AA	729	A	C5-C6-N1	7.05	121.23	117.70
21	AA	841	C	N3-C2-O2	-7.05	116.96	121.90
21	AA	848	C	N3-C2-O2	-7.05	116.96	121.90
21	AA	1293	C	N3-C2-O2	-7.05	116.96	121.90
21	AA	414	A	C5-C6-N1	7.05	121.22	117.70
21	AA	901	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1176	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	456	C	O4'-C1'-N1	7.05	113.84	108.20
54	BA	1308	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1899	A	N1-C6-N6	-7.05	114.37	118.60
55	BB	78	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	863	A	C5-C6-N1	7.05	121.22	117.70
21	AA	583	A	C5-C6-N1	7.05	121.22	117.70
21	AA	790	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1169	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1223	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	1328	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	1395	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	2020	A	C5-C6-N1	7.05	121.22	117.70
21	AA	906	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	2264	C	N3-C2-O2	-7.04	116.97	121.90
55	BB	88	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	356	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	401	C	O4'-C1'-N1	7.04	113.83	108.20
27	BE	69	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	1998	A	C5-C6-N1	7.04	121.22	117.70
21	AA	415	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2755	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	2211	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1240	U	O4'-C1'-N1	7.04	113.83	108.20
54	BA	1090	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1353	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1741	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	1786	A	C5-C6-N1	7.04	121.22	117.70
21	AA	448	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	928	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1387	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	1819	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	1152	A	N1-C6-N6	-7.03	114.38	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1289	A	C5-C6-N1	7.03	121.22	117.70
54	BA	957	C	N3-C2-O2	-7.03	116.98	121.90
55	BB	108	A	N1-C6-N6	-7.03	114.38	118.60
21	AA	366	A	C5-C6-N1	7.03	121.22	117.70
54	BA	183	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	217	A	C5-C6-N1	7.03	121.21	117.70
21	AA	320	A	C5-C6-N1	7.03	121.21	117.70
54	BA	1320	C	N1-C2-O2	7.03	123.12	118.90
54	BA	95	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	2199	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	730	A	C5-C6-N1	7.02	121.21	117.70
21	AA	44	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	270	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	2088	A	C5-C6-N1	7.02	121.21	117.70
54	BA	2600	A	C5-C6-N1	7.02	121.21	117.70
54	BA	2880	C	N3-C2-O2	-7.02	116.98	121.90
21	AA	853	C	N3-C2-O2	-7.02	116.99	121.90
54	BA	608	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1805	A	C5-C6-N1	7.02	121.21	117.70
54	BA	2346	A	C5-C6-N1	7.02	121.21	117.70
55	BB	46	A	C4-C5-C6	-7.02	113.49	117.00
21	AA	958	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1188	A	C5-C6-N1	7.02	121.21	117.70
24	A3	45	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	789	A	C5-C6-N1	7.02	121.21	117.70
54	BA	2767	C	N3-C2-O2	-7.02	116.99	121.90
21	AA	397	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	861	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	917	A	N1-C6-N6	-7.02	114.39	118.60
55	BB	52	A	C5-C6-N1	7.02	121.21	117.70
21	AA	572	A	C5-C6-N1	7.01	121.21	117.70
21	AA	872	A	O4'-C1'-N9	7.01	113.81	108.20
54	BA	2515	C	N3-C2-O2	-7.01	116.99	121.90
55	BB	66	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1402	U	O4'-C1'-N1	7.01	113.81	108.20
54	BA	2634	A	C5-C6-N1	7.01	121.21	117.70
54	BA	2298	A	C5-C6-N1	7.01	121.21	117.70
54	BA	2587	A	C5-C6-N1	7.01	121.21	117.70
54	BA	2902	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	42	A	C4-C5-C6	-7.01	113.50	117.00
54	BA	2456	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	1866	A	N1-C6-N6	-7.01	114.40	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	53	A	C5-C6-N1	7.00	121.20	117.70
54	BA	529	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	2096	C	N3-C2-O2	-7.00	117.00	121.90
15	AP	25	ARG	NE-CZ-NH1	7.00	123.80	120.30
21	AA	51	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	1103	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	1088	A	O4'-C1'-N9	7.00	113.80	108.20
54	BA	2377	A	C5-C6-N1	7.00	121.20	117.70
21	AA	72	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1572	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2101	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1304	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	837	C	N3-C2-O2	-6.99	117.00	121.90
21	AA	1111	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	820	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2753	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	685	A	N1-C6-N6	-6.99	114.41	118.60
21	AA	83	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	643	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	584	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	1067	A	C5-C6-N1	6.98	121.19	117.70
54	BA	590	A	C5-C6-N1	6.98	121.19	117.70
21	AA	958	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1630	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2632	A	C5-C6-N1	6.98	121.19	117.70
55	BB	53	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	1700	A	N1-C6-N6	-6.98	114.41	118.60
21	AA	339	C	N3-C2-O2	-6.98	117.02	121.90
21	AA	1410	A	C5-C6-N1	6.98	121.19	117.70
54	BA	734	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1583	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1808	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2886	A	N1-C6-N6	-6.98	114.41	118.60
21	AA	374	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	511	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	738	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	1204	A	N1-C6-N6	-6.97	114.42	118.60
27	BE	44	ARG	NE-CZ-NH1	6.97	123.79	120.30
48	BZ	30	ARG	NE-CZ-NH1	6.97	123.79	120.30
54	BA	382	A	C5-C6-N1	6.97	121.19	117.70
54	BA	575	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	1453	A	C5-C6-N1	6.97	121.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1605	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	1229	A	C5-C6-N1	6.97	121.19	117.70
54	BA	490	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	750	A	C5-C6-N1	6.97	121.19	117.70
21	AA	48	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	530	G	C1'-O4'-C4'	-6.97	104.33	109.90
21	AA	1410	A	N1-C6-N6	-6.97	114.42	118.60
50	B1	27	ARG	NE-CZ-NH1	6.97	123.78	120.30
54	BA	322	A	C5-C6-N1	6.97	121.19	117.70
54	BA	985	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	1127	A	C5-C6-N1	6.97	121.19	117.70
54	BA	163	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	28	A	C5-C6-N1	6.97	121.18	117.70
54	BA	195	A	C5-C6-N1	6.97	121.18	117.70
54	BA	905	A	C4-C5-C6	-6.97	113.52	117.00
55	BB	39	A	C5-C6-N1	6.97	121.18	117.70
54	BA	103	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2814	A	C5-C6-N1	6.96	121.18	117.70
21	AA	779	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	2706	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1036	A	C5-C6-N1	6.96	121.18	117.70
54	BA	454	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1043	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	1580	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	57	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	374	A	N1-C6-N6	-6.96	114.42	118.60
3	AD	46	ARG	NE-CZ-NH1	6.96	123.78	120.30
21	AA	777	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1101	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1871	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	2821	A	N1-C6-N6	-6.96	114.42	118.60
21	AA	80	A	N1-C6-N6	-6.96	114.43	118.60
21	AA	767	A	C5-C6-N1	6.96	121.18	117.70
54	BA	477	A	N1-C6-N6	-6.96	114.43	118.60
54	BA	1014	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1677	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	2829	A	C4-C5-C6	-6.96	113.52	117.00
4	AE	156	ARG	NE-CZ-NH1	6.96	123.78	120.30
21	AA	152	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1854	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	1976	U	O4'-C1'-N1	6.95	113.76	108.20
54	BA	2095	A	C5-C6-N1	6.95	121.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2751	G	O4'-C1'-N9	6.95	113.76	108.20
54	BA	142	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	2386	A	C4-C5-C6	-6.95	113.52	117.00
21	AA	243	A	C5-C6-N1	6.95	121.18	117.70
54	BA	2469	A	C5-C6-N1	6.95	121.18	117.70
54	BA	564	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	817	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	986	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	1237	A	O4'-C1'-N9	6.95	113.76	108.20
21	AA	43	C	N3-C2-O2	-6.95	117.04	121.90
21	AA	694	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1046	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1434	A	C5-C6-N1	6.95	121.17	117.70
54	BA	95	A	C5-C6-N1	6.94	121.17	117.70
21	AA	430	A	C5-C6-N1	6.94	121.17	117.70
21	AA	546	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	1067	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	1494	A	C4-C5-C6	-6.94	113.53	117.00
21	AA	780	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	1638	C	N3-C2-O2	-6.94	117.04	121.90
55	BB	52	A	C4-C5-C6	-6.94	113.53	117.00
45	BW	38	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	1785	A	C4-C5-C6	-6.94	113.53	117.00
21	AA	1339	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1854	A	C5-C6-N1	6.94	121.17	117.70
21	AA	192	A	C5-C6-N1	6.94	121.17	117.70
54	BA	147	C	N3-C2-O2	-6.94	117.05	121.90
21	AA	630	A	C5-C6-N1	6.93	121.17	117.70
22	A1	56	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	344	A	C5-C6-N1	6.93	121.17	117.70
54	BA	394	C	N3-C2-O2	-6.93	117.05	121.90
55	BB	97	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	918	A	C5-C6-N1	6.93	121.17	117.70
54	BA	203	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1170	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	1967	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	754	C	N1-C2-O2	6.93	123.06	118.90
21	AA	857	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	764	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	2810	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	618	G	O4'-C1'-N9	6.93	113.74	108.20
54	BA	1558	C	N3-C2-O2	-6.93	117.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	596	A	C5-C6-N1	6.92	121.16	117.70
54	BA	301	G	O4'-C1'-N9	6.92	113.74	108.20
54	BA	453	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1495	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1591	A	N1-C6-N6	-6.92	114.44	118.60
54	BA	2392	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	2776	A	C5-C6-N1	6.92	121.16	117.70
55	BB	27	C	N3-C2-O2	-6.92	117.05	121.90
21	AA	63	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	305	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	1345	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	1608	A	C5-C6-N1	6.92	121.16	117.70
55	BB	108	A	C5-C6-N1	6.92	121.16	117.70
21	AA	1336	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	1919	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2241	A	C5-C6-N1	6.92	121.16	117.70
54	BA	447	A	N1-C6-N6	-6.92	114.45	118.60
21	AA	303	A	N1-C6-N6	-6.92	114.45	118.60
21	AA	913	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	994	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1699	G	O4'-C1'-N9	6.92	113.73	108.20
54	BA	2097	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2547	A	O4'-C1'-N9	6.92	113.73	108.20
54	BA	2516	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2826	A	C5-C6-N1	6.92	121.16	117.70
21	AA	1044	A	C5-C6-N1	6.92	121.16	117.70
55	BB	104	A	C5-C6-N1	6.92	121.16	117.70
21	AA	743	A	C5-C6-N1	6.91	121.16	117.70
21	AA	864	A	C4-C5-C6	-6.91	113.54	117.00
54	BA	670	A	P-O3'-C3'	6.91	128.00	119.70
54	BA	900	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1803	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1821	A	C4-C5-C6	-6.91	113.54	117.00
54	BA	1969	A	C5-C6-N1	6.91	121.16	117.70
54	BA	2376	A	C5-C6-N1	6.91	121.16	117.70
21	AA	151	A	C5-C6-N1	6.91	121.16	117.70
21	AA	663	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1773	A	N1-C6-N6	-6.91	114.45	118.60
55	BB	99	A	C5-C6-N1	6.91	121.16	117.70
56	B5	53	ARG	NE-CZ-NH1	6.91	123.76	120.30
54	BA	1701	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2117	A	O4'-C1'-N9	6.91	113.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2662	A	C5-C6-N1	6.91	121.15	117.70
54	BA	2741	A	C5-C6-N1	6.91	121.15	117.70
54	BA	1547	C	N3-C2-O2	-6.91	117.07	121.90
54	BA	2070	A	C5-C6-N1	6.91	121.15	117.70
54	BA	2368	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	55	A	C5-C6-N1	6.90	121.15	117.70
54	BA	654	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1668	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	2177	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2352	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2577	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1434	A	O4'-C1'-N9	6.90	113.72	108.20
54	BA	995	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	1427	C	N3-C2-O2	-6.90	117.07	121.90
12	AM	102	LYS	C-N-CA	6.89	138.94	121.70
54	BA	1646	C	N3-C2-O2	-6.89	117.07	121.90
54	BA	1739	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	2439	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1142	A	C5-C6-N1	6.89	121.15	117.70
54	BA	734	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	1454	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	2033	A	C5-C6-N1	6.89	121.15	117.70
16	AQ	10	ARG	NE-CZ-NH1	6.89	123.74	120.30
21	AA	129	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1214	C	O4'-C1'-N1	6.89	113.71	108.20
54	BA	422	A	C5-C6-N1	6.89	121.14	117.70
54	BA	675	A	C5-C6-N1	6.89	121.14	117.70
54	BA	1359	A	C5-C6-N1	6.89	121.14	117.70
54	BA	299	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1261	A	C5-C6-N1	6.88	121.14	117.70
21	AA	1067	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	126	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	250	A	C5-C6-N1	6.88	121.14	117.70
21	AA	1096	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	195	A	N1-C6-N6	-6.88	114.47	118.60
54	BA	603	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	228	A	C5-C6-N1	6.88	121.14	117.70
21	AA	389	A	C5-C6-N1	6.88	121.14	117.70
21	AA	556	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	1349	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1396	A	C4-C5-C6	-6.88	113.56	117.00
36	BN	90	ARG	NE-CZ-NH1	6.88	123.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2616	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	2620	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	602	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1570	A	C5-C6-N1	6.88	121.14	117.70
21	AA	794	A	C5-C6-N1	6.88	121.14	117.70
54	BA	5	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	139	A	C5-C6-N1	6.87	121.14	117.70
21	AA	236	A	N1-C6-N6	-6.87	114.47	118.60
54	BA	751	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	1027	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	1369	C	N3-C2-O2	-6.87	117.09	121.90
39	BQ	91	ARG	NE-CZ-NH1	6.87	123.74	120.30
54	BA	632	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1635	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	2792	A	C4-C5-C6	-6.87	113.56	117.00
7	AH	127	TYR	CB-CG-CD2	-6.87	116.88	121.00
21	AA	1368	A	N1-C6-N6	-6.87	114.48	118.60
21	AA	1430	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	160	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1044	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1754	A	C5-C6-N1	6.87	121.13	117.70
21	AA	1176	A	C5-C6-N1	6.87	121.13	117.70
54	BA	2031	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1744	A	C5-C6-N1	6.87	121.13	117.70
54	BA	52	A	C5-C6-N1	6.86	121.13	117.70
54	BA	721	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	793	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	264	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	1480	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	1668	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2054	A	C5-C6-N1	6.86	121.13	117.70
21	AA	1080	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	345	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1815	A	C5-C6-N1	6.86	121.13	117.70
12	AM	86	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	941	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	728	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	1194	A	C4-C5-C6	-6.85	113.57	117.00
21	AA	1130	A	C5-C6-N1	6.85	121.13	117.70
54	BA	324	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	1032	A	N1-C6-N6	-6.85	114.49	118.60
54	BA	1590	A	N1-C6-N6	-6.85	114.49	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	689	C	N3-C2-O2	-6.85	117.10	121.90
21	AA	1407	C	N3-C2-O2	-6.85	117.11	121.90
54	BA	320	A	C5-C6-N1	6.85	121.12	117.70
54	BA	1017	G	O4'-C1'-N9	6.85	113.68	108.20
54	BA	1433	A	N1-C6-N6	-6.85	114.49	118.60
54	BA	1809	A	C5-C6-N1	6.85	121.12	117.70
54	BA	1918	A	C5-C6-N1	6.85	121.12	117.70
21	AA	1324	A	C5-C6-N1	6.84	121.12	117.70
54	BA	718	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1553	A	C5-C6-N1	6.84	121.12	117.70
21	AA	251	G	O4'-C1'-N9	6.84	113.67	108.20
21	AA	716	A	C5-C6-N1	6.84	121.12	117.70
55	BB	11	C	N3-C2-O2	-6.84	117.11	121.90
12	AM	56	ARG	NE-CZ-NH1	6.84	123.72	120.30
54	BA	1204	A	O4'-C1'-N9	6.84	113.67	108.20
54	BA	2059	A	N1-C6-N6	-6.84	114.50	118.60
55	BB	58	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	573	U	P-O3'-C3'	6.84	127.91	119.70
54	BA	2612	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	1082	A	C5-C6-N1	6.84	121.12	117.70
55	BB	43	C	N3-C2-O2	-6.84	117.11	121.90
55	BB	66	A	N1-C6-N6	-6.84	114.50	118.60
54	BA	1428	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	238	A	C5-C6-N1	6.83	121.12	117.70
21	AA	1465	A	C5-C6-N1	6.83	121.12	117.70
24	A3	42	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	727	A	C5-C6-N1	6.83	121.12	117.70
54	BA	941	A	C5-C6-N1	6.83	121.12	117.70
54	BA	1098	A	C5-C6-N1	6.83	121.12	117.70
54	BA	1900	A	C5-C6-N1	6.83	121.11	117.70
54	BA	2333	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2704	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	706	A	C5-C6-N1	6.83	121.11	117.70
54	BA	42	A	C5-C6-N1	6.83	121.11	117.70
54	BA	2506	U	O4'-C1'-N1	6.83	113.66	108.20
54	BA	2835	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1019	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	1508	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	374	A	C5-C6-N1	6.83	121.11	117.70
54	BA	1978	A	C5-C6-N1	6.83	121.11	117.70
54	BA	109	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	2089	C	N3-C2-O2	-6.82	117.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1652	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	342	C	N3-C2-O2	-6.82	117.12	121.90
43	BU	6	ARG	NE-CZ-NH2	6.82	123.71	120.30
54	BA	64	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	69	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	444	C	O4'-C1'-N1	6.82	113.66	108.20
54	BA	1676	A	N1-C6-N6	-6.82	114.51	118.60
21	AA	162	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	477	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	1046	A	C5-C6-N1	6.82	121.11	117.70
54	BA	226	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	244	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	2788	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	560	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	693	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	1597	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1916	A	C5-C6-N1	6.82	121.11	117.70
55	BB	94	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1997	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	2045	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	223	A	C5-C6-N1	6.81	121.11	117.70
54	BA	2288	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	2740	A	C5-C6-N1	6.81	121.11	117.70
54	BA	432	A	C5-C6-N1	6.81	121.11	117.70
3	AD	69	ARG	NE-CZ-NH1	6.81	123.70	120.30
54	BA	1054	A	C5-C6-N1	6.81	121.11	117.70
18	AS	36	ARG	NE-CZ-NH1	6.81	123.70	120.30
21	AA	155	A	N1-C6-N6	-6.81	114.52	118.60
21	AA	865	A	C5-C6-N1	6.81	121.10	117.70
54	BA	1254	A	C5-C6-N1	6.81	121.10	117.70
55	BB	30	C	N3-C2-O2	-6.81	117.14	121.90
54	BA	2354	C	N3-C2-O2	-6.81	117.14	121.90
21	AA	190	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	2227	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	2654	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	808	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	19	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	176	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1715	G	O4'-C1'-N9	6.80	113.64	108.20
21	AA	223	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	1366	A	N1-C6-N6	-6.80	114.52	118.60
21	AA	493	A	C4-C5-C6	-6.80	113.60	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1180	A	N1-C6-N6	-6.80	114.52	118.60
21	AA	1227	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1306	A	C5-C6-N1	6.80	121.10	117.70
47	BY	47	ARG	NE-CZ-NH1	6.80	123.70	120.30
54	BA	661	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	1932	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2497	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1409	C	N3-C2-O2	-6.80	117.14	121.90
24	A3	38	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	190	A	N1-C6-N6	-6.80	114.52	118.60
21	AA	300	A	C5-C6-N1	6.80	121.10	117.70
21	AA	579	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1431	A	C5-C6-N1	6.80	121.10	117.70
54	BA	844	A	C5-C6-N1	6.80	121.10	117.70
54	BA	990	A	C1'-O4'-C4'	-6.80	104.46	109.90
54	BA	1974	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	1805	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	2872	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	22	C	N1-C2-O2	6.79	122.97	118.90
21	AA	374	A	C5-C6-N1	6.79	121.09	117.70
54	BA	627	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	1335	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	787	A	C5-C6-N1	6.79	121.09	117.70
54	BA	1698	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	320	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	892	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	1250	A	C5-C6-N1	6.79	121.09	117.70
22	A1	9	A	N1-C6-N6	-6.79	114.53	118.60
54	BA	139	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	2628	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	2687	U	O4'-C1'-N1	6.79	113.63	108.20
21	AA	72	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	280	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	1441	A	C5-C6-N1	6.79	121.09	117.70
54	BA	362	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	371	A	C5-C6-N1	6.78	121.09	117.70
21	AA	913	A	C5-C6-N1	6.78	121.09	117.70
21	AA	1021	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1848	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	2225	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2778	A	C5-C6-N1	6.78	121.09	117.70
21	AA	264	C	N3-C2-O2	-6.78	117.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1521	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	142	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1764	C	O4'-C1'-N1	6.78	113.62	108.20
21	AA	335	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	815	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1400	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	492	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1928	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1962	C	N3-C2-O2	-6.78	117.15	121.90
43	BU	21	ARG	NE-CZ-NH1	6.78	123.69	120.30
21	AA	1275	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	703	U	O4'-C1'-N1	6.78	113.62	108.20
54	BA	981	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2432	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2274	A	C5-C6-N1	6.77	121.09	117.70
21	AA	946	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	969	A	C5-C6-N1	6.77	121.09	117.70
35	BM	18	ARG	NE-CZ-NH1	6.77	123.69	120.30
54	BA	723	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	1502	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	712	A	C4-C5-C6	-6.77	113.61	117.00
35	BM	10	ARG	NE-CZ-NH1	6.77	123.69	120.30
54	BA	749	A	N1-C6-N6	-6.77	114.54	118.60
54	BA	1040	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	480	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1637	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1705	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1912	A	C4-C5-C6	-6.77	113.62	117.00
54	BA	2749	A	C5-C6-N1	6.77	121.08	117.70
3	AD	13	ARG	NE-CZ-NH1	6.77	123.68	120.30
21	AA	19	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	872	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2060	A	C4-C5-C6	-6.76	113.62	117.00
17	AR	42	ARG	NE-CZ-NH1	-6.76	116.92	120.30
21	AA	781	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1247	A	C5-C6-N1	6.76	121.08	117.70
21	AA	630	A	N1-C6-N6	-6.76	114.55	118.60
54	BA	502	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1172	C	N3-C2-O2	-6.76	117.17	121.90
55	BB	36	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	782	A	C5-C6-N1	6.76	121.08	117.70
21	AA	825	A	C5-C6-N1	6.76	121.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	932	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	1384	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1843	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2388	A	C5-C6-N1	6.76	121.08	117.70
2	AC	71	ARG	NE-CZ-NH1	6.75	123.68	120.30
21	AA	1296	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	2874	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	528	A	N1-C6-N6	-6.75	114.55	118.60
54	BA	705	A	C5-C6-N1	6.75	121.08	117.70
54	BA	2531	A	C5-C6-N1	6.75	121.08	117.70
54	BA	2699	C	N3-C2-O2	-6.75	117.17	121.90
22	A1	66	A	C4-C5-C6	-6.75	113.62	117.00
28	BF	94	ARG	NE-CZ-NH1	6.75	123.67	120.30
54	BA	678	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	764	A	C5-C6-N1	6.75	121.08	117.70
54	BA	2781	A	C4-C5-C6	-6.75	113.62	117.00
50	B1	5	ARG	NE-CZ-NH2	-6.75	116.93	120.30
54	BA	5	A	C5-C6-N1	6.75	121.07	117.70
54	BA	626	A	C5-C6-N1	6.75	121.07	117.70
54	BA	2084	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	95	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	749	A	C5-C6-N1	6.75	121.07	117.70
21	AA	151	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	1192	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	130	A	C5'-C4'-C3'	-6.74	105.21	116.00
21	AA	796	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	1398	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1126	A	P-O3'-C3'	6.74	127.79	119.70
54	BA	1305	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	2270	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1291	C	N3-C2-O2	-6.74	117.18	121.90
38	BP	88	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	1260	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1276	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2342	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	419	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	747	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1360	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1706	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	873	A	N1-C6-N6	-6.74	114.56	118.60
21	AA	1254	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1329	A	C4-C5-C6	-6.74	113.63	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1239	A	C4-C5-C6	-6.73	113.63	117.00
54	BA	1654	A	C5-C6-N1	6.73	121.07	117.70
54	BA	2564	A	C5-C6-N1	6.73	121.07	117.70
21	AA	1251	A	C4-C5-C6	-6.73	113.63	117.00
54	BA	509	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2589	A	C4-C5-C6	-6.73	113.63	117.00
21	AA	940	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	1476	A	C5-C6-N1	6.73	121.06	117.70
54	BA	888	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2679	A	C4-C5-C6	-6.73	113.64	117.00
55	BB	92	C	N3-C2-O2	-6.73	117.19	121.90
24	A3	52	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2267	A	C5-C6-N1	6.73	121.06	117.70
54	BA	1194	A	C5-C6-N1	6.73	121.06	117.70
54	BA	1350	C	N1-C2-O2	6.73	122.94	118.90
54	BA	1469	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	1847	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	1924	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	507	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	765	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	1499	A	C5-C6-N1	6.72	121.06	117.70
23	A2	82	A	C5-C6-N1	6.72	121.06	117.70
54	BA	1953	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	949	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	412	A	C5-C6-N1	6.72	121.06	117.70
54	BA	839	U	O4'-C1'-N1	6.72	113.58	108.20
54	BA	2374	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	269	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	91	A	O4'-C1'-N9	6.72	113.58	108.20
54	BA	1246	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1306	C	O4'-C1'-N1	6.72	113.58	108.20
21	AA	50	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	655	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	1092	A	C5-C6-N1	6.72	121.06	117.70
54	BA	56	A	C5-C6-N1	6.72	121.06	117.70
54	BA	311	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1635	A	C5-C6-N1	6.72	121.06	117.70
21	AA	964	A	C5-C6-N1	6.71	121.06	117.70
54	BA	192	C	O4'-C1'-N1	6.71	113.57	108.20
54	BA	1437	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1586	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2114	A	C5-C6-N1	6.71	121.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2698	U	O4'-C1'-N1	6.71	113.57	108.20
21	AA	25	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	782	A	C5-C6-N1	6.71	121.06	117.70
24	A3	22	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1504	A	C5-C6-N1	6.71	121.06	117.70
54	BA	2534	A	C4-C5-C6	-6.71	113.64	117.00
21	AA	487	A	C5-C6-N1	6.71	121.06	117.70
21	AA	718	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1804	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1960	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1762	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2785	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	712	A	C5-C6-N1	6.71	121.05	117.70
54	BA	541	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1363	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1793	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	1196	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	1524	C	N3-C2-O2	-6.71	117.21	121.90
28	BF	70	ARG	NE-CZ-NH1	6.71	123.65	120.30
54	BA	482	A	C5-C6-N1	6.71	121.05	117.70
54	BA	742	A	C5-C6-N1	6.71	121.05	117.70
21	AA	1055	A	C5-C6-N1	6.71	121.05	117.70
21	AA	181	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1021	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1632	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2078	C	N3-C2-O2	-6.70	117.21	121.90
55	BB	115	A	C5-C6-N1	6.70	121.05	117.70
1	AB	62	ARG	NE-CZ-NH1	6.70	123.65	120.30
54	BA	1264	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	1397	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	960	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1387	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1940	U	O4'-C1'-N1	6.70	113.56	108.20
54	BA	2328	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2716	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	321	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	946	A	C5-C6-N1	6.70	121.05	117.70
21	AA	1170	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2014	A	C5-C6-N1	6.70	121.05	117.70
21	AA	576	C	N1-C2-O2	6.70	122.92	118.90
54	BA	414	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2199	A	C5-C6-N1	6.70	121.05	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AG	110	ARG	NE-CZ-NH1	6.70	123.65	120.30
22	A1	23	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	556	A	C5-C6-N1	6.70	121.05	117.70
54	BA	833	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1126	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1764	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2748	A	C5-C6-N1	6.70	121.05	117.70
54	BA	964	C	N3-C2-O2	-6.69	117.21	121.90
54	BA	197	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	209	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	272	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1265	A	O4'-C1'-N9	6.69	113.55	108.20
54	BA	457	A	C5-C6-N1	6.69	121.05	117.70
54	BA	737	C	O4'-C1'-N1	6.69	113.55	108.20
54	BA	1987	A	C5-C6-N1	6.69	121.05	117.70
21	AA	1197	A	C4-C5-C6	-6.69	113.66	117.00
22	A1	71	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	1749	A	C5-C6-N1	6.69	121.04	117.70
54	BA	2792	A	C5-C6-N1	6.69	121.04	117.70
43	BU	85	ARG	NE-CZ-NH1	6.69	123.64	120.30
54	BA	218	A	N1-C6-N6	-6.69	114.59	118.60
54	BA	2726	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	193	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	89	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2059	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2077	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	2503	A	P-O3'-C3'	6.68	127.72	119.70
55	BB	60	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	55	A	P-O3'-C3'	6.68	127.72	119.70
22	A1	6	A	C5-C6-N1	6.68	121.04	117.70
31	BI	126	ARG	NE-CZ-NH1	6.68	123.64	120.30
54	BA	722	A	C5-C6-N1	6.68	121.04	117.70
54	BA	972	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1745	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1363	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1285	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2471	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2560	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2825	G	N3-C2-N2	-6.68	115.22	119.90
21	AA	1230	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	74	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	1046	A	O4'-C1'-N9	6.68	113.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1175	A	C1'-O4'-C4'	-6.68	104.56	109.90
54	BA	1328	A	C4-C5-C6	-6.68	113.66	117.00
55	BB	50	A	C5-C6-N1	6.68	121.04	117.70
8	AI	94	ARG	NE-CZ-NH1	6.68	123.64	120.30
54	BA	2247	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2670	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1492	A	C5-C6-N1	6.68	121.04	117.70
54	BA	592	A	C4-C5-C6	-6.68	113.66	117.00
21	AA	507	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	695	A	C5-C6-N1	6.67	121.04	117.70
21	AA	1275	A	C5-C6-N1	6.67	121.04	117.70
21	AA	1394	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	1476	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	1529	G	O4'-C1'-N9	6.67	113.54	108.20
24	A3	29	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	97	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	330	A	C5-C6-N1	6.67	121.04	117.70
54	BA	699	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	1054	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	1937	A	O4'-C1'-N9	6.67	113.54	108.20
21	AA	164	G	O4'-C1'-N9	6.67	113.54	108.20
22	A1	73	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1498	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1528	A	C5-C6-N1	6.67	121.04	117.70
54	BA	2762	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1336	A	C5-C6-N1	6.67	121.03	117.70
54	BA	1427	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	1428	A	C5-C6-N1	6.67	121.03	117.70
33	BK	64	ARG	NE-CZ-NH1	6.67	123.63	120.30
54	BA	2001	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2858	C	N3-C2-O2	-6.67	117.23	121.90
19	AT	23	ARG	NE-CZ-NH1	6.67	123.63	120.30
54	BA	502	A	C5-C6-N1	6.67	121.03	117.70
54	BA	584	C	O4'-C1'-N1	6.67	113.53	108.20
54	BA	2205	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2649	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	547	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	753	A	C5-C6-N1	6.66	121.03	117.70
27	BE	88	ARG	NE-CZ-NH1	6.66	123.63	120.30
54	BA	281	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	565	C	N3-C2-O2	-6.66	117.23	121.90
54	BA	2579	C	N3-C2-O2	-6.66	117.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	303	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	587	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1717	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2019	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2412	A	C5-C6-N1	6.66	121.03	117.70
21	AA	972	C	O4'-C1'-N1	6.66	113.53	108.20
29	BG	68	ARG	NE-CZ-NH1	6.66	123.63	120.30
54	BA	156	A	C5-C6-N1	6.66	121.03	117.70
21	AA	327	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	1042	A	C5-C6-N1	6.66	121.03	117.70
54	BA	181	A	C5-C6-N1	6.66	121.03	117.70
21	AA	1069	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1550	C	O4'-C1'-N1	6.66	113.53	108.20
54	BA	2021	C	O4'-C1'-N1	6.66	113.53	108.20
54	BA	1395	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2114	A	C4-C5-C6	-6.66	113.67	117.00
11	AL	8	ARG	NE-CZ-NH1	6.65	123.63	120.30
25	BC	237	ARG	NE-CZ-NH1	6.65	123.63	120.30
21	AA	174	A	N1-C6-N6	-6.65	114.61	118.60
21	AA	221	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	1287	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	515	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1561	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	1429	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	66	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	457	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	735	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1384	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	2071	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1229	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	743	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	1443	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	2080	A	C5-C6-N1	6.65	121.02	117.70
54	BA	1383	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	1149	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	13	A	C5-C6-N1	6.64	121.02	117.70
54	BA	165	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1914	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2052	A	N1-C6-N6	-6.64	114.61	118.60
54	BA	2815	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	640	A	C4-C5-C6	-6.64	113.68	117.00
24	A3	63	C	N3-C2-O2	-6.64	117.25	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	191	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1690	A	C5-C6-N1	6.64	121.02	117.70
21	AA	1157	A	C5-C6-N1	6.64	121.02	117.70
28	BF	124	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	1313	U	N3-C2-O2	-6.64	117.55	122.20
54	BA	1648	U	O4'-C1'-N1	6.64	113.51	108.20
54	BA	2214	C	O4'-C1'-N1	6.64	113.51	108.20
54	BA	282	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2461	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1730	C	N1-C2-O2	6.64	122.88	118.90
21	AA	177	G	O4'-C1'-N9	6.63	113.51	108.20
21	AA	1396	A	C5-C6-N1	6.63	121.02	117.70
54	BA	105	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	867	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1205	A	O4'-C1'-N9	6.63	113.51	108.20
55	BB	90	C	O4'-C1'-N1	6.63	113.51	108.20
21	AA	496	A	N1-C6-N6	-6.63	114.62	118.60
21	AA	889	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	1105	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	116	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	216	A	C5-C6-N1	6.63	121.01	117.70
54	BA	352	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	1210	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	1383	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	2738	A	C5-C6-N1	6.63	121.01	117.70
24	A3	57	C	N3-C2-O2	-6.62	117.26	121.90
54	BA	251	A	N1-C6-N6	-6.62	114.62	118.60
21	AA	1201	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	1311	A	C5-C6-N1	6.62	121.01	117.70
29	BG	34	ARG	NE-CZ-NH1	6.62	123.61	120.30
54	BA	2660	A	C5-C6-N1	6.62	121.01	117.70
1	AB	207	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	1441	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1127	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1169	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2165	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	866	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1073	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2184	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	1195	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	1213	A	C5-C6-N1	6.62	121.01	117.70
54	BA	310	A	C5-C6-N1	6.62	121.01	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	514	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2899	A	N1-C6-N6	-6.62	114.63	118.60
21	AA	16	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	730	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	167	A	C5-C6-N1	6.62	121.01	117.70
21	AA	217	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	1161	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	418	C	N3-C2-O2	-6.62	117.27	121.90
24	A3	43	G	C1'-O4'-C4'	-6.61	104.61	109.90
47	BY	48	ARG	NE-CZ-NH2	6.61	123.61	120.30
21	AA	239	U	O4'-C1'-N1	6.61	113.49	108.20
54	BA	144	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	265	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	1321	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	2006	C	N3-C2-O2	-6.61	117.28	121.90
21	AA	186	C	N3-C2-O2	-6.61	117.28	121.90
21	AA	575	G	P-O3'-C3'	6.61	127.63	119.70
54	BA	792	A	N1-C6-N6	-6.61	114.64	118.60
54	BA	1156	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	193	U	O4'-C1'-N1	6.60	113.48	108.20
24	A3	73	A	C5-C6-N1	6.60	121.00	117.70
54	BA	609	A	C5-C6-N1	6.60	121.00	117.70
54	BA	2815	C	O4'-C1'-N1	6.60	113.48	108.20
21	AA	825	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	938	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	670	A	C5-C6-N1	6.60	121.00	117.70
54	BA	742	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1947	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	2527	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	211	G	O4'-C1'-N9	6.60	113.48	108.20
21	AA	366	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	127	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	26	A	C5-C6-N1	6.60	121.00	117.70
21	AA	452	A	C5-C6-N1	6.60	121.00	117.70
35	BM	40	ARG	NE-CZ-NH1	6.60	123.60	120.30
21	AA	1408	A	C5-C6-N1	6.59	121.00	117.70
24	A3	11	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	89	A	C4-C5-C6	-6.59	113.70	117.00
24	A3	66	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	623	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	633	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1268	A	C4-C5-C6	-6.59	113.70	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2275	C	N3-C2-O2	-6.59	117.28	121.90
21	AA	307	C	N1-C2-O2	6.59	122.86	118.90
24	A3	43	G	O4'-C1'-N9	6.59	113.47	108.20
54	BA	947	A	C5-C6-N1	6.59	121.00	117.70
21	AA	422	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1355	G	N3-C2-N2	-6.59	115.29	119.90
54	BA	1810	A	N1-C6-N6	-6.59	114.65	118.60
56	B5	164	ARG	NE-CZ-NH1	6.59	123.59	120.30
21	AA	694	A	N1-C6-N6	-6.59	114.65	118.60
54	BA	207	A	C4-C5-C6	-6.59	113.71	117.00
12	AM	92	ARG	NE-CZ-NH1	6.59	123.59	120.30
21	AA	329	A	C5-C6-N1	6.59	120.99	117.70
18	AS	80	ARG	NE-CZ-NH2	6.58	123.59	120.30
54	BA	348	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1879	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	1408	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	38	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1143	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1387	A	O4'-C1'-N9	6.58	113.47	108.20
54	BA	300	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	348	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2336	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2764	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2806	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	1248	A	C4-C5-C6	-6.58	113.71	117.00
24	A3	17	C	N1-C2-O2	6.58	122.85	118.90
54	BA	772	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1700	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1905	C	N3-C2-O2	-6.58	117.30	121.90
55	BB	73	A	C5-C6-N1	6.58	120.99	117.70
17	AR	60	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	1001	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1574	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	2426	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2450	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1109	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	439	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	1077	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	1152	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1274	A	C4-C5-C6	-6.57	113.71	117.00
36	BN	17	ARG	NE-CZ-NH1	6.57	123.59	120.30
54	BA	402	A	C5-C6-N1	6.57	120.99	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2900	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	599	A	C5-C6-N1	6.57	120.99	117.70
54	BA	602	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	982	C	N1-C2-O2	6.57	122.84	118.90
54	BA	1885	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	1927	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2606	C	N3-C2-O2	-6.57	117.30	121.90
24	A3	36	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	2668	G	O4'-C1'-N9	6.57	113.45	108.20
21	AA	172	A	C4-C5-C6	-6.57	113.72	117.00
21	AA	807	A	C5-C6-N1	6.57	120.98	117.70
54	BA	176	A	C4-C5-C6	-6.57	113.72	117.00
21	AA	143	A	C4-C5-C6	-6.57	113.72	117.00
21	AA	1097	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	1375	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2099	U	N3-C2-O2	-6.57	117.60	122.20
54	BA	2142	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2394	C	N3-C2-O2	-6.57	117.31	121.90
25	BC	155	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	1735	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1998	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2094	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2430	A	C4-C5-C6	-6.56	113.72	117.00
55	BB	39	A	C4-C5-C6	-6.56	113.72	117.00
2	AC	168	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	454	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1165	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	1324	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	1937	A	C5-C6-N1	6.56	120.98	117.70
21	AA	77	A	N1-C6-N6	-6.56	114.67	118.60
21	AA	1404	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1545	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1598	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2332	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2587	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	1119	C	N3-C2-O2	-6.55	117.31	121.90
22	A1	65	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	257	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1433	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	2317	A	C5-C6-N1	6.55	120.98	117.70
21	AA	784	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	1456	A	C5-C6-N1	6.55	120.98	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	866	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1754	A	C4-C5-C6	-6.55	113.72	117.00
9	AJ	9	ARG	NE-CZ-NH1	6.55	123.58	120.30
21	AA	349	A	C5-C6-N1	6.55	120.97	117.70
21	AA	624	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	719	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1584	U	N3-C2-O2	-6.55	117.61	122.20
54	BA	1717	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	309	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	342	A	C4-C5-C6	-6.55	113.73	117.00
21	AA	1114	C	N3-C2-O2	-6.55	117.32	121.90
27	BE	162	ARG	NE-CZ-NH1	6.55	123.57	120.30
54	BA	2307	G	N1-C6-O6	-6.55	115.97	119.90
21	AA	1246	A	N1-C6-N6	-6.54	114.67	118.60
21	AA	490	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	586	A	C5-C6-N1	6.54	120.97	117.70
54	BA	973	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1889	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2178	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	914	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	804	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1461	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1641	A	C5-C6-N1	6.54	120.97	117.70
2	AC	163	ARG	NE-CZ-NH1	6.54	123.57	120.30
21	AA	681	A	C5-C6-N1	6.54	120.97	117.70
21	AA	708	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	309	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	944	C	O4'-C1'-N1	6.54	113.43	108.20
54	BA	2381	A	C4-C5-C6	-6.54	113.73	117.00
55	BB	42	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	610	U	N3-C2-O2	-6.54	117.63	122.20
54	BA	2827	C	N3-C2-O2	-6.54	117.33	121.90
3	AD	25	ARG	NE-CZ-NH1	6.53	123.57	120.30
21	AA	414	A	C4-C5-C6	-6.53	113.73	117.00
21	AA	816	A	N1-C6-N6	-6.53	114.68	118.60
25	BC	51	ARG	NE-CZ-NH1	6.53	123.57	120.30
54	BA	531	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	964	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	1837	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	270	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	643	A	C5-C6-N1	6.53	120.97	117.70
21	AA	1510	C	N3-C2-O2	-6.53	117.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	199	A	C4-C5-C6	-6.53	113.74	117.00
51	B2	39	ARG	NE-CZ-NH1	6.53	123.56	120.30
21	AA	460	A	C5-C6-N1	6.53	120.96	117.70
54	BA	111	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	2700	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	311	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	655	A	C5-C6-N1	6.52	120.96	117.70
54	BA	2065	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	2700	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1144	A	C4-C5-C6	-6.52	113.74	117.00
55	BB	31	C	N3-C2-O2	-6.52	117.33	121.90
19	AT	9	ARG	NE-CZ-NH1	6.52	123.56	120.30
54	BA	621	A	C5-C6-N1	6.52	120.96	117.70
54	BA	960	A	N1-C6-N6	-6.52	114.69	118.60
54	BA	2435	A	C5-C6-N1	6.52	120.96	117.70
21	AA	129	A	N1-C6-N6	-6.52	114.69	118.60
21	AA	139	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	501	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1829	A	C4-C5-C6	-6.52	113.74	117.00
20	AU	17	ARG	NE-CZ-NH2	6.52	123.56	120.30
22	A1	61	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	849	A	C5-C6-N1	6.52	120.96	117.70
54	BA	901	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	389	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	749	A	C5-C6-N1	6.51	120.96	117.70
21	AA	802	A	C5-C6-N1	6.51	120.96	117.70
21	AA	1111	A	C5-C6-N1	6.51	120.96	117.70
54	BA	590	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	616	A	C5-C6-N1	6.51	120.96	117.70
54	BA	1600	C	N3-C2-O2	-6.51	117.34	121.90
56	B5	7	ARG	NE-CZ-NH1	6.51	123.56	120.30
21	AA	195	A	C5-C6-N1	6.51	120.96	117.70
21	AA	196	A	C4-C5-C6	-6.51	113.75	117.00
21	AA	288	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1532	A	C4-C5-C6	-6.51	113.74	117.00
11	AL	82	ARG	NE-CZ-NH1	6.51	123.56	120.30
21	AA	6	G	C1'-O4'-C4'	-6.51	104.69	109.90
54	BA	172	A	C5-C6-N1	6.51	120.95	117.70
54	BA	1626	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1686	C	O4'-C1'-N1	6.51	113.41	108.20
54	BA	1844	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1872	A	C5-C6-N1	6.51	120.95	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2875	C	N3-C2-O2	-6.51	117.34	121.90
16	AQ	76	ARG	NE-CZ-NH1	6.51	123.55	120.30
23	A2	93	U	C1'-O4'-C4'	-6.51	104.69	109.90
54	BA	1858	A	C4-C5-C6	-6.51	113.75	117.00
21	AA	155	A	C5-C6-N1	6.51	120.95	117.70
21	AA	623	C	N3-C2-O2	-6.51	117.35	121.90
54	BA	401	A	C5-C6-N1	6.51	120.95	117.70
54	BA	1262	A	C5-C6-N1	6.51	120.95	117.70
54	BA	1385	A	C5-C6-N1	6.51	120.95	117.70
54	BA	31	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	563	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2070	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2761	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	613	C	N3-C2-O2	-6.50	117.35	121.90
33	BK	98	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	1597	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1801	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2050	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	816	A	C5-C6-N1	6.50	120.95	117.70
53	B4	12	ARG	NE-CZ-NH1	-6.50	117.05	120.30
54	BA	196	A	C5-C6-N1	6.50	120.95	117.70
54	BA	330	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	613	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	680	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1276	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2013	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2380	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	608	A	C5-C6-N1	6.50	120.95	117.70
21	AA	998	C	N3-C2-O2	-6.50	117.35	121.90
22	A1	62	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1298	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	498	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	599	C	N3-C2-O2	-6.50	117.35	121.90
22	A1	35	A	C5-C6-N1	6.50	120.95	117.70
54	BA	241	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	471	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1593	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1655	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2267	A	N1-C6-N6	-6.50	114.70	118.60
21	AA	136	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	197	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	386	C	N3-C2-O2	-6.50	117.35	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	104	A	C5-C6-N1	6.50	120.95	117.70
54	BA	201	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2003	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1005	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	462	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2675	A	C5-C6-N1	6.49	120.95	117.70
54	BA	2675	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	766	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	1141	C	N3-C2-O2	-6.49	117.36	121.90
40	BR	90	ARG	NE-CZ-NH1	6.49	123.55	120.30
54	BA	821	A	C5-C6-N1	6.49	120.95	117.70
54	BA	1446	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2248	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	174	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	1016	A	C4-C5-C6	-6.49	113.76	117.00
21	AA	1216	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	846	U	O4'-C1'-N1	6.49	113.39	108.20
54	BA	990	A	C5-C6-N1	6.49	120.94	117.70
54	BA	199	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	1787	A	C5-C6-N1	6.49	120.94	117.70
21	AA	807	A	C4-C5-C6	-6.49	113.76	117.00
21	AA	1019	A	C5-C6-N1	6.49	120.94	117.70
37	BO	25	ARG	NE-CZ-NH1	6.49	123.54	120.30
54	BA	774	G	O4'-C1'-N9	6.49	113.39	108.20
54	BA	1481	U	O4'-C1'-N1	6.49	113.39	108.20
54	BA	1902	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2619	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	378	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	835	C	O4'-C1'-N1	6.48	113.39	108.20
54	BA	900	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2771	C	N3-C2-O2	-6.48	117.36	121.90
5	AF	45	ARG	NE-CZ-NH1	6.48	123.54	120.30
33	BK	17	ARG	NE-CZ-NH1	6.48	123.54	120.30
54	BA	517	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	2119	A	C5-C6-N1	6.48	120.94	117.70
51	B2	35	ARG	NE-CZ-NH1	6.48	123.54	120.30
3	AD	2	ARG	NE-CZ-NH1	6.48	123.54	120.30
8	AI	112	ARG	NE-CZ-NH1	6.48	123.54	120.30
13	AN	24	ARG	NE-CZ-NH1	6.47	123.54	120.30
54	BA	371	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	671	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2179	C	N3-C2-O2	-6.47	117.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2403	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	470	A	C5-C6-N1	6.47	120.94	117.70
21	AA	702	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	523	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1610	A	C5-C6-N1	6.47	120.94	117.70
54	BA	1722	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1810	A	C5-C6-N1	6.47	120.94	117.70
54	BA	1780	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1285	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	2147	A	C5-C6-N1	6.47	120.93	117.70
54	BA	84	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2434	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	131	A	C5-C6-N1	6.46	120.93	117.70
54	BA	699	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1110	A	N1-C6-N6	-6.46	114.72	118.60
21	AA	1271	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1367	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1462	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	167	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2424	C	N1-C2-O2	6.46	122.78	118.90
54	BA	2496	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1352	C	N3-C2-O2	-6.46	117.38	121.90
24	A3	44	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	2734	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1282	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1328	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	415	A	C5-C6-N1	6.46	120.93	117.70
54	BA	885	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1373	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1398	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1919	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1005	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1893	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2076	U	N3-C2-O2	-6.46	117.68	122.20
21	AA	855	U	O4'-C1'-N1	6.45	113.36	108.20
21	AA	1325	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	2634	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	2757	A	C5-C6-N1	6.45	120.93	117.70
54	BA	49	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	1039	A	C5-C6-N1	6.45	120.93	117.70
21	AA	432	A	C5-C6-N1	6.45	120.92	117.70
21	AA	1399	C	C1'-O4'-C4'	-6.45	104.74	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	151	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	637	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	936	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1420	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	2366	A	C5-C6-N1	6.45	120.92	117.70
54	BA	2637	U	O4'-C1'-N1	6.45	113.36	108.20
5	AF	44	ARG	NE-CZ-NH1	6.45	123.53	120.30
54	BA	310	A	N1-C6-N6	-6.45	114.73	118.60
54	BA	2335	A	C5-C6-N1	6.45	120.92	117.70
54	BA	2733	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	864	A	C5-C6-N1	6.45	120.92	117.70
54	BA	990	A	O4'-C1'-N9	6.45	113.36	108.20
54	BA	1053	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1403	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	295	C	N1-C2-O2	6.44	122.77	118.90
54	BA	1480	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2090	A	C5-C6-N1	6.44	120.92	117.70
54	BA	2268	A	C5-C6-N1	6.44	120.92	117.70
21	AA	220	G	N3-C2-N2	-6.44	115.39	119.90
21	AA	699	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	471	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2830	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	962	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	443	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1352	U	N3-C2-O2	-6.44	117.69	122.20
54	BA	1525	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1665	A	C5-C6-N1	6.44	120.92	117.70
54	BA	2215	C	O4'-C1'-N1	6.44	113.35	108.20
42	BT	6	ARG	NE-CZ-NH2	-6.44	117.08	120.30
54	BA	987	C	O4'-C1'-N1	6.44	113.35	108.20
21	AA	1045	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	513	A	N1-C6-N6	-6.44	114.74	118.60
54	BA	1795	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	1870	C	N1-C2-O2	6.44	122.76	118.90
54	BA	2284	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2340	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2512	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	1418	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	945	A	C4-C5-C6	-6.44	113.78	117.00
10	AK	52	ARG	NE-CZ-NH1	6.43	123.52	120.30
21	AA	873	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	907	A	C5-C6-N1	6.43	120.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1368	A	C4-C5-C6	-6.43	113.78	117.00
45	BW	13	ARG	NE-CZ-NH1	6.43	123.52	120.30
54	BA	149	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	1570	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	2662	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	608	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1952	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	192	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	233	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	586	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	1005	A	C4-C5-C6	-6.43	113.79	117.00
24	A3	22	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	118	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	497	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	810	U	O4'-C1'-N1	6.43	113.34	108.20
54	BA	998	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2082	A	C5-C6-N1	6.43	120.92	117.70
21	AA	1285	A	C5-C6-N1	6.43	120.91	117.70
54	BA	1032	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	2150	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	353	A	N1-C6-N6	-6.43	114.74	118.60
22	A1	74	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	788	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	928	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	2200	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2215	C	N3-C2-O2	-6.42	117.40	121.90
55	BB	114	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	1137	C	N3-C2-O2	-6.42	117.40	121.90
54	BA	351	C	N3-C2-O2	-6.42	117.41	121.90
55	BB	89	U	O4'-C1'-N1	6.42	113.34	108.20
21	AA	459	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	758	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1120	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1269	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	666	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2823	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	549	C	N1-C2-O2	6.42	122.75	118.90
21	AA	938	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	616	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	1323	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	2398	U	O4'-C1'-N1	6.42	113.33	108.20
21	AA	1344	C	N3-C2-O2	-6.42	117.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2094	A	C5-C6-N1	6.42	120.91	117.70
21	AA	392	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	1101	A	P-O3'-C3'	6.41	127.40	119.70
54	BA	1759	A	C5-C6-N1	6.41	120.91	117.70
54	BA	2715	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	403	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	626	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	1977	A	C4-C5-C6	-6.41	113.79	117.00
21	AA	16	A	C5-C6-N1	6.41	120.91	117.70
21	AA	1146	A	N1-C6-N6	-6.41	114.75	118.60
54	BA	505	A	C5-C6-N1	6.41	120.91	117.70
54	BA	582	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1579	A	N1-C6-N6	-6.41	114.75	118.60
21	AA	176	C	N3-C2-O2	-6.41	117.41	121.90
35	BM	16	ARG	NE-CZ-NH1	6.41	123.50	120.30
54	BA	352	A	C5-C6-N1	6.41	120.90	117.70
54	BA	802	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1565	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	991	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	2085	U	O4'-C1'-N1	6.41	113.33	108.20
54	BA	2901	C	N3-C2-O2	-6.41	117.42	121.90
21	AA	106	C	N3-C2-O2	-6.41	117.42	121.90
21	AA	131	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	856	C	N3-C2-O2	-6.41	117.42	121.90
24	A3	44	A	C5-C6-N1	6.41	120.90	117.70
54	BA	104	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	433	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	1076	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	1752	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	225	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	215	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	306	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1853	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2015	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2146	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2417	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2805	C	O4'-C1'-N1	6.40	113.32	108.20
21	AA	100	G	N1-C6-O6	-6.40	116.06	119.90
21	AA	179	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	76	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1956	U	O4'-C1'-N1	6.40	113.32	108.20
54	BA	1606	C	N1-C2-O2	6.40	122.74	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1513	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	1520	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	614	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	2338	C	N3-C2-O2	-6.40	117.42	121.90
55	BB	3	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	103	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	732	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	251	G	P-O3'-C3'	6.39	127.37	119.70
54	BA	943	A	C4-C5-C6	-6.39	113.80	117.00
15	AP	70	ARG	NE-CZ-NH1	6.39	123.50	120.30
21	AA	67	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	526	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	1035	A	N1-C6-N6	-6.39	114.77	118.60
54	BA	767	U	O4'-C1'-N1	6.39	113.31	108.20
54	BA	1084	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	2033	A	C4-C5-C6	-6.39	113.80	117.00
55	BB	59	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	1237	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2090	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	1501	C	N3-C2-O2	-6.39	117.43	121.90
24	A3	70	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	833	A	N1-C6-N6	-6.39	114.77	118.60
6	AG	142	ARG	NE-CZ-NH1	6.39	123.49	120.30
21	AA	536	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	595	C	N3-C2-O2	-6.39	117.43	121.90
11	AL	55	ARG	NE-CZ-NH1	6.39	123.49	120.30
21	AA	488	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	501	C	N1-C2-O2	6.39	122.73	118.90
21	AA	919	A	C5-C6-N1	6.39	120.89	117.70
54	BA	719	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1269	A	C4-C5-C6	-6.39	113.81	117.00
22	A1	30	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	1549	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2035	G	O4'-C1'-N9	6.38	113.31	108.20
21	AA	1388	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2555	U	O4'-C1'-N1	6.38	113.31	108.20
21	AA	1257	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	335	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	1822	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2032	G	O4'-C1'-N9	6.38	113.31	108.20
54	BA	2182	U	O4'-C1'-N1	6.38	113.31	108.20
54	BA	1508	A	C4-C5-C6	-6.38	113.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	34	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	680	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	912	C	N3-C2-O2	-6.38	117.44	121.90
24	A3	59	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	572	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1008	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1265	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2520	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	1110	A	C5-C6-N1	6.38	120.89	117.70
54	BA	382	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	449	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1092	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	1175	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1669	A	C5-C6-N1	6.38	120.89	117.70
54	BA	472	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1569	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2025	C	N1-C2-O2	6.38	122.72	118.90
54	BA	2339	C	N3-C2-O2	-6.38	117.44	121.90
18	AS	79	TYR	C-N-CA	6.37	137.63	121.70
21	AA	274	A	C4-C5-C6	-6.37	113.81	117.00
24	A3	43	G	N1-C6-O6	-6.37	116.08	119.90
54	BA	1936	A	P-O3'-C3'	6.37	127.35	119.70
54	BA	2750	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	175	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	679	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2443	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2598	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	1046	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	1050	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	1109	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	379	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1342	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	81	A	C4-C5-C6	-6.37	113.82	117.00
21	AA	207	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1010	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	1749	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	2226	C	O4'-C1'-N1	6.37	113.29	108.20
21	AA	518	C	O4'-C1'-N1	6.36	113.29	108.20
21	AA	1248	A	C5-C6-N1	6.36	120.88	117.70
21	AA	328	C	P-O3'-C3'	6.36	127.33	119.70
21	AA	1245	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	222	A	C4-C5-C6	-6.36	113.82	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	635	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	936	A	C5-C6-N1	6.36	120.88	117.70
54	BA	2088	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	845	A	O4'-C1'-N9	6.36	113.29	108.20
54	BA	1507	C	O4'-C1'-N1	6.36	113.29	108.20
54	BA	1958	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	53	A	C5-C6-N1	6.36	120.88	117.70
21	AA	1508	A	C5-C6-N1	6.36	120.88	117.70
21	AA	322	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	927	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	314	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	978	A	C5-C6-N1	6.35	120.88	117.70
54	BA	821	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	2314	A	N1-C6-N6	-6.35	114.79	118.60
21	AA	199	A	C5-C6-N1	6.35	120.88	117.70
21	AA	382	A	C5-C6-N1	6.35	120.88	117.70
21	AA	1163	A	C5-C6-N1	6.35	120.88	117.70
21	AA	1288	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	256	A	C5-C6-N1	6.35	120.88	117.70
54	BA	417	C	N3-C2-O2	-6.35	117.45	121.90
10	AK	92	ARG	NE-CZ-NH2	-6.35	117.12	120.30
21	AA	18	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	110	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	21	A	C5-C6-N1	6.35	120.88	117.70
54	BA	84	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	2064	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2153	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2766	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	286	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	1246	A	C5-C6-N1	6.35	120.87	117.70
21	AA	475	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	746	A	C5-C6-N1	6.35	120.87	117.70
21	AA	859	G	N1-C6-O6	-6.35	116.09	119.90
21	AA	253	A	C5-C6-N1	6.34	120.87	117.70
21	AA	931	C	N3-C2-O2	-6.34	117.46	121.90
32	BJ	99	ARG	NE-CZ-NH1	6.34	123.47	120.30
54	BA	1791	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1890	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	74	A	C5-C6-N1	6.34	120.87	117.70
54	BA	94	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	164	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	1169	A	C4-C5-C6	-6.34	113.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1327	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2441	U	O4'-C1'-N1	6.34	113.27	108.20
54	BA	2448	A	C4-C5-C6	-6.34	113.83	117.00
8	AI	105	ARG	NE-CZ-NH1	6.34	123.47	120.30
21	AA	1102	A	C5-C6-N1	6.34	120.87	117.70
54	BA	129	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	951	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	994	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2000	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	778	G	C8-N9-C4	-6.34	103.86	106.40
54	BA	1111	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1882	U	O4'-C1'-N1	6.33	113.27	108.20
54	BA	2805	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1389	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1512	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2134	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	2249	U	O4'-C1'-N1	6.33	113.27	108.20
54	BA	2411	A	C4-C5-C6	-6.33	113.83	117.00
21	AA	522	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1027	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	740	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1327	A	C5-C6-N1	6.33	120.87	117.70
8	AI	44	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	140	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	735	A	N1-C6-N6	-6.33	114.80	118.60
54	BA	2416	C	N3-C2-O2	-6.33	117.47	121.90
55	BB	49	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	78	A	C4-C5-C6	-6.33	113.83	117.00
21	AA	1171	A	C5-C6-N1	6.33	120.86	117.70
21	AA	1402	C	O4'-C1'-N1	6.33	113.26	108.20
37	BO	111	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	669	G	N3-C2-N2	-6.33	115.47	119.90
54	BA	816	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1129	A	C4-C5-C6	-6.33	113.84	117.00
7	AH	14	ARG	NE-CZ-NH1	6.33	123.46	120.30
55	BB	38	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	910	C	N3-C2-O2	-6.32	117.47	121.90
22	A1	72	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	56	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	336	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	368	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	624	C	N3-C2-O2	-6.32	117.47	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	835	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	1433	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	2295	C	N3-C2-O2	-6.32	117.47	121.90
21	AA	451	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	984	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	19	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1164	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	1990	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	1000	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2448	A	C5-C6-N1	6.32	120.86	117.70
1	AB	94	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	468	A	C5-C6-N1	6.32	120.86	117.70
21	AA	1237	C	N1-C2-O2	6.32	122.69	118.90
54	BA	886	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1684	G	N1-C6-O6	-6.32	116.11	119.90
54	BA	2531	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	899	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	174	U	O4'-C1'-N1	6.32	113.25	108.20
54	BA	1247	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	2103	C	N3-C2-O2	-6.32	117.48	121.90
55	BB	30	C	O4'-C1'-N1	6.32	113.25	108.20
55	BB	59	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1686	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1711	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	1466	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1553	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1986	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2800	A	C5-C6-N1	6.31	120.86	117.70
54	BA	2835	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	132	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1748	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2175	C	N3-C2-O2	-6.31	117.48	121.90
25	BC	42	ARG	NE-CZ-NH1	6.31	123.45	120.30
54	BA	917	A	C5-C6-N1	6.31	120.86	117.70
54	BA	1626	A	C5-C6-N1	6.31	120.86	117.70
21	AA	156	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	900	A	C4-C5-C6	-6.31	113.85	117.00
22	A1	17	U	O4'-C1'-N1	6.31	113.25	108.20
54	BA	1961	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2463	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2773	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	8	A	C4-C5-C6	-6.31	113.85	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	525	C	N3-C2-O2	-6.31	117.49	121.90
54	BA	1151	A	C4-C5-C6	-6.31	113.85	117.00
54	BA	1604	C	N3-C2-O2	-6.31	117.49	121.90
54	BA	1908	C	N3-C2-O2	-6.31	117.49	121.90
54	BA	2439	A	C4-C5-C6	-6.31	113.85	117.00
54	BA	1575	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1037	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	788	A	O4'-C1'-N9	6.30	113.24	108.20
54	BA	965	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	715	A	C5-C6-N1	6.30	120.85	117.70
21	AA	1484	C	N3-C2-O2	-6.30	117.49	121.90
24	A3	76	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	204	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	341	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2042	A	C4-C5-C6	-6.30	113.85	117.00
14	AO	88	ARG	NE-CZ-NH1	6.30	123.45	120.30
24	A3	62	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	355	U	O4'-C1'-N1	6.30	113.24	108.20
54	BA	1392	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1892	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2760	C	N3-C2-O2	-6.30	117.49	121.90
55	BB	63	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	535	A	C5-C6-N1	6.30	120.85	117.70
21	AA	735	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1132	C	N1-C2-O2	6.30	122.68	118.90
21	AA	1399	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	366	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	482	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	484	C	O4'-C1'-N1	6.30	113.24	108.20
54	BA	1114	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1167	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2063	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2273	A	C4-C5-C6	-6.30	113.85	117.00
55	BB	34	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	499	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	787	C	N1-C2-O2	6.29	122.68	118.90
54	BA	2301	C	N3-C2-O2	-6.29	117.49	121.90
54	BA	1146	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1348	C	N3-C2-O2	-6.29	117.49	121.90
1	AB	221	ARG	NE-CZ-NH1	6.29	123.45	120.30
11	AL	13	ARG	NE-CZ-NH1	6.29	123.45	120.30
21	AA	999	C	N3-C2-O2	-6.29	117.50	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1431	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	344	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	863	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	909	A	C4-C5-C6	-6.29	113.85	117.00
55	BB	17	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	919	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	792	A	C5-C6-N1	6.29	120.84	117.70
54	BA	1522	A	C5-C6-N1	6.29	120.84	117.70
21	AA	347	G	O4'-C1'-N9	6.29	113.23	108.20
54	BA	1609	A	C5-C6-N1	6.29	120.84	117.70
54	BA	1713	A	P-O3'-C3'	6.29	127.25	119.70
54	BA	2730	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	73	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1308	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	2565	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	418	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	750	C	N3-C2-O2	-6.28	117.50	121.90
34	BL	126	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	599	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1013	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1028	A	N1-C6-N6	-6.28	114.83	118.60
54	BA	2433	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1189	A	C5-C6-N1	6.28	120.84	117.70
54	BA	2332	C	O4'-C1'-N1	6.28	113.23	108.20
21	AA	338	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	563	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	795	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1203	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	893	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1479	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1293	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1895	C	N3-C2-O2	-6.28	117.51	121.90
8	AI	108	ARG	NE-CZ-NH2	-6.28	117.16	120.30
54	BA	280	U	N3-C2-O2	-6.28	117.81	122.20
54	BA	2541	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2736	A	C5-C6-N1	6.28	120.84	117.70
21	AA	1271	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	1371	G	O4'-C1'-N9	6.27	113.22	108.20
54	BA	2225	A	N1-C6-N6	-6.27	114.84	118.60
54	BA	2258	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	749	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	560	C	N3-C2-O2	-6.27	117.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1466	U	O4'-C1'-N1	6.27	113.22	108.20
54	BA	1515	A	C4-C5-C6	-6.27	113.86	117.00
24	A3	24	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	53	A	C4-C5-C6	-6.27	113.86	117.00
55	BB	91	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	109	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	2226	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2322	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	2601	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	411	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	934	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1261	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1477	A	C5-C6-N1	6.27	120.83	117.70
54	BA	1537	G	O4'-C1'-N9	6.27	113.21	108.20
54	BA	2196	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1272	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	2459	A	C4-C5-C6	-6.27	113.87	117.00
6	AG	137	ARG	NE-CZ-NH1	6.26	123.43	120.30
21	AA	30	U	C1'-O4'-C4'	-6.26	104.89	109.90
21	AA	189	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	554	A	C5-C6-N1	6.26	120.83	117.70
21	AA	631	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	968	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1786	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	614	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	994	A	C4-C5-C6	-6.26	113.87	117.00
39	BQ	12	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	877	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2594	C	N3-C2-O2	-6.26	117.52	121.90
12	AM	28	ARG	NE-CZ-NH1	6.26	123.43	120.30
21	AA	226	G	N3-C2-N2	-6.26	115.52	119.90
21	AA	1357	A	C5-C6-N1	6.26	120.83	117.70
21	AA	1534	A	C4-C5-C6	-6.26	113.87	117.00
22	A1	14	A	C5-C6-N1	6.26	120.83	117.70
54	BA	343	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1768	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2158	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2507	C	N3-C2-O2	-6.26	117.52	121.90
55	BB	70	C	N3-C2-O2	-6.26	117.52	121.90
25	BC	213	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	1571	A	C4-C5-C6	-6.26	113.87	117.00
22	A1	41	A	C4-C5-C6	-6.26	113.87	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AG	4	ARG	C-N-CA	6.26	137.34	121.70
54	BA	479	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1526	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2291	U	O4'-C1'-N1	6.26	113.21	108.20
54	BA	2753	A	C5-C6-N1	6.25	120.83	117.70
54	BA	691	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	1117	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	1142	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	1443	U	O4'-C1'-N1	6.25	113.20	108.20
54	BA	2037	A	C5-C6-N1	6.25	120.83	117.70
21	AA	1081	A	C5-C6-N1	6.25	120.83	117.70
21	AA	1082	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1261	C	O4'-C1'-N1	6.25	113.20	108.20
8	AI	108	ARG	NE-CZ-NH1	6.25	123.42	120.30
21	AA	313	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	901	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	1044	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1414	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	2396	G	N3-C2-N2	-6.25	115.53	119.90
54	BA	2482	A	C4-C5-C6	-6.25	113.88	117.00
55	BB	68	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	1011	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	1209	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	1469	C	O4'-C1'-N1	6.25	113.20	108.20
54	BA	1541	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	2772	C	N3-C2-O2	-6.25	117.53	121.90
1	AB	224	ARG	NE-CZ-NH1	6.25	123.42	120.30
21	AA	1063	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	20	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	1319	A	C5-C6-N1	6.24	120.82	117.70
54	BA	179	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	191	A	N1-C6-N6	-6.24	114.85	118.60
54	BA	1925	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2691	C	N3-C2-O2	-6.24	117.53	121.90
56	B5	71	ARG	NE-CZ-NH1	6.24	123.42	120.30
54	BA	1253	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1894	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	98	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1075	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2284	A	C5-C6-N1	6.24	120.82	117.70
54	BA	2741	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	985	C	N3-C2-O2	-6.24	117.53	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1163	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	231	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	727	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2108	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2468	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2806	C	O4'-C1'-N1	6.24	113.19	108.20
5	AF	25	TYR	CB-CG-CD2	-6.24	117.26	121.00
54	BA	2660	A	C1'-O4'-C4'	-6.24	104.91	109.90
54	BA	2712	C	N1-C2-O2	6.24	122.64	118.90
21	AA	602	A	C5-C6-N1	6.24	120.82	117.70
54	BA	420	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1934	C	N3-C2-O2	-6.24	117.54	121.90
55	BB	94	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1562	U	O4'-C1'-N1	6.23	113.19	108.20
54	BA	2800	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2861	U	O4'-C1'-N1	6.23	113.19	108.20
54	BA	32	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	620	G	C8-N9-C4	-6.23	103.91	106.40
21	AA	578	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2174	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	456	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	1147	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	20	U	O4'-C1'-N1	6.23	113.18	108.20
21	AA	1281	C	N1-C2-O2	6.23	122.64	118.90
54	BA	876	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1927	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	2451	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	2820	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	250	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	502	A	C4-C5-C6	-6.22	113.89	117.00
32	BJ	34	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	752	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	819	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1226	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	415	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1097	U	O4'-C1'-N1	6.22	113.18	108.20
54	BA	2058	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	984	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	294	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1234	C	N3-C2-O2	-6.22	117.55	121.90
46	BX	10	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	753	A	C4-C5-C6	-6.22	113.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2477	U	O4'-C1'-N1	6.22	113.17	108.20
21	AA	291	U	O4'-C1'-N1	6.22	113.17	108.20
22	A1	31	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	354	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1966	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	2589	A	C5-C6-N1	6.22	120.81	117.70
54	BA	2799	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	583	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	975	A	C4-C5-C6	-6.21	113.89	117.00
45	BW	24	ARG	NE-CZ-NH1	6.21	123.41	120.30
46	BX	27	ARG	NE-CZ-NH1	6.21	123.41	120.30
54	BA	146	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1306	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	514	C	N3-C2-O2	-6.21	117.55	121.90
24	A3	67	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1140	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2306	C	N3-C2-O2	-6.21	117.55	121.90
23	A2	79	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	478	A	C5-C6-N1	6.21	120.81	117.70
54	BA	1096	A	C4-C5-C6	-6.21	113.89	117.00
2	AC	130	ARG	NE-CZ-NH1	6.21	123.40	120.30
21	AA	161	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	970	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1140	C	N3-C2-O2	-6.21	117.55	121.90
24	A3	2	G	C3'-C2'-C1'	6.21	106.47	101.50
55	BB	47	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1529	G	N3-C4-C5	-6.21	125.50	128.60
28	BF	177	ARG	NE-CZ-NH2	6.21	123.40	120.30
54	BA	435	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	920	A	N1-C6-N6	-6.21	114.88	118.60
54	BA	2497	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	923	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	1303	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	996	A	C5-C6-N1	6.21	120.80	117.70
54	BA	1417	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	347	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	980	C	O4'-C1'-N1	6.20	113.16	108.20
24	A3	68	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1675	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1691	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	234	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	606	U	O4'-C1'-N1	6.20	113.16	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	436	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1357	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1992	G	N1-C6-O6	-6.20	116.18	119.90
21	AA	349	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2051	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	129	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	340	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2740	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	716	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	1713	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	1545	A	C4-C5-C6	-6.19	113.90	117.00
6	AG	101	ARG	NE-CZ-NH1	6.19	123.39	120.30
21	AA	611	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1171	A	C4-C5-C6	-6.19	113.91	117.00
25	BC	181	ARG	NE-CZ-NH1	6.19	123.39	120.30
54	BA	2036	C	C3'-C2'-C1'	6.19	106.45	101.50
21	AA	1201	A	P-O3'-C3'	6.19	127.13	119.70
23	A2	91	A	C5-C6-N1	6.19	120.79	117.70
54	BA	413	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	430	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	466	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	1260	A	C5-C6-N1	6.19	120.79	117.70
54	BA	2210	U	O4'-C1'-N1	6.19	113.15	108.20
54	BA	404	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	198	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	486	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	881	G	N1-C6-O6	-6.18	116.19	119.90
54	BA	918	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1957	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	673	A	C5-C6-N1	6.18	120.79	117.70
21	AA	1102	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	483	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1057	A	C5-C6-N1	6.18	120.79	117.70
21	AA	228	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	1317	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1864	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2300	C	O4'-C1'-N1	6.18	113.14	108.20
21	AA	32	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	724	G	N1-C6-O6	-6.18	116.19	119.90
54	BA	299	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	529	A	C5-C6-N1	6.18	120.79	117.70
21	AA	635	A	C4-C5-C6	-6.18	113.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	811	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	1191	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	91	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	361	G	N1-C6-O6	-6.18	116.19	119.90
54	BA	1349	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1942	C	N1-C2-O2	6.18	122.61	118.90
6	AG	77	ARG	NE-CZ-NH2	-6.17	117.21	120.30
54	BA	238	C	N3-C2-O2	-6.17	117.58	121.90
55	BB	110	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	200	U	O4'-C1'-N1	6.17	113.14	108.20
21	AA	47	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	1229	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	957	C	N1-C2-O2	6.17	122.60	118.90
54	BA	2558	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2887	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	489	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	513	C	O4'-C1'-N1	6.17	113.14	108.20
54	BA	569	U	O4'-C1'-N1	6.17	113.14	108.20
54	BA	1595	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2108	A	C5-C6-N1	6.17	120.78	117.70
54	BA	2161	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	461	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	806	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	825	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	1155	A	C5-C6-N1	6.17	120.78	117.70
54	BA	2813	A	C4-C5-C6	-6.17	113.92	117.00
22	A1	17	U	C1'-O4'-C4'	-6.17	104.97	109.90
55	BB	113	C	N3-C2-O2	-6.17	117.58	121.90
14	AO	83	ARG	NE-CZ-NH1	6.16	123.38	120.30
26	BD	128	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	1771	C	N3-C2-O2	-6.16	117.58	121.90
54	BA	1828	G	N1-C6-O6	-6.16	116.20	119.90
54	BA	1603	A	C5-C6-N1	6.16	120.78	117.70
54	BA	2486	C	N3-C2-O2	-6.16	117.59	121.90
55	BB	62	C	N1-C2-O2	6.16	122.60	118.90
21	AA	177	G	N3-C4-C5	-6.16	125.52	128.60
21	AA	865	A	C4-C5-C6	-6.16	113.92	117.00
22	A1	26	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	795	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2395	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2619	C	O4'-C1'-N1	6.16	113.13	108.20
54	BA	2824	C	N3-C2-O2	-6.16	117.59	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	237	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	315	G	N1-C6-O6	-6.16	116.20	119.90
54	BA	1639	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2206	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1577	C	N3-C2-O2	-6.16	117.59	121.90
24	A3	72	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	914	G	O4'-C1'-N9	6.16	113.12	108.20
54	BA	2135	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	797	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	883	C	N3-C2-O2	-6.15	117.59	121.90
24	A3	60	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1347	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	2426	A	C4-C5-C6	-6.15	113.92	117.00
6	AG	94	ARG	NE-CZ-NH1	6.15	123.38	120.30
21	AA	325	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	984	A	O4'-C1'-N9	6.15	113.12	108.20
54	BA	1502	A	C5-C6-N1	6.15	120.78	117.70
54	BA	1761	C	O4'-C1'-N1	6.15	113.12	108.20
54	BA	2540	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	53	A	N1-C6-N6	-6.15	114.91	118.60
21	AA	205	A	C4-C5-C6	-6.15	113.92	117.00
21	AA	496	A	C5-C6-N1	6.15	120.78	117.70
21	AA	504	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	790	A	C4-C5-C6	-6.15	113.92	117.00
24	A3	73	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1204	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1286	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	508	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	702	U	O4'-C1'-N1	6.15	113.12	108.20
54	BA	1169	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	2752	C	N1-C2-O2	6.15	122.59	118.90
21	AA	990	C	N1-C2-O2	6.15	122.59	118.90
54	BA	229	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	384	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	479	A	C5-C6-N1	6.15	120.77	117.70
54	BA	2539	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	2572	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	1234	U	O4'-C1'-N1	6.15	113.12	108.20
54	BA	404	A	N1-C6-N6	-6.14	114.91	118.60
54	BA	1320	C	O4'-C1'-N1	6.14	113.11	108.20
54	BA	1506	U	O4'-C1'-N1	6.14	113.12	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	785	G	N1-C6-O6	-6.14	116.22	119.90
54	BA	1552	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1569	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1809	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2020	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2142	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	876	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1672	A	C4-C5-C6	-6.14	113.93	117.00
56	B5	53	ARG	NE-CZ-NH2	-6.14	117.23	120.30
39	BQ	50	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	99	U	N3-C2-O2	-6.14	117.90	122.20
54	BA	208	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	815	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	823	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1548	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1901	A	C5-C6-N1	6.14	120.77	117.70
54	BA	2795	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	600	A	C4-C5-C6	-6.14	113.93	117.00
24	A3	58	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	897	C	O4'-C1'-N1	6.14	113.11	108.20
54	BA	948	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2047	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2350	C	N3-C2-O2	-6.14	117.61	121.90
21	AA	52	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	54	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	11	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1230	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	1518	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2560	A	C4-C5-C6	-6.13	113.93	117.00
21	AA	706	A	C4-C5-C6	-6.13	113.93	117.00
46	BX	2	ARG	NE-CZ-NH2	-6.13	117.23	120.30
54	BA	158	U	O4'-C1'-N1	6.13	113.11	108.20
21	AA	408	A	C5-C6-N1	6.13	120.77	117.70
54	BA	1499	C	N3-C2-O2	-6.13	117.61	121.90
55	BB	12	C	P-O3'-C3'	6.13	127.06	119.70
24	A3	14	A	N1-C6-N6	-6.13	114.92	118.60
21	AA	528	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	726	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	1289	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	73	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	320	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	423	A	C4-C5-C6	-6.13	113.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	794	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	958	U	O4'-C1'-N1	6.13	113.10	108.20
54	BA	2422	C	O4'-C1'-N1	6.13	113.10	108.20
21	AA	1346	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	399	U	O4'-C1'-N1	6.13	113.10	108.20
54	BA	540	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1746	A	C4-C5-C6	-6.13	113.94	117.00
4	AE	53	ARG	NE-CZ-NH1	6.12	123.36	120.30
21	AA	1434	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	381	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1676	A	C5-C6-N1	6.12	120.76	117.70
51	B2	28	ARG	NE-CZ-NH1	6.12	123.36	120.30
54	BA	1523	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	2129	C	N1-C2-O2	6.12	122.57	118.90
54	BA	2423	U	N3-C2-O2	-6.12	117.92	122.20
21	AA	153	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	518	C	C1'-O4'-C4'	-6.12	105.00	109.90
21	AA	633	G	N3-C2-N2	-6.12	115.62	119.90
54	BA	41	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	449	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	521	U	O4'-C1'-N1	6.12	113.09	108.20
54	BA	724	U	O4'-C1'-N1	6.12	113.09	108.20
54	BA	1101	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	2030	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2870	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	74	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	1428	A	C4-C5-C6	-6.12	113.94	117.00
36	BN	103	ARG	NE-CZ-NH1	6.12	123.36	120.30
54	BA	2530	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	239	U	C1'-O4'-C4'	-6.11	105.01	109.90
21	AA	1350	A	C4-C5-C6	-6.11	113.94	117.00
35	BM	114	ARG	NE-CZ-NH1	6.11	123.36	120.30
54	BA	550	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	890	C	N1-C2-O2	6.11	122.57	118.90
55	BB	50	A	C4-C5-C6	-6.11	113.94	117.00
56	B5	134	ARG	NE-CZ-NH1	6.11	123.36	120.30
22	A1	21	A	C4-C5-C6	-6.11	113.94	117.00
55	BB	35	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	408	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	1591	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	1848	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	2119	A	C4-C5-C6	-6.11	113.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2793	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	520	A	C5-C6-N1	6.11	120.75	117.70
24	A3	16	C	N1-C2-O2	6.11	122.56	118.90
54	BA	398	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	440	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	538	A	C5-C6-N1	6.11	120.75	117.70
54	BA	935	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1314	C	N1-C2-O2	6.11	122.56	118.90
54	BA	1399	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1495	A	C5-C6-N1	6.11	120.75	117.70
54	BA	851	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	2189	U	O4'-C1'-N1	6.11	113.08	108.20
21	AA	1100	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	334	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1055	A	C4-C5-C6	-6.10	113.95	117.00
24	A3	13	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	2191	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2899	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	400	C	N3-C2-O2	-6.10	117.63	121.90
22	A1	41	A	C5-C6-N1	6.10	120.75	117.70
54	BA	2336	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2855	C	N3-C2-O2	-6.10	117.63	121.90
55	BB	115	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	236	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	332	A	O4'-C1'-N9	6.10	113.08	108.20
54	BA	385	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	970	U	O4'-C1'-N1	6.10	113.08	108.20
2	AC	171	ARG	NE-CZ-NH1	6.10	123.35	120.30
21	AA	814	A	C5-C6-N1	6.10	120.75	117.70
54	BA	731	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	992	C	N1-C2-O2	6.10	122.56	118.90
21	AA	1208	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1259	C	N1-C2-O2	6.09	122.56	118.90
54	BA	32	C	O4'-C1'-N1	6.09	113.08	108.20
54	BA	2317	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	607	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	823	C	O4'-C1'-N1	6.09	113.07	108.20
54	BA	1932	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	1941	C	N1-C2-O2	6.09	122.56	118.90
54	BA	2392	A	C5-C6-N1	6.09	120.75	117.70
21	AA	290	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	213	A	C4-C5-C6	-6.09	113.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	395	U	O4'-C1'-N1	6.09	113.07	108.20
54	BA	1086	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	2222	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	58	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	240	C	N3-C2-O2	-6.09	117.64	121.90
48	BZ	37	ARG	NE-CZ-NH1	6.09	123.34	120.30
54	BA	475	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2202	U	O4'-C1'-N1	6.09	113.07	108.20
54	BA	2590	A	C6-C5-N7	6.09	136.56	132.30
54	BA	896	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1472	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	495	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	675	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	63	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	541	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2673	G	N3-C2-N2	-6.08	115.64	119.90
21	AA	802	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	983	A	N1-C6-N6	-6.08	114.95	118.60
21	AA	1060	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	2122	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	2551	C	N3-C2-O2	-6.08	117.64	121.90
55	BB	71	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	1306	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	1350	A	C5-C6-N1	6.08	120.74	117.70
54	BA	391	A	N1-C6-N6	-6.08	114.95	118.60
54	BA	686	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	1257	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2678	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	44	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	225	C	C4'-C3'-C2'	-6.08	96.52	102.60
54	BA	239	C	N1-C2-O2	6.08	122.55	118.90
54	BA	1049	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	1439	A	C5-C6-N1	6.08	120.74	117.70
21	AA	559	A	N1-C6-N6	-6.08	114.95	118.60
54	BA	1014	A	C5-C6-N1	6.08	120.74	117.70
54	BA	2261	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	673	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1300	G	C1'-O4'-C4'	-6.08	105.04	109.90
54	BA	1564	C	N3-C2-O2	-6.08	117.65	121.90
20	AU	33	ARG	NE-CZ-NH1	6.07	123.34	120.30
21	AA	149	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	64	A	C5-C6-N1	6.07	120.74	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	620	G	O4'-C1'-N9	6.07	113.06	108.20
54	BA	786	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2670	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	696	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	732	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2241	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	1001	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	1012	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	563	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	1023	U	O4'-C1'-N1	6.07	113.06	108.20
54	BA	1052	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1965	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1744	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	2324	U	O4'-C1'-N1	6.07	113.06	108.20
54	BA	2889	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	1360	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	758	C	N1-C2-O2	6.07	122.54	118.90
54	BA	1925	C	O4'-C1'-N1	6.07	113.05	108.20
54	BA	2359	C	N3-C2-O2	-6.07	117.65	121.90
20	AU	46	ARG	NE-CZ-NH2	6.07	123.33	120.30
21	AA	1092	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	655	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	1370	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2600	A	C4-C5-C6	-6.07	113.97	117.00
55	BB	88	C	N1-C2-O2	6.07	122.54	118.90
48	BZ	29	ARG	NE-CZ-NH2	-6.06	117.27	120.30
54	BA	806	C	O4'-C1'-N1	6.06	113.05	108.20
54	BA	854	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	676	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	858	G	O4'-C1'-N9	6.06	113.05	108.20
54	BA	1827	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	2762	C	O4'-C1'-N1	6.06	113.05	108.20
21	AA	178	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	530	G	O4'-C1'-N9	6.06	113.05	108.20
21	AA	948	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	1509	C	N3-C2-O2	-6.06	117.66	121.90
22	A1	6	A	C4-C5-C6	-6.06	113.97	117.00
37	BO	102	ARG	NE-CZ-NH2	-6.06	117.27	120.30
21	AA	60	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	687	A	C4-C5-C6	-6.06	113.97	117.00
24	A3	77	A	O4'-C1'-N9	6.06	113.05	108.20
54	BA	491	G	N1-C6-O6	-6.06	116.27	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1080	A	C5-C6-N1	6.06	120.73	117.70
54	BA	1214	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1263	U	C3'-C2'-C1'	6.06	106.35	101.50
54	BA	1757	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1899	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2646	C	N3-C2-O2	-6.06	117.66	121.90
55	BB	87	U	O4'-C1'-N1	6.06	113.05	108.20
21	AA	80	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	542	C	O4'-C1'-N1	6.06	113.05	108.20
54	BA	1981	A	C4-C5-C6	-6.06	113.97	117.00
55	BB	55	U	O4'-C1'-N1	6.06	113.05	108.20
21	AA	460	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2008	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	474	G	N1-C6-O6	-6.05	116.27	119.90
21	AA	1145	A	N1-C6-N6	-6.05	114.97	118.60
54	BA	1393	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1759	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	878	A	C4-C5-C6	-6.05	113.97	117.00
46	BX	17	ARG	NE-CZ-NH1	6.05	123.33	120.30
54	BA	903	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1832	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1070	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1302	A	C4-C5-C6	-6.05	113.98	117.00
21	AA	1412	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	165	A	C5-C6-N1	6.05	120.72	117.70
54	BA	611	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	2028	U	O4'-C1'-N1	6.04	113.04	108.20
21	AA	1101	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1314	C	N3-C2-O2	-6.04	117.67	121.90
22	A1	16	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	650	C	O4'-C1'-N1	6.04	113.03	108.20
54	BA	1243	C	N1-C2-O2	6.04	122.53	118.90
54	BA	2856	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	60	A	P-O3'-C3'	6.04	126.95	119.70
54	BA	244	A	C5-C6-N1	6.04	120.72	117.70
54	BA	436	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	668	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2469	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	274	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	274	C	O4'-C1'-N1	6.04	113.03	108.20
54	BA	650	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2023	C	N3-C2-O2	-6.04	117.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2841	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	882	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	3	U	O4'-C1'-N1	6.04	113.03	108.20
54	BA	781	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1208	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	468	A	O4'-C1'-N9	6.04	113.03	108.20
24	A3	1	C	N3-C2-O2	-6.04	117.67	121.90
9	AJ	48	ARG	NE-CZ-NH1	6.03	123.32	120.30
21	AA	651	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	184	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	196	A	O4'-C1'-N9	6.03	113.03	108.20
54	BA	2262	U	O4'-C1'-N1	6.03	113.03	108.20
55	BB	27	C	O4'-C1'-N1	6.03	113.03	108.20
21	AA	440	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	492	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2321	U	O4'-C1'-N1	6.03	113.03	108.20
21	AA	10	A	C5-C6-N1	6.03	120.72	117.70
21	AA	284	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	411	A	C5-C6-N1	6.03	120.72	117.70
49	B0	51	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	130	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	318	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1525	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	236	A	C5-C6-N1	6.03	120.71	117.70
21	AA	1093	A	C4-C5-C6	-6.03	113.99	117.00
26	BD	179	ARG	NE-CZ-NH2	-6.03	117.29	120.30
54	BA	1069	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	1278	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2412	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	2559	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	522	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	1503	A	C5-C6-N1	6.03	120.71	117.70
54	BA	1745	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	2346	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	1250	G	O4'-C1'-N9	6.02	113.02	108.20
13	AN	75	ARG	NE-CZ-NH1	6.02	123.31	120.30
21	AA	1507	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	453	A	O4'-C1'-N9	6.02	113.02	108.20
54	BA	1744	A	N1-C6-N6	-6.02	114.99	118.60
55	BB	45	A	C4-C5-C6	-6.02	113.99	117.00
10	AK	105	ARG	NE-CZ-NH1	6.02	123.31	120.30
54	BA	2420	C	N3-C2-O2	-6.02	117.69	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	470	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	156	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2407	A	C5-C6-N1	6.02	120.71	117.70
54	BA	1085	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1592	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1607	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1354	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2022	U	O4'-C1'-N1	6.02	113.01	108.20
54	BA	2062	A	O4'-C1'-N9	6.02	113.01	108.20
54	BA	2250	G	N3-C4-C5	-6.02	125.59	128.60
21	AA	373	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	660	C	N3-C2-O2	-6.01	117.69	121.90
26	BD	33	ARG	NE-CZ-NH1	6.01	123.31	120.30
54	BA	131	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	706	A	C5-C6-N1	6.01	120.71	117.70
54	BA	743	A	C6-C5-N7	6.01	136.51	132.30
54	BA	1021	A	C4-C5-C6	-6.01	113.99	117.00
37	BO	94	ARG	NE-CZ-NH1	6.01	123.31	120.30
54	BA	1158	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1189	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	2462	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2710	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2821	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	2859	G	O4'-C1'-N9	6.01	113.01	108.20
21	AA	10	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	1159	U	O4'-C1'-N1	6.01	113.01	108.20
54	BA	1205	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	2147	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	235	C	N3-C2-O2	-6.01	117.69	121.90
24	A3	43	G	C5'-C4'-O4'	6.01	116.31	109.10
8	AI	40	ARG	NE-CZ-NH1	6.01	123.30	120.30
26	BD	83	ARG	NE-CZ-NH1	6.00	123.30	120.30
51	B2	19	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	1994	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	7	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	121	G	C3'-C2'-C1'	6.00	106.30	101.50
54	BA	262	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	225	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2377	A	C6-C5-N7	6.00	136.50	132.30
54	BA	2882	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	1172	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1426	G	O4'-C1'-N9	6.00	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1123	U	O4'-C1'-N1	6.00	113.00	108.20
40	BR	21	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	443	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2080	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2183	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	698	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1357	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2160	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2774	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1039	A	N1-C6-N6	-6.00	115.00	118.60
54	BA	1366	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	576	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	461	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	933	A	C5-C6-N1	5.99	120.70	117.70
54	BA	2521	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	429	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	644	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1103	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	2036	C	N1-C2-O2	5.99	122.50	118.90
54	BA	2567	G	O4'-C1'-N9	5.99	112.99	108.20
55	BB	56	G	O4'-C1'-N9	5.99	112.99	108.20
21	AA	621	A	C4-C5-C6	-5.99	114.00	117.00
55	BB	109	A	C1'-O4'-C4'	-5.99	105.11	109.90
21	AA	246	A	C5-C6-N1	5.99	120.69	117.70
54	BA	106	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	463	G	N1-C6-O6	-5.99	116.31	119.90
54	BA	544	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1273	U	O4'-C1'-N1	5.99	112.99	108.20
21	AA	1285	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	812	C	N1-C2-O2	5.99	122.49	118.90
54	BA	1148	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	1625	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	501	A	N1-C6-N6	-5.99	115.01	118.60
54	BA	1106	G	O4'-C1'-N9	5.99	112.99	108.20
54	BA	1928	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	2212	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	2535	G	N3-C2-N2	-5.99	115.71	119.90
21	AA	238	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	372	G	N3-C4-C5	-5.98	125.61	128.60
54	BA	2101	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2703	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	327	A	C1'-O4'-C4'	-5.98	105.11	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1385	A	O4'-C1'-N9	5.98	112.98	108.20
54	BA	1732	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	2773	C	O4'-C1'-N1	5.98	112.98	108.20
54	BA	885	C	O4'-C1'-N1	5.98	112.98	108.20
54	BA	2840	C	N3-C2-O2	-5.98	117.72	121.90
3	AD	96	ARG	NE-CZ-NH1	5.98	123.29	120.30
54	BA	1080	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1783	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2635	A	C5-C6-N1	5.98	120.69	117.70
21	AA	767	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1157	A	C4-C5-C6	-5.98	114.01	117.00
37	BO	30	ARG	NE-CZ-NH1	5.98	123.29	120.30
54	BA	1877	A	C4-C5-C6	-5.98	114.01	117.00
8	AI	10	ARG	NE-CZ-NH1	5.97	123.29	120.30
54	BA	302	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	921	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1244	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	1825	U	O4'-C1'-N1	5.97	112.98	108.20
21	AA	482	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	493	A	O4'-C1'-N9	5.97	112.98	108.20
54	BA	1252	G	N3-C2-N2	-5.97	115.72	119.90
12	AM	112	ARG	NE-CZ-NH1	5.97	123.28	120.30
21	AA	564	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	739	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	1179	A	C4-C5-C6	-5.97	114.02	117.00
22	A1	51	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	418	C	O4'-C1'-N1	5.97	112.98	108.20
54	BA	1017	G	C1'-O4'-C4'	-5.97	105.12	109.90
54	BA	1821	A	C5-C6-N1	5.97	120.69	117.70
54	BA	1958	C	O4'-C1'-N1	5.97	112.98	108.20
54	BA	1963	U	O4'-C1'-N1	5.97	112.97	108.20
54	BA	2005	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2163	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2636	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	620	G	C2-N3-C4	5.97	114.88	111.90
54	BA	1489	C	N1-C2-O2	5.97	122.48	118.90
21	AA	1460	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	192	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2467	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	642	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1322	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1746	A	C5-C6-N1	5.96	120.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1868	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	2556	C	N1-C2-O2	5.96	122.48	118.90
54	BA	2672	U	O4'-C1'-N1	5.96	112.97	108.20
21	AA	479	U	O4'-C1'-N1	5.96	112.97	108.20
32	BJ	116	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	1100	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1866	A	C4-C5-C6	-5.96	114.02	117.00
14	AO	16	ARG	NE-CZ-NH1	5.96	123.28	120.30
21	AA	1066	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	453	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2176	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2682	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2704	C	N1-C2-O2	5.96	122.48	118.90
1	AB	112	ARG	NE-CZ-NH1	5.96	123.28	120.30
13	AN	63	ARG	NE-CZ-NH1	5.96	123.28	120.30
21	AA	1177	G	N3-C2-N2	-5.96	115.73	119.90
54	BA	2133	G	N1-C6-O6	-5.96	116.33	119.90
21	AA	1000	A	C4-C5-C6	-5.96	114.02	117.00
24	A3	40	C	N1-C2-O2	5.96	122.47	118.90
54	BA	145	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2283	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2581	G	N1-C6-O6	-5.96	116.33	119.90
21	AA	43	C	N1-C2-O2	5.95	122.47	118.90
54	BA	620	G	N3-C4-C5	-5.95	125.62	128.60
54	BA	1319	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	2171	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	1217	C	N1-C2-O2	5.95	122.47	118.90
54	BA	451	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	666	A	C5-C6-N1	5.95	120.68	117.70
54	BA	987	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	270	A	C5-C6-N1	5.95	120.67	117.70
21	AA	596	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	784	A	C5-C6-N1	5.95	120.67	117.70
21	AA	1098	C	N3-C2-O2	-5.95	117.73	121.90
38	BP	87	ARG	NE-CZ-NH1	5.95	123.28	120.30
54	BA	1287	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	2518	A	N1-C6-N6	-5.95	115.03	118.60
54	BA	2635	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	79	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	749	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1281	G	O4'-C1'-N9	5.95	112.96	108.20
54	BA	1708	C	N3-C2-O2	-5.95	117.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2207	C	N3-C2-O2	-5.95	117.74	121.90
18	AS	77	ARG	NE-CZ-NH1	5.95	123.27	120.30
54	BA	439	A	C5-C6-N1	5.95	120.67	117.70
54	BA	2278	A	C5-C6-N1	5.95	120.67	117.70
54	BA	2784	U	O4'-C1'-N1	5.95	112.96	108.20
8	AI	123	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	1617	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1793	C	N1-C2-O2	5.94	122.47	118.90
54	BA	1813	G	O4'-C1'-N9	5.94	112.95	108.20
54	BA	1838	C	N3-C2-O2	-5.94	117.74	121.90
2	AC	131	ARG	NE-CZ-NH1	5.94	123.27	120.30
21	AA	535	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	792	A	C4-C5-C6	-5.94	114.03	117.00
39	BQ	5	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	219	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	980	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1447	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1806	C	N1-C2-O2	5.94	122.47	118.90
54	BA	2644	G	O4'-C1'-N9	5.94	112.95	108.20
21	AA	969	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	782	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	902	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	961	C	N1-C2-O2	5.94	122.46	118.90
54	BA	2727	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	336	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	1179	A	C5-C6-N1	5.94	120.67	117.70
54	BA	210	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2164	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2657	A	C5-C6-N1	5.94	120.67	117.70
21	AA	456	A	C5-C6-N1	5.94	120.67	117.70
54	BA	1791	A	C4-C5-C6	-5.94	114.03	117.00
4	AE	137	ARG	NE-CZ-NH1	5.93	123.27	120.30
54	BA	1965	C	O4'-C1'-N1	5.93	112.95	108.20
54	BA	2009	A	C5-C6-N1	5.93	120.67	117.70
21	AA	116	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1000	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1772	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2676	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	2888	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	736	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	1307	A	C4-C5-C6	-5.93	114.03	117.00
55	BB	65	U	O4'-C1'-N1	5.93	112.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	11	G	N1-C6-O6	-5.93	116.34	119.90
21	AA	676	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1531	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	2073	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	2257	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	2868	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	229	C	O4'-C1'-N1	5.93	112.94	108.20
21	AA	719	C	N1-C2-O2	5.93	122.46	118.90
21	AA	935	A	C5-C6-N1	5.93	120.66	117.70
21	AA	1240	U	C1'-O4'-C4'	-5.93	105.16	109.90
21	AA	1297	G	C8-N9-C4	-5.93	104.03	106.40
54	BA	1590	A	C4-C5-C6	-5.93	114.04	117.00
21	AA	71	A	C6-C5-N7	5.92	136.45	132.30
54	BA	719	C	O4'-C1'-N1	5.92	112.94	108.20
21	AA	1302	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	1303	C	O4'-C1'-N1	5.92	112.94	108.20
21	AA	210	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	908	A	C5-C6-N1	5.92	120.66	117.70
54	BA	1018	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2009	A	C4-C5-C6	-5.92	114.04	117.00
22	A1	27	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	712	A	O4'-C1'-N9	5.92	112.94	108.20
21	AA	810	C	N3-C2-O2	-5.92	117.76	121.90
24	A3	26	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	346	A	O4'-C1'-N9	5.92	112.94	108.20
54	BA	840	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	1685	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	2879	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	686	U	O4'-C1'-N1	5.92	112.93	108.20
21	AA	1136	C	N1-C2-O2	5.92	122.45	118.90
21	AA	1378	C	N3-C2-O2	-5.92	117.76	121.90
35	BM	18	ARG	NE-CZ-NH2	-5.92	117.34	120.30
54	BA	87	U	O4'-C1'-N1	5.92	112.93	108.20
54	BA	756	A	C5-C6-N1	5.92	120.66	117.70
54	BA	1541	C	O4'-C1'-N1	5.92	112.93	108.20
54	BA	1918	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2079	U	O4'-C1'-N1	5.92	112.93	108.20
54	BA	2814	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	160	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	163	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	526	A	N1-C6-N6	-5.92	115.05	118.60
54	BA	1507	C	N3-C2-O2	-5.92	117.76	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	104	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	545	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	975	A	N1-C6-N6	-5.91	115.05	118.60
54	BA	1353	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	2611	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	249	C	O4'-C1'-N1	5.91	112.93	108.20
54	BA	1658	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	897	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	21	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	236	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	986	C	N1-C2-O2	5.91	122.44	118.90
9	AJ	62	ARG	NE-CZ-NH1	5.91	123.25	120.30
21	AA	298	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	452	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	609	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1221	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	2208	C	N3-C2-O2	-5.91	117.77	121.90
55	BB	46	A	C6-C5-N7	5.91	136.43	132.30
21	AA	1129	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	354	A	C4-C5-C6	-5.90	114.05	117.00
9	AJ	89	ARG	NE-CZ-NH1	5.90	123.25	120.30
21	AA	353	A	C1'-O4'-C4'	-5.90	105.18	109.90
21	AA	1004	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	377	G	N3-C2-N2	-5.90	115.77	119.90
54	BA	1451	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	2626	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1133	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	2860	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	839	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	723	C	N1-C2-O2	5.90	122.44	118.90
54	BA	1288	G	O4'-C1'-N9	5.90	112.92	108.20
54	BA	2232	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	2732	G	N3-C4-C5	-5.90	125.65	128.60
21	AA	1274	A	C4-C5-C6	-5.90	114.05	117.00
8	AI	32	ARG	NE-CZ-NH1	5.89	123.25	120.30
8	AI	121	ARG	NE-CZ-NH1	5.89	123.25	120.30
21	AA	124	C	N3-C2-O2	-5.89	117.77	121.90
21	AA	909	A	C5-C6-N1	5.89	120.65	117.70
21	AA	924	C	N1-C2-O2	5.89	122.44	118.90
21	AA	66	A	C4-C5-C6	-5.89	114.05	117.00
21	AA	503	C	N3-C2-O2	-5.89	117.78	121.90
43	BU	81	ARG	NE-CZ-NH1	5.89	123.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1007	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1200	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1644	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2071	A	C4-C5-C6	-5.89	114.05	117.00
38	BP	52	ARG	NE-CZ-NH1	5.89	123.25	120.30
54	BA	1292	G	O4'-C1'-N9	5.89	112.91	108.20
54	BA	314	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1284	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	1550	C	N3-C2-O2	-5.89	117.78	121.90
55	BB	37	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	1496	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	669	G	C3'-C2'-C1'	5.89	106.21	101.50
54	BA	750	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	1630	A	C6-C5-N7	5.89	136.42	132.30
54	BA	2440	C	N1-C2-O2	5.89	122.43	118.90
54	BA	441	U	O4'-C1'-N1	5.89	112.91	108.20
54	BA	444	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	456	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1773	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	1453	G	N3-C4-C5	-5.88	125.66	128.60
54	BA	1336	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2205	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2497	A	O4'-C1'-N9	5.88	112.91	108.20
54	BA	1646	C	N1-C2-O2	5.88	122.43	118.90
54	BA	2789	C	N3-C2-O2	-5.88	117.78	121.90
41	BS	8	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	1800	C	N3-C2-O2	-5.88	117.78	121.90
55	BB	92	C	O4'-C1'-N1	5.88	112.91	108.20
21	AA	66	A	C5-C6-N1	5.88	120.64	117.70
54	BA	509	C	N1-C2-O2	5.88	122.43	118.90
21	AA	164	G	N1-C6-O6	-5.88	116.37	119.90
21	AA	879	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1036	A	O4'-C1'-N9	5.88	112.90	108.20
54	BA	988	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1201	U	O4'-C1'-N1	5.88	112.90	108.20
54	BA	1262	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1656	C	N3-C2-O2	-5.88	117.78	121.90
23	A2	82	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	262	A	C5-C6-N1	5.88	120.64	117.70
54	BA	660	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	675	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	979	A	O4'-C1'-N9	5.88	112.90	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1665	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1949	G	N1-C6-O6	-5.88	116.38	119.90
54	BA	2665	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2240	U	O4'-C1'-N1	5.88	112.90	108.20
54	BA	2723	C	N1-C2-O2	5.88	122.42	118.90
54	BA	468	G	O4'-C1'-N9	5.87	112.90	108.20
54	BA	596	U	O4'-C1'-N1	5.87	112.90	108.20
54	BA	1121	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1735	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2428	G	C3'-C2'-C1'	5.87	106.20	101.50
54	BA	2896	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1536	C	N1-C2-O2	5.87	122.42	118.90
54	BA	2177	C	N1-C2-O2	5.87	122.42	118.90
54	BA	2432	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	312	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1788	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2320	U	N3-C2-O2	-5.87	118.09	122.20
54	BA	2690	U	O4'-C1'-N1	5.87	112.90	108.20
21	AA	188	C	N1-C2-O2	5.87	122.42	118.90
21	AA	1250	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	673	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2422	C	N1-C2-O2	5.87	122.42	118.90
54	BA	2458	G	N3-C4-C5	-5.87	125.67	128.60
54	BA	2734	A	C4-C5-C6	-5.87	114.07	117.00
25	BC	101	ARG	NE-CZ-NH1	5.87	123.23	120.30
54	BA	13	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	814	C	N3-C2-O2	-5.87	117.80	121.90
54	BA	2220	U	O4'-C1'-N1	5.87	112.89	108.20
8	AI	11	ARG	NE-CZ-NH1	5.86	123.23	120.30
21	AA	371	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1107	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1611	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2139	U	O4'-C1'-N1	5.86	112.89	108.20
54	BA	2561	U	O4'-C1'-N1	5.86	112.89	108.20
21	AA	996	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	670	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1975	G	O4'-C1'-N9	5.86	112.89	108.20
54	BA	2547	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	372	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1596	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	2173	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	426	C	N3-C2-O2	-5.86	117.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	775	G	O4'-C1'-N9	5.86	112.89	108.20
16	AQ	63	CYS	CA-C-N	5.86	130.09	117.20
54	BA	631	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1678	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1411	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	47	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	634	C	N3-C2-O2	-5.85	117.80	121.90
21	AA	1284	C	N3-C2-O2	-5.85	117.80	121.90
21	AA	271	C	N3-C2-O2	-5.85	117.80	121.90
21	AA	523	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	1035	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	1243	C	N3-C2-O2	-5.85	117.80	121.90
22	A1	38	A	N1-C6-N6	-5.85	115.09	118.60
24	A3	77	A	C1'-O4'-C4'	-5.85	105.22	109.90
24	A3	74	A	O4'-C1'-N9	5.85	112.88	108.20
54	BA	1784	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	2480	C	N3-C2-O2	-5.85	117.80	121.90
21	AA	477	C	N1-C2-O2	5.85	122.41	118.90
21	AA	595	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	8	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	485	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	1135	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	2095	A	C6-C5-N7	5.85	136.40	132.30
21	AA	248	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	741	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	692	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	937	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1654	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1552	A	O4'-C1'-N9	5.84	112.87	108.20
21	AA	1449	C	N3-C2-O2	-5.84	117.81	121.90
46	BX	44	ARG	NE-CZ-NH1	5.84	123.22	120.30
54	BA	421	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	898	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1183	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	1616	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	782	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	253	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1150	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	1185	G	O4'-C1'-N9	5.84	112.87	108.20
54	BA	2327	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	736	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	783	C	N3-C2-O2	-5.83	117.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B0	16	ARG	NE-CZ-NH1	5.83	123.22	120.30
21	AA	246	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	976	G	C3'-C2'-C1'	5.83	106.17	101.50
5	AF	38	ARG	NE-CZ-NH1	5.83	123.22	120.30
11	AL	109	ARG	NE-CZ-NH1	5.83	123.22	120.30
21	AA	1407	C	N1-C2-O2	5.83	122.40	118.90
24	A3	64	G	N1-C6-O6	-5.83	116.40	119.90
54	BA	460	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	1199	U	O4'-C1'-N1	5.83	112.86	108.20
54	BA	1781	U	O4'-C1'-N1	5.83	112.87	108.20
54	BA	2705	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	826	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1970	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	823	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1798	U	O4'-C1'-N1	5.83	112.86	108.20
54	BA	108	G	N1-C6-O6	-5.83	116.40	119.90
21	AA	1012	A	C5-C6-N1	5.83	120.61	117.70
55	BB	33	G	O4'-C1'-N9	5.83	112.86	108.20
21	AA	400	C	O4'-C1'-N1	5.82	112.86	108.20
21	AA	980	C	N3-C2-O2	-5.82	117.82	121.90
54	BA	1327	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1787	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	441	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2396	G	O4'-C1'-N9	5.82	112.86	108.20
12	AM	106	ARG	NE-CZ-NH1	5.82	123.21	120.30
21	AA	1447	A	O4'-C1'-N9	5.82	112.86	108.20
48	BZ	44	ARG	NE-CZ-NH1	5.82	123.21	120.30
54	BA	516	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1299	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	1340	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	718	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1145	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2717	C	N1-C2-O2	5.82	122.39	118.90
54	BA	789	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2456	C	N1-C2-O2	5.81	122.39	118.90
54	BA	2809	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	385	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	757	U	O4'-C1'-N1	5.81	112.85	108.20
21	AA	1014	A	C4-C5-C6	-5.81	114.09	117.00
22	A1	60	C	N1-C2-O2	5.81	122.39	118.90
16	AQ	64	ARG	NE-CZ-NH1	5.81	123.20	120.30
21	AA	1059	C	N1-C2-O2	5.81	122.39	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	838	C	N1-C2-O2	5.81	122.39	118.90
54	BA	1954	G	N1-C6-O6	-5.81	116.41	119.90
54	BA	2145	C	N1-C2-O2	5.81	122.39	118.90
31	BI	102	ARG	NE-CZ-NH1	5.81	123.20	120.30
54	BA	61	C	N1-C2-O2	5.81	122.39	118.90
54	BA	2385	C	O4'-C1'-N1	5.81	112.85	108.20
54	BA	2513	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	1900	A	C4-C5-C6	-5.81	114.10	117.00
20	AU	34	ARG	NE-CZ-NH1	5.80	123.20	120.30
21	AA	1319	A	C4-C5-C6	-5.80	114.10	117.00
36	BN	63	ARG	NE-CZ-NH2	-5.80	117.40	120.30
54	BA	305	C	N1-C2-O2	5.80	122.38	118.90
54	BA	1585	C	O4'-C1'-N1	5.80	112.84	108.20
21	AA	1519	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	525	U	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2678	C	O4'-C1'-N1	5.80	112.84	108.20
21	AA	108	G	N3-C4-C5	-5.80	125.70	128.60
21	AA	569	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1542	U	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2097	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2364	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	195	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1111	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	60	G	N3-C2-N2	-5.80	115.84	119.90
54	BA	2858	C	N1-C2-O2	5.80	122.38	118.90
21	AA	1110	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1614	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	510	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	513	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	602	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1502	A	C4-C5-C6	-5.80	114.10	117.00
38	BP	50	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	504	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	510	C	O4'-C1'-N1	5.80	112.84	108.20
54	BA	820	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2749	A	N1-C6-N6	-5.80	115.12	118.60
21	AA	744	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	690	G	N1-C6-O6	-5.79	116.42	119.90
54	BA	1929	G	N3-C2-N2	-5.79	115.84	119.90
22	A1	9	A	O4'-C1'-N9	5.79	112.83	108.20
54	BA	1143	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	1696	G	O4'-C1'-N9	5.79	112.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2471	A	C4-C5-C6	-5.79	114.10	117.00
21	AA	1152	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	756	A	C4-C5-C6	-5.79	114.11	117.00
12	AM	91	ARG	NE-CZ-NH1	5.79	123.19	120.30
21	AA	1213	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	1336	C	C1'-O4'-C4'	-5.79	105.27	109.90
54	BA	909	A	C5-C6-N1	5.79	120.59	117.70
54	BA	2808	G	N1-C6-O6	-5.79	116.43	119.90
54	BA	1909	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	2442	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	2026	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	360	U	O4'-C1'-N1	5.78	112.83	108.20
54	BA	402	A	C4-C5-C6	-5.78	114.11	117.00
55	BB	4	C	N3-C2-O2	-5.78	117.85	121.90
55	BB	111	U	O4'-C1'-N1	5.78	112.83	108.20
54	BA	16	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2358	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	959	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	177	G	O4'-C1'-N9	5.78	112.83	108.20
54	BA	1361	G	O4'-C1'-N9	5.78	112.82	108.20
54	BA	1528	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1815	A	C4-C5-C6	-5.78	114.11	117.00
4	AE	111	ARG	NE-CZ-NH1	5.78	123.19	120.30
21	AA	977	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1244	G	N1-C6-O6	-5.78	116.43	119.90
54	BA	161	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1369	G	C5'-C4'-O4'	5.78	116.03	109.10
54	BA	2092	U	N3-C2-O2	-5.78	118.16	122.20
54	BA	2736	A	C4-C5-C6	-5.78	114.11	117.00
56	B5	60	ARG	NE-CZ-NH1	5.78	123.19	120.30
21	AA	1410	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	323	C	O4'-C1'-N1	5.78	112.82	108.20
21	AA	243	A	C6-C5-N7	5.77	136.34	132.30
36	BN	22	ARG	NE-CZ-NH1	5.77	123.19	120.30
54	BA	323	C	N1-C2-O2	5.77	122.36	118.90
54	BA	562	U	O4'-C1'-N1	5.77	112.82	108.20
54	BA	946	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1081	U	O4'-C1'-N1	5.77	112.82	108.20
4	AE	44	ARG	NE-CZ-NH1	5.77	123.19	120.30
21	AA	108	G	N3-C2-N2	-5.77	115.86	119.90
28	BF	111	ARG	NE-CZ-NH1	5.77	123.19	120.30
54	BA	1315	C	N3-C2-O2	-5.77	117.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1778	U	O4'-C1'-N1	5.77	112.82	108.20
54	BA	2281	A	C6-C5-N7	5.77	136.34	132.30
54	BA	2785	C	O4'-C1'-N1	5.77	112.82	108.20
54	BA	556	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	1488	C	N3-C2-O2	-5.77	117.86	121.90
3	AD	52	VAL	C-N-CA	5.77	136.12	121.70
21	AA	1176	A	C6-C5-N7	5.77	136.34	132.30
21	AA	1366	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	152	A	C5-C6-N1	5.77	120.58	117.70
54	BA	1251	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1524	G	N3-C2-N2	-5.77	115.86	119.90
54	BA	2615	U	N3-C2-O2	-5.77	118.16	122.20
21	AA	272	C	N3-C2-O2	-5.77	117.86	121.90
49	B0	12	ARG	NE-CZ-NH1	5.77	123.18	120.30
54	BA	1395	A	O4'-C1'-N9	5.77	112.81	108.20
55	BB	66	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	393	A	C6-C5-N7	5.76	136.34	132.30
54	BA	2406	A	C4-C5-C6	-5.76	114.12	117.00
56	B5	9	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	2287	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	135	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	443	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	580	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	848	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	1104	C	N1-C2-O2	5.76	122.36	118.90
54	BA	1176	U	N3-C2-O2	-5.76	118.17	122.20
54	BA	1312	U	P-O3'-C3'	5.76	126.61	119.70
54	BA	2329	U	O4'-C1'-N1	5.76	112.81	108.20
21	AA	1170	A	C4-C5-C6	-5.76	114.12	117.00
38	BP	100	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	1662	U	O4'-C1'-N1	5.76	112.81	108.20
55	BB	19	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	1009	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2214	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	1249	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	226	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	715	A	N1-C6-N6	-5.76	115.15	118.60
54	BA	2272	U	N3-C2-O2	-5.76	118.17	122.20
54	BA	2466	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	557	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	59	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	355	C	N3-C2-O2	-5.75	117.87	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	430	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	972	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	1028	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2183	A	N1-C6-N6	-5.75	115.15	118.60
54	BA	672	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	1051	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	520	A	C4-C5-C6	-5.75	114.12	117.00
22	A1	23	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	897	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	2514	U	O4'-C1'-N1	5.75	112.80	108.20
55	BB	53	A	C4-C5-C6	-5.75	114.13	117.00
3	AD	127	ARG	NE-CZ-NH1	5.75	123.17	120.30
54	BA	905	A	C5-C6-N1	5.75	120.57	117.70
54	BA	1058	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	1072	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1462	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1582	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1879	C	N1-C2-O2	5.74	122.35	118.90
54	BA	228	C	N1-C2-O2	5.74	122.34	118.90
54	BA	281	C	N1-C2-O2	5.74	122.34	118.90
54	BA	1496	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	1280	A	C4-C5-C6	-5.74	114.13	117.00
34	BL	21	ARG	NE-CZ-NH2	5.74	123.17	120.30
54	BA	2492	U	N3-C2-O2	-5.74	118.18	122.20
21	AA	695	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	840	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	478	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1342	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1978	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2066	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	26	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	1492	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1618	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1974	C	O4'-C1'-N1	5.74	112.79	108.20
21	AA	1145	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1787	A	C3'-C2'-C1'	5.74	106.09	101.50
54	BA	282	A	C4-C5-C6	-5.73	114.13	117.00
54	BA	2011	U	O4'-C1'-N1	5.73	112.79	108.20
21	AA	582	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	1204	A	C5-C6-N1	5.73	120.57	117.70
45	BW	54	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	2395	C	O4'-C1'-N1	5.73	112.79	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	26	A	O4'-C1'-N9	5.73	112.78	108.20
21	AA	366	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	2886	A	O4'-C1'-N9	5.73	112.78	108.20
54	BA	167	A	N1-C6-N6	-5.73	115.16	118.60
54	BA	2511	U	O4'-C1'-N1	5.73	112.78	108.20
54	BA	2706	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	83	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	920	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1297	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1887	C	N1-C2-O2	5.73	122.34	118.90
54	BA	1937	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	645	C	N1-C2-O2	5.72	122.33	118.90
54	BA	717	C	O4'-C1'-N1	5.72	112.78	108.20
54	BA	847	U	N3-C2-O2	-5.72	118.19	122.20
54	BA	2326	C	N1-C2-O2	5.72	122.33	118.90
54	BA	2538	C	N3-C2-O2	-5.72	117.89	121.90
21	AA	1336	C	O4'-C1'-N1	5.72	112.78	108.20
21	AA	235	C	O4'-C1'-N1	5.72	112.78	108.20
21	AA	1117	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	1318	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	320	A	O4'-C1'-N9	5.72	112.78	108.20
54	BA	2385	C	N1-C2-O2	5.72	122.33	118.90
54	BA	2388	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1006	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	1393	A	O4'-C1'-N9	5.72	112.77	108.20
54	BA	2130	U	N3-C2-O2	-5.72	118.20	122.20
21	AA	1036	A	C4-C5-C6	-5.71	114.14	117.00
22	A1	25	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	1640	A	C4-C5-C6	-5.71	114.14	117.00
21	AA	686	U	C1'-O4'-C4'	-5.71	105.33	109.90
21	AA	1532	U	N3-C2-O2	-5.71	118.20	122.20
54	BA	542	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	1278	C	O4'-C1'-N1	5.71	112.77	108.20
54	BA	2759	G	N1-C6-O6	-5.71	116.47	119.90
21	AA	1151	A	C6-C5-N7	5.71	136.30	132.30
54	BA	37	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	911	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2282	G	O4'-C1'-N9	5.71	112.77	108.20
54	BA	2465	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	173	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1001	A	N1-C6-N6	-5.71	115.17	118.60
21	AA	33	A	C4-C5-C6	-5.71	114.15	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	573	A	C4-C5-C6	-5.71	114.15	117.00
30	BH	116	ARG	NE-CZ-NH1	5.71	123.15	120.30
54	BA	1330	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	1503	A	C6-C5-N7	5.71	136.29	132.30
54	BA	2768	U	O4'-C1'-N1	5.71	112.77	108.20
25	BC	257	ARG	NE-CZ-NH1	5.71	123.15	120.30
54	BA	1615	C	N1-C2-O2	5.71	122.32	118.90
54	BA	2404	U	O4'-C1'-N1	5.71	112.76	108.20
54	BA	116	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	128	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	1153	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	1219	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	405	U	N3-C2-O2	-5.70	118.21	122.20
21	AA	40	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	344	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	1462	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	172	A	C4-C5-C6	-5.70	114.15	117.00
5	AF	79	ARG	NE-CZ-NH1	5.70	123.15	120.30
5	AF	86	ARG	NE-CZ-NH1	5.70	123.15	120.30
21	AA	610	U	O4'-C1'-N1	5.70	112.76	108.20
21	AA	630	A	C4-C5-C6	-5.70	114.15	117.00
24	A3	42	C	N1-C2-O2	5.70	122.32	118.90
54	BA	1222	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	2110	G	N1-C6-O6	-5.69	116.48	119.90
54	BA	2902	C	N1-C2-O2	5.69	122.32	118.90
29	BG	2	ARG	NE-CZ-NH1	5.69	123.15	120.30
54	BA	514	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	852	U	O4'-C1'-N1	5.69	112.75	108.20
54	BA	1566	A	C3'-C2'-C1'	5.69	106.05	101.50
20	AU	44	ARG	NE-CZ-NH2	5.69	123.14	120.30
54	BA	147	C	N1-C2-O2	5.69	122.31	118.90
54	BA	873	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1254	A	C3'-C2'-C1'	5.69	106.05	101.50
54	BA	2311	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	620	G	N9-C4-C5	5.69	107.68	105.40
55	BB	18	G	N3-C2-N2	-5.69	115.92	119.90
54	BA	1888	G	O4'-C1'-N9	5.69	112.75	108.20
54	BA	1102	C	N3-C2-O2	-5.68	117.92	121.90
21	AA	49	U	O4'-C1'-N1	5.68	112.75	108.20
21	AA	1180	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	1465	A	C4-C5-C6	-5.68	114.16	117.00
25	BC	79	ARG	NE-CZ-NH1	5.68	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2225	A	O4'-C1'-N9	5.68	112.75	108.20
21	AA	1487	G	O4'-C1'-N9	5.68	112.75	108.20
54	BA	1396	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	2219	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	244	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1431	A	C4-C5-C6	-5.68	114.16	117.00
4	AE	92	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	1176	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	2590	A	O4'-C1'-N9	5.68	112.74	108.20
55	BB	93	C	N3-C2-O2	-5.68	117.93	121.90
54	BA	899	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	2620	C	N1-C2-O2	5.67	122.30	118.90
21	AA	909	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1803	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	2863	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	553	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	292	U	O4'-C1'-N1	5.67	112.74	108.20
54	BA	1155	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	1634	A	C4-C5-C6	-5.67	114.16	117.00
55	BB	33	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	1263	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1376	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	853	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1150	C	C4'-C3'-C2'	-5.67	96.93	102.60
54	BA	1309	G	C4'-C3'-C2'	-5.67	96.93	102.60
54	BA	1419	A	C4-C5-C6	-5.67	114.17	117.00
21	AA	478	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	445	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	791	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1360	G	O4'-C1'-N9	5.67	112.73	108.20
54	BA	2091	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	261	U	N3-C2-O2	-5.67	118.23	122.20
21	AA	1452	C	N1-C2-O2	5.67	122.30	118.90
24	A3	49	C	N3-C2-O2	-5.67	117.93	121.90
38	BP	97	TYR	CB-CG-CD2	-5.66	117.60	121.00
54	BA	14	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	946	C	C1'-O4'-C4'	-5.66	105.37	109.90
21	AA	860	A	C5-C6-N1	5.66	120.53	117.70
54	BA	173	A	C5-C6-N1	5.66	120.53	117.70
54	BA	2300	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1189	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	503	A	C4-C5-C6	-5.66	114.17	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	893	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	896	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	160	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2266	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2347	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	2658	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	635	C	C4'-C3'-C2'	-5.66	96.94	102.60
54	BA	1229	C	N1-C2-O2	5.66	122.29	118.90
21	AA	756	C	N1-C2-O2	5.65	122.29	118.90
21	AA	845	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1556	C	N3-C2-O2	-5.65	117.94	121.90
22	A1	48	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	1942	C	N3-C4-N4	-5.65	114.04	118.00
54	BA	2321	U	N3-C2-O2	-5.65	118.24	122.20
21	AA	492	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	697	U	O4'-C1'-N1	5.65	112.72	108.20
22	A1	75	C	N3-C2-O2	-5.65	117.94	121.90
37	BO	102	ARG	NE-CZ-NH1	5.65	123.12	120.30
54	BA	77	G	O4'-C1'-N9	5.65	112.72	108.20
54	BA	1547	C	N1-C2-O2	5.65	122.29	118.90
21	AA	53	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	57	G	C8-N9-C4	-5.65	104.14	106.40
21	AA	1362	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	1720	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1557	C	N1-C2-O2	5.65	122.29	118.90
54	BA	1881	C	N3-C2-O2	-5.65	117.95	121.90
4	AE	19	ARG	NE-CZ-NH1	5.64	123.12	120.30
55	BB	29	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	21	G	N1-C6-O6	-5.64	116.51	119.90
22	A1	70	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1254	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1704	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2364	C	O4'-C1'-N1	5.64	112.72	108.20
22	A1	35	A	C6-C5-N7	5.64	136.25	132.30
54	BA	143	C	O4'-C1'-N1	5.64	112.71	108.20
3	AD	187	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	217	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1840	G	N3-C4-C5	-5.64	125.78	128.60
54	BA	2837	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	1150	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	639	U	O4'-C1'-N1	5.64	112.71	108.20
54	BA	2232	C	O4'-C1'-N1	5.64	112.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	182	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	393	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1386	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1920	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	539	A	C5-C6-N1	5.63	120.52	117.70
21	AA	1467	C	N3-C2-O2	-5.63	117.95	121.90
54	BA	427	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	634	C	O4'-C1'-N1	5.63	112.71	108.20
54	BA	1161	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	1258	U	O4'-C1'-N1	5.63	112.71	108.20
22	A1	28	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	249	C	N1-C2-O2	5.63	122.28	118.90
54	BA	1434	A	C4-C5-C6	-5.63	114.18	117.00
6	AG	118	ARG	NE-CZ-NH1	5.63	123.11	120.30
54	BA	925	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	1128	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	1178	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	1943	U	N3-C2-O2	-5.63	118.26	122.20
54	BA	2602	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1530	G	C1'-O4'-C4'	-5.63	105.40	109.90
54	BA	646	U	O4'-C1'-N1	5.63	112.70	108.20
21	AA	635	A	C5-C6-N1	5.63	120.52	117.70
21	AA	1042	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1296	C	N1-C2-O2	5.63	122.28	118.90
54	BA	975	A	C4'-C3'-C2'	-5.63	96.97	102.60
54	BA	1593	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	2014	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	2313	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	232	G	N3-C2-N2	-5.63	115.96	119.90
21	AA	665	A	C1'-O4'-C4'	-5.63	105.40	109.90
21	AA	741	G	N1-C6-O6	-5.63	116.53	119.90
21	AA	1022	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	223	A	C6-C5-N7	5.62	136.24	132.30
21	AA	1481	U	O4'-C1'-N1	5.62	112.70	108.20
21	AA	487	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	39	G	O4'-C1'-N9	5.62	112.70	108.20
54	BA	71	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	717	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	2478	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2739	U	O4'-C1'-N1	5.62	112.70	108.20
54	BA	1705	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1999	C	N1-C2-O2	5.62	122.27	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1224	U	N3-C2-O2	-5.62	118.27	122.20
54	BA	1137	G	N1-C6-O6	-5.62	116.53	119.90
55	BB	118	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1537	G	C1'-O4'-C4'	-5.62	105.41	109.90
54	BA	1789	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2610	C	N1-C2-O2	5.62	122.27	118.90
54	BA	2628	C	N1-C2-O2	5.62	122.27	118.90
54	BA	2745	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	260	G	N3-C2-N2	-5.62	115.97	119.90
24	A3	10	G	N1-C6-O6	-5.62	116.53	119.90
26	BD	179	ARG	NE-CZ-NH1	5.62	123.11	120.30
21	AA	658	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	976	G	N1-C6-O6	-5.62	116.53	119.90
23	A2	91	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	932	C	O4'-C1'-N1	5.61	112.69	108.20
33	BK	30	ARG	NE-CZ-NH1	5.61	123.11	120.30
54	BA	28	A	O4'-C1'-N9	5.61	112.69	108.20
54	BA	179	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1019	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1301	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	1641	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	2247	A	C4-C5-C6	-5.61	114.19	117.00
55	BB	90	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	1363	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	1312	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1726	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1874	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	212	G	N1-C6-O6	-5.61	116.53	119.90
21	AA	483	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1185	G	C3'-C2'-C1'	5.61	105.99	101.50
54	BA	1561	C	N1-C2-O2	5.61	122.27	118.90
54	BA	2681	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	310	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	515	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	564	C	N1-C2-O2	5.61	122.27	118.90
54	BA	871	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2425	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	746	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	1423	G	N3-C2-N2	-5.61	115.98	119.90
54	BA	571	U	C1'-O4'-C4'	-5.61	105.42	109.90
54	BA	654	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	1090	A	C4-C5-C6	-5.61	114.20	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1128	G	O4'-C1'-N9	5.61	112.68	108.20
21	AA	533	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	2692	G	C4'-C3'-C2'	-5.60	97.00	102.60
23	A2	93	U	N3-C2-O2	-5.60	118.28	122.20
54	BA	803	U	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2655	G	N3-C4-C5	-5.60	125.80	128.60
21	AA	38	G	O3'-P-O5'	-5.60	93.36	104.00
54	BA	1238	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	1794	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	649	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	96	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	950	G	N3-C2-N2	-5.60	115.98	119.90
54	BA	1281	G	N1-C6-O6	-5.60	116.54	119.90
21	AA	656	G	N3-C2-N2	-5.60	115.98	119.90
21	AA	955	U	O4'-C1'-N1	5.60	112.68	108.20
54	BA	1510	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	1842	G	N1-C6-O6	-5.60	116.54	119.90
21	AA	693	G	N1-C6-O6	-5.59	116.54	119.90
54	BA	1669	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	2612	C	N1-C2-O2	5.59	122.26	118.90
21	AA	872	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	1533	C	N3-C4-C5	5.59	124.14	121.90
54	BA	722	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	285	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1347	G	O4'-C1'-N9	5.59	112.67	108.20
21	AA	1447	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	60	G	C1'-O4'-C4'	-5.59	105.43	109.90
54	BA	2720	U	O4'-C1'-N1	5.59	112.67	108.20
21	AA	1028	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2668	G	C3'-C2'-C1'	-5.59	97.03	101.50
55	BB	30	C	N1-C2-O2	5.59	122.25	118.90
21	AA	1261	A	N1-C6-N6	-5.58	115.25	118.60
54	BA	751	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2254	C	O4'-C1'-N1	5.58	112.67	108.20
21	AA	119	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	101	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	904	G	N1-C6-O6	-5.58	116.55	119.90
54	BA	1585	C	N1-C2-O2	5.58	122.25	118.90
55	BB	37	C	O4'-C1'-N1	5.58	112.67	108.20
21	AA	647	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	1378	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2021	C	N1-C2-O2	5.58	122.25	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2116	G	O4'-C4'-C3'	5.58	110.56	106.10
21	AA	868	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	1113	C	N1-C2-O2	5.58	122.25	118.90
54	BA	378	C	O4'-C1'-N1	5.58	112.66	108.20
55	BB	100	G	N1-C6-O6	-5.58	116.55	119.90
21	AA	572	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	890	G	N3-C4-C5	-5.58	125.81	128.60
23	A2	91	A	O4'-C1'-N9	5.58	112.66	108.20
54	BA	394	C	N1-C2-O2	5.58	122.25	118.90
54	BA	679	C	N3-C2-O2	-5.58	118.00	121.90
21	AA	574	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	808	C	N1-C2-O2	5.58	122.25	118.90
54	BA	2452	C	N3-C2-O2	-5.58	118.00	121.90
21	AA	344	A	C2-N3-C4	5.58	113.39	110.60
54	BA	1575	C	O4'-C1'-N1	5.58	112.66	108.20
15	AP	51	ARG	NE-CZ-NH1	5.57	123.09	120.30
21	AA	35	G	N3-C4-C5	-5.57	125.81	128.60
54	BA	1504	A	C4-C5-C6	-5.57	114.21	117.00
54	BA	2043	C	N3-C2-O2	-5.57	118.00	121.90
16	AQ	5	ARG	NE-CZ-NH2	-5.57	117.51	120.30
54	BA	166	U	O4'-C1'-N1	5.57	112.66	108.20
21	AA	936	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1637	A	C6-C5-N7	5.57	136.20	132.30
54	BA	2285	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	2548	U	O4'-C1'-N1	5.57	112.66	108.20
21	AA	44	A	C5-C6-N1	5.57	120.48	117.70
21	AA	913	A	P-O3'-C3'	5.57	126.38	119.70
54	BA	157	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	2376	A	C4-C5-C6	-5.57	114.22	117.00
16	AQ	63	CYS	O-C-N	-5.57	113.79	122.70
21	AA	252	U	C1'-O4'-C4'	-5.57	105.45	109.90
21	AA	316	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1551	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	742	G	C5-C6-N1	5.57	114.28	111.50
54	BA	761	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	1045	C	O4'-C1'-N1	5.57	112.65	108.20
54	BA	1901	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	1727	C	N3-C2-O2	-5.56	118.01	121.90
21	AA	1056	U	O4'-C1'-N1	5.56	112.65	108.20
54	BA	2113	U	N3-C2-O2	-5.56	118.31	122.20
2	AC	53	ARG	NE-CZ-NH1	5.56	123.08	120.30
21	AA	1071	C	N3-C2-O2	-5.56	118.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1174	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	1760	C	O4'-C1'-N1	5.56	112.65	108.20
21	AA	974	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	119	A	C6-C5-N7	5.56	136.19	132.30
54	BA	990	A	C5'-C4'-O4'	5.56	115.77	109.10
54	BA	1499	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	1833	C	N1-C2-O2	5.56	122.23	118.90
54	BA	2335	A	C4-C5-C6	-5.56	114.22	117.00
35	BM	59	ARG	NE-CZ-NH1	5.55	123.08	120.30
54	BA	1020	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	2112	G	N3-C4-C5	-5.55	125.82	128.60
54	BA	2657	A	C4-C5-C6	-5.55	114.22	117.00
21	AA	777	A	C4-C5-C6	-5.55	114.22	117.00
21	AA	1204	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	298	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	412	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1089	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1362	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	2039	U	O4'-C1'-N1	5.55	112.64	108.20
3	AD	164	ARG	NE-CZ-NH1	5.55	123.07	120.30
54	BA	857	G	N1-C6-O6	-5.55	116.57	119.90
21	AA	972	C	C1'-O4'-C4'	-5.54	105.46	109.90
54	BA	1453	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1647	U	C1'-O4'-C4'	-5.54	105.46	109.90
54	BA	326	G	O4'-C1'-N9	5.54	112.64	108.20
54	BA	2825	G	C8-N9-C4	-5.54	104.18	106.40
21	AA	300	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	1167	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	115	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	216	A	N1-C6-N6	-5.54	115.28	118.60
54	BA	2807	U	O4'-C1'-N1	5.54	112.63	108.20
10	AK	121	ARG	NE-CZ-NH1	5.54	123.07	120.30
22	A1	76	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	393	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	2308	G	P-O3'-C3'	5.54	126.35	119.70
54	BA	2564	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	505	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1849	G	O4'-C1'-N9	5.54	112.63	108.20
54	BA	2031	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2498	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	322	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2562	U	O4'-C1'-N1	5.54	112.63	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	233	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1063	G	C1'-O4'-C4'	-5.54	105.47	109.90
54	BA	1260	A	C6-C5-N7	5.54	136.17	132.30
54	BA	2296	U	C3'-C2'-C1'	5.54	105.93	101.50
21	AA	466	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	164	C	O4'-C1'-N1	5.53	112.63	108.20
21	AA	802	A	O4'-C1'-N9	5.53	112.62	108.20
54	BA	632	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	77	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1690	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1795	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	2180	U	N3-C2-O2	-5.53	118.33	122.20
21	AA	663	A	C4-C5-C6	-5.53	114.23	117.00
23	A2	80	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2726	A	C3'-C2'-C1'	5.53	105.92	101.50
54	BA	2853	C	N1-C2-O2	5.53	122.22	118.90
55	BB	80	U	O4'-C1'-N1	5.53	112.62	108.20
21	AA	266	G	O4'-C1'-N9	5.53	112.62	108.20
21	AA	395	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	831	A	C6-C5-N7	5.53	136.17	132.30
28	BF	79	ARG	NE-CZ-NH1	5.53	123.06	120.30
54	BA	677	A	O4'-C1'-N9	5.53	112.62	108.20
54	BA	983	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	2794	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2825	G	N3-C4-C5	-5.53	125.84	128.60
21	AA	47	C	C2-N3-C4	-5.53	117.14	119.90
54	BA	422	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	610	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	1148	U	C1'-O4'-C4'	-5.53	105.48	109.90
54	BA	1774	C	O4'-C1'-N1	5.53	112.62	108.20
21	AA	401	C	N3-C2-O2	-5.52	118.03	121.90
54	BA	316	C	N3-C2-O2	-5.52	118.03	121.90
54	BA	1520	U	O4'-C1'-N1	5.52	112.62	108.20
54	BA	2077	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2651	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	978	A	C4-C5-C6	-5.52	114.24	117.00
27	BE	69	ARG	NE-CZ-NH2	-5.52	117.54	120.30
54	BA	246	C	N3-C2-O2	-5.52	118.03	121.90
54	BA	581	C	N3-C2-O2	-5.52	118.03	121.90
54	BA	684	G	N3-C2-N2	-5.52	116.03	119.90
54	BA	1463	C	N3-C2-O2	-5.52	118.03	121.90
54	BA	1505	A	C6-C5-N7	5.52	136.16	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1612	C	N3-C2-O2	-5.52	118.03	121.90
54	BA	2819	G	N1-C6-O6	-5.52	116.59	119.90
54	BA	205	G	N1-C6-O6	-5.52	116.59	119.90
54	BA	1694	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	903	G	N1-C6-O6	-5.52	116.59	119.90
21	AA	1194	U	O4'-C1'-N1	5.52	112.61	108.20
21	AA	1400	C	N1-C2-O2	5.52	122.21	118.90
54	BA	1351	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	337	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	534	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	549	G	O4'-C1'-N9	5.52	112.61	108.20
54	BA	1490	A	N1-C6-N6	-5.52	115.29	118.60
54	BA	2195	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	2277	G	N1-C6-O6	-5.52	116.59	119.90
21	AA	1297	G	N7-C8-N9	5.51	115.86	113.10
54	BA	1012	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	2072	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	2758	A	C4-C5-C6	-5.51	114.24	117.00
24	A3	25	U	C3'-C2'-C1'	-5.51	97.09	101.50
21	AA	1252	A	N1-C6-N6	-5.51	115.29	118.60
47	BY	7	ARG	NE-CZ-NH2	-5.51	117.54	120.30
54	BA	528	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	737	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	2187	U	O4'-C1'-N1	5.51	112.61	108.20
21	AA	918	A	C4-C5-C6	-5.51	114.25	117.00
21	AA	1168	U	O4'-C1'-N1	5.51	112.61	108.20
22	A1	68	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	829	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	1300	G	N3-C2-N2	-5.51	116.04	119.90
54	BA	1872	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	1886	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	2703	C	O4'-C1'-N1	5.51	112.61	108.20
54	BA	646	U	N3-C2-O2	-5.51	118.35	122.20
55	BB	41	G	N1-C6-O6	-5.51	116.60	119.90
54	BA	1150	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	2362	C	N3-C2-O2	-5.50	118.05	121.90
8	AI	122	ARG	CD-NE-CZ	5.50	131.31	123.60
21	AA	560	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	933	A	O4'-C1'-N9	5.50	112.60	108.20
54	BA	1385	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1761	C	N1-C2-O2	5.50	122.20	118.90
21	AA	374	A	C4-C5-C6	-5.50	114.25	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	432	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	910	A	C6-C5-N7	5.50	136.15	132.30
54	BA	2458	G	O4'-C1'-N9	5.50	112.60	108.20
54	BA	1123	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	2483	C	N1-C2-O2	5.50	122.20	118.90
21	AA	976	G	O4'-C1'-N9	5.50	112.60	108.20
21	AA	1066	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	730	A	O4'-C1'-N9	5.50	112.60	108.20
54	BA	1063	G	O4'-C1'-N9	5.50	112.60	108.20
54	BA	1731	G	N3-C4-C5	-5.50	125.85	128.60
54	BA	2279	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	2554	U	O4'-C1'-N1	5.50	112.60	108.20
40	BR	78	ARG	NE-CZ-NH2	5.50	123.05	120.30
21	AA	182	A	C4-C5-C6	-5.49	114.25	117.00
21	AA	711	G	N1-C6-O6	-5.49	116.60	119.90
54	BA	2169	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	2298	A	C4-C5-C6	-5.49	114.25	117.00
36	BN	71	ARG	NE-CZ-NH1	5.49	123.05	120.30
54	BA	1936	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	2089	C	N1-C2-O2	5.49	122.19	118.90
54	BA	2661	G	N3-C2-N2	-5.49	116.06	119.90
21	AA	1080	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	211	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	737	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	289	G	N1-C6-O6	-5.49	116.61	119.90
12	AM	2	ARG	NE-CZ-NH2	5.49	123.04	120.30
54	BA	1802	A	C4-C5-C6	-5.49	114.26	117.00
21	AA	1225	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	1246	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1438	U	C2-N1-C1'	5.48	124.28	117.70
54	BA	1670	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	1748	C	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2132	U	N3-C2-O2	-5.48	118.36	122.20
21	AA	1265	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	1375	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	364	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	781	A	C4-C5-C6	-5.48	114.26	117.00
22	A1	36	C	N1-C2-O2	5.48	122.19	118.90
21	AA	167	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	141	G	O4'-C1'-N9	5.48	112.58	108.20
54	BA	1439	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2263	C	N3-C2-O2	-5.48	118.07	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2417	C	O4'-C1'-N1	5.48	112.58	108.20
54	BA	1289	C	N3-C2-O2	-5.48	118.07	121.90
54	BA	571	U	O4'-C1'-N1	5.47	112.58	108.20
21	AA	179	A	C3'-C2'-C1'	5.47	105.88	101.50
21	AA	548	G	N3-C2-N2	-5.47	116.07	119.90
21	AA	1489	G	N1-C6-O6	-5.47	116.62	119.90
24	A3	75	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	272	A	C4-C5-C6	-5.47	114.26	117.00
54	BA	1073	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	2044	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	2374	C	N1-C2-O2	5.47	122.18	118.90
21	AA	1311	A	C6-C5-N7	5.47	136.13	132.30
21	AA	71	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	2163	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	2275	C	O4'-C1'-N1	5.47	112.58	108.20
21	AA	437	U	O4'-C1'-N1	5.47	112.57	108.20
21	AA	496	A	C1'-O4'-C4'	-5.47	105.53	109.90
54	BA	1057	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	1992	G	C5-C6-N1	5.47	114.23	111.50
21	AA	1227	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	38	A	C4'-C3'-C2'	-5.47	97.13	102.60
54	BA	493	G	N3-C4-C5	-5.47	125.87	128.60
54	BA	765	C	N1-C2-O2	5.47	122.18	118.90
21	AA	394	G	N3-C4-C5	-5.46	125.87	128.60
29	BG	162	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	2268	A	N1-C6-N6	-5.46	115.32	118.60
21	AA	253	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1134	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1996	C	N1-C2-O2	5.46	122.18	118.90
21	AA	114	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	487	C	N1-C2-O2	5.46	122.18	118.90
54	BA	1796	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	2098	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	218	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	109	A	O4'-C1'-N9	5.46	112.57	108.20
21	AA	229	U	N3-C2-O2	-5.46	118.38	122.20
54	BA	48	G	C5'-C4'-C3'	-5.46	107.27	116.00
54	BA	1309	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	1497	U	O4'-C1'-N1	5.46	112.57	108.20
21	AA	1427	C	N1-C2-O2	5.46	122.17	118.90
27	BE	170	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
54	BA	428	A	C4-C5-C6	-5.46	114.27	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1270	C	N1-C2-O2	5.46	122.17	118.90
54	BA	2096	C	N1-C2-O2	5.46	122.17	118.90
21	AA	277	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	143	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	195	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	476	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	981	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	1118	C	N1-C2-O2	5.45	122.17	118.90
21	AA	120	A	C4-C5-C6	-5.45	114.27	117.00
21	AA	1146	A	C4-C5-C6	-5.45	114.27	117.00
21	AA	65	A	O4'-C1'-N9	5.45	112.56	108.20
21	AA	176	C	C1'-O4'-C4'	-5.45	105.54	109.90
21	AA	470	C	O4'-C1'-N1	5.45	112.56	108.20
21	AA	794	A	C6-C5-N7	5.45	136.12	132.30
54	BA	385	C	N1-C2-O2	5.45	122.17	118.90
54	BA	849	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2556	C	O4'-C1'-N1	5.45	112.56	108.20
21	AA	55	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	933	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	1292	G	C1'-O4'-C4'	-5.45	105.54	109.90
54	BA	1359	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	1535	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	1990	C	N1-C2-O2	5.45	122.17	118.90
54	BA	2575	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	357	C	N1-C2-O2	5.45	122.17	118.90
54	BA	1207	C	N3-C2-O2	-5.45	118.09	121.90
21	AA	36	C	N3-C2-O2	-5.45	118.09	121.90
21	AA	1493	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	543	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	2793	C	O4'-C1'-N1	5.45	112.56	108.20
21	AA	830	G	N3-C2-N2	-5.44	116.09	119.90
54	BA	998	C	O4'-C1'-N1	5.44	112.56	108.20
54	BA	1106	G	C8-N9-C4	-5.44	104.22	106.40
21	AA	618	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	1033	U	O4'-C1'-N1	5.44	112.56	108.20
54	BA	1818	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	2143	C	N3-C2-O2	-5.44	118.09	121.90
55	BB	73	A	C4-C5-C6	-5.44	114.28	117.00
41	BS	84	ARG	NE-CZ-NH1	5.44	123.02	120.30
54	BA	548	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	1530	G	N3-C2-N2	-5.44	116.09	119.90
21	AA	206	C	N3-C2-O2	-5.44	118.09	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A2	93	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	403	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	740	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	1947	C	N1-C2-O2	5.44	122.16	118.90
23	A2	84	G	O4'-C1'-N9	5.44	112.55	108.20
54	BA	6	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	2855	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	518	C	N1-C2-O2	5.43	122.16	118.90
22	A1	32	C	N3-C2-O2	-5.43	118.10	121.90
45	BW	10	ARG	NE-CZ-NH1	5.43	123.02	120.30
54	BA	1573	G	O4'-C1'-N9	5.43	112.55	108.20
21	AA	65	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	368	U	N3-C2-O2	-5.43	118.40	122.20
21	AA	601	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	1096	C	N1-C2-O2	5.43	122.16	118.90
21	AA	1228	C	O4'-C1'-N1	5.43	112.55	108.20
54	BA	912	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	1221	C	O4'-C1'-N1	5.43	112.55	108.20
21	AA	1155	A	C6-C5-N7	5.43	136.10	132.30
39	BQ	49	ARG	NE-CZ-NH2	-5.43	117.58	120.30
54	BA	2372	U	O4'-C1'-N1	5.43	112.55	108.20
54	BA	2498	C	O4'-C1'-N1	5.43	112.55	108.20
54	BA	2697	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	171	A	C6-C5-N7	5.43	136.10	132.30
54	BA	27	G	O4'-C1'-N9	5.43	112.54	108.20
54	BA	221	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	1719	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1837	C	N3-C4-N4	-5.43	114.20	118.00
54	BA	975	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	2789	C	O4'-C1'-N1	5.43	112.54	108.20
21	AA	55	A	C3'-C2'-C1'	-5.43	97.16	101.50
21	AA	264	C	N1-C2-O2	5.43	122.16	118.90
21	AA	1183	U	N3-C2-O2	-5.43	118.40	122.20
21	AA	1480	A	C4-C5-C6	-5.43	114.29	117.00
22	A1	11	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	2354	C	O4'-C1'-N1	5.43	112.54	108.20
21	AA	770	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	192	C	N3-C4-C5	5.42	124.07	121.90
54	BA	544	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	1030	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	2084	C	N1-C2-O2	5.42	122.15	118.90
39	BQ	91	ARG	NH1-CZ-NH2	-5.42	113.44	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	870	U	O4'-C1'-N1	5.42	112.54	108.20
55	BB	17	C	O4'-C1'-N1	5.42	112.54	108.20
21	AA	286	C	N1-C2-O2	5.42	122.15	118.90
21	AA	778	G	N7-C8-N9	5.42	115.81	113.10
21	AA	1423	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	500	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	2753	A	C6-C5-N7	5.42	136.09	132.30
54	BA	2769	U	O4'-C1'-N1	5.42	112.53	108.20
54	BA	1755	A	C6-C5-N7	5.42	136.09	132.30
21	AA	365	U	N3-C2-O2	-5.42	118.41	122.20
54	BA	254	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	1609	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1871	A	C6-C5-N7	5.42	136.09	132.30
54	BA	2380	C	N3-C4-C5	5.42	124.07	121.90
54	BA	662	G	O4'-C1'-N9	5.41	112.53	108.20
54	BA	1060	U	N3-C2-O2	-5.41	118.41	122.20
54	BA	1333	G	N1-C6-O6	-5.41	116.65	119.90
54	BA	2204	G	N3-C2-N2	-5.41	116.11	119.90
55	BB	28	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	1240	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1664	A	C3'-C2'-C1'	5.41	105.83	101.50
54	BA	2435	A	C4-C5-C6	-5.41	114.30	117.00
55	BB	107	G	C3'-C2'-C1'	5.41	105.83	101.50
54	BA	1875	G	N3-C2-N2	-5.41	116.11	119.90
54	BA	2030	A	C1'-O4'-C4'	-5.41	105.57	109.90
54	BA	2053	G	N1-C6-O6	-5.41	116.66	119.90
54	BA	2054	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	2314	A	C4-C5-C6	-5.41	114.30	117.00
3	AD	80	ARG	NE-CZ-NH2	-5.41	117.60	120.30
54	BA	257	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	403	U	O4'-C1'-N1	5.41	112.53	108.20
15	AP	35	ARG	NE-CZ-NH1	5.41	123.00	120.30
21	AA	729	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	1480	A	N9-C1'-C2'	-5.41	106.06	112.00
54	BA	1477	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1547	C	O4'-C1'-N1	5.41	112.52	108.20
54	BA	1574	C	N3-C4-C5	5.41	124.06	121.90
54	BA	1834	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2449	U	N3-C2-O2	-5.41	118.42	122.20
11	AL	98	ARG	NE-CZ-NH1	5.40	123.00	120.30
13	AN	53	ARG	NE-CZ-NH1	5.40	123.00	120.30
54	BA	2716	C	C4'-C3'-C2'	-5.40	97.20	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	15	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	382	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	1021	A	C6-C5-N7	5.40	136.08	132.30
54	BA	25	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	149	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	549	G	C3'-C2'-C1'	5.40	105.82	101.50
54	BA	1247	A	O4'-C1'-N9	5.40	112.52	108.20
54	BA	1295	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	1982	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2683	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	330	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	1273	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	930	G	N1-C6-O6	-5.40	116.66	119.90
21	AA	1130	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1533	C	N1-C2-O2	5.40	122.14	118.90
54	BA	2883	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	96	U	O4'-C1'-N1	5.40	112.52	108.20
21	AA	529	G	N1-C6-O6	-5.40	116.66	119.90
21	AA	960	U	N3-C2-O2	-5.40	118.42	122.20
54	BA	2812	G	N1-C6-O6	-5.40	116.66	119.90
55	BB	3	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	1605	C	N1-C2-O2	5.40	122.14	118.90
21	AA	377	G	O4'-C1'-N9	5.39	112.52	108.20
21	AA	1469	C	N1-C2-O2	5.39	122.14	118.90
54	BA	450	G	N3-C4-C5	-5.39	125.90	128.60
54	BA	640	C	N1-C2-O2	5.39	122.14	118.90
54	BA	2086	U	O4'-C1'-N1	5.39	112.52	108.20
54	BA	2394	C	O4'-C1'-N1	5.39	112.52	108.20
21	AA	1252	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	1064	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1174	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1916	A	C6-C5-N7	5.39	136.07	132.30
21	AA	466	A	O4'-C1'-N9	5.39	112.51	108.20
21	AA	1271	A	O4'-C1'-N9	5.39	112.51	108.20
33	BK	71	ARG	NE-CZ-NH1	5.39	123.00	120.30
21	AA	760	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	1665	A	O4'-C1'-N9	5.39	112.51	108.20
54	BA	2573	C	N1-C2-O2	5.39	122.13	118.90
21	AA	1310	G	N1-C6-O6	-5.39	116.67	119.90
23	A2	88	U	C1'-O4'-C4'	-5.39	105.59	109.90
54	BA	1290	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	1572	A	C4-C5-C6	-5.39	114.31	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	282	A	C6-C5-N7	5.39	136.07	132.30
33	BK	70	ARG	NE-CZ-NH1	5.39	122.99	120.30
54	BA	1118	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1493	C	N1-C2-O2	5.39	122.13	118.90
54	BA	1583	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	1940	U	N3-C2-O2	-5.39	118.43	122.20
21	AA	69	G	N3-C4-C5	-5.38	125.91	128.60
21	AA	1347	G	C4'-C3'-C2'	-5.38	97.22	102.60
11	AL	120	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BA	30	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	764	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1810	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	1038	C	N1-C2-O2	5.38	122.13	118.90
21	AA	25	C	N1-C2-O2	5.38	122.13	118.90
54	BA	1608	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	2669	G	C5'-C4'-O4'	5.38	115.56	109.10
14	AO	71	ARG	NE-CZ-NH1	5.38	122.99	120.30
21	AA	704	A	C6-C5-N7	5.38	136.06	132.30
21	AA	787	A	N1-C6-N6	-5.38	115.37	118.60
21	AA	995	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	353	C	N1-C2-O2	5.38	122.13	118.90
54	BA	549	G	N3-C4-C5	-5.38	125.91	128.60
54	BA	1039	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1072	C	N1-C2-O2	5.38	122.13	118.90
54	BA	1905	C	N1-C2-O2	5.38	122.13	118.90
54	BA	2501	C	N1-C2-O2	5.38	122.13	118.90
54	BA	51	G	O4'-C1'-N9	5.38	112.50	108.20
54	BA	1706	C	O4'-C1'-N1	5.38	112.50	108.20
21	AA	980	C	C3'-C2'-C1'	5.38	105.80	101.50
54	BA	203	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	60	G	O4'-C1'-N9	5.37	112.50	108.20
54	BA	275	C	N1-C2-O2	5.37	122.12	118.90
54	BA	1566	A	C4-C5-C6	-5.37	114.31	117.00
21	AA	1240	U	N3-C2-O2	-5.37	118.44	122.20
54	BA	969	G	N7-C8-N9	5.37	115.79	113.10
54	BA	1967	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2127	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	2260	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	714	G	N3-C2-N2	-5.37	116.14	119.90
55	BB	87	U	N3-C2-O2	-5.37	118.44	122.20
21	AA	579	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	622	A	C6-C5-N7	5.37	136.06	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	41	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	331	C	N1-C2-O2	5.37	122.12	118.90
54	BA	1771	C	N1-C2-O2	5.37	122.12	118.90
54	BA	191	A	C4-C5-C6	-5.37	114.32	117.00
14	AO	63	ARG	NE-CZ-NH1	5.37	122.98	120.30
21	AA	1501	C	N1-C2-O2	5.37	122.12	118.90
54	BA	383	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1391	U	O4'-C1'-N1	5.37	112.49	108.20
21	AA	415	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	934	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1226	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1367	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2078	C	N1-C2-O2	5.36	122.12	118.90
54	BA	2476	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	1147	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	1046	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	145	G	N1-C6-O6	-5.36	116.68	119.90
21	AA	837	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	267	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	821	A	C6-C5-N7	5.36	136.05	132.30
54	BA	1862	G	N1-C6-O6	-5.36	116.68	119.90
54	BA	959	A	C1'-O4'-C4'	-5.36	105.61	109.90
55	BB	33	G	N3-C2-N2	-5.36	116.15	119.90
21	AA	370	C	N1-C2-O2	5.36	122.11	118.90
54	BA	863	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2452	C	N3-C4-C5	5.36	124.04	121.90
21	AA	536	C	N1-C2-O2	5.36	122.11	118.90
54	BA	955	U	O4'-C1'-N1	5.36	112.48	108.20
54	BA	1760	C	N1-C2-O2	5.36	122.11	118.90
54	BA	1972	G	N1-C6-O6	-5.36	116.69	119.90
21	AA	111	G	O4'-C1'-N9	5.35	112.48	108.20
23	A2	80	C	N1-C2-O2	5.35	122.11	118.90
54	BA	791	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2046	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	2646	C	O4'-C1'-N1	5.35	112.48	108.20
21	AA	28	A	N1-C6-N6	-5.35	115.39	118.60
21	AA	354	G	N3-C2-N2	-5.35	116.15	119.90
54	BA	1048	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	1230	A	C1'-O4'-C4'	-5.35	105.62	109.90
54	BA	2627	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	2397	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	2632	A	C6-C5-N7	5.35	136.05	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1196	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	1681	G	O4'-C1'-N9	5.35	112.48	108.20
21	AA	1081	A	C4-C5-C6	-5.35	114.33	117.00
26	BD	141	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
54	BA	332	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	601	C	N1-C2-O2	5.35	122.11	118.90
54	BA	860	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2039	U	N3-C2-O2	-5.35	118.46	122.20
54	BA	2342	C	N1-C2-O2	5.35	122.11	118.90
55	BB	36	C	N1-C2-O2	5.35	122.11	118.90
54	BA	1343	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	1105	U	O4'-C1'-N1	5.34	112.48	108.20
54	BA	1331	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	1682	G	C3'-C2'-C1'	5.34	105.78	101.50
54	BA	2602	A	C1'-O4'-C4'	-5.34	105.62	109.90
21	AA	1128	C	N1-C2-O2	5.34	122.11	118.90
54	BA	1689	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2730	C	N1-C2-O2	5.34	122.11	118.90
1	AB	206	ILE	CA-C-N	5.34	128.95	117.20
21	AA	406	G	N3-C2-N2	-5.34	116.16	119.90
21	AA	694	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	968	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	1048	G	N1-C6-O6	-5.34	116.69	119.90
39	BQ	63	ARG	NE-CZ-NH2	-5.34	117.63	120.30
54	BA	2159	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	2232	C	C5'-C4'-O4'	5.34	115.51	109.10
54	BA	2342	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2470	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	1836	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	15	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	992	C	C5'-C4'-O4'	5.34	115.51	109.10
54	BA	1876	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2708	G	P-O3'-C3'	5.34	126.11	119.70
54	BA	2759	G	O4'-C1'-N9	5.34	112.47	108.20
25	BC	47	ARG	CD-NE-CZ	5.34	131.07	123.60
27	BE	61	ARG	NE-CZ-NH2	-5.34	117.63	120.30
54	BA	907	G	O4'-C1'-N9	5.34	112.47	108.20
54	BA	1043	C	N1-C2-O2	5.34	122.10	118.90
21	AA	993	G	N3-C4-C5	-5.33	125.93	128.60
21	AA	182	A	O4'-C1'-N9	5.33	112.47	108.20
21	AA	681	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	1448	C	N3-C2-O2	-5.33	118.17	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1186	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	1192	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	1682	G	O4'-C1'-N9	5.33	112.47	108.20
54	BA	1822	C	C4'-C3'-C2'	-5.33	97.27	102.60
54	BA	1983	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	1335	C	N1-C2-O2	5.33	122.10	118.90
21	AA	443	C	O4'-C1'-N1	5.33	112.46	108.20
34	BL	132	ARG	NE-CZ-NH1	5.33	122.97	120.30
54	BA	783	A	C6-C5-N7	5.33	136.03	132.30
54	BA	1073	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	1382	C	N3-C2-O2	-5.33	118.17	121.90
7	AH	76	ARG	NE-CZ-NH1	5.33	122.96	120.30
21	AA	148	G	O4'-C1'-N9	5.33	112.46	108.20
22	A1	29	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	464	U	C5-C6-N1	-5.33	120.04	122.70
54	BA	1481	U	N3-C2-O2	-5.33	118.47	122.20
54	BA	2074	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	2403	C	N1-C2-O2	5.33	122.09	118.90
54	BA	2897	U	O4'-C1'-N1	5.33	112.46	108.20
21	AA	75	G	N3-C2-N2	-5.32	116.17	119.90
21	AA	251	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	747	A	C6-C5-N7	5.32	136.02	132.30
21	AA	1218	C	N1-C2-O2	5.32	122.09	118.90
21	AA	1534	A	O4'-C1'-N9	5.32	112.46	108.20
54	BA	1041	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	186	C	N1-C2-O2	5.32	122.09	118.90
21	AA	625	U	O4'-C1'-N1	5.32	112.45	108.20
54	BA	2639	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	2755	C	N1-C2-O2	5.32	122.09	118.90
21	AA	254	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	1500	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	794	A	C3'-C2'-C1'	5.32	105.75	101.50
54	BA	1267	U	O4'-C1'-N1	5.32	112.45	108.20
54	BA	2062	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	1359	C	N1-C2-O2	5.31	122.09	118.90
54	BA	689	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	1332	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	1987	A	C6-C5-N7	5.31	136.02	132.30
21	AA	554	A	C4-C5-C6	-5.31	114.34	117.00
21	AA	801	U	O4'-C1'-N1	5.31	112.45	108.20
21	AA	805	C	N3-C2-O2	-5.31	118.18	121.90
21	AA	1301	U	O4'-C1'-N1	5.31	112.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	9	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	1843	C	O4'-C1'-N1	5.31	112.45	108.20
55	BB	26	C	N1-C2-O2	5.31	122.09	118.90
54	BA	2757	A	C4-C5-C6	-5.31	114.34	117.00
21	AA	128	G	N1-C6-O6	-5.31	116.72	119.90
54	BA	1270	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	47	C	N3-C4-C5	5.31	124.02	121.90
21	AA	764	C	N1-C2-O2	5.30	122.08	118.90
21	AA	779	C	N1-C2-O2	5.30	122.08	118.90
23	A2	80	C	P-O3'-C3'	5.30	126.06	119.70
54	BA	336	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	731	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2407	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	2617	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	259	G	N3-C2-N2	-5.30	116.19	119.90
24	A3	62	C	N1-C2-O2	5.30	122.08	118.90
21	AA	1320	C	C1'-O4'-C4'	-5.30	105.66	109.90
40	BR	80	ARG	CD-NE-CZ	5.30	131.02	123.60
54	BA	1856	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2215	C	N1-C2-O2	5.30	122.08	118.90
54	BA	2453	A	O4'-C1'-N9	5.30	112.44	108.20
21	AA	1053	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	1512	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	947	A	C6-C5-N7	5.30	136.01	132.30
54	BA	1554	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1633	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	1906	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	2221	G	C5-C6-N1	5.30	114.15	111.50
54	BA	2853	C	O4'-C1'-N1	5.30	112.44	108.20
55	BB	82	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	590	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	717	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	1103	C	N1-C2-O2	5.30	122.08	118.90
21	AA	934	C	N1-C2-O2	5.30	122.08	118.90
24	A3	1	C	N3-C4-C5	5.30	124.02	121.90
54	BA	915	C	N1-C2-O2	5.30	122.08	118.90
54	BA	1859	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	612	C	N3-C2-O2	-5.29	118.19	121.90
54	BA	2551	C	N1-C2-O2	5.29	122.08	118.90
54	BA	739	A	C4-C5-C6	-5.29	114.35	117.00
21	AA	539	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	817	C	C5'-C4'-O4'	5.29	115.45	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1439	A	C1'-O4'-C4'	-5.29	105.67	109.90
54	BA	2309	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	2344	U	N3-C2-O2	-5.29	118.50	122.20
54	BA	1498	C	N1-C2-O2	5.29	122.07	118.90
21	AA	315	A	O4'-C1'-N9	5.29	112.43	108.20
21	AA	981	U	O4'-C1'-N1	5.29	112.43	108.20
45	BW	19	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
54	BA	1076	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1512	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2058	A	O4'-C1'-N9	5.29	112.43	108.20
54	BA	2274	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	1670	C	O4'-C1'-N1	5.29	112.43	108.20
21	AA	862	C	N3-C2-O2	-5.29	118.20	121.90
21	AA	1032	G	O4'-C1'-N9	5.29	112.43	108.20
21	AA	1403	C	N1-C2-O2	5.29	122.07	118.90
21	AA	1484	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	501	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	837	C	N1-C2-O2	5.29	122.07	118.90
21	AA	509	A	C6-C5-N7	5.28	136.00	132.30
24	A3	63	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2788	C	N1-C2-O2	5.28	122.07	118.90
21	AA	1236	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1934	C	O4'-C1'-N1	5.28	112.43	108.20
25	BC	166	ARG	NE-CZ-NH1	5.28	122.94	120.30
54	BA	2087	G	O4'-C1'-N9	5.28	112.42	108.20
54	BA	1237	A	C1'-O4'-C4'	-5.28	105.68	109.90
54	BA	1797	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	2384	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2542	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	553	A	C5-C6-N1	5.28	120.34	117.70
54	BA	97	C	N1-C2-O2	5.28	122.07	118.90
54	BA	444	C	N1-C2-O2	5.28	122.07	118.90
54	BA	977	G	C5-C6-N1	5.28	114.14	111.50
54	BA	1706	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2368	C	N1-C2-O2	5.28	122.07	118.90
21	AA	122	G	C5-C6-N1	5.28	114.14	111.50
55	BB	57	A	C6-C5-N7	5.28	135.99	132.30
21	AA	705	G	N1-C6-O6	-5.27	116.74	119.90
24	A3	74	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	1544	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	1830	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	1924	C	N1-C2-O2	5.27	122.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2297	A	C4-C5-C6	-5.27	114.36	117.00
55	BB	20	G	C5'-C4'-O4'	5.27	115.43	109.10
55	BB	101	A	C4-C5-C6	-5.27	114.36	117.00
21	AA	670	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	28	A	C6-C5-N7	5.27	135.99	132.30
54	BA	1293	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	1996	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	2491	U	O4'-C1'-N1	5.27	112.42	108.20
3	AD	61	ARG	NE-CZ-NH1	5.27	122.93	120.30
21	AA	68	G	N3-C2-N2	-5.27	116.21	119.90
21	AA	971	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	177	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	366	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	990	A	C4-C5-C6	-5.27	114.37	117.00
28	BF	132	ARG	NE-CZ-NH1	5.27	122.93	120.30
21	AA	665	A	C6-C5-N7	5.26	135.99	132.30
21	AA	722	G	C5-C6-N1	5.26	114.13	111.50
21	AA	1320	C	N1-C2-O2	5.26	122.06	118.90
54	BA	517	C	N1-C2-O2	5.26	122.06	118.90
54	BA	1508	A	C1'-O4'-C4'	-5.26	105.69	109.90
21	AA	347	G	N3-C4-C5	-5.26	125.97	128.60
21	AA	556	C	N1-C2-O2	5.26	122.06	118.90
54	BA	467	G	N3-C4-C5	-5.26	125.97	128.60
21	AA	19	A	C6-C5-N7	5.26	135.98	132.30
21	AA	198	G	C5-C6-N1	5.26	114.13	111.50
21	AA	420	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	519	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	967	C	N1-C2-O2	5.26	122.06	118.90
54	BA	893	C	N1-C2-O2	5.26	122.06	118.90
54	BA	1473	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	2045	C	N1-C2-O2	5.26	122.06	118.90
54	BA	2767	C	N1-C2-O2	5.26	122.06	118.90
21	AA	449	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	1242	G	O4'-C1'-N9	5.26	112.41	108.20
21	AA	1322	C	N1-C2-O2	5.26	122.06	118.90
21	AA	1457	G	C5-C6-N1	5.26	114.13	111.50
54	BA	2034	U	C3'-C2'-C1'	5.26	105.71	101.50
54	BA	2196	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	2473	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	2641	G	N1-C6-O6	-5.26	116.75	119.90
54	BA	241	A	O4'-C1'-N9	5.26	112.41	108.20
54	BA	1029	A	C4-C5-C6	-5.26	114.37	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AL	93	ARG	NH1-CZ-NH2	-5.26	113.62	119.40
21	AA	1381	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	705	A	C4'-C3'-C2'	-5.26	97.34	102.60
54	BA	1558	C	N1-C2-O2	5.26	122.05	118.90
54	BA	2425	A	P-O3'-C3'	5.26	126.01	119.70
21	AA	1518	A	C6-C5-N7	5.25	135.98	132.30
54	BA	181	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	290	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2310	C	N3-C2-O2	-5.25	118.22	121.90
54	BA	2052	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	558	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2738	A	O4'-C1'-N9	5.25	112.40	108.20
22	A1	13	C	N3-C2-O2	-5.25	118.22	121.90
54	BA	125	A	C4-C5-C6	-5.25	114.38	117.00
21	AA	816	A	C4-C5-C6	-5.25	114.38	117.00
21	AA	962	C	N1-C2-O2	5.25	122.05	118.90
21	AA	1085	U	N3-C2-O2	-5.25	118.53	122.20
54	BA	620	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	1305	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1938	A	C4-C5-C6	-5.25	114.38	117.00
21	AA	169	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	575	G	O4'-C1'-N9	5.25	112.40	108.20
21	AA	618	C	C1'-O4'-C4'	-5.25	105.70	109.90
21	AA	637	C	N3-C2-O2	-5.25	118.23	121.90
21	AA	1297	G	N3-C4-C5	-5.25	125.98	128.60
21	AA	1200	C	N1-C2-O2	5.24	122.05	118.90
35	BM	55	ARG	NH1-CZ-NH2	-5.24	113.63	119.40
54	BA	345	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	2242	G	N1-C6-O6	-5.24	116.75	119.90
21	AA	1125	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2291	U	N3-C2-O2	-5.24	118.53	122.20
54	BA	2475	C	N3-C2-O2	-5.24	118.23	121.90
21	AA	1279	G	N3-C4-C5	-5.24	125.98	128.60
22	A1	20	G	N1-C6-O6	-5.24	116.75	119.90
24	A3	65	G	N1-C6-O6	-5.24	116.75	119.90
54	BA	506	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	971	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	1168	G	N1-C6-O6	-5.24	116.75	119.90
54	BA	1680	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2164	C	C3'-C2'-C1'	5.24	105.69	101.50
54	BA	2851	A	C6-C5-N7	5.24	135.97	132.30
54	BA	1400	U	O4'-C1'-N1	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2306	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2645	G	N3-C4-C5	-5.24	125.98	128.60
21	AA	380	G	N1-C6-O6	-5.24	116.76	119.90
21	AA	1275	A	C6-C5-N7	5.24	135.97	132.30
54	BA	2474	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	207	C	N1-C2-O2	5.24	122.04	118.90
21	AA	779	C	C1'-O4'-C4'	-5.24	105.71	109.90
22	A1	38	A	C4-C5-C6	-5.24	114.38	117.00
23	A2	81	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	372	G	C8-N9-C4	-5.24	104.31	106.40
54	BA	2307	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	2289	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	570	G	C8-N9-C4	-5.23	104.31	106.40
54	BA	1219	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	1236	G	N3-C2-N2	-5.23	116.24	119.90
54	BA	2200	C	C3'-C2'-C1'	5.23	105.69	101.50
14	AO	62	ARG	NE-CZ-NH1	5.23	122.92	120.30
21	AA	647	C	O4'-C1'-N1	5.23	112.38	108.20
21	AA	1273	C	O4'-C1'-N1	5.23	112.38	108.20
21	AA	1369	C	N1-C2-O2	5.23	122.04	118.90
54	BA	485	C	O4'-C1'-N1	5.23	112.39	108.20
54	BA	513	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	621	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	643	A	C6-C5-N7	5.23	135.96	132.30
54	BA	1387	A	C4-C5-C6	-5.23	114.38	117.00
54	BA	2517	C	N1-C2-O2	5.23	122.04	118.90
54	BA	2614	A	C6-C5-N7	5.23	135.96	132.30
21	AA	63	C	N1-C2-O2	5.23	122.04	118.90
21	AA	1067	A	C6-C5-N7	5.23	135.96	132.30
22	A1	57	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	50	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	452	G	N3-C4-C5	-5.23	125.98	128.60
21	AA	43	C	O4'-C1'-N1	5.23	112.38	108.20
21	AA	473	U	O4'-C1'-N1	5.23	112.38	108.20
21	AA	1032	G	N3-C2-N2	-5.23	116.24	119.90
24	A3	1	C	N1-C2-O2	5.23	122.04	118.90
54	BA	1625	C	N1-C2-O2	5.23	122.04	118.90
21	AA	275	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	138	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	1030	U	N3-C2-O2	-5.22	118.54	122.20
54	BA	715	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	979	A	C6-C5-N7	5.22	135.96	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1071	G	C3'-C2'-C1'	5.22	105.68	101.50
54	BA	2618	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	2765	A	C4-C5-C6	-5.22	114.39	117.00
55	BB	4	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	924	C	C6-N1-C2	-5.22	118.21	120.30
21	AA	1112	C	N3-C2-O2	-5.22	118.24	121.90
54	BA	1985	C	N3-C2-O2	-5.22	118.25	121.90
21	AA	234	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	334	C	N1-C2-O2	5.22	122.03	118.90
21	AA	1037	C	N1-C2-O2	5.22	122.03	118.90
54	BA	337	C	C4'-C3'-C2'	-5.22	97.38	102.60
54	BA	1198	U	N3-C2-O2	-5.22	118.55	122.20
21	AA	388	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	926	G	O4'-C1'-N9	5.22	112.37	108.20
21	AA	1263	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	527	C	C5'-C4'-C3'	-5.22	107.65	116.00
54	BA	532	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	2138	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	624	C	O4'-C1'-N1	5.22	112.37	108.20
21	AA	940	C	O4'-C1'-N1	5.22	112.37	108.20
54	BA	587	C	N1-C2-O2	5.22	122.03	118.90
54	BA	844	A	C6-C5-N7	5.22	135.95	132.30
54	BA	1638	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1985	C	O4'-C1'-N1	5.22	112.37	108.20
54	BA	2545	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	1251	A	C6-C5-N7	5.21	135.95	132.30
21	AA	1256	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	335	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2103	C	N1-C2-O2	5.21	122.03	118.90
21	AA	212	G	O4'-C1'-N9	5.21	112.37	108.20
21	AA	716	A	C6-C5-N7	5.21	135.95	132.30
54	BA	2776	A	C4-C5-C6	-5.21	114.39	117.00
21	AA	46	G	N1-C6-O6	-5.21	116.77	119.90
21	AA	1336	C	N1-C2-O2	5.21	122.03	118.90
54	BA	1893	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2201	G	N7-C8-N9	5.21	115.71	113.10
54	BA	2543	G	N3-C2-N2	-5.21	116.25	119.90
54	BA	2791	G	N3-C4-C5	-5.21	125.99	128.60
21	AA	1149	C	N1-C2-O2	5.21	122.03	118.90
21	AA	1008	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	259	G	N3-C4-C5	-5.21	126.00	128.60
54	BA	1172	C	O4'-C1'-N1	5.21	112.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2702	G	C5-C6-N1	5.21	114.11	111.50
55	BB	89	U	N3-C2-O2	-5.21	118.55	122.20
21	AA	398	U	O4'-C1'-N1	5.21	112.37	108.20
21	AA	720	C	N3-C2-O2	-5.21	118.26	121.90
24	A3	47	G	C5-C6-N1	5.21	114.10	111.50
54	BA	442	G	O4'-C1'-N9	5.21	112.37	108.20
54	BA	1216	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	1285	A	C4-C5-C6	-5.21	114.40	117.00
55	BB	23	G	N1-C6-O6	-5.21	116.78	119.90
36	BN	64	ARG	NE-CZ-NH1	5.21	122.90	120.30
39	BQ	47	ARG	NE-CZ-NH1	5.21	122.90	120.30
54	BA	2131	U	O4'-C1'-N1	5.21	112.36	108.20
54	BA	2752	C	O4'-C1'-N1	5.21	112.36	108.20
21	AA	72	A	C6-C5-N7	5.20	135.94	132.30
21	AA	352	C	C6-N1-C2	-5.20	118.22	120.30
21	AA	559	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	278	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2380	C	N1-C2-O2	5.20	122.02	118.90
54	BA	2420	C	O4'-C1'-N1	5.20	112.36	108.20
55	BB	27	C	N1-C2-O2	5.20	122.02	118.90
21	AA	1413	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1819	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2681	C	N1-C2-O2	5.20	122.02	118.90
21	AA	469	C	N1-C2-O2	5.20	122.02	118.90
21	AA	685	G	C8-N9-C4	-5.20	104.32	106.40
54	BA	1227	G	C5-C6-N1	5.20	114.10	111.50
54	BA	1851	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2738	A	C6-C5-N7	5.20	135.94	132.30
3	AD	62	ARG	NE-CZ-NH1	5.20	122.90	120.30
21	AA	832	G	C5-C6-N1	5.20	114.10	111.50
50	B1	5	ARG	NE-CZ-NH1	5.20	122.90	120.30
54	BA	610	C	N3-C2-O2	-5.20	118.26	121.90
54	BA	1110	G	C5-C6-N1	5.20	114.10	111.50
54	BA	2403	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	922	C	N1-C2-O2	5.20	122.02	118.90
54	BA	985	C	N1-C2-O2	5.20	122.02	118.90
54	BA	2264	C	O4'-C1'-N1	5.20	112.36	108.20
13	AN	9	ARG	NE-CZ-NH1	5.20	122.90	120.30
21	AA	778	G	N3-C2-N2	-5.20	116.26	119.90
14	AO	16	ARG	NE-CZ-NH2	-5.19	117.70	120.30
21	AA	1301	U	N3-C2-O2	-5.19	118.56	122.20
21	AA	1433	A	C6-C5-N7	5.19	135.94	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	19	G	N3-C2-N2	-5.19	116.26	119.90
39	BQ	69	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
54	BA	232	G	N1-C6-O6	-5.19	116.78	119.90
54	BA	249	C	N3-C4-C5	5.19	123.98	121.90
54	BA	2275	C	N1-C2-O2	5.19	122.02	118.90
54	BA	194	G	N1-C6-O6	-5.19	116.78	119.90
54	BA	1298	C	N1-C2-O2	5.19	122.02	118.90
54	BA	1703	G	N1-C6-O6	-5.19	116.78	119.90
54	BA	2427	C	N1-C2-O2	5.19	122.02	118.90
55	BB	19	C	O4'-C1'-N1	5.19	112.35	108.20
10	AK	68	ARG	NE-CZ-NH1	5.19	122.89	120.30
21	AA	818	G	N3-C4-C5	-5.19	126.00	128.60
54	BA	48	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	1929	G	C1'-O4'-C4'	-5.19	105.75	109.90
54	BA	2260	C	O4'-C1'-N1	5.19	112.35	108.20
55	BB	42	C	O4'-C1'-N1	5.19	112.35	108.20
21	AA	1162	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	288	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	477	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	991	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1823	G	C5'-C4'-O4'	5.19	115.33	109.10
21	AA	381	C	C5'-C4'-C3'	-5.19	107.70	116.00
21	AA	5	U	N3-C2-O2	-5.19	118.57	122.20
21	AA	733	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	2577	A	C4-C5-C6	-5.19	114.41	117.00
21	AA	341	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	15	G	O4'-C1'-N9	5.18	112.35	108.20
54	BA	931	U	N3-C2-O2	-5.18	118.57	122.20
54	BA	2037	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2084	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	2696	U	O4'-C1'-N1	5.18	112.35	108.20
21	AA	508	U	N3-C2-O2	-5.18	118.57	122.20
21	AA	806	C	N3-C2-O2	-5.18	118.27	121.90
21	AA	1448	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	141	G	N3-C4-C5	-5.18	126.01	128.60
21	AA	222	C	N3-C2-O2	-5.18	118.27	121.90
21	AA	1135	U	O4'-C1'-N1	5.18	112.34	108.20
21	AA	1370	G	O4'-C1'-N9	5.18	112.34	108.20
21	AA	1377	A	C6-C5-N7	5.18	135.93	132.30
54	BA	842	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	905	A	C6-C5-N7	5.18	135.93	132.30
54	BA	2254	C	N1-C2-O2	5.18	122.01	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AS	2	ARG	CD-NE-CZ	5.18	130.85	123.60
54	BA	1592	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	2893	A	C6-C5-N7	5.18	135.92	132.30
21	AA	1402	C	N3-C2-O2	-5.18	118.28	121.90
54	BA	346	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	686	U	C5'-C4'-C3'	-5.18	107.72	116.00
54	BA	707	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	1048	A	C5'-C4'-O4'	5.18	115.31	109.10
54	BA	1989	G	N3-C2-N2	-5.18	116.28	119.90
54	BA	2332	C	C3'-C2'-C1'	5.18	105.64	101.50
54	BA	2619	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1031	C	N1-C2-O2	5.17	122.00	118.90
21	AA	715	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	1095	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	2296	U	O4'-C1'-N1	5.17	112.34	108.20
11	AL	30	ARG	NE-CZ-NH1	5.17	122.89	120.30
21	AA	152	A	O4'-C1'-N9	5.17	112.34	108.20
21	AA	1238	A	C6-C5-N7	5.17	135.92	132.30
38	BP	112	ARG	NE-CZ-NH1	5.17	122.89	120.30
54	BA	463	G	O4'-C1'-N9	5.17	112.34	108.20
54	BA	598	U	O4'-C1'-N1	5.17	112.34	108.20
54	BA	2504	U	O4'-C1'-N1	5.17	112.34	108.20
17	AR	72	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
21	AA	822	U	O4'-C1'-N1	5.17	112.33	108.20
21	AA	985	C	N1-C2-O2	5.17	122.00	118.90
21	AA	1010	U	O4'-C1'-N1	5.17	112.33	108.20
21	AA	1293	C	N1-C2-O2	5.17	122.00	118.90
54	BA	636	G	N1-C6-O6	-5.17	116.80	119.90
11	AL	85	ARG	NE-CZ-NH1	5.17	122.88	120.30
21	AA	151	A	C6-C5-N7	5.17	135.92	132.30
54	BA	846	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	1280	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	2162	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	2167	U	O4'-C1'-N1	5.17	112.33	108.20
54	BA	2330	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	49	U	C5-C6-N1	-5.17	120.12	122.70
24	A3	64	G	C3'-C2'-C1'	5.17	105.63	101.50
54	BA	475	C	C5'-C4'-O4'	5.17	115.30	109.10
54	BA	1125	G	C3'-C2'-C1'	5.17	105.63	101.50
54	BA	2258	C	N1-C2-O2	5.17	122.00	118.90
54	BA	2576	G	N3-C4-C5	-5.17	126.02	128.60
21	AA	383	A	C6-C5-N7	5.16	135.91	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	778	G	N3-C4-C5	-5.16	126.02	128.60
54	BA	69	C	N1-C2-O2	5.16	122.00	118.90
54	BA	315	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	2638	G	N1-C6-O6	-5.16	116.80	119.90
10	AK	97	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BA	669	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	698	C	N3-C4-C5	5.16	123.96	121.90
54	BA	845	A	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	2095	A	O4'-C1'-N9	5.16	112.33	108.20
54	BA	2845	U	O4'-C1'-N1	5.16	112.33	108.20
55	BB	92	C	C3'-C2'-C1'	5.16	105.63	101.50
54	BA	662	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	833	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1778	U	C5'-C4'-O4'	5.16	115.29	109.10
55	BB	97	C	N1-C2-O2	5.16	122.00	118.90
21	AA	909	A	O4'-C1'-N9	5.16	112.33	108.20
54	BA	1414	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	359	G	N1-C6-O6	-5.16	116.81	119.90
21	AA	448	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	814	A	C4-C5-C6	-5.16	114.42	117.00
24	A3	68	C	N1-C2-O2	5.16	121.99	118.90
54	BA	211	C	O4'-C1'-N1	5.16	112.32	108.20
54	BA	1365	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	123	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	459	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	964	C	N1-C2-O2	5.15	121.99	118.90
54	BA	1603	A	C4-C5-C6	-5.15	114.42	117.00
21	AA	30	U	O4'-C1'-N1	5.15	112.32	108.20
21	AA	54	C	N1-C2-O2	5.15	121.99	118.90
21	AA	1443	C	N1-C2-O2	5.15	121.99	118.90
42	BT	3	ARG	NE-CZ-NH1	5.15	122.88	120.30
54	BA	34	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	484	C	N1-C2-O2	5.15	121.99	118.90
21	AA	419	C	N1-C2-O2	5.15	121.99	118.90
21	AA	821	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	868	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	1037	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1764	C	C5'-C4'-O4'	5.15	115.28	109.10
54	BA	2269	G	C5'-C4'-O4'	5.15	115.28	109.10
54	BA	2428	G	O4'-C4'-C3'	5.15	110.22	106.10
54	BA	2581	G	C5-C6-N1	5.15	114.08	111.50
54	BA	2778	A	C4-C5-C6	-5.15	114.42	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2828	G	C5-C6-N1	5.15	114.08	111.50
54	BA	959	A	C6-C5-N7	5.15	135.90	132.30
21	AA	512	U	O4'-C1'-N1	5.15	112.32	108.20
21	AA	1379	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	933	A	C4-C5-C6	-5.15	114.43	117.00
54	BA	1117	C	N1-C2-O2	5.15	121.99	118.90
21	AA	90	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	852	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1350	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	1650	A	C6-C5-N7	5.15	135.90	132.30
54	BA	1765	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	1788	C	O4'-C1'-N1	5.15	112.32	108.20
21	AA	1053	G	C3'-C2'-C1'	5.14	105.62	101.50
21	AA	1160	G	N3-C2-N2	-5.14	116.30	119.90
54	BA	253	C	O4'-C1'-N1	5.14	112.32	108.20
21	AA	1397	C	N1-C2-O2	5.14	121.98	118.90
54	BA	1828	G	C5-C6-N1	5.14	114.07	111.50
54	BA	2607	G	N1-C6-O6	-5.14	116.81	119.90
21	AA	363	A	C6-C5-N7	5.14	135.90	132.30
54	BA	800	A	C6-C5-N7	5.14	135.90	132.30
54	BA	1646	C	O4'-C1'-N1	5.14	112.31	108.20
21	AA	130	A	C6-C5-N7	5.14	135.90	132.30
21	AA	735	C	N1-C2-O2	5.14	121.98	118.90
21	AA	813	U	O4'-C1'-N1	5.14	112.31	108.20
21	AA	1137	C	N1-C2-O2	5.14	121.98	118.90
34	BL	21	ARG	NE-CZ-NH1	-5.14	117.73	120.30
54	BA	31	C	N1-C2-O2	5.14	121.98	118.90
54	BA	537	G	N7-C8-N9	5.14	115.67	113.10
54	BA	301	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	1051	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	1363	C	N1-C2-O2	5.14	121.98	118.90
54	BA	2566	A	C4-C5-C6	-5.14	114.43	117.00
21	AA	1333	A	C6-C5-N7	5.14	135.90	132.30
54	BA	114	U	O4'-C4'-C3'	5.14	110.21	106.10
54	BA	336	C	N1-C2-O2	5.14	121.98	118.90
54	BA	634	C	N1-C2-O2	5.14	121.98	118.90
54	BA	2106	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2652	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	330	A	O4'-C1'-N9	5.13	112.31	108.20
54	BA	2331	G	C3'-C2'-C1'	5.13	105.61	101.50
54	BA	2717	C	C5'-C4'-O4'	5.13	115.26	109.10
54	BA	33	C	N3-C2-O2	-5.13	118.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	388	G	N1-C6-O6	-5.13	116.82	119.90
20	AU	16	ARG	NE-CZ-NH1	5.13	122.87	120.30
21	AA	935	A	C4-C5-C6	-5.13	114.43	117.00
21	AA	1272	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	340	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	1911	U	O4'-C1'-N1	5.13	112.31	108.20
54	BA	2824	C	O4'-C1'-N1	5.13	112.31	108.20
21	AA	102	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	418	C	N1-C2-O2	5.13	121.98	118.90
54	BA	1841	U	O4'-C1'-N1	5.13	112.30	108.20
21	AA	753	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	243	U	O4'-C1'-N1	5.13	112.30	108.20
54	BA	1014	A	C6-C5-N7	5.13	135.89	132.30
54	BA	1509	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	156	C	N1-C2-O2	5.13	121.98	118.90
21	AA	1254	A	C6-C5-N7	5.13	135.89	132.30
21	AA	1287	A	C6-C5-N7	5.13	135.89	132.30
54	BA	502	A	C6-C5-N7	5.13	135.89	132.30
54	BA	774	G	C5-C6-N1	5.13	114.06	111.50
54	BA	1742	U	O4'-C1'-N1	5.13	112.30	108.20
54	BA	2400	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1092	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	2642	G	C4'-C3'-C2'	-5.12	97.47	102.60
27	BE	102	ARG	NE-CZ-NH2	-5.12	117.74	120.30
54	BA	1741	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1975	G	C5-C6-N1	5.12	114.06	111.50
21	AA	708	C	O4'-C1'-N1	5.12	112.30	108.20
22	A1	17	U	N3-C2-O2	-5.12	118.61	122.20
54	BA	17	G	O4'-C1'-N9	5.12	112.30	108.20
54	BA	765	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1172	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1699	G	N3-C4-C5	-5.12	126.04	128.60
54	BA	2428	G	C5-C6-N1	5.12	114.06	111.50
21	AA	1211	U	N3-C2-O2	-5.12	118.62	122.20
25	BC	51	ARG	NE-CZ-NH2	-5.12	117.74	120.30
54	BA	116	C	N1-C2-O2	5.12	121.97	118.90
21	AA	302	G	N3-C4-C5	-5.12	126.04	128.60
22	A1	59	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	805	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1884	G	O4'-C1'-N9	5.12	112.29	108.20
54	BA	2873	A	C4-C5-C6	-5.12	114.44	117.00
55	BB	79	G	N3-C4-C5	-5.12	126.04	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	817	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	1086	A	O4'-C1'-N9	5.12	112.29	108.20
21	AA	304	U	O4'-C1'-N1	5.12	112.29	108.20
21	AA	651	C	N1-C2-O2	5.12	121.97	118.90
54	BA	686	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	809	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	836	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1902	C	O4'-C1'-N1	5.12	112.29	108.20
21	AA	203	G	N1-C6-O6	-5.11	116.83	119.90
21	AA	915	A	C4-C5-C6	-5.11	114.44	117.00
21	AA	1483	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	854	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	996	A	C6-C5-N7	5.11	135.88	132.30
54	BA	2065	C	N1-C2-O2	5.11	121.97	118.90
54	BA	2170	A	C6-C5-N7	5.11	135.88	132.30
21	AA	912	C	N1-C2-O2	5.11	121.97	118.90
54	BA	1048	A	O4'-C1'-N9	5.11	112.29	108.20
21	AA	1040	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	1005	C	O4'-C1'-N1	5.11	112.29	108.20
55	BB	48	U	C5'-C4'-O4'	5.11	115.23	109.10
21	AA	532	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	99	U	C5'-C4'-O4'	5.11	115.23	109.10
54	BA	597	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	1607	C	O4'-C1'-N1	5.11	112.29	108.20
21	AA	611	C	N1-C2-O2	5.11	121.97	118.90
24	A3	35	C	N1-C2-O2	5.11	121.96	118.90
45	BW	76	ARG	NE-CZ-NH2	-5.11	117.75	120.30
54	BA	878	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	1025	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	2749	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	2850	A	C4-C5-C6	-5.11	114.45	117.00
21	AA	1069	C	N1-C2-O2	5.10	121.96	118.90
54	BA	1084	A	C6-C5-N7	5.10	135.87	132.30
54	BA	1230	A	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1470	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	1804	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2305	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	2811	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	2826	A	C5'-C4'-O4'	5.10	115.22	109.10
54	BA	2852	G	N3-C2-N2	-5.10	116.33	119.90
54	BA	2711	A	C6-C5-N7	5.10	135.87	132.30
13	AN	69	ARG	NE-CZ-NH1	5.10	122.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	388	G	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1237	C	N3-C4-C5	5.10	123.94	121.90
54	BA	1373	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2445	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	2890	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	993	G	C5-C6-N1	5.10	114.05	111.50
54	BA	1076	C	N1-C2-O2	5.10	121.96	118.90
54	BA	2692	G	C5-C6-N1	5.10	114.05	111.50
21	AA	193	C	N1-C2-O2	5.09	121.96	118.90
21	AA	796	C	N1-C2-O2	5.09	121.96	118.90
21	AA	917	G	C8-N9-C4	-5.09	104.36	106.40
21	AA	930	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	431	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1088	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	2131	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	1142	G	N3-C4-C5	-5.09	126.06	128.60
23	A2	91	A	C1'-O4'-C4'	-5.09	105.83	109.90
54	BA	57	C	N1-C2-O2	5.09	121.95	118.90
54	BA	641	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	1240	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	1341	G	O4'-C1'-N9	5.09	112.27	108.20
54	BA	2465	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2512	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	549	G	C8-N9-C4	-5.09	104.36	106.40
54	BA	957	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1079	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2386	A	C6-C5-N7	5.09	135.86	132.30
21	AA	704	A	C5-C6-N6	5.09	127.77	123.70
21	AA	810	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	20	C	N1-C2-O2	5.09	121.95	118.90
54	BA	1038	G	O4'-C1'-N9	5.09	112.27	108.20
54	BA	1510	G	O4'-C1'-N9	5.09	112.27	108.20
54	BA	2081	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2699	C	N1-C2-O2	5.09	121.95	118.90
21	AA	66	A	C5'-C4'-C3'	-5.08	107.86	116.00
21	AA	856	C	N1-C2-O2	5.08	121.95	118.90
54	BA	623	C	C5'-C4'-O4'	5.08	115.20	109.10
21	AA	198	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	416	U	O4'-C1'-N1	5.08	112.27	108.20
54	BA	748	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	872	U	O4'-C1'-N1	5.08	112.27	108.20
54	BA	1111	A	O4'-C1'-N9	5.08	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2755	C	O4'-C1'-N1	5.08	112.27	108.20
55	BB	26	C	N3-C4-C5	5.08	123.93	121.90
21	AA	219	U	N3-C2-O2	-5.08	118.64	122.20
21	AA	531	U	N3-C2-O2	-5.08	118.64	122.20
21	AA	532	A	O4'-C1'-N9	5.08	112.27	108.20
21	AA	1095	U	O4'-C1'-N1	5.08	112.27	108.20
21	AA	1342	C	N1-C2-O2	5.08	121.95	118.90
21	AA	1395	C	N1-C2-O2	5.08	121.95	118.90
30	BH	27	ARG	NE-CZ-NH1	5.08	122.84	120.30
54	BA	272	A	C1'-O4'-C4'	-5.08	105.83	109.90
54	BA	454	A	C6-C5-N7	5.08	135.86	132.30
54	BA	796	C	N1-C2-O2	5.08	121.95	118.90
54	BA	855	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2558	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2576	G	N3-C2-N2	-5.08	116.34	119.90
54	BA	2679	A	C6-C5-N7	5.08	135.86	132.30
55	BB	108	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	590	U	C5-C6-N1	-5.08	120.16	122.70
54	BA	462	C	N1-C2-O2	5.08	121.95	118.90
21	AA	112	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	96	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	620	G	C5-C6-N1	5.08	114.04	111.50
54	BA	2649	C	N1-C2-O2	5.08	121.95	118.90
54	BA	142	A	C6-C5-N7	5.08	135.85	132.30
54	BA	2810	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	860	A	N1-C6-N6	-5.08	115.55	118.60
25	BC	155	ARG	NE-CZ-NH2	-5.08	117.76	120.30
54	BA	669	G	C5-C6-N1	5.08	114.04	111.50
54	BA	989	G	P-O3'-C3'	5.08	125.79	119.70
54	BA	1253	A	O4'-C1'-N9	5.08	112.26	108.20
54	BA	2848	G	N1-C6-O6	-5.08	116.86	119.90
54	BA	2871	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	510	C	N1-C2-O2	5.07	121.94	118.90
54	BA	608	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	949	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1112	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1272	A	O4'-C1'-N9	5.07	112.26	108.20
54	BA	2751	G	N3-C2-N2	-5.07	116.35	119.90
21	AA	48	C	N1-C2-O2	5.07	121.94	118.90
21	AA	105	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1700	A	C4-C5-C6	-5.07	114.46	117.00
3	AD	145	ARG	NE-CZ-NH1	5.07	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	34	C	N1-C2-O2	5.07	121.94	118.90
21	AA	416	G	C5-C6-N1	5.07	114.03	111.50
54	BA	1064	C	N3-C2-O2	-5.07	118.35	121.90
52	B3	12	ARG	NE-CZ-NH1	5.07	122.83	120.30
54	BA	1871	A	C2-N3-C4	5.07	113.14	110.60
21	AA	932	C	C3'-C2'-C1'	5.07	105.55	101.50
54	BA	2579	C	N1-C2-O2	5.07	121.94	118.90
21	AA	956	U	O4'-C1'-N1	5.07	112.25	108.20
21	AA	1352	C	N1-C2-O2	5.07	121.94	118.90
54	BA	242	G	C5-C6-N1	5.07	114.03	111.50
54	BA	752	A	O4'-C1'-N9	5.07	112.25	108.20
54	BA	1895	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1925	C	N1-C2-O2	5.07	121.94	118.90
21	AA	331	G	N1-C6-O6	-5.06	116.86	119.90
2	AC	135	ARG	NE-CZ-NH1	5.06	122.83	120.30
21	AA	1049	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	1524	C	N1-C2-O2	5.06	121.94	118.90
54	BA	678	C	N1-C2-O2	5.06	121.94	118.90
54	BA	1406	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1922	G	C4'-C3'-C2'	-5.06	97.54	102.60
54	BA	790	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	979	A	C1'-O4'-C4'	-5.06	105.85	109.90
54	BA	2116	G	C3'-C2'-C1'	5.06	105.55	101.50
21	AA	953	G	N1-C6-O6	-5.06	116.86	119.90
22	A1	53	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	320	A	C6-C5-N7	5.06	135.84	132.30
54	BA	470	A	O4'-C1'-N9	5.06	112.25	108.20
54	BA	1892	C	O4'-C1'-N1	5.06	112.25	108.20
24	A3	76	C	N1-C2-O2	5.06	121.94	118.90
54	BA	401	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	906	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2160	C	N1-C2-O2	5.06	121.93	118.90
21	AA	799	G	N1-C6-O6	-5.06	116.87	119.90
54	BA	546	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	2616	C	N1-C2-O2	5.06	121.93	118.90
54	BA	2785	C	N1-C2-O2	5.06	121.93	118.90
21	AA	263	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	223	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	232	G	O4'-C1'-N9	5.05	112.24	108.20
54	BA	623	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	1667	G	C5-C6-N1	5.05	114.03	111.50
54	BA	2267	A	C4-C5-C6	-5.05	114.47	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2683	C	N3-C4-C5	5.05	123.92	121.90
54	BA	2518	A	C4-C5-C6	-5.05	114.47	117.00
55	BB	113	C	O4'-C1'-N1	5.05	112.24	108.20
55	BB	117	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	686	U	N1-C2-N3	5.05	117.93	114.90
21	AA	880	C	N1-C2-O2	5.05	121.93	118.90
21	AA	890	G	C5-C6-N1	5.05	114.03	111.50
23	A2	80	C	C1'-O4'-C4'	-5.05	105.86	109.90
25	BC	132	ARG	NE-CZ-NH1	5.05	122.83	120.30
54	BA	845	A	C6-C5-N7	5.05	135.84	132.30
54	BA	1077	A	C6-C5-N7	5.05	135.84	132.30
54	BA	2286	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	2902	C	O4'-C1'-N1	5.05	112.24	108.20
55	BB	96	G	O4'-C1'-N9	5.05	112.24	108.20
21	AA	1015	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	929	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	568	U	N3-C2-O2	-5.05	118.67	122.20
54	BA	1480	C	O4'-C1'-N1	5.05	112.24	108.20
21	AA	423	G	O4'-C1'-N9	5.05	112.24	108.20
21	AA	929	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	1532	U	N1-C1'-C2'	-5.05	106.45	112.00
54	BA	82	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	1149	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1177	G	O4'-C1'-N9	5.05	112.24	108.20
54	BA	2418	A	C6-C5-N7	5.05	135.83	132.30
21	AA	920	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	1632	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	1945	G	C3'-C2'-C1'	5.04	105.54	101.50
54	BA	2150	C	N1-C2-O2	5.04	121.93	118.90
21	AA	378	G	C1'-O4'-C4'	-5.04	105.86	109.90
54	BA	1233	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2626	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	164	G	O4'-C4'-C3'	5.04	110.13	106.10
21	AA	364	A	C6-C5-N7	5.04	135.83	132.30
21	AA	379	C	N1-C2-O2	5.04	121.92	118.90
21	AA	886	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	1642	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	1686	C	N1-C2-O2	5.04	121.92	118.90
54	BA	1843	C	N1-C2-O2	5.04	121.92	118.90
54	BA	2650	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	98	G	N3-C2-N2	-5.04	116.37	119.90
54	BA	2111	U	O4'-C1'-N1	5.04	112.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2126	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	2370	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2445	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2807	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	2852	G	N1-C6-O6	-5.04	116.88	119.90
21	AA	319	G	N1-C6-O6	-5.04	116.88	119.90
21	AA	1091	U	N3-C2-O2	-5.04	118.67	122.20
53	B4	24	ARG	NE-CZ-NH1	5.04	122.82	120.30
54	BA	932	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	1907	G	N1-C6-O6	-5.04	116.88	119.90
21	AA	951	G	C8-N9-C4	-5.04	104.39	106.40
21	AA	28	A	C4-C5-C6	-5.03	114.48	117.00
21	AA	73	C	N1-C2-O2	5.03	121.92	118.90
54	BA	1398	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2113	U	O4'-C1'-N1	5.03	112.23	108.20
54	BA	1795	C	N1-C2-O2	5.03	121.92	118.90
24	A3	39	A	C4-C5-C6	-5.03	114.48	117.00
40	BR	80	ARG	NE-CZ-NH2	-5.03	117.78	120.30
54	BA	240	C	N3-C4-C5	5.03	123.91	121.90
54	BA	972	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1519	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	1682	G	O4'-C4'-C3'	5.03	110.12	106.10
54	BA	2178	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2554	U	C5'-C4'-C3'	-5.03	107.95	116.00
54	BA	2792	A	C6-C5-N7	5.03	135.82	132.30
21	AA	1161	C	N1-C2-O2	5.03	121.92	118.90
24	A3	50	G	N1-C6-O6	-5.03	116.88	119.90
36	BN	86	ARG	NE-CZ-NH1	5.03	122.81	120.30
54	BA	268	C	N3-C2-O2	-5.03	118.38	121.90
54	BA	447	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	1438	U	N1-C1'-C2'	5.03	120.54	114.00
24	A3	20	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	1141	U	C3'-C2'-C1'	5.03	105.52	101.50
54	BA	1288	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	2858	C	C1'-O4'-C4'	-5.03	105.88	109.90
55	BB	63	C	O4'-C1'-N1	5.03	112.22	108.20
21	AA	818	G	C3'-C2'-C1'	5.03	105.52	101.50
22	A1	73	A	C6-C5-N7	5.03	135.82	132.30
54	BA	389	G	N3-C2-N2	-5.03	116.38	119.90
54	BA	1452	G	N1-C6-O6	-5.03	116.89	119.90
54	BA	1695	G	N3-C4-C5	-5.03	126.09	128.60
54	BA	1974	C	C3'-C2'-C1'	5.03	105.52	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2351	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	1421	G	N1-C6-O6	-5.02	116.89	119.90
23	A2	85	G	N3-C2-N2	-5.02	116.38	119.90
54	BA	598	U	C5-C6-N1	-5.02	120.19	122.70
54	BA	665	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1045	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2243	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	894	G	C5-C6-N1	5.02	114.01	111.50
21	AA	934	C	C1'-O4'-C4'	-5.02	105.88	109.90
26	BD	124	ARG	NE-CZ-NH2	-5.02	117.79	120.30
54	BA	291	G	C5'-C4'-C3'	-5.02	107.96	116.00
54	BA	455	C	N3-C2-O2	-5.02	118.38	121.90
54	BA	1236	G	O4'-C4'-C3'	5.02	110.12	106.10
54	BA	2506	U	C1'-O4'-C4'	-5.02	105.88	109.90
54	BA	285	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2472	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	136	C	N1-C2-O2	5.02	121.91	118.90
21	AA	1278	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	130	C	N1-C2-O2	5.02	121.91	118.90
54	BA	373	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	479	A	C6-C5-N7	5.02	135.81	132.30
54	BA	682	G	N3-C2-N2	-5.02	116.39	119.90
54	BA	869	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	57	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	599	A	O4'-C1'-N9	5.02	112.22	108.20
54	BA	1545	A	C6-C5-N7	5.02	135.81	132.30
54	BA	1664	A	N1-C6-N6	-5.02	115.59	118.60
54	BA	1969	A	C4-C5-C6	-5.02	114.49	117.00
6	AG	94	ARG	CD-NE-CZ	5.02	130.62	123.60
54	BA	851	C	N1-C2-O2	5.02	121.91	118.90
54	BA	865	C	N3-C2-O2	-5.02	118.39	121.90
21	AA	689	C	O4'-C1'-N1	5.01	112.21	108.20
22	A1	52	G	N1-C6-O6	-5.01	116.89	119.90
37	BO	13	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	492	A	C4'-C3'-C2'	-5.01	97.58	102.60
54	BA	1808	A	C4-C5-C6	-5.01	114.49	117.00
54	BA	1818	U	N3-C2-O2	-5.01	118.69	122.20
22	A1	30	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1682	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	2697	G	O4'-C1'-N9	5.01	112.21	108.20
21	AA	648	A	C6-C5-N7	5.01	135.81	132.30
21	AA	1400	C	N3-C4-C5	5.01	123.90	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	212	G	N3-C2-N2	-5.01	116.39	119.90
54	BA	435	C	O4'-C1'-N1	5.01	112.21	108.20
21	AA	335	C	N1-C2-O2	5.01	121.91	118.90
21	AA	1445	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	335	C	O4'-C1'-N1	5.01	112.21	108.20
54	BA	620	G	N1-C2-N2	5.01	120.71	116.20
54	BA	1357	C	N1-C2-O2	5.01	121.91	118.90
21	AA	543	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	452	G	C8-N9-C4	-5.01	104.40	106.40
22	A1	58	A	C4-C5-C6	-5.01	114.50	117.00
22	A1	59	U	O4'-C1'-N1	5.01	112.20	108.20
34	BL	60	ARG	CD-NE-CZ	5.01	130.61	123.60
54	BA	974	G	N3-C4-C5	-5.01	126.10	128.60
54	BA	994	C	O4'-C1'-N1	5.01	112.20	108.20
54	BA	1979	U	C4'-C3'-C2'	-5.01	97.59	102.60
54	BA	2238	G	N3-C4-C5	-5.01	126.10	128.60
54	BA	2238	G	N3-C2-N2	-5.01	116.39	119.90
54	BA	2338	C	O4'-C1'-N1	5.01	112.20	108.20
21	AA	330	C	N3-C4-C5	5.00	123.90	121.90
54	BA	2499	C	N3-C2-O2	-5.00	118.40	121.90
21	AA	941	G	N7-C8-N9	5.00	115.60	113.10
21	AA	1258	G	N3-C2-N2	-5.00	116.40	119.90
54	BA	1534	U	N3-C2-O2	-5.00	118.70	122.20
54	BA	1579	A	C4-C5-C6	-5.00	114.50	117.00
21	AA	960	U	C3'-C2'-C1'	5.00	105.50	101.50
54	BA	1583	A	C3'-C2'-C1'	5.00	105.50	101.50
54	BA	2286	G	C3'-C2'-C1'	5.00	105.50	101.50
54	BA	2338	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (1150) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	15	G	Sidechain
22	A1	20	G	Sidechain
22	A1	25	C	Sidechain
22	A1	28	C	Sidechain
22	A1	31	C	Sidechain
22	A1	44	G	Sidechain
22	A1	59	U	Sidechain
22	A1	6	A	Sidechain
22	A1	61	C	Sidechain

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Mol	Chain	Res	Type	Group
22	A1	9	A	Sidechain
23	A2	80	C	Sidechain
23	A2	83	U	Sidechain
23	A2	88	U	Sidechain
23	A2	89	U	Sidechain
24	A3	1	C	Sidechain
24	A3	10	G	Sidechain
24	A3	11	A	Sidechain
24	A3	19	G	Sidechain
24	A3	20	G	Sidechain
24	A3	28	U	Sidechain
24	A3	3	C	Sidechain
24	A3	30	G	Sidechain
24	A3	32	G	Sidechain
24	A3	5	G	Sidechain
24	A3	57	C	Sidechain
24	A3	60	A	Sidechain
24	A3	61	U	Sidechain
24	A3	65	G	Sidechain
24	A3	68	C	Sidechain
24	A3	69	C	Sidechain
24	A3	7	G	Sidechain
24	A3	75	C	Sidechain
24	A3	9	G	Sidechain
21	AA	1000	A	Sidechain
21	AA	1002	G	Sidechain
21	AA	1003	G	Sidechain
21	AA	1013	G	Sidechain
21	AA	1016	A	Sidechain
21	AA	1020	G	Sidechain
21	AA	1027	C	Sidechain
21	AA	1028	C	Sidechain
21	AA	1035	A	Sidechain
21	AA	1044	A	Sidechain
21	AA	1046	A	Sidechain
21	AA	1049	U	Sidechain
21	AA	1050	G	Sidechain
21	AA	1055	A	Sidechain
21	AA	1060	U	Sidechain
21	AA	1061	G	Sidechain
21	AA	1075	U	Sidechain
21	AA	1078	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1084	G	Sidechain
21	AA	1090	U	Sidechain
21	AA	1092	A	Sidechain
21	AA	1094	G	Sidechain
21	AA	1095	U	Sidechain
21	AA	11	G	Sidechain
21	AA	1101	A	Sidechain
21	AA	111	G	Sidechain
21	AA	1110	A	Sidechain
21	AA	1111	A	Sidechain
21	AA	1112	C	Sidechain
21	AA	1121	U	Sidechain
21	AA	1123	U	Sidechain
21	AA	113	G	Sidechain
21	AA	1130	A	Sidechain
21	AA	1131	G	Sidechain
21	AA	1132	C	Sidechain
21	AA	1144	G	Sidechain
21	AA	1145	A	Sidechain
21	AA	115	G	Sidechain
21	AA	1155	A	Sidechain
21	AA	1158	C	Sidechain
21	AA	1163	A	Sidechain
21	AA	1166	G	Sidechain
21	AA	117	G	Sidechain
21	AA	1178	G	Sidechain
21	AA	1181	G	Sidechain
21	AA	1187	G	Sidechain
21	AA	1194	U	Sidechain
21	AA	1198	G	Sidechain
21	AA	1208	C	Sidechain
21	AA	1214	C	Sidechain
21	AA	1221	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1223	C	Sidechain
21	AA	1226	C	Sidechain
21	AA	1228	C	Sidechain
21	AA	123	U	Sidechain
21	AA	1233	G	Sidechain
21	AA	1234	C	Sidechain
21	AA	1240	U	Sidechain
21	AA	1241	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1243	C	Sidechain
21	AA	1244	G	Sidechain
21	AA	1247	U	Sidechain
21	AA	1250	A	Sidechain
21	AA	1252	A	Sidechain
21	AA	1263	C	Sidechain
21	AA	1264	U	Sidechain
21	AA	1266	G	Sidechain
21	AA	1270	G	Sidechain
21	AA	1276	G	Sidechain
21	AA	1278	G	Sidechain
21	AA	128	G	Sidechain
21	AA	1281	C	Sidechain
21	AA	1283	U	Sidechain
21	AA	1294	G	Sidechain
21	AA	1298	U	Sidechain
21	AA	1301	U	Sidechain
21	AA	1303	C	Sidechain
21	AA	1305	G	Sidechain
21	AA	1312	G	Sidechain
21	AA	1313	U	Sidechain
21	AA	1316	G	Sidechain
21	AA	1320	C	Sidechain
21	AA	1331	G	Sidechain
21	AA	1332	A	Sidechain
21	AA	1334	G	Sidechain
21	AA	1340	A	Sidechain
21	AA	1345	U	Sidechain
21	AA	1356	G	Sidechain
21	AA	1363	A	Sidechain
21	AA	1364	U	Sidechain
21	AA	137	U	Sidechain
21	AA	1370	G	Sidechain
21	AA	1374	A	Sidechain
21	AA	1376	U	Sidechain
21	AA	1377	A	Sidechain
21	AA	1379	G	Sidechain
21	AA	138	G	Sidechain
21	AA	1381	U	Sidechain
21	AA	1391	U	Sidechain
21	AA	1397	C	Sidechain
21	AA	14	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1405	G	Sidechain
21	AA	1406	U	Sidechain
21	AA	1412	C	Sidechain
21	AA	1416	G	Sidechain
21	AA	142	G	Sidechain
21	AA	1423	G	Sidechain
21	AA	1431	A	Sidechain
21	AA	1437	A	Sidechain
21	AA	1438	G	Sidechain
21	AA	1439	G	Sidechain
21	AA	1441	A	Sidechain
21	AA	1445	U	Sidechain
21	AA	1446	A	Sidechain
21	AA	1448	C	Sidechain
21	AA	145	G	Sidechain
21	AA	1478	U	Sidechain
21	AA	1479	C	Sidechain
21	AA	1480	A	Sidechain
21	AA	1481	U	Sidechain
21	AA	1491	G	Sidechain
21	AA	1496	C	Sidechain
21	AA	1502	A	Sidechain
21	AA	1509	C	Sidechain
21	AA	1510	C	Sidechain
21	AA	1517	G	Sidechain
21	AA	1518	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1527	U	Sidechain
21	AA	1528	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1531	A	Sidechain
21	AA	1532	U	Sidechain
21	AA	1534	A	Sidechain
21	AA	155	A	Sidechain
21	AA	158	G	Sidechain
21	AA	159	G	Sidechain
21	AA	161	A	Sidechain
21	AA	164	G	Sidechain
21	AA	167	A	Sidechain
21	AA	173	U	Sidechain
21	AA	180	U	Sidechain
21	AA	185	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	187	G	Sidechain
21	AA	189	A	Sidechain
21	AA	19	A	Sidechain
21	AA	190	A	Sidechain
21	AA	191	G	Sidechain
21	AA	195	A	Sidechain
21	AA	197	A	Sidechain
21	AA	203	G	Sidechain
21	AA	205	A	Sidechain
21	AA	207	C	Sidechain
21	AA	208	U	Sidechain
21	AA	212	G	Sidechain
21	AA	22	G	Sidechain
21	AA	222	C	Sidechain
21	AA	224	U	Sidechain
21	AA	226	G	Sidechain
21	AA	228	A	Sidechain
21	AA	236	A	Sidechain
21	AA	237	G	Sidechain
21	AA	238	A	Sidechain
21	AA	240	G	Sidechain
21	AA	241	G	Sidechain
21	AA	242	G	Sidechain
21	AA	244	U	Sidechain
21	AA	250	A	Sidechain
21	AA	251	G	Sidechain
21	AA	254	G	Sidechain
21	AA	257	G	Sidechain
21	AA	26	A	Sidechain
21	AA	274	A	Sidechain
21	AA	278	G	Sidechain
21	AA	281	G	Sidechain
21	AA	285	C	Sidechain
21	AA	295	C	Sidechain
21	AA	297	G	Sidechain
21	AA	298	A	Sidechain
21	AA	308	C	Sidechain
21	AA	320	A	Sidechain
21	AA	321	A	Sidechain
21	AA	324	G	Sidechain
21	AA	326	G	Sidechain
21	AA	331	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	339	C	Sidechain
21	AA	345	C	Sidechain
21	AA	35	G	Sidechain
21	AA	353	A	Sidechain
21	AA	355	C	Sidechain
21	AA	356	A	Sidechain
21	AA	362	G	Sidechain
21	AA	372	C	Sidechain
21	AA	377	G	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	381	C	Sidechain
21	AA	383	A	Sidechain
21	AA	390	U	Sidechain
21	AA	391	G	Sidechain
21	AA	401	C	Sidechain
21	AA	405	U	Sidechain
21	AA	409	U	Sidechain
21	AA	413	G	Sidechain
21	AA	414	A	Sidechain
21	AA	42	G	Sidechain
21	AA	425	G	Sidechain
21	AA	429	U	Sidechain
21	AA	43	C	Sidechain
21	AA	434	U	Sidechain
21	AA	439	U	Sidechain
21	AA	448	A	Sidechain
21	AA	45	G	Sidechain
21	AA	464	U	Sidechain
21	AA	466	A	Sidechain
21	AA	467	U	Sidechain
21	AA	473	U	Sidechain
21	AA	475	C	Sidechain
21	AA	479	U	Sidechain
21	AA	48	C	Sidechain
21	AA	481	G	Sidechain
21	AA	485	U	Sidechain
21	AA	487	A	Sidechain
21	AA	490	C	Sidechain
21	AA	496	A	Sidechain
21	AA	497	G	Sidechain
21	AA	499	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	50	A	Sidechain
21	AA	505	G	Sidechain
21	AA	506	G	Sidechain
21	AA	508	U	Sidechain
21	AA	509	A	Sidechain
21	AA	51	A	Sidechain
21	AA	517	G	Sidechain
21	AA	518	C	Sidechain
21	AA	520	A	Sidechain
21	AA	525	C	Sidechain
21	AA	529	G	Sidechain
21	AA	530	G	Sidechain
21	AA	539	A	Sidechain
21	AA	540	G	Sidechain
21	AA	542	G	Sidechain
21	AA	548	G	Sidechain
21	AA	550	G	Sidechain
21	AA	552	U	Sidechain
21	AA	554	A	Sidechain
21	AA	562	U	Sidechain
21	AA	569	C	Sidechain
21	AA	57	G	Sidechain
21	AA	570	G	Sidechain
21	AA	577	G	Sidechain
21	AA	580	C	Sidechain
21	AA	585	G	Sidechain
21	AA	591	U	Sidechain
21	AA	592	G	Sidechain
21	AA	6	G	Sidechain
21	AA	60	A	Sidechain
21	AA	602	A	Sidechain
21	AA	605	U	Sidechain
21	AA	608	A	Sidechain
21	AA	612	C	Sidechain
21	AA	618	C	Sidechain
21	AA	620	C	Sidechain
21	AA	626	G	Sidechain
21	AA	633	G	Sidechain
21	AA	635	A	Sidechain
21	AA	642	A	Sidechain
21	AA	646	G	Sidechain
21	AA	65	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	654	G	Sidechain
21	AA	659	U	Sidechain
21	AA	664	G	Sidechain
21	AA	666	G	Sidechain
21	AA	676	A	Sidechain
21	AA	685	G	Sidechain
21	AA	69	G	Sidechain
21	AA	690	G	Sidechain
21	AA	691	G	Sidechain
21	AA	694	A	Sidechain
21	AA	7	A	Sidechain
21	AA	704	A	Sidechain
21	AA	707	U	Sidechain
21	AA	711	G	Sidechain
21	AA	714	G	Sidechain
21	AA	718	A	Sidechain
21	AA	719	C	Sidechain
21	AA	720	C	Sidechain
21	AA	722	G	Sidechain
21	AA	727	G	Sidechain
21	AA	735	C	Sidechain
21	AA	737	C	Sidechain
21	AA	739	C	Sidechain
21	AA	740	U	Sidechain
21	AA	741	G	Sidechain
21	AA	752	G	Sidechain
21	AA	753	A	Sidechain
21	AA	755	G	Sidechain
21	AA	76	G	Sidechain
21	AA	760	G	Sidechain
21	AA	765	G	Sidechain
21	AA	775	G	Sidechain
21	AA	776	G	Sidechain
21	AA	778	G	Sidechain
21	AA	781	A	Sidechain
21	AA	783	C	Sidechain
21	AA	785	G	Sidechain
21	AA	802	A	Sidechain
21	AA	807	A	Sidechain
21	AA	81	A	Sidechain
21	AA	812	G	Sidechain
21	AA	813	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	82	G	Sidechain
21	AA	823	C	Sidechain
21	AA	827	U	Sidechain
21	AA	828	U	Sidechain
21	AA	83	C	Sidechain
21	AA	841	C	Sidechain
21	AA	843	U	Sidechain
21	AA	844	G	Sidechain
21	AA	845	A	Sidechain
21	AA	849	G	Sidechain
21	AA	854	U	Sidechain
21	AA	861	G	Sidechain
21	AA	863	U	Sidechain
21	AA	868	C	Sidechain
21	AA	87	C	Sidechain
21	AA	871	U	Sidechain
21	AA	873	A	Sidechain
21	AA	880	C	Sidechain
21	AA	883	C	Sidechain
21	AA	885	G	Sidechain
21	AA	888	G	Sidechain
21	AA	891	U	Sidechain
21	AA	898	G	Sidechain
21	AA	90	C	Sidechain
21	AA	903	G	Sidechain
21	AA	909	A	Sidechain
21	AA	91	U	Sidechain
21	AA	917	G	Sidechain
21	AA	922	G	Sidechain
21	AA	925	G	Sidechain
21	AA	926	G	Sidechain
21	AA	928	G	Sidechain
21	AA	929	G	Sidechain
21	AA	932	C	Sidechain
21	AA	933	G	Sidechain
21	AA	935	A	Sidechain
21	AA	936	C	Sidechain
21	AA	94	G	Sidechain
21	AA	941	G	Sidechain
21	AA	944	G	Sidechain
21	AA	945	G	Sidechain
21	AA	946	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	962	C	Sidechain
21	AA	963	G	Sidechain
21	AA	964	A	Sidechain
21	AA	965	U	Sidechain
21	AA	971	G	Sidechain
21	AA	973	G	Sidechain
21	AA	98	A	Sidechain
21	AA	987	G	Sidechain
21	AA	988	G	Sidechain
21	AA	989	U	Sidechain
21	AA	99	C	Sidechain
21	AA	993	G	Sidechain
21	AA	994	A	Sidechain
21	AA	995	C	Sidechain
21	AA	998	C	Sidechain
2	AC	172	VAL	Peptide
6	AG	3	ARG	Sidechain
7	AH	76	ARG	Sidechain
52	B3	12	ARG	Sidechain
54	BA	1000	A	Sidechain
54	BA	1007	C	Sidechain
54	BA	1016	G	Sidechain
54	BA	1023	U	Sidechain
54	BA	1025	G	Sidechain
54	BA	1027	A	Sidechain
54	BA	1033	U	Sidechain
54	BA	1040	A	Sidechain
54	BA	1051	G	Sidechain
54	BA	1053	C	Sidechain
54	BA	1056	G	Sidechain
54	BA	1063	G	Sidechain
54	BA	1066	U	Sidechain
54	BA	1074	G	Sidechain
54	BA	1080	A	Sidechain
54	BA	1081	U	Sidechain
54	BA	1083	U	Sidechain
54	BA	1093	G	Sidechain
54	BA	1094	U	Sidechain
54	BA	1096	A	Sidechain
54	BA	1097	U	Sidechain
54	BA	1103	A	Sidechain
54	BA	1106	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1107	G	Sidechain
54	BA	1109	C	Sidechain
54	BA	111	A	Sidechain
54	BA	1115	G	Sidechain
54	BA	112	U	Sidechain
54	BA	1124	G	Sidechain
54	BA	1126	A	Sidechain
54	BA	1136	G	Sidechain
54	BA	1137	G	Sidechain
54	BA	1138	G	Sidechain
54	BA	1139	G	Sidechain
54	BA	114	U	Sidechain
54	BA	1146	C	Sidechain
54	BA	1147	A	Sidechain
54	BA	1151	A	Sidechain
54	BA	1153	C	Sidechain
54	BA	1160	G	Sidechain
54	BA	1164	C	Sidechain
54	BA	1169	A	Sidechain
54	BA	1171	G	Sidechain
54	BA	119	A	Sidechain
54	BA	1198	U	Sidechain
54	BA	1199	U	Sidechain
54	BA	1209	U	Sidechain
54	BA	1211	C	Sidechain
54	BA	1219	U	Sidechain
54	BA	1221	C	Sidechain
54	BA	1223	G	Sidechain
54	BA	1224	U	Sidechain
54	BA	1226	A	Sidechain
54	BA	1229	C	Sidechain
54	BA	123	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	1238	G	Sidechain
54	BA	1241	A	Sidechain
54	BA	1242	U	Sidechain
54	BA	1245	G	Sidechain
54	BA	1248	G	Sidechain
54	BA	1252	G	Sidechain
54	BA	1253	A	Sidechain
54	BA	1257	C	Sidechain
54	BA	1259	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1261	C	Sidechain
54	BA	1263	U	Sidechain
54	BA	1268	A	Sidechain
54	BA	1272	A	Sidechain
54	BA	1275	A	Sidechain
54	BA	1277	G	Sidechain
54	BA	1281	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	1291	C	Sidechain
54	BA	1292	G	Sidechain
54	BA	1294	U	Sidechain
54	BA	1296	G	Sidechain
54	BA	1299	G	Sidechain
54	BA	130	C	Sidechain
54	BA	1312	U	Sidechain
54	BA	132	G	Sidechain
54	BA	1322	A	Sidechain
54	BA	1323	C	Sidechain
54	BA	1324	G	Sidechain
54	BA	1328	A	Sidechain
54	BA	1336	A	Sidechain
54	BA	1338	G	Sidechain
54	BA	134	G	Sidechain
54	BA	1341	G	Sidechain
54	BA	1343	G	Sidechain
54	BA	1348	C	Sidechain
54	BA	1349	C	Sidechain
54	BA	1352	U	Sidechain
54	BA	1353	A	Sidechain
54	BA	1356	G	Sidechain
54	BA	1362	C	Sidechain
54	BA	1365	A	Sidechain
54	BA	1368	G	Sidechain
54	BA	1372	U	Sidechain
54	BA	1384	A	Sidechain
54	BA	1386	C	Sidechain
54	BA	1387	A	Sidechain
54	BA	1389	G	Sidechain
54	BA	1392	A	Sidechain
54	BA	1398	C	Sidechain
54	BA	1399	C	Sidechain
54	BA	141	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1418	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1427	A	Sidechain
54	BA	1431	A	Sidechain
54	BA	1434	A	Sidechain
54	BA	1437	C	Sidechain
54	BA	1439	A	Sidechain
54	BA	144	A	Sidechain
54	BA	1440	U	Sidechain
54	BA	1441	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1450	G	Sidechain
54	BA	1451	C	Sidechain
54	BA	1453	A	Sidechain
54	BA	1455	G	Sidechain
54	BA	1456	G	Sidechain
54	BA	1458	U	Sidechain
54	BA	1459	G	Sidechain
54	BA	146	A	Sidechain
54	BA	1461	C	Sidechain
54	BA	1465	G	Sidechain
54	BA	1471	G	Sidechain
54	BA	1476	U	Sidechain
54	BA	1477	A	Sidechain
54	BA	1478	G	Sidechain
54	BA	1483	G	Sidechain
54	BA	1488	C	Sidechain
54	BA	1492	G	Sidechain
54	BA	1494	A	Sidechain
54	BA	1495	A	Sidechain
54	BA	1498	C	Sidechain
54	BA	1508	A	Sidechain
54	BA	1523	U	Sidechain
54	BA	1530	G	Sidechain
54	BA	1534	U	Sidechain
54	BA	1535	A	Sidechain
54	BA	1538	G	Sidechain
54	BA	1540	G	Sidechain
54	BA	1546	G	Sidechain
54	BA	1550	C	Sidechain
54	BA	1552	A	Sidechain
54	BA	1553	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1567	G	Sidechain
54	BA	1572	A	Sidechain
54	BA	1573	G	Sidechain
54	BA	1577	C	Sidechain
54	BA	1579	A	Sidechain
54	BA	1580	A	Sidechain
54	BA	1581	G	Sidechain
54	BA	1585	C	Sidechain
54	BA	1593	A	Sidechain
54	BA	1595	C	Sidechain
54	BA	1601	G	Sidechain
54	BA	1608	A	Sidechain
54	BA	1614	A	Sidechain
54	BA	1618	A	Sidechain
54	BA	162	U	Sidechain
54	BA	1620	G	Sidechain
54	BA	1624	U	Sidechain
54	BA	1626	A	Sidechain
54	BA	1628	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1636	U	Sidechain
54	BA	1637	A	Sidechain
54	BA	1641	A	Sidechain
54	BA	1642	G	Sidechain
54	BA	1646	C	Sidechain
54	BA	1647	U	Sidechain
54	BA	1651	G	Sidechain
54	BA	1652	A	Sidechain
54	BA	1653	G	Sidechain
54	BA	1655	A	Sidechain
54	BA	1656	C	Sidechain
54	BA	1657	U	Sidechain
54	BA	1665	A	Sidechain
54	BA	1666	G	Sidechain
54	BA	1667	G	Sidechain
54	BA	1671	U	Sidechain
54	BA	1674	G	Sidechain
54	BA	168	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1680	U	Sidechain
54	BA	1683	U	Sidechain
54	BA	1685	C	Sidechain
54	BA	1693	U	Sidechain
54	BA	1698	A	Sidechain
54	BA	17	G	Sidechain
54	BA	1705	A	Sidechain
54	BA	1706	C	Sidechain
54	BA	1707	G	Sidechain
54	BA	1709	U	Sidechain
54	BA	1713	A	Sidechain
54	BA	1716	U	Sidechain
54	BA	1726	C	Sidechain
54	BA	1728	C	Sidechain
54	BA	1730	C	Sidechain
54	BA	1732	C	Sidechain
54	BA	1738	G	Sidechain
54	BA	1740	G	Sidechain
54	BA	1744	A	Sidechain
54	BA	1750	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1757	A	Sidechain
54	BA	176	A	Sidechain
54	BA	1763	G	Sidechain
54	BA	1769	U	Sidechain
54	BA	177	G	Sidechain
54	BA	1773	A	Sidechain
54	BA	1774	C	Sidechain
54	BA	1775	U	Sidechain
54	BA	1782	U	Sidechain
54	BA	1784	A	Sidechain
54	BA	1788	C	Sidechain
54	BA	1790	C	Sidechain
54	BA	1791	A	Sidechain
54	BA	1795	C	Sidechain
54	BA	1797	G	Sidechain
54	BA	180	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1804	C	Sidechain
54	BA	1805	A	Sidechain
54	BA	1807	G	Sidechain
54	BA	181	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1814	G	Sidechain
54	BA	1816	C	Sidechain
54	BA	1821	A	Sidechain
54	BA	1828	G	Sidechain
54	BA	1831	G	Sidechain
54	BA	1832	C	Sidechain
54	BA	1837	C	Sidechain
54	BA	1839	G	Sidechain
54	BA	1842	G	Sidechain
54	BA	1844	C	Sidechain
54	BA	1847	A	Sidechain
54	BA	1849	G	Sidechain
54	BA	1855	U	Sidechain
54	BA	1860	G	Sidechain
54	BA	1861	G	Sidechain
54	BA	1869	G	Sidechain
54	BA	1881	C	Sidechain
54	BA	1883	U	Sidechain
54	BA	1884	G	Sidechain
54	BA	189	G	Sidechain
54	BA	19	A	Sidechain
54	BA	190	A	Sidechain
54	BA	1906	G	Sidechain
54	BA	1910	G	Sidechain
54	BA	1916	A	Sidechain
54	BA	1927	A	Sidechain
54	BA	1931	U	Sidechain
54	BA	1932	A	Sidechain
54	BA	1933	G	Sidechain
54	BA	1937	A	Sidechain
54	BA	194	G	Sidechain
54	BA	1942	C	Sidechain
54	BA	1950	G	Sidechain
54	BA	1954	G	Sidechain
54	BA	1956	U	Sidechain
54	BA	1958	C	Sidechain
54	BA	1959	G	Sidechain
54	BA	196	A	Sidechain
54	BA	1960	A	Sidechain
54	BA	1969	A	Sidechain
54	BA	1972	G	Sidechain
54	BA	1974	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1979	U	Sidechain
54	BA	2006	C	Sidechain
54	BA	2009	A	Sidechain
54	BA	2014	A	Sidechain
54	BA	2018	G	Sidechain
54	BA	2028	U	Sidechain
54	BA	2029	G	Sidechain
54	BA	2032	G	Sidechain
54	BA	2034	U	Sidechain
54	BA	2035	G	Sidechain
54	BA	2043	C	Sidechain
54	BA	205	G	Sidechain
54	BA	2058	A	Sidechain
54	BA	2063	C	Sidechain
54	BA	2067	G	Sidechain
54	BA	207	A	Sidechain
54	BA	2070	A	Sidechain
54	BA	2086	U	Sidechain
54	BA	2089	C	Sidechain
54	BA	209	C	Sidechain
54	BA	2090	A	Sidechain
54	BA	2091	C	Sidechain
54	BA	2093	G	Sidechain
54	BA	2098	U	Sidechain
54	BA	2106	U	Sidechain
54	BA	2107	G	Sidechain
54	BA	2108	A	Sidechain
54	BA	211	C	Sidechain
54	BA	2112	G	Sidechain
54	BA	2113	U	Sidechain
54	BA	2115	G	Sidechain
54	BA	2120	G	Sidechain
54	BA	2127	G	Sidechain
54	BA	2129	C	Sidechain
54	BA	213	A	Sidechain
54	BA	2132	U	Sidechain
54	BA	2133	G	Sidechain
54	BA	2134	A	Sidechain
54	BA	2137	U	Sidechain
54	BA	2138	G	Sidechain
54	BA	2141	G	Sidechain
54	BA	2143	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2145	C	Sidechain
54	BA	2148	G	Sidechain
54	BA	2149	U	Sidechain
54	BA	2153	C	Sidechain
54	BA	2157	G	Sidechain
54	BA	2159	G	Sidechain
54	BA	2160	C	Sidechain
54	BA	2168	G	Sidechain
54	BA	2180	U	Sidechain
54	BA	2182	U	Sidechain
54	BA	2186	G	Sidechain
54	BA	2189	U	Sidechain
54	BA	2192	U	Sidechain
54	BA	2194	U	Sidechain
54	BA	2200	C	Sidechain
54	BA	2204	G	Sidechain
54	BA	2208	C	Sidechain
54	BA	221	A	Sidechain
54	BA	2211	A	Sidechain
54	BA	2215	C	Sidechain
54	BA	222	A	Sidechain
54	BA	2228	G	Sidechain
54	BA	2230	G	Sidechain
54	BA	2237	G	Sidechain
54	BA	2243	U	Sidechain
54	BA	2246	G	Sidechain
54	BA	2247	A	Sidechain
54	BA	2259	U	Sidechain
54	BA	2260	C	Sidechain
54	BA	2265	U	Sidechain
54	BA	2266	A	Sidechain
54	BA	227	A	Sidechain
54	BA	2282	G	Sidechain
54	BA	2289	G	Sidechain
54	BA	2293	G	Sidechain
54	BA	2296	U	Sidechain
54	BA	2300	C	Sidechain
54	BA	2301	C	Sidechain
54	BA	2305	U	Sidechain
54	BA	231	A	Sidechain
54	BA	2311	A	Sidechain
54	BA	2318	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2325	G	Sidechain
54	BA	2326	C	Sidechain
54	BA	2327	A	Sidechain
54	BA	2331	G	Sidechain
54	BA	2336	A	Sidechain
54	BA	2338	C	Sidechain
54	BA	2342	C	Sidechain
54	BA	2349	G	Sidechain
54	BA	2357	G	Sidechain
54	BA	2358	A	Sidechain
54	BA	2363	G	Sidechain
54	BA	2367	G	Sidechain
54	BA	2375	G	Sidechain
54	BA	2386	A	Sidechain
54	BA	2390	U	Sidechain
54	BA	2391	G	Sidechain
54	BA	2394	C	Sidechain
54	BA	2395	C	Sidechain
54	BA	24	G	Sidechain
54	BA	2402	U	Sidechain
54	BA	2408	U	Sidechain
54	BA	2415	G	Sidechain
54	BA	2428	G	Sidechain
54	BA	243	U	Sidechain
54	BA	244	A	Sidechain
54	BA	2444	G	Sidechain
54	BA	2447	G	Sidechain
54	BA	2448	A	Sidechain
54	BA	2454	G	Sidechain
54	BA	2458	G	Sidechain
54	BA	2460	U	Sidechain
54	BA	247	G	Sidechain
54	BA	2472	G	Sidechain
54	BA	2473	U	Sidechain
54	BA	2474	U	Sidechain
54	BA	2475	C	Sidechain
54	BA	2476	A	Sidechain
54	BA	2477	U	Sidechain
54	BA	2488	G	Sidechain
54	BA	2489	U	Sidechain
54	BA	249	C	Sidechain
54	BA	2491	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2494	G	Sidechain
54	BA	2496	C	Sidechain
54	BA	250	G	Sidechain
54	BA	2500	U	Sidechain
54	BA	2501	C	Sidechain
54	BA	2502	G	Sidechain
54	BA	2505	G	Sidechain
54	BA	2506	U	Sidechain
54	BA	2507	C	Sidechain
54	BA	2516	A	Sidechain
54	BA	2517	C	Sidechain
54	BA	2521	C	Sidechain
54	BA	2529	G	Sidechain
54	BA	2536	G	Sidechain
54	BA	2538	C	Sidechain
54	BA	2540	C	Sidechain
54	BA	2549	G	Sidechain
54	BA	2552	U	Sidechain
54	BA	2553	G	Sidechain
54	BA	2564	A	Sidechain
54	BA	2565	A	Sidechain
54	BA	2566	A	Sidechain
54	BA	2581	G	Sidechain
54	BA	2584	U	Sidechain
54	BA	2586	U	Sidechain
54	BA	2589	A	Sidechain
54	BA	2595	G	Sidechain
54	BA	2600	A	Sidechain
54	BA	2608	G	Sidechain
54	BA	2609	U	Sidechain
54	BA	2618	G	Sidechain
54	BA	2622	U	Sidechain
54	BA	2624	G	Sidechain
54	BA	2628	C	Sidechain
54	BA	2633	G	Sidechain
54	BA	2637	U	Sidechain
54	BA	264	C	Sidechain
54	BA	2645	G	Sidechain
54	BA	2649	C	Sidechain
54	BA	265	A	Sidechain
54	BA	2651	C	Sidechain
54	BA	2655	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2656	U	Sidechain
54	BA	2659	G	Sidechain
54	BA	2664	G	Sidechain
54	BA	2665	A	Sidechain
54	BA	2667	C	Sidechain
54	BA	2669	G	Sidechain
54	BA	2670	A	Sidechain
54	BA	2674	G	Sidechain
54	BA	2677	G	Sidechain
54	BA	268	C	Sidechain
54	BA	2680	U	Sidechain
54	BA	2681	C	Sidechain
54	BA	2682	A	Sidechain
54	BA	2683	C	Sidechain
54	BA	2702	G	Sidechain
54	BA	2706	A	Sidechain
54	BA	2710	C	Sidechain
54	BA	2711	A	Sidechain
54	BA	2712	C	Sidechain
54	BA	2714	G	Sidechain
54	BA	2727	A	Sidechain
54	BA	2729	G	Sidechain
54	BA	2731	G	Sidechain
54	BA	2735	G	Sidechain
54	BA	2751	G	Sidechain
54	BA	2753	A	Sidechain
54	BA	2756	U	Sidechain
54	BA	276	U	Sidechain
54	BA	2760	C	Sidechain
54	BA	2770	G	Sidechain
54	BA	278	A	Sidechain
54	BA	2781	A	Sidechain
54	BA	2784	U	Sidechain
54	BA	2785	C	Sidechain
54	BA	2786	U	Sidechain
54	BA	279	A	Sidechain
54	BA	2794	C	Sidechain
54	BA	2801	G	Sidechain
54	BA	2804	U	Sidechain
54	BA	2808	G	Sidechain
54	BA	2816	G	Sidechain
54	BA	2817	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	282	A	Sidechain
54	BA	2822	G	Sidechain
54	BA	2825	G	Sidechain
54	BA	2831	G	Sidechain
54	BA	2835	A	Sidechain
54	BA	2836	U	Sidechain
54	BA	2848	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2859	G	Sidechain
54	BA	2864	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	2874	C	Sidechain
54	BA	2875	C	Sidechain
54	BA	2876	G	Sidechain
54	BA	2883	A	Sidechain
54	BA	2886	A	Sidechain
54	BA	2889	C	Sidechain
54	BA	2891	U	Sidechain
54	BA	2892	G	Sidechain
54	BA	296	U	Sidechain
54	BA	298	G	Sidechain
54	BA	303	G	Sidechain
54	BA	304	U	Sidechain
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	311	A	Sidechain
54	BA	313	G	Sidechain
54	BA	314	C	Sidechain
54	BA	318	C	Sidechain
54	BA	319	G	Sidechain
54	BA	323	C	Sidechain
54	BA	331	C	Sidechain
54	BA	332	A	Sidechain
54	BA	333	G	Sidechain
54	BA	34	U	Sidechain
54	BA	341	C	Sidechain
54	BA	354	A	Sidechain
54	BA	360	U	Sidechain
54	BA	363	G	Sidechain
54	BA	364	C	Sidechain
54	BA	365	U	Sidechain
54	BA	372	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	379	G	Sidechain
54	BA	381	G	Sidechain
54	BA	387	U	Sidechain
54	BA	392	U	Sidechain
54	BA	394	C	Sidechain
54	BA	395	U	Sidechain
54	BA	4	U	Sidechain
54	BA	401	A	Sidechain
54	BA	406	G	Sidechain
54	BA	418	C	Sidechain
54	BA	419	U	Sidechain
54	BA	422	A	Sidechain
54	BA	423	A	Sidechain
54	BA	424	G	Sidechain
54	BA	434	U	Sidechain
54	BA	439	A	Sidechain
54	BA	44	A	Sidechain
54	BA	440	C	Sidechain
54	BA	446	G	Sidechain
54	BA	45	G	Sidechain
54	BA	450	G	Sidechain
54	BA	452	G	Sidechain
54	BA	455	C	Sidechain
54	BA	456	C	Sidechain
54	BA	458	G	Sidechain
54	BA	46	G	Sidechain
54	BA	460	A	Sidechain
54	BA	464	U	Sidechain
54	BA	472	A	Sidechain
54	BA	473	G	Sidechain
54	BA	474	G	Sidechain
54	BA	476	G	Sidechain
54	BA	479	A	Sidechain
54	BA	48	G	Sidechain
54	BA	481	G	Sidechain
54	BA	482	A	Sidechain
54	BA	488	G	Sidechain
54	BA	49	A	Sidechain
54	BA	491	G	Sidechain
54	BA	495	G	Sidechain
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	505	A	Sidechain
54	BA	506	G	Sidechain
54	BA	509	C	Sidechain
54	BA	51	G	Sidechain
54	BA	518	G	Sidechain
54	BA	525	U	Sidechain
54	BA	528	A	Sidechain
54	BA	529	A	Sidechain
54	BA	537	G	Sidechain
54	BA	541	A	Sidechain
54	BA	548	G	Sidechain
54	BA	55	G	Sidechain
54	BA	552	U	Sidechain
54	BA	556	A	Sidechain
54	BA	558	U	Sidechain
54	BA	56	A	Sidechain
54	BA	561	G	Sidechain
54	BA	567	U	Sidechain
54	BA	568	U	Sidechain
54	BA	570	G	Sidechain
54	BA	575	A	Sidechain
54	BA	577	G	Sidechain
54	BA	58	G	Sidechain
54	BA	581	C	Sidechain
54	BA	585	G	Sidechain
54	BA	588	U	Sidechain
54	BA	594	U	Sidechain
54	BA	606	U	Sidechain
54	BA	607	U	Sidechain
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	612	G	Sidechain
54	BA	617	G	Sidechain
54	BA	623	C	Sidechain
54	BA	63	A	Sidechain
54	BA	630	G	Sidechain
54	BA	631	A	Sidechain
54	BA	636	G	Sidechain
54	BA	640	C	Sidechain
54	BA	641	U	Sidechain
54	BA	642	U	Sidechain
54	BA	647	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	650	C	Sidechain
54	BA	653	U	Sidechain
54	BA	655	A	Sidechain
54	BA	656	G	Sidechain
54	BA	669	G	Sidechain
54	BA	670	A	Sidechain
54	BA	671	C	Sidechain
54	BA	674	G	Sidechain
54	BA	679	C	Sidechain
54	BA	682	G	Sidechain
54	BA	683	U	Sidechain
54	BA	686	U	Sidechain
54	BA	687	C	Sidechain
54	BA	69	C	Sidechain
54	BA	690	G	Sidechain
54	BA	698	C	Sidechain
54	BA	700	G	Sidechain
54	BA	703	U	Sidechain
54	BA	707	G	Sidechain
54	BA	71	A	Sidechain
54	BA	710	U	Sidechain
54	BA	714	U	Sidechain
54	BA	721	A	Sidechain
54	BA	724	U	Sidechain
54	BA	726	G	Sidechain
54	BA	727	A	Sidechain
54	BA	728	G	Sidechain
54	BA	729	G	Sidechain
54	BA	732	C	Sidechain
54	BA	74	A	Sidechain
54	BA	742	A	Sidechain
54	BA	744	U	Sidechain
54	BA	748	G	Sidechain
54	BA	759	G	Sidechain
54	BA	768	G	Sidechain
54	BA	77	G	Sidechain
54	BA	772	C	Sidechain
54	BA	775	G	Sidechain
54	BA	777	G	Sidechain
54	BA	779	U	Sidechain
54	BA	792	A	Sidechain
54	BA	795	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	800	A	Sidechain
54	BA	802	A	Sidechain
54	BA	809	G	Sidechain
54	BA	811	U	Sidechain
54	BA	820	A	Sidechain
54	BA	823	C	Sidechain
54	BA	827	U	Sidechain
54	BA	828	U	Sidechain
54	BA	83	A	Sidechain
54	BA	833	A	Sidechain
54	BA	834	G	Sidechain
54	BA	837	C	Sidechain
54	BA	845	A	Sidechain
54	BA	846	U	Sidechain
54	BA	847	U	Sidechain
54	BA	85	G	Sidechain
54	BA	852	U	Sidechain
54	BA	858	G	Sidechain
54	BA	859	G	Sidechain
54	BA	86	G	Sidechain
54	BA	864	G	Sidechain
54	BA	868	U	Sidechain
54	BA	869	G	Sidechain
54	BA	87	U	Sidechain
54	BA	871	U	Sidechain
54	BA	874	G	Sidechain
54	BA	875	G	Sidechain
54	BA	877	A	Sidechain
54	BA	884	U	Sidechain
54	BA	886	A	Sidechain
54	BA	892	A	Sidechain
54	BA	896	A	Sidechain
54	BA	900	A	Sidechain
54	BA	909	A	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	914	G	Sidechain
54	BA	92	U	Sidechain
54	BA	923	G	Sidechain
54	BA	930	G	Sidechain
54	BA	934	U	Sidechain
54	BA	936	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	94	A	Sidechain
54	BA	942	G	Sidechain
54	BA	945	A	Sidechain
54	BA	947	A	Sidechain
54	BA	949	G	Sidechain
54	BA	95	A	Sidechain
54	BA	950	G	Sidechain
54	BA	954	G	Sidechain
54	BA	956	G	Sidechain
54	BA	958	U	Sidechain
54	BA	962	G	Sidechain
54	BA	964	C	Sidechain
54	BA	972	A	Sidechain
54	BA	974	G	Sidechain
54	BA	975	A	Sidechain
54	BA	985	C	Sidechain
54	BA	986	C	Sidechain
54	BA	989	G	Sidechain
54	BA	993	G	Sidechain
54	BA	994	C	Sidechain
55	BB	10	G	Sidechain
55	BB	106	G	Sidechain
55	BB	115	A	Sidechain
55	BB	15	A	Sidechain
55	BB	18	G	Sidechain
55	BB	27	C	Sidechain
55	BB	32	U	Sidechain
55	BB	33	G	Sidechain
55	BB	34	A	Sidechain
55	BB	37	C	Sidechain
55	BB	38	C	Sidechain
55	BB	40	U	Sidechain
55	BB	43	C	Sidechain
55	BB	48	U	Sidechain
55	BB	50	A	Sidechain
55	BB	51	G	Sidechain
55	BB	59	A	Sidechain
55	BB	6	G	Sidechain
55	BB	64	G	Sidechain
55	BB	65	U	Sidechain
55	BB	69	G	Sidechain
55	BB	70	C	Sidechain

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Mol	Chain	Res	Type	Group
55	BB	72	G	Sidechain
55	BB	75	G	Sidechain
55	BB	76	G	Sidechain
55	BB	84	G	Sidechain
55	BB	87	U	Sidechain
55	BB	89	U	Sidechain
37	BO	36	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	2	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	1	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16520	2	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	1	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	1	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	2	0
39	BQ	947	0	1022	1	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	0	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	31345	1	0
55	BB	2504	0	1271	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	99663	11	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 (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BF:151:LEU:H	28:BF:151:LEU:HD13	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AJ:57:VAL:HG23	9:AJ:58:ASN:H	1.77	0.50
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.30	0.50
21:AA:565:U:H2'	21:AA:566:G:C8	2.48	0.47
21:AA:940:C:H2'	21:AA:941:G:C8	2.50	0.46
39:BQ:40:LYS:HE3	39:BQ:44:TYR:CZ	2.51	0.45
33:BK:119:ALA:H	33:BK:120:PRO:CD	2.32	0.43
38:BP:30:TRP:CD2	38:BP:37:LYS:HE2	2.53	0.43
54:BA:1256:G:H2'	54:BA:1257:C:C6	2.54	0.42
5:AF:94:HIS:CG	5:AF:95:ALA:N	2.89	0.41
38:BP:30:TRP:CE2	38:BP:37:LYS:HE2	2.55	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	198 (91%)	16 (7%)	4 (2%)	11	53
2	AC	205/208 (99%)	188 (92%)	8 (4%)	9 (4%)	3	33
3	AD	203/206 (98%)	182 (90%)	18 (9%)	3 (2%)	13	57
4	AE	150/152 (99%)	136 (91%)	8 (5%)	6 (4%)	4	35
5	AF	99/101 (98%)	84 (85%)	9 (9%)	6 (6%)	2	26
6	AG	150/152 (99%)	130 (87%)	14 (9%)	6 (4%)	4	35
7	AH	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	24	69
8	AI	126/128 (98%)	115 (91%)	9 (7%)	2 (2%)	12	56
9	AJ	98/100 (98%)	92 (94%)	2 (2%)	4 (4%)	3	35
10	AK	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	21	67
11	AL	121/124 (98%)	107 (88%)	13 (11%)	1 (1%)	24	69
12	AM	112/115 (97%)	98 (88%)	9 (8%)	5 (4%)	3	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	AN	98/101 (97%)	87 (89%)	10 (10%)	1 (1%)	19	65
14	AO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	16	61
15	AP	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	15	60
16	AQ	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	7	46
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	11	53
18	AS	79/81 (98%)	67 (85%)	9 (11%)	3 (4%)	4	37
19	AT	84/86 (98%)	78 (93%)	4 (5%)	2 (2%)	7	47
20	AU	51/53 (96%)	33 (65%)	14 (28%)	4 (8%)	1	20
25	BC	270/273 (99%)	237 (88%)	25 (9%)	8 (3%)	5	42
26	BD	207/209 (99%)	181 (87%)	17 (8%)	9 (4%)	3	34
27	BE	199/201 (99%)	180 (90%)	12 (6%)	7 (4%)	4	39
28	BF	176/179 (98%)	161 (92%)	8 (4%)	7 (4%)	4	35
29	BG	174/177 (98%)	158 (91%)	11 (6%)	5 (3%)	6	43
30	BH	147/149 (99%)	129 (88%)	15 (10%)	3 (2%)	9	51
31	BI	139/142 (98%)	132 (95%)	7 (5%)	0	100	100
32	BJ	140/142 (99%)	124 (89%)	11 (8%)	5 (4%)	4	38
33	BK	121/123 (98%)	103 (85%)	12 (10%)	6 (5%)	3	31
34	BL	141/144 (98%)	122 (86%)	10 (7%)	9 (6%)	2	25
35	BM	134/136 (98%)	121 (90%)	8 (6%)	5 (4%)	4	38
36	BN	119/121 (98%)	101 (85%)	17 (14%)	1 (1%)	24	69
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	21	67
38	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	6	45
39	BQ	115/118 (98%)	105 (91%)	7 (6%)	3 (3%)	7	45
40	BR	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	9	51
41	BS	108/110 (98%)	96 (89%)	8 (7%)	4 (4%)	4	38
42	BT	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	8	49
43	BU	101/104 (97%)	79 (78%)	16 (16%)	6 (6%)	2	27
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	64 (82%)	12 (15%)	2 (3%)	7	45
46	BX	75/79 (95%)	69 (92%)	6 (8%)	0	100	100
47	BY	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	12	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BZ	56/59 (95%)	47 (84%)	4 (7%)	5 (9%)	1	17
49	B0	54/57 (95%)	50 (93%)	2 (4%)	2 (4%)	4	38
50	B1	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	9	51
51	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
52	B3	62/65 (95%)	50 (81%)	8 (13%)	4 (6%)	1	25
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	205 (93%)	15 (7%)	1 (0%)	34	77
All	All	5876/6008 (98%)	5258 (90%)	453 (8%)	165 (3%)	10	44

All (165) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	206	ILE
2	AC	4	VAL
3	AD	54	LEU
4	AE	105	ILE
5	AF	59	TYR
6	AG	11	ILE
13	AN	63	ARG
18	AS	22	VAL
18	AS	79	TYR
26	BD	2	ILE
26	BD	51	THR
26	BD	77	ARG
26	BD	150	GLN
27	BE	70	SER
27	BE	79	ARG
28	BF	12	VAL
28	BF	103	ILE
30	BH	121	VAL
33	BK	32	TYR
33	BK	119	ALA
34	BL	21	ARG
34	BL	101	ILE
35	BM	36	VAL
42	BT	70	HIS
43	BU	57	ILE
1	AB	87	ASP
5	AF	10	VAL
6	AG	5	VAL

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Mol	Chain	Res	Type
6	AG	56	SER
6	AG	129	ASN
7	AH	77	VAL
8	AI	117	LEU
9	AJ	75	ASP
12	AM	11	HIS
12	AM	22	TYR
19	AT	3	ILE
20	AU	34	ARG
25	BC	136	VAL
26	BD	34	VAL
27	BE	94	GLN
27	BE	147	LEU
28	BF	136	ILE
30	BH	29	PHE
30	BH	67	ALA
34	BL	29	LYS
38	BP	32	VAL
38	BP	109	ILE
39	BQ	86	SER
39	BQ	87	VAL
40	BR	80	ARG
43	BU	43	LYS
48	BZ	3	THR
48	BZ	4	ILE
48	BZ	31	ILE
49	B0	13	GLY
52	B3	3	ILE
2	AC	159	ALA
2	AC	195	ILE
4	AE	103	GLY
5	AF	65	GLU
6	AG	60	ALA
6	AG	114	SER
8	AI	128	LYS
16	AQ	64	ARG
19	AT	42	ASP
25	BC	37	SER
25	BC	123	ILE
25	BC	191	LEU
25	BC	235	GLU
26	BD	20	VAL

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Mol	Chain	Res	Type
26	BD	201	LEU
27	BE	11	ALA
28	BF	46	LYS
29	BG	22	VAL
29	BG	113	ASP
32	BJ	15	TRP
34	BL	16	GLY
34	BL	65	GLY
35	BM	21	ALA
38	BP	74	GLN
41	BS	90	LYS
43	BU	45	GLN
45	BW	38	ARG
50	B1	6	GLU
1	AB	36	LYS
2	AC	65	VAL
2	AC	100	ILE
3	AD	28	ASP
4	AE	54	GLU
4	AE	104	ILE
4	AE	127	TYR
5	AF	82	ASP
5	AF	98	GLU
9	AJ	5	ARG
9	AJ	57	VAL
10	AK	12	ARG
11	AL	15	VAL
12	AM	104	ASN
12	AM	112	ARG
14	AO	86	LEU
15	AP	9	HIS
20	AU	47	ALA
25	BC	196	ASN
26	BD	55	LYS
27	BE	55	SER
27	BE	96	VAL
29	BG	8	VAL
29	BG	151	ARG
32	BJ	81	ILE
33	BK	103	VAL
33	BK	110	GLU
34	BL	36	LYS

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Mol	Chain	Res	Type
35	BM	62	LYS
35	BM	133	LYS
37	BO	23	ALA
39	BQ	10	ARG
40	BR	53	PHE
43	BU	74	ALA
48	BZ	9	THR
52	B3	31	ILE
2	AC	167	TYR
5	AF	6	ILE
12	AM	103	THR
18	AS	80	ARG
25	BC	99	GLU
26	BD	43	ASP
28	BF	122	ASP
28	BF	148	VAL
32	BJ	45	THR
32	BJ	64	VAL
36	BN	80	PHE
41	BS	33	LEU
41	BS	92	ARG
42	BT	2	ILE
43	BU	5	ARG
43	BU	40	LEU
47	BY	37	LEU
49	B0	27	LEU
52	B3	50	SER
56	B5	217	THR
3	AD	82	LYS
16	AQ	15	LYS
17	AR	20	ILE
34	BL	5	THR
34	BL	85	VAL
45	BW	70	VAL
4	AE	43	GLY
20	AU	27	VAL
33	BK	93	GLN
34	BL	55	MET
41	BS	96	ILE
48	BZ	32	GLY
1	AB	185	ILE
2	AC	172	VAL

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Mol	Chain	Res	Type
2	AC	194	VAL
9	AJ	42	LEU
25	BC	2	VAL
32	BJ	48	VAL
2	AC	206	ILE
20	AU	5	VAL
28	BF	123	GLY
33	BK	47	ILE
29	BG	116	LEU
35	BM	126	ILE
52	B3	44	ARG

### 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%)	175 (97%)	5 (3%)	51	78
2	AC	170/171 (99%)	166 (98%)	4 (2%)	57	82
3	AD	172/173 (99%)	168 (98%)	4 (2%)	58	83
4	AE	113/113 (100%)	112 (99%)	1 (1%)	84	93
5	AF	87/87 (100%)	85 (98%)	2 (2%)	58	83
6	AG	123/123 (100%)	121 (98%)	2 (2%)	70	88
7	AH	104/105 (99%)	102 (98%)	2 (2%)	65	86
8	AI	105/105 (100%)	100 (95%)	5 (5%)	31	67
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	88 (98%)	2 (2%)	60	83
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	90 (99%)	1 (1%)	80	91
13	AN	83/84 (99%)	82 (99%)	1 (1%)	78	90
14	AO	76/77 (99%)	75 (99%)	1 (1%)	76	89
15	AP	65/65 (100%)	63 (97%)	2 (3%)	47	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	212 (98%)	4 (2%)	65	86
26	BD	164/164 (100%)	161 (98%)	3 (2%)	66	87
27	BE	165/165 (100%)	161 (98%)	4 (2%)	57	82
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%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	107 (98%)	2 (2%)	66	87
32	BJ	116/116 (100%)	115 (99%)	1 (1%)	84	93
33	BK	103/103 (100%)	102 (99%)	1 (1%)	82	92
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	107 (98%)	2 (2%)	66	87
36	BN	100/100 (100%)	100 (100%)	0	100	100
37	BO	86/87 (99%)	83 (96%)	3 (4%)	43	74
38	BP	99/100 (99%)	97 (98%)	2 (2%)	63	85
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	80	91
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	91 (98%)	2 (2%)	60	83
42	BT	80/80 (100%)	79 (99%)	1 (1%)	76	89
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%)	55 (93%)	4 (7%)	20	57
46	BX	67/68 (98%)	66 (98%)	1 (2%)	72	88
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	61	84
50	B1	45/45 (100%)	45 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	B2	38/38 (100%)	37 (97%)	1 (3%)	54	80
52	B3	51/52 (98%)	50 (98%)	1 (2%)	63	85
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	170 (98%)	3 (2%)	68	87
All	All	4842/4870 (99%)	4763 (98%)	79 (2%)	72	88

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	22	TRP
1	AB	88	GLN
1	AB	92	ASN
1	AB	99	MET
1	AB	129	THR
2	AC	11	LEU
2	AC	35	ASP
2	AC	133	MET
2	AC	200	TRP
3	AD	39	GLN
3	AD	119	HIS
3	AD	139	ASN
3	AD	194	ILE
4	AE	152	VAL
5	AF	52	ASN
5	AF	61	LEU
6	AG	14	ASP
6	AG	59	GLU
7	AH	2	MET
7	AH	104	SER
8	AI	38	PHE
8	AI	41	GLU
8	AI	55	ASP
8	AI	105	ARG
8	AI	106	ASP
10	AK	36	ARG
10	AK	100	ASN
12	AM	53	ASP
13	AN	98	LYS
14	AO	48	ASP
15	AP	1	MET
15	AP	79	ASN

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Mol	Chain	Res	Type
25	BC	22	GLU
25	BC	175	LEU
25	BC	179	GLU
25	BC	191	LEU
26	BD	32	ASN
26	BD	43	ASP
26	BD	148	GLN
27	BE	7	ASP
27	BE	78	TRP
27	BE	168	ASP
27	BE	184	ASP
28	BF	15	LEU
28	BF	134	GLN
28	BF	151	LEU
29	BG	33	THR
29	BG	120	ILE
29	BG	154	GLU
31	BI	20	SER
31	BI	50	LYS
32	BJ	81	ILE
33	BK	32	TYR
35	BM	16	ARG
35	BM	97	GLN
37	BO	30	ARG
37	BO	38	GLN
37	BO	117	PHE
38	BP	50	ARG
38	BP	85	VAL
39	BQ	71	ASN
40	BR	23	GLU
41	BS	1	MET
41	BS	70	LYS
42	BT	34	VAL
43	BU	40	LEU
43	BU	46	LYS
44	BV	51	GLN
45	BW	38	ARG
45	BW	49	ASN
45	BW	55	ASP
45	BW	80	SER
46	BX	29	LEU
49	B0	2	VAL

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Mol	Chain	Res	Type
51	B2	19	ARG
52	B3	33	THR
56	B5	165	ASN
56	B5	215	SER
56	B5	217	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	AF	14	GLN
27	BE	46	GLN
35	BM	97	GLN
37	BO	29	HIS
49	B0	40	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	229 (14%)	86 (5%)
22	A1	73/76 (96%)	14 (19%)	5 (6%)
23	A2	15/15 (100%)	5 (33%)	4 (26%)
24	A3	76/77 (98%)	17 (22%)	6 (7%)
54	BA	2902/2903 (99%)	457 (15%)	117 (4%)
55	BB	116/118 (98%)	18 (15%)	4 (3%)
All	All	4711/4722 (99%)	740 (15%)	222 (4%)

All (740) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	27	G
21	AA	28	A
21	AA	32	A
21	AA	35	G
21	AA	36	C
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	49	U
21	AA	50	A

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Mol	Chain	Res	Type
21	AA	51	A
21	AA	55	A
21	AA	56	U
21	AA	61	G
21	AA	66	A
21	AA	69	G
21	AA	70	U
21	AA	86	G
21	AA	95	C
21	AA	108	G
21	AA	109	A
21	AA	120	A
21	AA	124	C
21	AA	130	A
21	AA	131	A
21	AA	144	G
21	AA	159	G
21	AA	165	G
21	AA	180	U
21	AA	183	C
21	AA	191	G
21	AA	198	G
21	AA	211	G
21	AA	214	C
21	AA	240	G
21	AA	244	U
21	AA	247	G
21	AA	251	G
21	AA	252	U
21	AA	258	G
21	AA	259	G
21	AA	266	G
21	AA	282	A
21	AA	289	G
21	AA	305	G
21	AA	306	A
21	AA	308	C
21	AA	316	C
21	AA	328	C
21	AA	329	A
21	AA	345	C
21	AA	352	C

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Mol	Chain	Res	Type
21	AA	353	A
21	AA	354	G
21	AA	367	U
21	AA	369	G
21	AA	372	C
21	AA	373	A
21	AA	381	C
21	AA	382	A
21	AA	383	A
21	AA	392	C
21	AA	397	A
21	AA	406	G
21	AA	412	A
21	AA	413	G
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	462	G
21	AA	463	U
21	AA	465	A
21	AA	466	A
21	AA	468	A
21	AA	493	A
21	AA	499	A
21	AA	511	C
21	AA	519	C
21	AA	524	G
21	AA	525	C
21	AA	527	G
21	AA	532	A
21	AA	547	A
21	AA	559	A
21	AA	560	A
21	AA	561	U
21	AA	563	A
21	AA	564	C
21	AA	565	U
21	AA	573	A
21	AA	576	C
21	AA	589	U
21	AA	607	A
21	AA	608	A

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Mol	Chain	Res	Type
21	AA	615	G
21	AA	632	U
21	AA	633	G
21	AA	653	U
21	AA	665	A
21	AA	687	A
21	AA	700	G
21	AA	704	A
21	AA	755	G
21	AA	761	G
21	AA	762	U
21	AA	764	C
21	AA	765	G
21	AA	777	A
21	AA	779	C
21	AA	794	A
21	AA	812	G
21	AA	816	A
21	AA	828	U
21	AA	841	C
21	AA	842	U
21	AA	843	U
21	AA	844	G
21	AA	845	A
21	AA	846	G
21	AA	913	A
21	AA	914	A
21	AA	926	G
21	AA	927	G
21	AA	933	G
21	AA	934	C
21	AA	935	A
21	AA	939	G
21	AA	942	G
21	AA	944	G
21	AA	959	A
21	AA	960	U
21	AA	961	U
21	AA	966	G
21	AA	968	A
21	AA	971	G
21	AA	976	G

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Mol	Chain	Res	Type
21	AA	977	A
21	AA	980	C
21	AA	981	U
21	AA	991	U
21	AA	993	G
21	AA	996	A
21	AA	1004	A
21	AA	1006	G
21	AA	1025	U
21	AA	1026	G
21	AA	1029	U
21	AA	1030	U
21	AA	1032	G
21	AA	1033	G
21	AA	1053	G
21	AA	1054	C
21	AA	1065	U
21	AA	1081	A
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1130	A
21	AA	1137	C
21	AA	1139	G
21	AA	1143	G
21	AA	1159	U
21	AA	1167	A
21	AA	1168	U
21	AA	1183	U
21	AA	1184	G
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1195	C
21	AA	1196	A
21	AA	1197	A
21	AA	1200	C
21	AA	1201	A
21	AA	1202	U
21	AA	1212	U
21	AA	1213	A

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Mol	Chain	Res	Type
21	AA	1215	G
21	AA	1224	U
21	AA	1225	A
21	AA	1227	A
21	AA	1228	C
21	AA	1229	A
21	AA	1240	U
21	AA	1256	A
21	AA	1257	A
21	AA	1264	U
21	AA	1265	C
21	AA	1279	G
21	AA	1280	A
21	AA	1282	C
21	AA	1285	A
21	AA	1286	U
21	AA	1300	G
21	AA	1301	U
21	AA	1303	C
21	AA	1304	G
21	AA	1305	G
21	AA	1306	A
21	AA	1312	G
21	AA	1320	C
21	AA	1335	U
21	AA	1336	C
21	AA	1337	G
21	AA	1346	A
21	AA	1347	G
21	AA	1378	C
21	AA	1379	G
21	AA	1381	U
21	AA	1423	G
21	AA	1429	A
21	AA	1430	A
21	AA	1446	A
21	AA	1460	C
21	AA	1468	A
21	AA	1481	U
21	AA	1499	A
21	AA	1502	A
21	AA	1503	A

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Mol	Chain	Res	Type
21	AA	1504	G
21	AA	1505	G
21	AA	1506	U
21	AA	1516	G
21	AA	1517	G
21	AA	1529	G
21	AA	1533	C
21	AA	1534	A
22	A1	7	4SU
22	A1	8	U
22	A1	16	C
22	A1	17	U
22	A1	19	G
22	A1	21	A
22	A1	25	C
22	A1	47	U
22	A1	56	C
22	A1	59	U
22	A1	60	C
22	A1	61	C
22	A1	75	C
22	A1	76	A
23	A2	80	C
23	A2	81	U
23	A2	89	U
23	A2	91	A
23	A2	93	U
24	A3	3	C
24	A3	10	G
24	A3	18	U
24	A3	20	G
24	A3	25	U
24	A3	40	C
24	A3	43	G
24	A3	48	U
24	A3	49	C
24	A3	61	U
24	A3	62	C
24	A3	64	G
24	A3	65	G
24	A3	73	A
24	A3	74	A

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Mol	Chain	Res	Type
24	A3	75	C
24	A3	77	A
54	BA	12	U
54	BA	20	C
54	BA	34	U
54	BA	45	G
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	83	A
54	BA	88	G
54	BA	91	A
54	BA	100	U
54	BA	101	A
54	BA	102	U
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	126	A
54	BA	138	U
54	BA	139	U
54	BA	147	C
54	BA	163	C
54	BA	164	C
54	BA	181	A
54	BA	196	A
54	BA	199	A
54	BA	200	U
54	BA	204	A
54	BA	216	A
54	BA	222	A
54	BA	230	G
54	BA	233	A
54	BA	242	G
54	BA	248	G
54	BA	255	A
54	BA	256	A
54	BA	266	G
54	BA	272	A
54	BA	273	G

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Mol	Chain	Res	Type
54	BA	277	G
54	BA	278	A
54	BA	279	A
54	BA	280	U
54	BA	294	A
54	BA	302	C
54	BA	316	C
54	BA	321	U
54	BA	323	C
54	BA	324	A
54	BA	330	A
54	BA	332	A
54	BA	333	G
54	BA	334	C
54	BA	346	A
54	BA	370	G
54	BA	373	U
54	BA	374	A
54	BA	386	G
54	BA	390	U
54	BA	396	G
54	BA	411	G
54	BA	412	A
54	BA	413	C
54	BA	428	A
54	BA	429	A
54	BA	451	U
54	BA	452	G
54	BA	453	A
54	BA	454	A
54	BA	455	C
54	BA	457	A
54	BA	475	C
54	BA	482	A
54	BA	483	A
54	BA	484	C
54	BA	501	A
54	BA	502	A
54	BA	504	A
54	BA	505	A
54	BA	509	C
54	BA	510	C

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Mol	Chain	Res	Type
54	BA	520	G
54	BA	527	C
54	BA	529	A
54	BA	530	G
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	546	U
54	BA	547	A
54	BA	548	G
54	BA	562	U
54	BA	563	A
54	BA	569	U
54	BA	573	U
54	BA	574	A
54	BA	590	A
54	BA	603	A
54	BA	615	U
54	BA	637	A
54	BA	644	A
54	BA	653	U
54	BA	654	A
54	BA	655	A
54	BA	670	A
54	BA	671	C
54	BA	672	C
54	BA	685	A
54	BA	686	U
54	BA	723	C
54	BA	728	G
54	BA	730	A
54	BA	745	G
54	BA	747	U
54	BA	748	G
54	BA	750	A
54	BA	751	A
54	BA	752	A
54	BA	758	C
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A

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Mol	Chain	Res	Type
54	BA	785	G
54	BA	789	A
54	BA	790	U
54	BA	791	C
54	BA	792	A
54	BA	801	G
54	BA	804	A
54	BA	805	G
54	BA	811	U
54	BA	812	C
54	BA	824	U
54	BA	827	U
54	BA	846	U
54	BA	869	G
54	BA	889	C
54	BA	890	C
54	BA	891	G
54	BA	897	C
54	BA	908	C
54	BA	910	A
54	BA	915	C
54	BA	932	U
54	BA	933	A
54	BA	941	A
54	BA	945	A
54	BA	946	C
54	BA	947	A
54	BA	951	C
54	BA	961	C
54	BA	962	G
54	BA	974	G
54	BA	975	A
54	BA	977	G
54	BA	983	A
54	BA	990	A
54	BA	1012	U
54	BA	1013	C
54	BA	1017	G
54	BA	1022	G
54	BA	1026	G
54	BA	1028	A
54	BA	1033	U

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Mol	Chain	Res	Type
54	BA	1034	G
54	BA	1044	C
54	BA	1045	C
54	BA	1055	G
54	BA	1063	G
54	BA	1070	A
54	BA	1071	G
54	BA	1072	C
54	BA	1073	A
54	BA	1076	C
54	BA	1088	A
54	BA	1089	A
54	BA	1090	A
54	BA	1091	G
54	BA	1096	A
54	BA	1112	G
54	BA	1127	A
54	BA	1128	G
54	BA	1129	A
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1142	A
54	BA	1148	U
54	BA	1158	C
54	BA	1176	U
54	BA	1177	G
54	BA	1189	A
54	BA	1204	A
54	BA	1211	C
54	BA	1220	G
54	BA	1224	U
54	BA	1230	A
54	BA	1236	G
54	BA	1237	A
54	BA	1253	A
54	BA	1266	G
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	1303	G
54	BA	1313	U
54	BA	1314	C
54	BA	1332	G
54	BA	1341	G
54	BA	1348	C
54	BA	1365	A
54	BA	1366	A
54	BA	1368	G
54	BA	1378	A
54	BA	1379	U
54	BA	1384	A
54	BA	1385	A
54	BA	1396	U
54	BA	1397	U
54	BA	1398	C
54	BA	1416	G
54	BA	1417	C
54	BA	1419	A
54	BA	1420	A
54	BA	1421	G
54	BA	1427	A
54	BA	1439	A
54	BA	1440	U
54	BA	1455	G
54	BA	1458	U
54	BA	1476	U
54	BA	1477	A
54	BA	1482	G
54	BA	1490	A
54	BA	1497	U
54	BA	1508	A
54	BA	1511	G
54	BA	1538	G
54	BA	1539	U
54	BA	1540	G
54	BA	1541	C
54	BA	1566	A
54	BA	1569	A

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Mol	Chain	Res	Type
54	BA	1578	U
54	BA	1585	C
54	BA	1598	A
54	BA	1602	U
54	BA	1603	A
54	BA	1608	A
54	BA	1616	A
54	BA	1618	A
54	BA	1622	G
54	BA	1626	A
54	BA	1639	C
54	BA	1646	C
54	BA	1648	U
54	BA	1664	A
54	BA	1669	A
54	BA	1670	C
54	BA	1674	G
54	BA	1701	A
54	BA	1713	A
54	BA	1714	U
54	BA	1715	G
54	BA	1730	C
54	BA	1731	G
54	BA	1733	G
54	BA	1739	A
54	BA	1745	A
54	BA	1758	U
54	BA	1764	C
54	BA	1773	A
54	BA	1776	G
54	BA	1786	A
54	BA	1787	A
54	BA	1800	C
54	BA	1801	A
54	BA	1808	A
54	BA	1816	C
54	BA	1821	A
54	BA	1829	A
54	BA	1848	A
54	BA	1900	A
54	BA	1901	A
54	BA	1906	G

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Mol	Chain	Res	Type
54	BA	1913	A
54	BA	1914	C
54	BA	1920	C
54	BA	1931	U
54	BA	1936	A
54	BA	1937	A
54	BA	1940	U
54	BA	1941	C
54	BA	1942	C
54	BA	1943	U
54	BA	1953	A
54	BA	1965	C
54	BA	1966	A
54	BA	1967	C
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1981	A
54	BA	1991	U
54	BA	1993	U
54	BA	1997	C
54	BA	2020	A
54	BA	2021	C
54	BA	2022	U
54	BA	2023	C
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2034	U
54	BA	2037	A
54	BA	2043	C
54	BA	2053	G
54	BA	2055	C
54	BA	2061	G
54	BA	2069	G
54	BA	2077	A
54	BA	2092	U
54	BA	2111	U
54	BA	2113	U
54	BA	2116	G
54	BA	2117	A
54	BA	2119	A

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Mol	Chain	Res	Type
54	BA	2127	G
54	BA	2133	G
54	BA	2138	G
54	BA	2159	G
54	BA	2160	C
54	BA	2164	C
54	BA	2165	C
54	BA	2173	A
54	BA	2174	C
54	BA	2181	U
54	BA	2198	A
54	BA	2203	U
54	BA	2204	G
54	BA	2211	A
54	BA	2212	A
54	BA	2213	U
54	BA	2225	A
54	BA	2238	G
54	BA	2250	G
54	BA	2251	G
54	BA	2267	A
54	BA	2269	G
54	BA	2270	A
54	BA	2275	C
54	BA	2283	C
54	BA	2287	A
54	BA	2296	U
54	BA	2297	A
54	BA	2305	U
54	BA	2309	A
54	BA	2310	C
54	BA	2311	A
54	BA	2312	U
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2332	C
54	BA	2333	A
54	BA	2334	U
54	BA	2335	A
54	BA	2339	C

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Mol	Chain	Res	Type
54	BA	2345	G
54	BA	2346	A
54	BA	2347	C
54	BA	2353	G
54	BA	2383	G
54	BA	2385	C
54	BA	2386	A
54	BA	2389	G
54	BA	2402	U
54	BA	2403	C
54	BA	2406	A
54	BA	2423	U
54	BA	2426	A
54	BA	2428	G
54	BA	2429	G
54	BA	2430	A
54	BA	2431	U
54	BA	2432	A
54	BA	2441	U
54	BA	2447	G
54	BA	2448	A
54	BA	2449	U
54	BA	2469	A
54	BA	2491	U
54	BA	2496	C
54	BA	2499	C
54	BA	2502	G
54	BA	2503	A
54	BA	2504	U
54	BA	2505	G
54	BA	2506	U
54	BA	2518	A
54	BA	2520	C
54	BA	2540	C
54	BA	2548	U
54	BA	2554	U
54	BA	2564	A
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2573	C
54	BA	2576	G

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Mol	Chain	Res	Type
54	BA	2578	G
54	BA	2596	U
54	BA	2609	U
54	BA	2610	C
54	BA	2613	U
54	BA	2615	U
54	BA	2616	C
54	BA	2645	G
54	BA	2646	C
54	BA	2655	G
54	BA	2669	G
54	BA	2683	C
54	BA	2689	U
54	BA	2690	U
54	BA	2707	U
54	BA	2709	G
54	BA	2718	G
54	BA	2729	G
54	BA	2751	G
54	BA	2755	C
54	BA	2761	A
54	BA	2765	A
54	BA	2766	A
54	BA	2777	G
54	BA	2778	A
54	BA	2779	U
54	BA	2780	G
54	BA	2791	G
54	BA	2797	U
54	BA	2798	U
54	BA	2799	A
54	BA	2801	G
54	BA	2816	G
54	BA	2823	A
54	BA	2850	A
54	BA	2868	A
54	BA	2876	G
54	BA	2884	U
54	BA	2895	G
55	BB	13	G
55	BB	15	A
55	BB	16	G

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Mol	Chain	Res	Type
55	BB	34	A
55	BB	35	C
55	BB	36	C
55	BB	42	C
55	BB	44	G
55	BB	45	A
55	BB	48	U
55	BB	51	G
55	BB	52	A
55	BB	67	G
55	BB	88	C
55	BB	89	U
55	BB	107	G
55	BB	108	A
55	BB	109	A

All (222) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	54	C
21	AA	55	A
21	AA	60	A
21	AA	66	A
21	AA	69	G
21	AA	70	U
21	AA	86	G
21	AA	164	G
21	AA	190	A
21	AA	227	G
21	AA	251	G
21	AA	258	G
21	AA	268	U
21	AA	289	G
21	AA	305	G
21	AA	327	A
21	AA	328	C
21	AA	352	C
21	AA	354	G
21	AA	368	U
21	AA	382	A
21	AA	406	G
21	AA	461	A

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Mol	Chain	Res	Type
21	AA	465	A
21	AA	505	G
21	AA	518	C
21	AA	519	C
21	AA	524	G
21	AA	563	A
21	AA	570	G
21	AA	575	G
21	AA	576	C
21	AA	607	A
21	AA	641	U
21	AA	659	U
21	AA	704	A
21	AA	761	G
21	AA	764	C
21	AA	778	G
21	AA	815	A
21	AA	827	U
21	AA	841	C
21	AA	843	U
21	AA	913	A
21	AA	932	C
21	AA	933	G
21	AA	959	A
21	AA	960	U
21	AA	978	A
21	AA	980	C
21	AA	991	U
21	AA	1003	G
21	AA	1025	U
21	AA	1029	U
21	AA	1032	G
21	AA	1053	G
21	AA	1101	A
21	AA	1112	C
21	AA	1124	G
21	AA	1129	C
21	AA	1152	A
21	AA	1181	G
21	AA	1183	U
21	AA	1190	G
21	AA	1195	C

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Mol	Chain	Res	Type
21	AA	1200	C
21	AA	1201	A
21	AA	1215	G
21	AA	1225	A
21	AA	1227	A
21	AA	1278	G
21	AA	1279	G
21	AA	1303	C
21	AA	1305	G
21	AA	1324	A
21	AA	1335	U
21	AA	1336	C
21	AA	1342	C
21	AA	1377	A
21	AA	1411	C
21	AA	1429	A
21	AA	1431	A
21	AA	1451	U
21	AA	1459	G
21	AA	1480	A
21	AA	1529	G
22	A1	7	4SU
22	A1	10	G
22	A1	56	C
22	A1	60	C
22	A1	75	C
23	A2	79	A
23	A2	80	C
23	A2	88	U
23	A2	91	A
24	A3	2	G
24	A3	10	G
24	A3	43	G
24	A3	61	U
24	A3	64	G
24	A3	73	A
54	BA	15	G
54	BA	60	G
54	BA	91	A
54	BA	118	A
54	BA	121	G
54	BA	125	A

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Mol	Chain	Res	Type
54	BA	138	U
54	BA	162	U
54	BA	163	C
54	BA	199	A
54	BA	221	A
54	BA	228	C
54	BA	255	A
54	BA	272	A
54	BA	276	U
54	BA	321	U
54	BA	330	A
54	BA	333	G
54	BA	372	G
54	BA	446	G
54	BA	452	G
54	BA	470	A
54	BA	482	A
54	BA	503	A
54	BA	509	C
54	BA	529	A
54	BA	530	G
54	BA	546	U
54	BA	547	A
54	BA	571	U
54	BA	573	U
54	BA	644	A
54	BA	653	U
54	BA	670	A
54	BA	750	A
54	BA	776	G
54	BA	791	C
54	BA	811	U
54	BA	889	C
54	BA	932	U
54	BA	945	A
54	BA	974	G
54	BA	989	G
54	BA	1045	C
54	BA	1070	A
54	BA	1090	A
54	BA	1095	A
54	BA	1126	A

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Mol	Chain	Res	Type
54	BA	1127	A
54	BA	1128	G
54	BA	1157	G
54	BA	1175	A
54	BA	1210	G
54	BA	1236	G
54	BA	1288	G
54	BA	1300	G
54	BA	1312	U
54	BA	1313	U
54	BA	1367	A
54	BA	1383	A
54	BA	1397	U
54	BA	1419	A
54	BA	1451	C
54	BA	1490	A
54	BA	1537	G
54	BA	1618	A
54	BA	1625	C
54	BA	1647	U
54	BA	1664	A
54	BA	1668	A
54	BA	1713	A
54	BA	1730	C
54	BA	1786	A
54	BA	1787	A
54	BA	1820	U
54	BA	1929	G
54	BA	1936	A
54	BA	1938	A
54	BA	1940	U
54	BA	1943	U
54	BA	1945	G
54	BA	2016	U
54	BA	2020	A
54	BA	2030	A
54	BA	2033	A
54	BA	2163	A
54	BA	2164	C
54	BA	2250	G
54	BA	2266	A
54	BA	2282	G

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Mol	Chain	Res	Type
54	BA	2286	G
54	BA	2296	U
54	BA	2312	U
54	BA	2332	C
54	BA	2385	C
54	BA	2389	G
54	BA	2391	G
54	BA	2425	A
54	BA	2428	G
54	BA	2430	A
54	BA	2447	G
54	BA	2495	G
54	BA	2503	A
54	BA	2505	G
54	BA	2564	A
54	BA	2565	A
54	BA	2602	A
54	BA	2612	C
54	BA	2615	U
54	BA	2645	G
54	BA	2689	U
54	BA	2708	G
54	BA	2726	A
54	BA	2776	A
54	BA	2777	G
54	BA	2780	G
54	BA	2826	A
55	BB	12	C
55	BB	51	G
55	BB	66	A
55	BB	107	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CM0	A1	34	22,23	15,26,27	1.90	3 (20%)	18,37,40	3.09	3 (16%)
22	6MZ	A1	37	22	17,25,26	0.95	1 (5%)	15,36,39	1.27	1 (6%)
22	7MG	A1	46	22	20,26,27	2.21	3 (15%)	23,39,42	2.11	2 (8%)
22	5MU	A1	54	22	13,22,23	1.04	1 (7%)	16,32,35	4.65	2 (12%)
22	PSU	A1	55	22	15,21,22	1.08	1 (6%)	16,30,33	3.50	4 (25%)
22	4SU	A1	7	22	12,21,22	0.94	0	15,30,33	2.24	2 (13%)
24	H2U	A3	21	24	17,21,22	1.42	2 (11%)	23,30,33	1.32	4 (17%)
24	OMC	A3	33	24	15,22,23	1.03	0	20,31,34	0.87	0
24	5MU	A3	55	24	13,22,23	1.14	1 (7%)	16,32,35	4.44	2 (12%)
24	PSU	A3	56	24	15,21,22	1.19	1 (6%)	16,30,33	3.46	5 (31%)
24	4SU	A3	8	24	12,21,22	1.18	2 (16%)	15,30,33	2.28	1 (6%)

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

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.31	1.33	1.45
22	A1	34	CM0	O5-C5	-5.83	1.25	1.37
24	A3	21	H2U	C4-N3	-3.40	1.32	1.37
24	A3	21	H2U	C2-N3	-3.25	1.31	1.38
22	A1	46	7MG	C8-N7	-2.77	1.30	1.43
22	A1	37	6MZ	C8-N7	-2.04	1.30	1.34
24	A3	8	4SU	O4'-C1'	2.02	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	56	PSU	C4-N3	2.25	1.37	1.33
22	A1	55	PSU	C4-N3	2.26	1.37	1.33
24	A3	8	4SU	C6-N1	2.32	1.38	1.35
22	A1	54	5MU	C4-N3	2.47	1.37	1.33
22	A1	34	CM0	C4-N3	2.60	1.37	1.33
22	A1	34	CM0	C4-C5	2.69	1.47	1.40
22	A1	46	7MG	C6-N1	2.72	1.37	1.33
24	A3	55	5MU	C4-N3	2.91	1.38	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-12.75	114.64	125.35
24	A3	55	5MU	C5-C4-N3	-12.43	114.92	125.35
24	A3	8	4SU	C5-C4-N3	-8.18	114.89	123.56
22	A1	7	4SU	C5-C4-N3	-7.70	115.39	123.56
22	A1	46	7MG	C5-C6-N1	-6.71	113.39	123.39
22	A1	55	PSU	C5-C6-N1	-3.24	119.86	124.38
22	A1	55	PSU	C5-C1'-C2'	-3.07	110.21	115.44
24	A3	56	PSU	C5-C1'-C2'	-3.06	110.23	115.44
24	A3	56	PSU	C5-C6-N1	-2.94	120.28	124.38
24	A3	56	PSU	C4'-O4'-C1'	-2.22	107.25	109.54
24	A3	21	H2U	O2-C2-N3	-2.20	117.11	121.44
22	A1	34	CM0	O4'-C1'-N1	2.10	112.09	108.10
24	A3	21	H2U	C5-C6-N1	2.24	113.22	110.76
22	A1	7	4SU	O4'-C4'-C3'	2.32	109.86	105.16
24	A3	21	H2U	C5-C4-N3	2.72	119.49	116.62
22	A1	34	CM0	C7-O5-C5	2.91	123.17	117.83
24	A3	56	PSU	O4'-C1'-C2'	3.04	107.98	104.69
24	A3	21	H2U	N3-C2-N1	3.08	119.49	116.64
22	A1	37	6MZ	C2-N1-C6	3.57	119.04	116.47
22	A1	55	PSU	O4'-C1'-C2'	3.83	108.83	104.69
22	A1	46	7MG	C6-N1-C2	6.77	123.81	115.88
22	A1	34	CM0	C4-N3-C2	12.05	125.22	115.16
22	A1	55	PSU	C4-N3-C2	12.20	125.33	115.16
24	A3	56	PSU	C4-N3-C2	12.28	125.40	115.16
24	A3	55	5MU	C4-N3-C2	12.30	125.42	115.16
22	A1	54	5MU	C4-N3-C2	13.14	126.12	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	VAL	A1	101	58,22	5,6,7	0.63	0	5,7,9	2.08	1 (20%)
58	FME	BA	3001	57	8,9,10	0.72	0	5,9,11	1.24	0

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-4.20	114.21	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.