



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:08 PM BST

PDB ID : 4V74  
EMDB ID: : EMD-1720  
Title : 70S-fMetVal-tRNAVal-tRNAfMet complex in hybrid pre-translocation state (pre5b)  
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 : 17.00 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

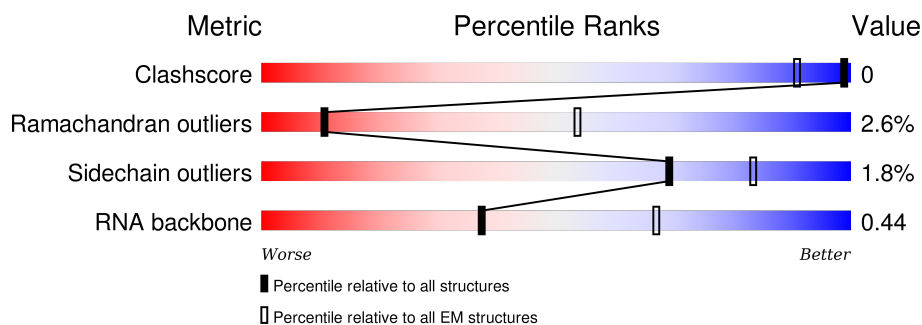
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 17.00 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.















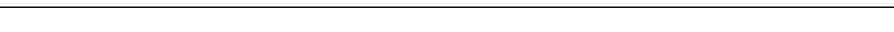

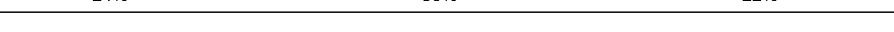
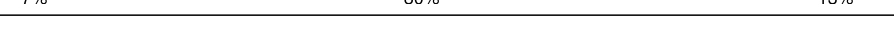
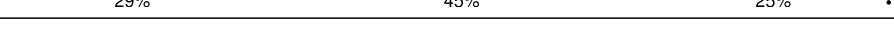





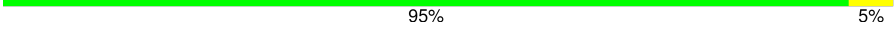


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	95% 5% •
2	AC	208	89% 10%
3	AD	206	88% 12%
4	AE	152	89% 11% •
5	AF	101	90% 9% •
6	AG	152	87% 13% •
7	AH	130	89% 10% •
8	AI	128	82% 16% •


















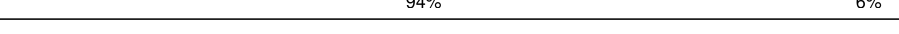



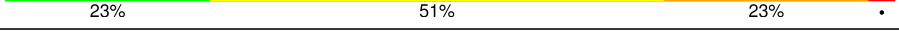
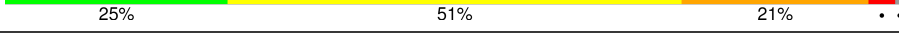
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Mol	Chain	Length	Quality of chain
9	AJ	100	 84% 15% .
10	AK	118	 92% 7% .
11	AL	124	 83% 15% ..
12	AM	115	 85% 14% .
13	AN	101	 86% 13% .
14	AO	89	 85% 13% .
15	AP	81	 84% 16%
16	AQ	82	 91% 9%
17	AR	57	 79% 21%
18	AS	81	 88% 11% .
19	AT	86	 93% 7%
20	AU	53	 79% 21%
21	AA	1533	 25% 49% 22% .
22	A1	76	 24% 50% 22% .
23	A2	15	 7% 80% 13%
24	A3	77	 29% 45% 25% .
25	BC	273	 87% 12%
26	BD	209	 90% 9%
27	BE	201	 91% 9%
28	BF	179	 89% 11% .
29	BG	177	 89% 11% .
30	BH	149	 95% 5%
31	BI	142	 94% 5% .
32	BJ	142	 90% 10%
33	BK	123	 88% 11% ..

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Mol	Chain	Length	Quality of chain
34	BL	144	
35	BM	136	
36	BN	121	
37	BO	117	
38	BP	115	
39	BQ	118	
40	BR	103	
41	BS	110	
42	BT	94	
43	BU	104	
44	BV	94	
45	BW	80	
46	BX	79	
47	BY	63	
48	BZ	59	
49	B0	57	
50	B1	52	
51	B2	46	
52	B3	65	
53	B4	38	
54	BA	2903	
55	BB	118	
56	B5	234	

## 2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

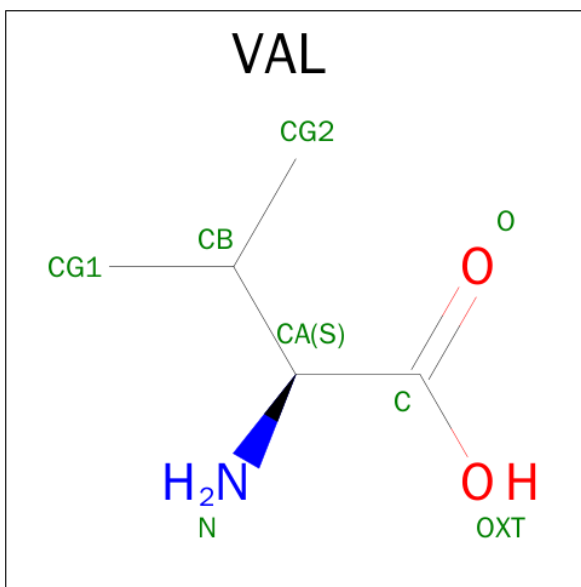
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

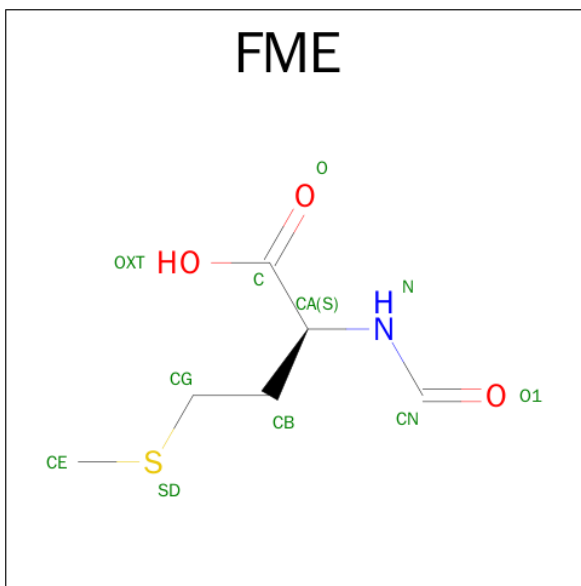
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



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

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



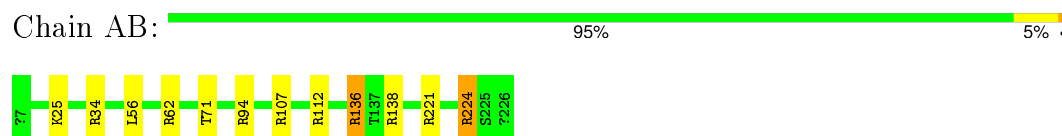
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



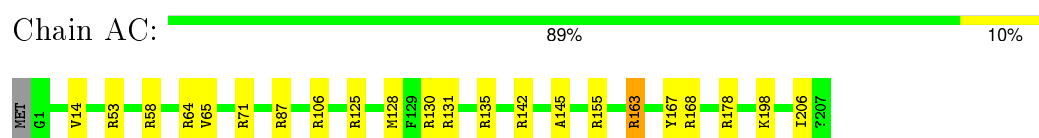
### 3 Residue-property plots

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

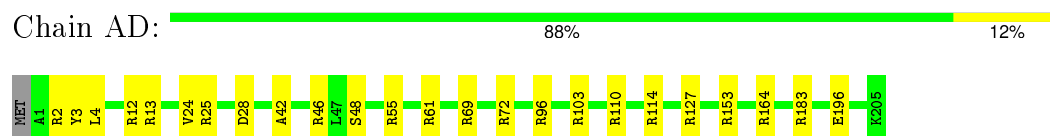
- Molecule 1: 30S ribosomal protein S2



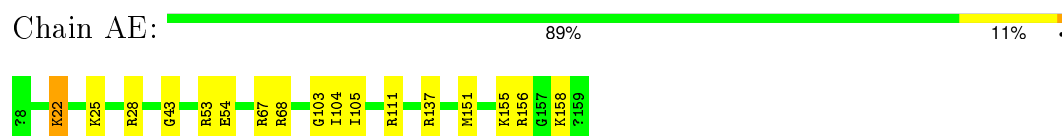
- Molecule 2: 30S ribosomal protein S3



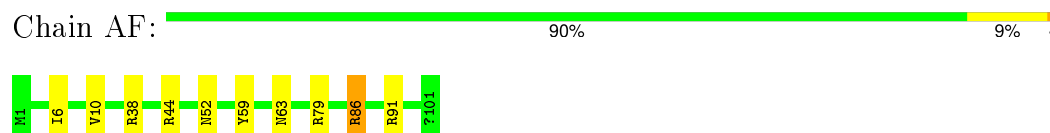
- Molecule 3: 30S ribosomal protein S4



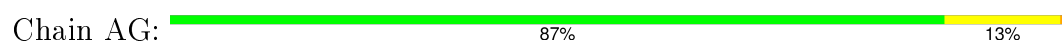
- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



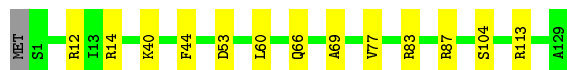
- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 89% 10%



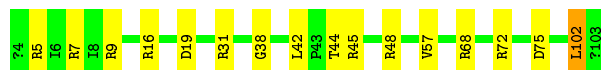
- Molecule 8: 30S ribosomal protein S9

Chain AI: 82% 16%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 84% 15%



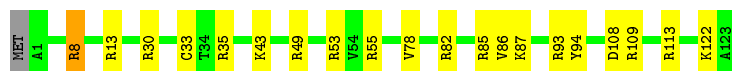
- Molecule 10: 30S ribosomal protein S11

Chain AK: 92% 7%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 83% 15%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%




- Molecule 13: 30S ribosomal protein S14

Chain AN: 86% 13%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  85% 13%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  84% 16%




- Molecule 16: 30S ribosomal protein S17

Chain AQ:  91% 9%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  79% 21%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  88% 11%




- Molecule 19: 30S ribosomal protein S20

Chain AT:  93% 7%



- Molecule 20: 30S ribosomal protein S21

Chain AU:  79% 21%



- Molecule 21: 16S ribosomal RNA

Chain AA:  25% 49% 22%

A1036	A1037	C1038	G1039	A1042	G1043	A1044	C1045	G1046	A1047	G1048	C1049	A1050	G1051	C1052	G1053	C1054	A1055	G1056	C1057	G1058	C1059	A1060	G1061	C1062	G1063	C1064	A1065	G1066	C1067	G1068	C1069	G1070	C1071	G1075	C1076	G1077	C1078	G1079	A1080	C1081	A1082	G1083	C1084	G1085	C1086	A1092	C1093	G1094	C1095	G1096	C1097	G1098	C1099	A1100	G1101	C1102	A1103	G1104	C1105	A1106	G1107	C1108	A1109	G1110	C1111	G1114	C1115	A1116	G1117	C1118	A1119	G1120	C1121	G1122	C1123	A1124	G1125	C1126	A1129	G1130	C1131	A1132	G1133	C1134	A1135	G1136	C1137	A1138	G1139	C1140	A1141	G1142	C1143	A1144	G1145	C1146	A1147	G1148	C1149	A1150	G1151	C1152	A1153	G1154	C1155	A1156	G1157	C1158	A1159	G1160	C1161	A1162	G1163	C1164	A1165	G1166	C1167	A1168	G1169	C1170	A1171	G1172	C1173	A1174	G1175	C1176	A1177	G1178	C1179	A1180	G1181	C1182	A1183	G1184	C1185	A1186	G1187	C1188	A1189	G1190	C1191	A1192	G1193	C1194	A1195	G1196	C1197	A1198	G1199	C1200	A1201	G1202	C1203	A1204	G1205	C1206	A1207	G1208	C1209	A1210	G1211	C1212	A1213	G1214	C1215	A1216	G1217	C1218	A1219	G1220	C1221	A1222	G1223	C1224	A1225	G1226	C1227	A1228	G1229	C1230	A1231	G1232	C1233	A1234	G1235	C1236	A1237	G1238	C1239	A1240	G1241	C1242	A1243	G1244	C1245	A1246	G1247	C1248	A1249	G1250	C1251	A1252	G1253	C1254	A1255	G1256	C1257	A1258	G1259	C1260	A1261	G1262	C1263	A1264	G1265	C1266	A1267	G1268	C1269	A1270	G1271	C1272	A1273	G1274	C1275	A1276	G1277	C1278	A1279	G1280	C1281	A1282	G1283	C1284	A1285	G1286	C1287	A1288	G1289	C1290	A1291	G1292	C1293	A1294	G1295	C1296	A1297	G1298	C1299	A1300	G1301	C1302	A1303	G1304	C1305	A1306	G1307	C1308	A1309	G1310	C1311	A1312	G1313	C1314	A1315	G1316	C1317	A1318	G1319	C1320	A1321	G1322	C1323	A1324	G1325	C1326	A1327	G1328	C1329	A1330	G1331	C1332	A1333	G1334	C1335	A1336	G1337	C1338	A1339	G1340	C1341	A1342	G1343	C1344	A1345	G1346	C1347	A1348	G1349	C1350	A1351	G1352	C1353	A1354	G1355	C1356	A1357	G1358	C1359	A1360	G1361	C1362	A1363	G1364	C1365	A1366	G1367	C1368	A1369	G1370	C1371	A1372	G1373	C1374	A1375	G1376	C1377	A1378	G1379	C1380	A1381	G1382	C1383	A1384	G1385	C1386	A1387	G1388	C1389	A1390	G1391	C1392	A1393	G1394	C1395	A1396	G1397	C1398	A1399	G1400	C1401	A1402	G1403	C1404	A1405	G1406	C1407	A1408	G1409	C1410	A1411	G1412	C1413	A1414	G1415	C1416	A1417	G1418	C1419	A1420	G1421	C1422	A1423	G1424	C1425	A1426	G1427	C1428	A1429	G1430	C1431	A1432	G1433	C1434	A1435	G1436	C1437	A1438	G1439	C1440	A1441	G1442	C1443	A1444	G1445	C1446	A1447	G1448	C1449	A1450	G1451	C1452	A1453	G1454	C1455	A1456	G1457	C1458	A1459	G1460	C1461	A1462	G1463	C1464	A1465	G1466	C1467	A1468	G1469	C1470	A1471	G1472	C1473	A1474	G1475	C1476	A1477	G1478	C1479	A1480	G1481	C1482	A1483	G1484	C1485	A1486	G1487	C1488	A1489	G1490	C1491	A1492	G1493	C1494	A1495	G1496	C1497	A1498	G1499	C1500	A1501	G1502	C1503	A1504	G1505	C1506	A1507	G1508	C1509	A1510	G1511	C1512	A1513	G1514	C1515	A1516	G1517	C1518	A1519	G1520	C1521	A1522	G1523	C1524	A1525	G1526	C1527	A1528	G1529	C1530	A1531	G1532	C1533	A1534	G1535	C1536	A1537	G1538	C1539	A1540	G1541	C1542	A1543	G1544	C1545	A1546	G1547	C1548	A1549	G1550	C1551	A1552	G1553	C1554	A1555	G1556	C1557	A1558	G1559	C1560	A1561	G1562	C1563	A1564	G1565	C1566	A1567	G1568	C1569	A1570	G1571	C1572	A1573	G1574	C1575	A1576	G1577	C1578	A1579	G1580	C1581	A1582	G1583	C1584	A1585	G1586	C1587	A1588	G1589	C1590	A1591	G1592	C1593	A1594	G1595	C1596	A1597	G1598	C1599	A1600	G1601	C1602	A1603	G1604	C1605	A1606	G1607	C1608	A1609	G1610	C1611	A1612	G1613	C1614	A1615	G1616	C1617	A1618	G1619	C1620	A1621	G1622	A1623	C1624	A1625	G1626	C1627	A1628	G1629	C1630	A1631	G1632	C1633	A1634	G1635	C1636	A1637	G1638	C1639	A1640	G1641	C1642	A1643	G1644	C1645	A1646	G1647	C1648	A1649	G1650	C1651	A1652	G1653	C1654	A1655	G1656	C1657	A1658	G1659	C1660	A1661	G1662	C1663	A1664	G1665	C1666	A1667	G1668	C1669	A1670	G1671	C1672	A1673	G1674	C1675	A1676	G1677	C1678	A1679	G1680	C1681	A1682	G1683	C1684	A1685	G1686	C1687	A1688	G1689	C1690	A1691	G1692	C1693	A1694	G1695	C1696	A1697	G1698	C1699	A1700	G1701	C1702	A1703	G1704	C1705	A1706	G1707	C1708	A1709	G1710	C1711	A1712	G1713	C1714	A1715	G1716	C1717	A1718	G1719	C1720	A1721	G1722	C1723	A1724	G1725	C1726	A1727	G1728	C1729	A1730	G1731	C1732	A1733	G1734	C1735	A1736	G1737	C1738	A1739	G1740	C1741	A1742	G1743	C1744	A1745	G1746	C1747	A1748	G1749	C1750	A1751	G1752	A1753	C1754	A1755	G1756	C1757	A1758	C1759	A1760	G1761	C1762	A1763	G1764	C1765	A1766	G1767	C1768	A1769	G1770	C1771	A1772	G1773	C1774	A1775	G1776	C1777	A1778	G1779	C1780	A1781	G1782	C1783	A1784	G1785	C1786	A1787	G1788	C1789	A1790	G1791	C1792	A1793	G1794	C1795	A1796	G1797	C1798	A1799	G1800	C1801	A1802	G1803	C1804	A1805	G1806	C1807	A1808	G1809	C1810	A1811	G1812	C1813	A1814	G1815	C1816	A1817	G1818	C1819	A1820	G1821	C1822	A1823	G1824	C1825	A1826	G1827	C1828	A1829	G1830	C1831	A1832	G1833	C1834	A1835	G1836	C1837	A1838	G1839	C1840	A1841	G1842	C1843	A1844	G1845	C1846	A1847	G1848	C1849	A1850	G1851	C1852	A1853	G1854	C1855	A1856	G1857	C1858	A1859	G1860	C1861	A1862	G1863	C1864	A1865	G1866	C1867	A1868	G1869	C1870	A1871	G1872	C1873	A1874	G1875	C1876	A1877	G1878	C1879	A1880	G1881	C1882	A1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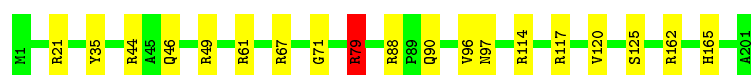
- Molecule 26: 50S ribosomal protein L3

Chain BD: 90% 9%



- Molecule 27: 50S ribosomal protein L4

Chain BE: 91% 9%



- Molecule 28: 50S ribosomal protein L5

Chain BF: 89% 11%



- Molecule 29: 50S ribosomal protein L6

Chain BG: 89% 11%



- Molecule 30: 50S ribosomal protein L9

Chain BH: 95% 5%



- Molecule 31: 50S ribosomal protein L11

Chain BI: 94% 5%



- Molecule 32: 50S ribosomal protein L13

Chain BJ: 90% 10%



- Molecule 33: 50S ribosomal protein L14

Chain BK: 88% 11% ..



- Molecule 34: 50S ribosomal protein L15

Chain BL: 85% 13% ..



- Molecule 35: 50S ribosomal protein L16

Chain BM: 85% 15%



- Molecule 36: 50S ribosomal protein L17

Chain BN: 87% 12% .



- Molecule 37: 50S ribosomal protein L18

Chain BO: 87% 11% ..



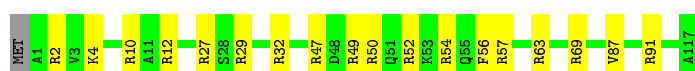
- Molecule 38: 50S ribosomal protein L19

Chain BP: 87% 12% .

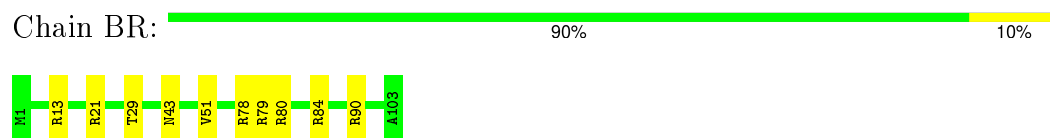


- Molecule 39: 50S ribosomal protein L20

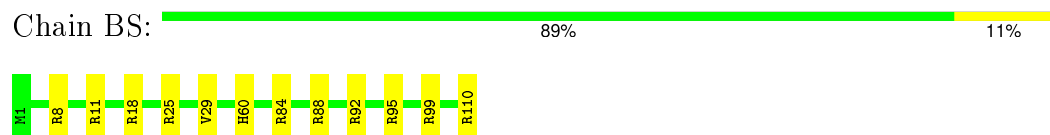
Chain BQ: 84% 15%



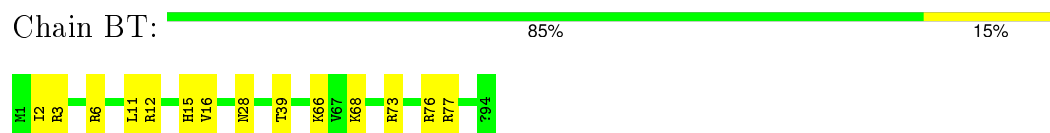
- Molecule 40: 50S ribosomal protein L21



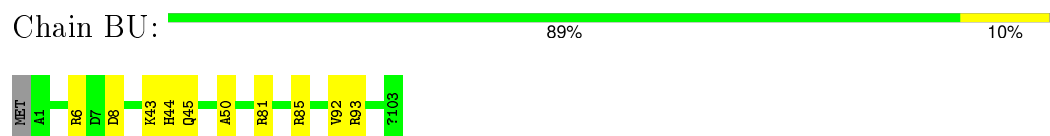
- Molecule 41: 50S ribosomal protein L22



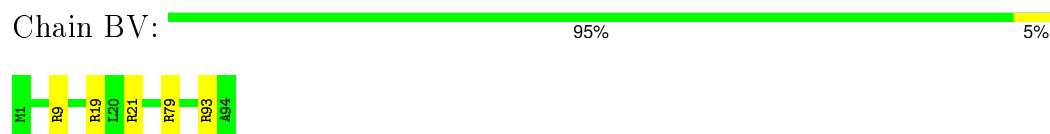
- Molecule 42: 50S ribosomal protein L23



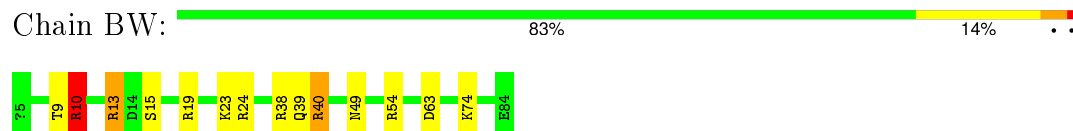
- Molecule 43: 50S ribosomal protein L24



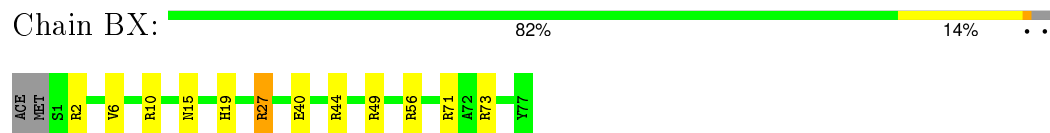
- Molecule 44: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L28




- Molecule 47: 50S ribosomal protein L29



Chain BY:  90% 10%




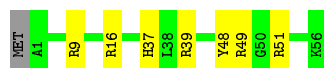
- Molecule 48: 50S ribosomal protein L30

Chain BZ:  83% 15%



- Molecule 49: 50S ribosomal protein L32

Chain B0:  86% 12%




- Molecule 50: 50S ribosomal protein L33

Chain B1:  94% 6%




- Molecule 51: 50S ribosomal protein L34

Chain B2:  78% 22%




- Molecule 52: 50S ribosomal protein L35

Chain B3:  85% 14%

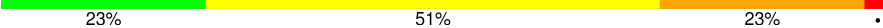


- Molecule 53: 50S ribosomal protein L36

Chain B4:  87% 13%

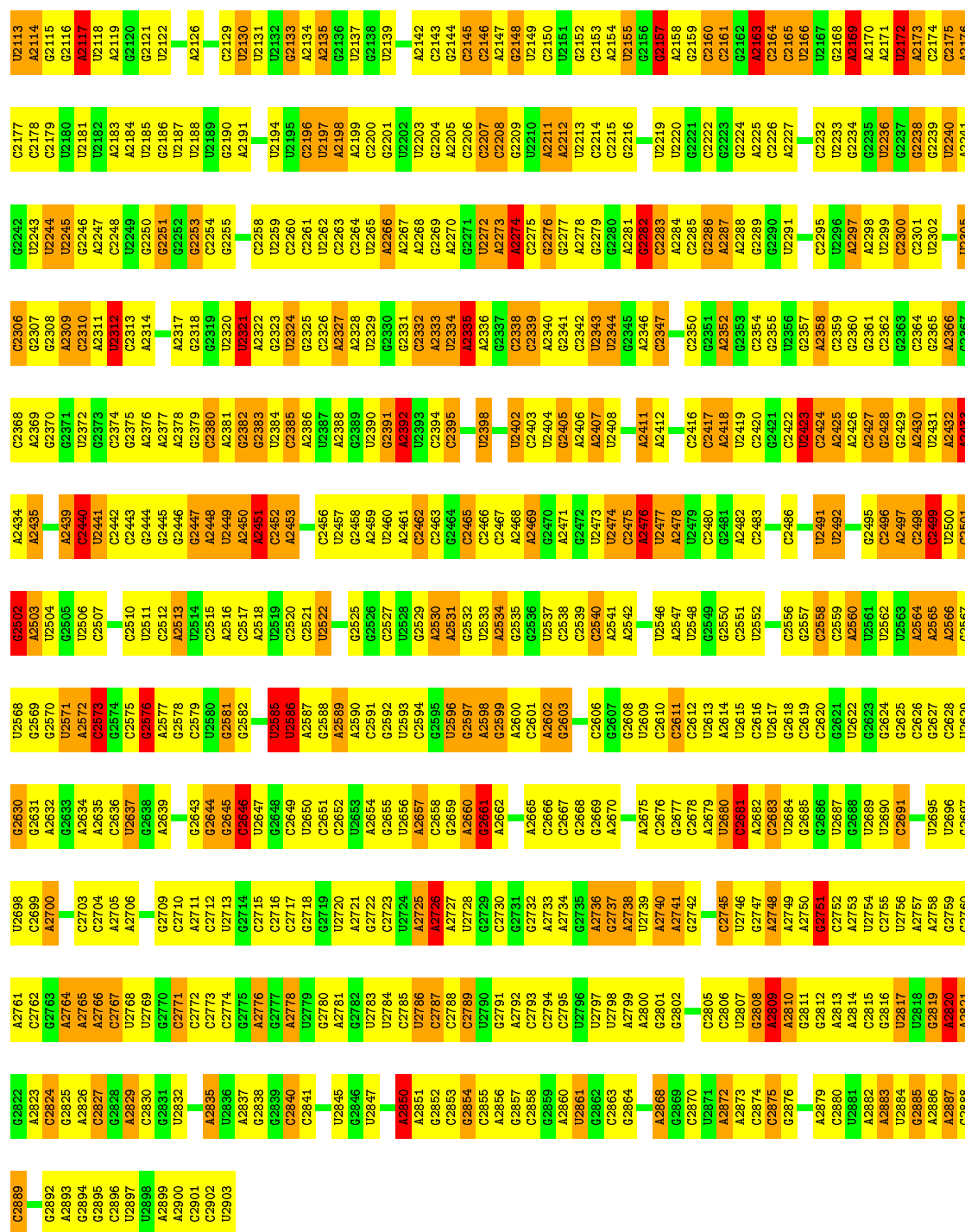


- Molecule 54: 23S ribosomal RNA

Chain BA:  23% 51% 23%

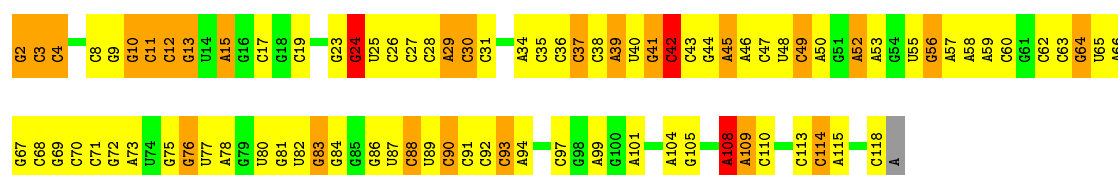
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A1027	G966	G904	C840	G776	U709	U642	U580	C517	U451	G388	A265	C201	A131	G68	G2
A1028	U967	A905	A843			A843	C581	G518	A452	G389	G266	U202		G69	U3
A1029	G968	U906	A844	U779	A715	A644	A582		A453	U390	C267	A203		G70	U4
G1030	G969	G907	A845	G780	A716	U645	G583	A521	A454	A391	C268	A204		A71	A5
G1031	U970	C908	A846	U781	C717	U646	C584	A522	A455	U392	C269	G205		U72	A6
A1032	G971	A909	U846	A782	A718	G647	C585	C523	A456	U393	A270	U206		A73	G7
A1033	A972	A910	U847	A783	C719		A586	G524	A457	C394	G271	A207		A74	C8
G1034	A973	A911	C848	G784	U720	C650	C587	G525	U458	U395	A272	C208		G75	G9
U1035	A974	G912	A849	C785	A721	U651	U588	A526	U459	C396	C273	C209		A76	C10
	A975	U913	U850	C786	A722	U652	U589	C527	U460	C397	C274	C210		A77	C11
		G914	C851	C787	G723	U653	U590	A528	C461	C398	C275	C211		U78	U12
A1039	G978	C915	U852	A788	U724	A654	U591	A529	C462	G400	U276	G212		C79	U13
A1040	A979	G916	C853	A789	G725	A655	A592	G530	G463	A401	G277	A213		G80	A14
C1043	A980	A917	C854	U790	G726	A656	U593	C531		A402	A278	G214		G81	G15
C1044	A981	A918	C855	C791	A727	U657	U594	A532	A466	U403	C279	G215		U82	C16
C1045	C982	U919	G856	U792	A727		C595	G533		U404	C280	A216		A83	A19
A1046	A983	A920	C857	A793	A730	C660	U596		A470	U405	C281	A217		A84	C20
G1047	A984	C921	C858	A794	C731	A661		G537	A471	G406	A282	A218			C21
A1048	C985	G922	C859	C795	C732		A599	A538	A472	G407	G283	A219		A89	A22
C1049	C986	G923	U860	C796	G733	G664	G600	G539	G473	G408	G284	G220		U90	C22
A1050	C987	G924	A861		A734	U665	C601	C540	A474	G409	G285	A221		A91	
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G1055	G992	U929	A866	U803	A739	A670	U606	U545	A479	C414	G291	A226		C96	C32
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A1057	C994	U931	U868	G905	U741	C672	A609	A547	C481	U416	A294	G228		G98	U34
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U1062	U999	A936	C874	U810	U747	A677	A613	U552	C486	C421	A300	A233		A103	G39
G1063	C1000	C937	G875	U811	G748	C678	A614	G553	C487	A422	G301			A104	C41
C1064		G938	C876	C812	A749	C679	U615	U554		A423	C302	C237		C105	C42
A1067	G1002	G939	A877	U813	A750	C680	A616	G555	C490		G303	C238		C106	A44
G1068	U1003	G940	A878	C814	A751	G681	G617	A556	C491	C426	C304	C239		G107	G43
A1069	C1004	A941		C815	A752			C557	A492	U427	U304	C239		G108	A44
A1070	U1005	G942	C881	C816	A753	U685	G620	U558	G493	A428	C305	C240		G109	G45
G1071	C1006	A943	C882	C817	U754	U686	A621	G559	A494	A429	U306	A241		G110	G46
A1072	C1007	C944	U883	C818	U755	C887	G622	C560	G495	A430	G307	G242		G111	C47
A1073	U1008	A945	U884	A819	U756	U688	C623	G561	C496	U431	G308	U243		C179	A111
A1074	A1009	C946	C885	A820	G757	A689	C624	U562	A497	A432	A309	A244		U114	G48
G1075	C1010	A947	A886	A821	C758	G900	G625	A563		C433	A310	G245		C115	A49
C1076	U1012	U948	U887	G822	G759	C691	A626	C564	G500	G434	G312	G246		C116	U50
A1077	C1013		C888	C823	G760	C692	A627	C565	A501	U373	G313	G247		G117	A52
U1078	A1014	C951	C889	U824	A761	A693	G628	U566	A502	A374	G314	G248		A118	G51
C1079	U1015		C890	A825	U762	U694	G629	U567	A503	G375	C314	C249		A119	A53
A1080	G1016	G954	C891		G763	G695	G630	U568	A504	G376	G315	G250		G188	A56
	G1017	U955	A892	U828	A764		A631	U569	A505	G377	C316	A251		G189	C57
U1083	U1018	G956	C893	A829	C765	C698	A632	G570	G506	C378	G317	G252		G190	G58
A1084	U1019	U958		G830	U766	A699	A633	U571	A507	G442	C318	C253		G191	U59
A1085	A1020	C959	C897	G831	U767	C700	C634	A443	A508	A443	G319	G254		U193	G60
A1086	A1021	A960	C898	U832		U703	C635	U573	C509	C444	A320	A255		G194	C61
G1087	G1022	C961	A899	A833	G770	G704	G636	A574	C510	C445	U321	A256		A126	U62
A1088	U1023	G962	A900	G834	G771	A705	A637	A575		G446	C322	C257		A127	A63
A1089	G1024	U963	A706	C835	C772	A706	G638	U576	A513	A447	C323			A196	A64
A1090	G1025	C964	G707	C838	G774		U639	G577	A514	U448	C324	A262		C198	U65
							C640	G578	A515	A449	G325	G263		A199	C66

A2051	G1984	G1993	G1861	G1797	G1733	G1671	A1608	G1546	G1483	U1415	C1349	A1286	C1221	G1157	G1091
A2052	C1985	C1924	G1862	U1798	G1734	A1672	A1609	C1547	U1484	G1416	C1350	A1287	U1222	C1158	C1092
G2053	C1986	G1925	G1863	G1799	A1735	G1673	A1610	A1548		C1417	C1351	G1288	G1223		U1093
A2054	A1987	U1926	U1864	C1800	G1736	G1674	C1611	A1549	U1487	G1418	U1352	C1289		C1161	U1094
C2055		A1927	U1865	A1801	G1737	C1675	G1612	C1550	C1489	A1419	A1353	C1291	A1226	G1163	A1095
G2056	G1990	A1928	A1866	A1802	G1738	C1676	G1613	A1551	C1489	A1420	A1354	C1291	G1227	G1164	A1096
G2057	U1991	G1929	G1867	A1803	A1739	A1677	A1614	A1552	A1490	G1421	G1355	G1292	G1228		U1097
A2058	G1992	U1930	C1868	C1804	A1739	A1678	C1615	A1553	G1491		G1356	C1293	C1229	A1165	A1098
A2059	U1993	U1931	G1869	A1805	C1741	A1679	A1616	U1554	G1492		C1357	U1294	A1230	G1166	G1099
A2060	C1994	A1932	C1870	C1806	U1742	G1680	C1617	G1555	C1493	A1427	G1358	C1295	U1231	C1167	C1100
G2061	U1995	G1933	A1871	G1807	G1743	G1681	A1618	C1556	A1494	A1428	G1359	G1296	G1232	G1168	U1101
A2062	C1996	C1934	A1872	A1808	A1744	G1682	G1619	C1557	A1495	C1428	G1360	C1297	G1233		C1102
C2063	C1997	G1935	G1873	A1809	A1745	G1683	G1620	C1558	A1496	G1429	G1361	C1298	C1233		A1103
C2064	A1998	A1936	C1874	A1810	A1746	G1684	U1621	U1559	U1497	G1430	C1362	G1299	G1236	G1171	C1104
C2065	C1999	A1937	G1875	G1811	U1747	C1685	G1622	G1560	C1498	A1431	C1363	G1300	A1237		
C2066	C2000	A1938	A1876	U1812	C1748	C1686	G1623	G1561	C1499	G1432	G1364	A1301	G1238	U1172	U1108
G2067	C2001	U1939	A1877	G1813	A1749		U1624	U1562	G1500	A1433	A1365	A1302	G1239	U1173	C1109
G2068	U1940	G1814	G1878	G1814		A1689	C1625	U1563	G1501	A1434	A1366	G1303	U1240	A1174	C1110
G2069	A2003	C1941	C1879	A1815	C1752	A1690	A1626	C1564	A1502	G1435	A1367	A1304	A1241	U1176	A1111
G2070	G2004	C1942	U1880	C1816	G1753	C1691	G1627	C1565	A1503	G1436		C1305	U1242		G1112
A2071	A2005	U1944	C1817	G1817	A1754	G1692	G1628	C1566	A1504	A1437	C1370	C1306	U1243	G1177	U1113
C2072	C2006	U1945	U1818	U1818	A1755	U1693	U1629	G1567	A1505	U1438	G1371	A1307	A1244	G1178	U1113
C2073	U2007	G1945	A1819	G1819	G1756	C1694	A1630	G1568	U1506	A1439	U1372	A1308	G1245	G1179	C1114
U2074	C2008	G1946	G1884	G1820	A1757	G1695	G1631	A1569	C1507	G1440	A1373		A1246		G1115
U2075	U2074	U1947	A1885	U1821	U1758	G1696	A1632	A1570	A1508	G1441		U1312	A1247	U1183	G1116
U2076	G1948	G1948	C1887	C1822	A1759	G1697	G1633	A1571	A1509	U1442	C1376		A1247	U1184	C1117
A2077	G1949	G1949	G1888	G1823	A1759	A1698	A1634	A1572	G1510			U1313		G1185	C1118
A2078	A2013	U1955	C1894	A1829	G1766	C1704	A1640	U1578			A1384	C1319	G1256	G1191	A1126
U2079	A2014	C1950	A1889	G1830	G1767	A1705	G1642	A1579	C1518	G1445	A1385	A1321	G1257	G1192	A1127
A2080	U2015	U1951	A1890	U1825	C1761	G1699	A1635	A1579	G1511	G1453	A1386	A1322	G1258	G1193	A1128
U2081	A2016	A1952	G1891	G1826	A1762	A1700	U1636	A1580	C1512	C1446	C1387	C1323	G1259	A1194	
U2082	U2017	A1953	C1892	U1827	G1764	G1702	G1643	G1581	U1520	C1447	G1388	G1324	A1260	G1195	A1129
A2082	G2018	G1954	C1893	G1828	U1765	G1703	C1638	C1582	G1521	G1456	G1388	G1324	C1261	C1196	
A2083	A2019	U1955	C1894	A1829	G1766	C1704	A1640	U1578	A1522	U1457	G1389	U1325	A1262	G1197	U1132
C2084	A2020	U1956	C1895	G1830	C1767	A1705	G1642	A1584	U1523	U1460	U1390	U1326	U1263	U1198	A1133
C2085	C2021	C1957	G1896	G1831	C1768	C1706	U1641	A1585	G1524	C1461	A1392	A1328	A1265	U1199	A1134
U2086	U2022	G1958	G1897	C1832	U1769	G1707	G1643	A1586	C1526	C1462	A1393	U1329	G1266	U1201	C1135
C2087	C2023	G1959	C1898	C1833	G1770	C1708	G1644	A1583	G1527	C1463	U1394	G1330	U1267	G1202	G1139
G2088	G2024	A1960	A1899	U1834	C1771		G1645	A1583	A1528	G1464	A1395	G1331	A1268	U1203	G1140
A2090	C2025	C1961	A1900	G1835	A1772	U1711	C1646	U1584	C1531		U1396	G1332	A1269	A1204	U1141
C2091	A2030	U1962	A1901	C1836	A1773	U1712	U1647	A1585	C1532		U1397	G1333	C1270	A1205	A1142
G2092	A2031	G1964	C1902	C1837	C1774	A1713	U1648	A1586	C1533	A1469	C1398	G1334	G1271	G1206	A1143
G2093	G2032	C1965	C1905	G1839	U1775	G1715	G1649	A1590	C1534		U1398	G1335	A1272	C1207	A1144
A2094	A2033	A1966	G1906	U1840	A1780	G1716	G1651	A1591	C1535		U1399	G1336	U1273	C1208	C1145
A2095	U2034	C1967	U1907	U1841	U1781	A1717	A1652	C1592	C1536	G1474	U1399	A1342	A1274	U1209	C1146
C2096	G2035	G1968	C1908	G1842	U1782	G1718	G1653	A1593	C1537		U1400	G1337	G1275	G1210	A1147
A2097	C2036	A1969	C1909	C1843	A1783	G1719	A1654	U1594	G1538	G1475	G1408	U1340	G1276	G1211	U1148
U2098	A2037	U1970	G1910	C1844	A1784	U1720	A1655	C1595	U1539	U1476	U1409	G1341	C1278	G1212	G1149
G2098	G2038	U1971	U1911		A1785	G1721	C1656	A1596	U1534	G1471	A1407	A1342		A1213	C1150
G2100	U2039	G1972	A1912		A1786	A1722	U1657	A1597	A1535	C1472	A1403			U1209	A1151
A2101	A2040	G1973	A1913	A1847	A1787	G1723	C1658	A1598	C1536	G1473	C1404	G1338	A1275	G1210	A1147
C2102	U2041	C1974	C1914	A1848	C1788	G1724	G1659	U1599	G1537	U1474		U1339	A1276	C1211	U1148
A2042	A2042	G1975	U1915	A1852	A1789	U1725		C1600	G1538	G1475	G1407	U1340	G1276	G1212	G1149
C2104	C2043	U1976	A1916	U1853	C1790	C1726	A1664	G1601	U1539	U1476	G1408	U1341	C1278	G1213	C1150
U2105	C2044	A1977	U1917	A1854	A1791	C1727	A1665	U1602	G1540	A1477	U1409			A1214	A1151
	C2045	A1978	A1918	U1855	G1792	C1728	G1666	A1603	C1541	G1478	G1410			G1281	C1152
	G2046		A1919	U1856	C1793	U1729	G1667	C1604	U1542	G1479	U1411	C1345	U1282	U1217	C1153
	C2047		C1920	G1857	A1794	C1730	A1668	C1605	G1543		U1412	G1346	G1283	G1218	G1154
	C2050	G1983	G1921	A1858	C1795	C1731	A1669	C1606	A1544	U1481	U1413	A1347	A1284	U1219	A1155
														G1220	A1156

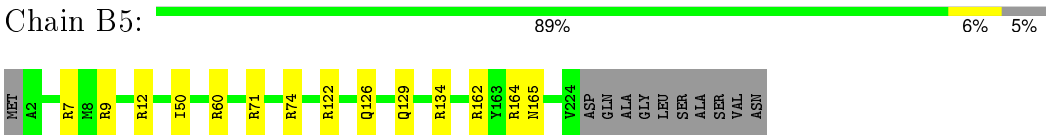


• Molecule 55: 5S ribosomal RNA

Chain BB:



- 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	3052	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	0.70	0/1736	1.07	11/2340 (0.5%)
10	AK	0.74	0/894	1.15	10/1207 (0.8%)
11	AL	0.76	0/969	1.23	15/1300 (1.2%)
12	AM	0.75	0/884	1.32	11/1181 (0.9%)
13	AN	0.77	0/817	1.26	12/1088 (1.1%)
14	AO	0.74	0/722	1.16	8/964 (0.8%)
15	AP	0.76	0/648	1.27	11/870 (1.3%)
16	AQ	0.70	0/658	1.06	4/883 (0.5%)
17	AR	0.81	0/463	1.29	10/623 (1.6%)
18	AS	0.76	0/653	1.13	7/879 (0.8%)
19	AT	0.68	0/672	1.05	5/890 (0.6%)
2	AC	0.72	0/1651	1.16	16/2225 (0.7%)
20	AU	0.83	0/431	1.44	8/572 (1.4%)
21	AA	1.53	1/36759 (0.0%)	2.22	1991/57346 (3.5%)
22	A1	1.53	0/1668	2.20	85/2595 (3.3%)
23	A2	1.47	0/343	2.25	15/531 (2.8%)
24	A3	1.53	0/1722	2.18	81/2685 (3.0%)
25	BC	0.74	0/2121	1.30	26/2852 (0.9%)
26	BD	0.68	0/1586	1.20	14/2134 (0.7%)
27	BE	0.67	0/1571	1.15	11/2113 (0.5%)
28	BF	0.74	0/1444	1.18	14/1937 (0.7%)
29	BG	0.69	0/1343	1.12	8/1816 (0.4%)
3	AD	0.77	0/1665	1.23	24/2227 (1.1%)
30	BH	0.65	0/1122	1.10	6/1515 (0.4%)
31	BI	0.65	0/1046	1.06	4/1410 (0.3%)
32	BJ	0.73	0/1152	1.16	8/1551 (0.5%)
33	BK	0.70	0/947	1.21	10/1268 (0.8%)
34	BL	0.73	0/1054	1.36	17/1403 (1.2%)
35	BM	0.74	0/1093	1.21	11/1460 (0.8%)
36	BN	0.77	0/973	1.36	15/1301 (1.2%)
37	BO	0.72	0/902	1.25	11/1209 (0.9%)
38	BP	0.75	0/929	1.27	8/1242 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.80	0/960	1.32	15/1278 (1.2%)
4	AE	0.70	0/1119	1.06	10/1506 (0.7%)
40	BR	0.70	0/829	1.22	7/1107 (0.6%)
41	BS	0.64	0/864	1.19	10/1156 (0.9%)
42	BT	0.65	0/744	1.19	7/994 (0.7%)
43	BU	0.68	0/787	1.10	4/1051 (0.4%)
44	BV	0.71	0/766	1.16	5/1025 (0.5%)
45	BW	0.77	0/604	1.36	9/799 (1.1%)
46	BX	0.75	0/635	1.28	10/848 (1.2%)
47	BY	0.65	0/510	1.17	5/677 (0.7%)
48	BZ	0.69	0/453	1.24	6/605 (1.0%)
49	B0	0.72	0/450	1.23	5/599 (0.8%)
5	AF	0.74	0/835	1.17	6/1128 (0.5%)
50	B1	0.73	0/417	1.05	2/556 (0.4%)
51	B2	0.81	0/380	1.49	11/498 (2.2%)
52	B3	0.72	0/513	1.23	5/676 (0.7%)
53	B4	0.68	0/303	1.24	4/397 (1.0%)
54	BA	1.41	2/69796 (0.0%)	2.21	4018/108888 (3.7%)
55	BB	1.42	0/2800	2.17	151/4367 (3.5%)
56	B5	0.64	0/1673	1.08	9/2255 (0.4%)
6	AG	0.74	0/1188	1.21	19/1593 (1.2%)
7	AH	0.70	0/989	1.08	5/1326 (0.4%)
8	AI	0.81	0/1035	1.34	20/1377 (1.5%)
9	AJ	0.69	0/797	1.23	13/1079 (1.2%)
All	All	1.28	3/160085 (0.0%)	2.00	6843/239402 (2.9%)

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
1	AB	0	1
14	AO	0	2
21	AA	0	368
22	A1	0	21
23	A2	0	4
24	A3	0	16
4	AE	0	1
43	BU	0	1
49	B0	0	1
54	BA	0	707

*Continued on next page...*



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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	25
All	All	0	1147

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	6	G	C2-N2	-5.63	1.28	1.34
54	BA	1568	G	C2-N2	-5.08	1.29	1.34
54	BA	2627	G	C2-N2	-5.01	1.29	1.34

All (6843) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1301	A	O4'-C1'-N9	17.59	122.27	108.20
54	BA	2126	A	O4'-C1'-N9	13.48	118.98	108.20
21	AA	547	A	N1-C6-N6	-12.92	110.85	118.60
54	BA	323	C	O4'-C1'-N1	12.84	118.47	108.20
54	BA	2199	A	N1-C6-N6	-12.76	110.94	118.60
21	AA	1362	A	N1-C6-N6	-12.39	111.16	118.60
54	BA	1069	A	N1-C6-N6	-12.35	111.19	118.60
54	BA	2810	A	N1-C6-N6	-12.29	111.23	118.60
54	BA	614	A	N1-C6-N6	-11.99	111.40	118.60
54	BA	1981	A	N1-C6-N6	-11.97	111.42	118.60
54	BA	933	A	N1-C6-N6	-11.94	111.44	118.60
54	BA	1591	A	N1-C6-N6	-11.92	111.45	118.60
21	AA	190	A	N1-C6-N6	-11.78	111.53	118.60
54	BA	382	A	N1-C6-N6	-11.78	111.53	118.60
54	BA	1205	A	N1-C6-N6	-11.77	111.54	118.60
54	BA	2134	A	N1-C6-N6	-11.75	111.55	118.60
54	BA	1523	U	O4'-C1'-N1	11.61	117.49	108.20
5	AF	91	ARG	NE-CZ-NH1	11.58	126.09	120.30
21	AA	1251	A	N1-C6-N6	-11.57	111.66	118.60
54	BA	1010	A	N1-C6-N6	-11.54	111.67	118.60
21	AA	172	A	N1-C6-N6	-11.51	111.69	118.60
54	BA	2572	A	N1-C6-N6	-11.49	111.70	118.60
54	BA	99	U	O4'-C1'-N1	11.44	117.35	108.20
54	BA	1427	A	N1-C6-N6	-11.42	111.75	118.60
21	AA	466	A	N1-C6-N6	-11.42	111.75	118.60
21	AA	746	A	N1-C6-N6	-11.41	111.75	118.60
21	AA	228	A	N1-C6-N6	-11.39	111.77	118.60
54	BA	1698	A	N1-C6-N6	-11.38	111.77	118.60
54	BA	1301	A	C1'-O4'-C4'	-11.36	100.81	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	432	A	N1-C6-N6	-11.36	111.79	118.60
54	BA	1940	U	O4'-C1'-N1	11.32	117.25	108.20
55	BB	94	A	N1-C6-N6	-11.25	111.85	118.60
54	BA	2267	A	N1-C6-N6	-11.25	111.85	118.60
54	BA	800	A	N1-C6-N6	-11.24	111.85	118.60
54	BA	53	A	N1-C6-N6	-11.23	111.86	118.60
55	BB	78	A	N1-C6-N6	-11.23	111.86	118.60
54	BA	2851	A	N1-C6-N6	-11.22	111.87	118.60
54	BA	197	A	N1-C6-N6	-11.20	111.88	118.60
54	BA	2097	A	N1-C6-N6	-11.20	111.88	118.60
21	AA	1480	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	53	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	1503	A	N1-C6-N6	-11.17	111.90	118.60
54	BA	1241	A	N1-C6-N6	-11.17	111.90	118.60
54	BA	1580	A	N1-C6-N6	-11.14	111.92	118.60
7	AH	87	ARG	NE-CZ-NH2	11.13	125.87	120.30
54	BA	2705	A	N1-C6-N6	-11.12	111.93	118.60
54	BA	575	A	N1-C6-N6	-11.09	111.95	118.60
21	AA	389	A	N1-C6-N6	-11.07	111.96	118.60
54	BA	2726	A	N1-C6-N6	-11.02	111.99	118.60
54	BA	1808	A	N1-C6-N6	-10.99	112.01	118.60
54	BA	125	A	N1-C6-N6	-10.97	112.02	118.60
54	BA	152	A	N1-C6-N6	-10.96	112.02	118.60
21	AA	630	A	N1-C6-N6	-10.95	112.03	118.60
54	BA	1746	A	N1-C6-N6	-10.93	112.04	118.60
54	BA	626	A	N1-C6-N6	-10.93	112.04	118.60
54	BA	181	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	2376	A	N1-C6-N6	-10.87	112.08	118.60
54	BA	2358	A	N1-C6-N6	-10.86	112.08	118.60
54	BA	1784	A	N1-C6-N6	-10.86	112.09	118.60
21	AA	1329	A	N1-C6-N6	-10.85	112.09	118.60
54	BA	2750	A	N1-C6-N6	-10.84	112.10	118.60
21	AA	1014	A	N1-C6-N6	-10.83	112.10	118.60
21	AA	1518	A	N1-C6-N6	-10.82	112.11	118.60
52	B3	39	ARG	NE-CZ-NH2	10.82	125.71	120.30
54	BA	764	A	N1-C6-N6	-10.81	112.11	118.60
54	BA	1317	G	O4'-C1'-N9	10.81	116.85	108.20
54	BA	1000	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	432	A	N1-C6-N6	-10.79	112.13	118.60
21	AA	937	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	1095	A	N1-C6-N6	-10.75	112.15	118.60
54	BA	324	A	N1-C6-N6	-10.72	112.17	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2814	A	N1-C6-N6	-10.72	112.17	118.60
21	AA	749	A	N1-C6-N6	-10.69	112.19	118.60
21	AA	665	A	N1-C6-N6	-10.68	112.19	118.60
54	BA	2614	A	N1-C6-N6	-10.66	112.20	118.60
21	AA	520	A	N1-C6-N6	-10.66	112.21	118.60
54	BA	1352	U	O4'-C1'-N1	10.64	116.71	108.20
40	BR	84	ARG	NE-CZ-NH1	10.63	125.62	120.30
54	BA	2099	U	O4'-C1'-N1	10.63	116.71	108.20
54	BA	609	A	N1-C6-N6	-10.61	112.23	118.60
21	AA	1289	A	N1-C6-N6	-10.59	112.25	118.60
54	BA	1033	U	O4'-C1'-N1	10.59	116.67	108.20
54	BA	2320	U	O4'-C1'-N1	10.59	116.67	108.20
54	BA	928	A	N1-C6-N6	-10.59	112.25	118.60
44	BV	9	ARG	NE-CZ-NH1	10.58	125.59	120.30
54	BA	2130	U	O4'-C1'-N1	10.58	116.67	108.20
54	BA	1713	A	N1-C6-N6	-10.58	112.25	118.60
54	BA	1858	A	N1-C6-N6	-10.58	112.25	118.60
21	AA	729	A	N1-C6-N6	-10.57	112.26	118.60
21	AA	784	A	N1-C6-N6	-10.56	112.27	118.60
54	BA	1365	A	N1-C6-N6	-10.55	112.27	118.60
54	BA	1553	A	N1-C6-N6	-10.54	112.28	118.60
54	BA	2711	A	N1-C6-N6	-10.53	112.28	118.60
12	AM	106	ARG	NE-CZ-NH1	10.51	125.56	120.30
54	BA	716	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	936	A	N1-C6-N6	-10.49	112.30	118.60
54	BA	101	A	N1-C6-N6	-10.49	112.31	118.60
21	AA	1201	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	1327	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	1021	A	N1-C6-N6	-10.46	112.32	118.60
54	BA	2748	A	N1-C6-N6	-10.46	112.32	118.60
54	BA	1919	A	N1-C6-N6	-10.46	112.33	118.60
21	AA	819	A	N1-C6-N6	-10.43	112.34	118.60
21	AA	120	A	N1-C6-N6	-10.42	112.34	118.60
21	AA	1434	A	N1-C6-N6	-10.41	112.36	118.60
54	BA	1434	A	N1-C6-N6	-10.41	112.36	118.60
54	BA	1597	A	N1-C6-N6	-10.41	112.36	118.60
54	BA	1937	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	2070	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	1301	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	2434	A	N1-C6-N6	-10.36	112.38	118.60
54	BA	761	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	1635	A	N1-C6-N6	-10.34	112.40	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	943	A	N1-C6-N6	-10.34	112.40	118.60
21	AA	151	A	N1-C6-N6	-10.33	112.40	118.60
54	BA	1494	A	N1-C6-N6	-10.31	112.41	118.60
21	AA	978	A	N1-C6-N6	-10.29	112.42	118.60
54	BA	1439	A	N1-C6-N6	-10.30	112.42	118.60
31	BI	102	ARG	NE-CZ-NH1	10.29	125.44	120.30
21	AA	780	A	N1-C6-N6	-10.29	112.43	118.60
54	BA	1509	A	N1-C6-N6	-10.28	112.43	118.60
54	BA	1302	A	N1-C6-N6	-10.28	112.43	118.60
21	AA	873	A	N1-C6-N6	-10.28	112.43	118.60
54	BA	2809	A	N1-C6-N6	-10.28	112.43	118.60
21	AA	353	A	N1-C6-N6	-10.27	112.44	118.60
21	AA	415	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	782	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	821	A	N1-C6-N6	-10.26	112.45	118.60
54	BA	2287	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	643	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	2751	G	O4'-C1'-N9	10.25	116.40	108.20
21	AA	51	A	N1-C6-N6	-10.24	112.45	118.60
54	BA	1630	A	N1-C6-N6	-10.23	112.46	118.60
38	BP	52	ARG	NE-CZ-NH1	10.22	125.41	120.30
21	AA	412	A	N1-C6-N6	-10.22	112.47	118.60
21	AA	1082	A	N1-C6-N6	-10.21	112.47	118.60
8	AI	79	ARG	NE-CZ-NH1	10.21	125.40	120.30
54	BA	2577	A	N1-C6-N6	-10.18	112.49	118.60
21	AA	1431	A	N1-C6-N6	-10.17	112.50	118.60
21	AA	414	A	N1-C6-N6	-10.17	112.50	118.60
21	AA	1363	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	2534	A	N1-C6-N6	-10.16	112.50	118.60
21	AA	1248	A	N1-C6-N6	-10.16	112.50	118.60
55	BB	109	A	N1-C6-N6	-10.16	112.51	118.60
14	AO	71	ARG	NE-CZ-NH1	10.15	125.38	120.30
54	BA	1755	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	263	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	1336	C	N3-C2-O2	-10.15	114.79	121.90
21	AA	338	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	1046	A	N1-C6-N6	-10.15	112.51	118.60
54	BA	2297	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	2346	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	1815	A	N1-C6-N6	-10.13	112.52	118.60
54	BA	2887	A	N1-C6-N6	-10.13	112.52	118.60
54	BA	483	A	N1-C6-N6	-10.13	112.52	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1953	A	N1-C6-N6	-10.11	112.53	118.60
21	AA	288	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	1952	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	2654	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	845	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	66	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	1393	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	1668	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	1717	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	1618	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	1085	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	1129	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	1966	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	345	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	1803	A	N1-C6-N6	-10.06	112.56	118.60
21	AA	959	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	1496	A	N1-C6-N6	-10.05	112.57	118.60
24	A3	74	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	2799	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	1067	A	N1-C6-N6	-10.04	112.57	118.60
54	BA	1508	A	N1-C6-N6	-10.04	112.57	118.60
54	BA	1610	A	O4'-C1'-N9	10.04	116.23	108.20
54	BA	1126	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	1678	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	1360	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	1318	A	N1-C6-N6	-10.02	112.59	118.60
56	B5	60	ARG	NE-CZ-NH2	10.02	125.31	120.30
54	BA	354	A	N1-C6-N6	-10.01	112.59	118.60
21	AA	1280	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	10	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	629	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	139	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	1794	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	539	A	N1-C6-N6	-9.99	112.60	118.60
42	BT	3	ARG	NE-CZ-NH1	9.99	125.30	120.30
54	BA	2560	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	1783	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	1213	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	1288	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	2835	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	320	A	N1-C6-N6	-9.97	112.62	118.60
34	BL	2	ARG	NE-CZ-NH2	9.97	125.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2108	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	152	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	274	A	N1-C6-N6	-9.96	112.63	118.60
21	AA	1152	A	N1-C6-N6	-9.96	112.63	118.60
21	AA	1204	A	N1-C6-N6	-9.96	112.63	118.60
21	AA	1408	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	945	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	782	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	784	G	O4'-C1'-N9	9.94	116.16	108.20
54	BA	1230	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	181	A	N1-C6-N6	-9.91	112.65	118.60
54	BA	941	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	5	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1762	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1453	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1943	U	O4'-C1'-N1	9.89	116.11	108.20
54	BA	2886	A	O4'-C1'-N9	9.89	116.11	108.20
21	AA	223	A	N1-C6-N6	-9.89	112.67	118.60
54	BA	925	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	1610	A	N1-C6-N6	-9.86	112.68	118.60
54	BA	1916	A	N1-C6-N6	-9.86	112.68	118.60
21	AA	510	A	N1-C6-N6	-9.86	112.69	118.60
21	AA	1044	A	N1-C6-N6	-9.86	112.69	118.60
21	AA	579	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	947	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	1147	A	N1-C6-N6	-9.85	112.69	118.60
55	BB	39	A	N1-C6-N6	-9.85	112.69	118.60
55	BB	66	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	44	A	N1-C6-N6	-9.84	112.69	118.60
54	BA	849	A	N1-C6-N6	-9.84	112.69	118.60
54	BA	654	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	216	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	927	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	1134	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	1067	A	N1-C6-N6	-9.82	112.70	118.60
54	BA	2665	A	N1-C6-N6	-9.82	112.71	118.60
21	AA	1171	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	160	A	N1-C6-N6	-9.81	112.71	118.60
21	AA	716	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	282	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	1552	A	O4'-C1'-N9	9.79	116.03	108.20
54	BA	675	A	N1-C6-N6	-9.77	112.74	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	250	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	1346	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	2518	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	1005	A	N1-C6-N6	-9.76	112.75	118.60
54	BA	2765	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	1586	A	N1-C6-N6	-9.73	112.76	118.60
39	BQ	29	ARG	NE-CZ-NH1	9.73	125.17	120.30
38	BP	38	ARG	NE-CZ-NH1	9.73	125.17	120.30
21	AA	969	A	N1-C6-N6	-9.73	112.77	118.60
2	AC	64	ARG	NE-CZ-NH1	9.72	125.16	120.30
23	A2	91	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	165	A	N1-C6-N6	-9.72	112.77	118.60
21	AA	1019	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	2169	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	126	A	N1-C6-N6	-9.71	112.78	118.60
55	BB	50	A	N1-C6-N6	-9.71	112.78	118.60
54	BA	608	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	2052	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	845	A	C1'-O4'-C4'	-9.70	102.14	109.90
54	BA	905	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1739	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1098	A	N1-C6-N6	-9.69	112.78	118.60
21	AA	622	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	111	A	N1-C6-N6	-9.69	112.79	118.60
21	AA	1287	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	2198	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	1433	A	N1-C6-N6	-9.68	112.80	118.60
54	BA	1284	A	N1-C6-N6	-9.67	112.80	118.60
21	AA	78	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	1340	U	O4'-C1'-N1	9.67	115.93	108.20
54	BA	1900	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	481	G	O4'-C1'-N9	9.65	115.92	108.20
43	BU	81	ARG	NE-CZ-NH1	9.64	125.12	120.30
54	BA	2268	A	N1-C6-N6	-9.64	112.81	118.60
54	BA	2634	A	N1-C6-N6	-9.64	112.81	118.60
21	AA	80	A	N1-C6-N6	-9.63	112.82	118.60
21	AA	1196	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2451	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2639	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	767	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1144	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	825	A	N1-C6-N6	-9.61	112.83	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	303	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	1490	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	1333	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	349	A	N1-C6-N6	-9.61	112.84	118.60
54	BA	119	A	N1-C6-N6	-9.61	112.84	118.60
54	BA	1570	A	N1-C6-N6	-9.60	112.84	118.60
21	AA	1493	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	2369	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	586	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	631	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	1175	A	N1-C6-N6	-9.59	112.85	118.60
25	BC	12	ARG	NE-CZ-NH1	9.59	125.09	120.30
24	A3	77	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	238	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	696	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	918	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	918	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	504	A	O4'-C1'-N9	9.57	115.85	108.20
54	BA	1237	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	2761	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	227	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	507	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	196	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	431	A	N1-C6-N6	-9.54	112.87	118.60
26	BD	77	ARG	NE-CZ-NH1	9.54	125.07	120.30
54	BA	300	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	668	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	213	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	171	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2886	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2309	A	N1-C6-N6	-9.52	112.89	118.60
21	AA	915	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2225	A	N1-C6-N6	-9.52	112.89	118.60
13	AN	24	ARG	NE-CZ-NH1	9.52	125.06	120.30
54	BA	781	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	693	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	71	A	N1-C6-N6	-9.50	112.90	118.60
22	A1	66	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	322	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	751	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	1616	A	N1-C6-N6	-9.48	112.91	118.60
7	AH	12	ARG	NE-CZ-NH1	9.47	125.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1394	A	N1-C6-N6	-9.47	112.92	118.60
41	BS	84	ARG	NE-CZ-NH1	9.47	125.04	120.30
54	BA	38	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	1133	A	N1-C6-N6	-9.46	112.92	118.60
21	AA	676	A	N1-C6-N6	-9.46	112.92	118.60
49	B0	16	ARG	NE-CZ-NH1	9.45	125.03	120.30
54	BA	2478	A	N1-C6-N6	-9.45	112.93	118.60
11	AL	109	ARG	NE-CZ-NH1	9.44	125.02	120.30
25	BC	237	ARG	NE-CZ-NH1	9.44	125.02	120.30
21	AA	441	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	1086	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	2088	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	975	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	2095	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	689	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	59	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	877	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	583	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1866	A	N1-C6-N6	-9.42	112.95	118.60
23	A2	79	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	19	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	1476	A	N1-C6-N6	-9.40	112.96	118.60
44	BV	79	ARG	NE-CZ-NH1	9.40	125.00	120.30
25	BC	68	ARG	NE-CZ-NH1	9.40	125.00	120.30
7	AH	14	ARG	NE-CZ-NH1	9.39	125.00	120.30
21	AA	1130	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	528	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	2381	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	306	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	8	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	1101	A	N1-C6-N6	-9.38	112.97	118.60
46	BX	56	ARG	NE-CZ-NH1	9.38	124.99	120.30
21	AA	1150	A	N1-C6-N6	-9.38	112.97	118.60
55	BB	52	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	715	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1226	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1264	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	65	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	1163	A	N1-C6-N6	-9.37	112.98	118.60
36	BN	96	ARG	NE-CZ-NH1	9.37	124.98	120.30
54	BA	633	A	N1-C6-N6	-9.37	112.98	118.60
51	B2	34	ARG	NE-CZ-NH1	9.36	124.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1847	A	N1-C6-N6	-9.36	112.99	118.60
21	AA	1254	A	N1-C6-N6	-9.35	112.99	118.60
21	AA	1534	A	N1-C6-N6	-9.35	112.99	118.60
21	AA	523	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1918	A	N1-C6-N6	-9.34	112.99	118.60
21	AA	600	A	N1-C6-N6	-9.34	113.00	118.60
21	AA	1433	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1010	A	C5-C6-N1	9.34	122.37	117.70
54	BA	2899	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	346	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	752	A	O4'-C1'-N9	9.33	115.66	108.20
54	BA	2476	A	N1-C6-N6	-9.32	113.00	118.60
22	A1	38	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	2158	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	2412	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	560	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	742	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	1640	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	2530	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	977	A	N1-C6-N6	-9.31	113.02	118.60
54	BA	788	A	N1-C6-N6	-9.31	113.02	118.60
3	AD	72	ARG	NE-CZ-NH1	9.30	124.95	120.30
21	AA	706	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	2721	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1328	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1634	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	750	A	N1-C6-N6	-9.30	113.02	118.60
41	BS	25	ARG	NE-CZ-NH1	9.29	124.95	120.30
54	BA	2058	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	1275	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	1534	U	O4'-C1'-N1	9.28	115.62	108.20
54	BA	1885	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2135	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	1690	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2868	A	N1-C6-N6	-9.28	113.03	118.60
47	BY	52	ARG	NE-CZ-NH1	9.27	124.94	120.30
54	BA	900	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1057	A	N1-C6-N6	-9.27	113.04	118.60
24	A3	77	A	C4-C5-C6	-9.25	112.38	117.00
54	BA	2386	A	N1-C6-N6	-9.24	113.06	118.60
21	AA	131	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	2170	A	N1-C6-N6	-9.23	113.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	279	A	N1-C6-N6	-9.23	113.06	118.60
54	BA	2513	A	N1-C6-N6	-9.22	113.06	118.60
54	BA	677	A	N1-C6-N6	-9.21	113.08	118.60
54	BA	74	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	1016	A	N1-C6-N6	-9.20	113.08	118.60
55	BB	99	A	N1-C6-N6	-9.20	113.08	118.60
1	AB	112	ARG	NE-CZ-NH1	9.19	124.90	120.30
21	AA	1093	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	1700	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	411	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	919	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	1311	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	1515	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	183	C	N3-C2-O2	-9.18	115.47	121.90
21	AA	250	A	C5-C6-N1	9.17	122.29	117.70
21	AA	935	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	1004	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	1179	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	89	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	734	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	1077	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	863	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	466	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1960	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2171	A	N1-C6-N6	-9.15	113.11	118.60
46	BX	27	ARG	NE-CZ-NH1	9.15	124.88	120.30
21	AA	807	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2377	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	718	A	N1-C6-N6	-9.14	113.11	118.60
54	BA	1301	A	C5'-C4'-O4'	9.14	120.07	109.10
54	BA	504	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	753	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1142	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2430	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1366	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1665	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2423	U	O4'-C1'-N1	9.12	115.49	108.20
54	BA	1970	A	N1-C6-N6	-9.11	113.13	118.60
26	BD	13	ARG	NE-CZ-NH1	9.11	124.86	120.30
54	BA	2340	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	2278	A	N1-C6-N6	-9.11	113.14	118.60
55	BB	46	A	N1-C6-N6	-9.11	113.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	53	ARG	NE-CZ-NH1	9.10	124.85	120.30
21	AA	655	A	N1-C6-N6	-9.10	113.14	118.60
40	BR	90	ARG	NE-CZ-NH2	9.10	124.85	120.30
54	BA	1679	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	315	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	1871	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2657	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	1029	A	N1-C6-N6	-9.09	113.14	118.60
54	BA	195	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	1492	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	2565	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	352	A	N1-C6-N6	-9.08	113.16	118.60
54	BA	1287	A	N1-C6-N6	-9.08	113.15	118.60
3	AD	61	ARG	NE-CZ-NH1	9.07	124.84	120.30
21	AA	673	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	1169	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	1419	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	990	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	2212	A	O4'-C1'-N9	9.07	115.46	108.20
21	AA	1219	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	28	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	493	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	975	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	2547	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	156	A	N1-C6-N6	-9.04	113.17	118.60
21	AA	1447	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	522	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	125	A	O4'-C1'-N9	9.04	115.43	108.20
21	AA	493	A	C5-C6-N1	9.03	122.22	117.70
54	BA	2031	A	O4'-C1'-N9	9.04	115.43	108.20
21	AA	675	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	140	C	N3-C2-O2	-9.03	115.58	121.90
54	BA	2333	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1127	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	2037	A	N1-C6-N6	-9.03	113.19	118.60
54	BA	217	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	81	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2191	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	627	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	1722	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2288	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2015	A	N1-C6-N6	-9.01	113.19	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1336	C	N1-C2-O2	9.01	124.31	118.90
21	AA	1289	A	C5-C6-N1	9.01	122.20	117.70
54	BA	1913	A	N1-C6-N6	-9.01	113.20	118.60
21	AA	98	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	753	A	N1-C6-N6	-9.00	113.20	118.60
12	AM	69	ARG	NE-CZ-NH1	9.00	124.80	120.30
54	BA	457	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1569	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	2062	A	N1-C6-N6	-8.99	113.21	118.60
24	A3	22	A	N1-C6-N6	-8.99	113.21	118.60
24	A3	36	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2031	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2531	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	448	A	N1-C6-N6	-8.97	113.22	118.60
24	A3	44	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1912	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	2589	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	2781	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	1239	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	1468	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	26	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1672	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	2741	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	960	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	205	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	373	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1080	A	N1-C6-N6	-8.96	113.23	118.60
21	AA	74	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	2005	A	N1-C6-N6	-8.95	113.23	118.60
55	BB	58	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	309	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	64	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	844	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	1246	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1701	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	374	A	N1-C6-N6	-8.94	113.24	118.60
27	BE	49	ARG	NE-CZ-NH1	8.94	124.77	120.30
28	BF	109	ARG	NE-CZ-NH1	8.93	124.76	120.30
54	BA	2328	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	161	A	N1-C6-N6	-8.92	113.25	118.60
2	AC	58	ARG	NE-CZ-NH1	8.91	124.76	120.30
54	BA	1390	U	O4'-C1'-N1	8.91	115.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	792	A	N1-C6-N6	-8.91	113.26	118.60
54	BA	101	A	O4'-C1'-N9	8.90	115.32	108.20
54	BA	1061	U	O4'-C1'-N1	8.90	115.32	108.20
54	BA	1614	A	N1-C6-N6	-8.90	113.26	118.60
24	A3	73	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	864	A	N1-C6-N6	-8.90	113.26	118.60
41	BS	92	ARG	NE-CZ-NH1	8.90	124.75	120.30
54	BA	1420	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2482	A	N1-C6-N6	-8.89	113.26	118.60
21	AA	336	A	N1-C6-N6	-8.89	113.27	118.60
32	BJ	13	ARG	NE-CZ-NH1	8.89	124.74	120.30
54	BA	2503	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	1502	A	N1-C6-N6	-8.88	113.27	118.60
24	A3	45	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	909	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	1339	A	N1-C6-N6	-8.88	113.27	118.60
26	BD	124	ARG	NE-CZ-NH1	8.88	124.74	120.30
21	AA	1238	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	695	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1262	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	478	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	233	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	661	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	347	G	O4'-C1'-N9	8.86	115.29	108.20
21	AA	728	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	1377	A	N1-C6-N6	-8.86	113.29	118.60
54	BA	1073	A	N1-C6-N6	-8.86	113.29	118.60
54	BA	2227	A	N1-C6-N6	-8.86	113.29	118.60
54	BA	472	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	1349	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	502	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	747	A	N1-C6-N6	-8.85	113.29	118.60
34	BL	132	ARG	NE-CZ-NH1	8.85	124.72	120.30
17	AR	56	ARG	NE-CZ-NH1	8.84	124.72	120.30
54	BA	497	A	N1-C6-N6	-8.84	113.29	118.60
54	BA	603	A	N1-C6-N6	-8.84	113.30	118.60
21	AA	1105	A	N1-C6-N6	-8.84	113.30	118.60
24	A3	39	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	2432	A	N1-C6-N6	-8.84	113.30	118.60
21	AA	1227	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	1694	C	N3-C2-O2	-8.84	115.72	121.90
21	AA	1250	A	N1-C6-N6	-8.83	113.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2750	A	O4'-C1'-N9	8.83	115.27	108.20
21	AA	192	A	N1-C6-N6	-8.83	113.30	118.60
2	AC	87	ARG	NE-CZ-NH1	8.83	124.71	120.30
54	BA	1084	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	2418	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	1551	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	596	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	681	A	N1-C6-N6	-8.81	113.31	118.60
22	A1	73	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	994	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	2241	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	42	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	1229	A	C1'-O4'-C4'	-8.80	102.86	109.90
54	BA	404	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	162	A	N1-C6-N6	-8.79	113.32	118.60
21	AA	179	A	N1-C6-N6	-8.79	113.32	118.60
21	AA	459	A	N1-C6-N6	-8.79	113.33	118.60
49	B0	9	ARG	NE-CZ-NH1	8.79	124.70	120.30
39	BQ	49	ARG	NE-CZ-NH1	8.79	124.70	120.30
21	AA	958	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	1368	A	N1-C6-N6	-8.79	113.33	118.60
1	AB	221	ARG	NE-CZ-NH1	8.78	124.69	120.30
54	BA	1285	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	872	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	1254	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	246	A	N1-C6-N6	-8.77	113.34	118.60
22	A1	6	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1664	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	913	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1384	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	792	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	663	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	984	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	1495	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	207	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	2706	A	N1-C6-N6	-8.76	113.35	118.60
21	AA	996	A	N1-C6-N6	-8.75	113.35	118.60
55	BB	29	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	1280	A	C5-C6-N1	8.75	122.07	117.70
54	BA	73	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1268	A	N1-C6-N6	-8.74	113.35	118.60
21	AA	182	A	N1-C6-N6	-8.74	113.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1434	A	O4'-C1'-N9	8.74	115.19	108.20
54	BA	2461	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	602	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1705	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	313	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	509	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	253	A	N1-C6-N6	-8.72	113.36	118.60
54	BA	1535	A	N1-C6-N6	-8.72	113.36	118.60
54	BA	2352	A	N1-C6-N6	-8.72	113.36	118.60
54	BA	637	A	N1-C6-N6	-8.72	113.37	118.60
37	BO	16	ARG	NE-CZ-NH1	8.72	124.66	120.30
36	BN	30	ARG	NE-CZ-NH1	8.72	124.66	120.30
21	AA	914	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	1288	G	O4'-C1'-N9	8.72	115.17	108.20
54	BA	1609	A	C5-C6-N1	8.72	122.06	117.70
54	BA	2425	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	364	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	833	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	2142	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	1063	G	O4'-C1'-N9	8.70	115.16	108.20
54	BA	2469	A	N1-C6-N6	-8.69	113.38	118.60
21	AA	498	A	N1-C6-N6	-8.69	113.38	118.60
54	BA	2564	A	N1-C6-N6	-8.69	113.38	118.60
9	AJ	48	ARG	NE-CZ-NH1	8.69	124.65	120.30
55	BB	108	A	N1-C6-N6	-8.69	113.39	118.60
47	BY	29	ARG	NE-CZ-NH1	8.69	124.64	120.30
21	AA	393	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	776	G	O4'-C1'-N9	8.68	115.14	108.20
54	BA	1987	A	N1-C6-N6	-8.68	113.39	118.60
8	AI	105	ARG	NE-CZ-NH1	8.68	124.64	120.30
54	BA	2497	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	2776	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	815	A	N1-C6-N6	-8.67	113.40	118.60
24	A3	38	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	655	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	103	A	N1-C6-N6	-8.67	113.40	118.60
3	AD	2	ARG	NE-CZ-NH1	8.66	124.63	120.30
21	AA	814	A	N1-C6-N6	-8.66	113.40	118.60
21	AA	845	A	N1-C6-N6	-8.66	113.40	118.60
21	AA	1146	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	861	A	N1-C6-N6	-8.66	113.40	118.60
21	AA	1191	A	N1-C6-N6	-8.66	113.40	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1256	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	699	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	1571	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	172	A	C5-C6-N1	8.65	122.02	117.70
24	A3	77	A	C5-C6-N1	8.65	122.03	117.70
21	AA	913	A	C5-C6-N1	8.64	122.02	117.70
54	BA	1027	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	2092	U	O4'-C1'-N1	8.64	115.11	108.20
54	BA	2503	A	O4'-C1'-N9	8.64	115.11	108.20
54	BA	1276	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	515	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	937	A	C5-C6-N1	8.63	122.02	117.70
22	A1	26	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	460	A	N1-C6-N6	-8.63	113.42	118.60
34	BL	78	ARG	NE-CZ-NH1	8.63	124.61	120.30
21	AA	55	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	77	A	N1-C6-N6	-8.62	113.42	118.60
54	BA	1070	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	829	A	O4'-C1'-N9	8.62	115.10	108.20
15	AP	28	ARG	NE-CZ-NH1	8.62	124.61	120.30
54	BA	2030	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	2675	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	1430	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	2388	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	1467	C	N3-C2-O2	-8.61	115.87	121.90
54	BA	2727	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	1773	A	N1-C6-N6	-8.61	113.44	118.60
22	A1	69	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	221	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	1201	A	C5-C6-N1	8.60	122.00	117.70
54	BA	2749	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	2432	A	C5-C6-N1	8.60	122.00	117.70
21	AA	243	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1821	A	N1-C6-N6	-8.60	113.44	118.60
2	AC	135	ARG	NE-CZ-NH1	8.59	124.59	120.30
54	BA	1504	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	2077	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	2740	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	712	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	1493	A	C5-C6-N1	8.59	121.99	117.70
55	BB	34	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	428	A	N1-C6-N6	-8.58	113.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	977	A	C5-C6-N1	8.58	121.99	117.70
21	AA	1012	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	144	A	N1-C6-N6	-8.58	113.45	118.60
12	AM	86	ARG	NE-CZ-NH1	8.57	124.58	120.30
21	AA	909	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	592	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2335	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	715	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	1183	U	O4'-C1'-N1	8.56	115.05	108.20
21	AA	183	C	O4'-C1'-N1	8.56	115.05	108.20
21	AA	759	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	1603	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	2882	A	N1-C6-N6	-8.56	113.47	118.60
54	BA	2628	C	N3-C2-O2	-8.56	115.91	121.90
54	BA	146	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	787	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	752	A	C5-C6-N1	8.55	121.97	117.70
54	BA	1632	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2602	A	N1-C6-N6	-8.55	113.47	118.60
6	AG	110	ARG	NE-CZ-NH1	8.55	124.57	120.30
21	AA	1216	A	C5-C6-N1	8.55	121.97	117.70
54	BA	2158	A	C5-C6-N1	8.55	121.97	117.70
21	AA	547	A	C5-C6-N1	8.55	121.97	117.70
54	BA	959	A	C5-C6-N1	8.54	121.97	117.70
54	BA	2212	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	1398	A	N1-C6-N6	-8.54	113.48	118.60
28	BF	91	ARG	NE-CZ-NH1	8.54	124.57	120.30
54	BA	1854	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	2516	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	1180	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	294	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	1156	A	N1-C6-N6	-8.53	113.48	118.60
55	BB	45	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	323	C	N3-C2-O2	-8.52	115.94	121.90
21	AA	1197	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	1522	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	1111	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	1176	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	503	A	N1-C6-N6	-8.51	113.50	118.60
21	AA	1021	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	896	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1439	A	O4'-C1'-N9	8.50	115.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1035	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	10	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	560	A	C5-C6-N1	8.49	121.94	117.70
54	BA	478	A	N1-C6-N6	-8.49	113.50	118.60
24	A3	60	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	356	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	694	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	1304	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	2666	C	O4'-C1'-N1	8.48	114.98	108.20
21	AA	974	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	226	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	1552	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	199	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	320	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	1126	A	C5-C6-N1	8.47	121.94	117.70
54	BA	1654	A	N1-C6-N6	-8.47	113.52	118.60
12	AM	91	ARG	NE-CZ-NH1	8.47	124.53	120.30
21	AA	766	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	2448	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	309	A	N1-C6-N6	-8.46	113.53	118.60
22	A1	16	C	N3-C2-O2	-8.46	115.98	121.90
3	AD	114	ARG	NE-CZ-NH1	8.45	124.53	120.30
54	BA	735	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	1650	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	430	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	1525	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	532	A	N1-C6-N6	-8.44	113.53	118.60
21	AA	1022	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	670	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	973	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	979	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	1608	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	602	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	981	A	C5-C6-N1	8.44	121.92	117.70
10	AK	36	ARG	NE-CZ-NH1	8.43	124.51	120.30
54	BA	677	A	C5-C6-N1	8.43	121.91	117.70
21	AA	1216	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	195	A	C5-C6-N1	8.43	121.91	117.70
54	BA	1913	A	C5-C6-N1	8.43	121.91	117.70
54	BA	1791	A	N1-C6-N6	-8.43	113.55	118.60
9	AJ	72	ARG	NE-CZ-NH1	8.42	124.51	120.30
21	AA	1155	A	N1-C6-N6	-8.42	113.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	56	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2450	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	397	A	N1-C6-N6	-8.42	113.55	118.60
36	BN	4	ARG	NE-CZ-NH1	8.42	124.51	120.30
21	AA	33	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	298	A	N1-C6-N6	-8.41	113.55	118.60
32	BJ	116	ARG	NE-CZ-NH1	8.41	124.51	120.30
54	BA	13	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	1396	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	1928	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	1932	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	2825	G	O4'-C1'-N9	8.41	114.93	108.20
54	BA	2820	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2435	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	127	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2753	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	794	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2071	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	1566	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	1609	A	N1-C6-N6	-8.39	113.57	118.60
21	AA	129	A	N1-C6-N6	-8.39	113.57	118.60
21	AA	1151	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	131	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	2808	G	O4'-C1'-N9	8.38	114.91	108.20
54	BA	2033	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	1350	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	1253	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	1428	A	N1-C6-N6	-8.38	113.58	118.60
21	AA	7	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	44	A	N1-C6-N6	-8.38	113.58	118.60
54	BA	1819	A	N1-C6-N6	-8.38	113.58	118.60
54	BA	2541	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	2778	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	845	A	C5-C6-N1	8.37	121.89	117.70
54	BA	2266	A	N1-C6-N6	-8.37	113.58	118.60
31	BI	126	ARG	NE-CZ-NH1	8.37	124.48	120.30
36	BN	90	ARG	NE-CZ-NH1	8.37	124.48	120.30
54	BA	422	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	344	A	N1-C6-N6	-8.36	113.58	118.60
9	AJ	7	ARG	NE-CZ-NH1	8.36	124.48	120.30
54	BA	1420	A	C5-C6-N1	8.36	121.88	117.70
54	BA	621	A	N1-C6-N6	-8.35	113.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1042	A	N1-C6-N6	-8.35	113.59	118.60
48	BZ	15	ARG	NE-CZ-NH1	8.35	124.48	120.30
21	AA	363	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	968	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	1535	A	C5-C6-N1	8.35	121.87	117.70
36	BN	8	ARG	NE-CZ-NH1	8.34	124.47	120.30
54	BA	453	A	N1-C6-N6	-8.34	113.59	118.60
17	AR	52	ARG	NE-CZ-NH1	8.34	124.47	120.30
21	AA	321	A	N1-C6-N6	-8.34	113.60	118.60
40	BR	79	ARG	NE-CZ-NH1	8.33	124.47	120.30
54	BA	739	A	C5-C6-N1	8.33	121.86	117.70
54	BA	2051	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	1027	C	N3-C2-O2	-8.33	116.07	121.90
21	AA	1046	A	C5-C6-N1	8.33	121.86	117.70
54	BA	1566	A	C5-C6-N1	8.33	121.86	117.70
54	BA	1791	A	C5-C6-N1	8.33	121.86	117.70
21	AA	149	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	49	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	804	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	1244	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	125	A	C5-C6-N1	8.31	121.86	117.70
41	BS	88	ARG	NE-CZ-NH2	8.31	124.46	120.30
54	BA	1032	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	1780	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2267	A	C5-C6-N1	8.31	121.86	117.70
54	BA	2468	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	599	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	959	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2471	A	N1-C6-N6	-8.30	113.62	118.60
55	BB	109	A	C5-C6-N1	8.30	121.85	117.70
8	AI	94	ARG	NE-CZ-NH1	8.30	124.45	120.30
21	AA	109	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	2163	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	1789	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	563	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	342	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	802	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1009	A	C5-C6-N1	8.29	121.84	117.70
54	BA	1205	A	C5-C6-N1	8.29	121.84	117.70
55	BB	53	A	C5-C6-N1	8.28	121.84	117.70
54	BA	1548	A	N1-C6-N6	-8.28	113.63	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	60	C	N3-C2-O2	-8.28	116.11	121.90
6	AG	108	ARG	NE-CZ-NH1	8.28	124.44	120.30
13	AN	69	ARG	NE-CZ-NH1	8.28	124.44	120.30
21	AA	371	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	91	A	C5-C6-N1	8.27	121.83	117.70
54	BA	1745	A	C5-C6-N1	8.27	121.83	117.70
21	AA	1246	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	547	A	C4-C5-C6	-8.26	112.87	117.00
54	BA	272	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	1652	A	N1-C6-N6	-8.26	113.64	118.60
8	AI	48	ARG	NE-CZ-NH1	8.26	124.43	120.30
21	AA	573	A	N1-C6-N6	-8.26	113.64	118.60
21	AA	967	C	N3-C2-O2	-8.26	116.12	121.90
54	BA	94	A	N1-C6-N6	-8.26	113.65	118.60
21	AA	72	A	N1-C6-N6	-8.25	113.65	118.60
37	BO	13	ARG	NE-CZ-NH1	8.25	124.43	120.30
54	BA	2042	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2850	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2450	A	C5-C6-N1	8.25	121.83	117.70
21	AA	1324	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2800	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	782	A	C5-C6-N1	8.24	121.82	117.70
54	BA	1641	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	1544	A	N1-C6-N6	-8.24	113.66	118.60
25	BC	220	ARG	NE-CZ-NH2	8.24	124.42	120.30
54	BA	2566	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	1321	A	C5-C6-N1	8.23	121.82	117.70
22	A1	41	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	1853	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	6	A	C5-C6-N1	8.23	121.81	117.70
54	BA	482	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2614	A	C4-C5-C6	-8.22	112.89	117.00
55	BB	15	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	152	A	C5-C6-N1	8.22	121.81	117.70
21	AA	704	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1390	U	C1'-O4'-C4'	-8.22	103.32	109.90
54	BA	176	A	C5-C6-N1	8.22	121.81	117.70
54	BA	1496	A	C5-C6-N1	8.22	121.81	117.70
54	BA	1552	A	C5-C6-N1	8.22	121.81	117.70
54	BA	2173	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	2070	A	C5-C6-N1	8.21	121.81	117.70
54	BA	2792	A	N1-C6-N6	-8.21	113.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2868	A	C5-C6-N1	8.21	121.81	117.70
21	AA	464	U	C1'-O4'-C4'	-8.21	103.33	109.90
21	AA	1500	A	N1-C6-N6	-8.21	113.68	118.60
36	BN	17	ARG	NE-CZ-NH1	8.20	124.40	120.30
54	BA	1522	A	C5-C6-N1	8.20	121.80	117.70
54	BA	2433	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1998	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1953	A	C5-C6-N1	8.20	121.80	117.70
21	AA	189	A	N1-C6-N6	-8.19	113.68	118.60
1	AB	34	ARG	NE-CZ-NH1	8.19	124.40	120.30
21	AA	325	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	1158	C	N3-C2-O2	-8.19	116.17	121.90
32	BJ	95	ARG	NE-CZ-NH2	8.19	124.40	120.30
54	BA	2646	C	N3-C2-O2	-8.19	116.17	121.90
54	BA	2879	A	C5-C6-N1	8.19	121.80	117.70
54	BA	705	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2199	A	C5-C6-N1	8.19	121.79	117.70
23	A2	91	A	C5-C6-N1	8.19	121.79	117.70
54	BA	2598	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	1200	C	N3-C2-O2	-8.19	116.17	121.90
54	BA	743	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1095	A	C5-C6-N1	8.18	121.79	117.70
54	BA	2406	A	N1-C6-N6	-8.18	113.69	118.60
19	AT	28	ARG	NE-CZ-NH1	8.18	124.39	120.30
21	AA	432	A	C5-C6-N1	8.17	121.79	117.70
54	BA	1028	A	C5-C6-N1	8.17	121.79	117.70
54	BA	299	A	C5-C6-N1	8.17	121.78	117.70
54	BA	1477	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	384	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	404	A	C5-C6-N1	8.16	121.78	117.70
54	BA	996	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1901	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	794	A	N1-C6-N6	-8.16	113.71	118.60
21	AA	1170	A	N1-C6-N6	-8.16	113.71	118.60
54	BA	1936	A	N1-C6-N6	-8.16	113.71	118.60
54	BA	526	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	2872	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1050	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	183	C	N1-C2-O2	8.15	123.79	118.90
54	BA	1378	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	626	A	C5-C6-N1	8.15	121.77	117.70
38	BP	112	ARG	NE-CZ-NH1	8.14	124.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1320	C	N3-C2-O2	-8.14	116.20	121.90
54	BA	6	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	983	A	N1-C6-N6	-8.14	113.72	118.60
52	B3	12	ARG	NE-CZ-NH1	8.13	124.37	120.30
21	AA	777	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	949	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	972	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	173	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1260	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	171	A	C5-C6-N1	8.13	121.76	117.70
54	BA	2094	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	222	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1442	U	O4'-C1'-N1	8.12	114.70	108.20
54	BA	2091	C	N3-C2-O2	-8.12	116.22	121.90
54	BA	1099	G	O4'-C1'-N9	8.12	114.69	108.20
21	AA	1317	C	N3-C2-O2	-8.11	116.22	121.90
54	BA	176	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	1110	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	1499	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	1054	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	1387	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	1146	A	C5-C6-N1	8.11	121.75	117.70
54	BA	514	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2205	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	648	A	N1-C6-N6	-8.11	113.74	118.60
21	AA	687	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	933	A	C5-C6-N1	8.10	121.75	117.70
54	BA	479	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1829	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	792	A	C5-C6-N1	8.10	121.75	117.70
21	AA	1067	A	C4-C5-C6	-8.10	112.95	117.00
25	BC	270	ARG	NE-CZ-NH1	8.10	124.35	120.30
21	AA	1252	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1383	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1847	A	O4'-C1'-N9	8.10	114.68	108.20
54	BA	1366	A	C5-C6-N1	8.10	121.75	117.70
54	BA	2635	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	468	A	N1-C6-N6	-8.09	113.74	118.60
21	AA	1117	A	N1-C6-N6	-8.09	113.75	118.60
21	AA	554	A	N1-C6-N6	-8.09	113.75	118.60
6	AG	78	ARG	NE-CZ-NH2	8.09	124.34	120.30
33	BK	31	ARG	NE-CZ-NH1	8.09	124.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1858	A	C5-C6-N1	8.09	121.74	117.70
21	AA	815	A	C5-C6-N1	8.09	121.74	117.70
55	BB	70	C	N3-C2-O2	-8.09	116.24	121.90
21	AA	1374	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	1700	A	C5-C6-N1	8.08	121.74	117.70
54	BA	1028	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	2541	A	C5-C6-N1	8.08	121.74	117.70
4	AE	111	ARG	NE-CZ-NH1	8.08	124.34	120.30
21	AA	167	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	728	A	C5-C6-N1	8.08	121.74	117.70
54	BA	2835	A	C5-C6-N1	8.08	121.74	117.70
21	AA	298	A	C5-C6-N1	8.07	121.74	117.70
54	BA	752	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2748	A	C5-C6-N1	8.07	121.74	117.70
54	BA	616	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	1089	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2154	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	1668	A	C5-C6-N1	8.07	121.73	117.70
3	AD	103	ARG	NE-CZ-NH1	8.07	124.33	120.30
21	AA	413	G	O4'-C1'-N9	8.07	114.65	108.20
54	BA	643	A	C5-C6-N1	8.07	121.73	117.70
54	BA	1809	A	C5-C6-N1	8.07	121.73	117.70
54	BA	2247	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2310	C	N3-C2-O2	-8.07	116.25	121.90
21	AA	602	A	C5-C6-N1	8.06	121.73	117.70
54	BA	1272	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	161	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	1009	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	1046	A	C5-C6-N1	8.06	121.73	117.70
21	AA	595	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	1698	A	C5-C6-N1	8.05	121.73	117.70
21	AA	878	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	199	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	609	A	C5-C6-N1	8.05	121.72	117.70
45	BW	19	ARG	NE-CZ-NH1	8.05	124.32	120.30
21	AA	702	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	1640	A	C5-C6-N1	8.05	121.72	117.70
54	BA	1308	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1981	A	O4'-C1'-N9	8.04	114.64	108.20
21	AA	155	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	1256	A	C5-C6-N1	8.04	121.72	117.70
21	AA	1157	A	N1-C6-N6	-8.04	113.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BG	34	ARG	NE-CZ-NH1	8.04	124.32	120.30
54	BA	1646	C	N3-C2-O2	-8.04	116.27	121.90
54	BA	2171	A	C5-C6-N1	8.04	121.72	117.70
54	BA	477	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	2725	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	328	C	N3-C2-O2	-8.03	116.28	121.90
54	BA	1759	A	C5-C6-N1	8.03	121.71	117.70
54	BA	1593	A	C5-C6-N1	8.03	121.71	117.70
21	AA	1418	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	14	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	1319	A	N1-C6-N6	-8.02	113.78	118.60
54	BA	718	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	60	A	N1-C6-N6	-8.02	113.79	118.60
43	BU	93	ARG	NE-CZ-NH1	8.02	124.31	120.30
54	BA	1772	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	101	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	2614	A	C5-C6-N1	8.01	121.71	117.70
21	AA	1225	A	C5-C6-N1	8.01	121.70	117.70
21	AA	238	A	C5-C6-N1	8.01	121.70	117.70
54	BA	63	A	N1-C6-N6	-8.00	113.80	118.60
45	BW	40	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	1503	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	1214	C	N3-C2-O2	-8.00	116.30	121.90
54	BA	1347	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1393	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2238	G	O4'-C1'-N9	8.00	114.60	108.20
54	BA	2281	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2176	A	C5-C6-N1	8.00	121.70	117.70
35	BM	114	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	1328	A	C5-C6-N1	8.00	121.70	117.70
21	AA	1286	U	O4'-C1'-N1	7.99	114.59	108.20
54	BA	689	A	C5-C6-N1	7.99	121.70	117.70
19	AT	24	ARG	NE-CZ-NH1	7.99	124.30	120.30
54	BA	1914	C	N3-C2-O2	-7.99	116.31	121.90
54	BA	2750	A	C5-C6-N1	7.99	121.69	117.70
1	AB	136	ARG	NE-CZ-NH1	7.99	124.29	120.30
21	AA	72	A	C5-C6-N1	7.99	121.69	117.70
21	AA	452	A	N1-C6-N6	-7.99	113.81	118.60
34	BL	21	ARG	NE-CZ-NH1	7.99	124.29	120.30
54	BA	685	A	C5-C6-N1	7.99	121.69	117.70
54	BA	1348	C	O4'-C1'-N1	7.99	114.59	108.20
54	BA	299	A	N1-C6-N6	-7.98	113.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AU	16	ARG	NE-CZ-NH1	7.98	124.29	120.30
54	BA	1336	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1490	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1583	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	2336	A	N1-C6-N6	-7.98	113.81	118.60
3	AD	46	ARG	NE-CZ-NH2	7.98	124.29	120.30
21	AA	607	A	C5-C6-N1	7.97	121.69	117.70
54	BA	118	A	N1-C6-N6	-7.97	113.81	118.60
54	BA	470	A	C5-C6-N1	7.97	121.69	117.70
21	AA	1081	A	N1-C6-N6	-7.97	113.82	118.60
36	BN	71	ARG	NE-CZ-NH1	7.97	124.28	120.30
54	BA	204	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	911	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	21	A	N1-C6-N6	-7.97	113.82	118.60
24	A3	58	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	845	A	O4'-C1'-N9	7.96	114.57	108.20
54	BA	1755	A	C4-C5-C6	-7.96	113.02	117.00
54	BA	2736	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	2899	A	C4-C5-C6	-7.96	113.02	117.00
38	BP	50	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	1286	A	N1-C6-N6	-7.96	113.83	118.60
54	BA	1509	A	C5-C6-N1	7.96	121.68	117.70
8	AI	11	ARG	NE-CZ-NH1	7.95	124.28	120.30
21	AA	1022	A	C5-C6-N1	7.95	121.68	117.70
21	AA	1229	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	303	A	C5-C6-N1	7.95	121.67	117.70
54	BA	83	A	N1-C6-N6	-7.95	113.83	118.60
45	BW	13	ARG	NE-CZ-NH1	7.95	124.27	120.30
54	BA	2660	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	1261	A	N1-C6-N6	-7.95	113.83	118.60
55	BB	78	A	C5-C6-N1	7.95	121.67	117.70
54	BA	781	A	C5-C6-N1	7.94	121.67	117.70
54	BA	945	A	C5-C6-N1	7.94	121.67	117.70
54	BA	1755	A	C5-C6-N1	7.94	121.67	117.70
55	BB	45	A	C5-C6-N1	7.94	121.67	117.70
54	BA	2829	A	N1-C6-N6	-7.94	113.84	118.60
24	A3	11	A	C5-C6-N1	7.93	121.67	117.70
54	BA	1744	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	332	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	983	A	C5-C6-N1	7.93	121.67	117.70
54	BA	2346	A	C5-C6-N1	7.93	121.67	117.70
21	AA	195	A	N1-C6-N6	-7.93	113.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	653	U	O4'-C1'-N1	7.93	114.54	108.20
54	BA	1532	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	676	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1143	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	2051	A	C5-C6-N1	7.93	121.66	117.70
21	AA	1257	A	N1-C6-N6	-7.92	113.84	118.60
54	BA	2883	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	1340	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	863	A	C5-C6-N1	7.92	121.66	117.70
54	BA	2758	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	1136	C	N3-C2-O2	-7.92	116.36	121.90
54	BA	415	A	N1-C6-N6	-7.92	113.85	118.60
22	A1	58	A	N1-C6-N6	-7.92	113.85	118.60
22	A1	66	A	C5-C6-N1	7.92	121.66	117.70
24	A3	45	A	C4-C5-C6	-7.92	113.04	117.00
22	A1	76	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	614	A	O4'-C1'-N9	7.91	114.53	108.20
54	BA	1307	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	1757	A	C5-C6-N1	7.91	121.66	117.70
54	BA	231	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	1553	A	C4-C5-C6	-7.91	113.05	117.00
54	BA	1745	A	N1-C6-N6	-7.91	113.85	118.60
55	BB	59	A	N1-C6-N6	-7.91	113.85	118.60
45	BW	10	ARG	NE-CZ-NH2	7.91	124.25	120.30
54	BA	645	C	N3-C2-O2	-7.91	116.36	121.90
54	BA	1204	A	C5-C6-N1	7.91	121.65	117.70
54	BA	482	A	C5-C6-N1	7.91	121.65	117.70
8	AI	32	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	265	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2632	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1195	C	N3-C2-O2	-7.90	116.37	121.90
55	BB	41	G	O4'-C1'-N9	7.90	114.52	108.20
25	BC	155	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	1847	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2358	A	C5-C6-N1	7.90	121.65	117.70
54	BA	574	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	2587	A	N1-C6-N6	-7.89	113.86	118.60
55	BB	88	C	N3-C2-O2	-7.89	116.37	121.90
54	BA	1336	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	647	G	N3-C2-N2	-7.89	114.38	119.90
54	BA	323	C	N1-C2-O2	7.89	123.63	118.90
54	BA	1505	A	N1-C6-N6	-7.89	113.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2198	A	C5-C6-N1	7.89	121.64	117.70
12	AM	56	ARG	NE-CZ-NH1	7.89	124.24	120.30
54	BA	368	A	N1-C6-N6	-7.89	113.87	118.60
54	BA	1253	A	C5-C6-N1	7.88	121.64	117.70
55	BB	73	A	N1-C6-N6	-7.88	113.87	118.60
21	AA	1302	C	N3-C2-O2	-7.88	116.38	121.90
21	AA	1434	A	C5-C6-N1	7.88	121.64	117.70
54	BA	158	U	O4'-C1'-N1	7.88	114.51	108.20
54	BA	522	A	C5-C6-N1	7.88	121.64	117.70
21	AA	300	A	N1-C6-N6	-7.88	113.87	118.60
51	B2	3	ARG	NE-CZ-NH2	7.88	124.24	120.30
54	BA	2826	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	382	A	C4-C5-C6	-7.88	113.06	117.00
54	BA	1579	A	C5-C6-N1	7.88	121.64	117.70
21	AA	85	U	N3-C2-O2	-7.87	116.69	122.20
54	BA	454	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	616	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1385	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	1437	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	1130	A	C5-C6-N1	7.87	121.64	117.70
21	AA	196	A	C5-C6-N1	7.87	121.63	117.70
21	AA	696	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1937	A	C5-C6-N1	7.87	121.63	117.70
54	BA	2451	A	C5-C6-N1	7.87	121.63	117.70
54	BA	2309	A	C5-C6-N1	7.87	121.63	117.70
54	BA	2598	A	C5-C6-N1	7.87	121.63	117.70
54	BA	1872	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	2307	G	O4'-C1'-N9	7.86	114.49	108.20
54	BA	2423	U	C1'-O4'-C4'	-7.86	103.61	109.90
54	BA	2873	A	N1-C6-N6	-7.86	113.88	118.60
21	AA	1036	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	504	A	C5-C6-N1	7.86	121.63	117.70
54	BA	783	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	1302	A	C5-C6-N1	7.86	121.63	117.70
54	BA	345	A	C5-C6-N1	7.86	121.63	117.70
24	A3	45	A	C5-C6-N1	7.86	121.63	117.70
54	BA	182	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	1669	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	981	A	N1-C6-N6	-7.85	113.89	118.60
21	AA	1376	U	O4'-C1'-N1	7.85	114.48	108.20
54	BA	2468	A	C5-C6-N1	7.85	121.63	117.70
25	BC	261	ARG	NE-CZ-NH2	7.85	124.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	975	A	C5-C6-N1	7.85	121.62	117.70
54	BA	1637	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2020	A	O4'-C1'-N9	7.85	114.48	108.20
54	BA	749	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2810	A	C5-C6-N1	7.85	121.62	117.70
21	AA	197	A	N1-C6-N6	-7.84	113.89	118.60
27	BE	117	ARG	NE-CZ-NH1	7.84	124.22	120.30
54	BA	362	A	C5-C6-N1	7.84	121.62	117.70
40	BR	78	ARG	NE-CZ-NH1	7.84	124.22	120.30
54	BA	1332	G	O4'-C1'-N9	7.84	114.47	108.20
54	BA	1314	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	1731	G	O4'-C1'-N9	7.83	114.47	108.20
21	AA	948	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	244	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1759	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	556	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1354	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	10	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1453	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1829	A	C5-C6-N1	7.83	121.61	117.70
20	AU	20	ARG	NE-CZ-NH1	7.83	124.21	120.30
21	AA	1219	A	C5-C6-N1	7.83	121.61	117.70
54	BA	280	U	O4'-C1'-N1	7.83	114.46	108.20
54	BA	2060	A	N1-C6-N6	-7.83	113.91	118.60
54	BA	2145	C	N3-C2-O2	-7.82	116.42	121.90
1	AB	107	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	1050	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1593	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	1383	A	C5-C6-N1	7.82	121.61	117.70
29	BG	152	ARG	NE-CZ-NH1	7.82	124.21	120.30
21	AA	914	A	C5-C6-N1	7.81	121.61	117.70
54	BA	2700	A	N1-C6-N6	-7.81	113.91	118.60
21	AA	906	A	C5-C6-N1	7.81	121.61	117.70
21	AA	1275	A	N1-C6-N6	-7.81	113.92	118.60
21	AA	1410	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	101	A	C5-C6-N1	7.81	121.61	117.70
21	AA	1109	C	N3-C2-O2	-7.81	116.44	121.90
54	BA	727	A	N1-C6-N6	-7.81	113.92	118.60
21	AA	262	A	C5-C6-N1	7.80	121.60	117.70
21	AA	704	A	C5-C6-N1	7.80	121.60	117.70
54	BA	2031	A	C5-C6-N1	7.80	121.60	117.70
54	BA	1069	A	C5-C6-N1	7.80	121.60	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	345	C	N3-C2-O2	-7.80	116.44	121.90
21	AA	353	A	C5-C6-N1	7.80	121.60	117.70
54	BA	1392	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	794	A	C5-C6-N1	7.80	121.60	117.70
21	AA	1285	A	N1-C6-N6	-7.80	113.92	118.60
22	A1	21	A	C5-C6-N1	7.80	121.60	117.70
54	BA	614	A	C5-C6-N1	7.80	121.60	117.70
54	BA	140	C	N1-C2-O2	7.79	123.58	118.90
15	AP	5	ARG	NE-CZ-NH1	7.79	124.20	120.30
21	AA	356	A	C5-C6-N1	7.79	121.59	117.70
54	BA	2369	A	C5-C6-N1	7.79	121.60	117.70
54	BA	2665	A	C5-C6-N1	7.79	121.59	117.70
21	AA	642	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	932	C	P-O3'-C3'	7.79	129.05	119.70
54	BA	620	G	O4'-C1'-N9	7.79	114.43	108.20
54	BA	2851	A	C4-C5-C6	-7.79	113.11	117.00
21	AA	50	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	729	A	C5-C6-N1	7.79	121.59	117.70
21	AA	795	C	N3-C2-O2	-7.79	116.45	121.90
21	AA	408	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	71	A	C5-C6-N1	7.79	121.59	117.70
54	BA	1359	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	2820	A	C5-C6-N1	7.79	121.59	117.70
21	AA	621	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	294	A	C5-C6-N1	7.78	121.59	117.70
54	BA	1067	A	C5-C6-N1	7.78	121.59	117.70
54	BA	1189	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	495	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	518	C	N3-C2-O2	-7.78	116.45	121.90
21	AA	1250	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1359	C	N3-C2-O2	-7.78	116.46	121.90
21	AA	1429	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	2670	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	160	A	N1-C6-N6	-7.78	113.94	118.60
48	BZ	29	ARG	NE-CZ-NH1	7.77	124.19	120.30
54	BA	1010	A	C4-C5-C6	-7.77	113.11	117.00
54	BA	2573	C	O4'-C1'-N1	7.77	114.42	108.20
54	BA	973	A	C5-C6-N1	7.77	121.59	117.70
54	BA	76	C	N3-C2-O2	-7.77	116.46	121.90
54	BA	972	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1876	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2164	C	N3-C2-O2	-7.77	116.46	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	466	A	C5-C6-N1	7.77	121.58	117.70
54	BA	52	A	N1-C6-N6	-7.77	113.94	118.60
55	BB	78	A	C4-C5-C6	-7.77	113.12	117.00
24	A3	60	A	C5-C6-N1	7.76	121.58	117.70
21	AA	676	A	C5-C6-N1	7.76	121.58	117.70
54	BA	910	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1762	A	C5-C6-N1	7.76	121.58	117.70
21	AA	160	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1048	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1871	A	C5-C6-N1	7.75	121.58	117.70
35	BM	59	ARG	NE-CZ-NH2	-7.75	116.42	120.30
54	BA	2823	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	764	A	C5-C6-N1	7.75	121.58	117.70
21	AA	1456	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	907	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1133	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1271	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	1413	A	N1-C6-N6	-7.74	113.95	118.60
37	BO	10	ARG	NE-CZ-NH1	7.74	124.17	120.30
54	BA	959	A	O4'-C1'-N9	7.74	114.39	108.20
54	BA	2781	A	C5-C6-N1	7.74	121.57	117.70
55	BB	92	C	O4'-C1'-N1	7.74	114.39	108.20
3	AD	69	ARG	NE-CZ-NH1	7.74	124.17	120.30
21	AA	48	C	N3-C2-O2	-7.74	116.49	121.90
21	AA	663	A	C5-C6-N1	7.74	121.57	117.70
54	BA	526	A	C5-C6-N1	7.74	121.57	117.70
21	AA	71	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	1403	C	N3-C2-O2	-7.73	116.49	121.90
24	A3	11	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	945	A	O4'-C1'-N9	7.73	114.39	108.20
54	BA	983	A	C5-C6-N1	7.73	121.57	117.70
2	AC	178	ARG	NE-CZ-NH1	7.73	124.17	120.30
21	AA	288	A	C5-C6-N1	7.73	121.57	117.70
54	BA	497	A	C5-C6-N1	7.73	121.56	117.70
54	BA	1652	A	C5-C6-N1	7.73	121.57	117.70
54	BA	1783	A	C5-C6-N1	7.73	121.56	117.70
54	BA	2786	U	O4'-C1'-N1	7.72	114.38	108.20
54	BA	2860	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2211	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2705	A	C5-C6-N1	7.72	121.56	117.70
21	AA	130	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	1054	C	N1-C2-O2	7.72	123.53	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1978	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2005	A	C5-C6-N1	7.72	121.56	117.70
55	BB	57	A	C5-C6-N1	7.72	121.56	117.70
21	AA	1004	A	C5-C6-N1	7.72	121.56	117.70
54	BA	984	A	C5-C6-N1	7.72	121.56	117.70
54	BA	50	U	O4'-C1'-N1	7.72	114.37	108.20
54	BA	1090	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	2474	U	O4'-C1'-N1	7.71	114.37	108.20
54	BA	73	A	C5-C6-N1	7.71	121.56	117.70
54	BA	626	A	C4-C5-C6	-7.71	113.14	117.00
54	BA	947	A	C5-C6-N1	7.71	121.56	117.70
54	BA	2130	U	N3-C2-O2	-7.71	116.80	122.20
21	AA	366	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	609	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	1301	A	C5-C6-N1	7.71	121.55	117.70
21	AA	129	A	C5-C6-N1	7.71	121.55	117.70
54	BA	91	A	O4'-C1'-N9	7.71	114.36	108.20
21	AA	865	A	N1-C6-N6	-7.71	113.98	118.60
24	A3	35	C	N3-C2-O2	-7.70	116.51	121.90
30	BH	68	ARG	NE-CZ-NH1	7.70	124.15	120.30
54	BA	1046	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1451	C	N3-C2-O2	-7.70	116.51	121.90
22	A1	38	A	C4-C5-C6	-7.70	113.15	117.00
54	BA	191	A	C5-C6-N1	7.70	121.55	117.70
54	BA	471	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	44	A	C4-C5-C6	-7.70	113.15	117.00
54	BA	666	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	16	A	N1-C6-N6	-7.69	113.98	118.60
21	AA	845	A	C5-C6-N1	7.69	121.55	117.70
54	BA	118	A	C5-C6-N1	7.69	121.55	117.70
54	BA	149	A	N1-C6-N6	-7.69	113.98	118.60
54	BA	1165	A	N1-C6-N6	-7.69	113.98	118.60
54	BA	382	A	C5-C6-N1	7.69	121.55	117.70
21	AA	274	A	C4-C5-C6	-7.69	113.16	117.00
54	BA	878	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	492	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	1615	C	N3-C2-O2	-7.69	116.52	121.90
21	AA	1225	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	1274	A	N1-C6-N6	-7.68	113.99	118.60
25	BC	51	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	219	A	N1-C6-N6	-7.68	113.99	118.60
11	AL	35	ARG	NE-CZ-NH1	7.68	124.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	432	A	C4-C5-C6	-7.68	113.16	117.00
54	BA	1590	A	N1-C6-N6	-7.68	113.99	118.60
9	AJ	16	ARG	NE-CZ-NH1	7.68	124.14	120.30
21	AA	982	U	P-O3'-C3'	7.68	128.91	119.70
8	AI	122	ARG	NE-CZ-NH2	7.68	124.14	120.30
54	BA	216	A	C5-C6-N1	7.68	121.54	117.70
54	BA	2682	A	N1-C6-N6	-7.68	113.99	118.60
14	AO	63	ARG	NE-CZ-NH1	7.67	124.14	120.30
21	AA	116	A	C5-C6-N1	7.67	121.54	117.70
54	BA	1395	A	C5-C6-N1	7.67	121.54	117.70
21	AA	720	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	2518	A	C5-C6-N1	7.67	121.54	117.70
22	A1	23	A	C5-C6-N1	7.67	121.53	117.70
21	AA	923	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1321	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	44	A	C5-C6-N1	7.67	121.53	117.70
21	AA	487	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	1969	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1229	A	C5-C6-N1	7.66	121.53	117.70
54	BA	1489	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	1991	U	O4'-C1'-N1	7.66	114.33	108.20
54	BA	2211	A	C5-C6-N1	7.66	121.53	117.70
21	AA	431	A	C5-C6-N1	7.66	121.53	117.70
54	BA	730	A	C5-C6-N1	7.66	121.53	117.70
48	BZ	37	ARG	NE-CZ-NH1	7.66	124.13	120.30
54	BA	196	A	C5-C6-N1	7.66	121.53	117.70
54	BA	889	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	1213	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	2191	A	C5-C6-N1	7.66	121.53	117.70
55	BB	12	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	1342	A	C5-C6-N1	7.65	121.53	117.70
21	AA	946	A	C5-C6-N1	7.65	121.53	117.70
2	AC	163	ARG	NE-CZ-NH1	7.65	124.12	120.30
21	AA	1101	A	C5-C6-N1	7.65	121.53	117.70
54	BA	514	A	C5-C6-N1	7.65	121.52	117.70
54	BA	547	A	N1-C6-N6	-7.65	114.01	118.60
21	AA	777	A	C5-C6-N1	7.65	121.52	117.70
54	BA	877	A	C5-C6-N1	7.65	121.52	117.70
54	BA	1927	A	N1-C6-N6	-7.65	114.01	118.60
3	AD	183	ARG	NE-CZ-NH1	7.64	124.12	120.30
54	BA	2823	A	C5-C6-N1	7.64	121.52	117.70
54	BA	513	A	N1-C6-N6	-7.64	114.01	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2814	A	C5-C6-N1	7.64	121.52	117.70
21	AA	978	A	C4-C5-C6	-7.64	113.18	117.00
54	BA	346	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2439	A	C5-C6-N1	7.64	121.52	117.70
54	BA	139	U	O4'-C1'-N1	7.64	114.31	108.20
54	BA	532	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	2059	A	C5-C6-N1	7.63	121.52	117.70
54	BA	181	A	C5-C6-N1	7.63	121.52	117.70
54	BA	2266	A	C5-C6-N1	7.63	121.52	117.70
21	AA	381	C	N3-C2-O2	-7.63	116.56	121.90
24	A3	73	A	C5-C6-N1	7.63	121.51	117.70
28	BF	29	ARG	NE-CZ-NH1	7.63	124.11	120.30
53	B4	24	ARG	NE-CZ-NH1	7.63	124.11	120.30
21	AA	501	C	N3-C2-O2	-7.63	116.56	121.90
54	BA	223	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	1363	A	C5-C6-N1	7.62	121.51	117.70
54	BA	374	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	753	A	C5-C6-N1	7.62	121.51	117.70
21	AA	790	A	C5-C6-N1	7.62	121.51	117.70
21	AA	961	U	O4'-C1'-N1	7.62	114.30	108.20
21	AA	1000	A	C5-C6-N1	7.62	121.51	117.70
21	AA	1236	A	C5-C6-N1	7.62	121.51	117.70
21	AA	89	U	O4'-C1'-N1	7.62	114.30	108.20
21	AA	747	A	C5-C6-N1	7.62	121.51	117.70
21	AA	1016	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1008	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1268	A	C5-C6-N1	7.62	121.51	117.70
21	AA	325	A	C5-C6-N1	7.61	121.51	117.70
54	BA	429	A	C5-C6-N1	7.61	121.51	117.70
54	BA	435	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	988	A	C5-C6-N1	7.61	121.51	117.70
54	BA	1705	A	C5-C6-N1	7.61	121.51	117.70
54	BA	2003	A	C5-C6-N1	7.61	121.51	117.70
27	BE	114	ARG	NE-CZ-NH1	7.61	124.11	120.30
54	BA	423	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	1022	G	O4'-C1'-N9	7.61	114.29	108.20
54	BA	2577	A	C5-C6-N1	7.61	121.51	117.70
6	AG	101	ARG	NE-CZ-NH1	7.61	124.11	120.30
54	BA	1129	A	C5-C6-N1	7.61	121.50	117.70
54	BA	2101	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	109	A	C1'-O4'-C4'	-7.61	103.82	109.90
54	BA	95	A	N1-C6-N6	-7.61	114.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2090	A	C5-C6-N1	7.61	121.50	117.70
54	BA	2394	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	2646	C	N1-C2-O2	7.60	123.46	118.90
21	AA	1394	A	C5-C6-N1	7.60	121.50	117.70
54	BA	1039	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	174	A	C5-C6-N1	7.60	121.50	117.70
21	AA	1492	A	C5-C6-N1	7.60	121.50	117.70
54	BA	2764	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	2766	A	C5-C6-N1	7.60	121.50	117.70
21	AA	205	A	C5-C6-N1	7.60	121.50	117.70
54	BA	179	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	1373	A	N1-C6-N6	-7.60	114.04	118.60
55	BB	39	A	C5-C6-N1	7.60	121.50	117.70
55	BB	115	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	1147	A	C5-C6-N1	7.60	121.50	117.70
54	BA	142	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	428	A	C5-C6-N1	7.59	121.50	117.70
21	AA	696	A	C4-C5-C6	-7.59	113.20	117.00
54	BA	1096	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	435	C	O4'-C1'-N1	7.59	114.27	108.20
54	BA	1711	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	1784	A	C5-C6-N1	7.59	121.49	117.70
21	AA	1519	A	C5-C6-N1	7.58	121.49	117.70
22	A1	38	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1007	C	N3-C2-O2	-7.58	116.59	121.90
21	AA	900	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1630	A	C4-C5-C6	-7.58	113.21	117.00
54	BA	1794	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1433	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1020	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	748	G	O4'-C1'-N9	7.58	114.26	108.20
54	BA	1211	C	N3-C2-O2	-7.58	116.59	121.90
21	AA	344	A	C5-C6-N1	7.58	121.49	117.70
21	AA	498	A	C5-C6-N1	7.58	121.49	117.70
21	AA	608	A	N1-C6-N6	-7.58	114.06	118.60
54	BA	2461	A	C5-C6-N1	7.58	121.49	117.70
9	AJ	9	ARG	NE-CZ-NH1	7.57	124.09	120.30
54	BA	685	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	751	A	O4'-C1'-N9	7.57	114.26	108.20
54	BA	1265	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1580	A	C5-C6-N1	7.57	121.49	117.70
54	BA	1872	A	C5-C6-N1	7.57	121.48	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2117	A	N1-C6-N6	-7.57	114.06	118.60
21	AA	7	A	C5-C6-N1	7.57	121.48	117.70
21	AA	80	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1528	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	1630	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1383	A	O4'-C1'-N9	7.56	114.25	108.20
21	AA	279	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2158	A	C4-C5-C6	-7.56	113.22	117.00
21	AA	280	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	457	A	C5-C6-N1	7.56	121.48	117.70
21	AA	1503	A	C5-C6-N1	7.56	121.48	117.70
54	BA	371	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	1549	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	2119	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	2451	A	C4-C5-C6	-7.56	113.22	117.00
54	BA	74	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2314	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2284	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	549	C	N3-C2-O2	-7.55	116.61	121.90
54	BA	1384	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2741	A	C5-C6-N1	7.55	121.47	117.70
2	AC	168	ARG	NE-CZ-NH1	7.55	124.07	120.30
21	AA	1269	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	706	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1145	A	C5-C6-N1	7.54	121.47	117.70
21	AA	1480	A	C4-C5-C6	-7.54	113.23	117.00
22	A1	26	A	C5-C6-N1	7.54	121.47	117.70
54	BA	119	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1352	U	N3-C2-O2	-7.54	116.92	122.20
54	BA	2117	A	C5-C6-N1	7.54	121.47	117.70
54	BA	2542	A	C5-C6-N1	7.54	121.47	117.70
22	A1	21	A	N1-C6-N6	-7.54	114.08	118.60
24	A3	74	A	C5-C6-N1	7.54	121.47	117.70
21	AA	574	A	C5-C6-N1	7.54	121.47	117.70
28	BF	149	ARG	NE-CZ-NH1	7.54	124.07	120.30
54	BA	1127	A	C5-C6-N1	7.54	121.47	117.70
54	BA	401	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	677	A	C4-C5-C6	-7.53	113.23	117.00
54	BA	2627	G	C1'-O4'-C4'	-7.53	103.87	109.90
54	BA	28	A	N1-C6-N6	-7.53	114.08	118.60
21	AA	1468	A	C5-C6-N1	7.53	121.47	117.70
54	BA	2060	A	C5-C6-N1	7.53	121.46	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	174	A	N1-C6-N6	-7.53	114.08	118.60
21	AA	1362	A	C5-C6-N1	7.53	121.46	117.70
21	AA	1102	A	N1-C6-N6	-7.53	114.08	118.60
24	A3	44	A	C5-C6-N1	7.53	121.46	117.70
54	BA	196	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	2893	A	C5-C6-N1	7.53	121.46	117.70
54	BA	1679	A	C5-C6-N1	7.52	121.46	117.70
54	BA	613	A	O4'-C1'-N9	7.52	114.22	108.20
54	BA	391	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1853	A	C5-C6-N1	7.52	121.46	117.70
54	BA	199	A	C5-C6-N1	7.52	121.46	117.70
54	BA	2392	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	665	A	C5-C6-N1	7.51	121.46	117.70
21	AA	1476	A	C5-C6-N1	7.51	121.46	117.70
35	BM	81	ARG	NE-CZ-NH2	7.51	124.06	120.30
21	AA	1226	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	505	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	892	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	130	A	C5-C6-N1	7.51	121.45	117.70
21	AA	151	A	C5-C6-N1	7.51	121.45	117.70
54	BA	1786	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2411	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2721	A	C5-C6-N1	7.51	121.45	117.70
21	AA	509	A	C5-C6-N1	7.51	121.45	117.70
44	BV	19	ARG	NE-CZ-NH1	7.51	124.05	120.30
54	BA	527	C	N3-C2-O2	-7.51	116.65	121.90
54	BA	538	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	157	C	O4'-C1'-N1	7.50	114.20	108.20
8	AI	118	ARG	NE-CZ-NH1	7.50	124.05	120.30
21	AA	263	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1518	A	C4-C5-C6	-7.50	113.25	117.00
30	BH	97	ARG	NE-CZ-NH1	7.50	124.05	120.30
21	AA	782	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1580	A	C4-C5-C6	-7.50	113.25	117.00
21	AA	320	A	C5-C6-N1	7.50	121.45	117.70
21	AA	909	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1054	C	N3-C2-O2	-7.50	116.65	121.90
54	BA	2611	C	N3-C2-O2	-7.50	116.65	121.90
6	AG	77	ARG	NE-CZ-NH1	7.49	124.05	120.30
21	AA	1019	A	C4-C5-C6	-7.49	113.25	117.00
21	AA	1163	A	C5-C6-N1	7.49	121.45	117.70
24	A3	38	A	C5-C6-N1	7.49	121.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1967	C	N3-C2-O2	-7.49	116.65	121.90
22	A1	56	C	N3-C2-O2	-7.49	116.66	121.90
54	BA	572	A	C5-C6-N1	7.49	121.45	117.70
21	AA	282	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	1134	A	C5-C6-N1	7.49	121.44	117.70
54	BA	563	A	C5-C6-N1	7.49	121.44	117.70
54	BA	654	A	C4-C5-C6	-7.49	113.26	117.00
54	BA	1244	A	C5-C6-N1	7.49	121.44	117.70
54	BA	927	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2733	A	C5-C6-N1	7.48	121.44	117.70
21	AA	313	A	C4-C5-C6	-7.48	113.26	117.00
21	AA	983	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	503	A	C5-C6-N1	7.48	121.44	117.70
54	BA	1496	A	C4-C5-C6	-7.48	113.26	117.00
54	BA	1000	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1353	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2126	A	N1-C6-N6	-7.47	114.11	118.60
54	BA	2270	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	941	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2288	A	C5-C6-N1	7.47	121.44	117.70
54	BA	631	A	C5-C6-N1	7.47	121.44	117.70
21	AA	546	A	C5-C6-N1	7.47	121.43	117.70
54	BA	163	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	1090	A	C5-C6-N1	7.47	121.44	117.70
21	AA	946	A	N1-C6-N6	-7.47	114.12	118.60
22	A1	14	A	N1-C6-N6	-7.47	114.12	118.60
35	BM	66	ARG	NE-CZ-NH1	7.47	124.03	120.30
54	BA	1194	A	C5-C6-N1	7.47	121.43	117.70
54	BA	947	A	C4-C5-C6	-7.46	113.27	117.00
54	BA	1005	C	N3-C2-O2	-7.46	116.67	121.90
54	BA	1544	A	C5-C6-N1	7.46	121.43	117.70
21	AA	8	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1938	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	2328	A	C5-C6-N1	7.46	121.43	117.70
12	AM	78	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	739	A	N1-C6-N6	-7.46	114.13	118.60
54	BA	229	C	N3-C2-O2	-7.45	116.68	121.90
54	BA	1933	G	O4'-C1'-N9	7.45	114.16	108.20
54	BA	1952	A	C5-C6-N1	7.45	121.43	117.70
54	BA	2666	C	N3-C2-O2	-7.45	116.68	121.90
21	AA	110	C	N3-C2-O2	-7.45	116.69	121.90
26	BD	169	ARG	NE-CZ-NH1	7.45	124.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2052	A	C4-C5-C6	-7.45	113.28	117.00
9	AJ	72	ARG	NE-CZ-NH2	-7.45	116.58	120.30
21	AA	1005	A	C5-C6-N1	7.45	121.42	117.70
21	AA	1362	A	C4-C5-C6	-7.45	113.28	117.00
21	AA	1447	A	C5-C6-N1	7.45	121.42	117.70
54	BA	998	C	N3-C2-O2	-7.45	116.69	121.90
21	AA	1534	A	C5-C6-N1	7.45	121.42	117.70
54	BA	362	A	N1-C6-N6	-7.45	114.13	118.60
5	AF	86	ARG	NE-CZ-NH1	7.45	124.02	120.30
15	AP	51	ARG	NE-CZ-NH1	7.45	124.02	120.30
21	AA	523	A	C5-C6-N1	7.45	121.42	117.70
21	AA	1200	C	N3-C2-O2	-7.45	116.69	121.90
29	BG	68	ARG	NE-CZ-NH1	7.45	124.02	120.30
54	BA	104	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	1137	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	918	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1021	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1142	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1735	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2499	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	2503	A	C5-C6-N1	7.44	121.42	117.70
54	BA	613	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2388	A	C5-C6-N1	7.44	121.42	117.70
21	AA	819	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	2900	A	C5-C6-N1	7.44	121.42	117.70
21	AA	831	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	131	A	C4-C5-C6	-7.43	113.28	117.00
21	AA	214	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	2183	A	C5-C6-N1	7.43	121.42	117.70
21	AA	430	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	814	A	C5-C6-N1	7.43	121.42	117.70
21	AA	938	A	N1-C6-N6	-7.43	114.14	118.60
34	BL	41	ARG	NE-CZ-NH1	-7.43	116.59	120.30
54	BA	460	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2407	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	2516	A	C5-C6-N1	7.43	121.42	117.70
54	BA	899	A	C5-C6-N1	7.43	121.41	117.70
54	BA	2856	A	C5-C6-N1	7.43	121.41	117.70
21	AA	864	A	C5-C6-N1	7.43	121.41	117.70
54	BA	1582	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	1722	A	C5-C6-N1	7.43	121.41	117.70
21	AA	55	A	C4-C5-C6	-7.42	113.29	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	414	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1111	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1513	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	730	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	222	A	C5-C6-N1	7.42	121.41	117.70
54	BA	347	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	1204	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	1460	U	O4'-C1'-N1	7.42	114.14	108.20
54	BA	1900	A	C5-C6-N1	7.42	121.41	117.70
21	AA	743	A	C5-C6-N1	7.42	121.41	117.70
54	BA	152	A	C4-C5-C6	-7.42	113.29	117.00
54	BA	776	G	N3-C2-N2	-7.42	114.71	119.90
21	AA	969	A	C5-C6-N1	7.42	121.41	117.70
23	A2	80	C	P-O3'-C3'	7.42	128.60	119.70
55	BB	52	A	C5-C6-N1	7.42	121.41	117.70
16	AQ	26	ARG	NE-CZ-NH1	7.42	124.01	120.30
25	BC	132	ARG	NE-CZ-NH2	-7.42	116.59	120.30
33	BK	30	ARG	NE-CZ-NH1	7.42	124.01	120.30
54	BA	2199	A	C4-C5-C6	-7.42	113.29	117.00
21	AA	535	A	C5-C6-N1	7.41	121.41	117.70
54	BA	2311	A	C5-C6-N1	7.41	121.41	117.70
33	BK	64	ARG	NE-CZ-NH1	7.41	124.01	120.30
3	AD	13	ARG	NE-CZ-NH1	7.41	124.00	120.30
18	AS	35	ARG	NE-CZ-NH1	7.41	124.00	120.30
21	AA	51	A	C5-C6-N1	7.41	121.41	117.70
21	AA	635	A	N1-C6-N6	-7.41	114.15	118.60
21	AA	1239	A	C5-C6-N1	7.41	121.41	117.70
54	BA	571	U	O4'-C1'-N1	7.41	114.13	108.20
54	BA	1962	C	N3-C2-O2	-7.41	116.71	121.90
54	BA	1241	A	C5-C6-N1	7.41	121.40	117.70
21	AA	718	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2711	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2765	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2809	A	C5-C6-N1	7.41	121.40	117.70
21	AA	119	A	N1-C6-N6	-7.41	114.16	118.60
21	AA	460	A	N1-C6-N6	-7.41	114.16	118.60
21	AA	640	A	C5-C6-N1	7.41	121.40	117.70
54	BA	1085	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2009	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	2887	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2317	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	81	A	C5-C6-N1	7.40	121.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	459	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1809	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	2213	U	O4'-C1'-N1	7.40	114.12	108.20
54	BA	2586	U	O4'-C1'-N1	7.40	114.12	108.20
54	BA	513	A	C5-C6-N1	7.40	121.40	117.70
21	AA	573	A	C5-C6-N1	7.40	121.40	117.70
54	BA	103	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2610	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	2639	A	C4-C5-C6	-7.40	113.30	117.00
55	BB	104	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	808	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	180	G	O4'-C1'-N9	7.40	114.12	108.20
54	BA	2602	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1105	A	C5-C6-N1	7.39	121.40	117.70
22	A1	9	A	C5-C6-N1	7.39	121.40	117.70
54	BA	602	A	C5-C6-N1	7.39	121.40	117.70
21	AA	78	A	C5-C6-N1	7.39	121.39	117.70
21	AA	532	A	C5-C6-N1	7.39	121.39	117.70
21	AA	630	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1545	A	N1-C6-N6	-7.39	114.17	118.60
21	AA	98	A	C5-C6-N1	7.39	121.39	117.70
54	BA	529	A	N1-C6-N6	-7.39	114.17	118.60
21	AA	702	A	C5-C6-N1	7.39	121.39	117.70
21	AA	1360	A	C5-C6-N1	7.39	121.39	117.70
54	BA	2497	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1655	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	1151	A	C5-C6-N1	7.38	121.39	117.70
54	BA	221	A	C5-C6-N1	7.38	121.39	117.70
54	BA	217	A	C5-C6-N1	7.38	121.39	117.70
21	AA	19	A	C5-C6-N1	7.38	121.39	117.70
21	AA	461	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1502	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	505	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	546	U	O4'-C1'-N1	7.38	114.10	108.20
54	BA	1754	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	2426	A	N1-C6-N6	-7.38	114.17	118.60
6	AG	118	ARG	NE-CZ-NH1	7.38	123.99	120.30
54	BA	1151	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	2251	G	O4'-C1'-N9	7.38	114.10	108.20
54	BA	1515	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1815	A	C4-C5-C6	-7.37	113.31	117.00
53	B4	12	ARG	NE-CZ-NH1	7.37	123.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	144	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1652	A	O4'-C1'-N9	7.37	114.10	108.20
54	BA	1689	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	2847	U	O4'-C1'-N1	7.37	114.10	108.20
6	AG	137	ARG	NE-CZ-NH1	7.37	123.98	120.30
54	BA	1590	A	C5-C6-N1	7.37	121.39	117.70
21	AA	1167	A	C5-C6-N1	7.37	121.38	117.70
54	BA	796	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	373	A	C5-C6-N1	7.37	121.38	117.70
21	AA	1333	A	C5-C6-N1	7.37	121.38	117.70
54	BA	740	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	2134	A	C4-C5-C6	-7.37	113.32	117.00
54	BA	2501	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	499	A	N1-C6-N6	-7.36	114.18	118.60
21	AA	975	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2449	U	O4'-C1'-N1	7.36	114.09	108.20
54	BA	2799	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2858	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	515	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2042	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1912	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2453	A	C5-C6-N1	7.36	121.38	117.70
3	AD	127	ARG	NE-CZ-NH1	7.36	123.98	120.30
21	AA	412	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1701	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2052	A	C5-C6-N1	7.36	121.38	117.70
21	AA	415	A	C5-C6-N1	7.35	121.38	117.70
24	A3	58	A	C5-C6-N1	7.35	121.38	117.70
32	BJ	34	ARG	NE-CZ-NH1	7.35	123.98	120.30
54	BA	156	A	C5-C6-N1	7.35	121.38	117.70
54	BA	1395	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1553	A	C5-C6-N1	7.35	121.38	117.70
54	BA	1717	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2856	A	N1-C6-N6	-7.35	114.19	118.60
17	AR	62	ARG	NE-CZ-NH1	7.35	123.97	120.30
21	AA	860	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1320	C	O4'-C1'-N1	7.35	114.08	108.20
21	AA	819	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1403	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1433	A	O4'-C1'-N9	7.34	114.08	108.20
54	BA	2062	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2883	A	C5-C6-N1	7.34	121.37	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	913	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	207	A	C5-C6-N1	7.34	121.37	117.70
24	A3	59	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	2310	C	O4'-C1'-N1	7.34	114.07	108.20
54	BA	2378	A	C5-C6-N1	7.34	121.37	117.70
54	BA	28	A	C5-C6-N1	7.34	121.37	117.70
21	AA	1280	A	O4'-C1'-N9	7.34	114.07	108.20
54	BA	706	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	1079	C	N3-C2-O2	-7.34	116.77	121.90
54	BA	2019	A	C5-C6-N1	7.34	121.37	117.70
54	BA	756	A	C5-C6-N1	7.33	121.37	117.70
54	BA	1088	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	2097	A	C4-C5-C6	-7.33	113.33	117.00
54	BA	2169	A	C5-C6-N1	7.33	121.37	117.70
21	AA	1394	A	C4-C5-C6	-7.33	113.33	117.00
54	BA	143	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	800	A	C4-C5-C6	-7.33	113.33	117.00
21	AA	364	A	C5-C6-N1	7.33	121.36	117.70
54	BA	878	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2551	C	N3-C2-O2	-7.33	116.77	121.90
14	AO	16	ARG	NE-CZ-NH1	7.33	123.96	120.30
21	AA	152	A	C4-C5-C6	-7.33	113.34	117.00
54	BA	197	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2054	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2340	A	C5-C6-N1	7.33	121.36	117.70
53	B4	19	ARG	NE-CZ-NH1	7.33	123.96	120.30
54	BA	443	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	1001	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	1322	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2639	A	C5-C6-N1	7.33	121.36	117.70
21	AA	235	C	N3-C2-O2	-7.32	116.77	121.90
54	BA	516	C	N3-C2-O2	-7.32	116.77	121.90
54	BA	1069	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	2147	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2670	A	C5-C6-N1	7.32	121.36	117.70
54	BA	603	A	C5-C6-N1	7.32	121.36	117.70
21	AA	1067	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1048	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	1070	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1531	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	255	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	1204	A	O4'-C1'-N9	7.32	114.06	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	473	U	P-O3'-C3'	7.32	128.48	119.70
21	AA	784	A	C4-C5-C6	-7.32	113.34	117.00
21	AA	915	A	C5-C6-N1	7.32	121.36	117.70
54	BA	69	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	311	A	C5-C6-N1	7.32	121.36	117.70
54	BA	789	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2212	A	C5-C6-N1	7.32	121.36	117.70
21	AA	807	A	C5-C6-N1	7.31	121.36	117.70
54	BA	1848	A	C5-C6-N1	7.31	121.36	117.70
21	AA	1219	A	C4-C5-C6	-7.31	113.34	117.00
54	BA	1000	A	C4-C5-C6	-7.31	113.34	117.00
54	BA	1175	A	C5-C6-N1	7.31	121.36	117.70
54	BA	402	A	C5-C6-N1	7.31	121.36	117.70
54	BA	541	A	C5-C6-N1	7.31	121.36	117.70
54	BA	721	A	N1-C6-N6	-7.31	114.22	118.60
54	BA	2459	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2725	A	C5-C6-N1	7.31	121.36	117.70
5	AF	44	ARG	NE-CZ-NH1	7.31	123.95	120.30
21	AA	1196	A	C5-C6-N1	7.31	121.35	117.70
54	BA	608	A	C5-C6-N1	7.31	121.35	117.70
54	BA	1246	A	C5-C6-N1	7.31	121.35	117.70
54	BA	1569	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1815	A	C5-C6-N1	7.30	121.35	117.70
54	BA	721	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2476	A	C5-C6-N1	7.30	121.35	117.70
37	BO	81	ARG	NE-CZ-NH1	7.30	123.95	120.30
54	BA	2114	A	N1-C6-N6	-7.30	114.22	118.60
21	AA	1014	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	829	A	C5-C6-N1	7.30	121.35	117.70
21	AA	441	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1346	A	C5-C6-N1	7.30	121.35	117.70
54	BA	34	U	O4'-C1'-N1	7.30	114.04	108.20
54	BA	1143	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1251	A	C5-C6-N1	7.29	121.35	117.70
21	AA	1507	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1398	C	N3-C2-O2	-7.29	116.79	121.90
20	AU	44	ARG	NE-CZ-NH1	7.29	123.95	120.30
54	BA	1532	A	C5-C6-N1	7.29	121.35	117.70
54	BA	2298	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	2358	A	C4-C5-C6	-7.29	113.35	117.00
54	BA	2667	C	N3-C2-O2	-7.29	116.80	121.90
21	AA	892	A	C5-C6-N1	7.29	121.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1378	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1801	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	2322	A	N1-C6-N6	-7.29	114.22	118.60
7	AH	113	ARG	NE-CZ-NH1	7.29	123.94	120.30
54	BA	2030	A	C5-C6-N1	7.29	121.34	117.70
54	BA	2899	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1180	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1431	A	C5-C6-N1	7.29	121.34	117.70
54	BA	896	A	C5-C6-N1	7.29	121.34	117.70
21	AA	978	A	C5-C6-N1	7.29	121.34	117.70
54	BA	2439	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	1470	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2721	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	582	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	1254	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	1322	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	1481	U	O4'-C1'-N1	7.28	114.02	108.20
54	BA	1505	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1918	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	590	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	750	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1375	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1775	U	O4'-C1'-N1	7.28	114.02	108.20
54	BA	155	A	N1-C6-N6	-7.27	114.24	118.60
54	BA	890	C	N3-C2-O2	-7.27	116.81	121.90
45	BW	54	ARG	NE-CZ-NH2	7.27	123.94	120.30
54	BA	654	A	C5-C6-N1	7.27	121.34	117.70
21	AA	919	A	C5-C6-N1	7.27	121.34	117.70
54	BA	613	A	N1-C6-N6	-7.27	114.24	118.60
12	AM	92	ARG	NE-CZ-NH1	7.27	123.94	120.30
54	BA	324	A	C5-C6-N1	7.27	121.33	117.70
54	BA	775	G	O4'-C1'-N9	7.27	114.02	108.20
54	BA	1938	A	C5-C6-N1	7.27	121.33	117.70
54	BA	2749	A	C5-C6-N1	7.27	121.33	117.70
3	AD	12	ARG	NE-CZ-NH1	7.27	123.93	120.30
54	BA	19	A	N1-C6-N6	-7.27	114.24	118.60
22	A1	35	A	C5-C6-N1	7.26	121.33	117.70
36	BN	86	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	1690	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2108	A	C5-C6-N1	7.26	121.33	117.70
21	AA	958	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1597	A	C5-C6-N1	7.26	121.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	109	A	C4-C5-C6	-7.26	113.37	117.00
21	AA	511	C	N3-C2-O2	-7.26	116.82	121.90
21	AA	243	A	C5-C6-N1	7.26	121.33	117.70
54	BA	472	A	C5-C6-N1	7.26	121.33	117.70
54	BA	866	A	N1-C6-N6	-7.26	114.25	118.60
54	BA	83	A	C5-C6-N1	7.25	121.33	117.70
21	AA	181	A	C5-C6-N1	7.25	121.33	117.70
21	AA	411	A	C5-C6-N1	7.25	121.33	117.70
22	A1	69	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1885	A	C5-C6-N1	7.25	121.33	117.70
21	AA	510	A	C5-C6-N1	7.25	121.33	117.70
21	AA	1500	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	1472	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	1413	A	N1-C6-N6	-7.25	114.25	118.60
21	AA	650	G	N3-C2-N2	-7.25	114.83	119.90
26	BD	128	ARG	NE-CZ-NH1	7.25	123.92	120.30
54	BA	2412	A	C5-C6-N1	7.25	121.32	117.70
54	BA	2565	A	C5-C6-N1	7.25	121.32	117.70
21	AA	1021	A	C5-C6-N1	7.25	121.32	117.70
54	BA	2070	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	2430	A	C5-C6-N1	7.25	121.32	117.70
10	AK	121	ARG	NE-CZ-NH1	7.24	123.92	120.30
54	BA	675	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1789	A	C5-C6-N1	7.24	121.32	117.70
25	BC	257	ARG	NE-CZ-NH1	7.24	123.92	120.30
54	BA	979	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1469	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1596	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	2660	A	C5-C6-N1	7.24	121.32	117.70
54	BA	845	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	637	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1586	A	C5-C6-N1	7.24	121.32	117.70
21	AA	161	A	C5-C6-N1	7.23	121.32	117.70
54	BA	2020	A	C1'-O4'-C4'	-7.23	104.11	109.90
54	BA	627	A	C5-C6-N1	7.23	121.31	117.70
54	BA	749	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1428	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	1549	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2893	A	N1-C6-N6	-7.23	114.26	118.60
21	AA	873	A	C5-C6-N1	7.23	121.31	117.70
54	BA	310	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	1894	C	O4'-C1'-N1	7.23	113.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2482	A	C5-C6-N1	7.23	121.31	117.70
12	AM	28	ARG	NE-CZ-NH1	7.23	123.91	120.30
21	AA	695	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1140	C	N3-C2-O2	-7.23	116.84	121.90
51	B2	28	ARG	NE-CZ-NH1	7.23	123.91	120.30
54	BA	522	A	C4-C5-C6	-7.23	113.39	117.00
21	AA	1377	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1469	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	480	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1103	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	1655	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1936	A	C5-C6-N1	7.22	121.31	117.70
21	AA	315	A	C5-C6-N1	7.22	121.31	117.70
21	AA	949	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1848	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	2434	A	C4-C5-C6	-7.22	113.39	117.00
55	BB	73	A	C5-C6-N1	7.22	121.31	117.70
21	AA	622	A	C5-C6-N1	7.22	121.31	117.70
39	BQ	10	ARG	NE-CZ-NH1	7.22	123.91	120.30
54	BA	279	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	53	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1609	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	149	A	C5-C6-N1	7.22	121.31	117.70
21	AA	780	A	C5-C6-N1	7.22	121.31	117.70
21	AA	938	A	C5-C6-N1	7.22	121.31	117.70
54	BA	311	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	1254	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2014	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2422	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	739	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	1014	A	C5-C6-N1	7.21	121.31	117.70
28	BF	132	ARG	NE-CZ-NH1	7.21	123.91	120.30
54	BA	490	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	899	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	5	A	C5-C6-N1	7.21	121.31	117.70
21	AA	228	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1035	A	C5-C6-N1	7.21	121.31	117.70
54	BA	371	A	C5-C6-N1	7.21	121.31	117.70
54	BA	886	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	1970	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2829	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1246	A	C4-C5-C6	-7.21	113.39	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2810	A	C4-C5-C6	-7.21	113.39	117.00
2	AC	130	ARG	NE-CZ-NH1	7.21	123.90	120.30
4	AE	156	ARG	NE-CZ-NH1	7.21	123.90	120.30
21	AA	1441	A	C5-C6-N1	7.21	121.31	117.70
54	BA	66	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	1634	A	C5-C6-N1	7.21	121.30	117.70
54	BA	2241	A	C4-C5-C6	-7.21	113.40	117.00
21	AA	285	C	N3-C2-O2	-7.21	116.86	121.90
21	AA	1352	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	420	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	572	A	N1-C6-N6	-7.21	114.28	118.60
21	AA	754	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	792	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1229	A	O4'-C1'-N9	7.20	113.96	108.20
54	BA	1427	A	C5-C6-N1	7.20	121.30	117.70
5	AF	79	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	104	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1877	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	2142	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1273	C	N3-C2-O2	-7.20	116.86	121.90
23	A2	82	A	C5-C6-N1	7.20	121.30	117.70
54	BA	804	A	C5-C6-N1	7.20	121.30	117.70
54	BA	838	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	1295	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	1326	U	O4'-C1'-N1	7.20	113.96	108.20
54	BA	1610	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2274	A	C5-C6-N1	7.20	121.30	117.70
21	AA	607	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	630	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	550	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	2003	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	2160	C	N3-C2-O2	-7.20	116.86	121.90
21	AA	1430	A	C5-C6-N1	7.19	121.30	117.70
54	BA	142	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2059	A	N1-C6-N6	-7.19	114.28	118.60
8	AI	40	ARG	NE-CZ-NH1	7.19	123.90	120.30
21	AA	729	A	C4-C5-C6	-7.19	113.41	117.00
54	BA	1434	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1572	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2478	A	C5-C6-N1	7.19	121.30	117.70
21	AA	370	C	N3-C2-O2	-7.19	116.87	121.90
21	AA	1357	A	C5-C6-N1	7.19	121.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	90	C	N3-C2-O2	-7.19	116.87	121.90
21	AA	397	A	C5-C6-N1	7.19	121.29	117.70
54	BA	272	A	C5-C6-N1	7.19	121.29	117.70
54	BA	344	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	401	A	C5-C6-N1	7.19	121.29	117.70
54	BA	901	C	N3-C2-O2	-7.19	116.87	121.90
54	BA	2327	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	2809	A	O4'-C1'-N9	7.19	113.95	108.20
21	AA	162	A	C5-C6-N1	7.18	121.29	117.70
56	B5	122	ARG	NE-CZ-NH1	7.18	123.89	120.30
54	BA	1977	A	N1-C6-N6	-7.18	114.29	118.60
21	AA	969	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	270	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	1340	U	N3-C2-O2	-7.18	117.17	122.20
54	BA	1889	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1899	A	N1-C6-N6	-7.18	114.29	118.60
21	AA	1239	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	322	A	C5-C6-N1	7.18	121.29	117.70
21	AA	487	A	C5-C6-N1	7.18	121.29	117.70
21	AA	927	G	C1'-O4'-C4'	-7.17	104.16	109.90
21	AA	1349	A	C5-C6-N1	7.17	121.29	117.70
54	BA	14	A	C5-C6-N1	7.17	121.29	117.70
21	AA	536	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	1130	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	960	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1013	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	2149	U	O4'-C1'-N1	7.17	113.94	108.20
21	AA	59	A	C5-C6-N1	7.17	121.28	117.70
21	AA	236	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2376	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2458	G	O4'-C1'-N9	7.17	113.94	108.20
54	BA	2682	A	C5-C6-N1	7.17	121.28	117.70
21	AA	199	A	C5-C6-N1	7.17	121.28	117.70
21	AA	363	A	C5-C6-N1	7.17	121.28	117.70
21	AA	1167	A	N1-C6-N6	-7.16	114.30	118.60
21	AA	1502	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2013	A	C5-C6-N1	7.16	121.28	117.70
21	AA	139	A	C5-C6-N1	7.16	121.28	117.70
54	BA	632	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2080	A	C5-C6-N1	7.16	121.28	117.70
21	AA	306	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	624	C	N3-C2-O2	-7.16	116.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	877	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	675	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2738	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2872	A	C5-C6-N1	7.16	121.28	117.70
21	AA	306	A	C5-C6-N1	7.16	121.28	117.70
21	AA	322	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	1286	A	C5-C6-N1	7.16	121.28	117.70
21	AA	768	A	N1-C6-N6	-7.15	114.31	118.60
1	AB	112	ARG	NE-CZ-NH2	-7.15	116.72	120.30
21	AA	857	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	693	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2054	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	2126	A	C5-C6-N1	7.15	121.28	117.70
55	BB	15	A	C5-C6-N1	7.15	121.28	117.70
21	AA	765	G	O4'-C1'-N9	7.15	113.92	108.20
24	A3	39	A	C5-C6-N1	7.15	121.28	117.70
54	BA	927	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	909	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1528	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2342	C	N3-C2-O2	-7.15	116.89	121.90
22	A1	76	A	C5-C6-N1	7.15	121.27	117.70
54	BA	131	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1156	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1342	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	1551	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1937	A	C4-C5-C6	-7.15	113.43	117.00
54	BA	126	A	C5-C6-N1	7.15	121.27	117.70
54	BA	911	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1694	C	N1-C2-O2	7.15	123.19	118.90
54	BA	1749	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	272	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	753	A	C5-C6-N1	7.14	121.27	117.70
21	AA	879	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	959	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1285	A	C5-C6-N1	7.14	121.27	117.70
54	BA	197	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	2566	A	C5-C6-N1	7.14	121.27	117.70
55	BB	57	A	N1-C6-N6	-7.14	114.31	118.60
21	AA	482	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1111	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	1135	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1598	A	N1-C6-N6	-7.14	114.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1616	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1785	A	N1-C6-N6	-7.14	114.31	118.60
21	AA	190	A	C5-C6-N1	7.14	121.27	117.70
45	BW	38	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	985	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1354	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2813	A	C5-C6-N1	7.14	121.27	117.70
21	AA	608	A	C5-C6-N1	7.14	121.27	117.70
54	BA	89	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2119	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2263	C	N3-C2-O2	-7.14	116.91	121.90
21	AA	1446	A	C5-C6-N1	7.13	121.27	117.70
21	AA	1465	A	C5-C6-N1	7.13	121.27	117.70
21	AA	559	A	C5-C6-N1	7.13	121.27	117.70
21	AA	802	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2734	A	C5-C6-N1	7.13	121.27	117.70
21	AA	533	A	C5-C6-N1	7.13	121.27	117.70
46	BX	49	ARG	NE-CZ-NH1	7.13	123.86	120.30
21	AA	768	A	C5-C6-N1	7.13	121.26	117.70
44	BV	21	ARG	NE-CZ-NH1	7.13	123.86	120.30
54	BA	1327	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2085	U	O4'-C1'-N1	7.13	113.90	108.20
22	A1	73	A	C5-C6-N1	7.13	121.26	117.70
28	BF	166	ARG	NE-CZ-NH1	7.13	123.86	120.30
54	BA	2776	A	C5-C6-N1	7.13	121.26	117.70
54	BA	2045	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	2541	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	2736	A	C5-C6-N1	7.12	121.26	117.70
54	BA	79	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	1607	C	O4'-C1'-N1	7.12	113.90	108.20
54	BA	1650	A	C5-C6-N1	7.12	121.26	117.70
21	AA	631	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	2377	A	C5-C6-N1	7.12	121.26	117.70
21	AA	435	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1150	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1408	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2297	A	C5-C6-N1	7.12	121.26	117.70
21	AA	994	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1155	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1916	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	499	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1299	A	N1-C6-N6	-7.12	114.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	160	A	C5-C6-N1	7.12	121.26	117.70
54	BA	866	A	C5-C6-N1	7.12	121.26	117.70
54	BA	982	C	N1-C2-O2	7.12	123.17	118.90
54	BA	1626	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1794	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	2716	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	109	A	C5-C6-N1	7.11	121.26	117.70
21	AA	315	A	C4-C5-C6	-7.11	113.44	117.00
54	BA	632	A	N1-C6-N6	-7.11	114.33	118.60
54	BA	2311	A	N1-C6-N6	-7.11	114.33	118.60
54	BA	2336	A	C5-C6-N1	7.11	121.26	117.70
54	BA	2058	A	C5-C6-N1	7.11	121.26	117.70
54	BA	1672	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2679	A	N1-C6-N6	-7.11	114.33	118.60
33	BK	108	ARG	NE-CZ-NH1	7.11	123.86	120.30
54	BA	1146	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	920	A	C5-C6-N1	7.11	121.25	117.70
54	BA	1086	A	C5-C6-N1	7.11	121.25	117.70
11	AL	82	ARG	NE-CZ-NH1	7.10	123.85	120.30
21	AA	1398	A	C5-C6-N1	7.10	121.25	117.70
54	BA	531	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	715	A	C5-C6-N1	7.10	121.25	117.70
54	BA	575	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	2134	A	C5-C6-N1	7.10	121.25	117.70
54	BA	816	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	1275	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2531	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2434	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2727	A	C5-C6-N1	7.10	121.25	117.70
21	AA	177	G	O4'-C1'-N9	7.10	113.88	108.20
21	AA	217	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	802	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	429	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	1155	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	866	C	N3-C2-O2	-7.09	116.93	121.90
21	AA	1093	A	C5-C6-N1	7.09	121.25	117.70
54	BA	449	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2814	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	203	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2227	A	C5-C6-N1	7.09	121.25	117.70
21	AA	55	A	C5-C6-N1	7.09	121.25	117.70
21	AA	746	A	C5-C6-N1	7.09	121.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	596	A	C5-C6-N1	7.09	121.25	117.70
21	AA	1170	A	C5-C6-N1	7.09	121.24	117.70
21	AA	1518	A	C5-C6-N1	7.09	121.24	117.70
54	BA	722	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1384	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2094	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2183	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	2418	A	C5-C6-N1	7.09	121.24	117.70
21	AA	1223	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	1364	U	O4'-C1'-N1	7.09	113.87	108.20
22	A1	58	A	C5-C6-N1	7.09	121.24	117.70
54	BA	218	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	1319	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	2632	A	C5-C6-N1	7.09	121.24	117.70
54	BA	2778	A	C5-C6-N1	7.09	121.24	117.70
55	BB	35	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	750	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	517	C	O4'-C1'-N1	7.08	113.87	108.20
21	AA	712	A	C5-C6-N1	7.08	121.24	117.70
21	AA	779	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	586	A	C5-C6-N1	7.08	121.24	117.70
54	BA	793	A	C5-C6-N1	7.08	121.24	117.70
54	BA	980	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	1916	A	C5-C6-N1	7.08	121.24	117.70
21	AA	26	A	C5-C6-N1	7.08	121.24	117.70
21	AA	382	A	C5-C6-N1	7.08	121.24	117.70
21	AA	572	A	N1-C6-N6	-7.08	114.35	118.60
21	AA	1192	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	1238	A	C5-C6-N1	7.08	121.24	117.70
25	BC	211	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	453	A	C5-C6-N1	7.08	121.24	117.70
54	BA	614	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	563	A	C5-C6-N1	7.08	121.24	117.70
21	AA	553	A	N1-C6-N6	-7.08	114.36	118.60
54	BA	10	A	C5-C6-N1	7.08	121.24	117.70
54	BA	49	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1800	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	1802	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1961	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	807	U	O4'-C1'-N1	7.07	113.86	108.20
54	BA	11	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1502	A	C5-C6-N1	7.07	121.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	886	A	C5-C6-N1	7.07	121.24	117.70
54	BA	1230	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	1243	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	496	A	C5-C6-N1	7.07	121.23	117.70
54	BA	915	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	1507	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	789	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	1366	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2761	A	C5-C6-N1	7.06	121.23	117.70
36	BN	2	ARG	NE-CZ-NH1	7.06	123.83	120.30
54	BA	213	A	C4-C5-C6	-7.06	113.47	117.00
10	AK	92	ARG	NE-CZ-NH1	7.06	123.83	120.30
21	AA	918	A	C5-C6-N1	7.06	121.23	117.70
21	AA	1382	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	1941	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	503	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2402	U	N3-C2-O2	-7.06	117.26	122.20
21	AA	74	A	C5-C6-N1	7.05	121.23	117.70
21	AA	456	A	C5-C6-N1	7.05	121.23	117.70
21	AA	600	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1029	A	C5-C6-N1	7.05	121.23	117.70
54	BA	204	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1302	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	1597	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	2314	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	2851	A	C5-C6-N1	7.05	121.23	117.70
21	AA	576	C	N3-C2-O2	-7.05	116.97	121.90
21	AA	1132	C	N3-C2-O2	-7.05	116.97	121.90
28	BF	79	ARG	NE-CZ-NH1	7.05	123.83	120.30
54	BA	262	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	903	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	2114	A	C5-C6-N1	7.05	121.22	117.70
21	AA	759	A	C5-C6-N1	7.05	121.22	117.70
54	BA	502	A	C5-C6-N1	7.05	121.22	117.70
54	BA	508	A	C5-C6-N1	7.05	121.22	117.70
54	BA	592	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2157	G	O4'-C1'-N9	7.05	113.84	108.20
55	BB	110	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	975	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	1508	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2471	A	C5-C6-N1	7.04	121.22	117.70
21	AA	143	A	C5-C6-N1	7.04	121.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1396	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1618	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2147	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	2748	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	2837	A	N1-C6-N6	-7.04	114.38	118.60
55	BB	39	A	C4-C5-C6	-7.04	113.48	117.00
16	AQ	61	ARG	NE-CZ-NH1	7.04	123.82	120.30
21	AA	998	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	681	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1513	A	C5-C6-N1	7.04	121.22	117.70
54	BA	279	A	C5-C6-N1	7.04	121.22	117.70
21	AA	737	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	255	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1092	C	N3-C2-O2	-7.04	116.97	121.90
55	BB	29	A	C5-C6-N1	7.04	121.22	117.70
21	AA	65	A	C5-C6-N1	7.04	121.22	117.70
21	AA	72	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	389	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2886	A	C5-C6-N1	7.04	121.22	117.70
21	AA	188	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	182	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1821	A	C4-C5-C6	-7.03	113.48	117.00
21	AA	814	A	C4-C5-C6	-7.03	113.48	117.00
21	AA	554	A	C5-C6-N1	7.03	121.22	117.70
21	AA	1080	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	631	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	2860	A	C5-C6-N1	7.03	121.22	117.70
11	AL	8	ARG	NE-CZ-NH1	7.03	123.81	120.30
21	AA	658	C	N3-C2-O2	-7.03	116.98	121.90
25	BC	101	ARG	NE-CZ-NH1	7.03	123.81	120.30
54	BA	241	A	C5-C6-N1	7.03	121.21	117.70
54	BA	1353	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	1757	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	2888	C	N3-C2-O2	-7.03	116.98	121.90
21	AA	327	A	N1-C6-N6	-7.03	114.39	118.60
54	BA	402	A	N1-C6-N6	-7.03	114.39	118.60
54	BA	477	A	C5-C6-N1	7.03	121.21	117.70
54	BA	2675	A	C5-C6-N1	7.03	121.21	117.70
21	AA	968	A	C5-C6-N1	7.02	121.21	117.70
23	A2	79	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1676	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	1805	A	N1-C6-N6	-7.02	114.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AP	35	ARG	NE-CZ-NH1	7.02	123.81	120.30
21	AA	468	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1092	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	853	C	N3-C2-O2	-7.02	116.99	121.90
21	AA	502	A	C5-C6-N1	7.02	121.21	117.70
54	BA	2309	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	2439	A	C1'-O4'-C4'	-7.02	104.29	109.90
5	AF	38	ARG	NE-CZ-NH1	7.02	123.81	120.30
21	AA	151	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	1470	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	340	A	C5-C6-N1	7.01	121.21	117.70
54	BA	456	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	1936	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2150	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	324	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2287	A	O4'-C1'-N9	7.01	113.81	108.20
21	AA	274	A	C5-C6-N1	7.01	121.20	117.70
21	AA	1306	A	C5-C6-N1	7.01	121.20	117.70
54	BA	302	C	N3-C2-O2	-7.01	116.99	121.90
37	BO	33	ARG	NE-CZ-NH2	7.01	123.80	120.30
54	BA	1669	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2835	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	382	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	1031	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	644	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	2542	A	N1-C6-N6	-7.00	114.40	118.60
22	A1	3	G	O4'-C1'-N9	7.00	113.80	108.20
21	AA	958	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	501	A	C5-C6-N1	7.00	121.20	117.70
54	BA	812	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2448	A	C5-C6-N1	7.00	121.20	117.70
55	BB	45	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	635	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1919	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2469	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2636	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	712	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	787	A	C5-C6-N1	7.00	121.20	117.70
21	AA	935	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	2097	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2711	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	539	A	C5-C6-N1	7.00	121.20	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2450	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	223	A	C5-C6-N1	6.99	121.20	117.70
54	BA	227	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	861	A	C5-C6-N1	6.99	121.20	117.70
54	BA	1403	A	N1-C6-N6	-6.99	114.40	118.60
54	BA	2095	A	C5-C6-N1	6.99	121.20	117.70
21	AA	1252	A	C5-C6-N1	6.99	121.20	117.70
54	BA	1678	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	1981	A	C5-C6-N1	6.99	121.20	117.70
55	BB	28	C	N3-C2-O2	-6.99	117.01	121.90
16	AQ	10	ARG	NE-CZ-NH1	6.99	123.80	120.30
54	BA	282	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	344	A	C5-C6-N1	6.99	121.19	117.70
54	BA	928	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	2706	A	C5-C6-N1	6.99	121.19	117.70
54	BA	111	A	C5-C6-N1	6.99	121.19	117.70
8	AI	121	ARG	NE-CZ-NH1	6.99	123.79	120.30
12	AM	108	ARG	NE-CZ-NH1	6.99	123.79	120.30
21	AA	221	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	364	A	C4-C5-C6	-6.99	113.51	117.00
21	AA	522	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	1574	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	329	A	C5-C6-N1	6.99	121.19	117.70
21	AA	1533	C	C1'-O4'-C4'	-6.99	104.31	109.90
34	BL	47	ARG	NE-CZ-NH1	6.99	123.79	120.30
54	BA	19	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1039	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2392	A	C5-C6-N1	6.99	121.19	117.70
21	AA	900	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	783	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2573	C	N3-C2-O2	-6.98	117.01	121.90
11	AL	49	ARG	NE-CZ-NH1	6.98	123.79	120.30
21	AA	620	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	751	A	C5-C6-N1	6.98	121.19	117.70
54	BA	920	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1237	A	C5-C6-N1	6.98	121.19	117.70
54	BA	564	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	1978	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2513	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2388	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	2813	A	N1-C6-N6	-6.98	114.41	118.60
21	AA	53	A	C4-C5-C6	-6.98	113.51	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	510	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	507	A	C5-C6-N1	6.98	121.19	117.70
21	AA	825	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	793	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	1833	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2572	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2757	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	1870	C	N3-C2-O2	-6.97	117.02	121.90
23	A2	89	U	O4'-C1'-N1	6.97	113.78	108.20
42	BT	12	ARG	NE-CZ-NH1	6.97	123.78	120.30
54	BA	1960	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	2333	A	C5-C6-N1	6.97	121.19	117.70
22	A1	69	A	C4-C5-C6	-6.97	113.52	117.00
14	AO	52	ARG	NE-CZ-NH1	6.97	123.78	120.30
21	AA	1499	A	C5-C6-N1	6.97	121.18	117.70
39	BQ	91	ARG	NE-CZ-NH1	6.97	123.78	120.30
54	BA	155	A	C5-C6-N1	6.97	121.18	117.70
54	BA	794	A	C5-C6-N1	6.97	121.18	117.70
54	BA	2019	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	2850	A	C5-C6-N1	6.97	121.18	117.70
21	AA	465	A	C5-C6-N1	6.96	121.18	117.70
54	BA	532	A	C5-C6-N1	6.96	121.18	117.70
54	BA	928	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1876	A	N1-C6-N6	-6.96	114.42	118.60
54	BA	2758	A	C5-C6-N1	6.96	121.18	117.70
22	A1	6	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2248	C	O4'-C1'-N1	6.96	113.77	108.20
54	BA	2547	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1093	A	C1'-O4'-C4'	-6.96	104.33	109.90
54	BA	1032	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1216	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	1395	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	716	A	C5-C6-N1	6.96	121.18	117.70
22	A1	28	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	1008	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1899	A	C5-C6-N1	6.96	121.18	117.70
54	BA	505	A	C5-C6-N1	6.96	121.18	117.70
54	BA	723	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	2215	C	N3-C2-O2	-6.96	117.03	121.90
13	AN	81	ARG	NE-CZ-NH1	6.96	123.78	120.30
54	BA	22	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	457	A	C4-C5-C6	-6.96	113.52	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1103	A	C5-C6-N1	6.96	121.18	117.70
20	AU	17	ARG	NE-CZ-NH1	6.95	123.78	120.30
21	AA	251	G	P-O3'-C3'	6.95	128.04	119.70
21	AA	383	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	1966	A	C5-C6-N1	6.95	121.18	117.70
21	AA	621	A	C5-C6-N1	6.95	121.18	117.70
21	AA	1357	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	1365	A	C4-C5-C6	-6.95	113.52	117.00
21	AA	321	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	732	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	599	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1754	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2108	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	456	A	N1-C6-N6	-6.95	114.43	118.60
46	BX	44	ARG	NE-CZ-NH1	6.95	123.77	120.30
54	BA	1251	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	835	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	2268	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2682	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	1092	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1264	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1504	A	C5-C6-N1	6.95	121.17	117.70
21	AA	1269	A	C5-C6-N1	6.94	121.17	117.70
54	BA	219	A	C5-C6-N1	6.94	121.17	117.70
21	AA	559	A	N1-C6-N6	-6.94	114.43	118.60
21	AA	66	A	C5-C6-N1	6.94	121.17	117.70
54	BA	802	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1111	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1365	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1300	G	P-O3'-C3'	6.94	128.03	119.70
54	BA	429	A	N1-C6-N6	-6.94	114.44	118.60
54	BA	673	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	2284	A	C5-C6-N1	6.94	121.17	117.70
21	AA	32	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1082	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	1735	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	209	U	O4'-C1'-N1	6.93	113.75	108.20
21	AA	451	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	758	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	1332	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1428	A	C5-C6-N1	6.93	121.17	117.70
21	AA	651	C	N3-C2-O2	-6.93	117.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1508	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	1096	A	C5-C6-N1	6.93	121.17	117.70
21	AA	195	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1251	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	1428	A	C4-C5-C6	-6.93	113.54	117.00
24	A3	42	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	1986	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	1089	A	C5-C6-N1	6.93	121.16	117.70
21	AA	120	A	C5-C6-N1	6.93	121.16	117.70
54	BA	2090	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	2096	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	2627	G	O4'-C1'-N9	6.93	113.74	108.20
54	BA	2815	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	366	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2171	A	C4-C5-C6	-6.92	113.54	117.00
5	AF	79	ARG	NE-CZ-NH2	-6.92	116.84	120.30
54	BA	42	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2340	A	C4-C5-C6	-6.92	113.54	117.00
55	BB	11	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	146	A	C5-C6-N1	6.92	121.16	117.70
54	BA	348	A	N1-C6-N6	-6.92	114.45	118.60
21	AA	167	A	C5-C6-N1	6.92	121.16	117.70
21	AA	563	A	N1-C6-N6	-6.92	114.45	118.60
49	B0	51	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	144	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	746	A	C4-C5-C6	-6.91	113.54	117.00
21	AA	1287	A	C5-C6-N1	6.91	121.16	117.70
54	BA	506	G	O4'-C1'-N9	6.91	113.73	108.20
54	BA	1877	A	C5-C6-N1	6.91	121.16	117.70
21	AA	1110	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1953	A	C4-C5-C6	-6.91	113.54	117.00
21	AA	640	A	N1-C6-N6	-6.91	114.45	118.60
21	AA	1151	A	C5-C6-N1	6.91	121.16	117.70
24	A3	22	A	C5-C6-N1	6.91	121.16	117.70
54	BA	920	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1942	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	2880	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	841	C	N3-C2-O2	-6.91	117.06	121.90
34	BL	41	ARG	NE-CZ-NH2	6.91	123.75	120.30
54	BA	1427	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2298	A	C5-C6-N1	6.91	121.15	117.70
55	BB	99	A	C5-C6-N1	6.91	121.15	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	106	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	910	C	N3-C2-O2	-6.91	117.07	121.90
21	AA	1339	A	C4-C5-C6	-6.91	113.55	117.00
27	BE	44	ARG	NE-CZ-NH1	6.91	123.75	120.30
54	BA	825	A	N1-C6-N6	-6.91	114.46	118.60
54	BA	1732	C	N3-C2-O2	-6.91	117.07	121.90
54	BA	2281	A	C5-C6-N1	6.91	121.15	117.70
54	BA	2666	C	N1-C2-O2	6.91	123.04	118.90
21	AA	321	A	C5-C6-N1	6.90	121.15	117.70
21	AA	706	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	1448	C	N3-C2-O2	-6.90	117.07	121.90
22	A1	66	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	192	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	1780	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2082	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2343	U	O4'-C1'-N1	6.90	113.72	108.20
54	BA	2418	A	C4-C5-C6	-6.90	113.55	117.00
24	A3	1	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	602	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	1019	A	C5-C6-N1	6.90	121.15	117.70
54	BA	643	A	O4'-C1'-N9	6.90	113.72	108.20
54	BA	2008	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2513	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	934	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	764	C	N3-C2-O2	-6.89	117.07	121.90
21	AA	1096	C	N3-C2-O2	-6.89	117.07	121.90
54	BA	1616	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	2427	C	N3-C2-O2	-6.89	117.07	121.90
21	AA	316	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	794	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	172	A	N1-C6-N6	-6.89	114.47	118.60
54	BA	727	A	C5-C6-N1	6.89	121.15	117.70
54	BA	944	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	982	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1040	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1894	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	300	A	C5-C6-N1	6.89	121.14	117.70
34	BL	123	ARG	NE-CZ-NH1	6.89	123.75	120.30
54	BA	1165	A	C5-C6-N1	6.89	121.15	117.70
21	AA	223	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	623	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1614	A	C5-C6-N1	6.89	121.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	44	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	2440	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1367	A	C5-C6-N1	6.89	121.14	117.70
54	BA	1866	A	C5-C6-N1	6.89	121.14	117.70
54	BA	1632	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2705	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	996	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1890	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	583	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1879	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	2635	A	C5-C6-N1	6.88	121.14	117.70
9	AJ	5	ARG	NE-CZ-NH1	6.88	123.74	120.30
21	AA	665	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2546	U	O4'-C1'-N1	6.88	113.70	108.20
54	BA	2868	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	878	A	C5-C6-N1	6.88	121.14	117.70
54	BA	146	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1895	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	338	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1201	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	71	A	O4'-C1'-N9	6.88	113.70	108.20
54	BA	103	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	541	A	N1-C6-N6	-6.88	114.47	118.60
54	BA	621	A	C5-C6-N1	6.88	121.14	117.70
56	B5	9	ARG	NE-CZ-NH1	6.88	123.74	120.30
21	AA	461	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	1375	A	N1-C6-N6	-6.88	114.47	118.60
54	BA	787	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1808	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1874	C	N3-C2-O2	-6.87	117.09	121.90
56	B5	7	ARG	NE-CZ-NH1	6.87	123.74	120.30
21	AA	339	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1088	A	C5-C6-N1	6.87	121.14	117.70
21	AA	298	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	386	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	695	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	1157	A	C5-C6-N1	6.87	121.14	117.70
21	AA	649	A	C5-C6-N1	6.87	121.13	117.70
54	BA	547	A	C5-C6-N1	6.87	121.14	117.70
54	BA	782	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	1676	A	C5-C6-N1	6.87	121.13	117.70
55	BB	29	A	C4-C5-C6	-6.87	113.57	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1496	C	N3-C2-O2	-6.87	117.09	121.90
22	A1	75	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1965	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	1476	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	2082	A	N1-C6-N6	-6.86	114.48	118.60
21	AA	533	A	N1-C6-N6	-6.86	114.48	118.60
32	BJ	37	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	1881	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2652	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	907	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1489	C	O4'-C1'-N1	6.86	113.69	108.20
54	BA	1566	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	1650	A	C4-C5-C6	-6.86	113.57	117.00
55	BB	58	A	C5-C6-N1	6.86	121.13	117.70
21	AA	13	U	C1'-O4'-C4'	-6.86	104.41	109.90
21	AA	496	A	N1-C6-N6	-6.86	114.48	118.60
21	AA	1046	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	910	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1247	A	C5-C6-N1	6.86	121.13	117.70
21	AA	228	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	612	C	N3-C2-O2	-6.86	117.10	121.90
22	A1	26	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	1350	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	839	U	O4'-C1'-N1	6.85	113.68	108.20
54	BA	1610	A	C1'-O4'-C4'	-6.85	104.42	109.90
54	BA	2386	A	C5-C6-N1	6.85	121.13	117.70
21	AA	192	A	C4-C5-C6	-6.85	113.57	117.00
21	AA	197	A	C5-C6-N1	6.85	121.13	117.70
54	BA	1746	A	C5-C6-N1	6.85	121.13	117.70
54	BA	1746	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	2015	A	C5-C6-N1	6.85	121.13	117.70
54	BA	2900	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	78	A	C4-C5-C6	-6.85	113.58	117.00
13	AN	61	ARG	NE-CZ-NH1	6.85	123.72	120.30
54	BA	1027	A	C5-C6-N1	6.85	121.12	117.70
54	BA	2327	A	C5-C6-N1	6.85	121.12	117.70
54	BA	2755	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	59	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	460	A	C5-C6-N1	6.85	121.12	117.70
54	BA	1918	A	C5-C6-N1	6.85	121.12	117.70
54	BA	2715	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	99	C	N3-C2-O2	-6.85	117.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	177	ARG	NE-CZ-NH1	6.85	123.72	120.30
54	BA	764	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	101	A	C5-C6-N1	6.84	121.12	117.70
21	AA	178	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	460	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1100	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1678	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1322	C	N3-C2-O2	-6.84	117.11	121.90
56	B5	12	ARG	NE-CZ-NH1	6.84	123.72	120.30
54	BA	270	A	C5-C6-N1	6.84	121.12	117.70
54	BA	951	C	O4'-C1'-N1	6.84	113.67	108.20
54	BA	1272	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2117	A	O4'-C1'-N9	6.84	113.67	108.20
21	AA	246	A	C5-C6-N1	6.84	121.12	117.70
21	AA	972	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	432	A	C5-C6-N1	6.84	121.12	117.70
55	BB	27	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	156	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	2535	G	N3-C2-N2	-6.84	115.11	119.90
9	AJ	45	ARG	NE-CZ-NH1	6.83	123.72	120.30
54	BA	497	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	637	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	1226	A	C5-C6-N1	6.83	121.12	117.70
21	AA	466	A	C4-C5-C6	-6.83	113.58	117.00
21	AA	860	A	C5-C6-N1	6.83	121.12	117.70
21	AA	932	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1081	A	C5-C6-N1	6.83	121.12	117.70
54	BA	905	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	2424	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	238	A	P-O3'-C3'	6.83	127.90	119.70
21	AA	347	G	C1'-O4'-C4'	-6.83	104.43	109.90
54	BA	2035	G	O4'-C1'-N9	6.83	113.67	108.20
21	AA	131	A	C5-C6-N1	6.83	121.11	117.70
54	BA	487	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	1020	A	C5-C6-N1	6.83	121.11	117.70
54	BA	1526	C	O4'-C1'-N1	6.83	113.66	108.20
54	BA	1677	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	435	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	1288	A	C5-C6-N1	6.83	121.11	117.70
54	BA	1393	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	1572	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	172	A	C4-C5-C6	-6.83	113.59	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	648	A	C5-C6-N1	6.83	121.11	117.70
54	BA	821	A	C5-C6-N1	6.83	121.11	117.70
54	BA	2433	A	C5-C6-N1	6.83	121.11	117.70
21	AA	408	A	C5-C6-N1	6.82	121.11	117.70
21	AA	583	A	C5-C6-N1	6.82	121.11	117.70
21	AA	1163	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	925	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1155	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2241	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2740	A	C5-C6-N1	6.82	121.11	117.70
21	AA	994	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1188	A	N1-C6-N6	-6.82	114.51	118.60
21	AA	1218	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	13	A	C5-C6-N1	6.82	121.11	117.70
55	BB	34	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	507	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	1194	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	2560	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	98	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	384	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1213	A	C5-C6-N1	6.82	121.11	117.70
21	AA	1299	A	C5-C6-N1	6.81	121.11	117.70
54	BA	2634	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	1439	A	C5-C6-N1	6.81	121.11	117.70
55	BB	52	A	C4-C5-C6	-6.81	113.59	117.00
21	AA	738	C	N3-C2-O2	-6.81	117.13	121.90
34	BL	48	ARG	NE-CZ-NH1	6.81	123.70	120.30
3	AD	164	ARG	NE-CZ-NH1	6.81	123.70	120.30
54	BA	1826	G	O4'-C1'-N9	6.81	113.65	108.20
54	BA	2507	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	16	A	C5-C6-N1	6.81	121.10	117.70
54	BA	1090	A	C4-C5-C6	-6.81	113.60	117.00
54	BA	2527	C	N3-C2-O2	-6.81	117.14	121.90
15	AP	5	ARG	NE-CZ-NH2	-6.81	116.90	120.30
54	BA	2716	C	O4'-C1'-N1	6.81	113.64	108.20
21	AA	974	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1169	A	N1-C6-N6	-6.80	114.52	118.60
21	AA	1410	A	C5-C6-N1	6.80	121.10	117.70
54	BA	10	A	C4-C5-C6	-6.80	113.60	117.00
2	AC	64	ARG	NE-CZ-NH2	-6.80	116.90	120.30
21	AA	1378	C	N3-C2-O2	-6.80	117.14	121.90
40	BR	13	ARG	NE-CZ-NH1	6.80	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	433	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	655	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1787	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2267	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	47	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	223	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1433	A	C5-C6-N1	6.80	121.10	117.70
55	BB	46	A	C5-C6-N1	6.80	121.10	117.70
54	BA	221	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	715	A	C4-C5-C6	-6.80	113.60	117.00
55	BB	59	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	781	A	C5-C6-N1	6.79	121.10	117.70
21	AA	1369	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	32	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	482	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	2403	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	2726	A	C5-C6-N1	6.79	121.10	117.70
21	AA	80	A	C4-C5-C6	-6.79	113.60	117.00
21	AA	472	U	C1'-O4'-C4'	-6.79	104.47	109.90
25	BC	176	ARG	NE-CZ-NH1	6.79	123.70	120.30
54	BA	1001	A	C5-C6-N1	6.79	121.10	117.70
54	BA	1064	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	1392	A	C5-C6-N1	6.79	121.10	117.70
54	BA	1584	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	2887	A	C4-C5-C6	-6.79	113.60	117.00
21	AA	1080	A	C5-C6-N1	6.79	121.09	117.70
54	BA	849	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	2281	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	1357	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	823	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	1433	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	2273	A	C5-C6-N1	6.79	121.09	117.70
21	AA	175	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	288	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	84	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1889	A	N1-C6-N6	-6.78	114.53	118.60
56	B5	134	ARG	NE-CZ-NH1	6.78	123.69	120.30
21	AA	906	A	N1-C6-N6	-6.78	114.53	118.60
21	AA	1374	A	C5-C6-N1	6.78	121.09	117.70
54	BA	466	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1244	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2752	C	N3-C2-O2	-6.78	117.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1169	A	C5-C6-N1	6.78	121.09	117.70
54	BA	705	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2335	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2602	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1004	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1051	C	N3-C2-O2	-6.78	117.15	121.90
24	A3	67	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	211	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	749	A	C5-C6-N1	6.78	121.09	117.70
21	AA	1066	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	1339	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2080	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	249	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	2014	A	N1-C6-N6	-6.78	114.53	118.60
21	AA	532	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	990	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2328	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	796	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	1500	A	C5-C6-N1	6.77	121.09	117.70
54	BA	650	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	900	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2510	C	O4'-C1'-N1	6.77	113.62	108.20
21	AA	1287	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	1494	A	C5-C6-N1	6.77	121.09	117.70
54	BA	1504	A	C4-C5-C6	-6.77	113.61	117.00
17	AR	72	ARG	NE-CZ-NH2	6.77	123.69	120.30
54	BA	1625	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	1635	A	C5-C6-N1	6.77	121.08	117.70
21	AA	345	C	N1-C2-O2	6.77	122.96	118.90
54	BA	278	A	C5-C6-N1	6.77	121.08	117.70
54	BA	706	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1700	A	C4-C5-C6	-6.77	113.62	117.00
54	BA	1912	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	1055	A	N1-C6-N6	-6.77	114.54	118.60
21	AA	1227	A	C5-C6-N1	6.77	121.08	117.70
21	AA	371	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	629	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	1102	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1276	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1772	A	C4-C5-C6	-6.76	113.62	117.00
55	BB	97	C	N3-C2-O2	-6.76	117.17	121.90
9	AJ	48	ARG	NE-CZ-NH2	-6.76	116.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2362	C	O4'-C1'-N1	6.76	113.61	108.20
21	AA	1257	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1437	A	C5-C6-N1	6.76	121.08	117.70
54	BA	423	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1359	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1509	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	334	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	694	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1012	A	C5-C6-N1	6.76	121.08	117.70
54	BA	320	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1054	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1200	C	O4'-C1'-N1	6.76	113.61	108.20
54	BA	1269	A	N1-C6-N6	-6.76	114.54	118.60
54	BA	1664	A	C5-C6-N1	6.76	121.08	117.70
21	AA	139	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	806	C	N3-C2-O2	-6.76	117.17	121.90
27	BE	21	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	2600	A	N1-C6-N6	-6.76	114.55	118.60
21	AA	374	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	893	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	817	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1114	C	N3-C2-O2	-6.76	117.17	121.90
55	BB	94	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1120	C	N3-C2-O2	-6.75	117.17	121.90
33	BK	78	ARG	NE-CZ-NH1	6.75	123.68	120.30
21	AA	451	A	C5-C6-N1	6.75	121.08	117.70
21	AA	968	A	O4'-C1'-N9	6.75	113.60	108.20
21	AA	578	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	579	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	1350	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1400	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	136	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	426	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	67	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	155	A	C5-C6-N1	6.75	121.07	117.70
54	BA	167	A	C5-C6-N1	6.75	121.07	117.70
54	BA	578	G	N3-C2-N2	-6.75	115.17	119.90
54	BA	917	A	C5-C6-N1	6.75	121.07	117.70
21	AA	25	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	192	A	C5-C6-N1	6.75	121.07	117.70
54	BA	21	A	C5-C6-N1	6.75	121.07	117.70
54	BA	439	A	N1-C6-N6	-6.75	114.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1987	A	C5-C6-N1	6.75	121.07	117.70
21	AA	81	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	1318	A	C5-C6-N1	6.74	121.07	117.70
54	BA	56	A	C5-C6-N1	6.74	121.07	117.70
54	BA	343	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1431	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1786	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2376	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2883	A	O4'-C1'-N9	6.74	113.59	108.20
8	AI	129	ARG	NE-CZ-NH2	6.74	123.67	120.30
21	AA	71	A	C5-C6-N1	6.74	121.07	117.70
21	AA	554	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1042	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1480	A	C5-C6-N1	6.74	121.07	117.70
24	A3	76	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	896	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2691	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	655	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1503	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	742	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1591	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2232	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	2577	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1285	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1632	A	C4-C5-C6	-6.74	113.63	117.00
23	A2	89	U	P-O3'-C3'	6.74	127.78	119.70
54	BA	544	C	N3-C2-O2	-6.74	117.19	121.90
54	BA	1868	C	N3-C2-O2	-6.74	117.19	121.90
24	A3	59	A	C5-C6-N1	6.73	121.07	117.70
21	AA	513	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	152	A	C5-C6-N1	6.73	121.07	117.70
21	AA	865	A	C5-C6-N1	6.73	121.06	117.70
39	BQ	32	ARG	NE-CZ-NH2	6.73	123.67	120.30
54	BA	2589	A	C4-C5-C6	-6.73	113.64	117.00
21	AA	349	A	C5-C6-N1	6.73	121.06	117.70
54	BA	99	U	N3-C2-O2	-6.73	117.49	122.20
54	BA	176	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	955	U	O4'-C1'-N1	6.73	113.58	108.20
54	BA	1591	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	2530	A	C5-C6-N1	6.73	121.06	117.70
21	AA	816	A	C5-C6-N1	6.73	121.06	117.70
54	BA	1276	A	C5-C6-N1	6.73	121.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	673	A	C5-C6-N1	6.72	121.06	117.70
21	AA	880	C	N3-C2-O2	-6.72	117.19	121.90
37	BO	25	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	586	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1465	G	N1-C6-O6	-6.72	115.87	119.90
54	BA	2366	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	2634	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2808	G	N3-C2-N2	-6.72	115.19	119.90
55	BB	101	A	C5-C6-N1	6.72	121.06	117.70
21	AA	944	G	P-O3'-C3'	6.72	127.77	119.70
54	BA	95	A	C5-C6-N1	6.72	121.06	117.70
54	BA	374	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2766	A	N1-C6-N6	-6.72	114.57	118.60
21	AA	270	A	C5-C6-N1	6.72	121.06	117.70
21	AA	313	A	C5-C6-N1	6.72	121.06	117.70
54	BA	644	A	C5-C6-N1	6.72	121.06	117.70
54	BA	1284	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2417	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	718	A	C5-C6-N1	6.72	121.06	117.70
54	BA	1070	A	O4'-C1'-N9	6.72	113.57	108.20
54	BA	1265	A	N1-C6-N6	-6.72	114.57	118.60
21	AA	1384	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	2291	U	O4'-C1'-N1	6.72	113.57	108.20
28	BF	111	ARG	NE-CZ-NH1	6.71	123.66	120.30
25	BC	132	ARG	NE-CZ-NH1	6.71	123.66	120.30
54	BA	1167	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	816	A	N1-C6-N6	-6.71	114.57	118.60
21	AA	1188	A	C5-C6-N1	6.71	121.06	117.70
54	BA	53	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1858	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2468	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	399	U	O4'-C1'-N1	6.71	113.57	108.20
54	BA	415	A	C5-C6-N1	6.71	121.06	117.70
54	BA	765	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1532	A	C4-C5-C6	-6.71	113.64	117.00
21	AA	1176	A	C5-C6-N1	6.71	121.05	117.70
54	BA	428	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	584	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1073	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1169	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	1919	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2179	C	N3-C2-O2	-6.71	117.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2243	U	O4'-C1'-N1	6.71	113.57	108.20
55	BB	89	U	O4'-C1'-N1	6.71	113.57	108.20
13	AN	65	ARG	NE-CZ-NH1	6.71	123.65	120.30
54	BA	422	A	C5-C6-N1	6.71	121.05	117.70
54	BA	575	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1006	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1802	A	N1-C6-N6	-6.71	114.58	118.60
54	BA	2590	A	N1-C6-N6	-6.71	114.58	118.60
22	A1	6	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	1350	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	1376	U	C1'-O4'-C4'	-6.70	104.54	109.90
54	BA	515	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1095	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1363	C	N3-C2-O2	-6.70	117.21	121.90
55	BB	43	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	574	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1664	A	C4-C5-C6	-6.70	113.65	117.00
32	BJ	27	ARG	NE-CZ-NH1	6.70	123.65	120.30
54	BA	1966	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	648	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	1069	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	1082	A	C5-C6-N1	6.70	121.05	117.70
44	BV	93	ARG	NE-CZ-NH1	6.70	123.65	120.30
47	BY	23	ARG	NE-CZ-NH1	6.70	123.65	120.30
54	BA	609	A	C5-C6-N1	6.70	121.05	117.70
54	BA	821	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2733	A	N1-C6-N6	-6.70	114.58	118.60
51	B2	33	ARG	NE-CZ-NH1	6.70	123.65	120.30
54	BA	281	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	1282	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1598	A	C5-C6-N1	6.70	121.05	117.70
21	AA	896	C	N3-C2-O2	-6.69	117.21	121.90
21	AA	253	A	C4-C5-C6	-6.69	113.65	117.00
21	AA	936	C	O4'-C1'-N1	6.69	113.55	108.20
21	AA	1413	A	C5-C6-N1	6.69	121.05	117.70
54	BA	352	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	668	A	C5-C6-N1	6.69	121.05	117.70
54	BA	2377	A	C4-C5-C6	-6.69	113.65	117.00
55	BB	8	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	238	A	C4-C5-C6	-6.69	113.66	117.00
22	A1	76	A	O4'-C1'-N9	6.69	113.55	108.20
54	BA	2207	C	N3-C2-O2	-6.69	117.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2486	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	92	U	O4'-C1'-N1	6.69	113.55	108.20
54	BA	1556	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	629	A	C5-C6-N1	6.69	121.04	117.70
21	AA	1502	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	201	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2025	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2675	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	2723	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2170	A	C5-C6-N1	6.69	121.04	117.70
54	BA	2234	G	O4'-C1'-N9	6.69	113.55	108.20
55	BB	42	C	N3-C2-O2	-6.69	117.22	121.90
55	BB	94	A	C4-C5-C6	-6.69	113.66	117.00
23	A2	91	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	2654	A	C5-C6-N1	6.68	121.04	117.70
21	AA	40	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	815	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	517	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1522	A	C4-C5-C6	-6.68	113.66	117.00
24	A3	14	A	C5-C6-N1	6.68	121.04	117.70
54	BA	795	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	1100	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1077	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	2840	C	N3-C2-O2	-6.68	117.22	121.90
8	AI	11	ARG	NE-CZ-NH2	-6.68	116.96	120.30
54	BA	1028	A	C4-C5-C6	-6.68	113.66	117.00
21	AA	681	A	C4-C5-C6	-6.68	113.66	117.00
21	AA	825	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1816	C	N3-C2-O2	-6.68	117.23	121.90
54	BA	2020	A	N1-C6-N6	-6.68	114.59	118.60
21	AA	1534	A	O4'-C1'-N9	6.67	113.54	108.20
36	BN	30	ARG	NE-CZ-NH2	-6.67	116.96	120.30
54	BA	737	C	O4'-C1'-N1	6.67	113.54	108.20
21	AA	564	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	687	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	1152	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	1314	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2594	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	459	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	790	A	N1-C6-N6	-6.67	114.60	118.60
26	BD	59	ARG	NE-CZ-NH1	6.67	123.63	120.30
54	BA	849	A	C5-C6-N1	6.67	121.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1209	U	C5'-C4'-O4'	6.67	117.10	109.10
54	BA	1382	G	C5'-C4'-C3'	-6.67	105.33	116.00
54	BA	2225	A	C5-C6-N1	6.67	121.03	117.70
54	BA	1513	U	O4'-C1'-N1	6.67	113.53	108.20
54	BA	1784	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	580	C	N3-C2-O2	-6.67	117.23	121.90
25	BC	181	ARG	NE-CZ-NH1	6.67	123.63	120.30
21	AA	130	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	256	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1385	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1477	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1535	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1890	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2088	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2411	A	C5-C6-N1	6.66	121.03	117.70
21	AA	649	A	N1-C6-N6	-6.66	114.60	118.60
21	AA	1210	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1447	A	O4'-C1'-N9	6.66	113.53	108.20
21	AA	58	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	129	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	1197	A	C5-C6-N1	6.66	121.03	117.70
54	BA	5	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	678	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1144	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2565	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	672	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1985	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	371	A	C5-C6-N1	6.66	121.03	117.70
21	AA	1063	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1389	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	56	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	634	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1708	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	2131	U	O4'-C1'-N1	6.66	113.53	108.20
54	BA	2628	C	N1-C2-O2	6.66	122.89	118.90
55	BB	62	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	309	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1583	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1837	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	2510	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	766	A	C5-C6-N1	6.65	121.03	117.70
54	BA	716	A	C5-C6-N1	6.65	121.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1080	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	2558	C	N3-C2-O2	-6.65	117.24	121.90
55	BB	50	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	520	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	1204	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	1076	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1305	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1612	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	634	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1172	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1173	U	O4'-C1'-N1	6.65	113.52	108.20
54	BA	2101	A	C5-C6-N1	6.65	121.03	117.70
54	BA	296	U	O4'-C1'-N1	6.65	113.52	108.20
54	BA	1175	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	1178	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	2173	A	C5-C6-N1	6.65	121.02	117.70
21	AA	1368	A	C5-C6-N1	6.65	121.02	117.70
54	BA	1677	A	C5-C6-N1	6.65	121.02	117.70
21	AA	336	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	1093	A	C4-C5-C6	-6.64	113.68	117.00
51	B2	39	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	1611	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	189	A	C5-C6-N1	6.64	121.02	117.70
21	AA	280	C	N1-C2-O2	6.64	122.89	118.90
21	AA	330	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	519	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	1183	U	C1'-O4'-C4'	-6.64	104.59	109.90
21	AA	1329	A	C5-C6-N1	6.64	121.02	117.70
21	AA	1510	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	48	C	N1-C2-O2	6.64	122.88	118.90
21	AA	156	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	1413	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1698	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	432	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1893	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2166	U	O4'-C1'-N1	6.64	113.51	108.20
54	BA	2359	C	N3-C2-O2	-6.64	117.25	121.90
25	BC	47	ARG	NE-CZ-NH1	6.63	123.62	120.30
54	BA	451	U	C1'-O4'-C4'	-6.63	104.59	109.90
54	BA	1048	A	C4-C5-C6	-6.63	113.68	117.00
54	BA	1773	A	C5-C6-N1	6.63	121.02	117.70
21	AA	419	C	N3-C2-O2	-6.63	117.26	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	937	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	1306	A	N1-C6-N6	-6.63	114.62	118.60
45	BW	24	ARG	NE-CZ-NH1	6.63	123.62	120.30
54	BA	97	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1039	A	C4-C5-C6	-6.63	113.68	117.00
54	BA	1417	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1793	C	N3-C2-O2	-6.63	117.26	121.90
19	AT	59	ARG	NE-CZ-NH2	6.63	123.61	120.30
35	BM	6	ARG	NE-CZ-NH2	6.63	123.61	120.30
54	BA	173	A	C4-C5-C6	-6.63	113.69	117.00
24	A3	3	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	231	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	767	U	O4'-C1'-N1	6.63	113.50	108.20
54	BA	1548	A	C5-C6-N1	6.63	121.01	117.70
54	BA	1892	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	2278	A	C5-C6-N1	6.63	121.01	117.70
54	BA	2601	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	1150	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	2154	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	478	A	C5-C6-N1	6.62	121.01	117.70
54	BA	19	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1738	G	O4'-C1'-N9	6.62	113.50	108.20
54	BA	2088	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	2135	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2471	A	C4-C5-C6	-6.62	113.69	117.00
8	AI	10	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	53	A	C5-C6-N1	6.62	121.01	117.70
22	A1	31	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	565	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1293	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1805	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1810	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1854	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2600	A	C5-C6-N1	6.62	121.01	117.70
21	AA	574	A	N1-C6-N6	-6.62	114.63	118.60
21	AA	1466	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	57	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1247	A	N1-C6-N6	-6.62	114.63	118.60
54	BA	1764	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	115	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1508	A	C5-C6-N1	6.61	121.01	117.70
54	BA	1541	C	N3-C2-O2	-6.61	117.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2077	A	C5-C6-N1	6.61	121.01	117.70
54	BA	661	A	C5-C6-N1	6.61	121.01	117.70
54	BA	666	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1836	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	310	A	C5-C6-N1	6.61	121.00	117.70
54	BA	540	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1067	A	C4-C5-C6	-6.61	113.69	117.00
21	AA	1277	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	352	A	C5-C6-N1	6.61	121.00	117.70
54	BA	501	A	N1-C6-N6	-6.61	114.64	118.60
54	BA	1713	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	32	A	N1-C6-N6	-6.60	114.64	118.60
21	AA	478	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1605	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	309	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1932	A	C5-C6-N1	6.60	121.00	117.70
54	BA	38	A	C5-C6-N1	6.60	121.00	117.70
54	BA	264	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1241	A	O4'-C1'-N9	6.60	113.48	108.20
54	BA	2054	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	2650	U	O4'-C1'-N1	6.60	113.48	108.20
21	AA	1261	A	C5-C6-N1	6.60	121.00	117.70
54	BA	270	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	825	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1274	A	N1-C6-N6	-6.59	114.64	118.60
54	BA	1606	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	1670	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	2261	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	1290	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	2879	A	O4'-C1'-N9	6.59	113.47	108.20
21	AA	179	A	C5-C6-N1	6.59	121.00	117.70
54	BA	47	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	52	A	C5-C6-N1	6.59	121.00	117.70
54	BA	299	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	735	A	C5-C6-N1	6.59	121.00	117.70
54	BA	945	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1127	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	1456	A	C5-C6-N1	6.59	121.00	117.70
54	BA	351	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1593	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1981	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	2717	C	N3-C2-O2	-6.59	117.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	373	A	C4-C5-C6	-6.59	113.71	117.00
54	BA	1416	G	O4'-C1'-N9	6.59	113.47	108.20
54	BA	2198	A	O4'-C1'-N9	6.59	113.47	108.20
54	BA	2774	C	O4'-C1'-N1	6.59	113.47	108.20
55	BB	115	A	C5-C6-N1	6.59	120.99	117.70
54	BA	1214	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	2432	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1363	A	C4-C5-C6	-6.58	113.71	117.00
35	BM	51	ARG	NE-CZ-NH1	6.58	123.59	120.30
51	B2	14	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	2632	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	171	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1022	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2227	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	264	C	N3-C2-O2	-6.58	117.30	121.90
21	AA	600	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	964	A	C5-C6-N1	6.58	120.99	117.70
54	BA	671	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	2283	C	O4'-C1'-N1	6.58	113.46	108.20
21	AA	279	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	936	C	N3-C2-O2	-6.58	117.30	121.90
24	A3	39	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	792	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1404	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1803	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2326	C	N3-C2-O2	-6.58	117.30	121.90
40	BR	80	ARG	NE-CZ-NH1	6.57	123.59	120.30
54	BA	1549	A	C4-C5-C6	-6.57	113.71	117.00
17	AR	63	TYR	CB-CG-CD1	-6.57	117.06	121.00
21	AA	77	A	C5-C6-N1	6.57	120.98	117.70
24	A3	36	A	C5-C6-N1	6.57	120.98	117.70
24	A3	63	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	596	U	O4'-C1'-N1	6.57	113.46	108.20
54	BA	1084	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2738	A	N1-C6-N6	-6.57	114.66	118.60
21	AA	83	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	60	A	C5-C6-N1	6.57	120.98	117.70
21	AA	329	A	N1-C6-N6	-6.57	114.66	118.60
21	AA	784	A	C5-C6-N1	6.57	120.98	117.70
21	AA	908	A	C5-C6-N1	6.57	120.98	117.70
21	AA	1511	G	N1-C6-O6	-6.57	115.96	119.90
54	BA	127	A	C5-C6-N1	6.57	120.98	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	635	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1084	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	1104	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1925	C	N3-C2-O2	-6.57	117.30	121.90
55	BB	34	A	C5-C6-N1	6.57	120.98	117.70
54	BA	1788	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2322	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2368	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	1228	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2000	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	23	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	193	C	N3-C2-O2	-6.56	117.31	121.90
42	BT	77	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	1051	G	O4'-C1'-N9	6.56	113.45	108.20
54	BA	2073	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	613	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2332	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2374	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2753	A	C5-C6-N1	6.56	120.98	117.70
25	BC	79	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	183	C	O4'-C1'-N1	6.56	113.45	108.20
54	BA	1246	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	1960	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2581	G	O4'-C1'-N9	6.56	113.45	108.20
54	BA	2764	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1944	U	O4'-C1'-N1	6.56	113.44	108.20
21	AA	489	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1281	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1341	U	O4'-C1'-N1	6.55	113.44	108.20
54	BA	748	G	C1'-O4'-C4'	-6.55	104.66	109.90
54	BA	1057	A	C5-C6-N1	6.55	120.98	117.70
54	BA	2589	A	C5-C6-N1	6.55	120.98	117.70
54	BA	2522	U	O4'-C1'-N1	6.55	113.44	108.20
21	AA	206	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	422	C	N3-C2-O2	-6.55	117.32	121.90
21	AA	1289	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	1360	A	C4-C5-C6	-6.55	113.73	117.00
48	BZ	30	ARG	NE-CZ-NH1	6.55	123.58	120.30
54	BA	346	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	1121	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2362	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2827	C	N3-C2-O2	-6.55	117.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1262	A	C5-C6-N1	6.55	120.97	117.70
54	BA	1796	U	O4'-C1'-N1	6.55	113.44	108.20
54	BA	2566	A	C4-C5-C6	-6.55	113.73	117.00
21	AA	338	A	C5-C6-N1	6.55	120.97	117.70
24	A3	70	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	216	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	2517	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	680	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	728	A	C4-C5-C6	-6.54	113.73	117.00
37	BO	25	ARG	NE-CZ-NH2	-6.54	117.03	120.30
54	BA	1085	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1819	A	C5-C6-N1	6.54	120.97	117.70
21	AA	1042	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1233	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1739	A	C5-C6-N1	6.54	120.97	117.70
54	BA	791	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1752	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	715	A	C5-C6-N1	6.54	120.97	117.70
21	AA	1113	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1914	C	N1-C2-O2	6.54	122.82	118.90
54	BA	2050	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	523	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	655	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	840	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	1634	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1652	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	119	A	C5-C6-N1	6.53	120.97	117.70
21	AA	234	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1155	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	251	A	C5-C6-N1	6.53	120.97	117.70
54	BA	854	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	675	A	C4-C5-C6	-6.53	113.73	117.00
21	AA	844	G	N3-C2-N2	-6.53	115.33	119.90
21	AA	1161	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1519	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	345	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	1260	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	1347	A	C5-C6-N1	6.53	120.97	117.70
54	BA	2119	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	177	G	O4'-C1'-N9	6.53	113.42	108.20
54	BA	471	A	C5-C6-N1	6.53	120.96	117.70
54	BA	925	A	C4-C5-C6	-6.53	113.74	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1745	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	2381	A	C5-C6-N1	6.53	120.96	117.70
54	BA	2738	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	936	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	2369	A	C4-C5-C6	-6.53	113.74	117.00
21	AA	1434	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2837	A	C5-C6-N1	6.52	120.96	117.70
11	AL	113	ARG	NE-CZ-NH1	6.52	123.56	120.30
54	BA	492	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1825	U	O4'-C1'-N1	6.52	113.42	108.20
54	BA	2343	U	C3'-C2'-C1'	6.52	106.72	101.50
54	BA	2534	A	C5-C6-N1	6.52	120.96	117.70
54	BA	2699	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	1771	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	647	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	1285	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1327	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	1055	A	C5-C6-N1	6.52	120.96	117.70
21	AA	1479	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	743	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1313	U	N3-C2-O2	-6.52	117.64	122.20
54	BA	1438	U	O4'-C1'-N1	6.52	113.42	108.20
54	BA	2829	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	633	A	C5-C6-N1	6.52	120.96	117.70
41	BS	95	ARG	NE-CZ-NH1	6.51	123.56	120.30
54	BA	1575	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	2095	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	393	A	C5-C6-N1	6.51	120.96	117.70
11	AL	53	ARG	NE-CZ-NH1	6.51	123.56	120.30
54	BA	398	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	640	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	116	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	167	A	N1-C6-N6	-6.51	114.69	118.60
54	BA	439	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1205	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	2560	A	C5-C6-N1	6.51	120.95	117.70
54	BA	2882	A	C4-C5-C6	-6.51	113.75	117.00
21	AA	1418	A	C5-C6-N1	6.51	120.95	117.70
54	BA	274	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	2009	A	C5-C6-N1	6.51	120.95	117.70
21	AA	1158	C	N1-C2-O2	6.51	122.80	118.90
54	BA	943	A	C5-C6-N1	6.51	120.95	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	430	A	C5-C6-N1	6.50	120.95	117.70
22	A1	25	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2163	A	C5-C6-N1	6.50	120.95	117.70
21	AA	614	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	649	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1011	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1156	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2726	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	553	A	C5-C6-N1	6.50	120.95	117.70
21	AA	559	A	O4'-C1'-N9	6.50	113.40	108.20
54	BA	968	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1123	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	959	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1271	A	C5-C6-N1	6.50	120.95	117.70
54	BA	64	A	C5-C6-N1	6.50	120.95	117.70
54	BA	340	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	980	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2635	A	C4-C5-C6	-6.50	113.75	117.00
55	BB	59	A	C5-C6-N1	6.50	120.95	117.70
11	AL	30	ARG	NE-CZ-NH1	6.50	123.55	120.30
21	AA	475	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1490	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1561	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1901	A	C5-C6-N1	6.50	120.95	117.70
55	BB	66	A	C5-C6-N1	6.50	120.95	117.70
54	BA	447	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	595	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2767	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	63	C	N3-C2-O2	-6.49	117.35	121.90
54	BA	1304	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1526	C	N3-C2-O2	-6.49	117.35	121.90
54	BA	2020	A	C5-C6-N1	6.49	120.95	117.70
55	BB	101	A	N1-C6-N6	-6.49	114.70	118.60
21	AA	85	U	O4'-C1'-N1	6.49	113.39	108.20
22	A1	35	A	N1-C6-N6	-6.49	114.70	118.60
54	BA	1413	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1414	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1689	A	C5-C6-N1	6.49	120.95	117.70
21	AA	190	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	1236	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	898	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1165	A	C4-C5-C6	-6.49	113.75	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	110	ARG	NE-CZ-NH1	6.49	123.54	120.30
18	AS	4	LEU	C-N-CA	6.49	137.92	121.70
21	AA	353	A	O4'-C1'-N9	6.49	113.39	108.20
54	BA	6	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	1608	A	C5-C6-N1	6.49	120.94	117.70
54	BA	2071	A	C5-C6-N1	6.49	120.94	117.70
54	BA	2649	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	915	A	C4-C5-C6	-6.49	113.76	117.00
21	AA	1160	G	O4'-C1'-N9	6.49	113.39	108.20
54	BA	1134	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	1262	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	1711	A	C5-C6-N1	6.49	120.94	117.70
21	AA	10	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	327	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1571	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2700	A	C5-C6-N1	6.48	120.94	117.70
21	AA	694	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	1036	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1259	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1614	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2191	A	C4-C5-C6	-6.48	113.76	117.00
2	AC	142	ARG	NE-CZ-NH1	6.48	123.54	120.30
54	BA	1768	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1974	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1656	C	N3-C2-O2	-6.48	117.37	121.90
54	BA	1669	A	C4-C5-C6	-6.48	113.76	117.00
24	A3	14	A	N1-C6-N6	-6.48	114.71	118.60
21	AA	349	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	335	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	637	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	718	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	1032	G	O4'-C1'-N9	6.47	113.38	108.20
54	BA	528	A	C5-C6-N1	6.47	120.94	117.70
54	BA	959	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1617	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1947	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2020	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1005	C	C3'-C2'-C1'	6.47	106.68	101.50
54	BA	1461	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1502	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	2154	A	C5-C6-N1	6.47	120.94	117.70
54	BA	2681	C	N3-C2-O2	-6.47	117.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	609	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	402	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1040	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	2753	A	C4-C5-C6	-6.47	113.77	117.00
55	BB	104	A	C5-C6-N1	6.47	120.94	117.70
21	AA	18	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1150	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	412	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	366	C	O4'-C1'-N1	6.47	113.37	108.20
54	BA	449	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	1603	A	C5-C6-N1	6.47	120.93	117.70
54	BA	1639	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1926	U	O4'-C1'-N1	6.47	113.37	108.20
54	BA	2768	U	O4'-C1'-N1	6.47	113.37	108.20
55	BB	108	A	C5-C6-N1	6.47	120.93	117.70
21	AA	795	C	N1-C2-O2	6.46	122.78	118.90
49	B0	49	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	693	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1203	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1443	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	72	U	O4'-C1'-N1	6.46	113.37	108.20
54	BA	1385	A	O4'-C1'-N9	6.46	113.37	108.20
54	BA	2175	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1214	A	C5-C6-N1	6.46	120.93	117.70
21	AA	495	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1128	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1713	A	C5-C6-N1	6.46	120.93	117.70
21	AA	411	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1208	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1399	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	608	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	2047	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2266	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	2407	A	C5-C6-N1	6.46	120.93	117.70
55	BB	36	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	820	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1373	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1152	A	C5-C6-N1	6.45	120.93	117.70
21	AA	1180	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	655	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	1654	A	C5-C6-N1	6.45	120.93	117.70
55	BB	17	C	N3-C2-O2	-6.45	117.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	29	A	O4'-C1'-N9	6.45	113.36	108.20
15	AP	14	ARG	NE-CZ-NH1	6.45	123.53	120.30
21	AA	1274	A	C5-C6-N1	6.45	120.92	117.70
54	BA	244	A	C5-C6-N1	6.45	120.92	117.70
54	BA	645	C	N1-C2-O2	6.45	122.77	118.90
54	BA	661	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1291	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1821	A	C5-C6-N1	6.45	120.93	117.70
21	AA	28	A	C5-C6-N1	6.45	120.92	117.70
54	BA	992	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1928	A	C5-C6-N1	6.45	120.92	117.70
54	BA	394	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1531	A	N1-C6-N6	-6.45	114.73	118.60
54	BA	734	A	C5-C6-N1	6.45	120.92	117.70
54	BA	2021	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	2539	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	435	A	C4-C5-C6	-6.44	113.78	117.00
55	BB	71	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	197	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	1213	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1404	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	383	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1078	U	N3-C2-O2	-6.44	117.69	122.20
54	BA	892	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1754	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2564	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	899	C	N3-C2-O2	-6.44	117.39	121.90
22	A1	11	C	N3-C2-O2	-6.44	117.39	121.90
34	BL	18	ARG	NE-CZ-NH1	6.44	123.52	120.30
21	AA	831	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	742	A	C4-C5-C6	-6.44	113.78	117.00
37	BO	94	ARG	NE-CZ-NH1	6.43	123.52	120.30
39	BQ	12	ARG	NE-CZ-NH2	6.43	123.52	120.30
21	AA	251	G	O4'-C1'-N9	6.43	113.34	108.20
21	AA	1045	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1307	A	C5-C6-N1	6.43	120.92	117.70
54	BA	2068	U	C1'-O4'-C4'	-6.43	104.75	109.90
54	BA	2205	A	C5-C6-N1	6.43	120.92	117.70
55	BB	15	A	O4'-C1'-N9	6.43	113.35	108.20
1	AB	62	ARG	NE-CZ-NH1	6.43	123.52	120.30
54	BA	357	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	668	A	C4-C5-C6	-6.43	113.78	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1452	G	N1-C6-O6	-6.43	116.04	119.90
54	BA	2273	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	2521	C	N3-C2-O2	-6.43	117.40	121.90
19	AT	17	ARG	NE-CZ-NH1	6.43	123.52	120.30
21	AA	54	C	N3-C2-O2	-6.43	117.40	121.90
27	BE	79	ARG	NE-CZ-NH1	6.43	123.52	120.30
54	BA	1888	G	O4'-C1'-N9	6.43	113.34	108.20
21	AA	560	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	595	A	C5-C6-N1	6.43	120.91	117.70
21	AA	1286	U	N3-C2-O2	-6.43	117.70	122.20
54	BA	1045	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	739	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	181	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	627	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2006	C	N3-C2-O2	-6.42	117.40	121.90
54	BA	1772	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2196	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	215	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1524	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1569	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1675	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	767	A	C5-C6-N1	6.42	120.91	117.70
21	AA	316	C	O4'-C1'-N1	6.42	113.33	108.20
21	AA	768	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	62	U	C1'-O4'-C4'	-6.41	104.77	109.90
54	BA	157	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1044	C	O4'-C1'-N1	6.41	113.33	108.20
54	BA	1571	A	C4-C5-C6	-6.41	113.79	117.00
55	BB	15	A	C4-C5-C6	-6.41	113.79	117.00
21	AA	743	A	N1-C6-N6	-6.41	114.75	118.60
21	AA	143	A	N1-C6-N6	-6.41	114.75	118.60
54	BA	227	A	C5-C6-N1	6.41	120.91	117.70
54	BA	1674	G	C3'-C2'-C1'	6.41	106.63	101.50
54	BA	404	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2033	A	C5-C6-N1	6.41	120.90	117.70
21	AA	44	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	431	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1674	G	N1-C6-O6	-6.41	116.06	119.90
21	AA	1117	A	C5-C6-N1	6.41	120.90	117.70
54	BA	1404	C	O4'-C1'-N1	6.41	113.33	108.20
54	BA	2170	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2703	C	O4'-C1'-N1	6.41	113.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	941	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1446	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1998	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	2403	C	O4'-C1'-N1	6.40	113.32	108.20
21	AA	421	U	O4'-C1'-N1	6.40	113.32	108.20
54	BA	109	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	354	A	C5-C6-N1	6.40	120.90	117.70
21	AA	952	U	O4'-C1'-N1	6.40	113.32	108.20
54	BA	322	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	74	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	1327	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	173	A	C5-C6-N1	6.40	120.90	117.70
54	BA	1330	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2795	C	N3-C2-O2	-6.40	117.42	121.90
24	A3	74	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1169	A	C5-C6-N1	6.40	120.90	117.70
54	BA	1287	A	C5-C6-N1	6.40	120.90	117.70
24	A3	17	C	N3-C2-O2	-6.39	117.42	121.90
24	A3	36	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	888	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	1385	A	C5-C6-N1	6.39	120.90	117.70
54	BA	2176	A	N1-C6-N6	-6.39	114.76	118.60
54	BA	2534	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	1296	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	603	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	1399	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	2761	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	1274	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	2443	C	N3-C2-O2	-6.39	117.43	121.90
3	AD	55	ARG	NE-CZ-NH1	6.39	123.49	120.30
54	BA	833	A	C5-C6-N1	6.39	120.89	117.70
54	BA	1396	U	O4'-C1'-N1	6.39	113.31	108.20
54	BA	1759	A	C4-C5-C6	-6.39	113.81	117.00
37	BO	111	ARG	NE-CZ-NH1	6.39	123.49	120.30
54	BA	182	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	240	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	692	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1140	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2287	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2406	A	C5-C6-N1	6.39	120.89	117.70
55	BB	73	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	111	A	C4-C5-C6	-6.38	113.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2453	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	2646	C	O4'-C1'-N1	6.38	113.31	108.20
21	AA	708	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	328	U	O4'-C1'-N1	6.38	113.31	108.20
54	BA	1548	A	C4-C5-C6	-6.38	113.81	117.00
24	A3	48	U	O4'-C1'-N1	6.38	113.31	108.20
39	BQ	27	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BA	118	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	529	A	C5-C6-N1	6.38	120.89	117.70
54	BA	610	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2350	C	O4'-C1'-N1	6.38	113.30	108.20
21	AA	448	A	C5-C6-N1	6.38	120.89	117.70
21	AA	883	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	1035	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	861	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1264	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1729	U	N3-C2-O2	-6.38	117.73	122.20
54	BA	1744	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2456	C	N3-C2-O2	-6.38	117.44	121.90
20	AU	32	ARG	NE-CZ-NH1	6.38	123.49	120.30
21	AA	873	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	278	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	716	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	621	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	226	A	C5-C6-N1	6.38	120.89	117.70
54	BA	125	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	183	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	209	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1349	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2051	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2462	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2547	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2800	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	572	A	C5-C6-N1	6.37	120.89	117.70
54	BA	1284	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2019	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	393	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	1367	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2425	A	C5-C6-N1	6.37	120.89	117.70
21	AA	176	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1171	A	C4-C5-C6	-6.37	113.82	117.00
26	BD	179	ARG	NE-CZ-NH1	6.37	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	301	G	O4'-C1'-N9	6.37	113.30	108.20
54	BA	675	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	685	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	1014	A	N1-C6-N6	-6.37	114.78	118.60
54	BA	1668	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	1760	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	412	A	N1-C6-N6	-6.37	114.78	118.60
54	BA	680	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1126	A	C4-C5-C6	-6.37	113.82	117.00
21	AA	1427	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	699	A	C5-C6-N1	6.36	120.88	117.70
54	BA	761	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1920	C	N3-C2-O2	-6.36	117.44	121.90
54	BA	418	C	O4'-C1'-N1	6.36	113.29	108.20
54	BA	1952	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2712	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	248	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	1246	A	C5-C6-N1	6.36	120.88	117.70
54	BA	676	A	C5-C6-N1	6.36	120.88	117.70
54	BA	819	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1392	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1419	A	C5-C6-N1	6.36	120.88	117.70
54	BA	73	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2037	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2103	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	507	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	623	C	N3-C2-O2	-6.36	117.45	121.90
22	A1	71	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1289	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1437	C	O4'-C1'-N1	6.36	113.28	108.20
54	BA	2590	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	917	A	N1-C6-N6	-6.36	114.79	118.60
54	BA	1987	A	C4-C5-C6	-6.36	113.82	117.00
56	B5	71	ARG	NE-CZ-NH1	6.36	123.48	120.30
24	A3	72	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	1810	A	N1-C6-N6	-6.35	114.79	118.60
54	BA	2099	U	N3-C2-O2	-6.35	117.75	122.20
54	BA	2469	A	C4-C5-C6	-6.35	113.82	117.00
55	BB	77	U	O4'-C1'-N1	6.35	113.28	108.20
24	A3	58	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	2476	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	2874	C	N3-C2-O2	-6.35	117.45	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	781	A	N1-C6-N6	-6.35	114.79	118.60
22	A1	73	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	145	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	653	U	N3-C2-O2	-6.35	117.75	122.20
54	BA	788	A	C5-C6-N1	6.35	120.87	117.70
21	AA	186	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	282	A	C5-C6-N1	6.35	120.87	117.70
21	AA	1179	A	C5-C6-N1	6.35	120.87	117.70
54	BA	2564	A	C5-C6-N1	6.35	120.87	117.70
21	AA	1248	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	1531	A	C5-C6-N1	6.35	120.87	117.70
54	BA	1428	C	O4'-C1'-N1	6.35	113.28	108.20
21	AA	132	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	236	A	N1-C6-N6	-6.34	114.79	118.60
21	AA	263	A	C4-C5-C6	-6.34	113.83	117.00
38	BP	102	ARG	NE-CZ-NH1	6.34	123.47	120.30
54	BA	1197	G	O4'-C1'-N9	6.34	113.28	108.20
54	BA	1208	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	478	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1142	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	1303	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1536	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1801	A	C5-C6-N1	6.34	120.87	117.70
54	BA	63	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	265	A	O4'-C1'-N9	6.34	113.27	108.20
54	BA	2077	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	1146	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	462	C	N3-C2-O2	-6.34	117.47	121.90
54	BA	504	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1278	C	O4'-C1'-N1	6.34	113.27	108.20
54	BA	1395	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	831	A	C5-C6-N1	6.33	120.87	117.70
21	AA	1329	A	C4-C5-C6	-6.33	113.83	117.00
25	BC	176	ARG	NE-CZ-NH2	-6.33	117.13	120.30
54	BA	1626	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	882	C	N3-C2-O2	-6.33	117.47	121.90
22	A1	48	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	233	A	C5-C6-N1	6.33	120.87	117.70
54	BA	2381	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	1143	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	1189	A	C5-C6-N1	6.33	120.86	117.70
54	BA	1268	A	C4-C5-C6	-6.33	113.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2902	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	328	C	N1-C2-O2	6.33	122.70	118.90
21	AA	374	A	C5-C6-N1	6.33	120.86	117.70
54	BA	105	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	582	A	C5-C6-N1	6.33	120.86	117.70
54	BA	2435	A	C5-C6-N1	6.33	120.86	117.70
21	AA	676	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	914	G	O4'-C1'-N9	6.33	113.26	108.20
54	BA	1285	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	2270	A	C5-C6-N1	6.33	120.86	117.70
55	BB	108	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	1462	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1889	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	2442	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	719	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1749	A	C5-C6-N1	6.33	120.86	117.70
54	BA	1843	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1977	A	C5-C6-N1	6.33	120.86	117.70
54	BA	2873	A	C5-C6-N1	6.33	120.86	117.70
2	AC	155	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	1172	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	510	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	670	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1288	G	N1-C6-O6	-6.32	116.11	119.90
54	BA	1565	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	1785	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2420	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	2459	A	N1-C6-N6	-6.32	114.81	118.60
54	BA	2497	A	C4-C5-C6	-6.32	113.84	117.00
10	AK	68	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	50	A	C5-C6-N1	6.32	120.86	117.70
24	A3	16	C	N3-C2-O2	-6.32	117.47	121.90
21	AA	207	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	624	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	844	A	C5-C6-N1	6.32	120.86	117.70
17	AR	62	ARG	NE-CZ-NH2	-6.32	117.14	120.30
54	BA	190	A	C5-C6-N1	6.32	120.86	117.70
21	AA	1110	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	353	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1769	U	O4'-C1'-N1	6.31	113.25	108.20
21	AA	498	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	1429	A	C5-C6-N1	6.31	120.86	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	21	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1044	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1353	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	31	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	418	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	539	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	557	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	599	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2197	U	O4'-C1'-N1	6.31	113.25	108.20
54	BA	1128	G	N3-C2-N2	-6.30	115.49	119.90
54	BA	1267	U	O4'-C1'-N1	6.30	113.24	108.20
21	AA	162	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1152	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2038	G	N1-C6-O6	-6.30	116.12	119.90
54	BA	2766	A	C4-C5-C6	-6.30	113.85	117.00
19	AT	9	ARG	NE-CZ-NH1	6.30	123.45	120.30
21	AA	1346	A	C4-C5-C6	-6.30	113.85	117.00
24	A3	11	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2163	A	O4'-C1'-N9	6.30	113.24	108.20
54	BA	2264	C	N3-C2-O2	-6.30	117.49	121.90
22	A1	27	C	N3-C2-O2	-6.30	117.49	121.90
41	BS	8	ARG	NE-CZ-NH1	6.30	123.45	120.30
54	BA	353	C	O4'-C1'-N1	6.30	113.24	108.20
54	BA	414	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	995	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	309	A	C5-C6-N1	6.30	120.85	117.70
21	AA	1502	A	O4'-C1'-N9	6.30	113.24	108.20
54	BA	2725	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	436	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1221	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1665	A	C5-C6-N1	6.30	120.85	117.70
21	AA	1317	C	N1-C2-O2	6.29	122.68	118.90
54	BA	1398	C	C3'-C2'-C1'	6.29	106.54	101.50
54	BA	1347	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	1871	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	1927	A	C5-C6-N1	6.29	120.85	117.70
22	A1	14	A	C5-C6-N1	6.29	120.84	117.70
54	BA	262	A	C5-C6-N1	6.29	120.85	117.70
54	BA	973	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	13	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	2031	A	C1'-O4'-C4'	-6.29	104.87	109.90
21	AA	179	A	C4-C5-C6	-6.29	113.86	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	262	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	356	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	126	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1388	G	O4'-C1'-N9	6.29	113.23	108.20
54	BA	1692	U	O4'-C1'-N1	6.29	113.23	108.20
55	BB	113	C	N3-C2-O2	-6.29	117.50	121.90
1	AB	94	ARG	NE-CZ-NH1	6.29	123.44	120.30
21	AA	1325	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	8	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	270	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1226	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	2288	A	C4-C5-C6	-6.29	113.86	117.00
22	A1	23	A	C4-C5-C6	-6.28	113.86	117.00
34	BL	60	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	265	A	N1-C6-N6	-6.28	114.83	118.60
54	BA	601	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	362	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	804	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1321	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2354	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1408	A	C4-C5-C6	-6.28	113.86	117.00
39	BQ	63	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	918	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1362	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1934	C	O4'-C1'-N1	6.28	113.22	108.20
18	AS	31	ARG	NE-CZ-NH1	6.28	123.44	120.30
26	BD	46	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	41	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	61	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	1117	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	1905	C	N3-C2-O2	-6.28	117.51	121.90
21	AA	573	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	779	C	N1-C2-O2	6.28	122.67	118.90
21	AA	1109	C	N1-C2-O2	6.28	122.67	118.90
31	BI	133	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	1686	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	780	A	C4-C5-C6	-6.27	113.86	117.00
39	BQ	52	ARG	NE-CZ-NH1	6.27	123.44	120.30
54	BA	2226	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	395	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1032	G	N1-C6-O6	-6.27	116.14	119.90
54	BA	1427	A	P-O3'-C3'	6.27	127.22	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2385	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	549	C	N1-C2-O2	6.27	122.66	118.90
21	AA	635	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	1260	A	C5-C6-N1	6.27	120.83	117.70
54	BA	1320	C	N1-C2-O2	6.27	122.66	118.90
54	BA	1706	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2657	A	C5-C6-N1	6.27	120.83	117.70
21	AA	545	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1451	C	N1-C2-O2	6.27	122.66	118.90
54	BA	2332	C	O4'-C1'-N1	6.27	113.21	108.20
54	BA	2395	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	645	C	O4'-C1'-N1	6.27	113.21	108.20
54	BA	2467	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1162	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	556	A	C5-C6-N1	6.26	120.83	117.70
54	BA	1370	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	308	C	N3-C2-O2	-6.26	117.52	121.90
50	B1	43	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	1158	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1940	U	C1'-O4'-C4'	-6.26	104.89	109.90
54	BA	1304	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2794	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2301	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2364	C	O4'-C1'-N1	6.26	113.21	108.20
54	BA	2480	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	1237	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	602	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1990	C	N3-C2-O2	-6.26	117.52	121.90
18	AS	80	ARG	NE-CZ-NH1	6.25	123.43	120.30
54	BA	199	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	213	A	C5-C6-N1	6.25	120.83	117.70
54	BA	1503	A	C5-C6-N1	6.25	120.83	117.70
54	BA	2787	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	312	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	414	A	C4-C5-C6	-6.25	113.88	117.00
22	A1	70	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	225	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1545	A	C5-C6-N1	6.25	120.83	117.70
54	BA	1943	U	N3-C2-O2	-6.25	117.82	122.20
54	BA	2001	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	1433	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	1507	A	C4-C5-C6	-6.25	113.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1525	A	C5-C6-N1	6.25	120.83	117.70
54	BA	1728	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	262	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	11	C	O4'-C1'-N1	6.25	113.20	108.20
54	BA	670	A	P-O3'-C3'	6.25	127.20	119.70
54	BA	2870	C	N3-C2-O2	-6.25	117.53	121.90
1	AB	138	ARG	NE-CZ-NH1	6.25	123.42	120.30
21	AA	756	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	439	A	C5-C6-N1	6.25	120.82	117.70
54	BA	479	A	C5-C6-N1	6.25	120.82	117.70
54	BA	508	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	620	G	N3-C4-C5	-6.25	125.48	128.60
54	BA	897	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1515	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1806	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	236	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	401	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	34	U	N3-C2-O2	-6.24	117.83	122.20
54	BA	348	A	C5-C6-N1	6.24	120.82	117.70
54	BA	454	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1382	G	O4'-C1'-N9	6.24	113.19	108.20
54	BA	1583	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	172	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1494	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1591	A	C1'-O4'-C4'	-6.24	104.91	109.90
54	BA	2300	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	6	G	N3-C2-N2	-6.24	115.53	119.90
21	AA	1407	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2178	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2188	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	2710	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	423	G	O4'-C1'-N9	6.24	113.19	108.20
21	AA	509	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1214	C	N1-C2-O2	6.24	122.64	118.90
54	BA	2439	A	O4'-C1'-N9	6.24	113.19	108.20
21	AA	1398	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1014	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1472	C	O4'-C1'-N1	6.24	113.19	108.20
54	BA	1998	A	C5-C6-N1	6.24	120.82	117.70
54	BA	2064	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1735	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2089	C	N3-C2-O2	-6.23	117.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	34	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	286	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	864	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	1059	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	525	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	807	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	1320	C	N3-C2-O2	-6.23	117.54	121.90
24	A3	29	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1415	U	O4'-C1'-N1	6.23	113.18	108.20
54	BA	1507	C	N3-C2-O2	-6.23	117.54	121.90
10	AK	12	ARG	NE-CZ-NH1	-6.23	117.19	120.30
54	BA	483	A	C5-C6-N1	6.23	120.81	117.70
54	BA	779	U	O4'-C1'-N1	6.23	113.18	108.20
54	BA	996	A	C4-C5-C6	-6.23	113.89	117.00
51	B2	12	ARG	NE-CZ-NH1	6.23	123.41	120.30
54	BA	523	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1069	C	O4'-C1'-N1	6.22	113.18	108.20
54	BA	238	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	330	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1312	U	P-O3'-C3'	6.22	127.17	119.70
54	BA	1585	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	1762	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	792	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1529	G	O4'-C1'-N9	6.22	113.18	108.20
54	BA	1866	A	C4-C5-C6	-6.22	113.89	117.00
24	A3	49	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2616	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	127	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	815	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1237	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1597	A	O4'-C1'-N9	6.22	113.18	108.20
54	BA	1908	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	267	C	N3-C2-O2	-6.22	117.55	121.90
25	BC	268	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	820	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	2883	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	167	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1250	A	C4-C5-C6	-6.22	113.89	117.00
28	BF	147	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	418	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2799	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1234	C	N3-C2-O2	-6.21	117.55	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1446	A	N1-C6-N6	-6.21	114.87	118.60
54	BA	89	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1705	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2347	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1012	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	933	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	972	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2222	C	O4'-C1'-N1	6.21	113.17	108.20
21	AA	744	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	846	G	C1'-O4'-C4'	-6.21	104.93	109.90
22	A1	70	C	P-O3'-C3'	6.21	127.15	119.70
54	BA	840	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	16	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	1105	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	461	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	679	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1027	C	N1-C2-O2	6.21	122.62	118.90
21	AA	1101	A	P-O3'-C3'	6.21	127.15	119.70
21	AA	1101	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	1429	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	124	G	N3-C2-N2	-6.21	115.55	119.90
54	BA	1447	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2352	A	C5-C6-N1	6.21	120.80	117.70
54	BA	2538	C	N3-C2-O2	-6.21	117.55	121.90
2	AC	125	ARG	NE-CZ-NH1	6.21	123.40	120.30
21	AA	817	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	314	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	964	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	1157	G	O4'-C1'-N9	6.21	113.17	108.20
54	BA	1983	G	N3-C2-N2	-6.21	115.56	119.90
12	AM	112	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	AA	1201	A	P-O3'-C3'	6.20	127.14	119.70
21	AA	1262	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1311	A	C5-C6-N1	6.20	120.80	117.70
21	AA	1501	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	604	G	C5'-C4'-O4'	6.20	116.55	109.10
54	BA	2059	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2426	A	C5-C6-N1	6.20	120.80	117.70
10	AK	127	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	BA	165	A	C5-C6-N1	6.20	120.80	117.70
54	BA	902	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1520	C	N3-C2-O2	-6.20	117.56	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1275	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1818	U	O4'-C1'-N1	6.20	113.16	108.20
21	AA	95	C	N3-C2-O2	-6.20	117.56	121.90
35	BM	59	ARG	NE-CZ-NH1	6.20	123.40	120.30
41	BS	18	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	BA	184	C	O4'-C1'-N1	6.20	113.16	108.20
54	BA	246	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	666	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1075	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1080	A	C5-C6-N1	6.20	120.80	117.70
54	BA	1969	A	C5-C6-N1	6.20	120.80	117.70
21	AA	1167	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1453	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	501	C	N1-C2-O2	6.20	122.62	118.90
21	AA	1319	A	C5-C6-N1	6.20	120.80	117.70
41	BS	11	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	BA	670	A	C5-C6-N1	6.20	120.80	117.70
54	BA	994	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	119	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	119	A	O4'-C1'-N9	6.19	113.16	108.20
54	BA	480	A	N1-C6-N6	-6.19	114.88	118.60
54	BA	2169	A	O4'-C1'-N9	6.19	113.16	108.20
21	AA	1248	A	C1'-O4'-C4'	-6.19	104.94	109.90
29	BG	169	ARG	NE-CZ-NH1	6.19	123.40	120.30
21	AA	1141	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1111	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	1970	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	1618	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	443	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1071	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1468	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	935	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	2558	C	O4'-C1'-N1	6.19	113.15	108.20
45	BW	74	LYS	C-N-CA	6.19	137.17	121.70
21	AA	1229	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	62	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	1978	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	123	U	C5'-C4'-C3'	-6.18	106.11	116.00
54	BA	269	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	758	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	761	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1070	A	C4-C5-C6	-6.18	113.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1240	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	1306	C	N3-C2-O2	-6.18	117.57	121.90
15	AP	70	ARG	NE-CZ-NH1	6.18	123.39	120.30
54	BA	609	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	735	C	N3-C2-O2	-6.18	117.57	121.90
22	A1	32	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	886	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2334	U	O4'-C1'-N1	6.18	113.14	108.20
22	A1	68	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	726	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1253	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	155	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	878	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	36	C	N3-C2-O2	-6.17	117.58	121.90
22	A1	41	A	C5-C6-N1	6.17	120.79	117.70
54	BA	282	A	C5-C6-N1	6.17	120.79	117.70
21	AA	52	C	N3-C2-O2	-6.17	117.58	121.90
39	BQ	2	ARG	NE-CZ-NH2	6.17	123.39	120.30
54	BA	957	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2165	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	893	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1996	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	272	C	N1-C2-O2	6.17	122.60	118.90
21	AA	1016	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	1196	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	384	A	C4-C5-C6	-6.17	113.92	117.00
55	BB	11	C	N1-C2-O2	6.17	122.60	118.90
21	AA	673	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	749	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	933	A	O4'-C1'-N9	6.17	113.13	108.20
29	BG	2	ARG	NE-CZ-NH1	6.17	123.38	120.30
54	BA	50	U	N3-C2-O2	-6.17	117.88	122.20
54	BA	2662	A	N1-C6-N6	-6.17	114.90	118.60
54	BA	1550	C	N3-C2-O2	-6.16	117.58	121.90
54	BA	873	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2478	A	C4-C5-C6	-6.16	113.92	117.00
10	AK	12	ARG	NE-CZ-NH2	6.16	123.38	120.30
54	BA	1378	A	O4'-C1'-N9	6.16	113.13	108.20
21	AA	961	U	C1'-O4'-C4'	-6.16	104.97	109.90
54	BA	1269	A	C5-C6-N1	6.16	120.78	117.70
54	BA	1582	C	N1-C2-O2	6.16	122.59	118.90
6	AG	52	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1832	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2005	A	C4-C5-C6	-6.16	113.92	117.00
24	A3	68	C	N3-C2-O2	-6.16	117.59	121.90
55	BB	87	U	O4'-C1'-N1	6.16	113.12	108.20
21	AA	1197	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	163	C	N1-C2-O2	6.15	122.59	118.90
54	BA	1261	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	135	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	719	C	N3-C2-O2	-6.15	117.59	121.90
43	BU	85	ARG	NE-CZ-NH1	6.15	123.38	120.30
54	BA	486	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2483	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1665	A	C4-C5-C6	-6.15	113.92	117.00
30	BH	51	ARG	NE-CZ-NH1	6.15	123.37	120.30
47	BY	48	ARG	NE-CZ-NH1	6.15	123.38	120.30
21	AA	1388	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	908	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	1367	A	N1-C6-N6	-6.15	114.91	118.60
54	BA	2626	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	2745	C	N3-C2-O2	-6.15	117.60	121.90
21	AA	1103	C	N3-C2-O2	-6.15	117.60	121.90
21	AA	1275	A	C5-C6-N1	6.14	120.77	117.70
54	BA	198	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	300	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1323	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1463	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1814	G	N1-C6-O6	-6.14	116.21	119.90
54	BA	2114	A	O4'-C1'-N9	6.14	113.11	108.20
21	AA	6	G	C1'-O4'-C4'	-6.14	104.99	109.90
8	AI	84	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	1780	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1924	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2425	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1248	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1972	G	N1-C6-O6	-6.14	116.22	119.90
21	AA	320	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1280	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	509	C	C1'-O4'-C4'	-6.14	104.99	109.90
54	BA	983	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1902	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	60	A	C4-C5-C6	-6.13	113.93	117.00
21	AA	663	A	C4-C5-C6	-6.13	113.93	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1412	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	582	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	587	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1808	A	O4'-C1'-N9	6.13	113.11	108.20
21	AA	87	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	579	A	C5-C6-N1	6.13	120.77	117.70
21	AA	1508	A	C4-C5-C6	-6.13	113.93	117.00
22	A1	30	C	N3-C2-O2	-6.13	117.61	121.90
22	A1	60	C	N1-C2-O2	6.13	122.58	118.90
54	BA	2283	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2781	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	233	A	C4-C5-C6	-6.13	113.94	117.00
55	BB	56	G	N1-C6-O6	-6.13	116.22	119.90
21	AA	33	A	C5-C6-N1	6.13	120.76	117.70
54	BA	36	G	N3-C2-N2	-6.13	115.61	119.90
54	BA	1999	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2320	U	N3-C2-O2	-6.13	117.91	122.20
54	BA	2452	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2591	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	1431	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	943	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	528	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	38	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2247	A	C5-C6-N1	6.12	120.76	117.70
54	BA	2875	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	120	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	1151	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2496	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	844	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	970	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	1050	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2366	A	C5-C6-N1	6.12	120.76	117.70
21	AA	1195	C	N1-C2-O2	6.12	122.57	118.90
54	BA	1166	G	N1-C6-O6	-6.12	116.23	119.90
54	BA	1994	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2416	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	147	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	633	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1351	C	O4'-C1'-N1	6.12	113.09	108.20
54	BA	1909	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2774	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	273	G	C1'-O4'-C4'	-6.11	105.01	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2176	A	C4-C5-C6	-6.11	113.94	117.00
21	AA	400	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	1044	A	C5-C6-N1	6.11	120.76	117.70
27	BE	61	ARG	NE-CZ-NH2	-6.11	117.25	120.30
54	BA	2466	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2901	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	94	A	C5-C6-N1	6.11	120.75	117.70
54	BA	378	C	N3-C2-O2	-6.11	117.62	121.90
55	BB	50	A	C5-C6-N1	6.11	120.75	117.70
21	AA	368	U	O4'-C1'-N1	6.11	113.08	108.20
21	AA	243	A	C4-C5-C6	-6.11	113.95	117.00
21	AA	415	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	241	A	N1-C6-N6	-6.11	114.94	118.60
54	BA	277	G	O4'-C1'-N9	6.11	113.08	108.20
54	BA	1021	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	1376	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	1957	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	2377	A	O4'-C1'-N9	6.11	113.08	108.20
54	BA	95	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	730	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	422	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	789	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1372	U	O4'-C1'-N1	6.10	113.08	108.20
21	AA	1238	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2030	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2321	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	478	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1049	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1761	C	N3-C2-O2	-6.10	117.63	121.90
49	B0	39	ARG	NE-CZ-NH2	6.09	123.35	120.30
54	BA	453	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	643	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	979	A	C4-C5-C6	-6.09	113.95	117.00
55	BB	70	C	N1-C2-O2	6.09	122.56	118.90
21	AA	607	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	1057	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	1098	A	C5-C6-N1	6.09	120.75	117.70
54	BA	2637	U	O4'-C1'-N1	6.09	113.07	108.20
22	A1	72	C	N3-C2-O2	-6.09	117.64	121.90
40	BR	21	ARG	NE-CZ-NH1	6.09	123.34	120.30
54	BA	63	A	C5-C6-N1	6.09	120.75	117.70
54	BA	1257	C	N3-C2-O2	-6.09	117.64	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	44	A	C5-C6-N1	6.09	120.74	117.70
6	AG	94	ARG	NE-CZ-NH1	6.09	123.34	120.30
21	AA	1245	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	932	U	O4'-C1'-N1	6.09	113.07	108.20
54	BA	1291	C	N1-C2-O2	6.09	122.55	118.90
55	BB	63	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	1398	C	N1-C2-O2	6.08	122.55	118.90
21	AA	1204	A	C5-C6-N1	6.08	120.74	117.70
21	AA	1318	A	C4-C5-C6	-6.08	113.96	117.00
26	BD	141	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	218	A	C5-C6-N1	6.08	120.74	117.70
54	BA	96	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	342	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2606	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	275	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	1161	C	O4'-C1'-N1	6.08	113.06	108.20
54	BA	2447	G	O4'-C1'-N9	6.08	113.06	108.20
54	BA	2463	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2695	U	O4'-C1'-N1	6.08	113.06	108.20
21	AA	35	G	P-O3'-C3'	6.08	126.99	119.70
21	AA	1136	C	N1-C2-O2	6.08	122.55	118.90
26	BD	83	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	1031	G	O4'-C1'-N9	6.08	113.06	108.20
54	BA	2037	A	C5-C6-N1	6.08	120.74	117.70
54	BA	2143	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2474	U	N3-C2-O2	-6.08	117.94	122.20
21	AA	379	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	788	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1469	A	N1-C6-N6	-6.08	114.95	118.60
54	BA	1787	A	N1-C6-N6	-6.08	114.95	118.60
54	BA	2559	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	101	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	490	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	922	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	2800	A	C5-C6-N1	6.08	120.74	117.70
21	AA	611	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	412	A	C5-C6-N1	6.07	120.74	117.70
54	BA	1547	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1801	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	382	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	853	C	N3-C2-O2	-6.07	117.65	121.90
55	BB	31	C	N3-C2-O2	-6.07	117.65	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	458	G	O4'-C1'-N9	6.07	113.06	108.20
54	BA	652	U	O4'-C1'-N1	6.07	113.06	108.20
54	BA	689	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	911	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	948	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1641	A	C5-C6-N1	6.07	120.73	117.70
54	BA	2161	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	520	A	C5-C6-N1	6.07	120.73	117.70
54	BA	2327	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	699	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	756	A	N1-C6-N6	-6.07	114.96	118.60
21	AA	1452	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	106	C	N3-C2-O2	-6.07	117.66	121.90
54	BA	1641	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	436	C	N3-C2-O2	-6.06	117.66	121.90
23	A2	82	A	N1-C6-N6	-6.06	114.96	118.60
54	BA	1230	A	C5-C6-N1	6.06	120.73	117.70
54	BA	2531	A	C4-C5-C6	-6.06	113.97	117.00
13	AN	85	ARG	NE-CZ-NH1	6.06	123.33	120.30
21	AA	1176	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1640	A	C4-C5-C6	-6.06	113.97	117.00
22	A1	65	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	988	A	N1-C6-N6	-6.06	114.96	118.60
54	BA	2587	A	C5-C6-N1	6.06	120.73	117.70
21	AA	8	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	307	C	C3'-C2'-C1'	6.06	106.35	101.50
21	AA	465	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1335	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1893	C	O4'-C1'-N1	6.06	113.05	108.20
54	BA	2058	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2407	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2651	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	935	A	C5-C6-N1	6.06	120.73	117.70
21	AA	946	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	1157	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	502	A	N1-C6-N6	-6.06	114.97	118.60
54	BA	1658	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	196	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	503	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	16	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	1161	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	325	A	C4-C5-C6	-6.05	113.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2435	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	687	A	C5-C6-N1	6.05	120.72	117.70
54	BA	430	A	C5-C6-N1	6.05	120.72	117.70
21	AA	1513	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	195	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1058	U	O4'-C1'-N1	6.05	113.04	108.20
54	BA	1387	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	2830	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	743	A	C4-C5-C6	-6.05	113.98	117.00
55	BB	30	C	N3-C2-O2	-6.05	117.67	121.90
41	BS	110	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	257	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	461	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1439	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1685	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2155	U	O4'-C1'-N1	6.04	113.03	108.20
1	AB	25	LYS	C-N-CA	6.04	136.81	121.70
54	BA	937	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1387	A	C5-C6-N1	6.04	120.72	117.70
3	AD	96	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	772	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1495	A	C4-C5-C6	-6.04	113.98	117.00
55	BB	91	C	N3-C2-O2	-6.04	117.67	121.90
6	AG	91	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	417	C	O4'-C1'-N1	6.04	113.03	108.20
54	BA	470	A	N1-C6-N6	-6.04	114.98	118.60
23	A2	87	U	O4'-C1'-N1	6.04	113.03	108.20
54	BA	1077	A	C5-C6-N1	6.04	120.72	117.70
21	AA	750	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	823	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1118	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2078	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2477	U	O4'-C1'-N1	6.03	113.03	108.20
54	BA	2773	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2811	G	O4'-C1'-N9	6.03	113.03	108.20
54	BA	2821	A	C5-C6-N1	6.03	120.72	117.70
54	BA	2174	C	N3-C2-O2	-6.03	117.68	121.90
10	AK	55	ARG	NE-CZ-NH2	6.03	123.32	120.30
21	AA	452	A	C5-C6-N1	6.03	120.72	117.70
54	BA	105	C	O4'-C1'-N1	6.03	113.02	108.20
21	AA	73	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	913	A	O4'-C1'-N9	6.03	113.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1822	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	271	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	763	G	N3-C2-N2	-6.03	115.68	119.90
54	BA	800	A	C5-C6-N1	6.03	120.71	117.70
54	BA	1072	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1552	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	427	U	O4'-C1'-N1	6.03	113.02	108.20
21	AA	1396	A	C4-C5-C6	-6.03	113.99	117.00
27	BE	88	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	851	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1270	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1577	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	253	C	N3-C2-O2	-6.02	117.68	121.90
54	BA	2313	C	N3-C2-O2	-6.02	117.68	121.90
21	AA	1032	G	N3-C4-C5	-6.02	125.59	128.60
54	BA	946	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	2498	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	2512	C	O4'-C1'-N1	6.02	113.02	108.20
21	AA	938	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	1044	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	596	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	1449	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1885	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2129	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	2338	C	N3-C2-O2	-6.02	117.69	121.90
22	A1	9	A	N1-C6-N6	-6.02	114.99	118.60
54	BA	380	G	O4'-C1'-N9	6.02	113.02	108.20
54	BA	1336	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1606	C	N1-C2-O2	6.02	122.51	118.90
54	BA	1900	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	819	A	N1-C6-N6	-6.02	114.99	118.60
55	BB	38	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	441	A	C4-C5-C6	-6.01	113.99	117.00
46	BX	10	ARG	NE-CZ-NH1	6.01	123.31	120.30
54	BA	553	G	N1-C6-O6	-6.01	116.29	119.90
54	BA	1694	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	753	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	488	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	979	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	66	C	N1-C2-O2	6.01	122.51	118.90
54	BA	423	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	477	A	C4-C5-C6	-6.01	113.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1595	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1638	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	766	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	972	C	O4'-C1'-N1	6.01	113.01	108.20
21	AA	996	A	C5-C6-N1	6.01	120.70	117.70
21	AA	1359	C	N1-C2-O2	6.01	122.51	118.90
22	A1	35	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	161	A	C5-C6-N1	6.01	120.70	117.70
54	BA	2636	C	O4'-C1'-N1	6.01	113.01	108.20
20	AU	30	GLU	C-N-CA	6.01	136.72	121.70
54	BA	447	A	C5-C6-N1	6.01	120.70	117.70
54	BA	531	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	1207	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1470	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2665	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	1477	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2190	G	N3-C2-N2	-6.01	115.70	119.90
54	BA	2386	A	C4-C5-C6	-6.01	114.00	117.00
24	A3	75	C	N3-C2-O2	-6.00	117.70	121.90
55	BB	87	U	C1'-O4'-C4'	-6.00	105.10	109.90
21	AA	65	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	845	A	C4-C5-C6	-6.00	114.00	117.00
22	A1	61	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1490	A	O4'-C1'-N9	6.00	113.00	108.20
54	BA	1715	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	2826	A	O4'-C1'-N9	6.00	113.00	108.20
54	BA	151	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1557	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2061	G	N3-C2-N2	-6.00	115.70	119.90
54	BA	2380	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2734	A	N1-C6-N6	-6.00	115.00	118.60
21	AA	422	C	O4'-C1'-N1	6.00	113.00	108.20
21	AA	1037	C	N3-C2-O2	-6.00	117.70	121.90
24	A3	26	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	981	A	C4-C5-C6	-6.00	114.00	117.00
13	AN	90	ARG	NE-CZ-NH1	6.00	123.30	120.30
21	AA	295	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1465	A	N1-C6-N6	-6.00	115.00	118.60
54	BA	2183	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2619	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	673	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	2103	C	O4'-C1'-N1	6.00	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2540	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2792	A	C5-C6-N1	6.00	120.70	117.70
55	BB	68	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2826	A	C5-C6-N1	6.00	120.70	117.70
21	AA	1209	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	1553	A	O4'-C1'-N9	5.99	113.00	108.20
54	BA	1627	G	C5'-C4'-O4'	5.99	116.29	109.10
21	AA	182	A	C5-C6-N1	5.99	120.70	117.70
54	BA	541	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1505	A	C4-C5-C6	-5.99	114.00	117.00
11	AL	13	ARG	NE-CZ-NH1	5.99	123.30	120.30
21	AA	502	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	918	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	528	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1354	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1528	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	2003	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	2084	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	721	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	199	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	767	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	781	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	872	A	C5-C6-N1	5.98	120.69	117.70
54	BA	1315	C	N3-C2-O2	-5.98	117.71	121.90
2	AC	53	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	26	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	546	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1499	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	315	G	N1-C6-O6	-5.98	116.31	119.90
21	AA	440	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	878	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1887	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	2187	U	O4'-C1'-N1	5.98	112.98	108.20
55	BB	53	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1179	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	787	C	N1-C2-O2	5.98	122.49	118.90
54	BA	892	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	15	G	N3-C2-N2	-5.98	115.72	119.90
21	AA	839	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	1243	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	563	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1144	A	C4-C5-C6	-5.98	114.01	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1378	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2206	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	1210	C	N1-C2-O2	5.98	122.49	118.90
54	BA	2101	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	747	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	481	G	C1'-O4'-C4'	-5.97	105.12	109.90
54	BA	1341	G	O4'-C1'-N9	5.97	112.98	108.20
54	BA	2262	U	O4'-C1'-N1	5.97	112.98	108.20
55	BB	12	C	N1-C2-O2	5.97	122.48	118.90
21	AA	1263	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	37	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1637	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	42	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	948	C	O4'-C1'-N1	5.97	112.97	108.20
55	BB	88	C	N1-C2-O2	5.97	122.48	118.90
21	AA	810	C	O4'-C1'-N1	5.97	112.97	108.20
54	BA	2142	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2612	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	552	U	O4'-C1'-N1	5.96	112.97	108.20
54	BA	1655	A	C4-C5-C6	-5.96	114.02	117.00
55	BB	66	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	1129	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	493	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	790	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	900	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1413	A	C5-C6-N1	5.96	120.68	117.70
54	BA	2205	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1717	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1783	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	940	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	1086	U	N3-C2-O2	-5.96	118.03	122.20
30	BH	116	ARG	NE-CZ-NH1	5.96	123.28	120.30
24	A3	22	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1056	G	N1-C6-O6	-5.96	116.33	119.90
55	BB	4	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2758	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	1040	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	2740	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	749	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	1411	C	N3-C2-O2	-5.95	117.73	121.90
25	BC	202	ARG	NE-CZ-NH1	5.95	123.28	120.30
21	AA	452	A	C4-C5-C6	-5.95	114.03	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	892	A	N1-C6-N6	-5.95	115.03	118.60
54	BA	1145	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1254	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	492	C	N3-C2-O2	-5.95	117.74	121.90
15	AP	31	ARG	NE-CZ-NH1	5.95	123.27	120.30
21	AA	110	C	N1-C2-O2	5.95	122.47	118.90
21	AA	535	A	N1-C6-N6	-5.95	115.03	118.60
21	AA	1112	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	28	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	2044	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1231	U	O4'-C1'-N1	5.94	112.95	108.20
54	BA	1564	C	N3-C2-O2	-5.94	117.74	121.90
9	AJ	68	ARG	NE-CZ-NH1	5.94	123.27	120.30
22	A1	23	A	N1-C6-N6	-5.94	115.03	118.60
54	BA	737	C	N3-C2-O2	-5.94	117.74	121.90
8	AI	112	ARG	NE-CZ-NH1	5.94	123.27	120.30
21	AA	341	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	766	A	C1'-O4'-C4'	-5.94	105.15	109.90
21	AA	1223	C	N1-C2-O2	5.94	122.46	118.90
54	BA	364	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	382	A	C6-C5-N7	5.94	136.46	132.30
54	BA	524	G	N1-C6-O6	-5.94	116.34	119.90
54	BA	1495	A	C5-C6-N1	5.94	120.67	117.70
21	AA	389	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	610	U	C1'-O4'-C4'	-5.94	105.15	109.90
54	BA	1809	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	34	C	P-O3'-C3'	5.94	126.82	119.70
21	AA	923	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	574	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	926	G	P-O3'-C3'	5.93	126.82	119.70
54	BA	2461	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2785	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	739	C	N1-C2-O2	5.93	122.46	118.90
21	AA	900	A	C4-C5-C6	-5.93	114.03	117.00
24	A3	59	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2789	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1225	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	1484	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1340	A	C5-C6-N1	5.93	120.67	117.70
24	A3	40	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	987	C	N3-C2-O2	-5.93	117.75	121.90
4	AE	68	ARG	NE-CZ-NH1	5.93	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	169	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	786	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	1554	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	2652	C	N1-C2-O2	5.93	122.46	118.90
6	AG	4	ARG	NE-CZ-NH1	5.93	123.26	120.30
33	BK	98	ARG	NE-CZ-NH1	5.93	123.26	120.30
54	BA	890	C	N1-C2-O2	5.93	122.46	118.90
21	AA	1293	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	2821	A	N1-C6-N6	-5.92	115.05	118.60
54	BA	1765	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2502	G	N1-C6-O6	-5.92	116.35	119.90
54	BA	1013	C	N1-C2-O2	5.92	122.45	118.90
54	BA	1099	G	N1-C6-O6	-5.92	116.35	119.90
54	BA	1493	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1730	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1784	A	O4'-C1'-N9	5.92	112.94	108.20
54	BA	2412	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2068	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2258	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	1191	A	C5-C6-N1	5.92	120.66	117.70
54	BA	936	A	C5-C6-N1	5.92	120.66	117.70
54	BA	1113	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	1790	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	2117	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	161	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	991	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	1518	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	2042	A	C4-C5-C6	-5.92	114.04	117.00
55	BB	108	A	O4'-C1'-N9	5.92	112.93	108.20
21	AA	865	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	965	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	526	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	962	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2658	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2679	A	C5-C6-N1	5.91	120.66	117.70
54	BA	960	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	2225	A	C4-C5-C6	-5.91	114.04	117.00
21	AA	960	U	O4'-C1'-N1	5.91	112.93	108.20
46	BX	27	ARG	NE-CZ-NH2	-5.91	117.34	120.30
54	BA	33	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1420	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1938	A	C4-C5-C6	-5.91	114.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	66	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	156	C	N3-C4-N4	-5.91	113.86	118.00
21	AA	316	C	C3'-C2'-C1'	5.91	106.23	101.50
54	BA	1551	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1592	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	465	A	N1-C6-N6	-5.91	115.06	118.60
54	BA	2070	A	O4'-C1'-N9	5.91	112.93	108.20
54	BA	2250	G	N1-C6-O6	-5.91	116.36	119.90
21	AA	469	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	1308	A	N1-C6-N6	-5.91	115.06	118.60
54	BA	1546	G	O4'-C1'-N9	5.91	112.92	108.20
54	BA	2590	A	C5-C6-N1	5.91	120.65	117.70
55	BB	58	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	71	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1437	C	N3-C2-O2	-5.90	117.77	121.90
13	AN	53	ARG	NE-CZ-NH1	5.90	123.25	120.30
54	BA	172	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	984	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1420	A	O4'-C1'-N9	5.90	112.92	108.20
21	AA	222	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	901	A	C5-C6-N1	5.90	120.65	117.70
21	AA	985	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1575	C	O4'-C1'-N1	5.90	112.92	108.20
21	AA	1418	A	C4-C5-C6	-5.90	114.05	117.00
15	AP	25	ARG	NE-CZ-NH1	5.90	123.25	120.30
21	AA	653	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	909	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	1114	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	219	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	611	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	253	A	C5-C6-N1	5.89	120.65	117.70
54	BA	79	C	N1-C2-O2	5.89	122.44	118.90
54	BA	703	U	O4'-C1'-N1	5.89	112.92	108.20
54	BA	912	C	N3-C2-O2	-5.89	117.77	121.90
54	BA	1795	C	N3-C2-O2	-5.89	117.77	121.90
54	BA	2579	C	N3-C2-O2	-5.89	117.77	121.90
21	AA	805	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	1302	C	N1-C2-O2	5.89	122.44	118.90
54	BA	679	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1271	G	O4'-C1'-N9	5.89	112.91	108.20
54	BA	1480	C	N3-C2-O2	-5.89	117.78	121.90
55	BB	60	C	N3-C2-O2	-5.89	117.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	315	A	C3'-C2'-C1'	5.89	106.21	101.50
21	AA	1368	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	806	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1933	G	N3-C4-C5	-5.89	125.65	128.60
9	AJ	31	ARG	NE-CZ-NH1	5.89	123.24	120.30
21	AA	19	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	811	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	949	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	162	U	N3-C2-O2	-5.89	118.08	122.20
54	BA	980	A	P-O3'-C3'	5.89	126.77	119.70
54	BA	1063	G	C1'-O4'-C4'	-5.89	105.19	109.90
54	BA	1073	A	O4'-C1'-N9	5.89	112.91	108.20
54	BA	2433	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	2654	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	1492	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	2184	A	C5-C6-N1	5.89	120.64	117.70
21	AA	51	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	626	A	C6-C5-N7	5.89	136.42	132.30
21	AA	1509	C	N3-C2-O2	-5.88	117.78	121.90
24	A3	24	C	N3-C2-O2	-5.88	117.78	121.90
39	BQ	47	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	1164	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	2772	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1288	G	C1'-O4'-C4'	-5.88	105.19	109.90
4	AE	137	ARG	NE-CZ-NH2	-5.88	117.36	120.30
21	AA	1379	G	N1-C6-O6	-5.88	116.37	119.90
24	A3	35	C	N1-C2-O2	5.88	122.43	118.90
54	BA	94	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1382	G	N3-C4-C5	-5.88	125.66	128.60
31	BI	64	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	1414	C	O4'-C1'-N1	5.88	112.90	108.20
21	AA	1028	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	1009	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2380	C	O4'-C1'-N1	5.88	112.90	108.20
54	BA	2645	G	O4'-C1'-N9	5.88	112.90	108.20
21	AA	610	U	N3-C2-O2	-5.88	118.09	122.20
21	AA	1271	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2793	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	83	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	546	U	C1'-O4'-C4'	-5.88	105.20	109.90
54	BA	660	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	1475	G	O4'-C1'-N9	5.88	112.90	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1704	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	1802	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2211	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2683	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	64	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	1512	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1646	C	N1-C2-O2	5.87	122.42	118.90
54	BA	2184	A	N1-C6-N6	-5.87	115.08	118.60
54	BA	2285	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	174	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	202	G	N1-C6-O6	-5.87	116.38	119.90
21	AA	866	C	N1-C2-O2	5.87	122.42	118.90
21	AA	1145	A	N1-C6-N6	-5.87	115.08	118.60
21	AA	1338	G	N1-C6-O6	-5.87	116.38	119.90
54	BA	2055	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	914	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2760	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1230	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	443	A	C5-C6-N1	5.87	120.63	117.70
54	BA	2825	G	N3-C4-C5	-5.87	125.67	128.60
52	B3	7	ARG	NE-CZ-NH1	5.87	123.23	120.30
21	AA	868	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1097	C	N3-C2-O2	-5.87	117.80	121.90
21	AA	1352	C	N1-C2-O2	5.87	122.42	118.90
24	A3	38	A	C4-C5-C6	-5.87	114.07	117.00
21	AA	334	C	N1-C2-O2	5.86	122.42	118.90
54	BA	2841	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	205	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1920	C	O4'-C1'-N1	5.86	112.89	108.20
21	AA	124	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	466	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	885	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2163	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1462	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1508	A	C4-C5-C6	-5.86	114.07	117.00
24	A3	66	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1830	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1167	C	O4'-C1'-N1	5.86	112.89	108.20
54	BA	2639	A	O4'-C1'-N9	5.86	112.88	108.20
54	BA	2741	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1111	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	398	C	O4'-C1'-N1	5.85	112.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	717	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	2181	U	O4'-C1'-N1	5.85	112.88	108.20
21	AA	116	A	N1-C6-N6	-5.85	115.09	118.60
21	AA	1081	A	C4-C5-C6	-5.85	114.07	117.00
22	A1	16	C	N1-C2-O2	5.85	122.41	118.90
39	BQ	69	ARG	NE-CZ-NH1	5.85	123.23	120.30
54	BA	1170	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	2614	A	C6-C5-N7	5.85	136.40	132.30
33	BK	70	ARG	NE-CZ-NH1	5.85	123.22	120.30
54	BA	2260	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	1133	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1417	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	1774	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2274	A	N1-C6-N6	-5.85	115.09	118.60
21	AA	1067	A	C6-C5-N7	5.85	136.39	132.30
54	BA	1206	G	N3-C2-N2	-5.85	115.81	119.90
54	BA	1654	A	C4-C5-C6	-5.85	114.08	117.00
21	AA	608	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	474	G	O4'-C1'-N9	5.85	112.88	108.20
54	BA	590	A	C5-C6-N1	5.85	120.62	117.70
54	BA	1634	A	O4'-C1'-N9	5.85	112.88	108.20
54	BA	1829	A	C4-C5-C6	-5.85	114.08	117.00
55	BB	92	C	N3-C2-O2	-5.85	117.81	121.90
21	AA	931	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1552	A	C1'-O4'-C4'	-5.84	105.22	109.90
54	BA	1603	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1644	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2096	C	O4'-C1'-N1	5.84	112.88	108.20
54	BA	2778	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	879	C	N1-C2-O2	5.84	122.41	118.90
54	BA	395	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	550	C	N1-C2-O2	5.84	122.41	118.90
54	BA	2194	U	O4'-C1'-N1	5.84	112.87	108.20
17	AR	47	ARG	NE-CZ-NH1	5.84	123.22	120.30
54	BA	251	A	N1-C6-N6	-5.84	115.10	118.60
18	AS	36	ARG	NE-CZ-NH2	5.84	123.22	120.30
21	AA	783	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	826	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	1145	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	1333	A	C4-C5-C6	-5.84	114.08	117.00
22	A1	59	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	184	C	N3-C2-O2	-5.84	117.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	930	G	O4'-C1'-N9	5.84	112.87	108.20
54	BA	2575	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	2670	A	C4-C5-C6	-5.84	114.08	117.00
6	AG	142	ARG	NE-CZ-NH1	5.84	123.22	120.30
54	BA	334	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	957	C	N1-C2-O2	5.84	122.40	118.90
54	BA	1789	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1054	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	2333	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	20	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2339	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2441	U	O4'-C1'-N1	5.83	112.87	108.20
21	AA	977	A	C4-C5-C6	-5.83	114.08	117.00
24	A3	60	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	905	A	C5-C6-N1	5.83	120.62	117.70
54	BA	1003	G	N1-C6-O6	-5.83	116.40	119.90
54	BA	2662	A	C5-C6-N1	5.83	120.62	117.70
55	BB	78	A	C6-C5-N7	5.83	136.38	132.30
54	BA	53	A	O4'-C1'-N9	5.83	112.86	108.20
54	BA	2173	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	487	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	459	U	O4'-C1'-N1	5.83	112.86	108.20
54	BA	527	C	N1-C2-O2	5.83	122.40	118.90
54	BA	1328	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	1431	A	N1-C6-N6	-5.83	115.10	118.60
54	BA	1741	C	N3-C2-O2	-5.83	117.82	121.90
22	A1	36	C	N3-C2-O2	-5.83	117.82	121.90
37	BO	9	ARG	NE-CZ-NH1	5.83	123.21	120.30
54	BA	2518	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	1311	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	222	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	231	A	C5-C6-N1	5.82	120.61	117.70
54	BA	434	U	O4'-C1'-N1	5.82	112.86	108.20
54	BA	2254	C	N3-C2-O2	-5.82	117.82	121.90
21	AA	770	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1507	C	O4'-C1'-N1	5.82	112.86	108.20
55	BB	52	A	O4'-C1'-N9	5.82	112.86	108.20
54	BA	210	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1600	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2788	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	277	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	368	A	C5-C6-N1	5.82	120.61	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2746	U	O4'-C1'-N1	5.82	112.86	108.20
21	AA	269	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1098	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1288	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1562	U	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2072	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	470	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1540	G	O4'-C1'-N9	5.82	112.85	108.20
54	BA	2060	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2146	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2882	A	C5-C6-N1	5.82	120.61	117.70
21	AA	381	C	O4'-C1'-N1	5.81	112.85	108.20
21	AA	990	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	1430	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	526	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1503	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1525	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2754	U	O4'-C1'-N1	5.81	112.85	108.20
21	AA	862	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	852	G	N1-C6-O6	-5.81	116.42	119.90
26	BD	169	ARG	NE-CZ-NH2	-5.81	117.40	120.30
54	BA	369	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	538	A	C5-C6-N1	5.81	120.60	117.70
54	BA	581	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2679	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	2720	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	2750	A	C4-C5-C6	-5.81	114.10	117.00
55	BB	64	G	N1-C6-O6	-5.81	116.42	119.90
54	BA	542	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1146	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2757	A	C5-C6-N1	5.80	120.60	117.70
21	AA	906	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	77	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	978	A	C6-C5-N7	5.80	136.36	132.30
21	AA	1217	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	1298	U	N3-C2-O2	-5.80	118.14	122.20
54	BA	267	C	N3-C2-O2	-5.80	117.84	121.90
27	BE	67	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	866	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2015	A	O4'-C1'-N9	5.80	112.84	108.20
54	BA	2458	G	N3-C4-C5	-5.80	125.70	128.60
55	BB	118	C	N3-C2-O2	-5.80	117.84	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2043	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	2222	C	N3-C2-O2	-5.80	117.84	121.90
28	BF	70	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	1690	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1447	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	829	A	N1-C6-N6	-5.79	115.12	118.60
54	BA	2177	C	N3-C2-O2	-5.79	117.84	121.90
55	BB	49	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	1117	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	698	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	1243	C	N1-C2-O2	5.79	122.38	118.90
54	BA	2312	U	N3-C2-O2	-5.79	118.14	122.20
54	BA	2556	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	816	A	C4-C5-C6	-5.79	114.10	117.00
21	AA	970	C	N3-C4-C5	5.79	124.22	121.90
54	BA	268	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	472	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	889	A	N1-C6-N6	-5.79	115.13	118.60
21	AA	927	G	O4'-C1'-N9	5.79	112.83	108.20
21	AA	460	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	167	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	990	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	704	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	894	G	N1-C6-O6	-5.78	116.43	119.90
21	AA	923	A	N1-C6-N6	-5.78	115.13	118.60
54	BA	1498	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	1758	U	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2651	C	O4'-C1'-N1	5.78	112.83	108.20
21	AA	1254	A	C5-C6-N1	5.78	120.59	117.70
54	BA	445	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2297	A	O4'-C1'-N9	5.78	112.83	108.20
21	AA	307	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	1005	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1469	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1894	C	N1-C2-O2	5.78	122.37	118.90
54	BA	2247	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2364	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2482	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	514	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	1913	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	844	G	N3-C4-C5	-5.78	125.71	128.60
54	BA	572	A	C4-C5-C6	-5.78	114.11	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1570	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1483	A	C5-C6-N1	5.78	120.59	117.70
54	BA	909	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2094	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2597	G	N1-C6-O6	-5.78	116.44	119.90
55	BB	115	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	131	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	426	C	O4'-C1'-N1	5.77	112.82	108.20
54	BA	994	C	N1-C2-O2	5.77	122.36	118.90
54	BA	1056	G	C5-C6-N1	5.77	114.39	111.50
54	BA	915	C	N1-C2-O2	5.77	122.36	118.90
54	BA	2512	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	975	A	C4-C5-C6	-5.77	114.11	117.00
21	AA	1188	A	C4-C5-C6	-5.77	114.11	117.00
24	A3	72	C	N1-C2-O2	5.77	122.36	118.90
34	BL	32	GLY	C-N-CA	5.77	136.13	121.70
54	BA	421	C	N3-C2-O2	-5.77	117.86	121.90
55	BB	93	C	N3-C2-O2	-5.77	117.86	121.90
51	B2	35	ARG	NE-CZ-NH1	5.77	123.18	120.30
54	BA	966	G	N1-C6-O6	-5.77	116.44	119.90
54	BA	1791	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	2314	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	339	C	N1-C2-O2	5.77	122.36	118.90
54	BA	160	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	592	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	2678	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	448	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	1170	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	1518	A	C6-C5-N7	5.76	136.34	132.30
54	BA	2036	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	2730	C	N3-C2-O2	-5.76	117.86	121.90
21	AA	177	G	N3-C4-C5	-5.76	125.72	128.60
21	AA	1001	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	164	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	980	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2853	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	876	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	1322	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2706	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2806	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	833	A	O4'-C1'-N9	5.76	112.81	108.20
21	AA	787	A	C4-C5-C6	-5.76	114.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	228	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	330	A	O4'-C1'-N9	5.76	112.81	108.20
54	BA	599	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	616	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1586	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	368	U	N3-C2-O2	-5.75	118.17	122.20
54	BA	1637	A	C5-C6-N1	5.75	120.58	117.70
21	AA	1031	C	N1-C2-O2	5.75	122.35	118.90
21	AA	1131	G	N3-C2-N2	-5.75	115.87	119.90
54	BA	272	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	320	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	1278	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	2411	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2483	C	O4'-C1'-N1	5.75	112.80	108.20
2	AC	131	ARG	NE-CZ-NH1	5.75	123.17	120.30
21	AA	919	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	336	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	433	C	N1-C2-O2	5.75	122.35	118.90
54	BA	678	C	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2091	C	N1-C2-O2	5.75	122.35	118.90
21	AA	980	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	41	G	N1-C6-O6	-5.75	116.45	119.90
21	AA	374	A	O4'-C1'-N9	5.75	112.80	108.20
21	AA	810	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	1214	C	C1'-O4'-C4'	-5.75	105.30	109.90
21	AA	1366	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	1804	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	702	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	999	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	1171	A	C5-C6-N1	5.75	120.57	117.70
54	BA	1848	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	547	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	2837	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	181	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	363	A	C4-C5-C6	-5.74	114.13	117.00
24	A3	73	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	191	A	N1-C6-N6	-5.74	115.15	118.60
54	BA	1147	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1351	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	2733	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	8	A	O4'-C1'-N9	5.74	112.79	108.20
54	BA	1030	C	N3-C2-O2	-5.74	117.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1176	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1487	U	O4'-C1'-N1	5.74	112.79	108.20
21	AA	35	G	O4'-C1'-N9	5.74	112.79	108.20
21	AA	385	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	1319	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	554	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1141	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1194	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	1342	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	1410	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	226	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2066	C	N3-C2-O2	-5.74	117.88	121.90
23	A2	80	C	N3-C2-O2	-5.74	117.89	121.90
54	BA	203	A	N1-C6-N6	-5.74	115.16	118.60
54	BA	1362	C	N1-C2-O2	5.74	122.34	118.90
54	BA	1379	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1153	C	N3-C2-O2	-5.73	117.89	121.90
55	BB	97	C	N1-C2-O2	5.73	122.34	118.90
21	AA	967	C	N1-C2-O2	5.73	122.34	118.90
54	BA	203	A	C4-C5-C6	-5.73	114.13	117.00
52	B3	39	ARG	NH1-CZ-NH2	-5.73	113.10	119.40
54	BA	921	C	N3-C2-O2	-5.73	117.89	121.90
17	AR	42	ARG	NE-CZ-NH1	5.73	123.16	120.30
54	BA	415	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1043	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2518	A	O4'-C1'-N9	5.73	112.78	108.20
13	AN	9	ARG	NE-CZ-NH1	5.73	123.16	120.30
21	AA	160	A	C4-C5-C6	-5.73	114.14	117.00
26	BD	15	PHE	CB-CG-CD1	-5.73	116.79	120.80
21	AA	482	A	N1-C6-N6	-5.72	115.17	118.60
21	AA	622	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	501	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1151	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	352	C	N3-C2-O2	-5.72	117.89	121.90
21	AA	979	C	N3-C2-O2	-5.72	117.89	121.90
22	A1	21	A	C4-C5-C6	-5.72	114.14	117.00
22	A1	62	C	N3-C2-O2	-5.72	117.89	121.90
39	BQ	49	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
54	BA	217	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1844	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	2305	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	1127	G	N1-C6-O6	-5.72	116.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2889	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	536	C	N1-C2-O2	5.72	122.33	118.90
54	BA	1686	C	O4'-C1'-N1	5.72	112.78	108.20
15	AP	8	ARG	NE-CZ-NH1	5.71	123.16	120.30
54	BA	1274	A	C5-C6-N1	5.71	120.56	117.70
21	AA	1284	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	910	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2762	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1456	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1155	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1241	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2771	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	944	G	N1-C6-O6	-5.71	116.47	119.90
55	BB	19	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	633	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1884	G	C3'-C2'-C1'	5.71	106.07	101.50
21	AA	582	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	14	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	1574	C	N3-C4-C5	5.71	124.18	121.90
54	BA	2039	U	O4'-C1'-N1	5.71	112.77	108.20
21	AA	309	A	C4-C5-C6	-5.71	114.15	117.00
21	AA	1102	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	2208	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	2900	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	347	A	C4-C5-C6	-5.70	114.15	117.00
23	A2	79	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	802	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1838	C	O4'-C1'-N1	5.70	112.76	108.20
21	AA	214	C	N1-C2-O2	5.70	122.32	118.90
29	BG	54	ARG	NE-CZ-NH1	5.70	123.15	120.30
54	BA	1847	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2715	C	N1-C2-O2	5.70	122.32	118.90
21	AA	642	A	C5-C6-N1	5.70	120.55	117.70
21	AA	1324	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	311	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	989	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1928	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2737	G	N1-C6-O6	-5.70	116.48	119.90
54	BA	2860	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1438	U	P-O3'-C3'	5.69	126.53	119.70
54	BA	2792	A	C4-C5-C6	-5.69	114.15	117.00
21	AA	285	C	N1-C2-O2	5.69	122.31	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	336	A	C5-C6-N1	5.69	120.55	117.70
21	AA	782	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2295	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	1261	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	687	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1434	A	C4-C5-C6	-5.69	114.16	117.00
21	AA	556	C	N3-C2-O2	-5.69	117.92	121.90
27	BE	61	ARG	NE-CZ-NH1	5.69	123.14	120.30
54	BA	1591	A	O4'-C1'-N9	5.69	112.75	108.20
54	BA	2600	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	740	C	N1-C2-O2	5.69	122.31	118.90
54	BA	794	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1565	C	O4'-C1'-N1	5.68	112.75	108.20
54	BA	2617	U	O4'-C1'-N1	5.68	112.75	108.20
21	AA	1182	G	N3-C2-N2	-5.68	115.92	119.90
21	AA	1369	C	N1-C2-O2	5.68	122.31	118.90
21	AA	1409	C	N3-C2-O2	-5.68	117.92	121.90
25	BC	216	ARG	NE-CZ-NH2	5.68	123.14	120.30
41	BS	99	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	277	G	N3-C4-C5	-5.68	125.76	128.60
21	AA	512	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	2850	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1596	A	C5-C6-N1	5.68	120.54	117.70
48	BZ	10	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	838	C	C5'-C4'-O4'	5.68	115.91	109.10
21	AA	625	U	O4'-C1'-N1	5.67	112.74	108.20
21	AA	1460	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	1500	A	C6-C5-N7	5.67	136.27	132.30
54	BA	337	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	347	A	C5-C6-N1	5.67	120.54	117.70
54	BA	2598	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	471	U	C1'-O4'-C4'	-5.67	105.36	109.90
22	A1	70	C	C5'-C4'-C3'	-5.67	106.92	116.00
54	BA	223	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1773	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1987	A	O4'-C1'-N9	5.67	112.74	108.20
54	BA	2317	A	C5-C6-N1	5.67	120.54	117.70
21	AA	28	A	C4-C5-C6	-5.67	114.17	117.00
32	BJ	99	ARG	NE-CZ-NH1	5.67	123.14	120.30
6	AG	95	ARG	NE-CZ-NH1	5.67	123.13	120.30
21	AA	897	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	140	C	N3-C4-N4	-5.67	114.03	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	285	G	O4'-C1'-N9	5.67	112.73	108.20
54	BA	558	U	O4'-C1'-N1	5.67	112.73	108.20
54	BA	731	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1075	C	O4'-C1'-N1	5.67	112.73	108.20
54	BA	1934	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2515	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	353	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2448	A	C4-C5-C6	-5.67	114.17	117.00
21	AA	392	C	N3-C2-O2	-5.67	117.94	121.90
54	BA	1001	A	C4-C5-C6	-5.67	114.17	117.00
39	BQ	54	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	161	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	440	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	752	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	884	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	2277	G	N1-C6-O6	-5.66	116.50	119.90
54	BA	2630	G	O4'-C1'-N9	5.66	112.73	108.20
54	BA	341	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	646	U	O4'-C1'-N1	5.66	112.73	108.20
21	AA	1397	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1441	A	N1-C6-N6	-5.66	115.20	118.60
22	A1	51	C	N3-C2-O2	-5.66	117.94	121.90
24	A3	52	C	N3-C2-O2	-5.66	117.94	121.90
30	BH	50	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	417	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1292	G	O4'-C1'-N9	5.66	112.73	108.20
54	BA	1570	A	C5-C6-N1	5.66	120.53	117.70
21	AA	89	U	N3-C2-O2	-5.66	118.24	122.20
21	AA	703	G	C3'-C2'-C1'	5.66	106.03	101.50
21	AA	716	A	C4-C5-C6	-5.66	114.17	117.00
46	BX	2	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	1027	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1086	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	348	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2465	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	35	G	C5'-C4'-C3'	-5.66	106.95	116.00
21	AA	1119	C	N3-C2-O2	-5.66	117.94	121.90
22	A1	51	C	O4'-C1'-N1	5.66	112.72	108.20
34	BL	48	ARG	NH1-CZ-NH2	-5.66	113.18	119.40
54	BA	147	C	O4'-C1'-N1	5.66	112.72	108.20
54	BA	149	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	475	C	O4'-C1'-N1	5.66	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	479	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1032	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1196	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1359	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1731	G	N3-C4-C5	-5.66	125.77	128.60
54	BA	1824	G	N1-C6-O6	-5.66	116.51	119.90
21	AA	250	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	863	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1585	C	O4'-C1'-N1	5.65	112.72	108.20
21	AA	403	C	N3-C2-O2	-5.65	117.94	121.90
22	A1	38	A	C6-C5-N7	5.65	136.25	132.30
54	BA	22	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1204	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1899	A	C4-C5-C6	-5.65	114.17	117.00
55	BB	37	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	838	C	N1-C2-O2	5.65	122.29	118.90
21	AA	233	C	N3-C2-O2	-5.65	117.95	121.90
54	BA	2261	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	835	C	N1-C2-O2	5.65	122.29	118.90
21	AA	467	U	N3-C2-O2	-5.64	118.25	122.20
21	AA	1305	G	N1-C6-O6	-5.64	116.51	119.90
54	BA	601	C	O4'-C1'-N1	5.64	112.72	108.20
21	AA	722	G	C5-C6-N1	5.64	114.32	111.50
54	BA	722	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	961	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2287	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1325	U	C1'-O4'-C4'	-5.64	105.39	109.90
21	AA	225	C	N3-C2-O2	-5.64	117.95	121.90
8	AI	44	ARG	NE-CZ-NH1	5.64	123.12	120.30
8	AI	17	ARG	NE-CZ-NH1	5.64	123.12	120.30
21	AA	777	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	76	C	N1-C2-O2	5.64	122.28	118.90
54	BA	2727	A	C4-C5-C6	-5.64	114.18	117.00
6	AG	101	ARG	NE-CZ-NH2	-5.63	117.48	120.30
7	AH	83	ARG	NE-CZ-NH1	5.63	123.12	120.30
21	AA	1533	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	1792	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	2024	G	N3-C2-N2	-5.63	115.96	119.90
22	A1	2	G	O4'-C1'-N9	5.63	112.71	108.20
54	BA	529	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	951	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	1064	C	N1-C2-O2	5.63	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2443	C	C4'-C3'-C2'	-5.63	96.97	102.60
54	BA	2530	A	C4-C5-C6	-5.63	114.18	117.00
56	B5	162	ARG	NE-CZ-NH1	5.63	123.12	120.30
21	AA	998	C	N1-C2-O2	5.63	122.28	118.90
54	BA	84	A	N1-C6-N6	-5.63	115.22	118.60
54	BA	2704	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	563	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1236	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1340	A	C4-C5-C6	-5.63	114.19	117.00
22	A1	56	C	N1-C2-O2	5.63	122.28	118.90
34	BL	48	ARG	NE-CZ-NH2	5.63	123.11	120.30
54	BA	1640	A	O4'-C1'-N9	5.63	112.70	108.20
54	BA	2378	A	N1-C6-N6	-5.63	115.22	118.60
54	BA	2749	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	270	A	C5'-C4'-C3'	-5.62	107.00	116.00
21	AA	270	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	303	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	239	C	N3-C2-O2	-5.62	117.96	121.90
21	AA	715	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2765	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1275	A	C4-C5-C6	-5.62	114.19	117.00
25	BC	174	ARG	NE-CZ-NH1	5.62	123.11	120.30
54	BA	1544	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2248	C	N3-C2-O2	-5.62	117.97	121.90
4	AE	67	ARG	NE-CZ-NH1	5.62	123.11	120.30
6	AG	3	ARG	NE-CZ-NH1	5.62	123.11	120.30
21	AA	856	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1718	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	2571	U	O4'-C1'-N1	5.62	112.69	108.20
21	AA	322	C	N1-C2-O2	5.61	122.27	118.90
54	BA	318	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1129	A	O4'-C1'-N9	5.61	112.69	108.20
21	AA	948	C	N1-C2-O2	5.61	122.27	118.90
54	BA	2268	A	C4-C5-C6	-5.61	114.19	117.00
21	AA	257	G	N1-C6-O6	-5.61	116.53	119.90
21	AA	483	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1888	G	N3-C4-C5	-5.61	125.80	128.60
54	BA	2306	C	N3-C2-O2	-5.61	117.97	121.90
55	BB	91	C	O4'-C1'-N1	5.61	112.69	108.20
21	AA	1107	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1538	G	N3-C2-N2	-5.61	115.97	119.90
21	AA	33	A	C4-C5-C6	-5.61	114.20	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	193	C	N1-C2-O2	5.61	122.26	118.90
21	AA	366	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	483	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	848	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	947	A	C6-C5-N7	5.61	136.22	132.30
54	BA	1645	G	C5-C6-N1	5.61	114.30	111.50
54	BA	1672	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	1827	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2270	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	423	G	N3-C4-C5	-5.61	125.80	128.60
54	BA	1061	U	N3-C2-O2	-5.61	118.28	122.20
54	BA	1295	C	N1-C2-O2	5.61	122.26	118.90
54	BA	1647	U	O4'-C1'-N1	5.61	112.68	108.20
54	BA	1747	U	O4'-C1'-N1	5.61	112.68	108.20
54	BA	2071	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	629	A	C6-C5-N7	5.60	136.22	132.30
54	BA	1774	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	2275	C	N3-C2-O2	-5.60	117.98	121.90
21	AA	643	C	N3-C2-O2	-5.60	117.98	121.90
22	A1	13	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	107	G	C5'-C4'-O4'	5.60	115.82	109.10
54	BA	1961	C	N1-C2-O2	5.60	122.26	118.90
54	BA	2302	U	O4'-C1'-N1	5.60	112.68	108.20
3	AD	25	ARG	NE-CZ-NH1	5.60	123.10	120.30
52	B3	7	ARG	NE-CZ-NH2	-5.60	117.50	120.30
54	BA	237	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	812	C	N1-C2-O2	5.60	122.26	118.90
54	BA	1052	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1598	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	2851	A	C6-C5-N7	5.60	136.22	132.30
54	BA	1729	U	O4'-C1'-N1	5.60	112.68	108.20
21	AA	984	C	N3-C2-O2	-5.60	117.98	121.90
21	AA	641	U	N3-C2-O2	-5.59	118.28	122.20
21	AA	1032	G	C8-N9-C4	-5.59	104.16	106.40
21	AA	1212	U	C1'-O4'-C4'	-5.59	105.42	109.90
54	BA	1236	G	O4'-C1'-N9	5.59	112.68	108.20
54	BA	581	C	O4'-C1'-N1	5.59	112.67	108.20
21	AA	1478	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	148	U	C3'-C2'-C1'	5.59	105.97	101.50
54	BA	1863	G	N1-C6-O6	-5.59	116.55	119.90
21	AA	419	C	N1-C2-O2	5.59	122.25	118.90
21	AA	1227	A	C4-C5-C6	-5.59	114.20	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BN	69	ARG	NE-CZ-NH1	5.59	123.09	120.30
54	BA	91	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	1088	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	2854	G	O4'-C1'-N9	5.59	112.67	108.20
21	AA	736	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1213	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	1265	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1448	C	C6-N1-C2	-5.59	118.06	120.30
54	BA	305	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2422	C	N1-C2-O2	5.59	122.25	118.90
54	BA	2453	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	329	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	1301	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	1360	G	N1-C6-O6	-5.59	116.55	119.90
54	BA	1679	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	2279	G	N1-C6-O6	-5.59	116.55	119.90
54	BA	1648	U	C5-C6-N1	-5.58	119.91	122.70
21	AA	508	U	N3-C2-O2	-5.58	118.29	122.20
54	BA	193	U	N3-C2-O2	-5.58	118.29	122.20
54	BA	731	C	C3'-C2'-C1'	5.58	105.97	101.50
54	BA	2687	U	O4'-C1'-N1	5.58	112.67	108.20
21	AA	428	G	O4'-C1'-N9	5.58	112.67	108.20
54	BA	237	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	998	C	N1-C2-O2	5.58	122.25	118.90
54	BA	1553	A	C6-C5-N7	5.58	136.21	132.30
54	BA	2215	C	N1-C2-O2	5.58	122.25	118.90
54	BA	2440	C	O4'-C1'-N1	5.58	112.66	108.20
54	BA	130	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	413	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	1342	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2419	U	O4'-C1'-N1	5.58	112.66	108.20
55	BB	35	C	N1-C2-O2	5.58	122.25	118.90
55	BB	47	C	N3-C2-O2	-5.58	118.00	121.90
22	A1	76	A	C4-C5-C6	-5.58	114.21	117.00
3	AD	69	ARG	NH1-CZ-NH2	-5.58	113.27	119.40
21	AA	106	C	C5'-C4'-O4'	5.58	115.79	109.10
21	AA	689	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	1102	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	2169	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	331	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1116	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	1608	A	C4-C5-C6	-5.57	114.21	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1741	C	N1-C2-O2	5.57	122.24	118.90
54	BA	2322	A	C4-C5-C6	-5.57	114.21	117.00
21	AA	703	G	O4'-C1'-N9	5.57	112.66	108.20
54	BA	1574	C	N1-C2-O2	5.57	122.24	118.90
21	AA	549	C	N3-C4-N4	-5.57	114.10	118.00
54	BA	2382	G	O4'-C1'-N9	5.57	112.66	108.20
21	AA	163	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	432	A	C6-C5-N7	5.57	136.20	132.30
21	AA	1108	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	2408	U	O4'-C1'-N1	5.57	112.66	108.20
21	AA	271	C	O4'-C1'-N1	5.57	112.65	108.20
21	AA	1124	G	O4'-C1'-N9	5.57	112.65	108.20
54	BA	1297	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1853	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	2656	U	O4'-C1'-N1	5.57	112.65	108.20
54	BA	2823	A	C3'-C2'-C1'	5.57	105.95	101.50
54	BA	1223	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	2838	G	O4'-C1'-N9	5.57	112.65	108.20
43	BU	81	ARG	NE-CZ-NH2	-5.56	117.52	120.30
21	AA	300	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	330	A	N1-C6-N6	-5.56	115.26	118.60
54	BA	1348	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1720	U	O4'-C1'-N1	5.56	112.65	108.20
54	BA	271	G	O4'-C1'-N9	5.56	112.65	108.20
54	BA	1005	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	2820	A	C4-C5-C6	-5.56	114.22	117.00
55	BB	43	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	1701	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1870	C	N1-C2-O2	5.56	122.23	118.90
21	AA	964	A	N1-C6-N6	-5.56	115.27	118.60
21	AA	1467	C	N1-C2-O2	5.56	122.23	118.90
54	BA	401	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1087	G	C3'-C2'-C1'	5.56	105.94	101.50
55	BB	86	G	N1-C6-O6	-5.56	116.57	119.90
21	AA	731	G	N3-C2-N2	-5.55	116.01	119.90
51	B2	21	ARG	NE-CZ-NH1	5.55	123.08	120.30
54	BA	560	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	876	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1200	C	N1-C2-O2	5.55	122.23	118.90
54	BA	1590	A	C4-C5-C6	-5.55	114.22	117.00
56	B5	74	ARG	NE-CZ-NH1	5.55	123.08	120.30
21	AA	1480	A	C6-C5-N7	5.55	136.19	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2232	C	N1-C2-O2	5.55	122.23	118.90
3	AD	153	ARG	NE-CZ-NH1	5.55	123.08	120.30
35	BM	55	ARG	NE-CZ-NH2	5.55	123.08	120.30
48	BZ	44	ARG	NE-CZ-NH1	5.55	123.08	120.30
54	BA	7	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	294	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	509	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	1306	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1967	C	N1-C2-O2	5.55	122.23	118.90
54	BA	2879	A	N1-C6-N6	-5.55	115.27	118.60
54	BA	2311	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	2475	C	N3-C2-O2	-5.55	118.02	121.90
21	AA	1349	A	C4-C5-C6	-5.55	114.23	117.00
33	BK	105	ARG	NE-CZ-NH1	5.55	123.07	120.30
54	BA	2014	A	C4-C5-C6	-5.55	114.23	117.00
21	AA	759	A	C4-C5-C6	-5.55	114.23	117.00
21	AA	1137	C	N1-C2-O2	5.55	122.23	118.90
54	BA	1534	U	N3-C2-O2	-5.55	118.32	122.20
2	AC	71	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	504	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	357	G	C3'-C2'-C1'	5.54	105.94	101.50
21	AA	653	U	N3-C2-O2	-5.54	118.32	122.20
54	BA	1955	U	O4'-C1'-N1	5.54	112.64	108.20
54	BA	2200	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	7	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	1296	C	N1-C2-O2	5.54	122.22	118.90
54	BA	2346	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2872	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1757	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2122	U	O4'-C1'-N1	5.54	112.63	108.20
54	BA	776	G	N9-C4-C5	5.54	107.61	105.40
50	B1	27	ARG	NE-CZ-NH1	5.54	123.07	120.30
54	BA	2214	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	1165	U	O4'-C1'-N1	5.54	112.63	108.20
24	A3	41	C	N3-C2-O2	-5.54	118.03	121.90
54	BA	244	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	119	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	212	G	O4'-C1'-N9	5.53	112.63	108.20
54	BA	632	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	722	A	O4'-C1'-N9	5.53	112.63	108.20
54	BA	2795	C	O4'-C1'-N1	5.53	112.63	108.20
21	AA	227	G	N1-C6-O6	-5.53	116.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1540	G	C5'-C4'-O4'	5.53	115.74	109.10
54	BA	2581	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	2153	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2520	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2717	C	N1-C2-O2	5.53	122.22	118.90
21	AA	660	C	N3-C2-O2	-5.53	118.03	121.90
47	BY	7	ARG	NE-CZ-NH1	5.53	123.06	120.30
54	BA	332	A	C5-C6-N1	5.53	120.46	117.70
54	BA	566	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	671	C	N1-C2-O2	5.53	122.22	118.90
54	BA	890	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	1239	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	1872	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	1881	C	N1-C2-O2	5.53	122.22	118.90
54	BA	2699	C	N1-C2-O2	5.53	122.22	118.90
21	AA	200	G	O4'-C1'-N9	5.53	112.62	108.20
54	BA	1630	A	C6-C5-N7	5.53	136.17	132.30
54	BA	2713	U	O4'-C1'-N1	5.52	112.62	108.20
54	BA	2784	U	O4'-C1'-N1	5.52	112.62	108.20
54	BA	876	C	N3-C2-O2	-5.52	118.03	121.90
54	BA	1073	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1123	C	O4'-C1'-N1	5.52	112.62	108.20
17	AR	56	ARG	NE-CZ-NH2	-5.52	117.54	120.30
21	AA	1534	A	C5'-C4'-C3'	-5.52	107.17	116.00
21	AA	945	G	C5-C6-N1	5.52	114.26	111.50
22	A1	41	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	166	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	824	U	C4'-C3'-C2'	-5.52	97.08	102.60
54	BA	1744	A	C4-C5-C6	-5.52	114.24	117.00
14	AO	88	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	AA	133	U	N3-C2-O2	-5.52	118.34	122.20
54	BA	606	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	785	G	N1-C6-O6	-5.52	116.59	119.90
54	BA	1591	A	C6-C5-N7	5.52	136.16	132.30
54	BA	2145	C	N1-C2-O2	5.52	122.21	118.90
54	BA	2562	U	O4'-C1'-N1	5.52	112.61	108.20
10	AK	52	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	AA	34	C	O4'-C1'-N1	5.52	112.61	108.20
21	AA	1000	A	N1-C6-N6	-5.52	115.29	118.60
21	AA	1021	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	1376	U	N3-C2-O2	-5.52	118.34	122.20
54	BA	1299	G	C3'-C2'-C1'	5.52	105.91	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	128	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	404	A	O4'-C1'-N9	5.51	112.61	108.20
54	BA	1371	G	N3-C2-N2	-5.51	116.04	119.90
54	BA	1722	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	2398	U	O4'-C1'-N1	5.51	112.61	108.20
21	AA	305	G	C3'-C2'-C1'	5.51	105.91	101.50
21	AA	595	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	2899	A	C6-C5-N7	5.51	136.16	132.30
4	AE	25	LYS	C-N-CA	5.51	133.87	122.30
21	AA	108	G	O4'-C1'-N9	5.51	112.61	108.20
21	AA	417	G	N1-C6-O6	-5.51	116.59	119.90
21	AA	760	G	N1-C6-O6	-5.51	116.59	119.90
21	AA	1534	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	455	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	1046	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	1070	A	C1'-O4'-C4'	-5.51	105.49	109.90
21	AA	848	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	279	A	C3'-C2'-C1'	5.51	105.91	101.50
54	BA	2278	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	1755	A	C6-C5-N7	5.51	136.16	132.30
21	AA	546	A	N1-C6-N6	-5.51	115.30	118.60
21	AA	1400	C	N1-C2-O2	5.51	122.20	118.90
54	BA	537	G	N1-C6-O6	-5.51	116.60	119.90
54	BA	1808	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	1862	G	N3-C2-N2	-5.51	116.05	119.90
54	BA	2723	C	N1-C2-O2	5.51	122.20	118.90
21	AA	85	U	C3'-C2'-C1'	5.50	105.90	101.50
54	BA	419	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	621	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1533	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1554	U	C3'-C2'-C1'	5.50	105.90	101.50
54	BA	1737	G	N3-C2-N2	-5.50	116.05	119.90
54	BA	1762	A	O4'-C1'-N9	5.50	112.60	108.20
21	AA	108	G	N3-C2-N2	-5.50	116.05	119.90
21	AA	151	A	C6-C5-N7	5.50	136.15	132.30
21	AA	714	G	N3-C4-C5	-5.50	125.85	128.60
21	AA	1269	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	84	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	120	U	N3-C2-O2	-5.50	118.35	122.20
54	BA	1876	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1961	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	243	U	O4'-C1'-N1	5.50	112.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2116	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	586	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	2272	U	N3-C2-O2	-5.50	118.35	122.20
21	AA	99	C	N1-C2-O2	5.50	122.20	118.90
21	AA	1344	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1109	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	2164	C	N1-C2-O2	5.50	122.20	118.90
21	AA	36	C	C5'-C4'-C3'	-5.50	107.21	116.00
21	AA	693	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	1266	G	C1'-O4'-C4'	-5.50	105.50	109.90
21	AA	869	G	C3'-C2'-C1'	5.49	105.89	101.50
54	BA	190	A	N1-C6-N6	-5.49	115.30	118.60
54	BA	1176	U	N3-C2-O2	-5.49	118.35	122.20
54	BA	1345	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	1489	C	N1-C2-O2	5.49	122.20	118.90
54	BA	355	U	O4'-C1'-N1	5.49	112.59	108.20
21	AA	912	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	970	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	337	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	1294	U	O4'-C1'-N1	5.49	112.59	108.20
21	AA	732	C	N1-C2-O2	5.49	122.19	118.90
21	AA	1249	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	1267	C	N3-C2-O2	-5.49	118.06	121.90
34	BL	33	ARG	NE-CZ-NH1	5.49	123.04	120.30
36	BN	71	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
54	BA	342	A	C5-C6-N1	5.49	120.44	117.70
54	BA	931	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	2033	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	2255	G	N3-C2-N2	-5.49	116.06	119.90
21	AA	1382	C	N1-C2-O2	5.49	122.19	118.90
26	BD	58	ASN	C-N-CA	5.49	135.42	121.70
54	BA	281	C	N1-C2-O2	5.49	122.19	118.90
21	AA	415	A	O4'-C1'-N9	5.49	112.59	108.20
21	AA	941	G	N9-C1'-C2'	-5.49	105.97	112.00
54	BA	823	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1213	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	2420	C	N1-C2-O2	5.49	122.19	118.90
54	BA	2537	U	C4'-C3'-C2'	-5.49	97.11	102.60
54	BA	2573	C	C1'-O4'-C4'	-5.49	105.51	109.90
54	BA	1877	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	13	U	O4'-C1'-N1	5.48	112.59	108.20
21	AA	760	G	O4'-C1'-N9	5.48	112.59	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	17	U	N3-C2-O2	-5.48	118.36	122.20
24	A3	62	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	339	U	O4'-C1'-N1	5.48	112.59	108.20
54	BA	393	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	1602	U	P-O3'-C3'	5.48	126.28	119.70
21	AA	857	C	N1-C2-O2	5.48	122.19	118.90
54	BA	1007	C	N1-C2-O2	5.48	122.19	118.90
54	BA	2447	G	C1'-O4'-C4'	-5.48	105.52	109.90
21	AA	143	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	982	C	O4'-C1'-N1	5.48	112.58	108.20
55	BB	69	G	N1-C6-O6	-5.48	116.61	119.90
21	AA	43	C	N3-C2-O2	-5.48	118.07	121.90
54	BA	1594	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	1898	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2426	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1781	U	N3-C2-O2	-5.48	118.37	122.20
54	BA	1967	C	O4'-C1'-N1	5.48	112.58	108.20
55	BB	104	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	96	U	O4'-C1'-N1	5.47	112.58	108.20
21	AA	1257	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	66	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	732	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	1272	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	92	U	O4'-C1'-N1	5.47	112.58	108.20
21	AA	520	A	C6-C5-N7	5.47	136.13	132.30
54	BA	168	G	N3-C2-N2	-5.47	116.07	119.90
54	BA	205	G	C5-C6-N1	5.47	114.24	111.50
54	BA	1794	A	C6-C5-N7	5.47	136.13	132.30
54	BA	2465	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	2596	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	2610	C	N1-C2-O2	5.47	122.18	118.90
21	AA	164	G	C1'-O4'-C4'	-5.47	105.53	109.90
54	BA	1386	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	832	G	N3-C2-N2	-5.47	116.07	119.90
54	BA	371	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	1509	A	O4'-C1'-N9	5.47	112.57	108.20
54	BA	1895	C	N1-C2-O2	5.47	122.18	118.90
54	BA	1895	C	O4'-C1'-N1	5.47	112.57	108.20
54	BA	2896	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	58	G	O4'-C1'-N9	5.46	112.57	108.20
54	BA	1129	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1152	C	O4'-C1'-N1	5.46	112.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2310	C	N1-C2-O2	5.46	122.18	118.90
54	BA	2527	C	N1-C2-O2	5.46	122.18	118.90
54	BA	2903	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1627	G	N3-C4-C5	-5.46	125.87	128.60
54	BA	2769	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	614	A	C1'-O4'-C4'	-5.46	105.53	109.90
54	BA	706	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	229	C	N1-C2-O2	5.46	122.18	118.90
54	BA	1936	A	P-O3'-C3'	5.46	126.25	119.70
13	AN	13	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	179	C	N1-C2-O2	5.46	122.17	118.90
54	BA	525	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1933	G	C8-N9-C4	-5.46	104.22	106.40
54	BA	2676	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	2885	G	N1-C6-O6	-5.46	116.62	119.90
21	AA	282	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	396	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	640	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	1039	G	N1-C6-O6	-5.46	116.63	119.90
21	AA	1531	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2434	A	C6-C5-N7	5.46	136.12	132.30
54	BA	676	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2212	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	429	U	C5-C6-N1	-5.45	119.97	122.70
25	BC	269	ARG	NE-CZ-NH1	5.45	123.03	120.30
54	BA	1020	A	C4-C5-C6	-5.45	114.27	117.00
6	AG	69	ARG	NE-CZ-NH1	5.45	123.03	120.30
16	AQ	76	ARG	NE-CZ-NH1	5.45	123.03	120.30
54	BA	364	C	N1-C2-O2	5.45	122.17	118.90
54	BA	1162	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	1409	U	O4'-C1'-N1	5.45	112.56	108.20
54	BA	2660	A	O4'-C1'-N9	5.45	112.56	108.20
54	BA	1854	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	923	G	N1-C6-O6	-5.45	116.63	119.90
11	AL	85	ARG	NE-CZ-NH1	5.45	123.02	120.30
21	AA	686	U	N3-C2-O2	-5.45	118.39	122.20
54	BA	881	G	N3-C2-N2	-5.45	116.09	119.90
54	BA	1580	A	C6-C5-N7	5.45	136.11	132.30
54	BA	1743	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	1799	G	N3-C4-C5	-5.45	125.88	128.60
54	BA	2734	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	1092	A	C4-C5-C6	-5.44	114.28	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	192	C	N1-C2-O2	5.44	122.17	118.90
54	BA	1291	C	N3-C4-C5	5.44	124.08	121.90
21	AA	37	U	N3-C2-O2	-5.44	118.39	122.20
21	AA	1000	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	1437	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1799	G	C8-N9-C4	-5.44	104.22	106.40
54	BA	2286	G	N1-C6-O6	-5.44	116.63	119.90
21	AA	156	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	503	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	372	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	2220	U	O4'-C1'-N1	5.44	112.55	108.20
21	AA	313	A	C6-C5-N7	5.44	136.11	132.30
21	AA	720	C	N1-C2-O2	5.44	122.16	118.90
21	AA	1099	G	C5-C6-N1	5.44	114.22	111.50
53	B4	4	ARG	NE-CZ-NH1	5.44	123.02	120.30
54	BA	882	G	N3-C2-N2	-5.44	116.09	119.90
54	BA	1012	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	1958	C	N3-C2-O2	-5.44	118.09	121.90
3	AD	42	ALA	C-N-CA	5.44	135.29	121.70
54	BA	492	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	831	G	C5-C6-N1	5.44	114.22	111.50
54	BA	1211	C	N1-C2-O2	5.44	122.16	118.90
21	AA	1251	A	C6-C5-N7	5.43	136.10	132.30
54	BA	175	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	2430	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	1194	U	N3-C2-O2	-5.43	118.40	122.20
21	AA	1324	A	C5-C6-N1	5.43	120.42	117.70
54	BA	443	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	2838	G	C4'-C3'-C2'	-5.43	97.17	102.60
18	AS	77	ARG	NE-CZ-NH1	5.43	123.02	120.30
21	AA	209	U	N3-C2-O2	-5.43	118.40	122.20
24	A3	42	C	N1-C2-O2	5.43	122.16	118.90
54	BA	1089	A	C3'-C2'-C1'	5.43	105.84	101.50
54	BA	1317	G	C1'-O4'-C4'	-5.43	105.56	109.90
54	BA	1519	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	2785	C	O4'-C1'-N1	5.43	112.55	108.20
21	AA	818	G	C5-C6-N1	5.43	114.22	111.50
54	BA	2459	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	274	A	C6-C5-N7	5.43	136.10	132.30
54	BA	1857	G	O4'-C1'-N9	5.43	112.54	108.20
21	AA	517	G	O4'-C1'-N9	5.43	112.54	108.20
21	AA	722	G	N3-C4-C5	-5.43	125.89	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	765	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	1020	G	N1-C6-O6	-5.43	116.64	119.90
22	A1	74	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	1748	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	2776	A	O4'-C1'-N9	5.43	112.54	108.20
54	BA	2838	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	1036	A	C4-C5-C6	-5.42	114.29	117.00
28	BF	94	ARG	NE-CZ-NH1	5.42	123.01	120.30
54	BA	1000	A	C1'-O4'-C4'	-5.42	105.56	109.90
54	BA	1367	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1542	U	O4'-C1'-N1	5.42	112.54	108.20
54	BA	2065	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	2889	C	O4'-C1'-N1	5.42	112.54	108.20
21	AA	845	A	C5'-C4'-O4'	5.42	115.61	109.10
54	BA	574	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2040	G	N3-C2-N2	-5.42	116.10	119.90
21	AA	560	A	C3'-C2'-C1'	5.42	105.84	101.50
21	AA	765	G	N3-C4-C5	-5.42	125.89	128.60
42	BT	73	ARG	NE-CZ-NH1	5.42	123.01	120.30
54	BA	81	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	556	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2066	C	O4'-C1'-N1	5.42	112.54	108.20
21	AA	108	G	N3-C4-C5	-5.42	125.89	128.60
21	AA	993	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	484	C	N3-C2-O2	-5.42	118.11	121.90
9	AJ	72	ARG	CD-NE-CZ	5.42	131.19	123.60
21	AA	1183	U	N3-C2-O2	-5.42	118.41	122.20
24	A3	16	C	C3'-C2'-C1'	5.42	105.84	101.50
54	BA	1101	U	O4'-C1'-N1	5.42	112.53	108.20
54	BA	1259	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	2700	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1377	A	C4-C5-C6	-5.42	114.29	117.00
35	BM	40	ARG	NE-CZ-NH1	5.42	123.01	120.30
54	BA	899	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2516	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2805	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	1794	A	O4'-C1'-N9	5.42	112.53	108.20
54	BA	2342	C	N1-C2-O2	5.41	122.15	118.90
54	BA	2760	C	N3-C4-C5	5.41	124.07	121.90
21	AA	430	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	300	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1233	C	O4'-C1'-N1	5.41	112.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1555	G	N3-C4-C5	-5.41	125.89	128.60
54	BA	1944	U	P-O3'-C3'	5.41	126.19	119.70
54	BA	1865	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2432	A	O4'-C1'-N9	5.41	112.53	108.20
55	BB	53	A	N1-C6-N6	-5.41	115.36	118.60
21	AA	1519	A	C4-C5-C6	-5.41	114.30	117.00
24	A3	67	C	N1-C2-O2	5.41	122.14	118.90
21	AA	575	G	P-O3'-C3'	5.41	126.19	119.70
21	AA	1080	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	1218	C	N1-C2-O2	5.41	122.14	118.90
54	BA	1089	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1398	C	O4'-C1'-N1	5.41	112.52	108.20
54	BA	1862	G	C8-N9-C4	-5.41	104.24	106.40
54	BA	2070	A	C6-C5-N7	5.41	136.08	132.30
54	BA	2080	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	818	G	N3-C4-C5	-5.40	125.90	128.60
21	AA	1129	C	C3'-C2'-C1'	5.40	105.82	101.50
28	BF	114	ARG	NE-CZ-NH1	5.40	123.00	120.30
54	BA	1786	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1832	C	C3'-C2'-C1'	5.40	105.82	101.50
55	BB	4	C	O4'-C1'-N1	5.40	112.52	108.20
13	AN	63	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	995	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	1226	C	N1-C2-O2	5.40	122.14	118.90
54	BA	503	A	C3'-C2'-C1'	5.40	105.82	101.50
54	BA	2134	A	C6-C5-N7	5.40	136.08	132.30
18	AS	54	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	124	C	C1'-O4'-C4'	-5.40	105.58	109.90
54	BA	615	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	1189	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1363	C	N1-C2-O2	5.40	122.14	118.90
4	AE	28	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	477	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	569	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	1579	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	1229	A	C5'-C4'-O4'	5.40	115.58	109.10
29	BG	94	ARG	NE-CZ-NH1	5.40	123.00	120.30
54	BA	1086	A	O4'-C1'-N9	5.40	112.52	108.20
54	BA	1536	C	N1-C2-O2	5.40	122.14	118.90
54	BA	1726	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	122	G	N3-C2-N2	-5.40	116.12	119.90
21	AA	924	C	N3-C2-O2	-5.40	118.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	827	U	N3-C2-O2	-5.39	118.42	122.20
21	AA	1192	C	N1-C2-O2	5.39	122.14	118.90
21	AA	1268	G	C5-C6-N1	5.39	114.20	111.50
54	BA	57	C	O4'-C1'-N1	5.39	112.52	108.20
54	BA	490	C	N1-C2-O2	5.39	122.14	118.90
54	BA	665	U	O4'-C1'-N1	5.39	112.52	108.20
54	BA	2499	C	O4'-C1'-N1	5.39	112.52	108.20
3	AD	153	ARG	NE-CZ-NH2	-5.39	117.60	120.30
21	AA	1453	G	N3-C4-C5	-5.39	125.90	128.60
54	BA	2511	U	O4'-C1'-N1	5.39	112.51	108.20
24	A3	57	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	33	C	O4'-C4'-C3'	5.39	110.41	106.10
54	BA	351	C	N1-C2-O2	5.39	122.14	118.90
54	BA	2112	G	N1-C6-O6	-5.39	116.67	119.90
8	AI	108	ARG	NE-CZ-NH1	5.39	122.99	120.30
21	AA	1099	G	N1-C6-O6	-5.39	116.67	119.90
21	AA	1156	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	2813	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	1812	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	2762	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1325	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1828	G	O4'-C1'-N9	5.39	112.51	108.20
21	AA	1224	U	N3-C2-O2	-5.38	118.43	122.20
21	AA	1259	C	N1-C2-O2	5.38	122.13	118.90
54	BA	2198	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	365	U	C1'-O4'-C4'	-5.38	105.59	109.90
54	BA	262	A	C4-C5-C6	-5.38	114.31	117.00
25	BC	100	ARG	NE-CZ-NH1	5.38	122.99	120.30
21	AA	118	U	N3-C2-O2	-5.38	118.43	122.20
54	BA	2667	C	N1-C2-O2	5.38	122.13	118.90
21	AA	372	C	N3-C2-O2	-5.38	118.14	121.90
21	AA	981	U	O4'-C1'-N1	5.38	112.50	108.20
24	A3	71	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	97	C	O4'-C1'-N1	5.38	112.50	108.20
54	BA	1121	C	O4'-C1'-N1	5.38	112.50	108.20
54	BA	2350	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	2611	C	N1-C2-O2	5.38	122.13	118.90
14	AO	57	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BA	143	C	N1-C2-O2	5.38	122.12	118.90
54	BA	420	C	N1-C2-O2	5.38	122.13	118.90
21	AA	1200	C	N1-C2-O2	5.38	122.12	118.90
21	AA	1487	G	C5-C6-N1	5.38	114.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1521	G	C5-C6-N1	5.38	114.19	111.50
54	BA	2856	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	726	G	N3-C4-C5	-5.37	125.91	128.60
54	BA	2062	A	C4-C5-C6	-5.37	114.31	117.00
55	BB	90	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	149	A	C4-C5-C6	-5.37	114.31	117.00
21	AA	907	A	C4-C5-C6	-5.37	114.31	117.00
24	A3	69	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	249	C	O4'-C1'-N1	5.37	112.50	108.20
21	AA	1150	A	C6-C5-N7	5.37	136.06	132.30
54	BA	2009	A	C4-C5-C6	-5.37	114.31	117.00
21	AA	171	A	C6-C5-N7	5.37	136.06	132.30
54	BA	1563	U	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2100	G	N3-C2-N2	-5.37	116.14	119.90
21	AA	35	G	N3-C4-C5	-5.37	125.92	128.60
21	AA	251	G	N3-C4-C5	-5.37	125.92	128.60
21	AA	1474	U	O4'-C1'-N1	5.37	112.49	108.20
32	BJ	69	ARG	NE-CZ-NH1	5.37	122.98	120.30
54	BA	1615	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2486	C	N1-C2-O2	5.37	122.12	118.90
54	BA	1628	G	N3-C2-N2	-5.36	116.15	119.90
54	BA	1644	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2680	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2861	U	O4'-C1'-N1	5.36	112.49	108.20
55	BB	89	U	N3-C2-O2	-5.36	118.45	122.20
21	AA	153	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	1532	U	C1'-O4'-C4'	-5.36	105.61	109.90
54	BA	2135	A	C4-C5-C6	-5.36	114.32	117.00
3	AD	103	ARG	CD-NE-CZ	5.36	131.10	123.60
21	AA	347	G	N3-C4-C5	-5.36	125.92	128.60
21	AA	1055	A	P-O3'-C3'	5.36	126.13	119.70
55	BB	41	G	N3-C4-C5	-5.36	125.92	128.60
21	AA	189	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2209	G	N1-C6-O6	-5.36	116.69	119.90
55	BB	101	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	456	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	1202	U	O4'-C1'-N1	5.36	112.49	108.20
21	AA	1346	A	C1'-O4'-C4'	-5.36	105.61	109.90
54	BA	141	G	N1-C6-O6	-5.36	116.69	119.90
54	BA	575	A	C6-C5-N7	5.36	136.05	132.30
54	BA	1969	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2458	G	C5-C6-N1	5.36	114.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	46	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	784	A	C6-C5-N7	5.36	136.05	132.30
21	AA	1294	G	N1-C6-O6	-5.36	116.69	119.90
21	AA	1403	C	N1-C2-O2	5.36	122.11	118.90
21	AA	1461	G	N1-C6-O6	-5.36	116.69	119.90
42	BT	6	ARG	NE-CZ-NH2	5.36	122.98	120.30
54	BA	1752	C	N1-C2-O2	5.36	122.11	118.90
54	BA	2711	A	C6-C5-N7	5.36	136.05	132.30
54	BA	2824	C	N3-C2-O2	-5.36	118.15	121.90
51	B2	34	ARG	NE-CZ-NH2	-5.35	117.62	120.30
21	AA	463	U	N3-C2-O2	-5.35	118.45	122.20
21	AA	806	C	C1'-O4'-C4'	-5.35	105.62	109.90
21	AA	1151	A	C5'-C4'-C3'	-5.35	107.44	116.00
54	BA	1053	C	N3-C2-O2	-5.35	118.15	121.90
54	BA	2286	G	C1'-O4'-C4'	-5.35	105.62	109.90
54	BA	2517	C	N1-C2-O2	5.35	122.11	118.90
21	AA	627	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	457	A	C6-C5-N7	5.35	136.05	132.30
54	BA	1011	G	O4'-C1'-N9	5.35	112.48	108.20
54	BA	1905	C	N1-C2-O2	5.35	122.11	118.90
21	AA	999	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	31	C	N1-C2-O2	5.35	122.11	118.90
54	BA	207	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	227	A	C6-C5-N7	5.35	136.04	132.30
54	BA	368	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	1175	A	C6-C5-N7	5.35	136.04	132.30
54	BA	1884	G	O4'-C1'-N9	5.35	112.48	108.20
21	AA	302	G	N1-C6-O6	-5.35	116.69	119.90
21	AA	512	U	C5-C6-N1	-5.35	120.03	122.70
21	AA	1169	A	C4-C5-C6	-5.35	114.33	117.00
28	BF	29	ARG	CD-NE-CZ	5.35	131.09	123.60
54	BA	74	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	502	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	787	C	N3-C4-C5	5.35	124.04	121.90
54	BA	2395	C	O4'-C1'-N1	5.35	112.48	108.20
55	BB	26	C	O4'-C1'-N1	5.35	112.48	108.20
14	AO	62	ARG	NE-CZ-NH1	5.35	122.97	120.30
21	AA	1048	G	N1-C6-O6	-5.35	116.69	119.90
34	BL	69	ARG	NE-CZ-NH1	5.35	122.97	120.30
21	AA	499	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	703	G	C8-N9-C4	-5.34	104.26	106.40
21	AA	1287	A	C6-C5-N7	5.34	136.04	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2321	U	N3-C2-O2	-5.34	118.46	122.20
21	AA	758	C	N1-C2-O2	5.34	122.11	118.90
24	A3	54	G	N3-C2-N2	-5.34	116.16	119.90
54	BA	12	U	O4'-C1'-N1	5.34	112.47	108.20
11	AL	55	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BA	724	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1122	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	2172	U	C1'-O4'-C4'	-5.34	105.63	109.90
54	BA	2620	C	N3-C2-O2	-5.34	118.16	121.90
55	BB	80	U	O4'-C1'-N1	5.34	112.47	108.20
21	AA	518	C	N1-C2-O2	5.34	122.10	118.90
54	BA	109	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	986	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1103	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	560	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1332	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	2394	C	N1-C2-O2	5.34	122.10	118.90
54	BA	2612	C	N1-C2-O2	5.34	122.10	118.90
21	AA	1216	A	O4'-C1'-N9	5.34	112.47	108.20
22	A1	4	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	441	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	783	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	901	C	N1-C2-O2	5.34	122.10	118.90
54	BA	336	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	2480	C	N1-C2-O2	5.33	122.10	118.90
21	AA	697	U	O4'-C1'-N1	5.33	112.47	108.20
21	AA	1190	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	49	A	O4'-C1'-N9	5.33	112.47	108.20
54	BA	338	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	1760	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	2275	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	2297	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	1217	C	C1'-O4'-C4'	-5.33	105.64	109.90
54	BA	2639	A	C6-C5-N7	5.33	136.03	132.30
54	BA	354	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	440	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	572	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	753	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	890	G	O4'-C1'-N9	5.33	112.46	108.20
54	BA	1604	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	1055	A	C4-C5-C6	-5.33	114.34	117.00
38	BP	97	TYR	CB-CG-CD2	-5.33	117.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	808	C	N1-C2-O2	5.33	122.10	118.90
54	BA	576	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	962	G	N3-C2-N2	-5.33	116.17	119.90
21	AA	86	G	N3-C4-C5	-5.32	125.94	128.60
21	AA	618	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	444	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	2439	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	355	C	N3-C2-O2	-5.32	118.17	121.90
21	AA	588	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	1046	A	C6-C5-N7	5.32	136.03	132.30
24	A3	77	A	C6-C5-N7	5.32	136.03	132.30
55	BB	19	C	O4'-C1'-N1	5.32	112.46	108.20
21	AA	654	G	N3-C2-N2	-5.32	116.18	119.90
21	AA	890	G	N3-C4-C5	-5.32	125.94	128.60
54	BA	1691	C	N3-C2-O2	-5.32	118.18	121.90
54	BA	2179	C	N1-C2-O2	5.32	122.09	118.90
22	A1	75	C	N1-C2-O2	5.32	122.09	118.90
20	AU	33	ARG	NE-CZ-NH1	5.32	122.96	120.30
39	BQ	57	ARG	NE-CZ-NH1	5.32	122.96	120.30
54	BA	544	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1217	U	O4'-C1'-N1	5.32	112.45	108.20
54	BA	2390	U	O4'-C1'-N1	5.32	112.45	108.20
54	BA	2826	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	149	A	C5'-C4'-O4'	5.32	115.48	109.10
54	BA	218	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	1245	G	N3-C2-N2	-5.32	116.18	119.90
54	BA	2880	C	N1-C2-O2	5.32	122.09	118.90
21	AA	316	C	N1-C2-O2	5.31	122.09	118.90
54	BA	2424	C	N1-C2-O2	5.31	122.09	118.90
21	AA	641	U	C3'-C2'-C1'	5.31	105.75	101.50
54	BA	672	C	N1-C2-O2	5.31	122.09	118.90
54	BA	1499	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	1819	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	2443	C	C5'-C4'-O4'	5.31	115.47	109.10
21	AA	5	U	N1-C2-N3	5.31	118.09	114.90
21	AA	559	A	C4-C5-C6	-5.31	114.34	117.00
33	BK	32	TYR	CB-CG-CD1	-5.31	117.81	121.00
54	BA	405	U	N3-C2-O2	-5.31	118.48	122.20
54	BA	1317	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	705	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	734	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	1098	A	C4-C5-C6	-5.31	114.34	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1967	C	N3-C4-C5	5.31	124.02	121.90
54	BA	1985	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	493	A	O4'-C1'-N9	5.31	112.45	108.20
21	AA	934	C	N1-C2-O2	5.31	122.08	118.90
54	BA	580	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1612	C	N1-C2-O2	5.31	122.08	118.90
54	BA	2457	U	O4'-C1'-N1	5.31	112.44	108.20
21	AA	1237	C	N1-C2-O2	5.31	122.08	118.90
54	BA	2284	A	C4-C5-C6	-5.31	114.35	117.00
21	AA	454	G	N3-C2-N2	-5.30	116.19	119.90
21	AA	535	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	922	G	N3-C4-C5	-5.30	125.95	128.60
54	BA	1488	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	2685	G	N3-C2-N2	-5.30	116.19	119.90
54	BA	1104	C	C5'-C4'-O4'	5.30	115.46	109.10
21	AA	438	U	N3-C2-O2	-5.30	118.49	122.20
21	AA	1222	G	N3-C2-N2	-5.30	116.19	119.90
46	BX	44	ARG	NE-CZ-NH2	-5.30	117.65	120.30
54	BA	2090	A	C4-C5-C6	-5.30	114.35	117.00
3	AD	48	SER	C-N-CA	5.30	134.95	121.70
21	AA	258	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	496	A	O4'-C1'-N9	5.30	112.44	108.20
54	BA	344	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1597	A	C6-C5-N7	5.30	136.01	132.30
21	AA	269	C	O4'-C1'-N1	5.30	112.44	108.20
21	AA	1446	A	O4'-C1'-N9	5.30	112.44	108.20
21	AA	1490	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	129	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	1286	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	1361	G	N1-C6-O6	-5.29	116.72	119.90
54	BA	324	A	C6-C5-N7	5.29	136.01	132.30
54	BA	2160	C	N1-C2-O2	5.29	122.08	118.90
21	AA	416	G	O4'-C1'-N9	5.29	112.44	108.20
54	BA	508	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	631	A	C6-C5-N7	5.29	136.01	132.30
54	BA	2776	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	2863	C	N3-C2-O2	-5.29	118.19	121.90
55	BB	13	G	N1-C6-O6	-5.29	116.72	119.90
9	AJ	16	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
21	AA	871	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1457	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2503	A	C4-C5-C6	-5.29	114.35	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2568	U	O4'-C1'-N1	5.29	112.43	108.20
21	AA	53	A	C6-C5-N7	5.29	136.00	132.30
21	AA	83	C	N1-C2-O2	5.29	122.07	118.90
21	AA	188	C	N1-C2-O2	5.29	122.07	118.90
54	BA	1977	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	480	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	601	C	N1-C2-O2	5.29	122.07	118.90
54	BA	1035	U	N3-C2-O2	-5.29	118.50	122.20
55	BB	28	C	N1-C2-O2	5.29	122.07	118.90
21	AA	236	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	790	U	C5-C6-N1	-5.29	120.06	122.70
54	BA	1014	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	1293	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1446	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1615	C	N1-C2-O2	5.29	122.07	118.90
54	BA	2240	U	O4'-C1'-N1	5.29	112.43	108.20
24	A3	74	A	O4'-C1'-N9	5.28	112.43	108.20
54	BA	359	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	2431	U	C5-C6-N1	-5.28	120.06	122.70
21	AA	1084	G	N1-C6-O6	-5.28	116.73	119.90
21	AA	1096	C	N1-C2-O2	5.28	122.07	118.90
54	BA	1227	G	O4'-C1'-N9	5.28	112.43	108.20
54	BA	1993	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2144	G	N1-C6-O6	-5.28	116.73	119.90
55	BB	44	G	N1-C6-O6	-5.28	116.73	119.90
21	AA	195	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	383	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	706	A	C6-C5-N7	5.28	136.00	132.30
21	AA	1190	G	P-O3'-C3'	5.28	126.04	119.70
54	BA	265	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	447	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	634	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	1288	G	N3-C4-C5	-5.28	125.96	128.60
54	BA	2443	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2601	C	N1-C2-O2	5.28	122.07	118.90
54	BA	405	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2155	U	N3-C2-O2	-5.28	118.50	122.20
54	BA	2627	G	N9-C4-C5	5.28	107.51	105.40
54	BA	2691	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2703	C	N3-C2-O2	-5.28	118.21	121.90
21	AA	216	U	N3-C2-O2	-5.28	118.51	122.20
21	AA	575	G	N1-C6-O6	-5.28	116.73	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1135	U	O4'-C1'-N1	5.28	112.42	108.20
21	AA	1479	C	C3'-C2'-C1'	5.28	105.72	101.50
35	BM	50	ARG	NE-CZ-NH1	5.28	122.94	120.30
54	BA	1157	G	N1-C6-O6	-5.28	116.73	119.90
21	AA	1132	C	N1-C2-O2	5.27	122.06	118.90
21	AA	57	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	391	A	N1-C6-N6	-5.27	115.44	118.60
54	BA	664	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	1000	A	C6-C5-N7	5.27	135.99	132.30
54	BA	1436	G	O4'-C1'-N9	5.27	112.42	108.20
54	BA	1659	G	N1-C6-O6	-5.27	116.74	119.90
21	AA	988	G	N3-C4-C5	-5.27	125.96	128.60
6	AG	110	ARG	NE-CZ-NH2	-5.27	117.67	120.30
21	AA	432	A	O4'-C1'-N9	5.27	112.42	108.20
21	AA	586	C	O4'-C1'-N1	5.27	112.42	108.20
21	AA	612	C	N1-C2-O2	5.27	122.06	118.90
21	AA	860	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	4	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	310	A	C4-C5-C6	-5.27	114.37	117.00
54	BA	430	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	516	C	N1-C2-O2	5.27	122.06	118.90
54	BA	1051	G	C1'-O4'-C4'	-5.27	105.69	109.90
54	BA	1412	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2023	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2530	A	C5'-C4'-C3'	-5.27	107.57	116.00
21	AA	699	C	N1-C2-O2	5.27	122.06	118.90
21	AA	1469	C	N1-C2-O2	5.27	122.06	118.90
54	BA	639	U	N3-C2-O2	-5.27	118.51	122.20
54	BA	1681	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	288	U	O4'-C1'-N1	5.27	112.41	108.20
11	AL	93	ARG	NE-CZ-NH1	5.26	122.93	120.30
21	AA	1033	G	O4'-C1'-N9	5.26	112.41	108.20
21	AA	1076	U	C5-C6-N1	-5.26	120.07	122.70
36	BN	22	ARG	NE-CZ-NH1	5.26	122.93	120.30
54	BA	251	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1433	A	C6-C5-N7	5.26	135.99	132.30
54	BA	2265	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	1412	C	O4'-C1'-N1	5.26	112.41	108.20
25	BC	62	ARG	NE-CZ-NH1	5.26	122.93	120.30
54	BA	1202	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	1500	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	751	A	C4-C5-C6	-5.26	114.37	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	932	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	1071	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	1478	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	1677	A	C4-C5-C6	-5.26	114.37	117.00
55	BB	69	G	O4'-C1'-N9	5.26	112.41	108.20
21	AA	1455	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	47	C	N1-C2-O2	5.26	122.06	118.90
54	BA	335	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	242	G	N1-C6-O6	-5.26	116.75	119.90
54	BA	1395	A	C1'-O4'-C4'	-5.26	105.69	109.90
54	BA	1558	C	N3-C2-O2	-5.26	118.22	121.90
54	BA	2097	A	C6-C5-N7	5.26	135.98	132.30
54	BA	2576	G	N3-C4-C5	-5.26	125.97	128.60
21	AA	593	U	C5-C6-N1	-5.26	120.07	122.70
21	AA	616	G	N3-C2-N2	-5.26	116.22	119.90
21	AA	1336	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	360	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	727	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1308	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2147	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	449	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	817	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2307	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	1054	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	1256	A	C4-C5-C6	-5.25	114.37	117.00
22	A1	25	C	N1-C2-O2	5.25	122.05	118.90
54	BA	759	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	1419	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	2491	U	N3-C2-O2	-5.25	118.52	122.20
54	BA	2576	G	C5-C6-N1	5.25	114.13	111.50
30	BH	27	ARG	NE-CZ-NH1	5.25	122.93	120.30
54	BA	1029	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	1269	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	2501	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2644	G	O4'-C1'-N9	5.25	112.40	108.20
21	AA	584	G	N3-C4-C5	-5.25	125.98	128.60
23	A2	87	U	C5-C6-N1	-5.25	120.08	122.70
54	BA	75	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	1524	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	547	A	C6-C5-N7	5.25	135.97	132.30
21	AA	665	A	C6-C5-N7	5.25	135.97	132.30
21	AA	797	C	N3-C2-O2	-5.25	118.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BO	102	ARG	NE-CZ-NH1	5.25	122.92	120.30
54	BA	888	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1625	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2214	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2329	U	N3-C2-O2	-5.25	118.53	122.20
54	BA	22	C	N1-C2-O2	5.25	122.05	118.90
54	BA	350	G	C5-C6-N1	5.25	114.12	111.50
54	BA	2627	G	N3-C2-N2	-5.25	116.23	119.90
21	AA	299	G	N1-C6-O6	-5.24	116.75	119.90
54	BA	1193	G	O4'-C4'-C3'	5.24	110.30	106.10
54	BA	814	C	N3-C2-O2	-5.24	118.23	121.90
54	BA	1768	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2391	G	O4'-C1'-N9	5.24	112.39	108.20
21	AA	792	A	C1'-O4'-C4'	-5.24	105.71	109.90
21	AA	1082	A	C6-C5-N7	5.24	135.97	132.30
21	AA	1284	C	N1-C2-O2	5.24	122.04	118.90
54	BA	445	C	N3-C4-C5	5.24	124.00	121.90
21	AA	531	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	818	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	1811	G	O4'-C1'-N9	5.24	112.39	108.20
54	BA	1815	A	C6-C5-N7	5.24	135.97	132.30
21	AA	1159	U	C1'-O4'-C4'	-5.23	105.71	109.90
12	AM	108	ARG	NE-CZ-NH2	-5.23	117.68	120.30
21	AA	148	G	C5-C6-N1	5.23	114.12	111.50
21	AA	935	A	C6-C5-N7	5.23	135.96	132.30
21	AA	1038	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	660	C	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2057	G	C5-C6-N1	5.23	114.12	111.50
54	BA	2105	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2807	U	C5-C6-N1	-5.23	120.08	122.70
21	AA	248	C	N1-C2-O2	5.23	122.04	118.90
21	AA	950	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	471	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	1298	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	2185	U	O4'-C1'-N1	5.23	112.38	108.20
54	BA	2318	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	306	A	C6-C5-N7	5.23	135.96	132.30
21	AA	381	C	N1-C2-O2	5.23	122.04	118.90
36	BN	46	ARG	NE-CZ-NH1	5.23	122.92	120.30
54	BA	456	C	N1-C2-O2	5.23	122.04	118.90
54	BA	1763	G	N3-C4-C5	-5.23	125.98	128.60
21	AA	385	C	O4'-C1'-N1	5.23	112.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	398	U	O4'-C1'-N1	5.23	112.38	108.20
21	AA	1250	A	C1'-O4'-C4'	-5.23	105.72	109.90
54	BA	1183	U	O4'-C1'-N1	5.23	112.38	108.20
21	AA	534	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	904	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	2575	C	N3-C2-O2	-5.23	118.24	121.90
55	BB	118	C	O4'-C1'-N1	5.23	112.38	108.20
21	AA	651	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1727	C	N3-C2-O2	-5.22	118.24	121.90
54	BA	2013	A	N1-C6-N6	-5.22	115.47	118.60
54	BA	2539	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2807	U	O4'-C1'-N1	5.22	112.38	108.20
55	BB	27	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	367	G	N3-C4-C5	-5.22	125.99	128.60
54	BA	849	A	C6-C5-N7	5.22	135.96	132.30
54	BA	1263	U	N3-C2-O2	-5.22	118.54	122.20
54	BA	2219	U	O4'-C1'-N1	5.22	112.38	108.20
55	BB	83	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	482	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	935	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2133	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	2551	C	N1-C2-O2	5.22	122.03	118.90
54	BA	681	G	N3-C4-C5	-5.22	125.99	128.60
54	BA	1595	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2418	A	C6-C5-N7	5.22	135.95	132.30
54	BA	2533	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	58	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	2599	G	N3-C4-C5	-5.22	125.99	128.60
11	AL	86	VAL	C-N-CA	5.22	134.74	121.70
21	AA	47	C	N1-C2-O2	5.22	122.03	118.90
54	BA	421	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1376	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1713	A	P-O3'-C3'	5.22	125.96	119.70
54	BA	2823	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	1395	C	N1-C2-O2	5.21	122.03	118.90
54	BA	331	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2024	G	O4'-C1'-N9	5.21	112.37	108.20
54	BA	2102	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	2144	G	C5-C6-N1	5.21	114.11	111.50
55	BB	24	G	O4'-C1'-N9	5.21	112.37	108.20
55	BB	76	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	1451	C	C2'-C3'-O3'	5.21	122.04	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1476	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2864	G	N1-C6-O6	-5.21	116.77	119.90
21	AA	405	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	529	A	C1'-O4'-C4'	-5.21	105.73	109.90
54	BA	530	G	O4'-C4'-C3'	5.21	110.27	106.10
54	BA	898	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2104	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2716	C	N1-C2-O2	5.21	122.03	118.90
11	AL	109	ARG	NE-CZ-NH2	-5.21	117.69	120.30
21	AA	246	A	C4-C5-C6	-5.21	114.39	117.00
21	AA	505	G	C5'-C4'-O4'	5.21	115.35	109.10
54	BA	1676	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	316	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	975	A	C6-C5-N7	5.21	135.95	132.30
54	BA	1572	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	1873	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	1881	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1994	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2092	U	N3-C2-O2	-5.21	118.55	122.20
35	BM	38	ARG	NE-CZ-NH1	5.21	122.90	120.30
54	BA	435	C	N1-C2-O2	5.21	122.02	118.90
54	BA	736	C	N3-C2-O2	-5.21	118.26	121.90
54	BA	855	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	885	C	O4'-C1'-N1	5.21	112.36	108.20
54	BA	919	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1670	C	N1-C2-O2	5.21	122.02	118.90
54	BA	2213	U	N3-C2-O2	-5.21	118.56	122.20
54	BA	1428	C	N1-C2-O2	5.21	122.02	118.90
54	BA	1694	C	N3-C4-N4	-5.21	114.36	118.00
54	BA	2814	A	C6-C5-N7	5.21	135.94	132.30
6	AG	125	ASP	CB-CG-OD2	5.20	122.98	118.30
21	AA	357	G	O4'-C1'-N9	5.20	112.36	108.20
54	BA	391	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	1454	C	N3-C2-O2	-5.20	118.26	121.90
54	BA	1574	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1997	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2245	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2652	C	O4'-C1'-N1	5.20	112.36	108.20
21	AA	1242	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	2697	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	342	C	N3-C2-O2	-5.20	118.26	121.90
21	AA	610	U	O4'-C1'-N1	5.20	112.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	31	C	N1-C2-O2	5.20	122.02	118.90
54	BA	452	G	C4'-C3'-C2'	-5.20	97.40	102.60
54	BA	2008	C	N1-C2-O2	5.20	122.02	118.90
21	AA	315	A	C6-C5-N7	5.20	135.94	132.30
54	BA	784	G	C1'-O4'-C4'	-5.20	105.74	109.90
54	BA	928	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1305	C	N1-C2-O2	5.20	122.02	118.90
54	BA	2658	C	O4'-C1'-N1	5.20	112.36	108.20
21	AA	1059	C	N1-C2-O2	5.19	122.02	118.90
22	A1	10	G	N1-C6-O6	-5.19	116.78	119.90
54	BA	15	G	O4'-C1'-N9	5.19	112.36	108.20
54	BA	692	C	N1-C2-O2	5.19	122.02	118.90
54	BA	49	A	C4-C5-C6	-5.19	114.40	117.00
55	BB	24	G	C3'-C2'-C1'	5.19	105.65	101.50
21	AA	1389	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1059	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	1803	A	C4-C5-C6	-5.19	114.40	117.00
21	AA	379	C	N1-C2-O2	5.19	122.01	118.90
34	BL	132	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
54	BA	2752	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	2812	G	C5'-C4'-C3'	-5.19	107.70	116.00
21	AA	597	G	N1-C6-O6	-5.19	116.79	119.90
46	BX	71	ARG	NE-CZ-NH1	5.19	122.89	120.30
54	BA	104	A	C4-C5-C6	-5.19	114.41	117.00
55	BB	99	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	208	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	452	G	N3-C4-C5	-5.19	126.01	128.60
54	BA	1473	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	1545	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	1564	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1704	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1600	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	1646	C	N3-C4-C5	5.18	123.97	121.90
54	BA	2114	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2333	A	C3'-C2'-C1'	5.18	105.65	101.50
54	BA	2657	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	237	G	C8-N9-C4	-5.18	104.33	106.40
21	AA	680	C	O4'-C1'-N1	5.18	112.34	108.20
21	AA	1064	G	N3-C4-C5	-5.18	126.01	128.60
21	AA	1379	G	N3-C2-N2	-5.18	116.27	119.90
54	BA	129	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	564	C	N1-C2-O2	5.18	122.01	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	793	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2696	U	O4'-C1'-N1	5.18	112.35	108.20
21	AA	1217	C	N3-C4-C5	5.18	123.97	121.90
26	BD	15	PHE	CB-CG-CD2	5.18	124.43	120.80
54	BA	114	U	N3-C2-O2	-5.18	118.57	122.20
54	BA	882	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	959	A	C4'-C3'-C2'	-5.18	97.42	102.60
24	A3	3	C	N1-C2-O2	5.18	122.01	118.90
54	BA	1675	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	2809	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	1066	C	N1-C2-O2	5.18	122.01	118.90
54	BA	100	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	191	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	196	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2040	G	N9-C4-C5	5.18	107.47	105.40
54	BA	2331	G	O4'-C1'-N9	5.18	112.34	108.20
21	AA	916	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	624	C	N1-C2-O2	5.18	122.01	118.90
54	BA	644	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	722	A	N1-C6-N6	-5.18	115.49	118.60
54	BA	2378	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	634	C	N1-C2-O2	5.17	122.00	118.90
21	AA	1487	G	N3-C2-N2	-5.17	116.28	119.90
54	BA	349	U	O4'-C1'-N1	5.17	112.34	108.20
54	BA	2015	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	2055	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	2362	C	C4'-C3'-C2'	-5.17	97.42	102.60
14	AO	71	ARG	NE-CZ-NH2	-5.17	117.71	120.30
21	AA	722	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	475	C	O4'-C1'-N1	5.17	112.34	108.20
21	AA	953	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	974	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	1350	C	N1-C2-O2	5.17	122.00	118.90
54	BA	67	U	O4'-C1'-N1	5.17	112.34	108.20
21	AA	187	G	C5-C6-N1	5.17	114.08	111.50
54	BA	1732	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1769	U	C4'-C3'-C2'	-5.17	97.43	102.60
55	BB	42	C	N1-C2-O2	5.17	122.00	118.90
21	AA	123	U	C3'-C2'-C1'	5.17	105.63	101.50
21	AA	182	A	C4-C5-C6	-5.17	114.42	117.00
21	AA	1042	A	C6-C5-N7	5.17	135.92	132.30
21	AA	1332	A	N1-C6-N6	-5.17	115.50	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2025	C	N1-C2-O2	5.17	122.00	118.90
54	BA	2137	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	2570	G	N3-C2-N2	-5.17	116.28	119.90
55	BB	12	C	O4'-C1'-N1	5.17	112.33	108.20
21	AA	733	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	1100	C	N1-C2-O2	5.17	122.00	118.90
54	BA	101	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1463	C	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1626	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	2384	U	C5'-C4'-C3'	-5.16	107.74	116.00
54	BA	2643	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	2661	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	2808	G	C1'-O4'-C4'	-5.16	105.77	109.90
54	BA	490	C	N3-C4-C5	5.16	123.97	121.90
23	A2	92	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	2585	U	N3-C2-O2	-5.16	118.59	122.20
8	AI	11	ARG	CD-NE-CZ	5.16	130.82	123.60
54	BA	10	A	O4'-C1'-N9	5.16	112.33	108.20
54	BA	43	G	N3-C2-N2	-5.16	116.29	119.90
54	BA	1680	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1749	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	2873	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	297	G	C5'-C4'-C3'	-5.16	107.75	116.00
54	BA	1893	C	N1-C2-O2	5.16	121.99	118.90
21	AA	1147	C	N3-C2-O2	-5.16	118.29	121.90
51	B2	19	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BA	211	C	O4'-C1'-N1	5.16	112.32	108.20
54	BA	297	G	O4'-C1'-N9	5.16	112.32	108.20
54	BA	514	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1079	C	O4'-C1'-N1	5.16	112.32	108.20
54	BA	1229	C	N3-C2-O2	-5.16	118.29	121.90
54	BA	2428	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	289	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	587	C	N1-C2-O2	5.15	121.99	118.90
3	AD	103	ARG	NE-CZ-NH2	-5.15	117.72	120.30
54	BA	1605	C	N1-C2-O2	5.15	121.99	118.90
54	BA	2199	A	O4'-C1'-N9	5.15	112.32	108.20
20	AU	30	GLU	CA-C-N	5.15	128.53	117.20
21	AA	250	A	C2-N3-C4	5.15	113.17	110.60
21	AA	1328	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	1399	C	N1-C2-O2	5.15	121.99	118.90
54	BA	1018	U	O4'-C1'-N1	5.15	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1051	C	N1-C2-O2	5.15	121.99	118.90
54	BA	69	C	N1-C2-O2	5.15	121.99	118.90
54	BA	834	G	N7-C8-N9	5.15	115.67	113.10
54	BA	2148	G	N3-C2-N2	-5.15	116.30	119.90
21	AA	749	A	C6-C5-N7	5.15	135.90	132.30
21	AA	1214	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	95	A	O4'-C1'-N9	5.15	112.32	108.20
54	BA	1576	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	1579	A	N1-C6-N6	-5.15	115.51	118.60
54	BA	1668	A	C6-C5-N7	5.15	135.90	132.30
54	BA	2456	C	C5'-C4'-O4'	5.15	115.28	109.10
21	AA	584	G	C5-C6-N1	5.15	114.07	111.50
21	AA	1233	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	70	G	C5-C6-N1	5.15	114.07	111.50
46	BX	73	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	394	C	N1-C2-O2	5.14	121.99	118.90
54	BA	1233	C	N1-C2-O2	5.14	121.99	118.90
54	BA	1411	U	O4'-C1'-N1	5.14	112.32	108.20
54	BA	1461	C	N1-C2-O2	5.14	121.99	118.90
54	BA	2462	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2619	C	N3-C2-O2	-5.14	118.30	121.90
55	BB	87	U	C5'-C4'-O4'	5.14	115.27	109.10
6	AG	4	ARG	C-N-CA	5.14	134.56	121.70
21	AA	126	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	242	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	1639	C	N1-C2-O2	5.14	121.99	118.90
54	BA	2041	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	32	C	N1-C2-O2	5.14	121.98	118.90
54	BA	250	G	N3-C2-N2	-5.14	116.30	119.90
55	BB	3	C	N3-C2-O2	-5.14	118.30	121.90
21	AA	86	G	O4'-C1'-N9	5.14	112.31	108.20
21	AA	163	C	P-O3'-C3'	5.14	125.87	119.70
21	AA	284	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	687	C	C4'-C3'-C2'	-5.14	97.46	102.60
54	BA	2298	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2608	G	C5-C6-N1	5.14	114.07	111.50
54	BA	2888	C	N1-C2-O2	5.14	121.98	118.90
21	AA	275	G	N3-C2-N2	-5.14	116.30	119.90
21	AA	1314	C	N1-C2-O2	5.14	121.98	118.90
54	BA	1078	U	O4'-C4'-C3'	5.14	110.21	106.10
54	BA	1666	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	1962	C	N1-C2-O2	5.14	121.98	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2618	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	2649	C	N1-C2-O2	5.14	121.98	118.90
21	AA	881	G	N3-C2-N2	-5.14	116.30	119.90
8	AI	48	ARG	NE-CZ-NH2	-5.13	117.73	120.30
54	BA	155	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	165	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	2052	A	C6-C5-N7	5.13	135.89	132.30
54	BA	2572	A	C4-C5-C6	-5.13	114.43	117.00
55	BB	55	U	O4'-C1'-N1	5.13	112.31	108.20
21	AA	453	G	C5-C6-N1	5.13	114.07	111.50
21	AA	631	C	N1-C2-O2	5.13	121.98	118.90
21	AA	1380	U	C5'-C4'-C3'	-5.13	107.79	116.00
54	BA	53	A	C6-C5-N7	5.13	135.89	132.30
54	BA	105	C	N1-C2-O2	5.13	121.98	118.90
54	BA	530	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1921	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2186	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2542	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	13	U	N3-C2-O2	-5.13	118.61	122.20
21	AA	510	A	C6-C5-N7	5.13	135.89	132.30
54	BA	530	G	N3-C4-C5	-5.13	126.03	128.60
54	BA	595	C	N1-C2-O2	5.13	121.98	118.90
54	BA	1005	C	N1-C2-O2	5.13	121.98	118.90
54	BA	1624	U	C5'-C4'-O4'	5.13	115.26	109.10
54	BA	1874	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2883	A	C1'-O4'-C4'	-5.13	105.80	109.90
21	AA	1191	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	1254	A	C6-C5-N7	5.13	135.89	132.30
54	BA	1006	C	C5'-C4'-O4'	5.13	115.25	109.10
54	BA	1357	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	1884	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2207	C	N1-C2-O2	5.13	121.98	118.90
21	AA	657	U	C5'-C4'-O4'	5.13	115.25	109.10
54	BA	1666	G	O4'-C1'-N9	5.13	112.30	108.20
54	BA	2581	G	N3-C4-C5	-5.13	126.04	128.60
21	AA	394	G	N3-C2-N2	-5.12	116.31	119.90
21	AA	1360	A	C6-C5-N7	5.12	135.89	132.30
29	BG	162	ARG	NE-CZ-NH1	5.12	122.86	120.30
54	BA	590	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1805	A	C4-C5-C6	-5.12	114.44	117.00
55	BB	114	C	N3-C2-O2	-5.12	118.31	121.90
4	AE	104	ILE	C-N-CA	5.12	134.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	350	G	N1-C6-O6	-5.12	116.83	119.90
22	A1	66	A	C6-C5-N7	5.12	135.89	132.30
54	BA	1115	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2603	G	N3-C4-C5	-5.12	126.04	128.60
21	AA	50	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	292	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1724	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1781	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	2805	C	O4'-C1'-N1	5.12	112.30	108.20
21	AA	338	A	C6-C5-N7	5.12	135.88	132.30
21	AA	669	G	O4'-C1'-N9	5.12	112.30	108.20
21	AA	1362	A	O4'-C1'-N9	5.12	112.29	108.20
21	AA	1364	U	N3-C2-O2	-5.12	118.62	122.20
22	A1	3	G	N1-C6-O6	-5.12	116.83	119.90
42	BT	3	ARG	NE-CZ-NH2	-5.12	117.74	120.30
54	BA	540	C	C4'-C3'-C2'	-5.12	97.48	102.60
54	BA	744	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	1950	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1997	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	2406	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2845	U	C5-C6-N1	-5.12	120.14	122.70
21	AA	861	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	144	A	C6-C5-N7	5.12	135.88	132.30
54	BA	758	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	810	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	1219	U	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2115	G	C8-N9-C4	-5.12	104.35	106.40
54	BA	2593	U	O4'-C1'-N1	5.12	112.29	108.20
21	AA	428	G	N3-C2-N2	-5.11	116.32	119.90
54	BA	1926	U	N3-C2-O2	-5.11	118.62	122.20
21	AA	1459	G	C5-C6-N1	5.11	114.06	111.50
54	BA	858	G	N3-C4-C5	-5.11	126.04	128.60
21	AA	883	C	N3-C4-N4	-5.11	114.42	118.00
21	AA	988	G	C8-N9-C4	-5.11	104.36	106.40
21	AA	1473	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	164	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	2062	A	O4'-C1'-N9	5.11	112.29	108.20
21	AA	1239	A	C6-C5-N7	5.11	135.88	132.30
21	AA	1406	U	C1'-O4'-C4'	-5.11	105.81	109.90
54	BA	686	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	955	U	C1'-O4'-C4'	-5.11	105.81	109.90
54	BA	1861	G	C4'-C3'-C2'	-5.11	97.49	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2238	G	N3-C4-C5	-5.11	126.05	128.60
21	AA	730	G	N1-C6-O6	-5.11	116.84	119.90
21	AA	1300	G	C5-C6-N1	5.11	114.05	111.50
22	A1	9	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	1407	G	N1-C6-O6	-5.11	116.84	119.90
54	BA	1715	G	C5-C6-N1	5.11	114.05	111.50
54	BA	732	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	828	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	1480	C	O4'-C1'-N1	5.10	112.28	108.20
3	AD	183	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
15	AP	79	ASN	C-N-CA	5.10	134.46	121.70
21	AA	605	U	C5-C6-N1	-5.10	120.15	122.70
21	AA	1108	G	C5-C6-N1	5.10	114.05	111.50
54	BA	903	C	N1-C2-O2	5.10	121.96	118.90
54	BA	927	A	C6-C5-N7	5.10	135.87	132.30
54	BA	1313	U	C3'-C2'-C1'	5.10	105.58	101.50
54	BA	1388	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	1861	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	2004	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	1474	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	201	G	N3-C2-N2	-5.10	116.33	119.90
21	AA	251	G	C3'-C2'-C1'	5.10	105.58	101.50
21	AA	370	C	N1-C2-O2	5.10	121.96	118.90
21	AA	485	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	764	C	N1-C2-O2	5.10	121.96	118.90
21	AA	872	A	C4-C5-C6	-5.10	114.45	117.00
38	BP	87	ARG	NE-CZ-NH1	5.10	122.85	120.30
54	BA	168	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	2795	C	N1-C2-O2	5.10	121.96	118.90
21	AA	310	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	1465	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	143	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2317	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2764	A	C4-C5-C6	-5.10	114.45	117.00
25	BC	47	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
54	BA	44	A	O4'-C1'-N9	5.10	112.28	108.20
54	BA	2748	A	C6-C5-N7	5.10	135.87	132.30
21	AA	25	C	N1-C2-O2	5.09	121.96	118.90
21	AA	271	C	C3'-C2'-C1'	5.09	105.58	101.50
21	AA	799	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	1856	U	N3-C2-O2	-5.09	118.63	122.20
54	BA	2855	C	N3-C2-O2	-5.09	118.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1331	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	1695	G	C3'-C2'-C1'	5.09	105.57	101.50
21	AA	46	G	N3-C2-N2	-5.09	116.34	119.90
21	AA	220	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	1787	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	2000	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2558	C	N1-C2-O2	5.09	121.95	118.90
54	BA	747	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	796	C	N1-C2-O2	5.09	121.95	118.90
54	BA	803	U	N1-C2-N3	5.09	117.95	114.90
54	BA	2239	G	C5-C6-N1	5.09	114.05	111.50
54	BA	2683	C	O4'-C1'-N1	5.09	112.27	108.20
10	AK	92	ARG	NE-CZ-NH2	-5.09	117.76	120.30
54	BA	1606	C	N3-C4-C5	5.09	123.94	121.90
54	BA	2072	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2594	C	N1-C2-O2	5.09	121.95	118.90
55	BB	8	C	N1-C2-O2	5.09	121.95	118.90
33	BK	17	ARG	NE-CZ-NH1	5.09	122.84	120.30
54	BA	816	C	N1-C2-O2	5.09	121.95	118.90
54	BA	1852	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1879	C	N1-C2-O2	5.09	121.95	118.90
55	BB	28	C	O4'-C1'-N1	5.09	112.27	108.20
21	AA	553	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1339	G	N3-C2-N2	-5.08	116.34	119.90
54	BA	2305	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	242	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1195	G	N7-C8-N9	5.08	115.64	113.10
54	BA	1599	U	O4'-C1'-N1	5.08	112.27	108.20
54	BA	2063	C	N3-C4-C5	5.08	123.93	121.90
54	BA	2858	C	N1-C2-O2	5.08	121.95	118.90
13	AN	81	ARG	NE-CZ-NH2	-5.08	117.76	120.30
38	BP	71	ARG	NE-CZ-NH1	5.08	122.84	120.30
54	BA	633	A	O4'-C1'-N9	5.08	112.26	108.20
54	BA	679	C	O4'-C1'-N1	5.08	112.27	108.20
54	BA	771	G	O4'-C1'-N9	5.08	112.26	108.20
54	BA	1123	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2466	C	N3-C4-N4	-5.08	114.44	118.00
54	BA	1833	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	239	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	301	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1050	A	O4'-C1'-N9	5.08	112.26	108.20
54	BA	2355	G	C5'-C4'-O4'	5.08	115.19	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	525	U	N3-C2-O2	-5.08	118.65	122.20
54	BA	1901	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1909	C	O4'-C1'-N1	5.08	112.26	108.20
17	AR	60	ARG	NE-CZ-NH1	5.08	122.84	120.30
21	AA	290	C	N3-C2-O2	-5.08	118.35	121.90
21	AA	1057	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	1223	C	N3-C4-C5	5.08	123.93	121.90
54	BA	1230	A	C6-C5-N7	5.08	135.85	132.30
4	AE	137	ARG	NE-CZ-NH1	5.07	122.84	120.30
21	AA	744	C	O4'-C1'-N1	5.07	112.26	108.20
54	BA	531	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1096	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	1120	G	C5-C6-N1	5.07	114.04	111.50
54	BA	1985	C	N1-C2-O2	5.07	121.94	118.90
54	BA	2199	A	C6-C5-N7	5.07	135.85	132.30
54	BA	2570	G	O4'-C1'-N9	5.07	112.26	108.20
54	BA	2819	G	C8-N9-C4	-5.07	104.37	106.40
55	BB	94	A	C6-C5-N7	5.07	135.85	132.30
21	AA	711	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2405	G	C5-C6-N1	5.07	114.04	111.50
21	AA	349	A	C6-C5-N7	5.07	135.85	132.30
21	AA	1303	C	N1-C2-O2	5.07	121.94	118.90
54	BA	974	G	N3-C2-N2	-5.07	116.35	119.90
54	BA	1483	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2506	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	672	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1340	U	P-O3'-C3'	5.07	125.78	119.70
21	AA	124	C	N1-C2-O2	5.07	121.94	118.90
54	BA	269	C	N1-C2-O2	5.07	121.94	118.90
54	BA	2063	C	O4'-C1'-N1	5.07	112.25	108.20
21	AA	1426	G	N3-C2-N2	-5.07	116.35	119.90
42	BT	76	ARG	NE-CZ-NH1	5.07	122.83	120.30
54	BA	181	A	C6-C5-N7	5.07	135.84	132.30
54	BA	678	C	N1-C2-O2	5.07	121.94	118.90
54	BA	865	C	N3-C4-C5	5.07	123.93	121.90
54	BA	939	G	C5-C6-N1	5.07	114.03	111.50
54	BA	2197	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	2622	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	2845	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2022	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	2736	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	131	A	C6-C5-N7	5.06	135.84	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	468	A	C1'-O4'-C4'	-5.06	105.85	109.90
21	AA	593	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1104	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2236	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2870	C	N1-C2-O2	5.06	121.94	118.90
21	AA	173	U	C1'-O4'-C4'	-5.06	105.85	109.90
21	AA	882	C	O4'-C1'-N1	5.06	112.25	108.20
21	AA	965	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	1378	C	N1-C2-O2	5.06	121.94	118.90
54	BA	179	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1864	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	2499	C	N3-C4-C5	5.06	123.92	121.90
55	BB	70	C	C5'-C4'-O4'	5.06	115.17	109.10
21	AA	1162	C	N1-C2-O2	5.06	121.93	118.90
21	AA	1512	U	N3-C2-O2	-5.06	118.66	122.20
45	BW	19	ARG	NE-CZ-NH2	-5.06	117.77	120.30
54	BA	1990	C	N1-C2-O2	5.06	121.93	118.90
21	AA	427	U	N3-C2-O2	-5.05	118.66	122.20
21	AA	948	C	C5'-C4'-O4'	5.05	115.17	109.10
24	A3	45	A	O4'-C1'-N9	5.05	112.24	108.20
54	BA	1227	G	C5-C6-N1	5.05	114.03	111.50
54	BA	2085	U	C5-C6-N1	-5.05	120.17	122.70
54	BA	2282	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	281	G	C3'-C2'-C1'	5.05	105.54	101.50
21	AA	493	A	C2-N3-C4	5.05	113.13	110.60
21	AA	1504	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	875	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	2372	U	C3'-C2'-C1'	-5.05	97.46	101.50
21	AA	200	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	545	C	N1-C2-O2	5.05	121.93	118.90
54	BA	364	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2250	G	C5-C6-N1	5.05	114.03	111.50
55	BB	71	C	O4'-C1'-N1	5.05	112.24	108.20
21	AA	526	C	N1-C2-O2	5.05	121.93	118.90
54	BA	640	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1140	C	C5'-C4'-O4'	5.05	115.16	109.10
54	BA	2385	C	N1-C2-O2	5.05	121.93	118.90
54	BA	497	A	C6-C5-N7	5.05	135.83	132.30
54	BA	1892	C	C6-N1-C2	-5.05	118.28	120.30
54	BA	2263	C	N1-C2-O2	5.05	121.93	118.90
54	BA	2759	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	1228	C	O4'-C1'-N1	5.04	112.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	14	A	C4-C5-C6	-5.04	114.48	117.00
24	A3	45	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1133	A	O4'-C1'-N9	5.04	112.24	108.20
21	AA	278	G	N1-C6-O6	-5.04	116.87	119.90
54	BA	197	A	C6-C5-N7	5.04	135.83	132.30
54	BA	988	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	2677	G	N1-C6-O6	-5.04	116.87	119.90
21	AA	40	C	N1-C2-O2	5.04	121.92	118.90
21	AA	495	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	538	G	N1-C6-O6	-5.04	116.88	119.90
21	AA	680	C	C1'-O4'-C4'	-5.04	105.87	109.90
21	AA	905	U	N3-C2-O2	-5.04	118.67	122.20
21	AA	1362	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1678	A	C6-C5-N7	5.04	135.83	132.30
21	AA	1231	G	N3-C2-N2	-5.04	116.37	119.90
21	AA	1443	C	N1-C2-O2	5.04	121.92	118.90
21	AA	429	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	819	A	C6-C5-N7	5.04	135.83	132.30
21	AA	923	A	C5'-C4'-C3'	-5.04	107.94	116.00
54	BA	552	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	765	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	295	C	N1-C2-O2	5.04	121.92	118.90
21	AA	583	A	C6-C5-N7	5.04	135.82	132.30
21	AA	821	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	772	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	1455	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	1531	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	1643	G	O4'-C1'-N9	5.04	112.23	108.20
11	AL	94	TYR	CB-CG-CD2	-5.03	117.98	121.00
21	AA	814	A	C6-C5-N7	5.03	135.82	132.30
21	AA	1494	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	522	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1366	A	C6-C5-N7	5.03	135.82	132.30
54	BA	646	U	N1-C2-N3	5.03	117.92	114.90
21	AA	927	G	C5'-C4'-O4'	5.03	115.14	109.10
21	AA	1161	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	188	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	691	C	N3-C2-O2	-5.03	118.38	121.90
54	BA	1992	G	N3-C2-N2	-5.03	116.38	119.90
54	BA	2417	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	2739	U	O4'-C1'-N1	5.03	112.22	108.20
21	AA	217	C	N1-C2-O2	5.03	121.92	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	318	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	1880	U	O4'-C1'-N1	5.03	112.22	108.20
2	AC	106	ARG	NE-CZ-NH1	5.03	122.81	120.30
24	A3	10	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	211	C	N1-C2-O2	5.03	121.92	118.90
54	BA	374	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	773	U	C5-C6-N1	-5.03	120.19	122.70
54	BA	1296	G	N3-C2-N2	-5.03	116.38	119.90
54	BA	1404	C	N1-C2-O2	5.03	121.92	118.90
21	AA	5	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	213	G	O4'-C1'-N9	5.03	112.22	108.20
21	AA	858	G	N1-C6-O6	-5.03	116.89	119.90
22	A1	43	G	C5-C6-N1	5.03	114.01	111.50
54	BA	461	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1119	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1352	U	C5'-C4'-O4'	5.03	115.13	109.10
54	BA	2682	A	C6-C5-N7	5.03	135.82	132.30
21	AA	78	A	C6-C5-N7	5.02	135.82	132.30
21	AA	796	C	N1-C2-O2	5.02	121.92	118.90
54	BA	479	A	C3'-C2'-C1'	-5.02	97.48	101.50
54	BA	1274	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	1351	C	N3-C4-N4	-5.02	114.48	118.00
21	AA	426	U	C5-C6-N1	-5.02	120.19	122.70
21	AA	920	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	588	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	970	U	C5'-C4'-O4'	5.02	115.13	109.10
54	BA	1209	U	N3-C2-O2	-5.02	118.68	122.20
21	AA	35	G	O3'-P-O5'	-5.02	94.46	104.00
22	A1	17	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	68	G	C5-C6-N1	5.02	114.01	111.50
21	AA	658	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1069	A	C6-C5-N7	5.02	135.81	132.30
54	BA	1191	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	1197	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	1585	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1818	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	2226	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	2244	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	108	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	869	G	C5-C6-N1	5.02	114.01	111.50
21	AA	982	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	81	G	O4'-C1'-N9	5.02	112.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	389	G	P-O3'-C3'	5.02	125.72	119.70
54	BA	787	C	N3-C4-N4	-5.02	114.49	118.00
21	AA	501	C	N3-C4-C5	5.02	123.91	121.90
21	AA	729	A	C6-C5-N7	5.02	135.81	132.30
54	BA	867	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	1305	C	N3-C4-C5	5.02	123.91	121.90
55	BB	2	G	N3-C4-C5	-5.02	126.09	128.60
1	AB	112	ARG	CD-NE-CZ	5.01	130.62	123.60
21	AA	637	C	N1-C2-O2	5.01	121.91	118.90
21	AA	800	G	N1-C6-O6	-5.01	116.89	119.90
27	BE	162	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	398	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1005	C	C6-N1-C2	-5.01	118.29	120.30
21	AA	561	U	C5-C6-N1	-5.01	120.19	122.70
54	BA	800	A	C6-C5-N7	5.01	135.81	132.30
54	BA	2365	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	1300	G	C1'-O4'-C4'	-5.01	105.89	109.90
54	BA	1068	G	N3-C4-C5	-5.01	126.09	128.60
54	BA	1974	C	O4'-C1'-N1	5.01	112.21	108.20
21	AA	961	U	N3-C2-O2	-5.01	118.69	122.20
21	AA	1405	G	N1-C6-O6	-5.01	116.89	119.90
36	BN	63	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	1832	C	N1-C2-O2	5.01	121.91	118.90
54	BA	2902	C	O4'-C1'-N1	5.01	112.21	108.20
21	AA	567	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	840	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1247	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	2018	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	122	G	O4'-C1'-N9	5.01	112.20	108.20
21	AA	149	A	C5-C6-N1	5.01	120.20	117.70
21	AA	802	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	639	U	C3'-C2'-C1'	5.01	105.50	101.50
54	BA	2370	G	N1-C6-O6	-5.01	116.90	119.90
55	BB	10	G	O4'-C1'-N9	5.01	112.21	108.20
54	BA	295	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	1307	A	C4-C5-C6	-5.00	114.50	117.00
54	BA	2601	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	206	C	N1-C2-O2	5.00	121.90	118.90
21	AA	1168	U	N3-C2-O2	-5.00	118.70	122.20
21	AA	1299	A	C4-C5-C6	-5.00	114.50	117.00
54	BA	1357	C	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1798	U	O4'-C1'-N1	5.00	112.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2525	G	N3-C2-N2	-5.00	116.40	119.90
21	AA	224	U	N3-C2-O2	-5.00	118.70	122.20
21	AA	1503	A	C6-C5-N7	5.00	135.80	132.30
22	A1	76	A	C8-N9-C4	-5.00	103.80	105.80
24	A3	7	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	408	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	481	G	C3'-C2'-C1'	5.00	105.50	101.50
54	BA	2115	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	2269	G	C5-C6-N1	5.00	114.00	111.50
55	BB	67	G	N3-C4-C5	-5.00	126.10	128.60

There are no chirality outliers.

All (1147) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	1	G	Sidechain
22	A1	11	C	Sidechain
22	A1	24	G	Sidechain
22	A1	3	G	Sidechain
22	A1	32	C	Sidechain
22	A1	33	U	Sidechain
22	A1	36	C	Sidechain
22	A1	38	A	Sidechain
22	A1	44	G	Sidechain
22	A1	49	G	Sidechain
22	A1	52	G	Sidechain
22	A1	6	A	Sidechain
22	A1	60	C	Sidechain
22	A1	63	G	Sidechain
22	A1	64	U	Sidechain
22	A1	65	C	Sidechain
22	A1	67	U	Sidechain
22	A1	71	C	Sidechain
22	A1	75	C	Sidechain
22	A1	76	A	Sidechain
22	A1	9	A	Sidechain
23	A2	80	C	Sidechain
23	A2	83	U	Sidechain
23	A2	86	U	Sidechain
23	A2	89	U	Sidechain
24	A3	1	C	Sidechain
24	A3	15	G	Sidechain

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Mol	Chain	Res	Type	Group
24	A3	17	C	Sidechain
24	A3	2	G	Sidechain
24	A3	28	U	Sidechain
24	A3	32	G	Sidechain
24	A3	35	C	Sidechain
24	A3	38	A	Sidechain
24	A3	42	C	Sidechain
24	A3	50	G	Sidechain
24	A3	61	U	Sidechain
24	A3	7	G	Sidechain
24	A3	71	G	Sidechain
24	A3	74	A	Sidechain
24	A3	75	C	Sidechain
24	A3	76	C	Sidechain
21	AA	100	G	Sidechain
21	AA	1010	U	Sidechain
21	AA	1013	G	Sidechain
21	AA	1025	U	Sidechain
21	AA	1028	C	Sidechain
21	AA	1029	U	Sidechain
21	AA	1038	C	Sidechain
21	AA	1044	A	Sidechain
21	AA	1046	A	Sidechain
21	AA	1048	G	Sidechain
21	AA	1053	G	Sidechain
21	AA	1054	C	Sidechain
21	AA	1066	C	Sidechain
21	AA	1075	U	Sidechain
21	AA	109	A	Sidechain
21	AA	1093	A	Sidechain
21	AA	1097	C	Sidechain
21	AA	110	C	Sidechain
21	AA	1108	G	Sidechain
21	AA	111	G	Sidechain
21	AA	1114	C	Sidechain
21	AA	1116	U	Sidechain
21	AA	1117	A	Sidechain
21	AA	1118	U	Sidechain
21	AA	1122	U	Sidechain
21	AA	1127	G	Sidechain
21	AA	1130	A	Sidechain
21	AA	1131	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1132	C	Sidechain
21	AA	1134	G	Sidechain
21	AA	1137	C	Sidechain
21	AA	1138	G	Sidechain
21	AA	1139	G	Sidechain
21	AA	114	U	Sidechain
21	AA	1140	C	Sidechain
21	AA	1142	G	Sidechain
21	AA	1144	G	Sidechain
21	AA	1149	C	Sidechain
21	AA	1155	A	Sidechain
21	AA	1162	C	Sidechain
21	AA	1177	G	Sidechain
21	AA	1178	G	Sidechain
21	AA	1189	U	Sidechain
21	AA	1193	G	Sidechain
21	AA	1200	C	Sidechain
21	AA	1206	G	Sidechain
21	AA	1207	G	Sidechain
21	AA	1211	U	Sidechain
21	AA	1212	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1214	C	Sidechain
21	AA	1216	A	Sidechain
21	AA	1217	C	Sidechain
21	AA	1218	C	Sidechain
21	AA	122	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1225	A	Sidechain
21	AA	1229	A	Sidechain
21	AA	1237	C	Sidechain
21	AA	1246	A	Sidechain
21	AA	1249	C	Sidechain
21	AA	1253	G	Sidechain
21	AA	126	G	Sidechain
21	AA	1260	G	Sidechain
21	AA	1263	C	Sidechain
21	AA	1267	C	Sidechain
21	AA	1269	A	Sidechain
21	AA	1273	C	Sidechain
21	AA	1274	A	Sidechain
21	AA	1278	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1299	A	Sidechain
21	AA	1300	G	Sidechain
21	AA	1302	C	Sidechain
21	AA	1305	G	Sidechain
21	AA	1312	G	Sidechain
21	AA	1321	U	Sidechain
21	AA	1324	A	Sidechain
21	AA	1328	C	Sidechain
21	AA	133	U	Sidechain
21	AA	1330	U	Sidechain
21	AA	1343	G	Sidechain
21	AA	1346	A	Sidechain
21	AA	1351	U	Sidechain
21	AA	1356	G	Sidechain
21	AA	1358	U	Sidechain
21	AA	1360	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	1366	C	Sidechain
21	AA	1370	G	Sidechain
21	AA	1372	U	Sidechain
21	AA	1380	U	Sidechain
21	AA	1381	U	Sidechain
21	AA	1382	C	Sidechain
21	AA	1385	G	Sidechain
21	AA	1391	U	Sidechain
21	AA	1392	G	Sidechain
21	AA	1397	C	Sidechain
21	AA	1398	A	Sidechain
21	AA	14	U	Sidechain
21	AA	1400	C	Sidechain
21	AA	1401	G	Sidechain
21	AA	1402	C	Sidechain
21	AA	1407	C	Sidechain
21	AA	1409	C	Sidechain
21	AA	1413	A	Sidechain
21	AA	1414	U	Sidechain
21	AA	1415	G	Sidechain
21	AA	1421	G	Sidechain
21	AA	1424	U	Sidechain
21	AA	1426	G	Sidechain
21	AA	1435	G	Sidechain
21	AA	1438	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	144	G	Sidechain
21	AA	1444	U	Sidechain
21	AA	1451	U	Sidechain
21	AA	1461	G	Sidechain
21	AA	1468	A	Sidechain
21	AA	1473	G	Sidechain
21	AA	1474	U	Sidechain
21	AA	1477	U	Sidechain
21	AA	1482	G	Sidechain
21	AA	1484	C	Sidechain
21	AA	1487	G	Sidechain
21	AA	15	G	Sidechain
21	AA	1500	A	Sidechain
21	AA	1502	A	Sidechain
21	AA	1503	A	Sidechain
21	AA	1505	G	Sidechain
21	AA	1509	C	Sidechain
21	AA	1511	G	Sidechain
21	AA	1513	A	Sidechain
21	AA	1515	G	Sidechain
21	AA	1519	A	Sidechain
21	AA	1526	G	Sidechain
21	AA	1527	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1530	G	Sidechain
21	AA	1533	C	Sidechain
21	AA	1534	A	Sidechain
21	AA	159	G	Sidechain
21	AA	161	A	Sidechain
21	AA	162	A	Sidechain
21	AA	164	G	Sidechain
21	AA	167	A	Sidechain
21	AA	17	U	Sidechain
21	AA	172	A	Sidechain
21	AA	173	U	Sidechain
21	AA	186	C	Sidechain
21	AA	187	G	Sidechain
21	AA	190	A	Sidechain
21	AA	198	G	Sidechain
21	AA	200	G	Sidechain
21	AA	207	C	Sidechain
21	AA	208	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	210	C	Sidechain
21	AA	215	C	Sidechain
21	AA	217	C	Sidechain
21	AA	220	G	Sidechain
21	AA	225	C	Sidechain
21	AA	233	C	Sidechain
21	AA	234	C	Sidechain
21	AA	235	C	Sidechain
21	AA	237	G	Sidechain
21	AA	241	G	Sidechain
21	AA	242	G	Sidechain
21	AA	244	U	Sidechain
21	AA	25	C	Sidechain
21	AA	250	A	Sidechain
21	AA	255	G	Sidechain
21	AA	265	G	Sidechain
21	AA	269	C	Sidechain
21	AA	273	U	Sidechain
21	AA	280	C	Sidechain
21	AA	281	G	Sidechain
21	AA	29	U	Sidechain
21	AA	292	G	Sidechain
21	AA	295	C	Sidechain
21	AA	298	A	Sidechain
21	AA	299	G	Sidechain
21	AA	305	G	Sidechain
21	AA	307	C	Sidechain
21	AA	310	G	Sidechain
21	AA	312	C	Sidechain
21	AA	317	U	Sidechain
21	AA	324	G	Sidechain
21	AA	33	A	Sidechain
21	AA	336	A	Sidechain
21	AA	337	G	Sidechain
21	AA	343	U	Sidechain
21	AA	347	G	Sidechain
21	AA	35	G	Sidechain
21	AA	350	G	Sidechain
21	AA	356	A	Sidechain
21	AA	359	G	Sidechain
21	AA	36	C	Sidechain
21	AA	361	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	367	U	Sidechain
21	AA	370	C	Sidechain
21	AA	372	C	Sidechain
21	AA	375	U	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	387	U	Sidechain
21	AA	388	G	Sidechain
21	AA	391	G	Sidechain
21	AA	398	U	Sidechain
21	AA	399	G	Sidechain
21	AA	404	G	Sidechain
21	AA	407	U	Sidechain
21	AA	413	G	Sidechain
21	AA	414	A	Sidechain
21	AA	419	C	Sidechain
21	AA	430	A	Sidechain
21	AA	436	C	Sidechain
21	AA	443	C	Sidechain
21	AA	446	G	Sidechain
21	AA	451	A	Sidechain
21	AA	455	G	Sidechain
21	AA	472	U	Sidechain
21	AA	478	A	Sidechain
21	AA	479	U	Sidechain
21	AA	481	G	Sidechain
21	AA	484	G	Sidechain
21	AA	485	U	Sidechain
21	AA	487	A	Sidechain
21	AA	491	G	Sidechain
21	AA	492	C	Sidechain
21	AA	493	A	Sidechain
21	AA	5	U	Sidechain
21	AA	506	G	Sidechain
21	AA	51	A	Sidechain
21	AA	513	C	Sidechain
21	AA	517	G	Sidechain
21	AA	519	C	Sidechain
21	AA	525	C	Sidechain
21	AA	529	G	Sidechain
21	AA	532	A	Sidechain
21	AA	546	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	55	A	Sidechain
21	AA	550	G	Sidechain
21	AA	554	A	Sidechain
21	AA	555	U	Sidechain
21	AA	558	G	Sidechain
21	AA	561	U	Sidechain
21	AA	565	U	Sidechain
21	AA	571	U	Sidechain
21	AA	572	A	Sidechain
21	AA	573	A	Sidechain
21	AA	581	G	Sidechain
21	AA	585	G	Sidechain
21	AA	595	A	Sidechain
21	AA	600	A	Sidechain
21	AA	604	G	Sidechain
21	AA	610	U	Sidechain
21	AA	611	C	Sidechain
21	AA	612	C	Sidechain
21	AA	622	A	Sidechain
21	AA	627	G	Sidechain
21	AA	628	G	Sidechain
21	AA	630	A	Sidechain
21	AA	635	A	Sidechain
21	AA	641	U	Sidechain
21	AA	642	A	Sidechain
21	AA	646	G	Sidechain
21	AA	650	G	Sidechain
21	AA	660	C	Sidechain
21	AA	661	G	Sidechain
21	AA	663	A	Sidechain
21	AA	666	G	Sidechain
21	AA	670	G	Sidechain
21	AA	675	A	Sidechain
21	AA	678	U	Sidechain
21	AA	682	G	Sidechain
21	AA	684	U	Sidechain
21	AA	685	G	Sidechain
21	AA	687	A	Sidechain
21	AA	689	C	Sidechain
21	AA	691	G	Sidechain
21	AA	693	G	Sidechain
21	AA	699	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	7	A	Sidechain
21	AA	701	U	Sidechain
21	AA	703	G	Sidechain
21	AA	704	A	Sidechain
21	AA	71	A	Sidechain
21	AA	712	A	Sidechain
21	AA	719	C	Sidechain
21	AA	720	C	Sidechain
21	AA	721	G	Sidechain
21	AA	732	C	Sidechain
21	AA	740	U	Sidechain
21	AA	741	G	Sidechain
21	AA	745	G	Sidechain
21	AA	750	C	Sidechain
21	AA	751	U	Sidechain
21	AA	752	G	Sidechain
21	AA	76	G	Sidechain
21	AA	760	G	Sidechain
21	AA	762	U	Sidechain
21	AA	765	G	Sidechain
21	AA	768	A	Sidechain
21	AA	769	G	Sidechain
21	AA	770	C	Sidechain
21	AA	771	G	Sidechain
21	AA	787	A	Sidechain
21	AA	791	G	Sidechain
21	AA	797	C	Sidechain
21	AA	8	A	Sidechain
21	AA	800	G	Sidechain
21	AA	802	A	Sidechain
21	AA	81	A	Sidechain
21	AA	812	G	Sidechain
21	AA	821	G	Sidechain
21	AA	822	U	Sidechain
21	AA	827	U	Sidechain
21	AA	828	U	Sidechain
21	AA	829	G	Sidechain
21	AA	83	C	Sidechain
21	AA	832	G	Sidechain
21	AA	833	G	Sidechain
21	AA	843	U	Sidechain
21	AA	852	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	86	G	Sidechain
21	AA	863	U	Sidechain
21	AA	869	G	Sidechain
21	AA	87	C	Sidechain
21	AA	870	U	Sidechain
21	AA	871	U	Sidechain
21	AA	873	A	Sidechain
21	AA	880	C	Sidechain
21	AA	887	G	Sidechain
21	AA	888	G	Sidechain
21	AA	898	G	Sidechain
21	AA	900	A	Sidechain
21	AA	907	A	Sidechain
21	AA	909	A	Sidechain
21	AA	913	A	Sidechain
21	AA	914	A	Sidechain
21	AA	917	G	Sidechain
21	AA	918	A	Sidechain
21	AA	920	U	Sidechain
21	AA	923	A	Sidechain
21	AA	927	G	Sidechain
21	AA	93	U	Sidechain
21	AA	932	C	Sidechain
21	AA	933	G	Sidechain
21	AA	938	A	Sidechain
21	AA	939	G	Sidechain
21	AA	94	G	Sidechain
21	AA	941	G	Sidechain
21	AA	944	G	Sidechain
21	AA	948	C	Sidechain
21	AA	949	A	Sidechain
21	AA	954	G	Sidechain
21	AA	956	U	Sidechain
21	AA	960	U	Sidechain
21	AA	970	C	Sidechain
21	AA	973	G	Sidechain
21	AA	976	G	Sidechain
21	AA	978	A	Sidechain
21	AA	982	U	Sidechain
21	AA	983	A	Sidechain
21	AA	984	C	Sidechain
21	AA	988	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	989	U	Sidechain
21	AA	99	C	Sidechain
21	AA	990	C	Sidechain
21	AA	998	C	Sidechain
1	AB	224	ARG	Sidechain
4	AE	22	LYS	Peptide
14	AO	48	ASP	Peptide
14	AO	68	TYR	Sidechain
49	B0	48	TYR	Sidechain
54	BA	100	U	Sidechain
54	BA	1000	A	Sidechain
54	BA	1009	A	Sidechain
54	BA	1013	C	Sidechain
54	BA	1016	G	Sidechain
54	BA	1022	G	Sidechain
54	BA	1026	G	Sidechain
54	BA	1027	A	Sidechain
54	BA	1028	A	Sidechain
54	BA	1030	C	Sidechain
54	BA	104	A	Sidechain
54	BA	1044	C	Sidechain
54	BA	1045	C	Sidechain
54	BA	1046	A	Sidechain
54	BA	1047	G	Sidechain
54	BA	1051	G	Sidechain
54	BA	1052	C	Sidechain
54	BA	1053	C	Sidechain
54	BA	1054	A	Sidechain
54	BA	1056	G	Sidechain
54	BA	1063	G	Sidechain
54	BA	1068	G	Sidechain
54	BA	107	G	Sidechain
54	BA	1071	G	Sidechain
54	BA	1074	G	Sidechain
54	BA	1075	C	Sidechain
54	BA	1076	C	Sidechain
54	BA	1083	U	Sidechain
54	BA	1090	A	Sidechain
54	BA	1093	G	Sidechain
54	BA	1099	G	Sidechain
54	BA	1108	U	Sidechain
54	BA	1111	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1115	G	Sidechain
54	BA	1121	C	Sidechain
54	BA	1129	A	Sidechain
54	BA	1135	C	Sidechain
54	BA	1139	G	Sidechain
54	BA	1142	A	Sidechain
54	BA	115	C	Sidechain
54	BA	1151	A	Sidechain
54	BA	1152	C	Sidechain
54	BA	1163	G	Sidechain
54	BA	1170	C	Sidechain
54	BA	1175	A	Sidechain
54	BA	1177	G	Sidechain
54	BA	1179	G	Sidechain
54	BA	1184	U	Sidechain
54	BA	1185	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1188	U	Sidechain
54	BA	1192	G	Sidechain
54	BA	1195	G	Sidechain
54	BA	1198	U	Sidechain
54	BA	1200	C	Sidechain
54	BA	1221	C	Sidechain
54	BA	1223	G	Sidechain
54	BA	1236	G	Sidechain
54	BA	124	G	Sidechain
54	BA	1244	A	Sidechain
54	BA	1254	A	Sidechain
54	BA	126	A	Sidechain
54	BA	1264	A	Sidechain
54	BA	1269	A	Sidechain
54	BA	1270	C	Sidechain
54	BA	1271	G	Sidechain
54	BA	1272	A	Sidechain
54	BA	1273	U	Sidechain
54	BA	1277	G	Sidechain
54	BA	1281	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	1287	A	Sidechain
54	BA	1299	G	Sidechain
54	BA	130	C	Sidechain
54	BA	1303	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1307	A	Sidechain
54	BA	1308	A	Sidechain
54	BA	1312	U	Sidechain
54	BA	1315	C	Sidechain
54	BA	1317	G	Sidechain
54	BA	1319	C	Sidechain
54	BA	1320	C	Sidechain
54	BA	1323	C	Sidechain
54	BA	1326	U	Sidechain
54	BA	1329	U	Sidechain
54	BA	1330	C	Sidechain
54	BA	1332	G	Sidechain
54	BA	1336	A	Sidechain
54	BA	1338	G	Sidechain
54	BA	1345	C	Sidechain
54	BA	1346	G	Sidechain
54	BA	1356	G	Sidechain
54	BA	1359	A	Sidechain
54	BA	136	G	Sidechain
54	BA	1360	G	Sidechain
54	BA	1361	G	Sidechain
54	BA	1362	C	Sidechain
54	BA	1366	A	Sidechain
54	BA	1373	A	Sidechain
54	BA	1376	C	Sidechain
54	BA	1388	G	Sidechain
54	BA	1392	A	Sidechain
54	BA	1393	A	Sidechain
54	BA	1399	C	Sidechain
54	BA	1410	G	Sidechain
54	BA	1416	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1429	G	Sidechain
54	BA	1435	G	Sidechain
54	BA	1438	U	Sidechain
54	BA	1445	G	Sidechain
54	BA	1457	U	Sidechain
54	BA	146	A	Sidechain
54	BA	1460	U	Sidechain
54	BA	1465	G	Sidechain
54	BA	1471	G	Sidechain
54	BA	1477	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1484	U	Sidechain
54	BA	1488	C	Sidechain
54	BA	1489	C	Sidechain
54	BA	1490	A	Sidechain
54	BA	1492	G	Sidechain
54	BA	1498	C	Sidechain
54	BA	15	G	Sidechain
54	BA	150	U	Sidechain
54	BA	1502	A	Sidechain
54	BA	1504	A	Sidechain
54	BA	1505	A	Sidechain
54	BA	1508	A	Sidechain
54	BA	1510	G	Sidechain
54	BA	152	A	Sidechain
54	BA	1522	A	Sidechain
54	BA	1525	A	Sidechain
54	BA	1535	A	Sidechain
54	BA	1543	G	Sidechain
54	BA	1546	G	Sidechain
54	BA	1548	A	Sidechain
54	BA	1551	A	Sidechain
54	BA	1553	A	Sidechain
54	BA	1555	G	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1565	C	Sidechain
54	BA	1567	G	Sidechain
54	BA	1569	A	Sidechain
54	BA	1573	G	Sidechain
54	BA	1580	A	Sidechain
54	BA	1584	U	Sidechain
54	BA	1595	C	Sidechain
54	BA	1599	U	Sidechain
54	BA	1600	C	Sidechain
54	BA	1601	G	Sidechain
54	BA	1606	C	Sidechain
54	BA	1612	C	Sidechain
54	BA	1615	C	Sidechain
54	BA	1616	A	Sidechain
54	BA	1620	G	Sidechain
54	BA	1621	U	Sidechain
54	BA	1622	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1623	G	Sidechain
54	BA	1627	G	Sidechain
54	BA	1628	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1633	G	Sidechain
54	BA	1634	A	Sidechain
54	BA	1635	A	Sidechain
54	BA	164	C	Sidechain
54	BA	1644	C	Sidechain
54	BA	1651	G	Sidechain
54	BA	1653	G	Sidechain
54	BA	1654	A	Sidechain
54	BA	1657	U	Sidechain
54	BA	1659	G	Sidechain
54	BA	1672	A	Sidechain
54	BA	1673	G	Sidechain
54	BA	1674	G	Sidechain
54	BA	168	G	Sidechain
54	BA	1680	U	Sidechain
54	BA	1682	G	Sidechain
54	BA	1683	U	Sidechain
54	BA	1686	C	Sidechain
54	BA	1697	G	Sidechain
54	BA	1699	G	Sidechain
54	BA	1703	G	Sidechain
54	BA	1705	A	Sidechain
54	BA	1707	G	Sidechain
54	BA	1708	C	Sidechain
54	BA	1713	A	Sidechain
54	BA	1716	U	Sidechain
54	BA	1719	G	Sidechain
54	BA	1721	G	Sidechain
54	BA	1724	G	Sidechain
54	BA	1725	U	Sidechain
54	BA	1729	U	Sidechain
54	BA	1735	A	Sidechain
54	BA	1736	U	Sidechain
54	BA	1737	G	Sidechain
54	BA	1738	G	Sidechain
54	BA	1740	G	Sidechain
54	BA	1743	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1746	A	Sidechain
54	BA	1748	C	Sidechain
54	BA	1753	G	Sidechain
54	BA	1758	U	Sidechain
54	BA	1762	A	Sidechain
54	BA	1767	G	Sidechain
54	BA	1774	C	Sidechain
54	BA	1781	U	Sidechain
54	BA	1790	C	Sidechain
54	BA	1796	U	Sidechain
54	BA	180	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1803	A	Sidechain
54	BA	1804	C	Sidechain
54	BA	1809	A	Sidechain
54	BA	1823	G	Sidechain
54	BA	1828	G	Sidechain
54	BA	1835	G	Sidechain
54	BA	1837	C	Sidechain
54	BA	1840	G	Sidechain
54	BA	1841	U	Sidechain
54	BA	1842	G	Sidechain
54	BA	1847	A	Sidechain
54	BA	1854	A	Sidechain
54	BA	1857	G	Sidechain
54	BA	1865	U	Sidechain
54	BA	1869	G	Sidechain
54	BA	1876	A	Sidechain
54	BA	1884	G	Sidechain
54	BA	1886	U	Sidechain
54	BA	1889	A	Sidechain
54	BA	189	G	Sidechain
54	BA	1890	A	Sidechain
54	BA	1891	G	Sidechain
54	BA	19	A	Sidechain
54	BA	190	A	Sidechain
54	BA	1908	C	Sidechain
54	BA	191	A	Sidechain
54	BA	1910	G	Sidechain
54	BA	1918	A	Sidechain
54	BA	1922	G	Sidechain
54	BA	1927	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1928	A	Sidechain
54	BA	1931	U	Sidechain
54	BA	1932	A	Sidechain
54	BA	1939	U	Sidechain
54	BA	1940	U	Sidechain
54	BA	1944	U	Sidechain
54	BA	1948	G	Sidechain
54	BA	1950	G	Sidechain
54	BA	1958	C	Sidechain
54	BA	1959	G	Sidechain
54	BA	1962	C	Sidechain
54	BA	197	A	Sidechain
54	BA	1973	G	Sidechain
54	BA	1976	U	Sidechain
54	BA	198	C	Sidechain
54	BA	1982	U	Sidechain
54	BA	1983	G	Sidechain
54	BA	1993	U	Sidechain
54	BA	1995	U	Sidechain
54	BA	1996	C	Sidechain
54	BA	20	C	Sidechain
54	BA	200	U	Sidechain
54	BA	2005	A	Sidechain
54	BA	2007	U	Sidechain
54	BA	2014	A	Sidechain
54	BA	2015	A	Sidechain
54	BA	2019	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2022	U	Sidechain
54	BA	2031	A	Sidechain
54	BA	2033	A	Sidechain
54	BA	2034	U	Sidechain
54	BA	2037	A	Sidechain
54	BA	2040	G	Sidechain
54	BA	2041	U	Sidechain
54	BA	2052	A	Sidechain
54	BA	206	U	Sidechain
54	BA	2061	G	Sidechain
54	BA	2064	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	2069	G	Sidechain
54	BA	2073	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2075	U	Sidechain
54	BA	2083	G	Sidechain
54	BA	2087	G	Sidechain
54	BA	2092	U	Sidechain
54	BA	210	C	Sidechain
54	BA	2103	C	Sidechain
54	BA	2104	C	Sidechain
54	BA	2113	U	Sidechain
54	BA	2114	A	Sidechain
54	BA	2117	A	Sidechain
54	BA	2121	G	Sidechain
54	BA	2130	U	Sidechain
54	BA	2135	A	Sidechain
54	BA	2139	U	Sidechain
54	BA	214	G	Sidechain
54	BA	215	G	Sidechain
54	BA	2152	G	Sidechain
54	BA	2155	U	Sidechain
54	BA	2157	G	Sidechain
54	BA	2161	C	Sidechain
54	BA	2163	A	Sidechain
54	BA	2165	C	Sidechain
54	BA	2166	U	Sidechain
54	BA	2168	G	Sidechain
54	BA	2169	A	Sidechain
54	BA	217	A	Sidechain
54	BA	2172	U	Sidechain
54	BA	2175	C	Sidechain
54	BA	2176	A	Sidechain
54	BA	218	A	Sidechain
54	BA	2196	C	Sidechain
54	BA	2197	U	Sidechain
54	BA	22	C	Sidechain
54	BA	2201	G	Sidechain
54	BA	2204	G	Sidechain
54	BA	2207	C	Sidechain
54	BA	2208	C	Sidechain
54	BA	2224	G	Sidechain
54	BA	2233	U	Sidechain
54	BA	2236	U	Sidechain
54	BA	2240	U	Sidechain
54	BA	2244	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2245	U	Sidechain
54	BA	2253	G	Sidechain
54	BA	2259	U	Sidechain
54	BA	2272	U	Sidechain
54	BA	2273	A	Sidechain
54	BA	2274	A	Sidechain
54	BA	2276	G	Sidechain
54	BA	228	C	Sidechain
54	BA	2282	G	Sidechain
54	BA	2289	G	Sidechain
54	BA	2299	U	Sidechain
54	BA	2300	C	Sidechain
54	BA	2306	C	Sidechain
54	BA	2308	G	Sidechain
54	BA	2310	C	Sidechain
54	BA	2312	U	Sidechain
54	BA	2321	U	Sidechain
54	BA	2323	G	Sidechain
54	BA	2324	U	Sidechain
54	BA	2327	A	Sidechain
54	BA	2332	C	Sidechain
54	BA	2335	A	Sidechain
54	BA	2338	C	Sidechain
54	BA	2341	G	Sidechain
54	BA	2344	U	Sidechain
54	BA	2352	A	Sidechain
54	BA	2357	G	Sidechain
54	BA	2358	A	Sidechain
54	BA	2360	G	Sidechain
54	BA	2361	G	Sidechain
54	BA	2366	A	Sidechain
54	BA	2375	G	Sidechain
54	BA	2379	G	Sidechain
54	BA	2380	C	Sidechain
54	BA	2382	G	Sidechain
54	BA	2383	G	Sidechain
54	BA	2391	G	Sidechain
54	BA	2392	A	Sidechain
54	BA	2395	C	Sidechain
54	BA	2398	U	Sidechain
54	BA	2404	U	Sidechain
54	BA	2405	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2411	A	Sidechain
54	BA	2417	C	Sidechain
54	BA	2418	A	Sidechain
54	BA	2423	U	Sidechain
54	BA	2424	C	Sidechain
54	BA	2427	C	Sidechain
54	BA	2433	A	Sidechain
54	BA	244	A	Sidechain
54	BA	2440	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2445	G	Sidechain
54	BA	2446	G	Sidechain
54	BA	2451	A	Sidechain
54	BA	2453	A	Sidechain
54	BA	2460	U	Sidechain
54	BA	2462	C	Sidechain
54	BA	2465	C	Sidechain
54	BA	2469	A	Sidechain
54	BA	2475	C	Sidechain
54	BA	2476	A	Sidechain
54	BA	2477	U	Sidechain
54	BA	2478	A	Sidechain
54	BA	248	G	Sidechain
54	BA	2492	U	Sidechain
54	BA	2495	G	Sidechain
54	BA	2496	C	Sidechain
54	BA	2497	A	Sidechain
54	BA	2498	C	Sidechain
54	BA	2499	C	Sidechain
54	BA	250	G	Sidechain
54	BA	2502	G	Sidechain
54	BA	2504	U	Sidechain
54	BA	2522	U	Sidechain
54	BA	2529	G	Sidechain
54	BA	2530	A	Sidechain
54	BA	2534	A	Sidechain
54	BA	254	G	Sidechain
54	BA	2540	C	Sidechain
54	BA	2548	U	Sidechain
54	BA	2550	G	Sidechain
54	BA	2552	U	Sidechain
54	BA	2557	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	256	A	Sidechain
54	BA	2560	A	Sidechain
54	BA	2569	G	Sidechain
54	BA	2571	U	Sidechain
54	BA	2573	C	Sidechain
54	BA	2576	G	Sidechain
54	BA	2581	G	Sidechain
54	BA	2582	G	Sidechain
54	BA	2585	U	Sidechain
54	BA	2586	U	Sidechain
54	BA	2588	G	Sidechain
54	BA	2589	A	Sidechain
54	BA	2597	G	Sidechain
54	BA	2598	A	Sidechain
54	BA	2611	C	Sidechain
54	BA	2615	U	Sidechain
54	BA	2624	G	Sidechain
54	BA	2625	G	Sidechain
54	BA	2629	U	Sidechain
54	BA	263	G	Sidechain
54	BA	2631	G	Sidechain
54	BA	2637	U	Sidechain
54	BA	264	C	Sidechain
54	BA	2646	C	Sidechain
54	BA	2647	U	Sidechain
54	BA	2657	A	Sidechain
54	BA	2659	G	Sidechain
54	BA	2661	G	Sidechain
54	BA	2668	G	Sidechain
54	BA	2680	U	Sidechain
54	BA	2681	C	Sidechain
54	BA	2683	C	Sidechain
54	BA	269	C	Sidechain
54	BA	2698	U	Sidechain
54	BA	270	A	Sidechain
54	BA	2700	A	Sidechain
54	BA	2709	G	Sidechain
54	BA	2722	G	Sidechain
54	BA	2725	A	Sidechain
54	BA	2726	A	Sidechain
54	BA	2728	U	Sidechain
54	BA	2732	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2737	G	Sidechain
54	BA	2738	A	Sidechain
54	BA	2740	A	Sidechain
54	BA	2741	A	Sidechain
54	BA	2742	G	Sidechain
54	BA	2745	C	Sidechain
54	BA	2747	G	Sidechain
54	BA	2748	A	Sidechain
54	BA	2751	G	Sidechain
54	BA	2756	U	Sidechain
54	BA	276	U	Sidechain
54	BA	2764	A	Sidechain
54	BA	2767	C	Sidechain
54	BA	277	G	Sidechain
54	BA	2771	C	Sidechain
54	BA	2776	A	Sidechain
54	BA	278	A	Sidechain
54	BA	2783	U	Sidechain
54	BA	2786	U	Sidechain
54	BA	2787	C	Sidechain
54	BA	2789	C	Sidechain
54	BA	2797	U	Sidechain
54	BA	2801	G	Sidechain
54	BA	2802	G	Sidechain
54	BA	2808	G	Sidechain
54	BA	2809	A	Sidechain
54	BA	2810	A	Sidechain
54	BA	2816	G	Sidechain
54	BA	2817	U	Sidechain
54	BA	2819	G	Sidechain
54	BA	2820	A	Sidechain
54	BA	2824	C	Sidechain
54	BA	2827	C	Sidechain
54	BA	2829	A	Sidechain
54	BA	283	G	Sidechain
54	BA	2832	U	Sidechain
54	BA	2835	A	Sidechain
54	BA	2840	C	Sidechain
54	BA	2850	A	Sidechain
54	BA	2852	G	Sidechain
54	BA	2854	G	Sidechain
54	BA	2857	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2868	A	Sidechain
54	BA	2872	A	Sidechain
54	BA	2875	C	Sidechain
54	BA	2883	A	Sidechain
54	BA	2884	U	Sidechain
54	BA	2885	G	Sidechain
54	BA	2887	A	Sidechain
54	BA	2889	C	Sidechain
54	BA	289	G	Sidechain
54	BA	2892	G	Sidechain
54	BA	2897	U	Sidechain
54	BA	291	G	Sidechain
54	BA	297	G	Sidechain
54	BA	3	U	Sidechain
54	BA	303	G	Sidechain
54	BA	305	C	Sidechain
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	31	C	Sidechain
54	BA	311	A	Sidechain
54	BA	313	G	Sidechain
54	BA	314	C	Sidechain
54	BA	317	G	Sidechain
54	BA	322	A	Sidechain
54	BA	323	C	Sidechain
54	BA	329	G	Sidechain
54	BA	33	C	Sidechain
54	BA	333	G	Sidechain
54	BA	356	G	Sidechain
54	BA	358	U	Sidechain
54	BA	359	G	Sidechain
54	BA	361	G	Sidechain
54	BA	363	G	Sidechain
54	BA	364	C	Sidechain
54	BA	365	U	Sidechain
54	BA	371	A	Sidechain
54	BA	373	U	Sidechain
54	BA	374	A	Sidechain
54	BA	376	G	Sidechain
54	BA	377	G	Sidechain
54	BA	379	G	Sidechain
54	BA	384	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	386	G	Sidechain
54	BA	39	G	Sidechain
54	BA	390	U	Sidechain
54	BA	394	C	Sidechain
54	BA	395	U	Sidechain
54	BA	40	U	Sidechain
54	BA	401	A	Sidechain
54	BA	402	A	Sidechain
54	BA	403	U	Sidechain
54	BA	405	U	Sidechain
54	BA	409	G	Sidechain
54	BA	418	C	Sidechain
54	BA	420	C	Sidechain
54	BA	423	A	Sidechain
54	BA	428	A	Sidechain
54	BA	43	G	Sidechain
54	BA	436	C	Sidechain
54	BA	439	A	Sidechain
54	BA	44	A	Sidechain
54	BA	440	C	Sidechain
54	BA	446	G	Sidechain
54	BA	449	A	Sidechain
54	BA	451	U	Sidechain
54	BA	452	G	Sidechain
54	BA	454	A	Sidechain
54	BA	458	G	Sidechain
54	BA	460	A	Sidechain
54	BA	463	G	Sidechain
54	BA	473	G	Sidechain
54	BA	476	G	Sidechain
54	BA	479	A	Sidechain
54	BA	48	G	Sidechain
54	BA	481	G	Sidechain
54	BA	484	C	Sidechain
54	BA	485	C	Sidechain
54	BA	491	G	Sidechain
54	BA	492	A	Sidechain
54	BA	493	G	Sidechain
54	BA	495	G	Sidechain
54	BA	496	G	Sidechain
54	BA	500	G	Sidechain
54	BA	517	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	521	U	Sidechain
54	BA	523	C	Sidechain
54	BA	524	G	Sidechain
54	BA	525	U	Sidechain
54	BA	526	A	Sidechain
54	BA	527	C	Sidechain
54	BA	528	A	Sidechain
54	BA	530	G	Sidechain
54	BA	551	G	Sidechain
54	BA	561	G	Sidechain
54	BA	568	U	Sidechain
54	BA	571	U	Sidechain
54	BA	572	A	Sidechain
54	BA	578	G	Sidechain
54	BA	579	G	Sidechain
54	BA	580	U	Sidechain
54	BA	582	A	Sidechain
54	BA	583	G	Sidechain
54	BA	587	C	Sidechain
54	BA	588	U	Sidechain
54	BA	590	A	Sidechain
54	BA	593	U	Sidechain
54	BA	606	U	Sidechain
54	BA	611	C	Sidechain
54	BA	614	A	Sidechain
54	BA	616	A	Sidechain
54	BA	617	G	Sidechain
54	BA	621	A	Sidechain
54	BA	630	G	Sidechain
54	BA	632	A	Sidechain
54	BA	633	A	Sidechain
54	BA	635	C	Sidechain
54	BA	636	G	Sidechain
54	BA	641	U	Sidechain
54	BA	645	C	Sidechain
54	BA	650	C	Sidechain
54	BA	652	U	Sidechain
54	BA	655	A	Sidechain
54	BA	656	G	Sidechain
54	BA	657	U	Sidechain
54	BA	669	G	Sidechain
54	BA	670	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	687	C	Sidechain
54	BA	690	G	Sidechain
54	BA	695	G	Sidechain
54	BA	700	G	Sidechain
54	BA	706	A	Sidechain
54	BA	707	G	Sidechain
54	BA	709	U	Sidechain
54	BA	718	A	Sidechain
54	BA	72	U	Sidechain
54	BA	724	U	Sidechain
54	BA	726	G	Sidechain
54	BA	727	A	Sidechain
54	BA	736	C	Sidechain
54	BA	738	G	Sidechain
54	BA	739	A	Sidechain
54	BA	74	A	Sidechain
54	BA	749	A	Sidechain
54	BA	75	G	Sidechain
54	BA	750	A	Sidechain
54	BA	754	U	Sidechain
54	BA	76	C	Sidechain
54	BA	761	A	Sidechain
54	BA	763	G	Sidechain
54	BA	765	C	Sidechain
54	BA	770	G	Sidechain
54	BA	772	C	Sidechain
54	BA	773	U	Sidechain
54	BA	775	G	Sidechain
54	BA	788	A	Sidechain
54	BA	790	U	Sidechain
54	BA	800	A	Sidechain
54	BA	808	G	Sidechain
54	BA	816	C	Sidechain
54	BA	829	A	Sidechain
54	BA	830	G	Sidechain
54	BA	835	C	Sidechain
54	BA	840	C	Sidechain
54	BA	841	G	Sidechain
54	BA	845	A	Sidechain
54	BA	846	U	Sidechain
54	BA	848	C	Sidechain
54	BA	850	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	851	C	Sidechain
54	BA	852	U	Sidechain
54	BA	855	G	Sidechain
54	BA	857	G	Sidechain
54	BA	859	G	Sidechain
54	BA	862	G	Sidechain
54	BA	864	G	Sidechain
54	BA	865	C	Sidechain
54	BA	869	G	Sidechain
54	BA	870	U	Sidechain
54	BA	875	G	Sidechain
54	BA	881	G	Sidechain
54	BA	882	G	Sidechain
54	BA	899	A	Sidechain
54	BA	905	A	Sidechain
54	BA	906	U	Sidechain
54	BA	907	G	Sidechain
54	BA	908	C	Sidechain
54	BA	912	C	Sidechain
54	BA	914	G	Sidechain
54	BA	92	U	Sidechain
54	BA	921	C	Sidechain
54	BA	922	C	Sidechain
54	BA	925	A	Sidechain
54	BA	926	G	Sidechain
54	BA	930	G	Sidechain
54	BA	932	U	Sidechain
54	BA	933	A	Sidechain
54	BA	934	U	Sidechain
54	BA	942	G	Sidechain
54	BA	954	G	Sidechain
54	BA	958	U	Sidechain
54	BA	960	A	Sidechain
54	BA	961	C	Sidechain
54	BA	962	G	Sidechain
54	BA	963	U	Sidechain
54	BA	969	G	Sidechain
54	BA	971	G	Sidechain
54	BA	979	A	Sidechain
54	BA	984	A	Sidechain
54	BA	986	C	Sidechain
54	BA	993	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	995	C	Sidechain
54	BA	998	C	Sidechain
55	BB	10	G	Sidechain
55	BB	105	G	Sidechain
55	BB	108	A	Sidechain
55	BB	114	C	Sidechain
55	BB	13	G	Sidechain
55	BB	23	G	Sidechain
55	BB	24	G	Sidechain
55	BB	29	A	Sidechain
55	BB	37	C	Sidechain
55	BB	39	A	Sidechain
55	BB	4	C	Sidechain
55	BB	40	U	Sidechain
55	BB	41	G	Sidechain
55	BB	42	C	Sidechain
55	BB	48	U	Sidechain
55	BB	49	C	Sidechain
55	BB	52	A	Sidechain
55	BB	64	G	Sidechain
55	BB	65	U	Sidechain
55	BB	72	G	Sidechain
55	BB	75	G	Sidechain
55	BB	76	G	Sidechain
55	BB	84	G	Sidechain
55	BB	9	G	Sidechain
55	BB	93	C	Sidechain
43	BU	6	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	1	0
5	AF	818	0	808	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	2	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16520	3	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	1	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	3	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	2	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	0
38	BP	917	0	965	1	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	1	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	31341	4	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	99659	17	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BL:30:THR:HG21	34:BL:36:LYS:H	1.72	0.54
54:BA:388:G:H2'	54:BA:389:G:H3'	1.91	0.52
42:BT:15:HIS:CG	42:BT:16:VAL:H	2.29	0.50
21:AA:1054:C:C6	23:A2:89:U:H1'	2.48	0.48
37:BO:53:THR:HG21	37:BO:70:ALA:HB1	1.98	0.46
38:BP:95:LYS:HE2	54:BA:2718:G:O3'	2.17	0.45
35:BM:34:LYS:HE3	35:BM:131:VAL:HG11	1.99	0.44
33:BK:119:ALA:H	33:BK:120:PRO:CD	2.31	0.44
21:AA:865:A:H2'	21:AA:866:C:C6	2.55	0.42
7:AH:60:LEU:H	7:AH:60:LEU:HD23	1.84	0.41
21:AA:1517:G:H2'	21:AA:1518:A:C8	2.56	0.41
35:BM:14:LYS:HE3	54:BA:958:U:C2	2.56	0.41
4:AE:155:LYS:HE3	7:AH:44:PHE:CE1	2.56	0.41
45:BW:9:THR:HB	45:BW:10:ARG:HA	2.02	0.41
54:BA:833:A:H2'	54:BA:834:G:C8	2.56	0.41
33:BK:105:ARG:NE	33:BK:105:ARG:H	2.20	0.40
33:BK:119:ALA:H	33:BK:120:PRO:HD2	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	200 (92%)	17 (8%)	1 (0%)	34	77
2	AC	205/208 (99%)	184 (90%)	15 (7%)	6 (3%)	6	43
3	AD	203/206 (98%)	185 (91%)	14 (7%)	4 (2%)	9	51
4	AE	150/152 (99%)	134 (89%)	10 (7%)	6 (4%)	4	35
5	AF	99/101 (98%)	80 (81%)	13 (13%)	6 (6%)	2	26
6	AG	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	6	45
7	AH	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	7	47
8	AI	126/128 (98%)	107 (85%)	15 (12%)	4 (3%)	5	41
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	2	30
10	AK	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	11	55
11	AL	121/124 (98%)	107 (88%)	8 (7%)	6 (5%)	3	31
12	AM	112/115 (97%)	94 (84%)	13 (12%)	5 (4%)	3	33
13	AN	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
14	AO	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	16	61
15	AP	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	4	37
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	AR	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	11	53
18	AS	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	4	37
19	AT	84/86 (98%)	76 (90%)	8 (10%)	0	100	100
20	AU	51/53 (96%)	32 (63%)	15 (29%)	4 (8%)	1	20
25	BC	270/273 (99%)	238 (88%)	25 (9%)	7 (3%)	7	45
26	BD	207/209 (99%)	185 (89%)	17 (8%)	5 (2%)	7	47
27	BE	199/201 (99%)	171 (86%)	20 (10%)	8 (4%)	4	35
28	BF	176/179 (98%)	155 (88%)	17 (10%)	4 (2%)	8	48
29	BG	174/177 (98%)	155 (89%)	12 (7%)	7 (4%)	4	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BH	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	26	71
31	BI	139/142 (98%)	125 (90%)	12 (9%)	2 (1%)	14	58
32	BJ	140/142 (99%)	126 (90%)	11 (8%)	3 (2%)	9	50
33	BK	121/123 (98%)	107 (88%)	10 (8%)	4 (3%)	5	40
34	BL	141/144 (98%)	124 (88%)	11 (8%)	6 (4%)	3	34
35	BM	134/136 (98%)	115 (86%)	14 (10%)	5 (4%)	4	38
36	BN	119/121 (98%)	105 (88%)	11 (9%)	3 (2%)	7	46
37	BO	114/117 (97%)	108 (95%)	3 (3%)	3 (3%)	7	45
38	BP	112/115 (97%)	92 (82%)	17 (15%)	3 (3%)	6	45
39	BQ	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	11	55
40	BR	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	5	42
41	BS	108/110 (98%)	105 (97%)	2 (2%)	1 (1%)	21	67
42	BT	92/94 (98%)	80 (87%)	6 (6%)	6 (6%)	1	25
43	BU	101/104 (97%)	83 (82%)	14 (14%)	4 (4%)	4	35
44	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
45	BW	78/80 (98%)	59 (76%)	17 (22%)	2 (3%)	7	45
46	BX	75/79 (95%)	68 (91%)	3 (4%)	4 (5%)	2	29
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	49 (88%)	4 (7%)	3 (5%)	2	29
49	B0	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
50	B1	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
51	B2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
52	B3	62/65 (95%)	54 (87%)	5 (8%)	3 (5%)	3	32
53	B4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	6	44
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	34	77
All	All	5876/6008 (98%)	5245 (89%)	476 (8%)	155 (3%)	11	45

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	224	ARG
2	AC	14	VAL
5	AF	86	ARG

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Mol	Chain	Res	Type
15	AP	11	ALA
15	AP	17	TYR
18	AS	4	LEU
25	BC	191	LEU
26	BD	2	ILE
27	BE	96	VAL
28	BF	12	VAL
29	BG	8	VAL
33	BK	103	VAL
33	BK	119	ALA
34	BL	29	LYS
43	BU	45	GLN
56	B5	50	ILE
2	AC	65	VAL
3	AD	24	VAL
4	AE	158	LYS
5	AF	10	VAL
5	AF	52	ASN
5	AF	63	ASN
6	AG	9	ARG
6	AG	56	SER
8	AI	115	VAL
8	AI	120	ALA
9	AJ	75	ASP
11	AL	33	CYS
11	AL	78	VAL
11	AL	108	ASP
14	AO	45	HIS
18	AS	5	LYS
20	AU	25	ALA
25	BC	36	ASN
29	BG	16	VAL
29	BG	22	VAL
29	BG	59	ASP
30	BH	67	ALA
31	BI	135	MET
32	BJ	48	VAL
32	BJ	72	LYS
32	BJ	81	ILE
34	BL	33	ARG
34	BL	34	GLY
34	BL	36	LYS

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Mol	Chain	Res	Type
34	BL	94	THR
35	BM	36	VAL
35	BM	70	ASP
35	BM	123	LYS
36	BN	110	MET
37	BO	89	ASP
39	BQ	87	VAL
42	BT	11	LEU
42	BT	39	THR
42	BT	66	LYS
42	BT	68	LYS
43	BU	50	ALA
43	BU	92	VAL
46	BX	27	ARG
52	B3	3	ILE
3	AD	3	TYR
3	AD	4	LEU
4	AE	43	GLY
4	AE	54	GLU
6	AG	60	ALA
7	AH	53	ASP
7	AH	69	ALA
9	AJ	102	LEU
10	AK	117	HIS
12	AM	21	ILE
17	AR	21	ASP
18	AS	33	TRP
20	AU	27	VAL
25	BC	189	ALA
25	BC	196	ASN
26	BD	60	VAL
26	BD	112	THR
26	BD	119	ALA
27	BE	46	GLN
27	BE	71	GLY
27	BE	97	ASN
27	BE	120	VAL
28	BF	46	LYS
28	BF	116	LEU
33	BK	22	ILE
35	BM	21	ALA
35	BM	58	LYS

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Mol	Chain	Res	Type
36	BN	2	ARG
37	BO	23	ALA
37	BO	102	ARG
38	BP	31	VAL
40	BR	43	ASN
42	BT	2	ILE
43	BU	43	LYS
45	BW	15	SER
52	B3	25	HIS
2	AC	145	ALA
2	AC	163	ARG
2	AC	167	TYR
3	AD	28	ASP
4	AE	105	ILE
5	AF	59	TYR
8	AI	42	THR
8	AI	55	ASP
11	AL	87	LYS
11	AL	122	LYS
12	AM	22	TYR
20	AU	24	LYS
25	BC	109	LEU
27	BE	165	HIS
33	BK	2	ILE
38	BP	86	LYS
40	BR	51	VAL
45	BW	23	LYS
2	AC	206	ILE
4	AE	22	LYS
5	AF	6	ILE
6	AG	5	VAL
10	AK	12	ARG
12	AM	11	HIS
15	AP	26	ASN
27	BE	79	ARG
27	BE	90	GLN
36	BN	66	ALA
39	BQ	4	LYS
42	BT	28	ASN
48	BZ	3	THR
48	BZ	4	ILE
52	B3	35	LYS

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Mol	Chain	Res	Type
29	BG	164	ALA
31	BI	31	GLY
40	BR	29	THR
46	BX	19	HIS
46	BX	40	GLU
48	BZ	9	THR
4	AE	103	GLY
9	AJ	57	VAL
26	BD	73	VAL
29	BG	9	VAL
7	AH	77	VAL
25	BC	136	VAL
28	BF	136	ILE
34	BL	55	MET
46	BX	6	VAL
9	AJ	38	GLY
12	AM	66	GLY
20	AU	13	VAL
29	BG	116	LEU
53	B4	16	ILE
9	AJ	42	LEU
12	AM	3	ILE
25	BC	53	ILE
41	BS	29	VAL
11	AL	43	LYS
38	BP	32	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	177 (98%)	3 (2%)	68	87
2	AC	170/171 (99%)	168 (99%)	2 (1%)	78	90
3	AD	172/173 (99%)	171 (99%)	1 (1%)	90	95
4	AE	113/113 (100%)	112 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	86	94
7	AH	104/105 (99%)	101 (97%)	3 (3%)	50	78
8	AI	105/105 (100%)	101 (96%)	4 (4%)	40	73
9	AJ	86/86 (100%)	83 (96%)	3 (4%)	43	74
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	102 (99%)	1 (1%)	82	92
12	AM	91/92 (99%)	90 (99%)	1 (1%)	80	91
13	AN	83/84 (99%)	81 (98%)	2 (2%)	57	82
14	AO	76/77 (99%)	74 (97%)	2 (3%)	54	80
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	71 (96%)	3 (4%)	37	71
17	AR	48/48 (100%)	45 (94%)	3 (6%)	22	59
18	AS	70/70 (100%)	69 (99%)	1 (1%)	74	89
19	AT	65/65 (100%)	64 (98%)	1 (2%)	72	88
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	51	78
26	BD	164/164 (100%)	160 (98%)	4 (2%)	57	82
27	BE	165/165 (100%)	162 (98%)	3 (2%)	66	87
28	BF	149/150 (99%)	147 (99%)	2 (1%)	76	89
29	BG	137/138 (99%)	133 (97%)	4 (3%)	50	78
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	108 (99%)	1 (1%)	84	93
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	54	80
33	BK	103/103 (100%)	102 (99%)	1 (1%)	82	92
34	BL	102/103 (99%)	100 (98%)	2 (2%)	63	85
35	BM	109/109 (100%)	107 (98%)	2 (2%)	66	87
36	BN	100/100 (100%)	99 (99%)	1 (1%)	82	92
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	97 (98%)	2 (2%)	63	85
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BR	84/84 (100%)	84 (100%)	0	100	100
41	BS	93/93 (100%)	92 (99%)	1 (1%)	80	91
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	57	82
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	53 (90%)	6 (10%)	9	37
46	BX	67/68 (98%)	66 (98%)	1 (2%)	72	88
47	BY	55/55 (100%)	54 (98%)	1 (2%)	66	87
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%)	44 (98%)	1 (2%)	60	83
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	48 (94%)	3 (6%)	24	61
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	169 (98%)	4 (2%)	58	83
All	All	4842/4870 (99%)	4757 (98%)	85 (2%)	69	87

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	56	LEU
1	AB	71	THR
1	AB	136	ARG
2	AC	128	MET
2	AC	198	LYS
3	AD	196	GLU
4	AE	151	MET
6	AG	56	SER
7	AH	40	LYS
7	AH	66	GLN
7	AH	104	SER
8	AI	41	GLU
8	AI	42	THR
8	AI	105	ARG
8	AI	125	GLN
9	AJ	19	ASP
9	AJ	44	THR

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Mol	Chain	Res	Type
9	AJ	102	LEU
11	AL	8	ARG
12	AM	81	ASP
13	AN	41	ARG
13	AN	42	TRP
14	AO	19	ASN
14	AO	46	LYS
16	AQ	7	LEU
16	AQ	17	GLU
16	AQ	43	LEU
17	AR	32	ILE
17	AR	66	LEU
17	AR	69	TYR
18	AS	78	THR
19	AT	27	MET
25	BC	47	ARG
25	BC	50	THR
25	BC	86	ARG
25	BC	123	ILE
25	BC	194	VAL
25	BC	229	HIS
26	BD	15	PHE
26	BD	33	ARG
26	BD	154	LYS
26	BD	200	ASP
27	BE	35	TYR
27	BE	79	ARG
27	BE	125	SER
28	BF	80	GLN
28	BF	124	ARG
29	BG	148	ARG
29	BG	163	TYR
29	BG	165	ASP
29	BG	166	GLU
31	BI	110	GLN
32	BJ	9	GLU
32	BJ	14	ASP
32	BJ	24	THR
33	BK	105	ARG
34	BL	4	ASN
34	BL	93	ASN
35	BM	1	MET

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Mol	Chain	Res	Type
35	BM	97	GLN
36	BN	37	THR
38	BP	105	LYS
38	BP	108	ARG
39	BQ	50	ARG
39	BQ	56	PHE
41	BS	60	HIS
43	BU	8	ASP
43	BU	44	HIS
45	BW	10	ARG
45	BW	13	ARG
45	BW	39	GLN
45	BW	40	ARG
45	BW	49	ASN
45	BW	63	ASP
46	BX	15	ASN
47	BY	26	PHE
49	B0	37	HIS
50	B1	20	TYR
52	B3	37	THR
52	B3	38	LYS
52	B3	53	ASP
56	B5	126	GLN
56	B5	129	GLN
56	B5	164	ARG
56	B5	165	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
12	AM	104	ASN
44	BV	88	HIS
46	BX	15	ASN
49	B0	41	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	248 (16%)	86 (5%)
22	A1	73/76 (96%)	15 (20%)	7 (9%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	A2	14/15 (93%)	5 (35%)	3 (21%)
24	A3	76/77 (98%)	13 (17%)	5 (6%)
54	BA	2902/2903 (99%)	464 (15%)	110 (3%)
55	BB	117/118 (99%)	15 (12%)	4 (3%)
All	All	4712/4722 (99%)	760 (16%)	215 (4%)

All (760) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	16	A
21	AA	28	A
21	AA	32	A
21	AA	35	G
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	52	C
21	AA	54	C
21	AA	56	U
21	AA	66	A
21	AA	67	C
21	AA	71	A
21	AA	81	A
21	AA	86	G
21	AA	90	C
21	AA	91	U
21	AA	95	C
21	AA	110	C
21	AA	121	U
21	AA	124	C
21	AA	131	A
21	AA	144	G
21	AA	163	C
21	AA	164	G
21	AA	168	G
21	AA	198	G
21	AA	207	C

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Mol	Chain	Res	Type
21	AA	212	G
21	AA	213	G
21	AA	214	C
21	AA	236	A
21	AA	238	A
21	AA	239	U
21	AA	240	G
21	AA	244	U
21	AA	245	U
21	AA	247	G
21	AA	250	A
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	267	C
21	AA	272	C
21	AA	279	A
21	AA	289	G
21	AA	293	G
21	AA	307	C
21	AA	308	C
21	AA	315	A
21	AA	316	C
21	AA	317	U
21	AA	328	C
21	AA	329	A
21	AA	344	A
21	AA	345	C
21	AA	347	G
21	AA	352	C
21	AA	353	A
21	AA	354	G
21	AA	358	U
21	AA	361	G
21	AA	367	U
21	AA	372	C
21	AA	381	C
21	AA	384	G
21	AA	389	A
21	AA	397	A
21	AA	412	A
21	AA	413	G

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Mol	Chain	Res	Type
21	AA	414	A
21	AA	415	A
21	AA	422	C
21	AA	424	G
21	AA	428	G
21	AA	429	U
21	AA	458	U
21	AA	461	A
21	AA	462	G
21	AA	464	U
21	AA	472	U
21	AA	474	G
21	AA	484	G
21	AA	496	A
21	AA	499	A
21	AA	511	C
21	AA	527	G
21	AA	533	A
21	AA	547	A
21	AA	559	A
21	AA	560	A
21	AA	561	U
21	AA	562	U
21	AA	564	C
21	AA	566	G
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	577	G
21	AA	607	A
21	AA	608	A
21	AA	618	C
21	AA	619	U
21	AA	620	C
21	AA	626	G
21	AA	632	U
21	AA	633	G
21	AA	653	U
21	AA	659	U
21	AA	663	A
21	AA	664	G

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Mol	Chain	Res	Type
21	AA	714	G
21	AA	718	A
21	AA	731	G
21	AA	755	G
21	AA	777	A
21	AA	794	A
21	AA	812	G
21	AA	815	A
21	AA	816	A
21	AA	817	C
21	AA	819	A
21	AA	822	U
21	AA	828	U
21	AA	841	C
21	AA	843	U
21	AA	845	A
21	AA	846	G
21	AA	872	A
21	AA	885	G
21	AA	890	G
21	AA	902	G
21	AA	918	A
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	945	G
21	AA	958	A
21	AA	959	A
21	AA	960	U
21	AA	961	U
21	AA	962	C
21	AA	964	A
21	AA	965	U
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	972	C
21	AA	975	A
21	AA	977	A

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Mol	Chain	Res	Type
21	AA	980	C
21	AA	983	A
21	AA	992	U
21	AA	993	G
21	AA	994	A
21	AA	996	A
21	AA	1004	A
21	AA	1006	G
21	AA	1026	G
21	AA	1028	C
21	AA	1032	G
21	AA	1033	G
21	AA	1049	U
21	AA	1053	G
21	AA	1054	C
21	AA	1055	A
21	AA	1056	U
21	AA	1061	G
21	AA	1065	U
21	AA	1068	G
21	AA	1081	A
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1124	G
21	AA	1125	U
21	AA	1130	A
21	AA	1137	C
21	AA	1139	G
21	AA	1143	G
21	AA	1159	U
21	AA	1161	C
21	AA	1167	A
21	AA	1168	U
21	AA	1169	A
21	AA	1183	U
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1193	G
21	AA	1202	U

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Mol	Chain	Res	Type
21	AA	1203	C
21	AA	1212	U
21	AA	1213	A
21	AA	1217	C
21	AA	1221	G
21	AA	1224	U
21	AA	1225	A
21	AA	1227	A
21	AA	1232	U
21	AA	1240	U
21	AA	1241	G
21	AA	1256	A
21	AA	1257	A
21	AA	1260	G
21	AA	1267	C
21	AA	1278	G
21	AA	1280	A
21	AA	1281	C
21	AA	1286	U
21	AA	1302	C
21	AA	1303	C
21	AA	1307	U
21	AA	1308	U
21	AA	1317	C
21	AA	1319	A
21	AA	1320	C
21	AA	1321	U
21	AA	1323	G
21	AA	1329	A
21	AA	1338	G
21	AA	1346	A
21	AA	1360	A
21	AA	1363	A
21	AA	1378	C
21	AA	1394	A
21	AA	1397	C
21	AA	1401	G
21	AA	1402	C
21	AA	1413	A
21	AA	1432	G
21	AA	1447	A
21	AA	1460	C

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Mol	Chain	Res	Type
21	AA	1503	A
21	AA	1505	G
21	AA	1506	U
21	AA	1529	G
21	AA	1530	G
22	A1	3	G
22	A1	10	G
22	A1	17	U
22	A1	19	G
22	A1	44	G
22	A1	45	G
22	A1	46	7MG
22	A1	47	U
22	A1	49	G
22	A1	59	U
22	A1	61	C
22	A1	70	C
22	A1	71	C
22	A1	74	C
22	A1	76	A
23	A2	81	U
23	A2	85	G
23	A2	89	U
23	A2	90	U
23	A2	93	U
24	A3	2	G
24	A3	9	G
24	A3	18	U
24	A3	20	G
24	A3	31	G
24	A3	48	U
24	A3	49	C
24	A3	60	A
24	A3	61	U
24	A3	63	C
24	A3	73	A
24	A3	74	A
24	A3	77	A
54	BA	15	G
54	BA	29	U
54	BA	34	U
54	BA	45	G

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Mol	Chain	Res	Type
54	BA	60	G
54	BA	62	U
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	77	G
54	BA	100	U
54	BA	101	A
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	128	C
54	BA	139	U
54	BA	141	G
54	BA	142	A
54	BA	143	C
54	BA	165	A
54	BA	180	G
54	BA	181	A
54	BA	196	A
54	BA	199	A
54	BA	200	U
54	BA	205	G
54	BA	206	U
54	BA	216	A
54	BA	221	A
54	BA	222	A
54	BA	230	G
54	BA	233	A
54	BA	245	G
54	BA	248	G
54	BA	271	G
54	BA	272	A
54	BA	273	G
54	BA	275	C
54	BA	278	A
54	BA	279	A
54	BA	283	G
54	BA	297	G
54	BA	316	C

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Mol	Chain	Res	Type
54	BA	323	C
54	BA	324	A
54	BA	325	G
54	BA	330	A
54	BA	331	C
54	BA	333	G
54	BA	346	A
54	BA	365	U
54	BA	372	G
54	BA	373	U
54	BA	374	A
54	BA	389	G
54	BA	390	U
54	BA	403	U
54	BA	404	A
54	BA	405	U
54	BA	406	G
54	BA	411	G
54	BA	413	C
54	BA	430	A
54	BA	436	C
54	BA	443	A
54	BA	444	C
54	BA	450	G
54	BA	451	U
54	BA	453	A
54	BA	457	A
54	BA	475	C
54	BA	481	G
54	BA	482	A
54	BA	491	G
54	BA	504	A
54	BA	505	A
54	BA	507	A
54	BA	518	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

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Mol	Chain	Res	Type
54	BA	547	A
54	BA	548	G
54	BA	563	A
54	BA	571	U
54	BA	572	A
54	BA	573	U
54	BA	587	C
54	BA	603	A
54	BA	615	U
54	BA	616	A
54	BA	620	G
54	BA	621	A
54	BA	628	G
54	BA	637	A
54	BA	644	A
54	BA	653	U
54	BA	654	A
54	BA	671	C
54	BA	672	C
54	BA	686	U
54	BA	706	A
54	BA	719	C
54	BA	732	C
54	BA	736	C
54	BA	747	U
54	BA	748	G
54	BA	751	A
54	BA	752	A
54	BA	775	G
54	BA	776	G
54	BA	781	A
54	BA	782	A
54	BA	784	G
54	BA	788	A
54	BA	789	A
54	BA	791	C
54	BA	793	A
54	BA	799	G
54	BA	800	A
54	BA	805	G
54	BA	830	G
54	BA	846	U

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Mol	Chain	Res	Type
54	BA	847	U
54	BA	848	C
54	BA	853	C
54	BA	854	C
54	BA	888	C
54	BA	889	C
54	BA	890	C
54	BA	891	G
54	BA	910	A
54	BA	912	C
54	BA	915	C
54	BA	931	U
54	BA	932	U
54	BA	933	A
54	BA	941	A
54	BA	945	A
54	BA	946	C
54	BA	955	U
54	BA	958	U
54	BA	959	A
54	BA	981	A
54	BA	983	A
54	BA	984	A
54	BA	996	A
54	BA	999	U
54	BA	1000	A
54	BA	1005	C
54	BA	1006	C
54	BA	1012	U
54	BA	1024	G
54	BA	1026	G
54	BA	1033	U
54	BA	1044	C
54	BA	1046	A
54	BA	1047	G
54	BA	1051	G
54	BA	1057	A
54	BA	1063	G
54	BA	1067	A
54	BA	1070	A
54	BA	1072	C
54	BA	1073	A

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Mol	Chain	Res	Type
54	BA	1076	C
54	BA	1087	G
54	BA	1088	A
54	BA	1089	A
54	BA	1094	U
54	BA	1096	A
54	BA	1109	C
54	BA	1110	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	1155	A
54	BA	1157	G
54	BA	1158	C
54	BA	1175	A
54	BA	1176	U
54	BA	1186	G
54	BA	1204	A
54	BA	1206	G
54	BA	1227	G
54	BA	1237	A
54	BA	1238	G
54	BA	1242	U
54	BA	1245	G
54	BA	1256	G
54	BA	1265	A
54	BA	1275	A
54	BA	1276	A
54	BA	1287	A
54	BA	1288	G
54	BA	1289	C
54	BA	1292	G
54	BA	1293	C
54	BA	1300	G
54	BA	1301	A
54	BA	1302	A
54	BA	1313	U
54	BA	1317	G
54	BA	1322	A

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Mol	Chain	Res	Type
54	BA	1325	U
54	BA	1329	U
54	BA	1330	C
54	BA	1333	G
54	BA	1341	G
54	BA	1365	A
54	BA	1378	A
54	BA	1379	U
54	BA	1383	A
54	BA	1385	A
54	BA	1389	G
54	BA	1390	U
54	BA	1398	C
54	BA	1399	C
54	BA	1416	G
54	BA	1417	C
54	BA	1420	A
54	BA	1421	G
54	BA	1428	C
54	BA	1439	A
54	BA	1440	U
54	BA	1452	G
54	BA	1455	G
54	BA	1482	G
54	BA	1490	A
54	BA	1491	G
54	BA	1493	C
54	BA	1523	U
54	BA	1524	G
54	BA	1532	A
54	BA	1535	A
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1540	G
54	BA	1555	G
54	BA	1568	G
54	BA	1578	U
54	BA	1591	A
54	BA	1598	A
54	BA	1603	A
54	BA	1607	C

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Mol	Chain	Res	Type
54	BA	1610	A
54	BA	1611	C
54	BA	1616	A
54	BA	1618	A
54	BA	1627	G
54	BA	1647	U
54	BA	1648	U
54	BA	1651	G
54	BA	1652	A
54	BA	1654	A
54	BA	1655	A
54	BA	1664	A
54	BA	1670	C
54	BA	1674	G
54	BA	1675	C
54	BA	1693	U
54	BA	1696	G
54	BA	1699	G
54	BA	1700	A
54	BA	1701	A
54	BA	1707	G
54	BA	1713	A
54	BA	1714	U
54	BA	1730	C
54	BA	1731	G
54	BA	1733	G
54	BA	1763	G
54	BA	1764	C
54	BA	1773	A
54	BA	1775	U
54	BA	1780	A
54	BA	1782	U
54	BA	1783	A
54	BA	1784	A
54	BA	1791	A
54	BA	1797	G
54	BA	1800	C
54	BA	1808	A
54	BA	1809	A
54	BA	1815	A
54	BA	1816	C
54	BA	1817	G

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Mol	Chain	Res	Type
54	BA	1821	A
54	BA	1835	G
54	BA	1858	A
54	BA	1870	C
54	BA	1871	A
54	BA	1873	G
54	BA	1877	A
54	BA	1886	U
54	BA	1896	G
54	BA	1906	G
54	BA	1916	A
54	BA	1919	A
54	BA	1926	U
54	BA	1929	G
54	BA	1930	G
54	BA	1937	A
54	BA	1938	A
54	BA	1945	G
54	BA	1955	U
54	BA	1963	U
54	BA	1964	G
54	BA	1967	C
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1982	U
54	BA	1993	U
54	BA	1997	C
54	BA	2016	U
54	BA	2023	C
54	BA	2030	A
54	BA	2043	C
54	BA	2047	C
54	BA	2052	A
54	BA	2055	C
54	BA	2061	G
54	BA	2062	A
54	BA	2069	G
54	BA	2076	U
54	BA	2077	A
54	BA	2090	A
54	BA	2092	U

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Mol	Chain	Res	Type
54	BA	2093	G
54	BA	2111	U
54	BA	2113	U
54	BA	2117	A
54	BA	2118	U
54	BA	2133	G
54	BA	2145	C
54	BA	2146	C
54	BA	2148	G
54	BA	2157	G
54	BA	2159	G
54	BA	2160	C
54	BA	2163	A
54	BA	2164	C
54	BA	2169	A
54	BA	2172	U
54	BA	2173	A
54	BA	2198	A
54	BA	2203	U
54	BA	2211	A
54	BA	2212	A
54	BA	2216	G
54	BA	2238	G
54	BA	2246	G
54	BA	2253	G
54	BA	2266	A
54	BA	2274	A
54	BA	2276	G
54	BA	2283	C
54	BA	2286	G
54	BA	2287	A
54	BA	2297	A
54	BA	2305	U
54	BA	2309	A
54	BA	2312	U
54	BA	2321	U
54	BA	2325	G
54	BA	2333	A
54	BA	2334	U
54	BA	2335	A
54	BA	2339	C
54	BA	2343	U

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Mol	Chain	Res	Type
54	BA	2344	U
54	BA	2347	C
54	BA	2383	G
54	BA	2385	C
54	BA	2392	A
54	BA	2402	U
54	BA	2407	A
54	BA	2425	A
54	BA	2428	G
54	BA	2429	G
54	BA	2430	A
54	BA	2432	A
54	BA	2433	A
54	BA	2435	A
54	BA	2439	A
54	BA	2440	C
54	BA	2441	U
54	BA	2447	G
54	BA	2448	A
54	BA	2449	U
54	BA	2450	A
54	BA	2452	C
54	BA	2473	U
54	BA	2474	U
54	BA	2476	A
54	BA	2491	U
54	BA	2492	U
54	BA	2499	C
54	BA	2500	U
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2513	A
54	BA	2531	A
54	BA	2532	G
54	BA	2558	C
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2572	A
54	BA	2573	C
54	BA	2576	G

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Mol	Chain	Res	Type
54	BA	2578	G
54	BA	2585	U
54	BA	2586	U
54	BA	2592	G
54	BA	2596	U
54	BA	2599	G
54	BA	2602	A
54	BA	2603	G
54	BA	2609	U
54	BA	2613	U
54	BA	2630	G
54	BA	2644	G
54	BA	2645	G
54	BA	2646	C
54	BA	2655	G
54	BA	2660	A
54	BA	2661	G
54	BA	2669	G
54	BA	2681	C
54	BA	2684	U
54	BA	2689	U
54	BA	2690	U
54	BA	2691	C
54	BA	2736	A
54	BA	2751	G
54	BA	2765	A
54	BA	2766	A
54	BA	2778	A
54	BA	2780	G
54	BA	2791	G
54	BA	2798	U
54	BA	2809	A
54	BA	2817	U
54	BA	2820	A
54	BA	2821	A
54	BA	2850	A
54	BA	2861	U
54	BA	2876	G
54	BA	2894	G
54	BA	2895	G
55	BB	3	C
55	BB	11	C

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Mol	Chain	Res	Type
55	BB	12	C
55	BB	15	A
55	BB	25	U
55	BB	30	C
55	BB	42	C
55	BB	45	A
55	BB	81	G
55	BB	82	U
55	BB	83	G
55	BB	88	C
55	BB	90	C
55	BB	108	A
55	BB	109	A

All (215) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	15	G
21	AA	32	A
21	AA	34	C
21	AA	51	A
21	AA	66	A
21	AA	71	A
21	AA	90	C
21	AA	109	A
21	AA	120	A
21	AA	123	U
21	AA	162	A
21	AA	163	C
21	AA	206	C
21	AA	212	G
21	AA	235	C
21	AA	238	A
21	AA	243	A
21	AA	251	G
21	AA	271	C
21	AA	307	C
21	AA	315	A
21	AA	316	C

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Mol	Chain	Res	Type
21	AA	327	A
21	AA	329	A
21	AA	343	U
21	AA	351	G
21	AA	354	G
21	AA	414	A
21	AA	462	G
21	AA	464	U
21	AA	472	U
21	AA	473	U
21	AA	496	A
21	AA	499	A
21	AA	531	U
21	AA	532	A
21	AA	559	A
21	AA	560	A
21	AA	575	G
21	AA	607	A
21	AA	610	U
21	AA	632	U
21	AA	641	U
21	AA	659	U
21	AA	663	A
21	AA	844	G
21	AA	869	G
21	AA	872	A
21	AA	884	U
21	AA	913	A
21	AA	926	G
21	AA	932	C
21	AA	944	G
21	AA	964	A
21	AA	982	U
21	AA	1032	G
21	AA	1054	C
21	AA	1066	C
21	AA	1080	A
21	AA	1092	A
21	AA	1101	A
21	AA	1123	U
21	AA	1124	G
21	AA	1129	C

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Mol	Chain	Res	Type
21	AA	1137	C
21	AA	1139	G
21	AA	1159	U
21	AA	1168	U
21	AA	1187	G
21	AA	1190	G
21	AA	1201	A
21	AA	1212	U
21	AA	1231	G
21	AA	1241	G
21	AA	1298	U
21	AA	1300	G
21	AA	1345	U
21	AA	1346	A
21	AA	1365	G
21	AA	1401	G
21	AA	1459	G
21	AA	1505	G
21	AA	1533	C
22	A1	10	G
22	A1	15	G
22	A1	19	G
22	A1	45	G
22	A1	46	7MG
22	A1	49	G
22	A1	70	C
23	A2	80	C
23	A2	88	U
23	A2	89	U
24	A3	16	C
24	A3	19	G
24	A3	47	G
24	A3	60	A
24	A3	62	C
54	BA	33	C
54	BA	60	G
54	BA	121	G
54	BA	125	A
54	BA	177	G
54	BA	199	A
54	BA	205	G
54	BA	221	A

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Mol	Chain	Res	Type
54	BA	222	A
54	BA	278	A
54	BA	279	A
54	BA	323	C
54	BA	332	A
54	BA	345	A
54	BA	389	G
54	BA	403	U
54	BA	448	U
54	BA	481	G
54	BA	529	A
54	BA	531	C
54	BA	546	U
54	BA	570	G
54	BA	571	U
54	BA	614	A
54	BA	615	U
54	BA	620	G
54	BA	643	A
54	BA	645	C
54	BA	652	U
54	BA	670	A
54	BA	685	A
54	BA	847	U
54	BA	853	C
54	BA	933	A
54	BA	954	G
54	BA	957	C
54	BA	978	G
54	BA	980	A
54	BA	983	A
54	BA	1005	C
54	BA	1069	A
54	BA	1070	A
54	BA	1087	G
54	BA	1099	G
54	BA	1109	C
54	BA	1185	G
54	BA	1287	A
54	BA	1288	G
54	BA	1299	G
54	BA	1300	G

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Mol	Chain	Res	Type
54	BA	1312	U
54	BA	1324	G
54	BA	1325	U
54	BA	1332	G
54	BA	1340	U
54	BA	1379	U
54	BA	1398	C
54	BA	1420	A
54	BA	1427	A
54	BA	1439	A
54	BA	1451	C
54	BA	1455	G
54	BA	1554	U
54	BA	1602	U
54	BA	1610	A
54	BA	1625	C
54	BA	1647	U
54	BA	1654	A
54	BA	1674	G
54	BA	1695	G
54	BA	1706	C
54	BA	1713	A
54	BA	1730	C
54	BA	1731	G
54	BA	1781	U
54	BA	1783	A
54	BA	1787	A
54	BA	1808	A
54	BA	1816	C
54	BA	1876	A
54	BA	1913	A
54	BA	1936	A
54	BA	1938	A
54	BA	1963	U
54	BA	1970	A
54	BA	2030	A
54	BA	2051	A
54	BA	2092	U
54	BA	2111	U
54	BA	2145	C
54	BA	2163	A
54	BA	2172	U

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Mol	Chain	Res	Type
54	BA	2251	G
54	BA	2282	G
54	BA	2286	G
54	BA	2324	U
54	BA	2343	U
54	BA	2423	U
54	BA	2430	A
54	BA	2439	A
54	BA	2451	A
54	BA	2491	U
54	BA	2500	U
54	BA	2502	G
54	BA	2531	A
54	BA	2564	A
54	BA	2585	U
54	BA	2689	U
54	BA	2726	A
54	BA	2894	G
55	BB	2	G
55	BB	24	G
55	BB	56	G
55	BB	81	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	21,22	15,26,27	1.92	3 (20%)	18,37,40	3.16	4 (22%)
22	6MZ	A1	37	22	17,25,26	0.99	1 (5%)	15,36,39	1.09	1 (6%)
22	7MG	A1	46	22	20,26,27	2.19	3 (15%)	23,39,42	2.14	2 (8%)
22	5MU	A1	54	22	13,22,23	1.21	2 (15%)	16,32,35	4.75	2 (12%)
22	PSU	A1	55	22	15,21,22	1.03	1 (6%)	16,30,33	3.32	5 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	4SU	A1	7	22	12,21,22	1.10	1 (8%)	15,30,33	2.24	3 (20%)
24	H2U	A3	21	24	17,21,22	1.45	2 (11%)	23,30,33	1.29	4 (17%)
24	OMC	A3	33	24	15,22,23	1.13	0	20,31,34	1.07	1 (5%)
24	5MU	A3	55	24	13,22,23	1.06	1 (7%)	16,32,35	4.45	2 (12%)
24	PSU	A3	56	24	15,21,22	1.35	2 (13%)	16,30,33	3.44	4 (25%)
24	4SU	A3	8	24	12,21,22	1.19	2 (16%)	15,30,33	2.20	1 (6%)

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

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.13	1.33	1.45
22	A1	34	CM0	O5-C5	-6.17	1.25	1.37
24	A3	21	H2U	C4-N3	-3.55	1.31	1.37
24	A3	21	H2U	C2-N3	-3.36	1.31	1.38
22	A1	46	7MG	C8-N7	-2.68	1.31	1.43
22	A1	37	6MZ	C8-N7	-2.36	1.30	1.34
24	A3	56	PSU	O4'-C1'	-2.03	1.41	1.44
22	A1	34	CM0	C4-N3	2.15	1.36	1.33
24	A3	8	4SU	O4'-C1'	2.17	1.44	1.41
22	A1	7	4SU	C6-N1	2.24	1.38	1.35
24	A3	8	4SU	C6-N1	2.34	1.38	1.35
22	A1	55	PSU	C4-N3	2.40	1.37	1.33
22	A1	54	5MU	O4'-C1'	2.43	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	54	5MU	C4-N3	2.46	1.37	1.33
24	A3	55	5MU	C4-N3	2.60	1.37	1.33
22	A1	34	CM0	C4-C5	2.68	1.47	1.40
22	A1	46	7MG	C6-N1	2.69	1.37	1.33
24	A3	56	PSU	C4-N3	2.76	1.38	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-13.21	114.26	125.35
24	A3	55	5MU	C5-C4-N3	-12.35	114.98	125.35
24	A3	8	4SU	C5-C4-N3	-7.81	115.28	123.56
22	A1	7	4SU	C5-C4-N3	-7.11	116.02	123.56
22	A1	46	7MG	C5-C6-N1	-6.89	113.14	123.39
22	A1	55	PSU	C5-C1'-C2'	-3.75	109.07	115.44
22	A1	7	4SU	C4'-O4'-C1'	-3.28	106.17	109.64
22	A1	55	PSU	C5-C6-N1	-2.96	120.25	124.38
24	A3	56	PSU	C5-C6-N1	-2.94	120.28	124.38
24	A3	33	OMC	C4'-O4'-C1'	-2.86	106.62	109.64
22	A1	34	CM0	C4'-O4'-C1'	-2.33	107.17	109.64
22	A1	55	PSU	C4'-O4'-C1'	-2.25	107.23	109.54
24	A3	56	PSU	O2'-C2'-C1'	-2.24	107.06	111.93
24	A3	21	H2U	C5-C4-N3	2.01	118.75	116.62
22	A1	34	CM0	O5-C7-C8	2.10	112.35	108.01
22	A1	7	4SU	O4'-C4'-C3'	2.11	109.43	105.16
24	A3	21	H2U	C4-N3-C2	2.43	127.97	125.77
24	A3	21	H2U	C5-C6-N1	2.47	113.47	110.76
22	A1	34	CM0	O5-C5-C4	2.62	118.75	115.20
22	A1	55	PSU	O4'-C1'-C2'	2.89	107.82	104.69
22	A1	37	6MZ	C2-N1-C6	2.94	118.58	116.47
24	A3	21	H2U	N3-C2-N1	3.28	119.68	116.64
24	A3	56	PSU	O4'-C1'-C2'	3.97	108.98	104.69
22	A1	46	7MG	C6-N1-C2	6.78	123.82	115.88
22	A1	55	PSU	C4-N3-C2	11.47	124.73	115.16
22	A1	34	CM0	C4-N3-C2	12.27	125.40	115.16
24	A3	55	5MU	C4-N3-C2	12.32	125.44	115.16
24	A3	56	PSU	C4-N3-C2	12.37	125.47	115.16
22	A1	54	5MU	C4-N3-C2	13.05	126.05	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	VAL	A1	101	58,22	5,6,7	0.63	0	5,7,9	2.26	2 (40%)
58	FME	BA	3001	57	8,9,10	0.61	0	5,9,11	1.37	1 (20%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-3.85	115.18	125.69
58	BA	3001	FME	O1-CN-N	-2.29	121.30	124.80
57	A1	101	VAL	C-CA-N	3.27	117.17	109.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.