



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:11 PM BST

PDB ID : 4V79  
EMDB ID: : EMD-1723  
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post3b)  
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 : 15.00 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

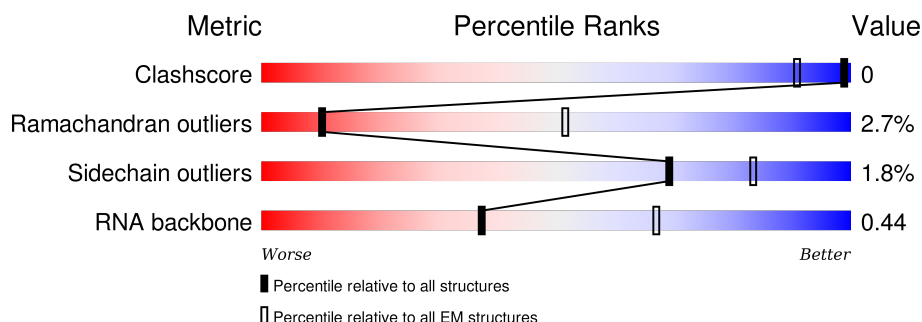
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 15.00 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.














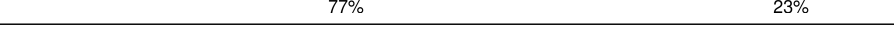
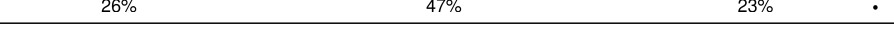






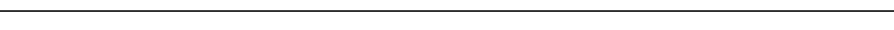

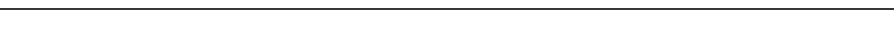
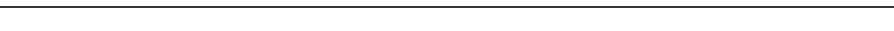


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	
2	AC	208	
3	AD	206	
4	AE	152	
5	AF	101	
6	AG	152	
7	AH	130	
8	AI	128	









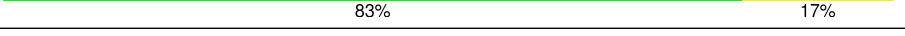

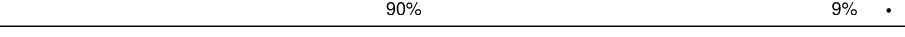
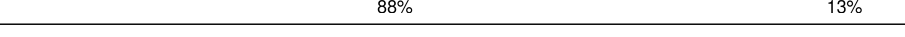

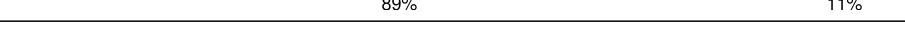




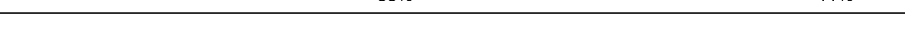



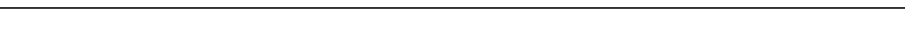
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Mol	Chain	Length	Quality of chain
9	AJ	100	 84% 16%
10	AK	118	 92% 8%
11	AL	124	 85% 15% .
12	AM	115	 86% 13% .
13	AN	101	 82% 17% .
14	AO	89	 85% 13% .
15	AP	81	 91% 9%
16	AQ	82	 90% 10%
17	AR	57	 89% 11%
18	AS	81	 89% 11%
19	AT	86	 90% 10%
20	AU	53	 77% 23%
21	AA	1533	 26% 47% 23% .
22	A1	76	 28% 57% 14% .
23	A2	15	 20% 40% 20% 20%
24	A3	77	 26% 55% 19%
25	BC	273	 87% 12% .
26	BD	209	 92% 8%
27	BE	201	 86% 12% .
28	BF	179	 89% 10% .
29	BG	177	 91% 8% ..
30	BH	149	 93% 7%
31	BI	142	 95% . .
32	BJ	142	 94% 6%
33	BK	123	 89% 9% .

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Mol	Chain	Length	Quality of chain
34	BL	144	 83% 15% ..
35	BM	136	 89% 10% .
36	BN	121	 88% 12% .
37	BO	117	 86% 11% ..
38	BP	115	 87% 10% ...
39	BQ	118	 89% 9% ..
40	BR	103	 89% 11%
41	BS	110	 91% 9%
42	BT	94	 83% 17%
43	BU	104	 86% 13% ..
44	BV	94	 90% 9% .
45	BW	80	 88% 13%
46	BX	79	 78% 18% ..
47	BY	63	 89% 11%
48	BZ	59	 90% 7% ..
49	B0	57	 84% 12% ..
50	B1	52	 85% 15%
51	B2	46	 76% 24%
52	B3	65	 88% 11% .
53	B4	38	 87% 8% 5%
54	BA	2903	 22% 51% 23% .
55	BB	118	 22% 53% 19% 6% .
56	B5	234	 90% 5% 5%

## 2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

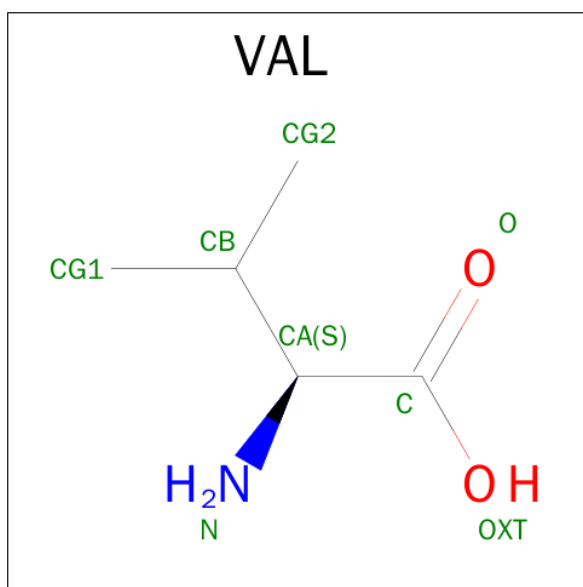
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

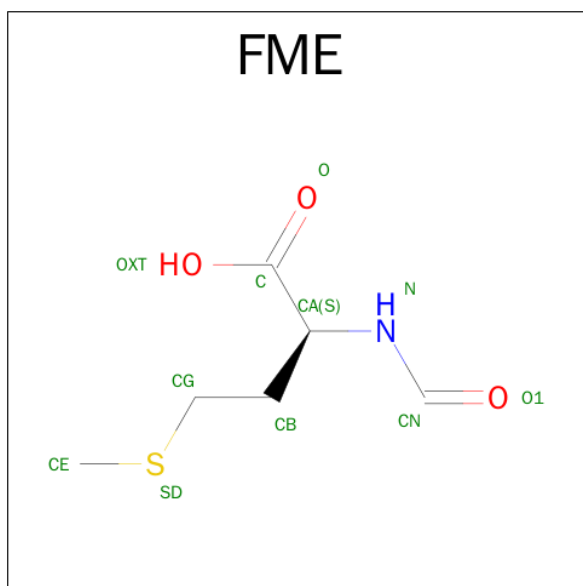
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



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

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



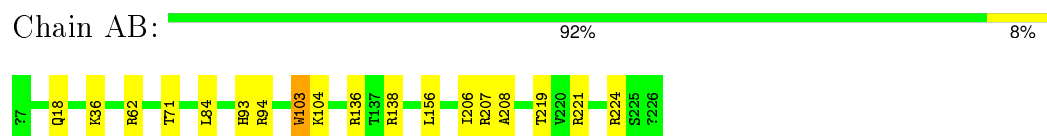
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



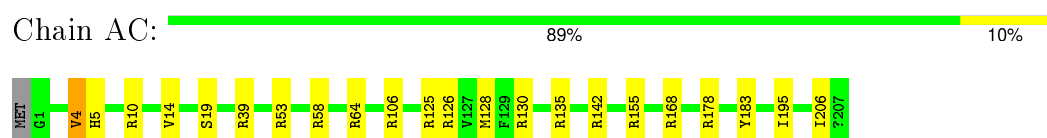
### 3 Residue-property plots

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

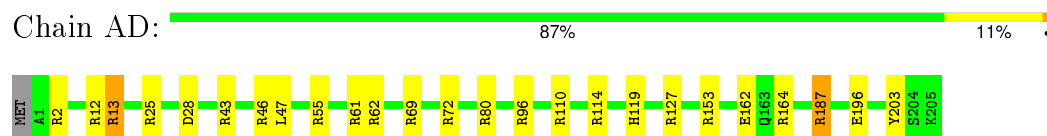
- Molecule 1: 30S ribosomal protein S2



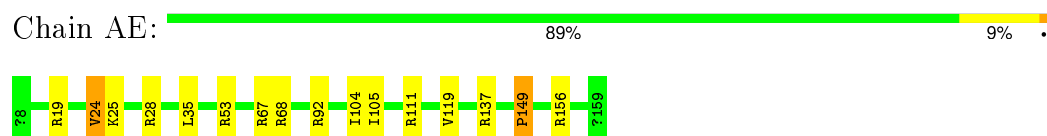
- Molecule 2: 30S ribosomal protein S3



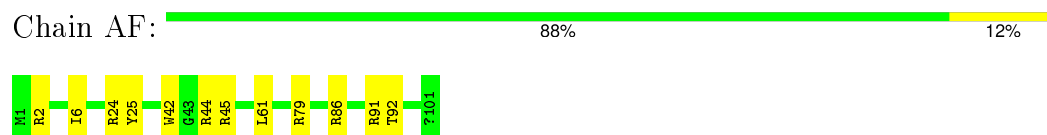
- Molecule 3: 30S ribosomal protein S4



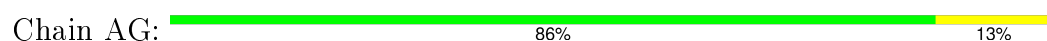
- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 7%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 85% 15%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 84% 16%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 92% 8%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 85% 15%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 86% 13%

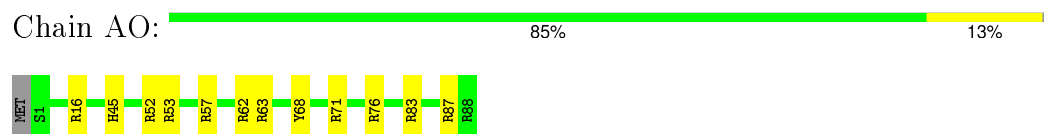


- Molecule 13: 30S ribosomal protein S14

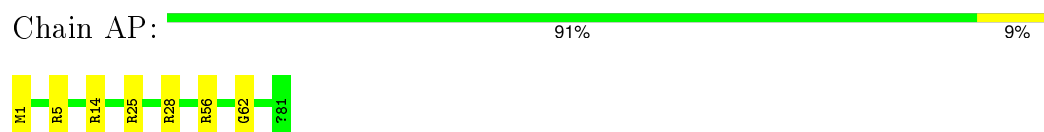
Chain AN: 82% 17%



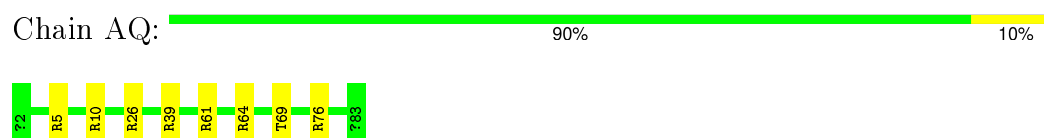
- Molecule 14: 30S ribosomal protein S15



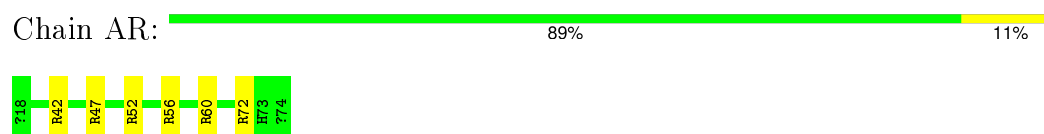
- Molecule 15: 30S ribosomal protein S16



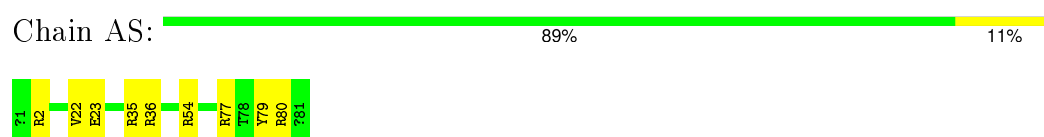
- Molecule 16: 30S ribosomal protein S17



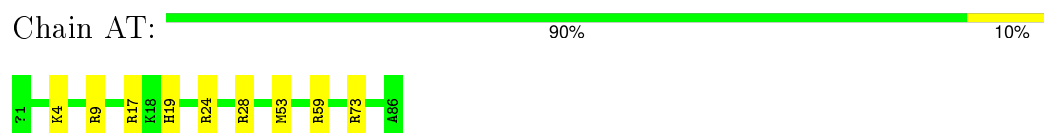
- Molecule 17: 30S ribosomal protein S18



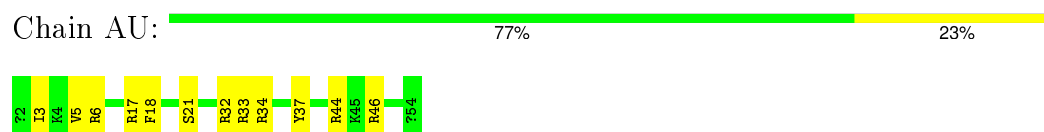
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



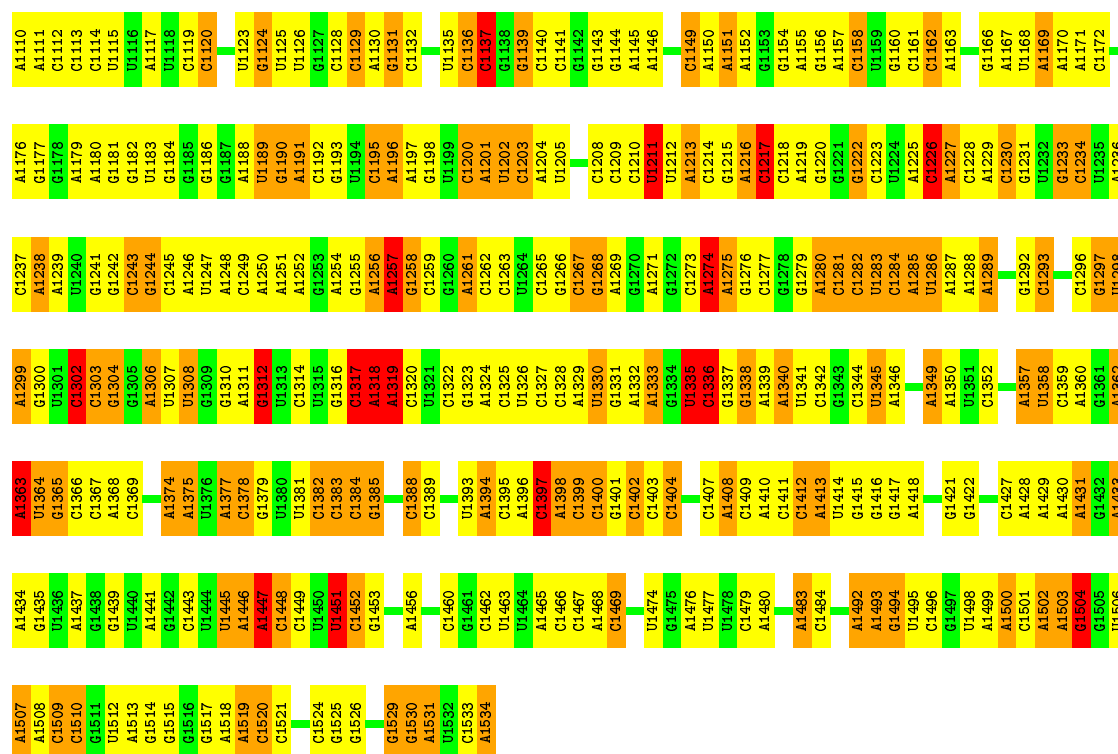
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA

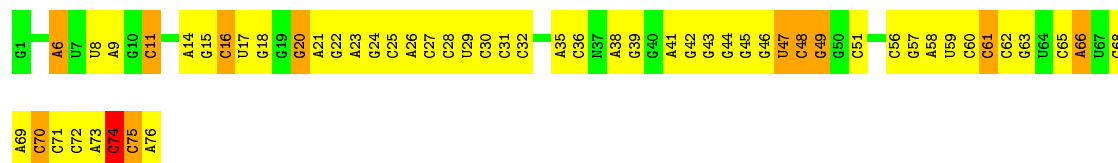


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C980	U981	A982	A983	C984	C985	U986	G987	G988	U989	C990	U991	G992	G993	A994	C995	A996	U997	C998	C999	A1000	C1001	C1002	A1003	A1004	A1005	U1006	C1007	U1008	U1009	A1010	A1011	A1012	G1013	G1014	G1015	U1016	U1017	G1018	U1019	A1020	A1021	A1022	U1025	G1026	C1027	C1028	U1029	U1030	C1031	G1032	A1033	C1034	A1035	A1036	C1037	C1038	G1039									
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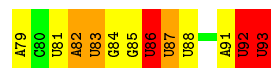
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 28% 57% 14%



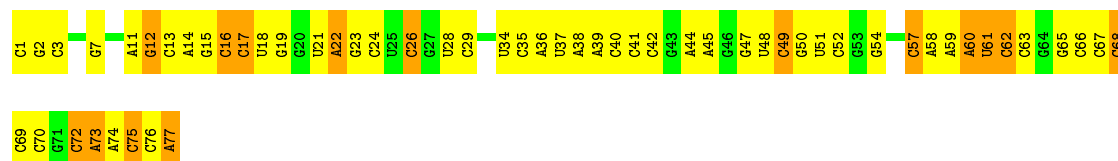
• Molecule 23: 5'-R(\*AP\*CP\*UP\*AP\*UP\*GP\*GP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*U)-3'

Chain A2: 20% 40% 20% 20%

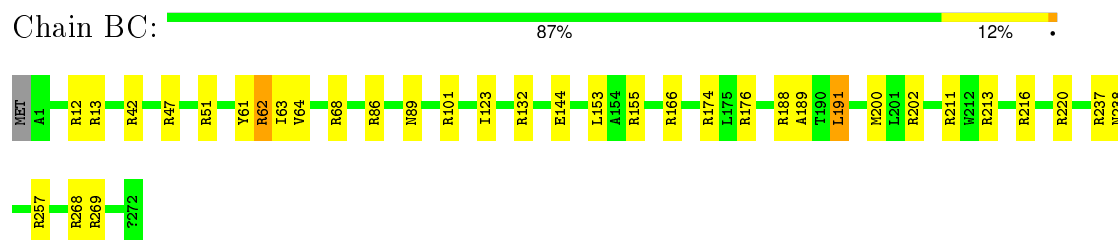


• Molecule 24: tRNA-fMet

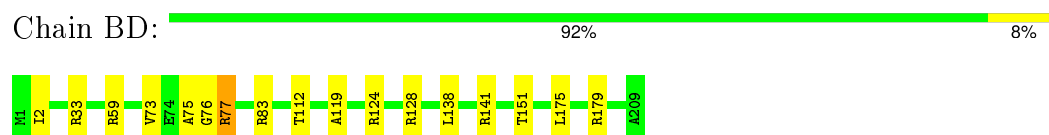
Chain A3: 26% 55% 19%



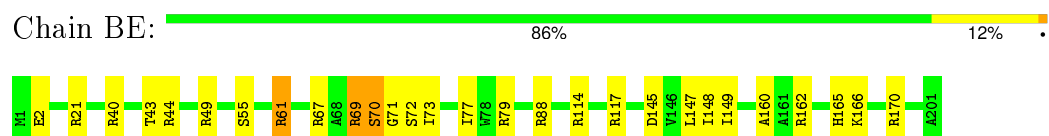
• Molecule 25: 50S ribosomal protein L2



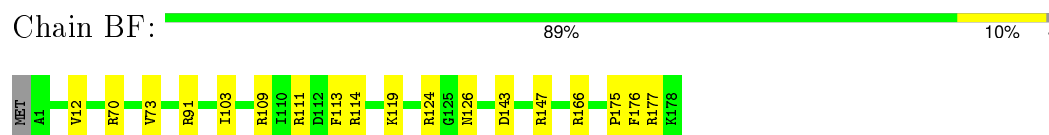
- Molecule 26: 50S ribosomal protein L3



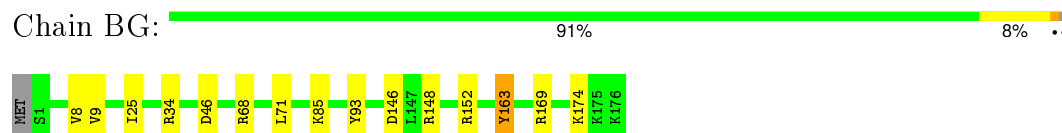
- Molecule 27: 50S ribosomal protein L4



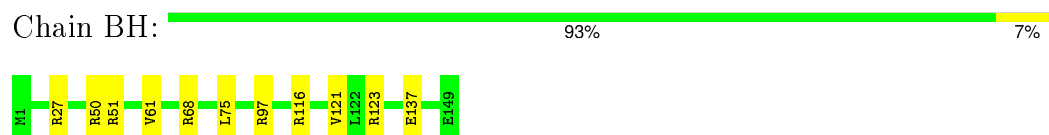
- Molecule 28: 50S ribosomal protein L5



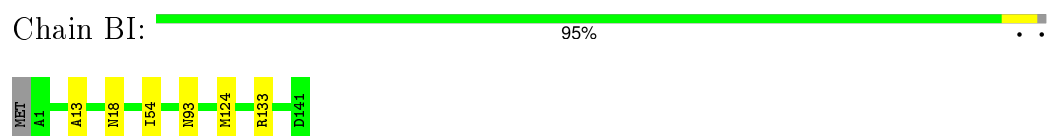
- Molecule 29: 50S ribosomal protein L6



- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L11



- Molecule 32: 50S ribosomal protein L13

Chain BJ:  94% 6%




- Molecule 33: 50S ribosomal protein L14

Chain BK:  89% 9% .



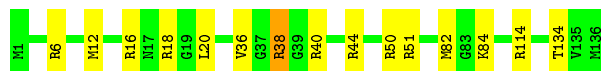
- Molecule 34: 50S ribosomal protein L15

Chain BL:  83% 15% ..




- Molecule 35: 50S ribosomal protein L16

Chain BM:  89% 10% .



- Molecule 36: 50S ribosomal protein L17

Chain BN:  88% 12% .




- Molecule 37: 50S ribosomal protein L18

Chain BO:  86% 11% ..



- Molecule 38: 50S ribosomal protein L19

Chain BP:  87% 10% ...



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  89% 9% ..



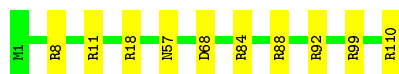
- Molecule 40: 50S ribosomal protein L21

Chain BR: 89% 11%



- Molecule 41: 50S ribosomal protein L22

Chain BS: 91% 9%



- Molecule 42: 50S ribosomal protein L23

Chain BT: 83% 17%



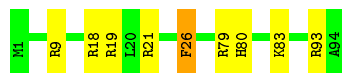
- Molecule 43: 50S ribosomal protein L24

Chain BU: 86% 13% ..



- Molecule 44: 50S ribosomal protein L25

Chain BV: 90% 9% .



- Molecule 45: 50S ribosomal protein L27

Chain BW: 88% 13%



- Molecule 46: 50S ribosomal protein L28

Chain BX: 78% 18% ..





- Molecule 47: 50S ribosomal protein L29

Chain BY:  89% 11%




- Molecule 48: 50S ribosomal protein L30

Chain BZ:  90% 7% ..




- Molecule 49: 50S ribosomal protein L32

Chain B0:  84% 12% ..




- Molecule 50: 50S ribosomal protein L33

Chain B1:  85% 15%




- Molecule 51: 50S ribosomal protein L34

Chain B2:  76% 24%




- Molecule 52: 50S ribosomal protein L35

Chain B3:  88% 11% .



- Molecule 53: 50S ribosomal protein L36

Chain B4:  87% 8% 5%

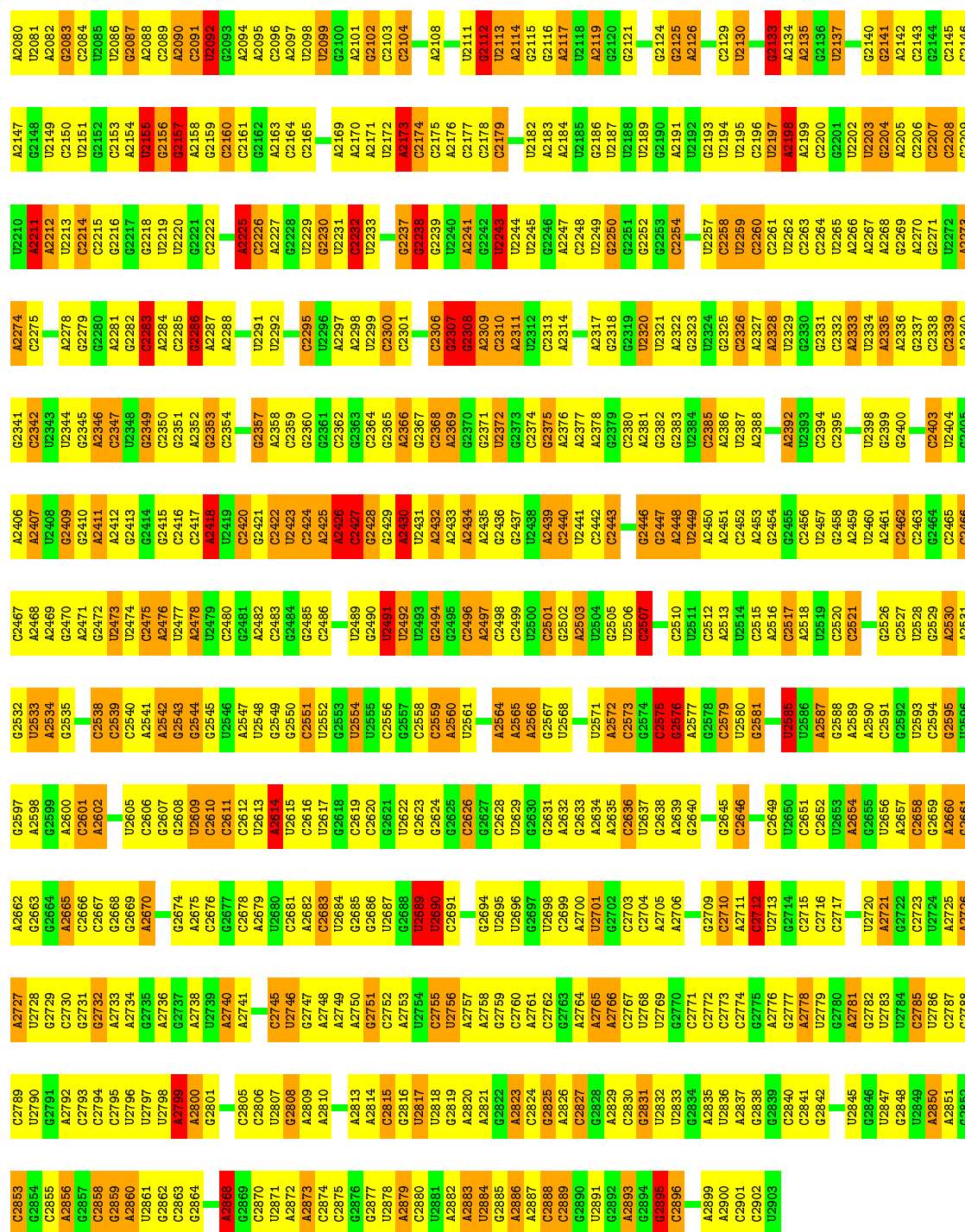


- Molecule 54: 23S ribosomal RNA

Chain BA:  22% 51% 23% .

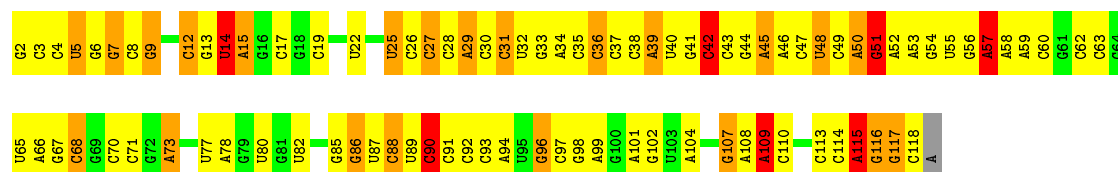
G1011	A947	C885	A820	U755	U694	C585	A504	G376	C316	C253	C192	A127	A64	G1
U1012	C948	A886	A821	A756	G695	G589	A805	G377	G317	G254	C128	C128	U65	G2
C1013	G949	U887	G822	G757	G696	U589	G506	G378	C318	A255	A195	C129	C66	U3
A1014	C951	C888	C823	G758	G697	G570	A507	G379	C319	A256	A196	C130	G13	U4
U1015	G952	C889	U824	G759	C698	U571	A508	C380	A320	A257	A197	A131	C69	A5
U1018	G953	G891	U825	G760	A699	A572	C509	A382	U321	G258	C198	U135	G70	A6
A1019	U826	A892	U827	A761	G700	U573	C510	C383	A322	U135	A199	U135	A71	G7
U1020	U828	A893	U829	G762	G701	A574	U511	A384	C323	A282	U200	G136	A72	G8
A1021	U829	U894	U830	G763	U702	A575	G512	C385	A324	G263	C201	U139	U73	G9
G1022	U830	U895	U831	A764	U703	U576	A513	G386	G325	C264	U202	U139	A74	A10
U1023	G831	A896	G832	G765	G704	G577	A514	U387	G326	A265	U203	A140	G75	C11
G1024	U832	A897	U833	U766	A705	U578	A515	G388	G327	G266	A204	G141	G76	U12
G1025	A833	C898	A834	U767	G706	C581	C516	G389	U328	C267	G205	A142	G77	U13
A1026	U834	A899	G834	U772	G707	A582	C517	U390	G329	C268	U206	C143	U78	A14
A1027	A835	A900	U835	U773	U708	G583	G518	A391	A330	C269	A207	A144	C79	G15
C1028	U836	C901	U836	G774	U709	U584	A519	U392	C331	A270	C208	C145	G80	C16
A1029	G837	C902	G837	G775	U710	G585	G520	C393	A332	A271	C209	A146	G81	C17
G1030	C838	C903	U838	G776	G711	A586	U521	C394	G333	A272	C210	C147	A83	U18
G1031	U839	G904	U839	G777	U714	C587	A522	U395	C334	G273	C211	U148	A84	A19
A1032	C840	A905	C840	G778	A715	U588	C523	G396	C335	C274	G212	A149	G85	C20
U1033	G841	U906	G841	U779	A716	A590	A526	U397	C336	C275	A213	U150	G86	A21
G1037	U842	C907	U842	G780	C717	U591	C527	C398	C337	U276	G214	A151	U87	G22
A1038	A844	C908	A844	A781	A718	A592	A528	G400	U339	A278	A216	U153	U88	G23
A1039	A845	A909	A845	A782	C719	G593	A529	A401	A340	A279	A217	U154	U90	G24
A1040	U846	A911	U846	A783	U720	C595	G530	A402	C341	U280	A218	A155	A91	G25
C1043	U847	C912	U847	G784	A721	U596	C531	U403	A342	C281	A219	A156	U92	G26
C1045	A848	C913	C848	G785	A722	U597	A532	A404	C343	C282	G220	C157	U93	A28
A1046	U849	U913	U849	G786	C723	U598	G533	U405	A344	U290	A221	U158	A94	A29
G1047	U850	C914	U850	C787	U724	A599	U534	G408	A345	G285	A222	G159	A95	A30
A1050	A851	C915	C851	A788	G725	G600	G535	A346	A346	U286	A223	A160	C96	G31
G1051	A852	G916	U852	A789	G726	C601	G536	A347	A347	G287	U224	A161	C97	G32
C1052	U853	A917	C853	U790	A727	A602	G537	A348	U349	U288	C225	U162	U98	C33
C1053	C854	U918	C854	G791	G728	A603	A538	A412	C350	G289	A226	C163	U99	U34
A1054	G857	C920	G857	A792	G729	G604	G539	C413	C351	G291	C228	C164	U100	G35
G1055	U858	C921	U858	A793	A730	G605	C540	C414	A352	U292	C229	U165	A101	G36
A1056	G859	C922	G859	C731	C732	U606	C541	A415	A353	U293	G230	A167	U102	C37
C1057	U860	A925	U860	G733	G733	A608	G543	U416	C353	U294	A231	A168	A103	A38
U1058	A861	G926	A861	A734	A734	A609	C544	C417	U355	U295	G232	G168	A104	C41
G1059	U862	C927	G862	A735	A735	C610	U545	U418	G356	U296	A233	U170	C105	A42
C1063	U863	A928	U863	C736	C736	C611	U546	C420	C357	G297	U234	U171	C106	A43
C1064	C864	U929	C864	A737	G737	G612	C547	C421	U358	U298	U235	A172	G108	A44
U1065	A865	G930	A865	A738	G738	A613	G548	A422	C359	A299	C236	A173	C109	A45
G1066	U866	U931	U866	C739	A739	A614	G549	A423	U360	A300	C237	U174	G110	G46
A1067	C867	U932	C867	C740	G740	U615	C550	A424	A362	G301	C238	G175	A111	C47
C1068	U868	U933	U868	U741	U741	A616	G551	G425	A363	G302	C239	A176	U112	G48
A1069	G869	U934	G869	A742	A742	G488	U552	C426	G363	G303	C240	G177	U113	A49
G1070	U870	C935	U870	G881	G743	G489	U553	U427	C364	U304	A241	G178	U114	U50
C1071	U871	A936	U871	U883	U744	G490	U554	A428	U365	C305	G242	C179	U115	G51
A1072	U872	G937	U872	G884	G745	A491	G555	A429	C366	U306	U243	G180	C116	A52
G1073	U873	U938	U873	A885	U746	A492	A556	A430	G367	G307	A244	A181	G117	A53
C1074	C876	G942	C876	U886	U747	G496	U557	U431	A368	G308	G245	A182	A118	A56
A1075	U877	A941	U877	U887	U748	C623	C558	A432	U369	A309	C246	C183	A119	G57
G1076	A878	U943	A878	C814	A749	G625	G559	C433	G370	A310	G247	C184	U120	G58
C1077	C815	C944	C815	C815	A750	A626	C560	U434	A371	A311	G248	G188	G122	C61
A1078	C816	C945	C816	C817	A751	G627	G561	C435	G372	G312	C249	G189	A125	U62
C1079	C817	A946	C817	U752	A752	U628	U562	C436	U373	G313	G250	A190	A126	A63
A1080	G818	C947	G818	A753	A753	G629	A563	A374	G375	G315	G252	A191		
C1076	U754	A893	U754	U754	U754	G630	C564	A439						

A2015	A1963	C1768	A1640	A1579	C1518	G1455	U1391	C1330	U1267	A1205	A1142	A1077
U2016	G1994	U1769	A1641	A1580	G1519	G1456	A1392	G1331	A1268	G1205	A1143	U1078
U2017	G1985	C1706	G1642	G1581	A1522	U1457	A1393	G1332	A1269	C1208	A1144	C1079
G2018	C1894	G1770	G1643	C1582	A1523	U1458	A1394	G1333	C1270	C1209	C1145	A1080
A2019	C1895	C1708	G1644	A1583	G1524	G1459	A1395	G1334	A1271	U1210	C1146	U1081
A2020	C1896	A1772	G1645	U1584	G1525	U1460	A1396	C1335	A1272	G1211	A1147	U1082
C2021	G1897	C1774	G1646	C1585	A1526	C1461	A1397	A1336	U1273	C1211	U1148	U1083
U2022	U1898	U1775	U1647	A1586	G1527	C1462	C1398	G1337	A1274	G1212	U1149	A1084
C2023	G1776	G1776	U1648	G1587	A1528	C1463	C1399	G1338	A1275	A1213	G1149	A1085
G2024	U1777	U1714	G1649	U1588	A1529			G1339	A1276	A1214	C1150	A1086
C2025	U1714		A1650	U1589	G1530			G1340	G1277	G1215	C1151	G1087
			G1651	A1590	G1531	U1466	U1402	G1341	C1278	G1216	G1152	A1088
U2028	A1717	A1780	G1652	A1591	C1531	U1467	A1403	G1342		U1217	G1153	A1089
G2029	G1718	U1781	G1653	C1592	A1532	U1468	U1404	G1343		G1216	A1155	A1090
A2030	U1719	U1782	A1654	A1593	C1533	A1469	U1405	G1344	G1281	U1219	A1156	G1091
A2031	G1720	G1783	G1655	U1594	G1534	U1470	A1406	G1345	U1282	G1220	G1157	C1092
C2032	A1721	A1784	G1656	C1595	A1535	G1471	A1407	C1346	U1283	G1221	C1158	G1093
A2033	G1722	G1785	U1657	A1596	G1536	G1472	G1408	G1347	A1284	U1222	U1159	U1094
U2034	A1723	A1786	C1658	A1597	G1537	G1473	U1409	A1348	A1285	G1223	U1160	A1095
G2035	G1724	U1787		U1598	G1538	U1474	G1410	C1349	A1286	U1224	G1161	A1096
C2036	U1725	C1788	G1661	A1599	U1539	G1475		C1350	A1287	G1225		U1097
A2037	C1726	C1726		G1600	G1540	U1476	A1413	G1351	G1288	A1226	C1164	A1098
	C1727		A1664	G1601	C1541	A1477	U1415	C1352	C1289		A1165	G1099
G2040	C1728	C1728	G1665	U1602	U1542	U1480	G1416	A1353	C1291	C1230	C1167	C1100
A2042	U1729	U1730	G1666	A1603	G1543	U1481	C1417	A1354	G1292	A1230	G1168	U1101
C2043	G1731	C1730	G1667	C1604	A1544	G1482	G1418	G1355	C1293	U1231		C1102
A2044	C1732	G1731	A1668	G1605	A1545	G1483	A1419	G1356	U1294	G1232	A1169	A1103
C2045	G1733	C1732	G1669	C1606	G1546	U1484	A1420	C1357	C1295	C1233	C1170	C1104
	G1734	G1733	C1670	C1607	C1547	U1485	G1421	G1358	G1296	U1234	G1171	
G2046	G1735	G1734	A1671	A1608	A1548	U1486	G1422	A1359	C1297	G1235	C1172	U1108
C2047	A1735	A1735	A1672	A1609	A1549	U1487	G1423	G1360	G1298	G1236	U1173	C1109
G2048	G1736	G1735	G1673	A1610	G1550	C1488	G1424	G1361	C1299	A1237	U1174	G1110
C2049	U1738	C1800	G1674	C1611	A1551	U1489	U1425	G1362	G1300	G1238	A1175	A1111
A2050	A1739	A1801	C1675	G1612	A1552	A1490	G1426	C1363	A1301	G1239	U1176	G1112
A2051	G1740	A1802	A1676	G1613	U1553	G1491	A1427	G1364	A1302	U1240	G1177	U1113
A2052	C1741	A1803	A1677	A1614	U1554	G1492	C1428	A1365	G1303	A1241	C1178	C1114
G2053	U1742	C1804	A1678	C1615	G1555	G1493	G1429	A1366	A1304	U1242	G1179	
A2054	G1743	A1805	A1679	A1616	C1556	A1494	G1430	A1367	C1305	C1243	U1180	C1117
	A1744	C1806		C1617	C1557	U1495	A1431	G1368	C1306	A1244	U1181	C1118
	A1745	C1807	G1682	A1618	C1558	A1496	G1432	G1369	A1307	G1245	G1182	
A2058	U1746	A1808	G1683	G1619	U1559	U1497	A1433	C1370	A1308	A1246	G1185	C1121
A2059	U1747	A1809	G1684	G1620	G1560	C1498	A1434	G1371	G1309	G1247	G1186	G1122
A2060	C1748	A1810	C1685	G1621	C1561	U1499	G1435	U1372	G1310	G1248	G1187	C1123
G2061	A1749	A1811	C1686	G1622	U1562		G1436	A1373	U1249	U1249	G1187	
A2062	G1750	U1812		G1623	C1563		U1437	G1374	G1311	G1250	U1188	A1126
	U1751		A1689	U1624	U1563	A1502	C1438	U1375	U1312	C1251	A1189	A1127
A2068	C1752	A1815	G1695	A1625	C1564	A1503	U1439	C1376	U1313	G1252	G1189	G1128
C2064	G1753	A1816	A1690	A1626	C1565	A1504	A1439	G1377	G1314	A1253	G1190	A1129
C2065	C1754	G1817	C1691	G1627	A1566	A1505	U1440	G1378	C1315	A1254	G1191	
A2066	A1755	U1818	U1692	G1628	G1567	U1506	G1441	U1379		A1254	A1194	U1130
	U1756	A1819	U1693	U1629	G1568	C1507	U1442	U1379	G1319	U1255	A1195	G1131
A2070	G1756	C1820	C1694	A1630	A1569	A1508			C1320	G1256	G1196	U1132
A2071	U1757	U1820	G1695	G1631	A1570	A1509	C1446	G1382	A1321	C1257	A1197	A1133
C2072	A1758	A1821	G1696	A1632	A1571	A1510	C1447	A1383	A1322	A1260	G1197	A1134
C2073	U1759	G1822	G1697	G1633	A1572	G1511	G1448	A1384	C1323	A1261	C1198	C1135
A2074	C1760	A1823	A1698	A1634	C1573	G1512	G1449	A1385	G1324	C1261	U1199	G1136
G2075	G1761	C1824	G1699	A1635	U1574	U1513	G1450	A1386	U1325	A1262	G1200	G1137
U2076	C1762	U1825	A1700	U1636	C1575	G1514	C1451	A1387	U1326	U1263	U1201	G1138
A2077	G1763	G1826	A1701	A1637	U1576	A1515	G1452	A1388	A1327	A1264	G1202	G1139
C2078	C1764	G1827	G1702	C1638	U1577	G1516	A1453	G1389	A1265	A1265	U1203	C1140
U2079		G1828	G1703	C1639	U1578	G1517	C1454	U1390	U1329	G1266	A1204	U1141




• Molecule 55: 5S ribosomal RNA

Chain BB: 22% 53% 19% 6%



- Molecule 56: 50S ribosomal protein L1

Chain B5:  90% 5% 5%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	5083	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	0.69	0/1736	1.03	9/2340 (0.4%)
10	AK	0.73	0/894	1.13	9/1207 (0.7%)
11	AL	0.74	0/969	1.26	15/1300 (1.2%)
12	AM	0.74	0/884	1.34	17/1181 (1.4%)
13	AN	0.77	0/817	1.28	13/1088 (1.2%)
14	AO	0.70	0/722	1.21	11/964 (1.1%)
15	AP	0.76	0/648	1.24	6/870 (0.7%)
16	AQ	0.66	0/658	1.16	9/883 (1.0%)
17	AR	0.81	0/463	1.25	6/623 (1.0%)
18	AS	0.74	0/653	1.22	7/879 (0.8%)
19	AT	0.66	0/672	1.13	7/890 (0.8%)
2	AC	0.72	0/1651	1.15	18/2225 (0.8%)
20	AU	0.80	0/431	1.42	8/572 (1.4%)
21	AA	1.55	5/36759 (0.0%)	2.21	1980/57346 (3.5%)
22	A1	1.56	0/1668	2.21	89/2595 (3.4%)
23	A2	1.41	0/343	2.12	13/531 (2.4%)
24	A3	1.56	0/1722	2.23	97/2685 (3.6%)
25	BC	0.74	0/2121	1.29	28/2852 (1.0%)
26	BD	0.67	0/1586	1.13	9/2134 (0.4%)
27	BE	0.66	0/1571	1.19	15/2113 (0.7%)
28	BF	0.72	0/1444	1.16	10/1937 (0.5%)
29	BG	0.67	0/1343	1.16	7/1816 (0.4%)
3	AD	0.75	0/1665	1.22	19/2227 (0.9%)
30	BH	0.64	0/1122	1.12	8/1515 (0.5%)
31	BI	0.65	0/1046	1.04	1/1410 (0.1%)
32	BJ	0.72	0/1152	1.18	12/1551 (0.8%)
33	BK	0.72	0/947	1.25	10/1268 (0.8%)
34	BL	0.73	0/1054	1.43	15/1403 (1.1%)
35	BM	0.73	0/1093	1.21	9/1460 (0.6%)
36	BN	0.74	0/973	1.34	16/1301 (1.2%)
37	BO	0.72	0/902	1.27	13/1209 (1.1%)
38	BP	0.73	0/929	1.28	13/1242 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.77	0/960	1.33	11/1278 (0.9%)
4	AE	0.69	0/1119	1.14	13/1506 (0.9%)
40	BR	0.71	0/829	1.19	6/1107 (0.5%)
41	BS	0.64	0/864	1.19	9/1156 (0.8%)
42	BT	0.65	0/744	1.21	6/994 (0.6%)
43	BU	0.68	0/787	1.17	6/1051 (0.6%)
44	BV	0.69	0/766	1.14	6/1025 (0.6%)
45	BW	0.74	0/604	1.22	4/799 (0.5%)
46	BX	0.75	0/635	1.38	8/848 (0.9%)
47	BY	0.67	0/510	1.21	6/677 (0.9%)
48	BZ	0.68	0/453	1.18	4/605 (0.7%)
49	B0	0.72	0/450	1.25	5/599 (0.8%)
5	AF	0.72	0/835	1.12	9/1128 (0.8%)
50	B1	0.68	0/417	1.12	2/556 (0.4%)
51	B2	0.81	0/380	1.45	9/498 (1.8%)
52	B3	0.70	0/513	1.17	6/676 (0.9%)
53	B4	0.70	0/303	1.29	3/397 (0.8%)
54	BA	1.43	5/69796 (0.0%)	2.22	4096/108888 (3.8%)
55	BB	1.45	0/2800	2.19	160/4367 (3.7%)
56	B5	0.64	0/1673	1.07	8/2255 (0.4%)
6	AG	0.73	0/1188	1.25	18/1593 (1.1%)
7	AH	0.68	0/989	1.09	8/1326 (0.6%)
8	AI	0.79	0/1035	1.25	16/1377 (1.2%)
9	AJ	0.71	0/797	1.19	11/1079 (1.0%)
All	All	1.30	10/160085 (0.0%)	2.00	6929/239402 (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
21	AA	0	359
22	A1	0	16
23	A2	0	5
24	A3	0	8
3	AD	0	1
36	BN	0	1
37	BO	0	1
38	BP	0	2
46	BX	0	1
54	BA	0	692

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	29
All	All	0	1115

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1200	C	C4-N4	-5.60	1.28	1.33
54	BA	1526	C	C4-N4	-5.22	1.29	1.33
54	BA	2000	C	C4-N4	-5.18	1.29	1.33
21	AA	339	C	C4-N4	-5.17	1.29	1.33
54	BA	867	C	C4-N4	-5.15	1.29	1.33
54	BA	2073	C	C4-N4	-5.13	1.29	1.33
21	AA	311	C	C4-N4	-5.12	1.29	1.33
21	AA	1501	C	C4-N4	-5.08	1.29	1.33
54	BA	2532	G	C2-N2	-5.03	1.29	1.34
21	AA	27	G	C2-N2	-5.01	1.29	1.34

All (6929) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1981	A	O4'-C1'-N9	13.97	119.37	108.20
21	AA	1191	A	N1-C6-N6	-13.33	110.60	118.60
24	A3	60	A	N1-C6-N6	-13.05	110.77	118.60
54	BA	323	C	O4'-C1'-N1	12.75	118.40	108.20
21	AA	520	A	N1-C6-N6	-12.44	111.14	118.60
54	BA	983	A	N1-C6-N6	-12.32	111.21	118.60
21	AA	1251	A	N1-C6-N6	-12.17	111.30	118.60
54	BA	265	A	O4'-C1'-N9	12.09	117.87	108.20
54	BA	479	A	N1-C6-N6	-11.89	111.47	118.60
54	BA	1268	A	N1-C6-N6	-11.88	111.47	118.60
21	AA	1101	A	N1-C6-N6	-11.86	111.49	118.60
54	BA	2076	U	O4'-C1'-N1	11.81	117.65	108.20
21	AA	1289	A	N1-C6-N6	-11.72	111.57	118.60
21	AA	382	A	N1-C6-N6	-11.66	111.61	118.60
21	AA	162	A	N1-C6-N6	-11.64	111.61	118.60
54	BA	99	U	O4'-C1'-N1	11.64	117.52	108.20
21	AA	729	A	N1-C6-N6	-11.62	111.63	118.60
54	BA	63	A	N1-C6-N6	-11.61	111.63	118.60
21	AA	1500	A	N1-C6-N6	-11.61	111.64	118.60
54	BA	2366	A	N1-C6-N6	-11.59	111.64	118.60
21	AA	1363	A	N1-C6-N6	-11.55	111.67	118.60
54	BA	2198	A	N1-C6-N6	-11.52	111.69	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2307	G	O4'-C1'-N9	11.50	117.40	108.20
54	BA	716	A	N1-C6-N6	-11.43	111.74	118.60
54	BA	1347	A	N1-C6-N6	-11.37	111.78	118.60
54	BA	2829	A	N1-C6-N6	-11.36	111.78	118.60
24	A3	11	A	N1-C6-N6	-11.35	111.79	118.60
54	BA	1854	A	N1-C6-N6	-11.34	111.80	118.60
21	AA	794	A	N1-C6-N6	-11.33	111.80	118.60
54	BA	2541	A	N1-C6-N6	-11.33	111.80	118.60
54	BA	1784	A	N1-C6-N6	-11.31	111.81	118.60
54	BA	1635	A	N1-C6-N6	-11.27	111.83	118.60
21	AA	72	A	N1-C6-N6	-11.27	111.84	118.60
54	BA	1815	A	N1-C6-N6	-11.25	111.85	118.60
54	BA	1943	U	O4'-C1'-N1	11.25	117.20	108.20
24	A3	77	A	N1-C6-N6	-11.24	111.86	118.60
21	AA	554	A	N1-C6-N6	-11.21	111.87	118.60
54	BA	2435	A	N1-C6-N6	-11.18	111.89	118.60
54	BA	2478	A	N1-C6-N6	-11.16	111.90	118.60
54	BA	219	A	N1-C6-N6	-11.09	111.94	118.60
54	BA	2020	A	N1-C6-N6	-11.07	111.96	118.60
21	AA	523	A	N1-C6-N6	-11.07	111.96	118.60
54	BA	2602	A	N1-C6-N6	-11.07	111.96	118.60
54	BA	2516	A	N1-C6-N6	-11.06	111.96	118.60
54	BA	1495	A	N1-C6-N6	-11.06	111.97	118.60
54	BA	2333	A	N1-C6-N6	-11.04	111.98	118.60
54	BA	614	A	O4'-C1'-N9	11.03	117.02	108.20
54	BA	1596	A	N1-C6-N6	-11.02	111.99	118.60
54	BA	2765	A	N1-C6-N6	-11.02	111.99	118.60
54	BA	2882	A	N1-C6-N6	-11.01	111.99	118.60
21	AA	189	A	N1-C6-N6	-10.99	112.00	118.60
54	BA	1069	A	N1-C6-N6	-10.99	112.01	118.60
54	BA	1801	A	N1-C6-N6	-10.96	112.02	118.60
35	BM	38	ARG	NE-CZ-NH1	10.94	125.77	120.30
54	BA	1690	A	N1-C6-N6	-10.94	112.03	118.60
21	AA	152	A	N1-C6-N6	-10.93	112.04	118.60
54	BA	1014	A	N1-C6-N6	-10.92	112.05	118.60
22	A1	59	U	O4'-C1'-N1	10.90	116.92	108.20
21	AA	704	A	N1-C6-N6	-10.90	112.06	118.60
54	BA	2327	A	N1-C6-N6	-10.89	112.06	118.60
15	AP	5	ARG	NE-CZ-NH1	10.87	125.74	120.30
21	AA	1155	A	N1-C6-N6	-10.87	112.08	118.60
54	BA	2682	A	N1-C6-N6	-10.86	112.08	118.60
54	BA	2560	A	N1-C6-N6	-10.84	112.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2266	A	N1-C6-N6	-10.82	112.11	118.60
3	AD	69	ARG	NE-CZ-NH1	10.80	125.70	120.30
54	BA	2665	A	N1-C6-N6	-10.80	112.12	118.60
21	AA	6	G	O4'-C1'-N9	10.80	116.84	108.20
55	BB	94	A	N1-C6-N6	-10.78	112.13	118.60
21	AA	1318	A	N1-C6-N6	-10.78	112.14	118.60
21	AA	28	A	N1-C6-N6	-10.77	112.14	118.60
54	BA	2114	A	N1-C6-N6	-10.77	112.14	118.60
54	BA	1127	A	N1-C6-N6	-10.73	112.16	118.60
54	BA	2883	A	N1-C6-N6	-10.70	112.18	118.60
54	BA	2547	A	N1-C6-N6	-10.70	112.18	118.60
21	AA	665	A	N1-C6-N6	-10.69	112.18	118.60
54	BA	2418	A	N1-C6-N6	-10.68	112.19	118.60
21	AA	274	A	N1-C6-N6	-10.68	112.19	118.60
54	BA	910	A	N1-C6-N6	-10.68	112.19	118.60
29	BG	169	ARG	NE-CZ-NH1	10.66	125.63	120.30
21	AA	325	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1086	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1679	A	N1-C6-N6	-10.64	112.21	118.60
54	BA	2748	A	N1-C6-N6	-10.62	112.23	118.60
54	BA	1523	U	O4'-C1'-N1	10.62	116.69	108.20
54	BA	546	U	O4'-C1'-N1	10.62	116.69	108.20
54	BA	2675	A	N1-C6-N6	-10.60	112.24	118.60
21	AA	196	A	N1-C6-N6	-10.59	112.25	118.60
21	AA	546	A	N1-C6-N6	-10.58	112.25	118.60
54	BA	1494	A	N1-C6-N6	-10.56	112.27	118.60
54	BA	2564	A	N1-C6-N6	-10.55	112.27	118.60
54	BA	975	A	N1-C6-N6	-10.50	112.30	118.60
27	BE	114	ARG	NE-CZ-NH1	10.50	125.55	120.30
54	BA	1544	A	N1-C6-N6	-10.49	112.30	118.60
54	BA	2163	A	N1-C6-N6	-10.49	112.30	118.60
54	BA	6	A	N1-C6-N6	-10.49	112.31	118.60
21	AA	435	A	N1-C6-N6	-10.48	112.31	118.60
54	BA	1285	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	241	A	N1-C6-N6	-10.46	112.32	118.60
21	AA	452	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	119	A	N1-C6-N6	-10.43	112.34	118.60
21	AA	130	A	N1-C6-N6	-10.41	112.35	118.60
54	BA	1932	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	1287	A	N1-C6-N6	-10.39	112.36	118.60
54	BA	1637	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	2309	A	N1-C6-N6	-10.36	112.38	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1287	A	N1-C6-N6	-10.36	112.38	118.60
54	BA	1700	A	N1-C6-N6	-10.36	112.39	118.60
21	AA	1333	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	1342	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	959	A	N1-C6-N6	-10.34	112.40	118.60
54	BA	670	A	N1-C6-N6	-10.34	112.40	118.60
21	AA	499	A	N1-C6-N6	-10.34	112.40	118.60
54	BA	1551	A	N1-C6-N6	-10.33	112.40	118.60
54	BA	1618	A	N1-C6-N6	-10.33	112.40	118.60
54	BA	2287	A	N1-C6-N6	-10.33	112.40	118.60
54	BA	1783	A	N1-C6-N6	-10.33	112.40	118.60
54	BA	2657	A	N1-C6-N6	-10.32	112.41	118.60
54	BA	294	A	N1-C6-N6	-10.31	112.42	118.60
54	BA	941	A	N1-C6-N6	-10.31	112.42	118.60
54	BA	931	U	O4'-C1'-N1	10.28	116.43	108.20
54	BA	1327	A	N1-C6-N6	-10.28	112.43	118.60
21	AA	167	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	111	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	1655	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	2734	A	N1-C6-N6	-10.26	112.45	118.60
54	BA	2530	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	933	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	1960	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	2858	C	N3-C2-O2	-10.24	114.73	121.90
21	AA	1360	A	N1-C6-N6	-10.23	112.46	118.60
54	BA	160	A	N1-C6-N6	-10.22	112.47	118.60
21	AA	718	A	N1-C6-N6	-10.22	112.47	118.60
21	AA	315	A	N1-C6-N6	-10.21	112.47	118.60
54	BA	2750	A	N1-C6-N6	-10.21	112.47	118.60
39	BQ	47	ARG	NE-CZ-NH1	10.21	125.40	120.30
54	BA	2211	A	N1-C6-N6	-10.21	112.48	118.60
21	AA	50	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	2788	C	N3-C2-O2	-10.19	114.77	121.90
54	BA	1754	A	N1-C6-N6	-10.18	112.49	118.60
21	AA	831	A	N1-C6-N6	-10.17	112.50	118.60
21	AA	1044	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	280	U	O4'-C1'-N1	10.15	116.32	108.20
21	AA	1329	A	N1-C6-N6	-10.14	112.51	118.60
34	BL	132	ARG	NE-CZ-NH1	10.14	125.37	120.30
21	AA	313	A	N1-C6-N6	-10.14	112.52	118.60
21	AA	539	A	N1-C6-N6	-10.13	112.52	118.60
54	BA	2339	C	O4'-C1'-N1	10.12	116.29	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	675	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	1699	G	O4'-C1'-N9	10.11	116.28	108.20
54	BA	981	A	N1-C6-N6	-10.09	112.54	118.60
21	AA	563	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	1332	G	O4'-C1'-N9	10.09	116.27	108.20
54	BA	1794	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	1762	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	2776	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	21	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	800	A	N1-C6-N6	-10.06	112.56	118.60
21	AA	460	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	2726	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	8	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	1493	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	1028	A	N1-C6-N6	-10.04	112.57	118.60
54	BA	2476	A	N1-C6-N6	-10.04	112.57	118.60
21	AA	59	A	N1-C6-N6	-10.04	112.58	118.60
21	AA	1396	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	56	A	N1-C6-N6	-10.02	112.59	118.60
54	BA	2893	A	N1-C6-N6	-10.02	112.59	118.60
54	BA	199	A	N1-C6-N6	-10.01	112.59	118.60
54	BA	447	A	N1-C6-N6	-10.01	112.59	118.60
24	A3	74	A	N1-C6-N6	-10.01	112.59	118.60
21	AA	621	A	N1-C6-N6	-10.01	112.60	118.60
54	BA	1606	C	O4'-C1'-N1	10.01	116.20	108.20
54	BA	899	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	441	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	896	A	N1-C6-N6	-9.99	112.60	118.60
54	BA	173	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	1591	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	125	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	2547	A	O4'-C1'-N9	9.96	116.17	108.20
54	BA	621	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	1275	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	988	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	1261	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	288	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	321	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	1789	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	203	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	721	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	466	A	N1-C6-N6	-9.92	112.65	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1169	A	N1-C6-N6	-9.91	112.65	118.60
54	BA	1308	A	N1-C6-N6	-9.91	112.65	118.60
54	BA	38	A	N1-C6-N6	-9.91	112.66	118.60
21	AA	1093	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1889	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	635	A	N1-C6-N6	-9.90	112.66	118.60
24	A3	22	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	677	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1142	A	N1-C6-N6	-9.89	112.67	118.60
26	BD	141	ARG	NE-CZ-NH1	9.89	125.24	120.30
54	BA	699	A	N1-C6-N6	-9.89	112.67	118.60
54	BA	2173	A	N1-C6-N6	-9.88	112.67	118.60
25	BC	12	ARG	NE-CZ-NH1	9.88	125.24	120.30
54	BA	432	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	83	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	2589	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	574	A	N1-C6-N6	-9.87	112.67	118.60
54	BA	1735	A	N1-C6-N6	-9.88	112.67	118.60
21	AA	1227	A	N1-C6-N6	-9.87	112.68	118.60
46	BX	73	ARG	NE-CZ-NH1	9.87	125.23	120.30
54	BA	374	A	N1-C6-N6	-9.86	112.68	118.60
54	BA	1532	A	N1-C6-N6	-9.86	112.69	118.60
54	BA	643	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	2274	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	1569	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	1265	A	N1-C6-N6	-9.84	112.69	118.60
54	BA	2679	A	N1-C6-N6	-9.84	112.69	118.60
21	AA	356	A	N1-C6-N6	-9.84	112.70	118.60
21	AA	1250	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	2005	A	N1-C6-N6	-9.83	112.70	118.60
21	AA	155	A	N1-C6-N6	-9.82	112.71	118.60
45	BW	10	ARG	NE-CZ-NH1	9.82	125.21	120.30
54	BA	1336	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	727	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	2461	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	933	A	O4'-C1'-N9	9.80	116.04	108.20
54	BA	2433	A	N1-C6-N6	-9.79	112.72	118.60
54	BA	849	A	N1-C6-N6	-9.79	112.73	118.60
54	BA	1272	A	N1-C6-N6	-9.79	112.73	118.60
54	BA	1378	A	N1-C6-N6	-9.78	112.73	118.60
21	AA	1158	C	N3-C2-O2	-9.78	115.06	121.90
54	BA	2104	C	N3-C2-O2	-9.77	115.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	960	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	1439	A	N1-C6-N6	-9.77	112.74	118.60
22	A1	35	A	N1-C6-N6	-9.76	112.75	118.60
54	BA	661	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	2727	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	1676	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2566	A	N1-C6-N6	-9.73	112.76	118.60
21	AA	1434	A	N1-C6-N6	-9.73	112.76	118.60
21	AA	696	A	N1-C6-N6	-9.73	112.76	118.60
37	BO	15	ARG	NE-CZ-NH1	9.73	125.16	120.30
39	BQ	57	ARG	NE-CZ-NH1	9.72	125.16	120.30
21	AA	766	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	915	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	1036	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	10	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	2088	A	N1-C6-N6	-9.70	112.78	118.60
18	AS	80	ARG	NE-CZ-NH1	9.69	125.14	120.30
54	BA	10	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	1088	A	N1-C6-N6	-9.69	112.79	118.60
55	BB	109	A	N1-C6-N6	-9.69	112.79	118.60
21	AA	579	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	354	A	N1-C6-N6	-9.67	112.80	118.60
22	A1	69	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	2297	A	N1-C6-N6	-9.66	112.80	118.60
21	AA	7	A	N1-C6-N6	-9.66	112.81	118.60
14	AO	76	ARG	NE-CZ-NH1	9.64	125.12	120.30
54	BA	1253	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	2886	A	O4'-C1'-N9	9.63	115.91	108.20
54	BA	2766	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	1745	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	914	A	N1-C6-N6	-9.62	112.83	118.60
55	BB	39	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	199	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	802	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1490	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	547	A	N1-C6-N6	-9.61	112.84	118.60
54	BA	474	G	O4'-C1'-N9	9.60	115.88	108.20
54	BA	2670	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	1640	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	2503	A	O4'-C1'-N9	9.59	115.87	108.20
21	AA	706	A	N1-C6-N6	-9.59	112.85	118.60
21	AA	1082	A	N1-C6-N6	-9.57	112.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1981	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	633	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	1938	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	1286	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	616	A	N1-C6-N6	-9.56	112.87	118.60
54	BA	2030	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	1254	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	227	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	278	A	N1-C6-N6	-9.54	112.88	118.60
39	BQ	5	ARG	NE-CZ-NH1	9.53	125.06	120.30
54	BA	412	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2800	A	N1-C6-N6	-9.53	112.89	118.60
54	BA	1672	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	443	A	N1-C6-N6	-9.52	112.89	118.60
21	AA	602	A	N1-C6-N6	-9.52	112.89	118.60
21	AA	1016	A	N1-C6-N6	-9.52	112.89	118.60
21	AA	456	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	752	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	1304	A	N1-C6-N6	-9.52	112.89	118.60
21	AA	825	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	231	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	2108	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	2176	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	460	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	1073	A	N1-C6-N6	-9.51	112.90	118.60
21	AA	383	A	N1-C6-N6	-9.51	112.90	118.60
21	AA	101	A	N1-C6-N6	-9.50	112.90	118.60
21	AA	622	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	94	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	528	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	653	U	O4'-C1'-N1	9.50	115.80	108.20
3	AD	164	ARG	NE-CZ-NH1	9.49	125.04	120.30
21	AA	262	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	2711	A	N1-C6-N6	-9.48	112.91	118.60
33	BK	78	ARG	NE-CZ-NH1	9.48	125.04	120.30
34	BL	78	ARG	NE-CZ-NH1	9.48	125.04	120.30
54	BA	2377	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	753	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1912	A	N1-C6-N6	-9.47	112.92	118.60
51	B2	35	ARG	NE-CZ-NH1	9.47	125.03	120.30
54	BA	1966	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	303	A	N1-C6-N6	-9.46	112.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1307	A	N1-C6-N6	-9.46	112.92	118.60
21	AA	1158	C	N1-C2-O2	9.46	124.58	118.90
29	BG	68	ARG	NE-CZ-NH1	9.46	125.03	120.30
54	BA	590	A	N1-C6-N6	-9.46	112.93	118.60
55	BB	34	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1529	G	O4'-C1'-N9	9.45	115.76	108.20
54	BA	2425	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	348	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	1248	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	66	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	1176	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	877	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	2392	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	886	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	507	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	864	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	459	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	533	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	833	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	860	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	28	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	1366	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	1916	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	1269	A	N1-C6-N6	-9.40	112.96	118.60
22	A1	76	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	626	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	1451	C	O4'-C1'-N1	9.39	115.71	108.20
54	BA	819	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	223	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	2169	A	O4'-C1'-N9	9.38	115.70	108.20
54	BA	2654	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	613	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	55	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1009	A	N1-C6-N6	-9.37	112.98	118.60
16	AQ	64	ARG	NE-CZ-NH1	9.37	124.98	120.30
54	BA	14	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1359	A	N1-C6-N6	-9.36	112.98	118.60
21	AA	1503	A	N1-C6-N6	-9.36	112.98	118.60
21	AA	1067	A	N1-C6-N6	-9.36	112.98	118.60
21	AA	432	A	N1-C6-N6	-9.36	112.99	118.60
54	BA	1127	A	O4'-C1'-N9	9.35	115.68	108.20
21	AA	181	A	N1-C6-N6	-9.34	113.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	393	A	N1-C6-N6	-9.34	113.00	118.60
21	AA	465	A	N1-C6-N6	-9.34	113.00	118.60
21	AA	607	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	2565	A	N1-C6-N6	-9.32	113.01	118.60
24	A3	44	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	44	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	1744	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	1749	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	408	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	1468	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	1610	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	1216	A	N1-C6-N6	-9.31	113.02	118.60
54	BA	371	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	453	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	2015	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	977	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	2590	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	91	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	1321	A	N1-C6-N6	-9.29	113.03	118.60
50	B1	27	ARG	NE-CZ-NH1	9.27	124.93	120.30
54	BA	2158	A	N1-C6-N6	-9.27	113.04	118.60
55	BB	45	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1493	C	N3-C2-O2	-9.26	115.42	121.90
21	AA	1531	A	N1-C6-N6	-9.26	113.05	118.60
54	BA	1230	A	N1-C6-N6	-9.25	113.05	118.60
35	BM	40	ARG	NE-CZ-NH1	9.25	124.92	120.30
54	BA	1940	U	O4'-C1'-N1	9.25	115.60	108.20
54	BA	2278	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	401	A	N1-C6-N6	-9.24	113.05	118.60
25	BC	211	ARG	NE-CZ-NH1	9.24	124.92	120.30
54	BA	1757	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	366	A	N1-C6-N6	-9.23	113.06	118.60
55	BB	115	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	780	A	N1-C6-N6	-9.23	113.06	118.60
22	A1	47	U	O4'-C1'-N1	9.23	115.58	108.20
54	BA	1919	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	310	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	866	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	2101	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	1519	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	572	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	300	A	N1-C6-N6	-9.20	113.08	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1652	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	510	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	340	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	706	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	222	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	2781	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	1301	A	O4'-C1'-N9	9.19	115.55	108.20
21	AA	119	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	861	A	N1-C6-N6	-9.18	113.09	118.60
21	AA	109	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	279	A	N1-C6-N6	-9.18	113.09	118.60
21	AA	1080	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1084	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	2814	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	1413	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	226	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	2117	A	O4'-C1'-N9	9.17	115.53	108.20
40	BR	21	ARG	NE-CZ-NH1	9.16	124.88	120.30
54	BA	2700	A	N1-C6-N6	-9.16	113.10	118.60
7	AH	116	ARG	NE-CZ-NH1	9.16	124.88	120.30
21	AA	655	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	514	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	936	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	300	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	964	A	N1-C6-N6	-9.15	113.11	118.60
36	BN	96	ARG	NE-CZ-NH1	9.15	124.87	120.30
54	BA	127	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	218	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	130	A	C1'-O4'-C4'	-9.14	102.59	109.90
21	AA	26	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	1508	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	1586	A	N1-C6-N6	-9.13	113.12	118.60
32	BJ	99	ARG	NE-CZ-NH1	9.13	124.86	120.30
54	BA	1010	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	195	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	1346	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2858	C	O4'-C1'-N1	9.12	115.50	108.20
54	BA	2317	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	329	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	648	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	501	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	654	A	N1-C6-N6	-9.11	113.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2666	C	N3-C2-O2	-9.11	115.53	121.90
54	BA	1590	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	1848	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	44	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	984	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	947	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	352	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	2013	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	655	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	141	G	O4'-C1'-N9	9.06	115.45	108.20
54	BA	2287	A	O4'-C1'-N9	9.06	115.45	108.20
54	BA	1847	A	N1-C6-N6	-9.06	113.17	118.60
21	AA	1213	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	1525	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	1677	A	N1-C6-N6	-9.06	113.17	118.60
21	AA	197	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	637	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	1408	A	N1-C6-N6	-9.05	113.17	118.60
46	BX	26	ARG	NE-CZ-NH2	9.04	124.82	120.30
25	BC	62	ARG	NE-CZ-NH1	9.04	124.82	120.30
54	BA	104	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	1871	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2600	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	1570	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	2094	A	N1-C6-N6	-9.03	113.18	118.60
7	AH	14	ARG	NE-CZ-NH1	9.02	124.81	120.30
21	AA	487	A	N1-C6-N6	-9.02	113.19	118.60
55	BB	104	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	182	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2887	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2705	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	1441	A	N1-C6-N6	-9.01	113.19	118.60
55	BB	66	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	1365	A	N1-C6-N6	-9.01	113.20	118.60
54	BA	204	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	728	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	793	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1936	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	1171	A	N1-C6-N6	-8.99	113.20	118.60
54	BA	644	A	C5-C6-N1	8.99	122.19	117.70
54	BA	1096	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	1419	A	N1-C6-N6	-8.99	113.21	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BD	59	ARG	NE-CZ-NH1	8.98	124.79	120.30
55	BB	50	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	16	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	389	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	1130	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	1518	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	1668	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	777	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	2147	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	2614	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	975	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	33	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	262	A	C5-C6-N1	8.96	122.18	117.70
43	BU	85	ARG	NE-CZ-NH1	8.96	124.78	120.30
54	BA	272	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1383	A	N1-C6-N6	-8.96	113.22	118.60
22	A1	73	A	N1-C6-N6	-8.96	113.23	118.60
21	AA	364	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	2741	A	N1-C6-N6	-8.95	113.23	118.60
21	AA	336	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	423	A	N1-C6-N6	-8.95	113.23	118.60
8	AI	98	ARG	NE-CZ-NH1	8.94	124.77	120.30
54	BA	750	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	505	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	2646	C	O4'-C1'-N1	8.94	115.35	108.20
21	AA	478	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	872	A	C1'-O4'-C4'	-8.93	102.75	109.90
21	AA	1431	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	1609	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	2635	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	1791	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	582	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	1252	A	N1-C6-N6	-8.93	113.25	118.60
1	AB	224	ARG	NE-CZ-NH1	8.92	124.76	120.30
21	AA	1357	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	1552	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	1000	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	1952	A	N1-C6-N6	-8.92	113.25	118.60
21	AA	174	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	346	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	2434	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	2764	A	N1-C6-N6	-8.91	113.25	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1367	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1505	A	N1-C6-N6	-8.91	113.26	118.60
21	AA	1021	A	N1-C6-N6	-8.89	113.27	118.60
54	BA	2051	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	270	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	535	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	1400	C	N3-C2-O2	-8.88	115.68	121.90
21	AA	349	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	911	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	2411	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	630	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	608	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	1105	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1928	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	743	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1205	A	O4'-C1'-N9	8.87	115.29	108.20
54	BA	213	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	2453	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	820	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	2095	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	2587	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	572	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	906	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	294	A	C5-C6-N1	8.84	122.12	117.70
54	BA	1214	A	N1-C6-N6	-8.84	113.29	118.60
54	BA	1970	A	N1-C6-N6	-8.84	113.30	118.60
29	BG	148	ARG	NE-CZ-NH1	8.84	124.72	120.30
21	AA	344	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	1508	A	O4'-C1'-N9	8.83	115.27	108.20
54	BA	2388	A	N1-C6-N6	-8.83	113.30	118.60
17	AR	60	ARG	NE-CZ-NH1	8.83	124.72	120.30
54	BA	1871	A	C5-C6-N1	8.83	122.11	117.70
54	BA	2534	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	2738	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	781	A	N1-C6-N6	-8.82	113.31	118.60
24	A3	11	A	C5-C6-N1	8.82	122.11	117.70
54	BA	477	A	C5-C6-N1	8.82	122.11	117.70
54	BA	347	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	919	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	272	A	O4'-C1'-N9	8.81	115.25	108.20
55	BB	34	A	C5-C6-N1	8.81	122.11	117.70
54	BA	101	A	N1-C6-N6	-8.80	113.32	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	531	C	O4'-C1'-N1	8.80	115.24	108.20
21	AA	792	A	O4'-C1'-N9	8.80	115.24	108.20
21	AA	749	A	N1-C6-N6	-8.79	113.32	118.60
54	BA	1535	A	N1-C6-N6	-8.79	113.32	118.60
21	AA	631	C	N3-C2-O2	-8.79	115.75	121.90
55	BB	15	A	O4'-C1'-N9	8.79	115.23	108.20
21	AA	759	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1451	C	N3-C2-O2	-8.79	115.75	121.90
21	AA	968	A	N1-C6-N6	-8.78	113.33	118.60
39	BQ	63	ARG	NE-CZ-NH1	8.79	124.69	120.30
54	BA	472	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	602	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	1394	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	1626	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2059	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2458	G	O4'-C1'-N9	8.78	115.22	108.20
54	BA	2154	A	N1-C6-N6	-8.78	113.33	118.60
18	AS	77	ARG	NE-CZ-NH1	8.77	124.69	120.30
21	AA	509	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2212	A	O4'-C1'-N9	8.77	115.22	108.20
54	BA	2706	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	1004	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	497	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2639	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	889	A	N1-C6-N6	-8.76	113.35	118.60
55	BB	108	A	N1-C6-N6	-8.76	113.35	118.60
21	AA	1163	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	332	A	N1-C6-N6	-8.75	113.35	118.60
24	A3	3	C	N3-C2-O2	-8.74	115.78	121.90
54	BA	825	A	N1-C6-N6	-8.74	113.35	118.60
21	AA	98	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1603	A	N1-C6-N6	-8.74	113.36	118.60
22	A1	6	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1393	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	429	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	751	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	1204	A	N1-C6-N6	-8.72	113.36	118.60
21	AA	787	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	872	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	396	C	N3-C2-O2	-8.71	115.80	121.90
38	BP	52	ARG	NE-CZ-NH1	8.71	124.66	120.30
42	BT	76	ARG	NE-CZ-NH1	8.71	124.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1254	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	913	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	783	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	689	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	1276	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	1597	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	722	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	216	A	N1-C6-N6	-8.69	113.38	118.60
54	BA	2471	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	1274	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	179	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	814	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1248	G	O4'-C1'-N9	8.68	115.14	108.20
54	BA	603	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	784	G	O4'-C1'-N9	8.67	115.14	108.20
54	BA	1705	A	N1-C6-N6	-8.67	113.39	118.60
54	BA	1205	A	N1-C6-N6	-8.67	113.40	118.60
12	AM	70	ARG	NE-CZ-NH1	8.67	124.64	120.30
54	BA	1634	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	282	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	1246	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	2071	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	746	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	747	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	1216	A	O4'-C1'-N9	8.65	115.12	108.20
27	BE	21	ARG	NE-CZ-NH1	8.65	124.62	120.30
54	BA	161	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	1395	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	574	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	1453	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	2736	A	N1-C6-N6	-8.64	113.41	118.60
2	AC	64	ARG	NE-CZ-NH1	8.64	124.62	120.30
55	BB	58	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	2721	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	151	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	1012	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1129	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	2602	A	C5-C6-N1	8.63	122.01	117.70
54	BA	2733	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	2336	A	N1-C6-N6	-8.63	113.42	118.60
4	AE	111	ARG	NE-CZ-NH1	8.62	124.61	120.30
25	BC	188	ARG	NE-CZ-NH1	8.62	124.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2825	G	O4'-C1'-N9	8.62	115.09	108.20
21	AA	1219	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	1821	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	782	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	1978	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	1615	C	N3-C2-O2	-8.61	115.88	121.90
21	AA	371	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	1496	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	1133	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	174	A	C5-C6-N1	8.60	122.00	117.70
21	AA	493	A	C5-C6-N1	8.60	122.00	117.70
21	AA	816	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1502	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	749	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	1054	C	N3-C2-O2	-8.59	115.89	121.90
23	A2	79	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	1056	G	O4'-C1'-N9	8.59	115.07	108.20
21	AA	139	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	195	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	490	C	N3-C2-O2	-8.58	115.89	121.90
54	BA	1354	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	2450	A	N1-C6-N6	-8.58	113.45	118.60
17	AR	56	ARG	NE-CZ-NH1	8.58	124.59	120.30
21	AA	1446	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	1201	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	49	A	O4'-C1'-N9	8.57	115.06	108.20
21	AA	1339	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	155	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	1501	C	N3-C2-O2	-8.57	115.90	121.90
54	BA	1987	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	270	A	N1-C6-N6	-8.56	113.46	118.60
39	BQ	29	ARG	NE-CZ-NH2	8.56	124.58	120.30
12	AM	2	ARG	NE-CZ-NH2	8.55	124.58	120.30
54	BA	1678	A	N1-C6-N6	-8.56	113.47	118.60
21	AA	784	A	C5-C6-N1	8.55	121.98	117.70
21	AA	889	A	C5-C6-N1	8.55	121.97	117.70
21	AA	1288	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	632	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	553	A	N1-C6-N6	-8.55	113.47	118.60
25	BC	51	ARG	NE-CZ-NH1	8.55	124.57	120.30
54	BA	1175	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	1805	A	N1-C6-N6	-8.55	113.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AI	121	ARG	NE-CZ-NH1	8.55	124.57	120.30
54	BA	181	A	N1-C6-N6	-8.55	113.47	118.60
24	A3	36	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	1632	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	1591	A	C5-C6-N1	8.54	121.97	117.70
54	BA	1785	A	N1-C6-N6	-8.54	113.47	118.60
55	BB	14	U	O4'-C1'-N1	8.54	115.03	108.20
21	AA	1340	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	687	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	547	A	C5-C6-N1	8.53	121.96	117.70
55	BB	57	A	C5-C6-N1	8.53	121.97	117.70
54	BA	984	A	O4'-C1'-N9	8.53	115.02	108.20
21	AA	958	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	1188	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	1486	U	O4'-C1'-N1	8.52	115.02	108.20
54	BA	1522	A	C5-C6-N1	8.52	121.96	117.70
21	AA	1285	A	C5-C6-N1	8.52	121.96	117.70
46	BX	44	ARG	NE-CZ-NH1	8.51	124.56	120.30
54	BA	362	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	933	A	C5-C6-N1	8.51	121.96	117.70
21	AA	675	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	1299	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1899	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	363	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1583	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	820	A	C5-C6-N1	8.50	121.95	117.70
54	BA	2104	C	N1-C2-O2	8.50	124.00	118.90
2	AC	178	ARG	NE-CZ-NH1	8.50	124.55	120.30
21	AA	790	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1872	A	N1-C6-N6	-8.50	113.50	118.60
44	BV	9	ARG	NE-CZ-NH1	8.50	124.55	120.30
13	AN	75	ARG	NE-CZ-NH1	8.50	124.55	120.30
21	AA	1465	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	2792	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	342	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	935	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	1375	A	C5-C6-N1	8.49	121.94	117.70
21	AA	80	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	1714	U	O4'-C1'-N1	8.49	114.99	108.20
19	AT	9	ARG	NE-CZ-NH1	8.48	124.54	120.30
54	BA	1711	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	1492	A	N1-C6-N6	-8.48	113.51	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	666	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	2169	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	196	A	C5-C6-N1	8.47	121.94	117.70
54	BA	508	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	2082	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	251	A	N1-C6-N6	-8.47	113.52	118.60
21	AA	938	A	N1-C6-N6	-8.47	113.52	118.60
21	AA	994	A	C5-C6-N1	8.47	121.94	117.70
21	AA	1398	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	13	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	2009	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	2328	A	N1-C6-N6	-8.47	113.52	118.60
47	BY	48	ARG	NE-CZ-NH1	8.46	124.53	120.30
54	BA	2468	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	900	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	144	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	2879	A	C5-C6-N1	8.46	121.93	117.70
54	BA	528	A	O4'-C1'-N9	8.46	114.97	108.20
21	AA	197	A	C5-C6-N1	8.45	121.93	117.70
21	AA	573	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	2145	C	N3-C2-O2	-8.45	115.98	121.90
7	AH	12	ARG	NE-CZ-NH1	8.45	124.53	120.30
21	AA	1022	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	599	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2542	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	322	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	1774	C	N3-C2-O2	-8.44	115.99	121.90
54	BA	515	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	702	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	739	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	1147	A	N1-C6-N6	-8.44	113.54	118.60
12	AM	86	ARG	NE-CZ-NH1	8.43	124.52	120.30
54	BA	1135	C	N3-C2-O2	-8.43	116.00	121.90
54	BA	2886	A	N1-C6-N6	-8.43	113.54	118.60
12	AM	112	ARG	NE-CZ-NH1	8.43	124.52	120.30
21	AA	1022	A	C5-C6-N1	8.43	121.92	117.70
54	BA	404	A	N1-C6-N6	-8.43	113.54	118.60
21	AA	182	A	C5-C6-N1	8.43	121.91	117.70
21	AA	676	A	N1-C6-N6	-8.43	113.55	118.60
21	AA	1508	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	1156	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2872	A	N1-C6-N6	-8.42	113.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1322	A	N1-C6-N6	-8.41	113.55	118.60
33	BK	64	ARG	NE-CZ-NH1	8.41	124.50	120.30
54	BA	990	A	N1-C6-N6	-8.41	113.56	118.60
55	BB	59	A	N1-C6-N6	-8.41	113.56	118.60
21	AA	1004	A	C5-C6-N1	8.40	121.90	117.70
54	BA	483	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	1253	A	C5-C6-N1	8.40	121.90	117.70
19	AT	17	ARG	NE-CZ-NH2	8.40	124.50	120.30
21	AA	78	A	N1-C6-N6	-8.40	113.56	118.60
44	BV	79	ARG	NE-CZ-NH1	8.40	124.50	120.30
54	BA	644	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	767	A	N1-C6-N6	-8.39	113.56	118.60
21	AA	865	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2063	C	N3-C2-O2	-8.39	116.03	121.90
21	AA	279	A	N1-C6-N6	-8.39	113.57	118.60
56	B5	71	ARG	NE-CZ-NH1	8.38	124.49	120.30
21	AA	338	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	1046	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	262	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	161	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	1081	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	753	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	807	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	1267	C	N3-C2-O2	-8.37	116.04	121.90
54	BA	980	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	2314	A	N1-C6-N6	-8.37	113.58	118.60
5	AF	24	ARG	NE-CZ-NH1	8.37	124.48	120.30
18	AS	54	ARG	NE-CZ-NH1	8.36	124.48	120.30
21	AA	448	A	N1-C6-N6	-8.36	113.58	118.60
21	AA	546	A	C5-C6-N1	8.36	121.88	117.70
54	BA	2746	U	O4'-C1'-N1	8.36	114.89	108.20
54	BA	788	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	2366	A	C5-C6-N1	8.36	121.88	117.70
21	AA	19	A	N1-C6-N6	-8.36	113.59	118.60
21	AA	815	A	N1-C6-N6	-8.36	113.59	118.60
54	BA	52	A	N1-C6-N6	-8.36	113.59	118.60
54	BA	244	A	N1-C6-N6	-8.36	113.59	118.60
54	BA	2778	A	N1-C6-N6	-8.35	113.59	118.60
55	BB	15	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1150	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	279	A	C5-C6-N1	8.35	121.87	117.70
54	BA	2267	A	N1-C6-N6	-8.35	113.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	927	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	1528	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	2886	A	C5-C6-N1	8.35	121.87	117.70
22	A1	41	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	845	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	1321	A	O4'-C1'-N9	8.34	114.87	108.20
54	BA	2753	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	466	A	N1-C6-N6	-8.34	113.60	118.60
1	AB	221	ARG	NE-CZ-NH1	8.34	124.47	120.30
54	BA	2135	A	N1-C6-N6	-8.34	113.60	118.60
21	AA	1054	C	C1'-O4'-C4'	-8.34	103.23	109.90
54	BA	730	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	2060	A	O4'-C1'-N9	8.34	114.87	108.20
32	BJ	35	ARG	NE-CZ-NH1	8.34	124.47	120.30
54	BA	1580	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	2169	A	C5-C6-N1	8.34	121.87	117.70
21	AA	1428	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	126	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	457	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1732	C	N3-C2-O2	-8.33	116.07	121.90
21	AA	482	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1439	A	O4'-C1'-N9	8.33	114.86	108.20
21	AA	892	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	1152	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	482	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	499	A	C5-C6-N1	8.32	121.86	117.70
21	AA	935	A	C5-C6-N1	8.32	121.86	117.70
54	BA	2054	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	1387	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	249	C	N3-C2-O2	-8.32	116.08	121.90
54	BA	2860	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	246	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	673	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	1073	A	C5-C6-N1	8.31	121.86	117.70
54	BA	324	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	1151	A	N1-C6-N6	-8.31	113.61	118.60
36	BN	86	ARG	NE-CZ-NH1	8.31	124.45	120.30
54	BA	508	A	C5-C6-N1	8.30	121.85	117.70
54	BA	783	A	C5-C6-N1	8.30	121.85	117.70
21	AA	1280	A	N1-C6-N6	-8.30	113.62	118.60
48	BZ	30	ARG	NE-CZ-NH2	8.30	124.45	120.30
54	BA	1194	A	N1-C6-N6	-8.30	113.62	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	918	A	N1-C6-N6	-8.30	113.62	118.60
21	AA	493	A	N1-C6-N6	-8.29	113.62	118.60
21	AA	937	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	2352	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	1544	A	C5-C6-N1	8.29	121.84	117.70
21	AA	1368	A	N1-C6-N6	-8.28	113.63	118.60
3	AD	46	ARG	NE-CZ-NH1	8.28	124.44	120.30
21	AA	466	A	C5-C6-N1	8.28	121.84	117.70
54	BA	982	C	N3-C2-O2	-8.28	116.10	121.90
21	AA	71	A	C5-C6-N1	8.28	121.84	117.70
21	AA	120	A	C5-C6-N1	8.28	121.84	117.70
21	AA	1377	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	119	A	C5-C6-N1	8.28	121.84	117.70
54	BA	2501	C	N3-C2-O2	-8.28	116.11	121.90
54	BA	161	A	C5-C6-N1	8.28	121.84	117.70
54	BA	1126	A	N1-C6-N6	-8.28	113.64	118.60
54	BA	1787	A	C5-C6-N1	8.28	121.84	117.70
8	AI	44	ARG	NE-CZ-NH1	8.27	124.44	120.30
21	AA	979	C	N3-C2-O2	-8.27	116.11	121.90
54	BA	415	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	2097	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	2451	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	53	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	694	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	1213	A	C5-C6-N1	8.27	121.83	117.70
54	BA	1755	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	1815	A	C5-C6-N1	8.27	121.83	117.70
21	AA	1151	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	1238	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	715	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	1559	U	O4'-C1'-N1	8.26	114.81	108.20
54	BA	2114	A	C5-C6-N1	8.26	121.83	117.70
54	BA	345	A	C5-C6-N1	8.26	121.83	117.70
54	BA	1070	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	2114	A	C4-C5-C6	-8.26	112.87	117.00
54	BA	2212	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	73	A	C5-C6-N1	8.26	121.83	117.70
54	BA	422	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	1001	A	N1-C6-N6	-8.26	113.65	118.60
21	AA	263	A	N1-C6-N6	-8.26	113.65	118.60
54	BA	371	A	C5-C6-N1	8.26	121.83	117.70
23	A2	91	A	N1-C6-N6	-8.25	113.65	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	71	A	N1-C6-N6	-8.25	113.65	118.60
21	AA	1225	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2799	A	N1-C6-N6	-8.25	113.65	118.60
3	AD	80	ARG	NE-CZ-NH1	8.24	124.42	120.30
8	AI	48	ARG	NE-CZ-NH1	8.24	124.42	120.30
22	A1	74	C	O4'-C1'-N1	8.24	114.79	108.20
37	BO	94	ARG	NE-CZ-NH1	8.24	124.42	120.30
21	AA	1429	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	2711	A	C5-C6-N1	8.24	121.82	117.70
21	AA	681	A	N1-C6-N6	-8.24	113.66	118.60
34	BL	60	ARG	NE-CZ-NH1	8.24	124.42	120.30
54	BA	2900	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	151	A	C5-C6-N1	8.23	121.82	117.70
21	AA	884	U	C1'-O4'-C4'	-8.23	103.31	109.90
22	A1	74	C	N3-C2-O2	-8.23	116.14	121.90
54	BA	233	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	428	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	146	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2868	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	694	A	C5-C6-N1	8.23	121.81	117.70
24	A3	39	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	643	A	O4'-C1'-N9	8.23	114.78	108.20
54	BA	1032	A	C5-C6-N1	8.23	121.81	117.70
54	BA	323	C	N3-C2-O2	-8.22	116.14	121.90
54	BA	2425	A	C5-C6-N1	8.22	121.81	117.70
54	BA	734	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	256	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	2051	A	C5-C6-N1	8.22	121.81	117.70
6	AG	9	ARG	NE-CZ-NH1	8.21	124.41	120.30
22	A1	16	C	N3-C2-O2	-8.21	116.15	121.90
21	AA	110	C	N3-C2-O2	-8.21	116.15	121.90
54	BA	996	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	89	A	N1-C6-N6	-8.21	113.67	118.60
21	AA	794	A	C5-C6-N1	8.21	121.80	117.70
54	BA	727	A	C5-C6-N1	8.21	121.81	117.70
54	BA	602	A	C5-C6-N1	8.21	121.80	117.70
54	BA	909	A	N1-C6-N6	-8.20	113.68	118.60
55	BB	66	A	C5-C6-N1	8.20	121.80	117.70
54	BA	294	A	C4-C5-C6	-8.20	112.90	117.00
54	BA	1664	A	C5-C6-N1	8.20	121.80	117.70
54	BA	2450	A	C5-C6-N1	8.20	121.80	117.70
21	AA	1285	A	N1-C6-N6	-8.20	113.68	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	149	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	346	A	C5-C6-N1	8.20	121.80	117.70
54	BA	1268	A	C5-C6-N1	8.19	121.80	117.70
21	AA	1503	A	C5-C6-N1	8.19	121.80	117.70
21	AA	959	A	C5-C6-N1	8.19	121.80	117.70
54	BA	118	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2158	A	C5-C6-N1	8.19	121.80	117.70
21	AA	1046	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	1413	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	1628	G	O4'-C1'-N9	8.19	114.75	108.20
21	AA	1269	A	C5-C6-N1	8.19	121.79	117.70
21	AA	1111	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	139	U	O4'-C1'-N1	8.18	114.74	108.20
54	BA	2134	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	477	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1552	A	O4'-C1'-N9	8.17	114.74	108.20
54	BA	1566	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2117	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	1048	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	1069	A	O4'-C1'-N9	8.17	114.73	108.20
54	BA	1877	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2378	A	N1-C6-N6	-8.17	113.70	118.60
55	BB	37	C	N3-C2-O2	-8.17	116.18	121.90
21	AA	1375	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	532	A	C5-C6-N1	8.16	121.78	117.70
54	BA	412	A	C5-C6-N1	8.16	121.78	117.70
21	AA	72	A	C5-C6-N1	8.16	121.78	117.70
21	AA	250	A	N1-C6-N6	-8.16	113.71	118.60
21	AA	1225	A	C5-C6-N1	8.16	121.78	117.70
54	BA	1490	A	C5-C6-N1	8.16	121.78	117.70
54	BA	270	A	C5-C6-N1	8.15	121.78	117.70
54	BA	1226	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1545	A	N1-C6-N6	-8.15	113.71	118.60
23	A2	82	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	91	A	C5-C6-N1	8.15	121.77	117.70
54	BA	2225	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	73	A	N1-C6-N6	-8.14	113.71	118.60
55	BB	45	A	C5-C6-N1	8.14	121.77	117.70
54	BA	1403	A	N1-C6-N6	-8.14	113.71	118.60
24	A3	77	A	C5-C6-N1	8.14	121.77	117.70
11	AL	30	ARG	NE-CZ-NH1	8.14	124.37	120.30
54	BA	44	A	C5-C6-N1	8.14	121.77	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	142	A	N1-C6-N6	-8.14	113.72	118.60
21	AA	1311	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	671	C	N3-C2-O2	-8.14	116.20	121.90
54	BA	804	A	N1-C6-N6	-8.13	113.72	118.60
14	AO	63	ARG	NE-CZ-NH1	8.13	124.37	120.30
21	AA	1000	A	N1-C6-N6	-8.13	113.72	118.60
55	BB	34	A	C4-C5-C6	-8.13	112.94	117.00
21	AA	1014	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1247	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	905	A	N1-C6-N6	-8.13	113.72	118.60
38	BP	50	ARG	NE-CZ-NH1	8.12	124.36	120.30
54	BA	877	A	C5-C6-N1	8.12	121.76	117.70
54	BA	1672	A	C5-C6-N1	8.12	121.76	117.70
21	AA	1281	C	N3-C2-O2	-8.12	116.22	121.90
33	BK	30	ARG	NE-CZ-NH1	8.12	124.36	120.30
54	BA	910	A	C5-C6-N1	8.12	121.76	117.70
54	BA	1494	A	C5-C6-N1	8.12	121.76	117.70
54	BA	538	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2042	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2758	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2879	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	344	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	1237	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	2281	A	C4-C5-C6	-8.11	112.95	117.00
21	AA	792	A	C1'-O4'-C4'	-8.10	103.42	109.90
21	AA	1110	A	C5-C6-N1	8.10	121.75	117.70
22	A1	26	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1829	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1787	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	2660	A	C5-C6-N1	8.10	121.75	117.70
54	BA	74	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	1274	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	71	A	N1-C6-N6	-8.09	113.74	118.60
21	AA	560	A	N1-C6-N6	-8.09	113.75	118.60
22	A1	38	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2516	A	C5-C6-N1	8.09	121.75	117.70
54	BA	507	A	C5-C6-N1	8.09	121.74	117.70
21	AA	1101	A	C5-C6-N1	8.08	121.74	117.70
21	AA	970	C	N3-C2-O2	-8.08	116.24	121.90
54	BA	1608	A	N1-C6-N6	-8.08	113.75	118.60
40	BR	80	ARG	NE-CZ-NH1	8.08	124.34	120.30
54	BA	156	A	N1-C6-N6	-8.08	113.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	396	C	N1-C2-O2	8.07	123.75	118.90
21	AA	665	A	C4-C5-C6	-8.07	112.97	117.00
54	BA	2407	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	1759	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	719	C	N3-C2-O2	-8.06	116.26	121.90
36	BN	69	ARG	NE-CZ-NH1	8.06	124.33	120.30
54	BA	2052	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	1134	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	309	A	C5-C6-N1	8.05	121.73	117.70
21	AA	1437	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	547	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	243	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	1246	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	1362	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	435	C	N3-C2-O2	-8.05	116.27	121.90
54	BA	586	A	C5-C6-N1	8.05	121.72	117.70
54	BA	668	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	2298	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	2893	A	C5-C6-N1	8.05	121.73	117.70
21	AA	767	A	C5-C6-N1	8.05	121.72	117.70
54	BA	941	A	C5-C6-N1	8.05	121.72	117.70
54	BA	1262	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	2788	C	N1-C2-O2	8.05	123.73	118.90
54	BA	513	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	1918	A	N1-C6-N6	-8.05	113.77	118.60
2	AC	10	ARG	NE-CZ-NH1	8.05	124.32	120.30
21	AA	1377	A	C5-C6-N1	8.05	121.72	117.70
21	AA	1384	C	O4'-C1'-N1	8.04	114.64	108.20
36	BN	118	ARG	NE-CZ-NH1	8.04	124.32	120.30
54	BA	428	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1213	A	N1-C6-N6	-8.04	113.77	118.60
21	AA	575	G	C1'-O4'-C4'	-8.04	103.47	109.90
21	AA	1157	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	223	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	715	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	1789	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1551	A	C5-C6-N1	8.04	121.72	117.70
21	AA	665	A	C5-C6-N1	8.03	121.72	117.70
41	BS	18	ARG	NE-CZ-NH1	8.03	124.32	120.30
21	AA	1257	A	C5-C6-N1	8.03	121.72	117.70
54	BA	2820	A	O4'-C1'-N9	8.03	114.63	108.20
21	AA	532	A	N1-C6-N6	-8.03	113.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1786	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	729	A	C5-C6-N1	8.03	121.71	117.70
24	A3	39	A	C5-C6-N1	8.03	121.71	117.70
54	BA	1802	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2147	A	C5-C6-N1	8.03	121.72	117.70
54	BA	2813	A	C5-C6-N1	8.03	121.71	117.70
54	BA	2094	A	C5-C6-N1	8.03	121.71	117.70
21	AA	546	A	C4-C5-C6	-8.02	112.99	117.00
54	BA	1469	A	N1-C6-N6	-8.02	113.79	118.60
56	B5	12	ARG	NE-CZ-NH1	8.02	124.31	120.30
21	AA	1320	C	N3-C2-O2	-8.02	116.29	121.90
54	BA	1384	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	2335	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	526	A	C5-C6-N1	8.01	121.71	117.70
54	BA	1603	A	C5-C6-N1	8.01	121.71	117.70
2	AC	155	ARG	NE-CZ-NH1	8.01	124.30	120.30
54	BA	1965	C	O4'-C1'-N1	8.01	114.61	108.20
54	BA	2376	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	330	A	C5-C6-N1	8.01	121.70	117.70
54	BA	2516	A	O4'-C1'-N9	8.01	114.61	108.20
21	AA	1413	A	C5-C6-N1	8.00	121.70	117.70
24	A3	45	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	402	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2369	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2274	A	C5-C6-N1	8.00	121.70	117.70
54	BA	1913	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	974	A	C5-C6-N1	8.00	121.70	117.70
34	BL	48	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	1143	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1544	A	C4-C5-C6	-8.00	113.00	117.00
54	BA	2163	A	C5-C6-N1	7.99	121.70	117.70
54	BA	2422	C	N3-C2-O2	-7.99	116.30	121.90
54	BA	2632	A	N1-C6-N6	-7.99	113.80	118.60
24	A3	3	C	N1-C2-O2	7.99	123.69	118.90
54	BA	1419	A	C5-C6-N1	7.99	121.69	117.70
54	BA	1780	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	1534	U	O4'-C1'-N1	7.98	114.59	108.20
54	BA	1302	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	872	A	O4'-C1'-N9	7.98	114.58	108.20
54	BA	470	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	449	A	C5-C6-N1	7.97	121.69	117.70
54	BA	586	A	N1-C6-N6	-7.97	113.82	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1021	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	1384	A	C5-C6-N1	7.97	121.69	117.70
21	AA	397	A	C5-C6-N1	7.97	121.69	117.70
21	AA	663	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	327	A	C5-C6-N1	7.97	121.68	117.70
54	BA	2426	A	C5-C6-N1	7.97	121.68	117.70
54	BA	332	A	C5-C6-N1	7.96	121.68	117.70
54	BA	892	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	1890	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1609	A	C5-C6-N1	7.96	121.68	117.70
21	AA	1197	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	221	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	454	A	N1-C6-N6	-7.96	113.82	118.60
25	BC	86	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	925	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1713	A	N1-C6-N6	-7.96	113.83	118.60
54	BA	2406	A	N1-C6-N6	-7.96	113.83	118.60
21	AA	1044	A	C5-C6-N1	7.95	121.68	117.70
39	BQ	91	ARG	NE-CZ-NH1	7.95	124.28	120.30
54	BA	165	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	2340	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	163	C	O4'-C1'-N1	7.95	114.56	108.20
54	BA	1402	U	O4'-C1'-N1	7.95	114.56	108.20
21	AA	262	A	C1'-O4'-C4'	-7.95	103.54	109.90
21	AA	1271	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1593	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	2042	A	C5-C6-N1	7.95	121.67	117.70
54	BA	2761	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	492	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	821	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	2199	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	2281	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	563	A	C5-C6-N1	7.94	121.67	117.70
54	BA	2386	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	177	G	O4'-C1'-N9	7.94	114.55	108.20
54	BA	1373	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	1582	C	O4'-C1'-N1	7.94	114.55	108.20
54	BA	1809	A	N1-C6-N6	-7.94	113.83	118.60
21	AA	1239	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	1606	C	N3-C2-O2	-7.94	116.34	121.90
54	BA	216	A	C5-C6-N1	7.93	121.67	117.70
54	BA	449	A	N1-C6-N6	-7.93	113.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2547	A	C5-C6-N1	7.93	121.67	117.70
54	BA	439	A	N1-C6-N6	-7.93	113.84	118.60
37	BO	7	ARG	NE-CZ-NH1	7.93	124.27	120.30
54	BA	2459	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	716	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	2738	A	C5-C6-N1	7.93	121.66	117.70
54	BA	2198	A	C5-C6-N1	7.93	121.66	117.70
54	BA	2426	A	N1-C6-N6	-7.93	113.84	118.60
35	BM	114	ARG	NE-CZ-NH1	7.93	124.26	120.30
54	BA	330	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	2126	A	C5-C6-N1	7.93	121.66	117.70
54	BA	2191	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	74	A	N1-C6-N6	-7.92	113.84	118.60
21	AA	640	A	N1-C6-N6	-7.92	113.84	118.60
21	AA	583	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	53	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1515	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	2346	A	N1-C6-N6	-7.92	113.85	118.60
29	BG	34	ARG	NE-CZ-NH1	7.92	124.26	120.30
54	BA	1395	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1522	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1819	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	2813	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	1251	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1470	A	N1-C6-N6	-7.92	113.85	118.60
24	A3	73	A	C5-C6-N1	7.91	121.66	117.70
54	BA	1551	A	C4-C5-C6	-7.91	113.04	117.00
54	BA	2126	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	1535	A	C5-C6-N1	7.91	121.66	117.70
54	BA	2104	C	O4'-C1'-N1	7.91	114.53	108.20
54	BA	2173	A	C5-C6-N1	7.91	121.66	117.70
54	BA	2191	A	C5-C6-N1	7.91	121.66	117.70
54	BA	2281	A	C5-C6-N1	7.91	121.66	117.70
10	AK	52	ARG	NE-CZ-NH1	7.91	124.26	120.30
21	AA	777	A	C5-C6-N1	7.91	121.66	117.70
21	AA	1180	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	743	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	984	A	C5-C6-N1	7.91	121.66	117.70
54	BA	1359	A	C5-C6-N1	7.91	121.66	117.70
21	AA	274	A	C5-C6-N1	7.91	121.65	117.70
21	AA	1146	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	1890	A	N1-C6-N6	-7.91	113.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	47	C	N3-C2-O2	-7.91	116.37	121.90
21	AA	1280	A	C5-C6-N1	7.91	121.65	117.70
21	AA	1339	A	C5-C6-N1	7.91	121.65	117.70
54	BA	2513	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	1773	A	N1-C6-N6	-7.90	113.86	118.60
24	A3	74	A	C5-C6-N1	7.90	121.65	117.70
54	BA	264	C	N3-C2-O2	-7.90	116.37	121.90
21	AA	977	A	C5-C6-N1	7.90	121.65	117.70
54	BA	163	C	N3-C2-O2	-7.90	116.37	121.90
21	AA	54	C	P-O3'-C3'	7.90	129.18	119.70
55	BB	35	C	N3-C2-O2	-7.90	116.37	121.90
21	AA	995	C	N3-C2-O2	-7.89	116.37	121.90
21	AA	1128	C	N3-C2-O2	-7.89	116.37	121.90
54	BA	160	A	C5-C6-N1	7.89	121.65	117.70
54	BA	2126	A	O4'-C1'-N9	7.89	114.52	108.20
54	BA	2564	A	C5-C6-N1	7.89	121.65	117.70
21	AA	495	A	N1-C6-N6	-7.89	113.87	118.60
21	AA	60	A	C5-C6-N1	7.89	121.64	117.70
21	AA	978	A	N1-C6-N6	-7.88	113.87	118.60
21	AA	1229	A	C5-C6-N1	7.88	121.64	117.70
54	BA	541	A	N1-C6-N6	-7.88	113.87	118.60
24	A3	58	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	515	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1876	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	2518	A	N1-C6-N6	-7.88	113.87	118.60
25	BC	269	ARG	NE-CZ-NH2	-7.88	116.36	120.30
21	AA	130	A	C5-C6-N1	7.88	121.64	117.70
54	BA	282	A	C5-C6-N1	7.87	121.64	117.70
54	BA	981	A	O4'-C1'-N9	7.87	114.50	108.20
54	BA	149	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	2205	A	N1-C6-N6	-7.87	113.88	118.60
55	BB	78	A	C5-C6-N1	7.87	121.63	117.70
21	AA	7	A	C5-C6-N1	7.87	121.63	117.70
21	AA	998	C	N3-C2-O2	-7.87	116.39	121.90
54	BA	575	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	800	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1301	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1570	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1204	A	O4'-C1'-N9	7.86	114.49	108.20
54	BA	1611	C	N3-C2-O2	-7.86	116.40	121.90
21	AA	1513	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	472	A	C5-C6-N1	7.86	121.63	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AI	17	ARG	NE-CZ-NH1	7.86	124.23	120.30
21	AA	32	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	1410	G	O4'-C1'-N9	7.86	114.49	108.20
21	AA	1289	A	C5-C6-N1	7.86	121.63	117.70
21	AA	1456	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	1028	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2031	A	C5-C6-N1	7.86	121.63	117.70
21	AA	935	A	C4-C5-C6	-7.85	113.07	117.00
21	AA	1520	C	N3-C2-O2	-7.85	116.41	121.90
35	BM	50	ARG	NE-CZ-NH1	7.85	124.22	120.30
54	BA	802	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	979	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	627	A	C5-C6-N1	7.84	121.62	117.70
21	AA	119	A	C5-C6-N1	7.84	121.62	117.70
37	BO	13	ARG	NE-CZ-NH1	7.84	124.22	120.30
54	BA	1126	A	C5-C6-N1	7.84	121.62	117.70
21	AA	968	A	C5-C6-N1	7.84	121.62	117.70
20	AU	46	ARG	NE-CZ-NH1	7.83	124.22	120.30
54	BA	1558	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	1040	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	2829	A	C4-C5-C6	-7.83	113.08	117.00
21	AA	412	A	C5-C6-N1	7.83	121.62	117.70
54	BA	503	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1597	A	C5-C6-N1	7.83	121.61	117.70
21	AA	1179	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	172	A	N1-C6-N6	-7.83	113.91	118.60
24	A3	59	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1095	A	N1-C6-N6	-7.83	113.91	118.60
54	BA	240	C	N3-C2-O2	-7.82	116.42	121.90
25	BC	213	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	611	C	O4'-C1'-N1	7.82	114.46	108.20
21	AA	1256	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	522	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	1755	A	C5-C6-N1	7.81	121.61	117.70
3	AD	55	ARG	NE-CZ-NH1	7.81	124.21	120.30
21	AA	51	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	2183	A	N1-C6-N6	-7.81	113.91	118.60
21	AA	787	A	C5-C6-N1	7.81	121.60	117.70
21	AA	412	A	N1-C6-N6	-7.81	113.92	118.60
54	BA	2771	C	N3-C2-O2	-7.81	116.44	121.90
21	AA	282	A	N1-C6-N6	-7.81	113.92	118.60
21	AA	81	A	N1-C6-N6	-7.80	113.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	264	C	N3-C2-O2	-7.80	116.44	121.90
54	BA	2020	A	C5-C6-N1	7.80	121.60	117.70
25	BC	269	ARG	NE-CZ-NH1	7.80	124.20	120.30
6	AG	9	ARG	NE-CZ-NH2	-7.80	116.40	120.30
54	BA	265	A	N1-C6-N6	-7.80	113.92	118.60
40	BR	84	ARG	NE-CZ-NH2	7.80	124.20	120.30
54	BA	95	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	479	A	C5-C6-N1	7.80	121.60	117.70
54	BA	2531	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	2712	C	N3-C2-O2	-7.79	116.44	121.90
21	AA	451	A	C5-C6-N1	7.79	121.60	117.70
54	BA	309	A	C5-C6-N1	7.79	121.59	117.70
54	BA	2856	A	N1-C6-N6	-7.79	113.92	118.60
21	AA	131	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	994	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	1467	C	N3-C2-O2	-7.79	116.45	121.90
22	A1	56	C	N3-C2-O2	-7.79	116.45	121.90
54	BA	1810	A	N1-C6-N6	-7.79	113.93	118.60
5	AF	2	ARG	NE-CZ-NH1	7.79	124.19	120.30
30	BH	27	ARG	NE-CZ-NH1	7.79	124.19	120.30
54	BA	718	A	O4'-C1'-N9	7.79	114.43	108.20
54	BA	1953	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	2376	A	C5-C6-N1	7.79	121.59	117.70
54	BA	2829	A	C5-C6-N1	7.78	121.59	117.70
54	BA	609	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	2614	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2740	A	C5-C6-N1	7.78	121.59	117.70
21	AA	67	C	N3-C2-O2	-7.78	116.46	121.90
21	AA	673	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2189	U	O4'-C1'-N1	7.78	114.42	108.20
19	AT	73	ARG	NE-CZ-NH1	7.78	124.19	120.30
21	AA	1082	A	C5-C6-N1	7.77	121.59	117.70
54	BA	2080	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	2094	A	C4-C5-C6	-7.77	113.11	117.00
21	AA	502	A	C5-C6-N1	7.77	121.58	117.70
45	BW	38	ARG	NE-CZ-NH1	7.77	124.19	120.30
54	BA	1175	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1616	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	2033	A	N1-C6-N6	-7.77	113.94	118.60
55	BB	27	C	N3-C2-O2	-7.77	116.46	121.90
21	AA	796	C	N3-C2-O2	-7.77	116.46	121.90
21	AA	959	A	N1-C6-N6	-7.76	113.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	415	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	321	A	C4-C5-C6	-7.76	113.12	117.00
21	AA	1483	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	311	A	N1-C6-N6	-7.76	113.95	118.60
21	AA	26	A	C5-C6-N1	7.75	121.58	117.70
21	AA	221	C	N3-C2-O2	-7.75	116.47	121.90
21	AA	1238	A	C5-C6-N1	7.75	121.58	117.70
24	A3	1	C	N3-C2-O2	-7.75	116.47	121.90
54	BA	614	A	C5-C6-N1	7.75	121.58	117.70
55	BB	78	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	1203	C	N3-C2-O2	-7.75	116.47	121.90
21	AA	344	A	C5-C6-N1	7.75	121.58	117.70
54	BA	794	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1050	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2019	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	742	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1745	A	C4-C5-C6	-7.75	113.13	117.00
54	BA	2005	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1257	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1308	A	C5-C6-N1	7.75	121.57	117.70
54	BA	2350	C	O4'-C1'-N1	7.75	114.40	108.20
54	BA	2667	C	N3-C2-O2	-7.75	116.48	121.90
54	BA	2740	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	118	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2821	A	N1-C6-N6	-7.74	113.95	118.60
21	AA	501	C	N3-C2-O2	-7.74	116.48	121.90
21	AA	969	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	1701	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	1383	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1549	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	1433	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	2211	A	C5-C6-N1	7.74	121.57	117.70
21	AA	621	A	C5-C6-N1	7.73	121.57	117.70
21	AA	901	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	907	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	718	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	6	A	C5-C6-N1	7.73	121.56	117.70
54	BA	2758	A	C5-C6-N1	7.73	121.56	117.70
27	BE	67	ARG	NE-CZ-NH1	7.72	124.16	120.30
34	BL	18	ARG	NE-CZ-NH1	7.72	124.16	120.30
54	BA	2565	A	C5-C6-N1	7.72	121.56	117.70
21	AA	1216	A	C5-C6-N1	7.72	121.56	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AC	178	ARG	NE-CZ-NH2	-7.72	116.44	120.30
21	AA	1130	A	C5-C6-N1	7.72	121.56	117.70
21	AA	1329	A	C4-C5-C6	-7.72	113.14	117.00
54	BA	1583	A	C5-C6-N1	7.72	121.56	117.70
54	BA	2184	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2037	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	807	A	C5-C6-N1	7.72	121.56	117.70
21	AA	938	A	C5-C6-N1	7.72	121.56	117.70
54	BA	49	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	2850	A	C5-C6-N1	7.71	121.56	117.70
21	AA	649	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	1410	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	1349	C	N3-C2-O2	-7.71	116.51	121.90
9	AJ	5	ARG	NE-CZ-NH1	7.70	124.15	120.30
54	BA	2507	C	N3-C2-O2	-7.70	116.51	121.90
21	AA	969	A	C5-C6-N1	7.70	121.55	117.70
54	BA	574	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1552	A	C5-C6-N1	7.70	121.55	117.70
21	AA	901	A	C5-C6-N1	7.70	121.55	117.70
25	BC	101	ARG	NE-CZ-NH1	7.70	124.15	120.30
21	AA	98	A	C5-C6-N1	7.70	121.55	117.70
21	AA	802	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1046	A	C5-C6-N1	7.70	121.55	117.70
16	AQ	26	ARG	NE-CZ-NH1	7.69	124.14	120.30
21	AA	1200	C	N3-C4-C5	7.69	124.98	121.90
33	BK	70	ARG	NE-CZ-NH1	7.69	124.14	120.30
54	BA	599	A	C5-C6-N1	7.69	121.55	117.70
54	BA	661	A	C4-C5-C6	-7.69	113.16	117.00
54	BA	2266	A	C5-C6-N1	7.69	121.55	117.70
53	B4	24	ARG	NE-CZ-NH1	7.69	124.14	120.30
54	BA	94	A	C5-C6-N1	7.69	121.54	117.70
54	BA	355	U	O4'-C1'-N1	7.69	114.35	108.20
54	BA	514	A	C5-C6-N1	7.69	121.54	117.70
54	BA	1096	A	C5-C6-N1	7.69	121.54	117.70
21	AA	1200	C	N3-C2-O2	-7.69	116.52	121.90
54	BA	878	A	C5-C6-N1	7.69	121.54	117.70
21	AA	596	A	N1-C6-N6	-7.68	113.99	118.60
25	BC	220	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	2858	C	N1-C2-O2	7.68	123.51	118.90
21	AA	631	C	N1-C2-O2	7.68	123.51	118.90
54	BA	1428	C	N3-C2-O2	-7.68	116.52	121.90
54	BA	1630	A	N1-C6-N6	-7.68	113.99	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	59	A	C5-C6-N1	7.68	121.54	117.70
21	AA	50	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1431	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	1912	A	C5-C6-N1	7.68	121.54	117.70
21	AA	1468	A	C5-C6-N1	7.68	121.54	117.70
24	A3	22	A	C5-C6-N1	7.67	121.54	117.70
54	BA	643	A	C5-C6-N1	7.67	121.54	117.70
54	BA	1626	A	C4-C5-C6	-7.67	113.16	117.00
54	BA	404	A	C5-C6-N1	7.67	121.54	117.70
21	AA	712	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	915	A	C5-C6-N1	7.67	121.54	117.70
54	BA	829	A	C5-C6-N1	7.67	121.53	117.70
3	AD	96	ARG	NE-CZ-NH1	7.67	124.14	120.30
21	AA	461	A	N1-C6-N6	-7.67	114.00	118.60
22	A1	59	U	C1'-O4'-C4'	-7.67	103.77	109.90
54	BA	347	A	C5-C6-N1	7.67	121.53	117.70
21	AA	65	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1626	A	C5-C6-N1	7.67	121.53	117.70
54	BA	2270	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	217	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2060	A	C5-C6-N1	7.66	121.53	117.70
27	BE	162	ARG	NE-CZ-NH1	7.66	124.13	120.30
21	AA	792	A	N1-C6-N6	-7.66	114.00	118.60
22	A1	21	A	N1-C6-N6	-7.66	114.00	118.60
21	AA	583	A	C5-C6-N1	7.66	121.53	117.70
54	BA	197	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	1717	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	1901	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	541	A	C4-C5-C6	-7.66	113.17	117.00
54	BA	1054	A	N1-C6-N6	-7.65	114.01	118.60
9	AJ	48	ARG	NE-CZ-NH1	7.65	124.13	120.30
54	BA	668	A	C5-C6-N1	7.65	121.53	117.70
54	BA	1275	A	C5-C6-N1	7.65	121.53	117.70
54	BA	2430	A	C5-C6-N1	7.65	121.52	117.70
3	AD	2	ARG	NE-CZ-NH1	7.65	124.12	120.30
21	AA	946	A	C5-C6-N1	7.65	121.52	117.70
54	BA	2333	A	C5-C6-N1	7.65	121.52	117.70
54	BA	2682	A	C5-C6-N1	7.65	121.52	117.70
54	BA	456	C	N3-C2-O2	-7.64	116.55	121.90
54	BA	2478	A	C5-C6-N1	7.64	121.52	117.70
21	AA	243	A	C5-C6-N1	7.64	121.52	117.70
21	AA	1500	A	C5-C6-N1	7.64	121.52	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1877	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2060	A	N1-C6-N6	-7.64	114.01	118.60
54	BA	2809	A	N1-C6-N6	-7.64	114.01	118.60
21	AA	1507	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	487	A	C5-C6-N1	7.64	121.52	117.70
54	BA	685	A	C5-C6-N1	7.64	121.52	117.70
6	AG	77	ARG	NE-CZ-NH2	7.64	124.12	120.30
55	BB	39	A	C5-C6-N1	7.63	121.52	117.70
21	AA	937	A	C5-C6-N1	7.63	121.52	117.70
21	AA	1492	A	C5-C6-N1	7.63	121.52	117.70
41	BS	92	ARG	NE-CZ-NH1	7.63	124.12	120.30
21	AA	48	C	N3-C2-O2	-7.63	116.56	121.90
21	AA	167	A	C5-C6-N1	7.63	121.52	117.70
11	AL	98	ARG	NE-CZ-NH1	7.63	124.11	120.30
15	AP	14	ARG	NE-CZ-NH1	7.63	124.11	120.30
30	BH	116	ARG	NE-CZ-NH1	7.63	124.11	120.30
54	BA	685	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	205	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	2406	A	C5-C6-N1	7.63	121.51	117.70
21	AA	397	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	482	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1057	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2879	A	O4'-C1'-N9	7.62	114.30	108.20
21	AA	353	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	535	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1502	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1607	C	N3-C2-O2	-7.62	116.56	121.90
54	BA	2273	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1264	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	502	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	513	A	C5-C6-N1	7.61	121.51	117.70
54	BA	631	A	C5-C6-N1	7.61	121.51	117.70
54	BA	1532	A	C4-C5-C6	-7.61	113.19	117.00
54	BA	2112	G	O4'-C1'-N9	7.61	114.29	108.20
21	AA	363	A	C5-C6-N1	7.61	121.50	117.70
54	BA	152	A	N1-C6-N6	-7.61	114.04	118.60
54	BA	2448	A	N1-C6-N6	-7.61	114.03	118.60
42	BT	6	ARG	NE-CZ-NH2	7.61	124.10	120.30
54	BA	886	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1085	A	N1-C6-N6	-7.61	114.04	118.60
54	BA	1937	A	N1-C6-N6	-7.61	114.04	118.60
54	BA	1969	A	N1-C6-N6	-7.61	114.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2165	C	N3-C2-O2	-7.61	116.58	121.90
54	BA	2155	U	O4'-C1'-N1	7.60	114.28	108.20
54	BA	2820	A	C5-C6-N1	7.60	121.50	117.70
54	BA	1678	A	C5-C6-N1	7.60	121.50	117.70
54	BA	2174	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	1265	A	C5-C6-N1	7.60	121.50	117.70
21	AA	190	A	C5-C6-N1	7.60	121.50	117.70
21	AA	1369	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	2077	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1698	A	C5-C6-N1	7.59	121.50	117.70
54	BA	299	A	N1-C6-N6	-7.59	114.05	118.60
21	AA	328	C	N3-C2-O2	-7.59	116.59	121.90
54	BA	706	A	C5-C6-N1	7.59	121.49	117.70
54	BA	752	A	C5-C6-N1	7.59	121.49	117.70
54	BA	1609	A	C1'-O4'-C4'	-7.59	103.83	109.90
21	AA	435	A	C4-C5-C6	-7.58	113.21	117.00
21	AA	1384	C	P-O3'-C3'	7.58	128.80	119.70
54	BA	217	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	627	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	503	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1275	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	2451	A	C5-C6-N1	7.58	121.49	117.70
21	AA	129	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1067	A	C5-C6-N1	7.58	121.49	117.70
54	BA	792	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	1809	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1040	A	C5-C6-N1	7.57	121.49	117.70
54	BA	1894	C	N3-C2-O2	-7.57	116.60	121.90
22	A1	38	A	C5-C6-N1	7.57	121.49	117.70
54	BA	2469	A	C5-C6-N1	7.57	121.49	117.70
21	AA	1374	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	735	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1669	A	C5-C6-N1	7.57	121.49	117.70
54	BA	2598	A	N1-C6-N6	-7.57	114.06	118.60
8	AI	122	ARG	NE-CZ-NH1	7.57	124.08	120.30
21	AA	648	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1382	G	O4'-C1'-N9	7.57	114.25	108.20
54	BA	2566	A	C5-C6-N1	7.57	121.48	117.70
21	AA	320	A	C5-C6-N1	7.57	121.48	117.70
21	AA	572	A	C5-C6-N1	7.57	121.48	117.70
54	BA	2506	U	O4'-C1'-N1	7.57	114.25	108.20
21	AA	363	A	C4-C5-C6	-7.57	113.22	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	374	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1322	A	C5-C6-N1	7.56	121.48	117.70
54	BA	637	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1665	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	2430	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	960	A	C5-C6-N1	7.56	121.48	117.70
21	AA	607	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1205	A	C5-C6-N1	7.56	121.48	117.70
3	AD	110	ARG	NE-CZ-NH1	7.56	124.08	120.30
54	BA	540	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	878	A	N1-C6-N6	-7.56	114.06	118.60
21	AA	1283	U	N3-C2-O2	-7.55	116.91	122.20
54	BA	877	A	C4-C5-C6	-7.55	113.22	117.00
54	BA	293	U	O4'-C1'-N1	7.55	114.24	108.20
54	BA	522	A	C5-C6-N1	7.55	121.48	117.70
54	BA	988	A	C5-C6-N1	7.55	121.48	117.70
54	BA	1189	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1133	A	C5-C6-N1	7.55	121.47	117.70
54	BA	1757	A	C5-C6-N1	7.55	121.47	117.70
54	BA	1762	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2542	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2823	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	595	A	N1-C6-N6	-7.55	114.07	118.60
24	A3	47	G	C1'-O4'-C4'	-7.55	103.86	109.90
54	BA	1103	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1610	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1548	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1889	A	C5-C6-N1	7.54	121.47	117.70
21	AA	459	A	C5-C6-N1	7.54	121.47	117.70
21	AA	704	A	C5-C6-N1	7.54	121.47	117.70
3	AD	43	ARG	NE-CZ-NH1	7.54	124.07	120.30
21	AA	307	C	N3-C2-O2	-7.54	116.62	121.90
21	AA	1014	A	C5-C6-N1	7.54	121.47	117.70
21	AA	1303	C	N3-C2-O2	-7.54	116.62	121.90
54	BA	197	A	C5-C6-N1	7.54	121.47	117.70
54	BA	2835	A	N1-C6-N6	-7.54	114.08	118.60
8	AI	40	ARG	NE-CZ-NH1	7.54	124.07	120.30
21	AA	298	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	329	A	C5-C6-N1	7.54	121.47	117.70
21	AA	622	A	C5-C6-N1	7.53	121.47	117.70
54	BA	199	A	C5-C6-N1	7.53	121.47	117.70
54	BA	2311	A	C5-C6-N1	7.53	121.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1214	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	606	U	O4'-C1'-N1	7.53	114.22	108.20
21	AA	1352	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	460	A	C5-C6-N1	7.53	121.46	117.70
24	A3	60	A	C4-C5-C6	-7.53	113.24	117.00
12	AM	91	ARG	NE-CZ-NH2	-7.53	116.54	120.30
21	AA	1092	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	278	A	C5-C6-N1	7.53	121.46	117.70
21	AA	1149	C	N3-C2-O2	-7.52	116.63	121.90
54	BA	560	C	N3-C2-O2	-7.52	116.63	121.90
54	BA	507	A	C4-C5-C6	-7.52	113.24	117.00
22	A1	16	C	O4'-C1'-N1	7.52	114.22	108.20
21	AA	263	A	C5-C6-N1	7.52	121.46	117.70
21	AA	373	A	C5-C6-N1	7.52	121.46	117.70
21	AA	411	A	C5-C6-N1	7.52	121.46	117.70
54	BA	2377	A	C5-C6-N1	7.52	121.46	117.70
4	AE	156	ARG	NE-CZ-NH2	7.52	124.06	120.30
54	BA	1020	A	C5-C6-N1	7.52	121.46	117.70
54	BA	2547	A	C4-C5-C6	-7.52	113.24	117.00
21	AA	1000	A	C5-C6-N1	7.52	121.46	117.70
54	BA	2781	A	C5-C6-N1	7.51	121.46	117.70
21	AA	1145	A	C5-C6-N1	7.51	121.46	117.70
54	BA	1307	A	C5-C6-N1	7.51	121.46	117.70
54	BA	1885	A	C5-C6-N1	7.51	121.46	117.70
3	AD	12	ARG	NE-CZ-NH1	7.51	124.06	120.30
54	BA	1321	A	C5-C6-N1	7.51	121.46	117.70
21	AA	1146	A	C5-C6-N1	7.51	121.45	117.70
21	AA	1350	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	1504	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2749	A	C5-C6-N1	7.51	121.45	117.70
24	A3	57	C	N3-C2-O2	-7.51	116.64	121.90
21	AA	1176	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2015	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2667	C	O4'-C1'-N1	7.50	114.20	108.20
7	AH	87	ARG	NE-CZ-NH2	7.50	124.05	120.30
21	AA	250	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1274	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1306	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	829	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	2059	A	C5-C6-N1	7.50	121.45	117.70
6	AG	69	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	2748	A	C5-C6-N1	7.50	121.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1084	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2590	A	C5-C6-N1	7.50	121.45	117.70
21	AA	116	A	C5-C6-N1	7.50	121.45	117.70
54	BA	272	A	C1'-O4'-C4'	-7.50	103.90	109.90
54	BA	827	U	O4'-C1'-N1	7.50	114.20	108.20
54	BA	1679	A	C4-C5-C6	-7.50	113.25	117.00
21	AA	1152	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1396	A	C4-C5-C6	-7.50	113.25	117.00
21	AA	609	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	2635	A	C5-C6-N1	7.50	121.45	117.70
21	AA	282	A	C5-C6-N1	7.49	121.45	117.70
21	AA	1246	A	C5-C6-N1	7.49	121.45	117.70
21	AA	1359	C	N3-C2-O2	-7.49	116.65	121.90
54	BA	1347	A	C5-C6-N1	7.49	121.45	117.70
21	AA	814	A	C5-C6-N1	7.49	121.45	117.70
54	BA	196	A	C5-C6-N1	7.49	121.45	117.70
21	AA	1360	A	C5-C6-N1	7.49	121.44	117.70
34	BL	123	ARG	NE-CZ-NH1	7.49	124.05	120.30
54	BA	1378	A	C5-C6-N1	7.49	121.44	117.70
24	A3	38	A	C5-C6-N1	7.49	121.44	117.70
54	BA	902	C	N3-C2-O2	-7.49	116.66	121.90
55	BB	108	A	C5-C6-N1	7.49	121.44	117.70
21	AA	1005	A	N1-C6-N6	-7.49	114.11	118.60
21	AA	272	C	N3-C2-O2	-7.48	116.66	121.90
21	AA	1082	A	C4-C5-C6	-7.48	113.26	117.00
54	BA	961	C	N3-C2-O2	-7.48	116.66	121.90
54	BA	1103	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2030	A	C5-C6-N1	7.48	121.44	117.70
21	AA	452	A	C4-C5-C6	-7.48	113.26	117.00
24	A3	73	A	N1-C6-N6	-7.48	114.11	118.60
25	BC	132	ARG	NE-CZ-NH1	7.48	124.04	120.30
54	BA	1302	A	C5-C6-N1	7.48	121.44	117.70
54	BA	63	A	C5-C6-N1	7.48	121.44	117.70
54	BA	676	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	1165	A	N1-C6-N6	-7.48	114.11	118.60
21	AA	262	A	C4-C5-C6	-7.48	113.26	117.00
21	AA	996	A	C5-C6-N1	7.48	121.44	117.70
21	AA	1446	A	C5-C6-N1	7.48	121.44	117.70
54	BA	529	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	1086	A	C5-C6-N1	7.48	121.44	117.70
3	AD	61	ARG	NE-CZ-NH1	7.47	124.04	120.30
9	AJ	72	ARG	NE-CZ-NH1	7.47	124.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	771	G	C1'-O4'-C4'	-7.47	103.92	109.90
54	BA	1701	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2516	A	C4-C5-C6	-7.47	113.26	117.00
54	BA	2577	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2606	C	O4'-C1'-N1	7.47	114.18	108.20
21	AA	1349	A	N1-C6-N6	-7.47	114.12	118.60
24	A3	3	C	O4'-C1'-N1	7.47	114.18	108.20
54	BA	221	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2326	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	2835	A	C5-C6-N1	7.47	121.44	117.70
21	AA	520	A	C4-C5-C6	-7.47	113.27	117.00
54	BA	1899	A	C5-C6-N1	7.47	121.44	117.70
21	AA	1211	U	O4'-C1'-N1	7.47	114.17	108.20
21	AA	1363	A	C5-C6-N1	7.47	121.43	117.70
21	AA	315	A	C5-C6-N1	7.46	121.43	117.70
24	A3	16	C	N3-C2-O2	-7.46	116.67	121.90
54	BA	456	C	N1-C2-O2	7.46	123.38	118.90
54	BA	2749	A	N1-C6-N6	-7.46	114.12	118.60
41	BS	88	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	1039	A	C5-C6-N1	7.46	121.43	117.70
21	AA	414	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1132	C	N3-C2-O2	-7.46	116.68	121.90
54	BA	226	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2070	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	2750	A	C5-C6-N1	7.46	121.43	117.70
54	BA	497	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1439	A	C5-C6-N1	7.46	121.43	117.70
21	AA	85	U	N3-C2-O2	-7.46	116.98	122.20
37	BO	25	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	352	A	C4-C5-C6	-7.46	113.27	117.00
54	BA	195	A	C5-C6-N1	7.46	121.43	117.70
54	BA	412	A	C4-C5-C6	-7.46	113.27	117.00
54	BA	1490	A	O4'-C1'-N9	7.46	114.17	108.20
54	BA	1784	A	C5-C6-N1	7.46	121.43	117.70
21	AA	466	A	O4'-C1'-N9	7.46	114.16	108.20
23	A2	82	A	C5-C6-N1	7.46	121.43	117.70
6	AG	137	ARG	NE-CZ-NH1	7.45	124.03	120.30
21	AA	1042	A	C5-C6-N1	7.45	121.43	117.70
54	BA	144	A	C5-C6-N1	7.45	121.43	117.70
54	BA	1981	A	C5-C6-N1	7.45	121.43	117.70
30	BH	50	ARG	NE-CZ-NH1	7.45	124.03	120.30
24	A3	11	A	C4-C5-C6	-7.45	113.28	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	974	G	O4'-C1'-N9	7.45	114.16	108.20
21	AA	768	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	60	A	N1-C6-N6	-7.44	114.13	118.60
21	AA	152	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1579	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2422	C	N1-C2-O2	7.44	123.37	118.90
22	A1	66	A	N1-C6-N6	-7.44	114.14	118.60
24	A3	59	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	802	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2270	A	C5-C6-N1	7.44	121.42	117.70
21	AA	59	A	C5-C6-N1	7.43	121.42	117.70
21	AA	1408	A	C5-C6-N1	7.43	121.42	117.70
55	BB	46	A	C5-C6-N1	7.43	121.42	117.70
1	AB	206	ILE	C-N-CA	7.43	140.28	121.70
54	BA	371	A	C4-C5-C6	-7.43	113.28	117.00
54	BA	478	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	147	C	O4'-C1'-N1	7.43	114.14	108.20
21	AA	321	A	C5-C6-N1	7.43	121.41	117.70
21	AA	1155	A	C4-C5-C6	-7.43	113.29	117.00
54	BA	789	A	C5-C6-N1	7.43	121.41	117.70
54	BA	1264	A	C5-C6-N1	7.43	121.41	117.70
21	AA	1080	A	C5-C6-N1	7.42	121.41	117.70
54	BA	634	C	N3-C2-O2	-7.42	116.70	121.90
54	BA	2572	A	C5-C6-N1	7.42	121.41	117.70
54	BA	323	C	N1-C2-O2	7.42	123.35	118.90
54	BA	2814	A	C4-C5-C6	-7.42	113.29	117.00
1	AB	136	ARG	NE-CZ-NH1	7.42	124.01	120.30
54	BA	504	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	972	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	2424	C	N3-C2-O2	-7.42	116.70	121.90
54	BA	1566	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1236	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	143	C	C1'-O4'-C4'	-7.42	103.97	109.90
54	BA	207	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	819	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1251	A	C4-C5-C6	-7.42	113.29	117.00
21	AA	1394	A	C5-C6-N1	7.42	121.41	117.70
54	BA	176	A	C5-C6-N1	7.42	121.41	117.70
21	AA	841	C	N3-C2-O2	-7.41	116.71	121.90
54	BA	632	A	C5-C6-N1	7.41	121.41	117.70
21	AA	197	A	C4-C5-C6	-7.41	113.30	117.00
54	BA	334	C	O4'-C1'-N1	7.41	114.13	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1504	A	N1-C6-N6	-7.41	114.15	118.60
54	BA	1705	A	C5-C6-N1	7.41	121.41	117.70
21	AA	949	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	1459	G	O4'-C1'-N9	7.41	114.13	108.20
54	BA	2826	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	2765	A	C5-C6-N1	7.41	121.40	117.70
54	BA	689	A	C5-C6-N1	7.41	121.40	117.70
54	BA	972	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2453	A	C5-C6-N1	7.41	121.40	117.70
21	AA	1096	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	661	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1011	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	821	A	C5-C6-N1	7.40	121.40	117.70
54	BA	889	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	250	A	P-O3'-C3'	7.40	128.58	119.70
54	BA	1572	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1655	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1819	A	C5-C6-N1	7.40	121.40	117.70
21	AA	160	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	415	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1314	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	274	A	C4-C5-C6	-7.40	113.30	117.00
45	BW	24	ARG	NE-CZ-NH1	7.39	124.00	120.30
54	BA	613	A	C5-C6-N1	7.39	121.40	117.70
54	BA	204	A	C5-C6-N1	7.39	121.40	117.70
21	AA	306	A	C5-C6-N1	7.39	121.39	117.70
21	AA	1229	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	19	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	83	A	C5-C6-N1	7.39	121.40	117.70
54	BA	1893	C	N3-C2-O2	-7.39	116.73	121.90
54	BA	2154	A	O4'-C1'-N9	7.39	114.11	108.20
21	AA	77	A	C5-C6-N1	7.39	121.39	117.70
54	BA	849	A	C5-C6-N1	7.39	121.39	117.70
54	BA	2450	A	C4-C5-C6	-7.39	113.31	117.00
54	BA	1493	C	N1-C2-O2	7.39	123.33	118.90
11	AL	85	ARG	NE-CZ-NH1	7.39	123.99	120.30
21	AA	306	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	152	A	C5-C6-N1	7.39	121.39	117.70
54	BA	526	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	1040	A	C4-C5-C6	-7.39	113.31	117.00
54	BA	1287	A	C5-C6-N1	7.39	121.39	117.70
21	AA	1332	A	C5-C6-N1	7.38	121.39	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	352	A	C5-C6-N1	7.38	121.39	117.70
21	AA	149	A	C5-C6-N1	7.38	121.39	117.70
24	A3	58	A	C5-C6-N1	7.38	121.39	117.70
54	BA	182	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	1354	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1606	C	C1'-O4'-C4'	-7.38	104.00	109.90
21	AA	716	A	C5-C6-N1	7.38	121.39	117.70
21	AA	718	A	C5-C6-N1	7.38	121.39	117.70
54	BA	432	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1274	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2868	A	C5-C6-N1	7.38	121.39	117.70
2	AC	126	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	983	A	N1-C6-N6	-7.38	114.17	118.60
21	AA	794	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	2108	A	C4-C5-C6	-7.38	113.31	117.00
11	AL	13	ARG	NE-CZ-NH1	7.37	123.99	120.30
54	BA	56	A	C5-C6-N1	7.37	121.39	117.70
21	AA	383	A	C5-C6-N1	7.37	121.39	117.70
21	AA	1256	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1801	A	C5-C6-N1	7.37	121.39	117.70
21	AA	934	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	750	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2014	A	C5-C6-N1	7.37	121.39	117.70
21	AA	465	A	C5-C6-N1	7.37	121.38	117.70
21	AA	909	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	344	A	C5-C6-N1	7.37	121.38	117.70
54	BA	1525	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1048	A	C5-C6-N1	7.37	121.38	117.70
54	BA	1508	A	C5-C6-N1	7.37	121.38	117.70
54	BA	501	A	C5-C6-N1	7.37	121.38	117.70
54	BA	2573	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	928	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	941	A	C4-C5-C6	-7.36	113.32	117.00
55	BB	113	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	2482	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	743	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1155	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	479	A	C4-C5-C6	-7.36	113.32	117.00
54	BA	2288	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	2031	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	1689	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	1344	C	N3-C2-O2	-7.35	116.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1357	A	C5-C6-N1	7.35	121.38	117.70
54	BA	443	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2378	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2657	A	C5-C6-N1	7.35	121.38	117.70
21	AA	1192	C	N3-C2-O2	-7.35	116.76	121.90
54	BA	111	A	C5-C6-N1	7.35	121.37	117.70
54	BA	8	C	N3-C2-O2	-7.35	116.76	121.90
54	BA	753	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1654	A	N1-C6-N6	-7.34	114.19	118.60
54	BA	2757	A	C5-C6-N1	7.34	121.37	117.70
55	BB	115	A	C5-C6-N1	7.34	121.37	117.70
21	AA	819	A	C5-C6-N1	7.34	121.37	117.70
54	BA	721	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1305	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2899	A	N1-C6-N6	-7.34	114.20	118.60
21	AA	451	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	2778	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2614	A	C4-C5-C6	-7.34	113.33	117.00
21	AA	28	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	547	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2117	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1548	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	441	A	C5-C6-N1	7.33	121.37	117.70
21	AA	815	A	C5-C6-N1	7.33	121.37	117.70
54	BA	1156	A	C5-C6-N1	7.33	121.37	117.70
54	BA	1161	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	1453	A	C5-C6-N1	7.33	121.37	117.70
54	BA	1713	A	C5-C6-N1	7.33	121.37	117.70
54	BA	1900	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	686	U	O4'-C1'-N1	7.33	114.06	108.20
21	AA	729	A	C4-C5-C6	-7.33	113.34	117.00
54	BA	817	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	1029	A	C5-C6-N1	7.33	121.36	117.70
54	BA	1353	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	461	A	C5-C6-N1	7.33	121.36	117.70
54	BA	1786	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2725	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	120	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	1059	C	N3-C2-O2	-7.32	116.77	121.90
54	BA	354	A	C5-C6-N1	7.32	121.36	117.70
54	BA	587	C	O4'-C1'-N1	7.32	114.06	108.20
54	BA	793	A	C5-C6-N1	7.32	121.36	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2711	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	2022	U	O4'-C1'-N1	7.32	114.06	108.20
54	BA	2003	A	C5-C6-N1	7.32	121.36	117.70
21	AA	303	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	1008	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	1169	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2088	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2090	A	N1-C6-N6	-7.32	114.21	118.60
5	AF	2	ARG	NE-CZ-NH2	-7.31	116.64	120.30
21	AA	1046	A	C5-C6-N1	7.31	121.36	117.70
21	AA	210	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	382	A	N1-C6-N6	-7.31	114.21	118.60
54	BA	1749	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2577	A	N1-C6-N6	-7.31	114.21	118.60
49	B0	51	ARG	NE-CZ-NH1	7.31	123.95	120.30
46	BX	36	ARG	NE-CZ-NH1	7.31	123.95	120.30
54	BA	20	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	2566	A	C4-C5-C6	-7.31	113.35	117.00
21	AA	395	C	N3-C2-O2	-7.31	116.79	121.90
54	BA	608	A	C5-C6-N1	7.31	121.35	117.70
21	AA	136	C	N3-C2-O2	-7.30	116.79	121.90
21	AA	1250	A	C5-C6-N1	7.30	121.35	117.70
55	BB	36	C	N3-C2-O2	-7.30	116.79	121.90
11	AL	109	ARG	NE-CZ-NH1	7.30	123.95	120.30
21	AA	876	C	N3-C2-O2	-7.30	116.79	121.90
24	A3	14	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1640	A	C5-C6-N1	7.30	121.35	117.70
21	AA	681	A	C5-C6-N1	7.30	121.35	117.70
54	BA	415	A	C5-C6-N1	7.30	121.35	117.70
54	BA	946	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	1070	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1780	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1191	A	C5-C6-N1	7.30	121.35	117.70
21	AA	913	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	1553	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2158	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	2476	A	C5-C6-N1	7.30	121.35	117.70
10	AK	127	ARG	NE-CZ-NH1	7.29	123.95	120.30
54	BA	6	A	C4-C5-C6	-7.29	113.35	117.00
12	AM	108	ARG	NE-CZ-NH1	7.29	123.95	120.30
54	BA	1537	G	O4'-C1'-N9	7.29	114.03	108.20
54	BA	1919	A	C5-C6-N1	7.29	121.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	145	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	423	A	C5-C6-N1	7.29	121.35	117.70
54	BA	440	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	900	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	142	A	C5-C6-N1	7.29	121.34	117.70
54	BA	1000	A	C5-C6-N1	7.29	121.34	117.70
12	AM	78	ARG	NE-CZ-NH1	7.29	123.94	120.30
54	BA	516	C	O4'-C1'-N1	7.29	114.03	108.20
54	BA	980	A	C5-C6-N1	7.29	121.34	117.70
21	AA	468	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	196	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	575	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1145	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	901	C	N3-C2-O2	-7.29	116.80	121.90
19	AT	24	ARG	NE-CZ-NH1	7.28	123.94	120.30
54	BA	2795	C	N3-C2-O2	-7.28	116.80	121.90
21	AA	1227	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2590	A	C4-C5-C6	-7.28	113.36	117.00
24	A3	49	C	N3-C2-O2	-7.28	116.80	121.90
54	BA	911	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1411	C	N3-C2-O2	-7.28	116.81	121.90
21	AA	308	C	N3-C2-O2	-7.28	116.81	121.90
54	BA	981	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2082	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2632	A	C5-C6-N1	7.28	121.34	117.70
21	AA	109	A	C5-C6-N1	7.28	121.34	117.70
54	BA	44	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	2639	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1427	A	P-O3'-C3'	7.27	128.43	119.70
54	BA	1509	A	N1-C6-N6	-7.27	114.23	118.60
21	AA	160	A	C5-C6-N1	7.27	121.34	117.70
54	BA	914	G	O4'-C1'-N9	7.27	114.02	108.20
21	AA	432	A	C5-C6-N1	7.27	121.34	117.70
47	BY	23	ARG	NE-CZ-NH1	7.27	123.94	120.30
54	BA	794	A	C5-C6-N1	7.27	121.33	117.70
13	AN	41	ARG	NE-CZ-NH1	7.27	123.94	120.30
21	AA	1137	C	N3-C2-O2	-7.27	116.81	121.90
21	AA	1349	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1328	A	N1-C6-N6	-7.27	114.24	118.60
54	BA	2826	A	C5-C6-N1	7.27	121.33	117.70
21	AA	579	A	C5-C6-N1	7.27	121.33	117.70
54	BA	915	C	N3-C2-O2	-7.27	116.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2560	A	C4-C5-C6	-7.27	113.37	117.00
21	AA	576	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	191	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1853	A	N1-C6-N6	-7.27	114.24	118.60
21	AA	181	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2452	C	N3-C2-O2	-7.26	116.81	121.90
21	AA	195	A	C5-C6-N1	7.26	121.33	117.70
54	BA	257	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	844	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	207	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2589	A	C5-C6-N1	7.26	121.33	117.70
54	BA	722	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2518	A	C5-C6-N1	7.26	121.33	117.70
23	A2	91	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1420	A	O4'-C1'-N9	7.26	114.00	108.20
54	BA	2404	U	O4'-C1'-N1	7.26	114.00	108.20
54	BA	718	A	C5-C6-N1	7.25	121.33	117.70
21	AA	167	A	C4-C5-C6	-7.25	113.37	117.00
54	BA	716	A	C5-C6-N1	7.25	121.33	117.70
21	AA	1502	A	C5-C6-N1	7.25	121.33	117.70
54	BA	655	A	C5-C6-N1	7.25	121.33	117.70
21	AA	171	A	N1-C6-N6	-7.25	114.25	118.60
21	AA	228	A	C5-C6-N1	7.25	121.33	117.70
21	AA	946	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	257	C	O4'-C1'-N1	7.25	114.00	108.20
54	BA	2670	A	C4-C5-C6	-7.25	113.38	117.00
21	AA	554	A	C5-C6-N1	7.25	121.32	117.70
54	BA	223	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1214	A	C5-C6-N1	7.25	121.32	117.70
54	BA	2725	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1772	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	2809	A	C5-C6-N1	7.25	121.32	117.70
54	BA	910	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	1155	A	C5-C6-N1	7.25	121.32	117.70
21	AA	1111	A	C5-C6-N1	7.24	121.32	117.70
22	A1	69	A	C5-C6-N1	7.24	121.32	117.70
47	BY	47	ARG	NE-CZ-NH1	7.24	123.92	120.30
54	BA	320	A	N1-C6-N6	-7.24	114.25	118.60
54	BA	621	A	C5-C6-N1	7.24	121.32	117.70
21	AA	238	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2071	A	C5-C6-N1	7.24	121.32	117.70
21	AA	55	A	C5-C6-N1	7.24	121.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	431	A	N1-C6-N6	-7.24	114.26	118.60
21	AA	840	C	N3-C2-O2	-7.24	116.83	121.90
21	AA	1066	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	28	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2328	A	C5-C6-N1	7.24	121.32	117.70
21	AA	205	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2058	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1291	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	1226	A	C5-C6-N1	7.23	121.32	117.70
54	BA	95	A	C5-C6-N1	7.23	121.32	117.70
54	BA	309	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	2439	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	888	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	792	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1480	A	N1-C6-N6	-7.23	114.26	118.60
22	A1	69	A	C4-C5-C6	-7.23	113.39	117.00
54	BA	64	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	1269	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	1284	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	2005	A	C4-C5-C6	-7.23	113.39	117.00
54	BA	844	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1176	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	251	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1927	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	1098	A	N1-C6-N6	-7.22	114.27	118.60
21	AA	975	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1353	A	C5-C6-N1	7.22	121.31	117.70
21	AA	1236	A	C5-C6-N1	7.22	121.31	117.70
54	BA	848	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	1952	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2340	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1586	A	C5-C6-N1	7.22	121.31	117.70
36	BN	46	ARG	NE-CZ-NH1	7.22	123.91	120.30
54	BA	706	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	1794	A	C4-C5-C6	-7.22	113.39	117.00
21	AA	649	A	C5-C6-N1	7.21	121.31	117.70
37	BO	30	ARG	NE-CZ-NH1	7.21	123.91	120.30
10	AK	121	ARG	NE-CZ-NH1	7.21	123.91	120.30
21	AA	560	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1216	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	16	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	1344	U	O4'-C1'-N1	7.21	113.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2534	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1213	A	C5-C6-N1	7.21	121.31	117.70
22	A1	14	A	N1-C6-N6	-7.21	114.28	118.60
54	BA	693	A	N1-C6-N6	-7.21	114.28	118.60
54	BA	781	A	C5-C6-N1	7.21	121.30	117.70
54	BA	1089	A	C5-C6-N1	7.21	121.30	117.70
54	BA	2513	A	C5-C6-N1	7.21	121.30	117.70
54	BA	10	A	C5-C6-N1	7.21	121.30	117.70
54	BA	1700	A	C5-C6-N1	7.21	121.30	117.70
21	AA	199	A	C5-C6-N1	7.20	121.30	117.70
25	BC	216	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	626	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2727	A	C5-C6-N1	7.20	121.30	117.70
55	BB	52	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	129	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	1456	A	C5-C6-N1	7.20	121.30	117.70
24	A3	36	A	C5-C6-N1	7.20	121.30	117.70
54	BA	384	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	482	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1144	A	C5-C6-N1	7.20	121.30	117.70
55	BB	52	A	C5-C6-N1	7.20	121.30	117.70
21	AA	329	A	C4-C5-C6	-7.20	113.40	117.00
46	BX	17	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	201	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	1690	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	2366	A	C4-C5-C6	-7.20	113.40	117.00
3	AD	153	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	225	C	O4'-C1'-N1	7.20	113.96	108.20
54	BA	804	A	C5-C6-N1	7.20	121.30	117.70
54	BA	979	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1495	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1833	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	2311	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	371	A	C5-C6-N1	7.19	121.30	117.70
21	AA	1534	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1932	A	C5-C6-N1	7.19	121.30	117.70
21	AA	949	A	C4-C5-C6	-7.19	113.40	117.00
21	AA	1252	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1794	A	C5-C6-N1	7.19	121.30	117.70
17	AR	42	ARG	NE-CZ-NH1	7.19	123.89	120.30
54	BA	975	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2342	C	N3-C2-O2	-7.19	116.87	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	298	A	C5-C6-N1	7.19	121.29	117.70
54	BA	478	A	C5-C6-N1	7.19	121.29	117.70
54	BA	1579	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	1650	A	N1-C6-N6	-7.19	114.29	118.60
21	AA	53	A	C5-C6-N1	7.19	121.29	117.70
54	BA	1142	A	C5-C6-N1	7.19	121.29	117.70
54	BA	1580	A	C5-C6-N1	7.19	121.29	117.70
54	BA	1978	A	C4-C5-C6	-7.19	113.41	117.00
54	BA	2346	A	C5-C6-N1	7.19	121.29	117.70
21	AA	101	A	C4-C5-C6	-7.19	113.41	117.00
54	BA	1744	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2368	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	2757	A	N1-C6-N6	-7.18	114.29	118.60
21	AA	66	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	320	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	149	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1610	A	O4'-C1'-N9	7.18	113.95	108.20
54	BA	1423	G	O4'-C1'-N9	7.18	113.94	108.20
54	BA	401	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1913	A	C5-C6-N1	7.18	121.29	117.70
54	BA	453	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1853	A	C5-C6-N1	7.18	121.29	117.70
21	AA	192	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1163	A	C5-C6-N1	7.17	121.29	117.70
50	B1	5	ARG	NE-CZ-NH2	7.17	123.89	120.30
21	AA	6	G	C1'-O4'-C4'	-7.17	104.16	109.90
54	BA	1570	A	C4-C5-C6	-7.17	113.41	117.00
21	AA	1448	C	N3-C2-O2	-7.17	116.88	121.90
24	A3	17	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	1084	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	2054	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2274	A	C4-C5-C6	-7.17	113.42	117.00
55	BB	115	A	C4-C5-C6	-7.17	113.41	117.00
1	AB	94	ARG	NE-CZ-NH1	7.17	123.89	120.30
54	BA	833	A	C5-C6-N1	7.17	121.28	117.70
54	BA	982	C	N1-C2-O2	7.17	123.20	118.90
54	BA	2665	A	C5-C6-N1	7.17	121.28	117.70
55	BB	109	A	C5-C6-N1	7.17	121.28	117.70
21	AA	819	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	146	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2329	U	O4'-C1'-N1	7.17	113.94	108.20
54	BA	2726	A	C4-C5-C6	-7.17	113.42	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AG	94	ARG	NE-CZ-NH1	7.17	123.88	120.30
54	BA	37	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	1431	A	C5-C6-N1	7.17	121.28	117.70
27	BE	170	ARG	NE-CZ-NH1	7.17	123.88	120.30
54	BA	2896	C	N3-C2-O2	-7.17	116.89	121.90
21	AA	831	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	908	A	C5-C6-N1	7.16	121.28	117.70
21	AA	1507	A	C4-C5-C6	-7.16	113.42	117.00
54	BA	675	A	C5-C6-N1	7.16	121.28	117.70
54	BA	1272	A	C5-C6-N1	7.16	121.28	117.70
54	BA	1698	A	N1-C6-N6	-7.16	114.30	118.60
54	BA	2660	A	N1-C6-N6	-7.16	114.30	118.60
21	AA	695	A	N1-C6-N6	-7.16	114.30	118.60
21	AA	1031	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	1241	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2394	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	1171	A	C5-C6-N1	7.16	121.28	117.70
21	AA	1531	A	C5-C6-N1	7.16	121.28	117.70
54	BA	1590	A	C5-C6-N1	7.16	121.28	117.70
21	AA	238	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	814	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	2764	A	C5-C6-N1	7.16	121.28	117.70
21	AA	559	A	C5-C6-N1	7.16	121.28	117.70
21	AA	747	A	C5-C6-N1	7.16	121.28	117.70
54	BA	241	A	C5-C6-N1	7.16	121.28	117.70
54	BA	362	A	C5-C6-N1	7.16	121.28	117.70
54	BA	896	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1872	A	C5-C6-N1	7.15	121.28	117.70
54	BA	528	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1675	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	1754	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1214	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	1571	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2873	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	205	A	C4-C5-C6	-7.15	113.43	117.00
21	AA	780	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2284	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	635	C	N3-C2-O2	-7.15	116.90	121.90
54	BA	1866	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	1403	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1044	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1170	C	O4'-C1'-N1	7.14	113.92	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2055	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	2327	A	C5-C6-N1	7.14	121.27	117.70
11	AL	55	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	300	A	C5-C6-N1	7.14	121.27	117.70
54	BA	447	A	C5-C6-N1	7.14	121.27	117.70
54	BA	481	G	O4'-C1'-N9	7.14	113.91	108.20
54	BA	1039	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	2418	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	2602	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	478	A	C5-C6-N1	7.14	121.27	117.70
21	AA	695	A	C5-C6-N1	7.14	121.27	117.70
54	BA	101	A	C5-C6-N1	7.14	121.27	117.70
21	AA	559	A	N1-C6-N6	-7.14	114.32	118.60
21	AA	1434	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1347	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1420	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1772	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1502	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	2751	G	O4'-C1'-N9	7.14	113.91	108.20
54	BA	2411	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1080	A	N1-C6-N6	-7.13	114.32	118.60
55	BB	15	A	C5-C6-N1	7.13	121.27	117.70
54	BA	176	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	309	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	313	A	C5-C6-N1	7.13	121.26	117.70
38	BP	20	ARG	NE-CZ-NH1	7.13	123.86	120.30
54	BA	191	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	8	A	C5-C6-N1	7.13	121.26	117.70
21	AA	995	C	N1-C2-O2	7.13	123.18	118.90
54	BA	1598	A	C5-C6-N1	7.13	121.26	117.70
54	BA	2278	A	C5-C6-N1	7.13	121.26	117.70
54	BA	2497	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	2541	A	C5-C6-N1	7.13	121.26	117.70
55	BB	46	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	1395	C	N3-C2-O2	-7.12	116.91	121.90
22	A1	23	A	C5-C6-N1	7.12	121.26	117.70
54	BA	844	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	909	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1969	A	C5-C6-N1	7.12	121.26	117.70
54	BA	244	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	782	A	N1-C6-N6	-7.12	114.33	118.60
21	AA	1045	C	N3-C2-O2	-7.12	116.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AP	25	ARG	NE-CZ-NH1	7.12	123.86	120.30
21	AA	687	A	C5-C6-N1	7.12	121.26	117.70
44	BV	21	ARG	NE-CZ-NH1	7.12	123.86	120.30
54	BA	195	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	1603	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	673	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	1285	A	C5-C6-N1	7.12	121.26	117.70
55	BB	101	A	C5-C6-N1	7.12	121.26	117.70
21	AA	300	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1265	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	152	A	C4-C5-C6	-7.11	113.44	117.00
21	AA	236	A	C5-C6-N1	7.11	121.26	117.70
21	AA	312	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	1496	A	C5-C6-N1	7.11	121.26	117.70
54	BA	2101	A	C5-C6-N1	7.11	121.26	117.70
54	BA	1899	A	C4-C5-C6	-7.11	113.44	117.00
21	AA	533	A	C5-C6-N1	7.11	121.25	117.70
36	BN	2	ARG	NE-CZ-NH1	7.11	123.85	120.30
54	BA	2119	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	993	G	O4'-C1'-N9	7.11	113.89	108.20
54	BA	1854	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2776	A	C5-C6-N1	7.11	121.25	117.70
21	AA	1286	U	O4'-C1'-N1	7.11	113.89	108.20
21	AA	161	A	C5-C6-N1	7.10	121.25	117.70
28	BF	124	ARG	NE-CZ-NH1	7.10	123.85	120.30
21	AA	336	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1407	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	400	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	825	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	873	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	1328	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1876	A	C5-C6-N1	7.10	121.25	117.70
2	AC	125	ARG	NE-CZ-NH1	7.10	123.85	120.30
21	AA	6	G	P-O3'-C3'	7.10	128.22	119.70
21	AA	573	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1730	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	1977	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1393	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2496	C	N3-C2-O2	-7.09	116.94	121.90
9	AJ	7	ARG	NE-CZ-NH1	7.09	123.85	120.30
9	AJ	89	ARG	NE-CZ-NH1	7.09	123.85	120.30
21	AA	382	A	C5-C6-N1	7.09	121.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1518	A	C4-C5-C6	-7.09	113.45	117.00
22	A1	41	A	C5-C6-N1	7.09	121.25	117.70
37	BO	81	ARG	NE-CZ-NH1	7.09	123.85	120.30
54	BA	2732	G	O4'-C1'-N9	7.09	113.87	108.20
55	BB	53	A	N1-C6-N6	-7.09	114.35	118.60
4	AE	67	ARG	NE-CZ-NH1	7.09	123.84	120.30
21	AA	77	A	N1-C6-N6	-7.08	114.35	118.60
21	AA	825	A	C5-C6-N1	7.08	121.24	117.70
21	AA	1306	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2154	A	C5-C6-N1	7.08	121.24	117.70
49	B0	15	ARG	NE-CZ-NH2	7.08	123.84	120.30
55	BB	99	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2741	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2899	A	C5-C6-N1	7.08	121.24	117.70
21	AA	629	A	N1-C6-N6	-7.08	114.35	118.60
21	AA	744	C	N3-C2-O2	-7.08	116.95	121.90
21	AA	1493	A	C4-C5-C6	-7.08	113.46	117.00
49	B0	9	ARG	NE-CZ-NH1	7.08	123.84	120.30
55	BB	118	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	1042	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	94	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	728	A	C5-C6-N1	7.08	121.24	117.70
36	BN	2	ARG	NE-CZ-NH2	-7.08	116.76	120.30
54	BA	428	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	1789	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	95	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	393	A	C5-C6-N1	7.07	121.24	117.70
54	BA	2073	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	2853	C	N3-C2-O2	-7.07	116.95	121.90
11	AL	53	ARG	NE-CZ-NH1	7.07	123.84	120.30
54	BA	2882	A	C4-C5-C6	-7.07	113.46	117.00
21	AA	782	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1089	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	1289	A	C4-C5-C6	-7.07	113.47	117.00
48	BZ	15	ARG	NE-CZ-NH1	7.07	123.83	120.30
54	BA	63	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	863	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1067	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	1268	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	2314	A	C5-C6-N1	7.07	121.23	117.70
22	A1	66	A	C5-C6-N1	7.07	121.23	117.70
54	BA	84	A	C5-C6-N1	7.07	121.23	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	244	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2309	A	C5-C6-N1	7.07	121.23	117.70
54	BA	320	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1916	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2610	C	N3-C2-O2	-7.06	116.95	121.90
54	BA	1145	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	2856	A	C5-C6-N1	7.06	121.23	117.70
21	AA	246	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2635	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2009	A	C5-C6-N1	7.06	121.23	117.70
54	BA	50	U	O4'-C1'-N1	7.06	113.85	108.20
54	BA	2856	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	174	A	C4-C5-C6	-7.06	113.47	117.00
14	AO	57	ARG	NE-CZ-NH1	7.05	123.83	120.30
21	AA	608	A	C5-C6-N1	7.05	121.23	117.70
21	AA	1037	C	N3-C2-O2	-7.05	116.96	121.90
21	AA	1188	A	C5-C6-N1	7.05	121.23	117.70
22	A1	76	A	C5-C6-N1	7.05	121.23	117.70
21	AA	1101	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	11	C	N3-C2-O2	-7.05	116.96	121.90
54	BA	1069	A	C5-C6-N1	7.05	121.23	117.70
54	BA	430	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2521	C	N3-C2-O2	-7.05	116.97	121.90
22	A1	58	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2241	A	N1-C6-N6	-7.05	114.37	118.60
21	AA	171	A	C5-C6-N1	7.05	121.22	117.70
21	AA	978	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1147	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1247	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1787	A	C4-C5-C6	-7.05	113.48	117.00
54	BA	1815	A	C4-C5-C6	-7.05	113.48	117.00
54	BA	2799	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1217	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	1010	A	C5-C6-N1	7.04	121.22	117.70
21	AA	712	A	C5-C6-N1	7.04	121.22	117.70
21	AA	746	A	C5-C6-N1	7.04	121.22	117.70
44	BV	93	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	172	A	N1-C6-N6	-7.04	114.37	118.60
54	BA	2883	A	C5-C6-N1	7.04	121.22	117.70
21	AA	964	A	C5-C6-N1	7.04	121.22	117.70
54	BA	734	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1600	C	N3-C2-O2	-7.04	116.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1640	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	523	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	1866	A	C5-C6-N1	7.04	121.22	117.70
21	AA	236	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	1112	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	1413	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	1634	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1668	A	C5-C6-N1	7.04	121.22	117.70
21	AA	87	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	131	A	C5-C6-N1	7.04	121.22	117.70
21	AA	749	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	103	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	1469	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1848	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2787	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	2902	C	N3-C2-O2	-7.04	116.98	121.90
54	BA	935	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1129	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2598	A	C5-C6-N1	7.03	121.22	117.70
54	BA	572	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1783	A	C4-C5-C6	-7.03	113.48	117.00
19	AT	59	ARG	NE-CZ-NH1	7.03	123.82	120.30
21	AA	708	C	N3-C2-O2	-7.03	116.98	121.90
21	AA	1462	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1233	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	2810	A	C5-C6-N1	7.03	121.22	117.70
21	AA	892	A	C5-C6-N1	7.03	121.21	117.70
21	AA	1204	A	N1-C6-N6	-7.03	114.38	118.60
21	AA	1311	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2227	A	N1-C6-N6	-7.03	114.38	118.60
21	AA	143	A	N1-C6-N6	-7.03	114.38	118.60
21	AA	609	A	C5-C6-N1	7.03	121.21	117.70
54	BA	147	C	C1'-O4'-C4'	-7.03	104.28	109.90
54	BA	2821	A	C5-C6-N1	7.03	121.21	117.70
21	AA	750	C	N3-C2-O2	-7.03	116.98	121.90
22	A1	38	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	1086	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	1997	C	O4'-C1'-N1	7.03	113.82	108.20
21	AA	364	A	C5-C6-N1	7.02	121.21	117.70
21	AA	883	C	N3-C2-O2	-7.02	116.98	121.90
21	AA	196	A	C4-C5-C6	-7.02	113.49	117.00
21	AA	498	A	C5-C6-N1	7.02	121.21	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	768	A	C5-C6-N1	7.02	121.21	117.70
32	BJ	69	ARG	NE-CZ-NH1	7.02	123.81	120.30
54	BA	2589	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	2748	A	C4-C5-C6	-7.02	113.49	117.00
10	AK	92	ARG	NE-CZ-NH1	7.02	123.81	120.30
21	AA	1396	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1534	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	1881	C	N3-C2-O2	-7.02	116.99	121.90
54	BA	2381	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	2815	C	N3-C2-O2	-7.02	116.99	121.90
22	A1	48	C	N3-C2-O2	-7.02	116.99	121.90
54	BA	1885	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	2634	A	C5-C6-N1	7.02	121.21	117.70
21	AA	983	A	C5-C6-N1	7.01	121.21	117.70
54	BA	340	A	C5-C6-N1	7.01	121.21	117.70
13	AN	63	ARG	NE-CZ-NH1	7.01	123.81	120.30
21	AA	502	A	N1-C6-N6	-7.01	114.39	118.60
24	A3	14	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	1773	A	C5-C6-N1	7.01	121.20	117.70
18	AS	35	ARG	NE-CZ-NH1	7.01	123.80	120.30
54	BA	1470	A	C5-C6-N1	7.01	121.20	117.70
21	AA	179	A	C5-C6-N1	7.00	121.20	117.70
54	BA	61	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	1144	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	2814	A	C5-C6-N1	7.00	121.20	117.70
54	BA	541	A	C5-C6-N1	7.00	121.20	117.70
54	BA	505	A	C5-C6-N1	7.00	121.20	117.70
55	BB	53	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1427	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1614	A	C5-C6-N1	7.00	121.20	117.70
21	AA	949	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1676	A	C5-C6-N1	7.00	121.20	117.70
21	AA	67	C	N1-C2-O2	7.00	123.10	118.90
21	AA	1248	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1244	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	452	A	C5-C6-N1	6.99	121.20	117.70
54	BA	222	A	C5-C6-N1	6.99	121.20	117.70
54	BA	2503	A	N1-C6-N6	-6.99	114.40	118.60
18	AS	36	ARG	NE-CZ-NH2	6.99	123.80	120.30
54	BA	1134	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1144	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	2700	A	C5-C6-N1	6.99	121.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1429	A	C5-C6-N1	6.99	121.19	117.70
22	A1	75	C	N3-C2-O2	-6.99	117.01	121.90
38	BP	87	ARG	NE-CZ-NH1	6.99	123.80	120.30
38	BP	92	ARG	NE-CZ-NH1	6.99	123.79	120.30
54	BA	299	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1433	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	2581	G	O4'-C1'-N9	6.99	113.79	108.20
21	AA	16	A	C5-C6-N1	6.99	121.19	117.70
22	A1	60	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	1427	A	N1-C6-N6	-6.99	114.41	118.60
21	AA	328	C	N1-C2-O2	6.99	123.09	118.90
54	BA	182	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2435	A	C5-C6-N1	6.99	121.19	117.70
54	BA	616	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1008	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1291	C	O4'-C1'-N1	6.98	113.79	108.20
21	AA	80	A	C5-C6-N1	6.98	121.19	117.70
21	AA	1201	A	P-O3'-C3'	6.98	128.08	119.70
21	AA	1519	A	C5-C6-N1	6.98	121.19	117.70
43	BU	6	ARG	NE-CZ-NH2	6.98	123.79	120.30
54	BA	723	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	1286	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2171	A	C5-C6-N1	6.98	121.19	117.70
21	AA	906	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2823	A	C5-C6-N1	6.98	121.19	117.70
55	BB	58	A	C5-C6-N1	6.98	121.19	117.70
21	AA	217	C	N3-C2-O2	-6.98	117.02	121.90
21	AA	1519	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	529	A	C5-C6-N1	6.98	121.19	117.70
8	AI	108	ARG	NE-CZ-NH1	6.98	123.79	120.30
21	AA	808	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	34	U	O4'-C1'-N1	6.98	113.78	108.20
54	BA	345	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	527	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	2202	U	O4'-C1'-N1	6.98	113.78	108.20
54	BA	2322	A	N1-C6-N6	-6.98	114.41	118.60
4	AE	92	ARG	NE-CZ-NH1	6.97	123.79	120.30
21	AA	519	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	630	A	C5-C6-N1	6.97	121.19	117.70
21	AA	805	C	N3-C2-O2	-6.97	117.02	121.90
28	BF	166	ARG	NE-CZ-NH1	6.97	123.79	120.30
54	BA	928	A	C5-C6-N1	6.97	121.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2820	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	861	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1366	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2468	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	28	A	C5-C6-N1	6.97	121.19	117.70
21	AA	996	A	N1-C6-N6	-6.97	114.42	118.60
24	A3	75	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	1965	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2161	C	N3-C2-O2	-6.97	117.02	121.90
55	BB	47	C	O4'-C1'-N1	6.97	113.78	108.20
54	BA	228	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	393	A	C4-C5-C6	-6.97	113.52	117.00
21	AA	1169	A	C5-C6-N1	6.97	121.18	117.70
21	AA	1170	A	C5-C6-N1	6.97	121.18	117.70
54	BA	460	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	190	A	C5-C6-N1	6.96	121.18	117.70
54	BA	845	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2062	A	N1-C6-N6	-6.96	114.42	118.60
54	BA	2275	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	820	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1650	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1900	A	C5-C6-N1	6.96	121.18	117.70
55	BB	39	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	1285	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	739	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1932	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	791	C	N3-C2-O2	-6.96	117.03	121.90
3	AD	187	ARG	NE-CZ-NH1	6.96	123.78	120.30
21	AA	1191	A	C4-C5-C6	-6.96	113.52	117.00
22	A1	74	C	N1-C2-O2	6.96	123.08	118.90
54	BA	104	A	C5-C6-N1	6.96	121.18	117.70
54	BA	161	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	219	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1028	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	2058	A	N1-C6-N6	-6.96	114.42	118.60
54	BA	1088	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2433	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2435	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	663	A	C5-C6-N1	6.95	121.18	117.70
21	AA	1055	A	C5-C6-N1	6.95	121.18	117.70
35	BM	44	ARG	NE-CZ-NH1	6.95	123.78	120.30
54	BA	2432	A	N1-C6-N6	-6.95	114.43	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2705	A	C5-C6-N1	6.95	121.18	117.70
54	BA	127	A	C5-C6-N1	6.95	121.17	117.70
54	BA	310	A	C5-C6-N1	6.95	121.17	117.70
54	BA	470	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1067	A	C5-C6-N1	6.95	121.17	117.70
21	AA	66	A	C5-C6-N1	6.95	121.17	117.70
21	AA	574	A	C5-C6-N1	6.95	121.17	117.70
21	AA	1329	A	C5-C6-N1	6.95	121.17	117.70
54	BA	603	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1591	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	19	A	C5-C6-N1	6.95	121.17	117.70
44	BV	19	ARG	NE-CZ-NH1	6.95	123.77	120.30
54	BA	2662	A	N1-C6-N6	-6.95	114.43	118.60
21	AA	366	A	C5-C6-N1	6.95	121.17	117.70
21	AA	784	A	N1-C6-N6	-6.95	114.43	118.60
21	AA	807	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	466	A	C5-C6-N1	6.95	121.17	117.70
54	BA	959	A	C5-C6-N1	6.94	121.17	117.70
21	AA	831	A	C5-C6-N1	6.94	121.17	117.70
21	AA	1493	A	C5-C6-N1	6.94	121.17	117.70
54	BA	936	A	C4-C5-C6	-6.94	113.53	117.00
21	AA	1258	G	C1'-O4'-C4'	-6.94	104.35	109.90
54	BA	422	A	C5-C6-N1	6.94	121.17	117.70
21	AA	706	A	C5-C6-N1	6.94	121.17	117.70
54	BA	821	A	C4-C5-C6	-6.94	113.53	117.00
27	BE	79	ARG	NE-CZ-NH1	6.94	123.77	120.30
21	AA	345	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	592	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	670	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1791	A	C5-C6-N1	6.93	121.17	117.70
54	BA	2052	A	C5-C6-N1	6.93	121.17	117.70
21	AA	131	A	C5-C6-N1	6.93	121.17	117.70
21	AA	878	A	N1-C6-N6	-6.93	114.44	118.60
30	BH	123	ARG	NE-CZ-NH1	6.93	123.77	120.30
54	BA	457	A	C5-C6-N1	6.93	121.17	117.70
54	BA	2092	U	O4'-C1'-N1	6.93	113.75	108.20
54	BA	2273	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	2628	C	N3-C2-O2	-6.93	117.05	121.90
55	BB	43	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	387	U	O4'-C1'-N1	6.93	113.74	108.20
54	BA	645	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	716	A	C4-C5-C6	-6.93	113.53	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1760	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	1035	A	C5-C6-N1	6.93	121.16	117.70
54	BA	91	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	1032	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	1289	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	1545	A	C5-C6-N1	6.93	121.17	117.70
22	A1	26	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	911	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	2706	A	C5-C6-N1	6.93	121.16	117.70
21	AA	1093	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	633	A	C5-C6-N1	6.93	121.16	117.70
54	BA	1652	A	C5-C6-N1	6.93	121.16	117.70
54	BA	1858	A	C5-C6-N1	6.93	121.16	117.70
21	AA	1167	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1569	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2248	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	387	U	C1'-O4'-C4'	-6.92	104.36	109.90
21	AA	139	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1705	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	2232	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	348	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1050	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	1262	A	O4'-C1'-N9	6.92	113.74	108.20
21	AA	1418	A	N1-C6-N6	-6.92	114.45	118.60
30	BH	97	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	1342	A	C5-C6-N1	6.92	121.16	117.70
21	AA	19	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	2675	A	C5-C6-N1	6.92	121.16	117.70
54	BA	265	A	C5-C6-N1	6.91	121.16	117.70
54	BA	627	A	C4-C5-C6	-6.91	113.54	117.00
54	BA	1373	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1625	C	N3-C2-O2	-6.91	117.06	121.90
55	BB	97	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	532	A	C5-C6-N1	6.91	121.16	117.70
21	AA	483	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	21	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	79	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	1301	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1606	C	N1-C2-O2	6.91	123.05	118.90
21	AA	422	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	1027	A	C5-C6-N1	6.91	121.15	117.70
54	BA	1152	C	N3-C2-O2	-6.91	117.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1596	A	C5-C6-N1	6.91	121.15	117.70
54	BA	1413	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	1739	A	N1-C6-N6	-6.91	114.46	118.60
54	BA	2352	A	C5-C6-N1	6.91	121.15	117.70
54	BA	103	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1532	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2003	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	262	A	C5-C6-N1	6.90	121.15	117.70
54	BA	480	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1260	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2135	A	C5-C6-N1	6.90	121.15	117.70
21	AA	235	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	694	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	1219	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	311	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1392	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	1953	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2666	C	O4'-C1'-N1	6.90	113.72	108.20
21	AA	349	A	C5-C6-N1	6.90	121.15	117.70
21	AA	602	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1261	A	C5-C6-N1	6.90	121.15	117.70
39	BQ	32	ARG	NE-CZ-NH1	6.90	123.75	120.30
54	BA	1420	A	N1-C6-N6	-6.90	114.46	118.60
21	AA	575	G	O4'-C1'-N9	6.90	113.72	108.20
54	BA	1230	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1387	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2418	A	C5-C6-N1	6.90	121.15	117.70
21	AA	726	C	N3-C2-O2	-6.89	117.07	121.90
21	AA	931	C	N3-C2-O2	-6.89	117.07	121.90
21	AA	1117	A	N1-C6-N6	-6.89	114.46	118.60
21	AA	1518	A	C5-C6-N1	6.89	121.15	117.70
54	BA	908	C	N3-C2-O2	-6.89	117.07	121.90
54	BA	947	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1320	C	N3-C2-O2	-6.89	117.07	121.90
54	BA	2417	C	N3-C2-O2	-6.89	117.07	121.90
54	BA	614	A	N1-C6-N6	-6.89	114.47	118.60
54	BA	936	A	C5-C6-N1	6.89	121.15	117.70
54	BA	2191	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	2425	A	C4-C5-C6	-6.89	113.55	117.00
21	AA	51	A	C5-C6-N1	6.89	121.14	117.70
21	AA	622	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	1597	A	C4-C5-C6	-6.89	113.56	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2080	A	C5-C6-N1	6.89	121.14	117.70
54	BA	84	A	N1-C6-N6	-6.89	114.47	118.60
54	BA	1664	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	1746	A	N1-C6-N6	-6.89	114.47	118.60
21	AA	328	C	O4'-C1'-N1	6.89	113.71	108.20
54	BA	1938	A	O4'-C1'-N9	6.89	113.71	108.20
54	BA	975	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1073	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	914	A	C5-C6-N1	6.88	121.14	117.70
54	BA	382	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	432	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	124	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	151	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1382	C	N3-C2-O2	-6.88	117.08	121.90
24	A3	39	A	C4-C5-C6	-6.88	113.56	117.00
38	BP	71	ARG	NE-CZ-NH1	6.88	123.74	120.30
21	AA	1271	A	C5-C6-N1	6.88	121.14	117.70
54	BA	943	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1958	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	642	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	826	C	N3-C2-O2	-6.88	117.09	121.90
36	BN	71	ARG	NE-CZ-NH1	6.88	123.74	120.30
54	BA	74	A	C5-C6-N1	6.88	121.14	117.70
21	AA	1044	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	1111	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	1593	A	C5-C6-N1	6.87	121.14	117.70
54	BA	587	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	727	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	2606	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	958	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	1494	A	C4-C5-C6	-6.87	113.56	117.00
16	AQ	76	ARG	NE-CZ-NH1	6.87	123.73	120.30
21	AA	743	A	C4-C5-C6	-6.87	113.57	117.00
43	BU	5	ARG	NE-CZ-NH1	6.87	123.73	120.30
54	BA	322	A	O4'-C1'-N9	6.87	113.69	108.20
54	BA	1870	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	2284	A	C5-C6-N1	6.87	121.14	117.70
54	BA	2813	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	909	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	1126	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	1679	A	C5-C6-N1	6.87	121.13	117.70
54	BA	2147	A	C4-C5-C6	-6.87	113.57	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	81	A	C5-C6-N1	6.87	121.13	117.70
21	AA	162	A	C5-C6-N1	6.87	121.13	117.70
21	AA	189	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1837	C	N3-C2-O2	-6.87	117.09	121.90
6	AG	91	ARG	NE-CZ-NH1	6.86	123.73	120.30
33	BK	98	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	1564	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	1757	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	233	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1847	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2020	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	26	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	140	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	382	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2268	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	1278	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	72	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	440	C	O4'-C1'-N1	6.86	113.68	108.20
54	BA	2160	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2171	A	N1-C6-N6	-6.85	114.49	118.60
20	AU	17	ARG	NE-CZ-NH1	6.85	123.73	120.30
21	AA	108	G	O4'-C1'-N9	6.85	113.68	108.20
54	BA	1365	A	C5-C6-N1	6.85	121.13	117.70
54	BA	1821	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	2298	A	C5-C6-N1	6.85	121.13	117.70
54	BA	925	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	2134	A	C5-C6-N1	6.85	121.12	117.70
54	BA	2734	A	C5-C6-N1	6.85	121.12	117.70
21	AA	430	A	C5-C6-N1	6.85	121.12	117.70
54	BA	71	A	C5-C6-N1	6.85	121.12	117.70
21	AA	253	A	N1-C6-N6	-6.84	114.49	118.60
21	AA	749	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1225	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	2560	A	C5-C6-N1	6.84	121.12	117.70
54	BA	290	U	O4'-C1'-N1	6.84	113.67	108.20
2	AC	106	ARG	NE-CZ-NH1	6.84	123.72	120.30
13	AN	90	ARG	NE-CZ-NH1	6.84	123.72	120.30
21	AA	743	A	C5-C6-N1	6.84	121.12	117.70
54	BA	756	A	C5-C6-N1	6.84	121.12	117.70
54	BA	764	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1413	A	C5-C6-N1	6.84	121.12	117.70
21	AA	795	C	N3-C2-O2	-6.84	117.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	678	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1528	A	C5-C6-N1	6.84	121.12	117.70
54	BA	717	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	423	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	739	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1130	U	O4'-C1'-N1	6.84	113.67	108.20
54	BA	1553	A	N1-C6-N6	-6.84	114.50	118.60
55	BB	59	A	C4-C5-C6	-6.84	113.58	117.00
24	A3	38	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	183	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	1515	A	C5-C6-N1	6.83	121.12	117.70
54	BA	1608	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2726	A	C5-C6-N1	6.83	121.12	117.70
21	AA	766	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1035	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	1938	A	C5-C6-N1	6.83	121.12	117.70
54	BA	1713	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	2453	A	C4-C5-C6	-6.83	113.58	117.00
55	BB	63	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1248	A	C4-C5-C6	-6.83	113.58	117.00
32	BJ	37	ARG	NE-CZ-NH1	6.83	123.71	120.30
21	AA	547	A	C4-C5-C6	-6.83	113.59	117.00
21	AA	1362	A	C5-C6-N1	6.83	121.11	117.70
22	A1	72	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	1098	A	C5-C6-N1	6.83	121.11	117.70
24	A3	68	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	240	C	N1-C2-O2	6.83	123.00	118.90
54	BA	1598	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	2072	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	2227	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1180	A	C5-C6-N1	6.82	121.11	117.70
22	A1	26	A	C5-C6-N1	6.82	121.11	117.70
54	BA	556	A	N1-C6-N6	-6.82	114.50	118.60
54	BA	590	A	C4-C5-C6	-6.82	113.59	117.00
16	AQ	39	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	1970	A	C5-C6-N1	6.82	121.11	117.70
15	AP	56	ARG	NE-CZ-NH1	6.82	123.71	120.30
21	AA	386	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	564	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	842	U	O4'-C1'-N1	6.82	113.66	108.20
32	BJ	34	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	457	A	C4-C5-C6	-6.82	113.59	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	624	C	N3-C2-O2	-6.82	117.13	121.90
22	A1	23	A	N1-C6-N6	-6.82	114.51	118.60
21	AA	1483	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2339	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	2682	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	2901	C	N3-C2-O2	-6.82	117.13	121.90
55	BB	29	A	C5-C6-N1	6.82	121.11	117.70
54	BA	945	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1434	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1769	U	O4'-C1'-N1	6.82	113.65	108.20
54	BA	2308	G	O4'-C1'-N9	6.82	113.65	108.20
54	BA	2872	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1999	C	N3-C2-O2	-6.81	117.13	121.90
22	A1	6	A	C5-C6-N1	6.81	121.11	117.70
54	BA	1167	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	2761	A	C5-C6-N1	6.81	121.11	117.70
54	BA	2792	A	C5-C6-N1	6.81	121.11	117.70
54	BA	998	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	1476	A	N1-C6-N6	-6.81	114.51	118.60
54	BA	2175	C	N3-C2-O2	-6.81	117.14	121.90
54	BA	2317	A	C5-C6-N1	6.81	121.10	117.70
54	BA	2649	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	607	A	C4-C5-C6	-6.81	113.60	117.00
21	AA	23	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	1398	A	C5-C6-N1	6.80	121.10	117.70
54	BA	64	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2247	A	N1-C6-N6	-6.80	114.52	118.60
54	BA	2700	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	872	A	C5-C6-N1	6.80	121.10	117.70
21	AA	496	A	N1-C6-N6	-6.80	114.52	118.60
54	BA	483	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2021	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	2378	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	1130	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	966	G	N1-C6-O6	-6.80	115.82	119.90
54	BA	2019	A	C5-C6-N1	6.80	121.10	117.70
54	BA	219	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	2666	C	N1-C2-O2	6.79	122.98	118.90
21	AA	495	A	C5-C6-N1	6.79	121.10	117.70
54	BA	145	C	O4'-C1'-N1	6.79	113.63	108.20
54	BA	1802	A	C5-C6-N1	6.79	121.09	117.70
54	BA	2733	A	C5-C6-N1	6.79	121.10	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	860	A	C5-C6-N1	6.79	121.09	117.70
22	A1	16	C	N1-C2-O2	6.79	122.97	118.90
54	BA	368	A	C5-C6-N1	6.79	121.09	117.70
54	BA	1204	A	C5-C6-N1	6.79	121.09	117.70
21	AA	1274	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	1146	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	1616	A	C5-C6-N1	6.79	121.09	117.70
21	AA	1021	A	C5-C6-N1	6.79	121.09	117.70
54	BA	1618	A	C5-C6-N1	6.79	121.09	117.70
21	AA	325	A	C5-C6-N1	6.79	121.09	117.70
21	AA	1136	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	666	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	817	C	N1-C2-O2	6.79	122.97	118.90
54	BA	1810	A	C5-C6-N1	6.79	121.09	117.70
54	BA	2358	A	C5-C6-N1	6.79	121.09	117.70
54	BA	2381	A	C5-C6-N1	6.79	121.09	117.70
21	AA	468	A	C5-C6-N1	6.78	121.09	117.70
21	AA	1500	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	761	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	2900	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	990	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1276	A	C5-C6-N1	6.78	121.09	117.70
11	AL	113	ARG	NE-CZ-NH1	6.78	123.69	120.30
21	AA	385	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	1618	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	1669	A	N1-C6-N6	-6.78	114.53	118.60
21	AA	706	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1465	A	C5-C6-N1	6.78	121.09	117.70
54	BA	582	A	C5-C6-N1	6.78	121.09	117.70
54	BA	886	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	497	A	C4-C5-C6	-6.78	113.61	117.00
55	BB	73	A	N1-C6-N6	-6.78	114.53	118.60
4	AE	137	ARG	NE-CZ-NH1	6.78	123.69	120.30
21	AA	271	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	1318	A	C4-C5-C6	-6.77	113.61	117.00
55	BB	29	A	N1-C6-N6	-6.77	114.53	118.60
21	AA	845	A	C1'-O4'-C4'	-6.77	104.48	109.90
21	AA	1110	A	N1-C6-N6	-6.77	114.54	118.60
54	BA	912	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	2336	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2439	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2440	C	N3-C2-O2	-6.77	117.16	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1151	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	324	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1477	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2388	A	C5-C6-N1	6.77	121.08	117.70
21	AA	1502	A	N1-C6-N6	-6.77	114.54	118.60
54	BA	231	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1638	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	1859	U	O4'-C1'-N1	6.77	113.61	108.20
21	AA	228	A	N1-C6-N6	-6.76	114.54	118.60
21	AA	431	A	C5-C6-N1	6.76	121.08	117.70
21	AA	510	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1275	A	C5-C6-N1	6.76	121.08	117.70
54	BA	111	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	198	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	574	A	O4'-C1'-N9	6.76	113.61	108.20
54	BA	693	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1690	A	C5-C6-N1	6.76	121.08	117.70
54	BA	2285	C	O4'-C1'-N1	6.76	113.61	108.20
14	AO	76	ARG	NE-CZ-NH2	-6.76	116.92	120.30
54	BA	492	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1677	A	C5-C6-N1	6.76	121.08	117.70
13	AN	81	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	753	A	C5-C6-N1	6.76	121.08	117.70
54	BA	250	G	O4'-C1'-N9	6.76	113.61	108.20
54	BA	631	A	N1-C6-N6	-6.76	114.54	118.60
54	BA	1143	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1433	A	C5-C6-N1	6.76	121.08	117.70
54	BA	433	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	282	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	972	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1644	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	171	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	768	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	749	A	C5-C6-N1	6.75	121.08	117.70
21	AA	845	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	2585	U	O4'-C1'-N1	6.75	113.60	108.20
21	AA	1327	C	N3-C2-O2	-6.75	117.17	121.90
47	BY	29	ARG	NE-CZ-NH1	6.75	123.68	120.30
54	BA	1722	A	N1-C6-N6	-6.75	114.55	118.60
54	BA	2062	A	C5-C6-N1	6.75	121.08	117.70
21	AA	262	A	O4'-C1'-N9	6.75	113.60	108.20
21	AA	924	C	N3-C2-O2	-6.75	117.17	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1318	A	C5-C6-N1	6.75	121.08	117.70
54	BA	705	A	C5-C6-N1	6.75	121.08	117.70
21	AA	560	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	1521	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	1530	G	C1'-O4'-C4'	-6.75	104.50	109.90
54	BA	996	A	C5-C6-N1	6.75	121.07	117.70
54	BA	1284	A	C5-C6-N1	6.75	121.07	117.70
21	AA	1219	A	C5-C6-N1	6.75	121.07	117.70
21	AA	1402	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	1678	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	2205	A	C5-C6-N1	6.75	121.07	117.70
21	AA	1067	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1507	A	C5-C6-N1	6.74	121.07	117.70
54	BA	368	A	N1-C6-N6	-6.74	114.55	118.60
54	BA	792	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1211	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1178	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1616	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2805	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	280	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	429	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	430	A	N1-C6-N6	-6.74	114.56	118.60
54	BA	624	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1509	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1217	C	O4'-C1'-N1	6.74	113.59	108.20
21	AA	658	C	N3-C2-O2	-6.74	117.19	121.90
54	BA	2108	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2565	A	C4-C5-C6	-6.73	113.63	117.00
24	A3	60	A	C5-C6-N1	6.73	121.07	117.70
54	BA	227	A	C5-C6-N1	6.73	121.07	117.70
54	BA	269	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	480	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	750	A	C4-C5-C6	-6.73	113.63	117.00
54	BA	838	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2417	C	O4'-C1'-N1	6.73	113.59	108.20
21	AA	1022	A	C4-C5-C6	-6.73	113.64	117.00
21	AA	190	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	1557	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2101	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	1635	A	C5-C6-N1	6.73	121.06	117.70
21	AA	554	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	1127	A	C5-C6-N1	6.73	121.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1962	C	N3-C2-O2	-6.73	117.19	121.90
34	BL	4	ASN	C-N-CA	6.72	138.51	121.70
54	BA	478	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1451	C	N1-C2-O2	6.72	122.93	118.90
54	BA	2196	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	2616	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	1652	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1892	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	2347	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	2534	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	1157	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	203	A	C5-C6-N1	6.72	121.06	117.70
21	AA	1322	C	N3-C2-O2	-6.72	117.20	121.90
21	AA	1333	A	C5-C6-N1	6.72	121.06	117.70
21	AA	1430	A	C5-C6-N1	6.72	121.06	117.70
22	A1	32	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	487	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	724	U	O4'-C1'-N1	6.72	113.58	108.20
54	BA	779	U	O4'-C1'-N1	6.72	113.58	108.20
52	B3	29	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	925	A	N1-C6-N6	-6.72	114.57	118.60
21	AA	44	A	C5-C6-N1	6.72	121.06	117.70
21	AA	279	A	C5-C6-N1	6.72	121.06	117.70
32	BJ	95	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	789	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	2142	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2266	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2600	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	355	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1632	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1960	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	927	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1095	A	C5-C6-N1	6.71	121.06	117.70
21	AA	1109	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	1476	A	C5-C6-N1	6.71	121.06	117.70
54	BA	73	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1982	U	O4'-C1'-N1	6.71	113.57	108.20
54	BA	354	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	866	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1045	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	900	A	C5-C6-N1	6.71	121.05	117.70
21	AA	1384	C	N3-C2-O2	-6.71	117.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	637	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	1287	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	1960	A	C5-C6-N1	6.71	121.05	117.70
34	BL	41	ARG	NE-CZ-NH1	6.71	123.65	120.30
54	BA	1614	A	N1-C6-N6	-6.71	114.58	118.60
54	BA	2482	A	C5-C6-N1	6.71	121.05	117.70
21	AA	1157	A	C5-C6-N1	6.70	121.05	117.70
54	BA	397	U	O4'-C1'-N1	6.70	113.56	108.20
54	BA	1160	G	N3-C2-N2	-6.70	115.21	119.90
54	BA	1574	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2809	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	53	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	913	A	C5-C6-N1	6.70	121.05	117.70
21	AA	1447	A	C5-C6-N1	6.70	121.05	117.70
21	AA	754	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	792	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	1117	A	C5-C6-N1	6.70	121.05	117.70
54	BA	47	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1615	C	N1-C2-O2	6.70	122.92	118.90
26	BD	59	ARG	NE-CZ-NH2	-6.69	116.95	120.30
54	BA	2547	A	C1'-O4'-C4'	-6.69	104.55	109.90
21	AA	889	A	C4-C5-C6	-6.69	113.65	117.00
21	AA	1340	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1269	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1367	A	C5-C6-N1	6.69	121.05	117.70
54	BA	384	A	C5-C6-N1	6.69	121.05	117.70
54	BA	892	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	1013	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	1978	A	C5-C6-N1	6.69	121.05	117.70
54	BA	2736	A	C5-C6-N1	6.69	121.05	117.70
16	AQ	61	ARG	NE-CZ-NH1	6.69	123.64	120.30
30	BH	68	ARG	NE-CZ-NH1	6.69	123.64	120.30
54	BA	163	C	N1-C2-O2	6.69	122.91	118.90
54	BA	995	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2392	A	C5-C6-N1	6.69	121.05	117.70
21	AA	50	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	38	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	2178	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	1759	A	C5-C6-N1	6.68	121.04	117.70
55	BB	38	C	N3-C2-O2	-6.68	117.22	121.90
3	AD	25	ARG	NE-CZ-NH1	6.68	123.64	120.30
21	AA	1160	G	N3-C2-N2	-6.68	115.22	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	33	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	510	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	2207	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	40	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	499	A	C4-C5-C6	-6.68	113.66	117.00
21	AA	1016	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1609	A	O4'-C1'-N9	6.68	113.55	108.20
54	BA	2469	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	825	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1843	C	N3-C2-O2	-6.68	117.23	121.90
21	AA	414	A	N1-C6-N6	-6.68	114.59	118.60
21	AA	1114	C	N3-C2-O2	-6.68	117.23	121.90
24	A3	22	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	342	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2214	C	N3-C2-O2	-6.68	117.23	121.90
21	AA	1081	A	C5-C6-N1	6.67	121.04	117.70
54	BA	95	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	1085	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1254	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1404	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2314	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	212	G	O4'-C1'-N9	6.67	113.54	108.20
21	AA	1324	A	N1-C6-N6	-6.67	114.60	118.60
33	BK	108	ARG	NE-CZ-NH1	6.67	123.64	120.30
54	BA	2433	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	432	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	1908	C	N3-C2-O2	-6.67	117.23	121.90
20	AU	33	ARG	NE-CZ-NH1	6.67	123.63	120.30
21	AA	295	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	498	A	N1-C6-N6	-6.67	114.60	118.60
54	BA	2374	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2119	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2799	A	O4'-C1'-N9	6.67	113.53	108.20
54	BA	2800	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2893	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	243	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	781	A	N1-C6-N6	-6.67	114.60	118.60
54	BA	1711	A	C5-C6-N1	6.67	121.03	117.70
22	A1	11	C	N3-C2-O2	-6.66	117.24	121.90
25	BC	176	ARG	NE-CZ-NH1	6.66	123.63	120.30
54	BA	144	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2426	A	C4-C5-C6	-6.66	113.67	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	125	A	C5-C6-N1	6.66	121.03	117.70
54	BA	200	U	O4'-C1'-N1	6.66	113.53	108.20
21	AA	65	A	N1-C6-N6	-6.66	114.60	118.60
54	BA	781	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1001	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1844	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	2654	A	C5-C6-N1	6.66	121.03	117.70
21	AA	525	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1092	A	C5-C6-N1	6.66	121.03	117.70
33	BK	49	ARG	NE-CZ-NH1	6.66	123.63	120.30
54	BA	2377	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	176	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2745	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1119	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	279	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	364	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	938	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	1283	U	O4'-C1'-N1	6.65	113.52	108.20
54	BA	1783	A	C5-C6-N1	6.65	121.03	117.70
21	AA	286	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	272	A	C5-C6-N1	6.65	121.03	117.70
54	BA	322	A	C5-C6-N1	6.65	121.03	117.70
54	BA	532	A	N1-C6-N6	-6.65	114.61	118.60
54	BA	650	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	2527	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1694	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	139	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	1197	A	C5-C6-N1	6.65	121.02	117.70
36	BN	4	ARG	NE-CZ-NH1	6.65	123.62	120.30
54	BA	1009	A	C5-C6-N1	6.65	121.02	117.70
55	BB	65	U	O4'-C1'-N1	6.65	113.52	108.20
54	BA	52	A	C5-C6-N1	6.65	121.02	117.70
54	BA	1241	A	N1-C6-N6	-6.65	114.61	118.60
54	BA	439	A	C5-C6-N1	6.64	121.02	117.70
8	AI	105	ARG	NE-CZ-NH1	6.64	123.62	120.30
21	AA	130	A	O4'-C1'-N9	6.64	113.52	108.20
21	AA	637	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	919	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	1328	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	221	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	787	C	N3-C2-O2	-6.64	117.25	121.90
55	BB	57	A	N1-C6-N6	-6.64	114.61	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	157	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	629	A	C5-C6-N1	6.64	121.02	117.70
21	AA	787	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	880	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	14	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1784	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2146	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2403	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	574	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	947	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1966	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2380	C	O4'-C1'-N1	6.64	113.51	108.20
54	BA	2462	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	472	A	C4-C5-C6	-6.63	113.68	117.00
54	BA	502	A	C5-C6-N1	6.63	121.02	117.70
54	BA	599	A	C4-C5-C6	-6.63	113.68	117.00
54	BA	1735	A	C5-C6-N1	6.63	121.02	117.70
54	BA	2014	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	2882	A	C5-C6-N1	6.63	121.02	117.70
21	AA	845	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	1937	A	C5-C6-N1	6.63	121.02	117.70
21	AA	702	A	C5-C6-N1	6.63	121.02	117.70
54	BA	115	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	675	A	C5-C6-N1	6.63	121.02	117.70
21	AA	1510	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	666	A	C5-C6-N1	6.63	121.02	117.70
21	AA	441	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	2090	A	C5-C6-N1	6.63	121.02	117.70
21	AA	936	C	N3-C2-O2	-6.63	117.26	121.90
24	A3	45	A	C5-C6-N1	6.63	121.01	117.70
54	BA	1323	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1791	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	2169	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	2451	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	1254	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	1378	C	N3-C2-O2	-6.62	117.26	121.90
54	BA	199	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1396	U	O4'-C1'-N1	6.62	113.50	108.20
54	BA	1592	C	N3-C2-O2	-6.62	117.26	121.90
54	BA	2600	A	C5-C6-N1	6.62	121.01	117.70
21	AA	816	A	C5-C6-N1	6.62	121.01	117.70
21	AA	1237	C	N3-C2-O2	-6.62	117.26	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1263	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	97	C	O4'-C1'-N1	6.62	113.50	108.20
54	BA	644	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	391	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	155	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	443	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	2013	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1505	A	C5-C6-N1	6.62	121.01	117.70
20	AU	34	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	306	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	448	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2416	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	507	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	1533	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1536	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1686	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	2699	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	958	A	C5-C6-N1	6.61	121.01	117.70
21	AA	1246	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	53	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1901	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	2766	A	C5-C6-N1	6.61	121.00	117.70
54	BA	2800	A	C4-C5-C6	-6.61	113.69	117.00
21	AA	771	G	O4'-C1'-N9	6.61	113.49	108.20
21	AA	263	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	520	A	C5-C6-N1	6.61	121.00	117.70
21	AA	865	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1057	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1901	A	C5-C6-N1	6.61	121.00	117.70
54	BA	927	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	882	C	N3-C4-N4	-6.60	113.38	118.00
54	BA	374	A	C5-C6-N1	6.60	121.00	117.70
55	BB	9	G	O4'-C1'-N9	6.60	113.48	108.20
21	AA	816	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	165	A	C5-C6-N1	6.60	121.00	117.70
54	BA	213	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1304	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1433	A	C5-C6-N1	6.60	121.00	117.70
54	BA	21	A	C5-C6-N1	6.60	121.00	117.70
54	BA	342	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1816	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	1374	A	C5-C6-N1	6.60	121.00	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2011	U	O4'-C1'-N1	6.60	113.48	108.20
54	BA	2468	A	C5-C6-N1	6.60	121.00	117.70
21	AA	635	A	C5-C6-N1	6.59	121.00	117.70
21	AA	765	G	O4'-C1'-N9	6.59	113.48	108.20
21	AA	1036	A	C5-C6-N1	6.59	121.00	117.70
21	AA	1277	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	1077	A	N1-C6-N6	-6.59	114.64	118.60
54	BA	2412	A	C5-C6-N1	6.59	121.00	117.70
55	BB	109	A	C4-C5-C6	-6.59	113.70	117.00
24	A3	58	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	397	A	C4-C5-C6	-6.59	113.70	117.00
26	BD	83	ARG	NE-CZ-NH1	6.59	123.60	120.30
21	AA	1273	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	721	A	C4-C5-C6	-6.59	113.71	117.00
54	BA	2538	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	648	A	C4-C5-C6	-6.59	113.71	117.00
21	AA	864	A	C5-C6-N1	6.59	120.99	117.70
21	AA	1360	A	C4-C5-C6	-6.59	113.71	117.00
21	AA	1501	C	N1-C2-O2	6.59	122.85	118.90
54	BA	1768	C	O4'-C1'-N1	6.59	113.47	108.20
54	BA	2270	A	C4-C5-C6	-6.59	113.71	117.00
21	AA	1383	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	155	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1134	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1392	A	C5-C6-N1	6.58	120.99	117.70
54	BA	173	A	C5-C6-N1	6.58	120.99	117.70
54	BA	899	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1111	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1561	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	1302	C	N3-C2-O2	-6.58	117.29	121.90
12	AM	22	TYR	CB-CG-CD2	-6.58	117.05	121.00
12	AM	106	ARG	NE-CZ-NH1	6.58	123.59	120.30
21	AA	155	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2749	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2887	A	C5-C6-N1	6.58	120.99	117.70
6	AG	101	ARG	NE-CZ-NH1	6.58	123.59	120.30
21	AA	1102	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1090	A	N1-C6-N6	-6.58	114.66	118.60
54	BA	1275	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	2142	A	C5-C6-N1	6.57	120.99	117.70
21	AA	32	A	C5-C6-N1	6.57	120.99	117.70
54	BA	2841	C	N3-C2-O2	-6.57	117.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AC	168	ARG	NE-CZ-NH1	6.57	123.58	120.30
13	AN	53	ARG	NE-CZ-NH1	6.57	123.58	120.30
21	AA	270	A	C5-C6-N1	6.57	120.98	117.70
25	BC	47	ARG	NE-CZ-NH1	6.57	123.58	120.30
54	BA	389	G	N3-C2-N2	-6.57	115.30	119.90
54	BA	2679	A	C4-C5-C6	-6.57	113.72	117.00
21	AA	83	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	1001	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	992	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	143	A	C5-C6-N1	6.57	120.98	117.70
21	AA	759	A	C5-C6-N1	6.57	120.98	117.70
21	AA	1469	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	623	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	900	A	C5-C6-N1	6.57	120.98	117.70
21	AA	55	A	C4-C5-C6	-6.57	113.72	117.00
21	AA	492	C	N3-C2-O2	-6.57	117.31	121.90
54	BA	1260	A	N1-C6-N6	-6.57	114.66	118.60
21	AA	563	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	974	A	N1-C6-N6	-6.56	114.66	118.60
21	AA	1155	A	C5-C6-N1	6.56	120.98	117.70
54	BA	796	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1070	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	1293	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2222	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	980	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	106	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	223	A	C5-C6-N1	6.56	120.98	117.70
54	BA	239	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	715	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	943	A	N1-C6-N6	-6.56	114.67	118.60
54	BA	1304	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2225	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2517	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2564	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	1299	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2077	A	N1-C6-N6	-6.56	114.67	118.60
12	AM	91	ARG	NE-CZ-NH1	6.55	123.58	120.30
21	AA	1027	C	N3-C2-O2	-6.55	117.31	121.90
11	AL	82	ARG	NE-CZ-NH1	6.55	123.58	120.30
21	AA	338	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	608	A	N1-C6-N6	-6.55	114.67	118.60
55	BB	28	C	N3-C2-O2	-6.55	117.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1035	A	C4-C5-C6	-6.55	113.72	117.00
24	A3	29	C	N3-C2-O2	-6.55	117.31	121.90
29	BG	163	TYR	CB-CG-CD1	-6.55	117.07	121.00
41	BS	110	ARG	NE-CZ-NH1	6.55	123.58	120.30
54	BA	1070	A	O4'-C1'-N9	6.55	113.44	108.20
54	BA	2170	A	N1-C6-N6	-6.55	114.67	118.60
21	AA	130	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	806	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	1774	C	O4'-C1'-N1	6.55	113.44	108.20
54	BA	28	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	347	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	2679	A	C5-C6-N1	6.55	120.97	117.70
21	AA	349	A	C4-C5-C6	-6.54	113.73	117.00
22	A1	58	A	N1-C6-N6	-6.54	114.67	118.60
54	BA	983	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1104	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1123	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1879	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	1410	A	C5-C6-N1	6.54	120.97	117.70
23	A2	82	A	O4'-C1'-N9	6.54	113.43	108.20
24	A3	44	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	357	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	429	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1512	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	2868	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	270	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	1170	A	N1-C6-N6	-6.54	114.68	118.60
54	BA	2015	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2288	A	C5-C6-N1	6.54	120.97	117.70
21	AA	163	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	57	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	819	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1284	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	720	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1349	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	471	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	475	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	704	A	C4-C5-C6	-6.53	113.73	117.00
21	AA	1171	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	1385	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	1447	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1548	A	C4-C5-C6	-6.53	113.73	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2407	A	C5-C6-N1	6.53	120.97	117.70
55	BB	66	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	812	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1829	A	C5-C6-N1	6.53	120.97	117.70
54	BA	2670	A	C5-C6-N1	6.53	120.96	117.70
42	BT	77	ARG	NE-CZ-NH1	6.53	123.56	120.30
54	BA	504	A	C5-C6-N1	6.53	120.96	117.70
54	BA	1262	A	C5-C6-N1	6.53	120.96	117.70
54	BA	2142	A	N1-C6-N6	-6.53	114.69	118.60
21	AA	336	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	1259	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	1412	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	1509	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	1006	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	234	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	315	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	643	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	1317	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	1368	A	C5-C6-N1	6.52	120.96	117.70
54	BA	2065	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	2125	G	O4'-C1'-N9	6.52	113.42	108.20
54	BA	591	U	O4'-C1'-N1	6.52	113.42	108.20
54	BA	1054	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1370	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	2723	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	2889	C	N3-C2-O2	-6.52	117.34	121.90
1	AB	62	ARG	NE-CZ-NH1	6.52	123.56	120.30
21	AA	1100	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	1441	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1007	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	2805	C	O4'-C1'-N1	6.52	113.41	108.20
54	BA	1732	C	N1-C2-O2	6.52	122.81	118.90
55	BB	31	C	N3-C2-O2	-6.52	117.34	121.90
14	AO	53	ARG	NE-CZ-NH1	6.51	123.56	120.30
21	AA	1097	C	N3-C2-O2	-6.51	117.34	121.90
40	BR	79	ARG	NE-CZ-NH1	6.51	123.56	120.30
54	BA	1711	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	2037	A	C5-C6-N1	6.51	120.96	117.70
54	BA	2497	A	C5-C6-N1	6.51	120.96	117.70
54	BA	2705	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	536	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1549	A	C5-C6-N1	6.51	120.95	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2587	A	C5-C6-N1	6.51	120.95	117.70
54	BA	264	C	N1-C2-O2	6.51	122.81	118.90
21	AA	1203	C	N1-C2-O2	6.51	122.80	118.90
22	A1	25	C	N3-C2-O2	-6.51	117.35	121.90
54	BA	426	C	O4'-C1'-N1	6.51	113.41	108.20
54	BA	2532	G	N1-C6-O6	-6.51	116.00	119.90
21	AA	54	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1503	A	N1-C6-N6	-6.50	114.70	118.60
18	AS	22	VAL	C-N-CA	6.50	137.96	121.70
21	AA	78	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	460	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2268	A	C5-C6-N1	6.50	120.95	117.70
55	BB	26	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2306	C	N3-C2-O2	-6.50	117.35	121.90
22	A1	45	G	N3-C2-N2	-6.50	115.35	119.90
54	BA	1785	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1803	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2184	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	612	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	1004	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	179	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1188	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1492	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	515	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	671	C	N1-C2-O2	6.50	122.80	118.90
54	BA	1092	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1856	U	O4'-C1'-N1	6.50	113.40	108.20
21	AA	553	A	C5-C6-N1	6.49	120.95	117.70
54	BA	668	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1961	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2594	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	767	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	484	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	590	A	C5-C6-N1	6.49	120.94	117.70
54	BA	2153	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1339	G	N3-C2-N2	-6.49	115.36	119.90
54	BA	1458	U	O4'-C1'-N1	6.49	113.39	108.20
54	BA	1547	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	975	A	C4-C5-C6	-6.49	113.76	117.00
21	AA	1093	A	C5-C6-N1	6.49	120.94	117.70
54	BA	2267	A	C5-C6-N1	6.49	120.94	117.70
54	BA	2515	C	N3-C2-O2	-6.49	117.36	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	37	C	N1-C2-O2	6.49	122.79	118.90
5	AF	91	ARG	NE-CZ-NH2	6.49	123.54	120.30
54	BA	825	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	1165	A	C5-C6-N1	6.49	120.94	117.70
54	BA	1700	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	2350	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2461	A	C4-C5-C6	-6.49	113.76	117.00
15	AP	28	ARG	NE-CZ-NH1	6.48	123.54	120.30
54	BA	339	U	O4'-C1'-N1	6.48	113.39	108.20
54	BA	2507	C	N1-C2-O2	6.48	122.79	118.90
54	BA	2510	C	N3-C2-O2	-6.48	117.36	121.90
55	BB	25	U	O4'-C1'-N1	6.48	113.39	108.20
21	AA	233	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	696	A	C4-C5-C6	-6.48	113.76	117.00
23	A2	86	U	O4'-C1'-N1	6.48	113.38	108.20
54	BA	330	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	421	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	654	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1961	C	O4'-C1'-N1	6.48	113.38	108.20
54	BA	2047	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	162	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	399	U	O4'-C1'-N1	6.48	113.38	108.20
54	BA	1741	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	342	C	N3-C2-O2	-6.48	117.37	121.90
21	AA	475	C	N3-C2-O2	-6.48	117.37	121.90
21	AA	915	A	C4-C5-C6	-6.48	113.76	117.00
24	A3	44	A	C5-C6-N1	6.48	120.94	117.70
54	BA	426	C	N3-C2-O2	-6.48	117.37	121.90
54	BA	991	C	N3-C2-O2	-6.48	117.37	121.90
54	BA	1064	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1934	C	O4'-C1'-N1	6.48	113.38	108.20
21	AA	487	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	907	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1102	A	N1-C6-N6	-6.48	114.71	118.60
54	BA	1111	A	N1-C6-N6	-6.48	114.72	118.60
54	BA	449	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	640	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	761	A	C5-C6-N1	6.47	120.94	117.70
54	BA	1905	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2000	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2030	A	C4-C5-C6	-6.47	113.76	117.00
55	BB	68	C	O4'-C1'-N1	6.47	113.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	578	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1350	A	C5-C6-N1	6.47	120.94	117.70
54	BA	1735	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	300	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	2154	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	469	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1028	C	N3-C2-O2	-6.47	117.37	121.90
24	A3	70	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2078	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2471	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	2900	A	C5-C6-N1	6.47	120.94	117.70
54	BA	2364	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2556	C	N3-C2-O2	-6.47	117.37	121.90
18	AS	2	ARG	NE-CZ-NH1	6.47	123.53	120.30
21	AA	373	A	N1-C6-N6	-6.47	114.72	118.60
21	AA	502	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	1428	A	C5-C6-N1	6.47	120.93	117.70
54	BA	786	C	N3-C2-O2	-6.47	117.37	121.90
55	BB	101	A	N1-C6-N6	-6.47	114.72	118.60
21	AA	1105	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1137	C	C1'-O4'-C4'	-6.46	104.73	109.90
24	A3	63	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	569	U	O4'-C1'-N1	6.46	113.37	108.20
54	BA	1764	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2184	A	C5-C6-N1	6.46	120.93	117.70
55	BB	73	A	C5-C6-N1	6.46	120.93	117.70
28	BF	91	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	1585	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1630	A	C5-C6-N1	6.46	120.93	117.70
21	AA	443	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	621	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	655	A	C5-C6-N1	6.46	120.93	117.70
54	BA	152	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1005	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2499	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1336	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1363	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2051	A	C4-C5-C6	-6.46	113.77	117.00
9	AJ	45	ARG	NE-CZ-NH2	6.46	123.53	120.30
21	AA	797	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	391	A	N1-C6-N6	-6.46	114.73	118.60
54	BA	556	A	C5-C6-N1	6.46	120.93	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	945	A	N1-C6-N6	-6.46	114.73	118.60
54	BA	1077	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1141	U	C3'-C2'-C1'	6.46	106.67	101.50
54	BA	1918	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2176	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2297	A	C5-C6-N1	6.46	120.93	117.70
55	BB	80	U	O4'-C1'-N1	6.46	113.36	108.20
8	AI	94	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	2283	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2781	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1293	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	1990	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	120	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	391	A	C5-C6-N1	6.45	120.93	117.70
54	BA	1771	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	2278	A	C4-C5-C6	-6.45	113.77	117.00
21	AA	1261	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	2327	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	435	A	C5-C6-N1	6.45	120.92	117.70
21	AA	1345	U	C1'-O4'-C4'	-6.45	104.74	109.90
54	BA	505	A	C4-C5-C6	-6.45	113.78	117.00
55	BB	60	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1014	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	135	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	765	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	845	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1691	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1836	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1998	A	C5-C6-N1	6.45	120.92	117.70
54	BA	2291	U	O4'-C1'-N1	6.44	113.36	108.20
48	BZ	29	ARG	NE-CZ-NH1	6.44	123.52	120.30
54	BA	2461	A	C5-C6-N1	6.44	120.92	117.70
22	A1	56	C	N1-C2-O2	6.44	122.76	118.90
45	BW	76	ARG	NE-CZ-NH1	6.44	123.52	120.30
54	BA	1264	A	C4-C5-C6	-6.44	113.78	117.00
11	AL	8	ARG	NE-CZ-NH1	6.44	123.52	120.30
21	AA	7	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	251	G	P-O3'-C3'	6.44	127.42	119.70
21	AA	673	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	878	A	C5-C6-N1	6.44	120.92	117.70
22	A1	68	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	143	C	N3-C2-O2	-6.44	117.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1920	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2226	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	104	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	1449	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	1452	C	N3-C2-O2	-6.43	117.39	121.90
21	AA	1468	A	C4-C5-C6	-6.43	113.78	117.00
51	B2	34	ARG	NE-CZ-NH1	6.43	123.52	120.30
54	BA	1350	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	401	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	173	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	675	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	752	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	2310	C	N3-C2-O2	-6.43	117.40	121.90
36	BN	103	ARG	NE-CZ-NH1	6.43	123.52	120.30
54	BA	301	G	C1'-O4'-C4'	-6.43	104.75	109.90
54	BA	1749	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1998	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	1545	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	1572	A	C5-C6-N1	6.43	120.92	117.70
21	AA	223	A	C4-C5-C6	-6.43	113.79	117.00
38	BP	88	ARG	NE-CZ-NH1	6.43	123.51	120.30
54	BA	1747	U	O4'-C1'-N1	6.43	113.34	108.20
21	AA	912	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	1409	C	N3-C2-O2	-6.43	117.40	121.90
35	BM	16	ARG	NE-CZ-NH1	6.43	123.51	120.30
38	BP	108	ARG	NE-CZ-NH1	6.43	123.51	120.30
54	BA	523	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	699	A	C5-C6-N1	6.43	120.91	117.70
54	BA	1488	C	O4'-C1'-N1	6.43	113.34	108.20
54	BA	1610	A	C4-C5-C6	-6.43	113.79	117.00
56	B5	7	ARG	NE-CZ-NH1	6.43	123.51	120.30
54	BA	672	C	N3-C2-O2	-6.42	117.40	121.90
54	BA	676	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1169	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2678	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	322	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	1210	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1460	C	N3-C2-O2	-6.42	117.40	121.90
54	BA	2510	C	O4'-C1'-N1	6.42	113.34	108.20
21	AA	1375	A	C4-C5-C6	-6.42	113.79	117.00
41	BS	8	ARG	NE-CZ-NH1	6.42	123.51	120.30
21	AA	460	A	C4-C5-C6	-6.42	113.79	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	756	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	335	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1993	U	O4'-C1'-N1	6.42	113.33	108.20
54	BA	2689	U	O4'-C1'-N1	6.42	113.33	108.20
21	AA	539	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1346	A	C5-C6-N1	6.42	120.91	117.70
22	A1	51	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	84	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	172	A	C5-C6-N1	6.42	120.91	117.70
21	AA	600	A	C5-C6-N1	6.42	120.91	117.70
55	BB	78	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	74	A	C4-C5-C6	-6.41	113.79	117.00
42	BT	69	ARG	NE-CZ-NH1	6.41	123.51	120.30
54	BA	233	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	1909	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	2287	A	C5-C6-N1	6.41	120.91	117.70
54	BA	2459	A	C5-C6-N1	6.41	120.91	117.70
20	AU	6	ARG	NE-CZ-NH1	6.41	123.51	120.30
21	AA	728	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	892	A	C5-C6-N1	6.41	120.91	117.70
12	AM	56	ARG	NE-CZ-NH1	6.41	123.51	120.30
21	AA	549	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	687	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	878	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	129	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	601	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1140	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	2615	U	O4'-C1'-N1	6.41	113.33	108.20
7	AH	113	ARG	NE-CZ-NH1	6.41	123.50	120.30
21	AA	1021	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2703	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	2860	A	C5-C6-N1	6.41	120.90	117.70
21	AA	899	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	217	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	870	U	O4'-C1'-N1	6.41	113.32	108.20
54	BA	1635	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1803	A	N1-C6-N6	-6.40	114.76	118.60
54	BA	2531	A	C5-C6-N1	6.40	120.90	117.70
27	BE	117	ARG	NE-CZ-NH1	6.40	123.50	120.30
21	AA	16	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	1151	A	C5-C6-N1	6.40	120.90	117.70
54	BA	196	A	O4'-C1'-N9	6.40	113.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	256	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	920	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2150	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2626	C	O4'-C1'-N1	6.40	113.32	108.20
55	BB	94	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	379	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	1377	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1808	A	N1-C6-N6	-6.40	114.76	118.60
55	BB	12	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	83	A	O4'-C1'-N9	6.40	113.32	108.20
26	BD	33	ARG	NE-CZ-NH1	6.40	123.50	120.30
54	BA	2333	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	1201	A	C4-C5-C6	-6.39	113.80	117.00
38	BP	92	ARG	NE-CZ-NH2	-6.39	117.10	120.30
54	BA	2646	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	1593	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	2261	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	837	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1963	U	O4'-C1'-N1	6.39	113.31	108.20
54	BA	471	A	C5-C6-N1	6.39	120.89	117.70
54	BA	184	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1830	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1958	C	N3-C4-C5	6.39	124.45	121.90
54	BA	2767	C	O4'-C1'-N1	6.39	113.31	108.20
21	AA	356	A	C5-C6-N1	6.38	120.89	117.70
21	AA	1336	C	N3-C2-O2	-6.38	117.43	121.90
25	BC	155	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BA	1153	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	1327	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1607	C	O4'-C1'-N1	6.38	113.31	108.20
54	BA	2129	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	865	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	454	A	C5-C6-N1	6.38	120.89	117.70
21	AA	583	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	1508	A	C5-C6-N1	6.38	120.89	117.70
34	BL	2	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BA	126	A	C5-C6-N1	6.38	120.89	117.70
54	BA	181	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1307	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2164	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	351	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	1670	C	N3-C2-O2	-6.38	117.43	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	93	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2837	A	C5-C6-N1	6.38	120.89	117.70
21	AA	655	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	856	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	984	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	1269	A	C4-C5-C6	-6.38	113.81	117.00
34	BL	21	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BA	301	G	O4'-C1'-N9	6.38	113.30	108.20
54	BA	1156	A	C4-C5-C6	-6.38	113.81	117.00
11	AL	93	ARG	NE-CZ-NH1	6.38	123.49	120.30
51	B2	3	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BA	960	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1100	C	N3-C2-O2	-6.38	117.44	121.90
55	BB	89	U	O4'-C1'-N1	6.38	113.30	108.20
21	AA	996	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2597	G	O4'-C1'-N9	6.37	113.30	108.20
54	BA	602	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	1805	A	C5-C6-N1	6.37	120.89	117.70
54	BA	2220	U	O4'-C1'-N1	6.37	113.30	108.20
54	BA	2796	U	O4'-C1'-N1	6.37	113.30	108.20
22	A1	6	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	742	A	C5-C6-N1	6.37	120.89	117.70
54	BA	968	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1717	A	C5-C6-N1	6.37	120.88	117.70
21	AA	651	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	893	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	36	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	338	A	C5-C6-N1	6.37	120.88	117.70
54	BA	1672	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	2332	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2572	A	N1-C6-N6	-6.37	114.78	118.60
21	AA	189	A	C4-C5-C6	-6.36	113.82	117.00
24	A3	24	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	795	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	861	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1136	G	N3-C4-C5	-6.36	125.42	128.60
54	BA	1480	C	N3-C2-O2	-6.36	117.44	121.90
54	BA	1605	C	N3-C2-O2	-6.36	117.44	121.90
54	BA	2102	G	N1-C6-O6	-6.36	116.08	119.90
21	AA	1239	A	C5-C6-N1	6.36	120.88	117.70
54	BA	109	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	218	A	C5-C6-N1	6.36	120.88	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	660	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1118	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1372	U	O4'-C1'-N1	6.36	113.29	108.20
54	BA	1793	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2205	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2476	A	C4-C5-C6	-6.36	113.82	117.00
38	BP	38	ARG	NE-CZ-NH1	6.36	123.48	120.30
54	BA	1577	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	10	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	696	A	C5-C6-N1	6.36	120.88	117.70
21	AA	1200	C	C2-N3-C4	-6.36	116.72	119.90
54	BA	1632	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1936	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2006	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	353	A	C5-C6-N1	6.36	120.88	117.70
21	AA	579	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	1218	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1230	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2767	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	751	A	C5-C6-N1	6.35	120.88	117.70
21	AA	873	A	C5-C6-N1	6.35	120.88	117.70
54	BA	987	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	1722	A	C5-C6-N1	6.35	120.88	117.70
21	AA	742	G	N3-C2-N2	-6.35	115.45	119.90
21	AA	1279	G	N3-C2-N2	-6.35	115.45	119.90
54	BA	705	A	N1-C6-N6	-6.35	114.79	118.60
54	BA	1079	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2322	A	C5-C6-N1	6.35	120.88	117.70
54	BA	2425	A	C1'-O4'-C4'	-6.35	104.82	109.90
21	AA	248	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	1404	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	600	A	N1-C6-N6	-6.35	114.79	118.60
21	AA	844	G	O4'-C1'-N9	6.35	113.28	108.20
21	AA	1128	C	N1-C2-O2	6.35	122.71	118.90
54	BA	89	A	C5-C6-N1	6.35	120.87	117.70
54	BA	462	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	1654	A	C5-C6-N1	6.35	120.87	117.70
54	BA	346	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	588	U	O4'-C1'-N1	6.34	113.28	108.20
54	BA	1406	U	O4'-C1'-N1	6.34	113.28	108.20
55	BB	41	G	O4'-C1'-N9	6.34	113.28	108.20
16	AQ	5	ARG	NE-CZ-NH1	6.34	123.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	790	A	C5-C6-N1	6.34	120.87	117.70
21	AA	1137	C	O4'-C1'-N1	6.34	113.27	108.20
22	A1	62	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	31	C	O4'-C1'-N1	6.34	113.27	108.20
54	BA	1002	G	O4'-C1'-N9	6.34	113.27	108.20
54	BA	1043	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1189	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1209	U	N3-C2-O2	-6.34	117.76	122.20
54	BA	2043	C	O4'-C1'-N1	6.34	113.27	108.20
21	AA	599	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	736	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1226	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	2434	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	2662	A	C5-C6-N1	6.34	120.87	117.70
54	BA	2858	C	C6-N1-C2	-6.34	117.76	120.30
21	AA	930	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	1480	A	C5-C6-N1	6.34	120.87	117.70
54	BA	268	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2222	C	O4'-C1'-N1	6.34	113.27	108.20
54	BA	2753	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	848	C	N3-C2-O2	-6.34	117.47	121.90
21	AA	1298	U	C1'-O4'-C4'	-6.34	104.83	109.90
28	BF	147	ARG	NE-CZ-NH1	6.34	123.47	120.30
54	BA	691	C	N3-C2-O2	-6.34	117.47	121.90
54	BA	1075	C	O4'-C1'-N1	6.34	113.27	108.20
54	BA	1957	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2483	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2665	A	C4-C5-C6	-6.34	113.83	117.00
11	AL	49	ARG	NE-CZ-NH1	6.33	123.47	120.30
21	AA	735	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	923	A	C5-C6-N1	6.33	120.87	117.70
54	BA	160	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	1266	G	O4'-C1'-N9	6.33	113.27	108.20
19	AT	28	ARG	NE-CZ-NH1	6.33	123.47	120.30
55	BB	104	A	C5-C6-N1	6.33	120.87	117.70
21	AA	1252	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	1530	G	N1-C6-O6	-6.33	116.10	119.90
54	BA	192	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1822	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2498	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2861	U	O4'-C1'-N1	6.33	113.26	108.20
54	BA	2870	C	N3-C2-O2	-6.33	117.47	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	456	A	C5-C6-N1	6.33	120.86	117.70
54	BA	2018	G	O4'-C1'-N9	6.33	113.26	108.20
21	AA	288	A	C5-C6-N1	6.33	120.86	117.70
54	BA	179	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1739	A	C5-C6-N1	6.33	120.86	117.70
21	AA	676	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1889	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1954	G	N1-C6-O6	-6.32	116.11	119.90
54	BA	2824	C	N3-C2-O2	-6.32	117.47	121.90
43	BU	93	ARG	NE-CZ-NH1	6.32	123.46	120.30
54	BA	2052	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	2170	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2721	A	C5-C6-N1	6.32	120.86	117.70
21	AA	408	A	C5-C6-N1	6.32	120.86	117.70
21	AA	419	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	411	A	N1-C6-N6	-6.32	114.81	118.60
21	AA	1418	A	C5-C6-N1	6.32	120.86	117.70
22	A1	14	A	C5-C6-N1	6.32	120.86	117.70
54	BA	13	A	C5-C6-N1	6.32	120.86	117.70
54	BA	732	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	1052	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2326	C	N1-C2-O2	6.32	122.69	118.90
54	BA	2530	A	C5-C6-N1	6.32	120.86	117.70
54	BA	167	A	C5-C6-N1	6.32	120.86	117.70
54	BA	677	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1590	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	1227	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	131	A	N1-C6-N6	-6.31	114.81	118.60
54	BA	764	A	N1-C6-N6	-6.31	114.81	118.60
54	BA	1748	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1927	A	C5-C6-N1	6.31	120.86	117.70
54	BA	2369	A	C5-C6-N1	6.31	120.86	117.70
54	BA	1366	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	2321	U	O4'-C1'-N1	6.31	113.25	108.20
54	BA	2338	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	383	A	C4-C5-C6	-6.31	113.84	117.00
43	BU	21	ARG	NE-CZ-NH1	6.31	123.45	120.30
54	BA	231	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	455	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2231	U	O4'-C1'-N1	6.31	113.25	108.20
55	BB	70	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	225	C	N3-C2-O2	-6.31	117.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	58	A	C4-C5-C6	-6.31	113.85	117.00
21	AA	74	A	C5-C6-N1	6.30	120.85	117.70
54	BA	890	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1174	U	O4'-C1'-N1	6.30	113.24	108.20
54	BA	1285	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1617	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2211	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2386	A	C5-C6-N1	6.30	120.85	117.70
54	BA	1133	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2888	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	110	C	N1-C2-O2	6.30	122.68	118.90
21	AA	330	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	522	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1364	U	N3-C2-O2	-6.30	117.79	122.20
54	BA	592	A	C5-C6-N1	6.30	120.85	117.70
54	BA	983	A	O4'-C1'-N9	6.30	113.24	108.20
54	BA	2434	A	C5-C6-N1	6.30	120.85	117.70
21	AA	356	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	853	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	149	A	C5-C6-N1	6.30	120.85	117.70
54	BA	255	A	C5-C6-N1	6.30	120.85	117.70
54	BA	1925	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2165	C	N1-C2-O2	6.30	122.68	118.90
55	BB	92	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	67	C	O4'-C1'-N1	6.30	113.24	108.20
21	AA	764	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1499	A	C5-C6-N1	6.30	120.85	117.70
54	BA	655	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2448	A	C5-C6-N1	6.30	120.85	117.70
21	AA	811	C	O4'-C1'-N1	6.30	113.24	108.20
21	AA	1245	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	22	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	106	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1708	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2753	A	C5-C6-N1	6.30	120.85	117.70
22	A1	21	A	C5-C6-N1	6.29	120.85	117.70
54	BA	974	G	N3-C4-C5	-6.29	125.45	128.60
54	BA	1858	A	N1-C6-N6	-6.29	114.82	118.60
54	BA	1966	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	177	G	N3-C4-C5	-6.29	125.45	128.60
21	AA	545	C	N3-C2-O2	-6.29	117.49	121.90
37	BO	9	ARG	NE-CZ-NH1	6.29	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	227	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	470	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	937	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	147	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	183	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	847	U	N3-C2-O2	-6.29	117.80	122.20
54	BA	32	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2369	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	34	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	207	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	613	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2734	A	C4-C5-C6	-6.29	113.86	117.00
55	BB	99	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	1434	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	1804	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	944	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1261	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1319	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2392	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	2725	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	47	C	N1-C2-O2	6.28	122.67	118.90
21	AA	1437	A	C5-C6-N1	6.28	120.84	117.70
54	BA	785	G	N1-C6-O6	-6.28	116.13	119.90
54	BA	1466	U	O4'-C1'-N1	6.28	113.23	108.20
54	BA	1612	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2597	G	N3-C2-N2	-6.28	115.50	119.90
55	BB	88	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2358	A	N1-C6-N6	-6.28	114.83	118.60
21	AA	373	A	C4-C5-C6	-6.28	113.86	117.00
24	A3	26	C	N3-C2-O2	-6.28	117.50	121.90
25	BC	202	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	563	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1367	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1772	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1819	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	618	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1143	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	732	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	860	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	1429	A	C4-C5-C6	-6.28	113.86	117.00
22	A1	66	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	984	A	C4-C5-C6	-6.28	113.86	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2198	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	256	A	C5-C6-N1	6.27	120.84	117.70
54	BA	586	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	1641	A	N1-C6-N6	-6.27	114.84	118.60
54	BA	1854	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	2503	A	C5-C6-N1	6.27	120.84	117.70
21	AA	509	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	1267	C	N1-C2-O2	6.27	122.66	118.90
54	BA	2619	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2685	G	N1-C6-O6	-6.27	116.14	119.90
54	BA	414	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	517	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	715	A	C5-C6-N1	6.27	120.83	117.70
54	BA	730	A	C5-C6-N1	6.27	120.83	117.70
54	BA	965	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1223	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1237	A	O4'-C1'-N9	6.27	113.21	108.20
54	BA	1808	A	O4'-C1'-N9	6.27	113.21	108.20
54	BA	1916	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	2520	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	90	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	13	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2760	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	845	A	C5-C6-N1	6.26	120.83	117.70
21	AA	1513	A	C5-C6-N1	6.26	120.83	117.70
54	BA	1196	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2741	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	1146	A	C4-C5-C6	-6.26	113.87	117.00
23	A2	79	A	C5-C6-N1	6.26	120.83	117.70
52	B3	12	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	229	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	267	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1531	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2740	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	654	A	O4'-C1'-N9	6.26	113.21	108.20
54	BA	1327	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	18	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1149	G	O4'-C1'-N9	6.26	113.20	108.20
54	BA	1656	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2362	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	917	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	2254	C	N3-C2-O2	-6.25	117.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	71	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	815	A	C4-C5-C6	-6.25	113.87	117.00
21	AA	1141	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	527	C	P-O3'-C3'	6.25	127.20	119.70
54	BA	767	U	O4'-C1'-N1	6.25	113.20	108.20
21	AA	802	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	820	U	P-O3'-C3'	6.25	127.20	119.70
54	BA	788	A	C5-C6-N1	6.25	120.83	117.70
54	BA	959	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	2543	G	C5'-C4'-C3'	-6.25	106.00	116.00
21	AA	78	A	C5-C6-N1	6.25	120.83	117.70
21	AA	498	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	882	C	O4'-C1'-N1	6.25	113.20	108.20
54	BA	1699	G	N3-C2-N2	-6.25	115.53	119.90
54	BA	2530	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2614	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	1147	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1403	A	C4-C5-C6	-6.25	113.88	117.00
10	AK	55	ARG	NE-CZ-NH1	6.25	123.42	120.30
22	A1	65	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	456	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	511	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	1513	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1704	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2163	A	O4'-C1'-N9	6.24	113.19	108.20
55	BB	46	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	290	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	325	A	C4-C5-C6	-6.24	113.88	117.00
25	BC	166	ARG	NE-CZ-NH1	6.24	123.42	120.30
54	BA	1322	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	161	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	303	A	C5-C6-N1	6.24	120.82	117.70
21	AA	1303	C	C6-N1-C2	-6.24	117.81	120.30
54	BA	1231	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	1252	G	O4'-C1'-N9	6.24	113.19	108.20
54	BA	456	C	O4'-C1'-N1	6.24	113.19	108.20
54	BA	1033	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	2850	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	101	A	C5-C6-N1	6.24	120.82	117.70
54	BA	66	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	829	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2095	A	C4-C5-C6	-6.24	113.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	193	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	522	A	C4-C5-C6	-6.23	113.88	117.00
7	AH	80	PRO	C-N-CA	6.23	135.39	122.30
21	AA	503	C	N3-C2-O2	-6.23	117.54	121.90
24	A3	73	A	C4-C5-C6	-6.23	113.88	117.00
24	A3	76	C	N3-C2-O2	-6.23	117.54	121.90
51	B2	19	ARG	NE-CZ-NH1	6.23	123.42	120.30
54	BA	42	A	N1-C6-N6	-6.23	114.86	118.60
54	BA	835	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	675	A	C4-C5-C6	-6.23	113.89	117.00
22	A1	28	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	119	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	2792	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	695	A	C4-C5-C6	-6.23	113.89	117.00
37	BO	33	ARG	NE-CZ-NH1	6.23	123.42	120.30
54	BA	1056	G	N3-C2-N2	-6.23	115.54	119.90
21	AA	250	A	O4'-C1'-N9	6.23	113.18	108.20
54	BA	1089	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	1806	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2359	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	459	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	362	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	815	C	O4'-C1'-N1	6.22	113.18	108.20
54	BA	816	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	1639	C	N3-C2-O2	-6.22	117.54	121.90
24	A3	35	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	204	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	242	G	O4'-C1'-N9	6.22	113.18	108.20
54	BA	509	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	1288	G	N3-C4-C5	-6.22	125.49	128.60
54	BA	1607	C	N1-C2-O2	6.22	122.63	118.90
54	BA	2054	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	2097	A	C5-C6-N1	6.22	120.81	117.70
54	BA	2636	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2826	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1306	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	2806	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	580	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	1000	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1689	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1745	A	C5-C6-N1	6.22	120.81	117.70
54	BA	2309	A	C4-C5-C6	-6.22	113.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2547	A	C6-C5-N7	6.22	136.65	132.30
21	AA	679	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	810	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2463	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	59	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	985	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1244	A	C5-C6-N1	6.21	120.81	117.70
5	AF	79	ARG	NE-CZ-NH1	6.21	123.41	120.30
54	BA	2332	C	O4'-C1'-N1	6.21	113.17	108.20
55	BB	108	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	382	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	602	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2091	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2764	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	1244	G	N1-C6-O6	-6.21	116.17	119.90
54	BA	1076	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1503	A	C5-C6-N1	6.21	120.80	117.70
21	AA	316	C	N3-C2-O2	-6.21	117.56	121.90
22	A1	73	A	C5-C6-N1	6.21	120.80	117.70
54	BA	348	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1785	A	C5-C6-N1	6.21	120.80	117.70
54	BA	1646	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1167	A	N1-C6-N6	-6.20	114.88	118.60
21	AA	1256	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1466	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	318	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1274	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1399	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1868	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2579	C	N3-C2-O2	-6.20	117.56	121.90
55	BB	49	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	538	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1936	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2072	C	O4'-C1'-N1	6.20	113.16	108.20
11	AL	120	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	AA	215	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	488	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	969	A	C4-C5-C6	-6.20	113.90	117.00
22	A1	9	A	N1-C6-N6	-6.20	114.88	118.60
54	BA	2755	C	N3-C2-O2	-6.20	117.56	121.90
55	BB	62	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	896	C	N3-C2-O2	-6.20	117.56	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2559	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2768	U	O4'-C1'-N1	6.20	113.16	108.20
21	AA	663	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1503	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1253	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	364	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	403	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	635	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1340	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1433	A	C4-C5-C6	-6.20	113.90	117.00
24	A3	77	A	C4-C5-C6	-6.20	113.90	117.00
28	BF	109	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	BA	190	A	N1-C6-N6	-6.20	114.88	118.60
54	BA	280	U	N3-C2-O2	-6.20	117.86	122.20
21	AA	1298	U	O4'-C1'-N1	6.19	113.16	108.20
54	BA	758	C	N3-C2-O2	-6.19	117.56	121.90
21	AA	1447	A	N1-C6-N6	-6.19	114.88	118.60
54	BA	1427	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	1525	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	1809	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	2471	A	C5-C6-N1	6.19	120.80	117.70
54	BA	2687	U	O4'-C1'-N1	6.19	113.15	108.20
21	AA	132	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	882	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1399	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	782	A	C5-C6-N1	6.19	120.80	117.70
26	BD	124	ARG	NE-CZ-NH1	6.19	123.39	120.30
54	BA	557	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	2840	C	N3-C2-O2	-6.19	117.57	121.90
3	AD	13	ARG	NE-CZ-NH1	6.19	123.39	120.30
21	AA	192	A	N1-C6-N6	-6.19	114.89	118.60
54	BA	2395	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	381	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	528	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1871	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2772	C	N3-C2-O2	-6.18	117.57	121.90
55	BB	82	U	O4'-C1'-N1	6.18	113.15	108.20
14	AO	71	ARG	NE-CZ-NH1	6.18	123.39	120.30
54	BA	274	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	854	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	983	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1200	C	N3-C2-O2	-6.18	117.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1541	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1676	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2212	A	C5-C6-N1	6.18	120.79	117.70
21	AA	372	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1630	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1799	G	P-O3'-C3'	6.18	127.12	119.70
41	BS	84	ARG	NE-CZ-NH1	6.18	123.39	120.30
54	BA	546	U	N3-C2-O2	-6.18	117.87	122.20
54	BA	903	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1582	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	1055	A	N1-C6-N6	-6.18	114.89	118.60
54	BA	1005	C	O4'-C1'-N1	6.18	113.14	108.20
21	AA	987	G	N1-C6-O6	-6.18	116.19	119.90
36	BN	12	ARG	NE-CZ-NH1	6.18	123.39	120.30
3	AD	114	ARG	NE-CZ-NH1	6.17	123.39	120.30
21	AA	674	G	N3-C2-N2	-6.17	115.58	119.90
21	AA	739	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	101	A	O4'-C1'-N9	6.17	113.14	108.20
54	BA	2710	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	128	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	436	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	714	G	N3-C2-N2	-6.17	115.58	119.90
54	BA	945	A	O4'-C1'-N9	6.17	113.14	108.20
54	BA	1942	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2354	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2432	A	C5-C6-N1	6.17	120.79	117.70
54	BA	2526	G	N1-C6-O6	-6.17	116.20	119.90
54	BA	223	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	962	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1164	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1462	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2657	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	2883	A	O4'-C1'-N9	6.17	113.14	108.20
21	AA	288	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	573	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	640	A	C5-C6-N1	6.17	120.78	117.70
21	AA	823	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	968	A	C4-C5-C6	-6.17	113.92	117.00
43	BU	81	ARG	NE-CZ-NH1	6.17	123.38	120.30
54	BA	1461	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2506	U	N3-C2-O2	-6.17	117.88	122.20
55	BB	37	C	O4'-C1'-N1	6.17	113.13	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1477	A	N1-C6-N6	-6.17	114.90	118.60
54	BA	1834	U	O4'-C1'-N1	6.17	113.13	108.20
54	BA	2765	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	535	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	1230	C	N3-C2-O2	-6.16	117.58	121.90
54	BA	1048	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1665	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	2206	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	205	G	O4'-C1'-N9	6.16	113.13	108.20
54	BA	420	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	448	U	O4'-C1'-N1	6.16	113.13	108.20
54	BA	1495	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1596	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	857	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	1319	A	N1-C6-N6	-6.16	114.90	118.60
54	BA	19	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1027	A	N1-C6-N6	-6.16	114.90	118.60
54	BA	2033	A	C5-C6-N1	6.16	120.78	117.70
21	AA	510	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	712	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	1063	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	1190	G	P-O3'-C3'	6.16	127.09	119.70
54	BA	208	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	337	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	772	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1808	A	C5-C6-N1	6.16	120.78	117.70
54	BA	1963	U	N3-C2-O2	-6.16	117.89	122.20
54	BA	2119	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	2712	C	N1-C2-O2	6.16	122.59	118.90
21	AA	477	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	998	C	N1-C2-O2	6.16	122.59	118.90
44	BV	18	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	849	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	917	A	C5-C6-N1	6.16	120.78	117.70
54	BA	2587	A	C4-C5-C6	-6.16	113.92	117.00
55	BB	14	U	N3-C2-O2	-6.16	117.89	122.20
21	AA	918	A	C5-C6-N1	6.16	120.78	117.70
54	BA	2873	A	C5-C6-N1	6.16	120.78	117.70
21	AA	909	A	C5-C6-N1	6.15	120.78	117.70
54	BA	38	A	C5-C6-N1	6.15	120.78	117.70
54	BA	1172	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2059	A	C4-C5-C6	-6.15	113.92	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1036	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	2491	U	O4'-C1'-N1	6.15	113.12	108.20
54	BA	2870	C	O4'-C1'-N1	6.15	113.12	108.20
21	AA	99	C	N3-C2-O2	-6.15	117.59	121.90
52	B3	39	ARG	NE-CZ-NH1	6.15	123.38	120.30
54	BA	404	A	O4'-C1'-N9	6.15	113.12	108.20
54	BA	677	A	C5-C6-N1	6.15	120.78	117.70
54	BA	1382	G	N3-C4-C5	-6.15	125.53	128.60
3	AD	127	ARG	NE-CZ-NH1	6.15	123.38	120.30
54	BA	130	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	1403	A	C5-C6-N1	6.15	120.78	117.70
54	BA	1417	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1938	A	C4-C5-C6	-6.15	113.92	117.00
21	AA	780	A	C4-C5-C6	-6.15	113.93	117.00
21	AA	1101	A	P-O3'-C3'	6.15	127.08	119.70
21	AA	1441	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	827	U	N3-C2-O2	-6.15	117.90	122.20
54	BA	2720	U	O4'-C1'-N1	6.15	113.12	108.20
54	BA	2736	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	2887	A	C4-C5-C6	-6.15	113.93	117.00
21	AA	1196	A	C5-C6-N1	6.15	120.77	117.70
21	AA	58	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	1214	C	N1-C2-O2	6.14	122.59	118.90
54	BA	382	A	P-O3'-C3'	6.14	127.07	119.70
54	BA	980	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2001	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	937	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1223	G	N1-C6-O6	-6.14	116.22	119.90
54	BA	477	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2654	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	967	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	1069	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	1217	C	C1'-O4'-C4'	-6.14	104.99	109.90
54	BA	1801	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1943	U	N3-C2-O2	-6.14	117.90	122.20
21	AA	777	A	C4-C5-C6	-6.14	113.93	117.00
25	BC	42	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	563	A	N1-C6-N6	-6.14	114.92	118.60
54	BA	951	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1021	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1277	G	N1-C6-O6	-6.14	116.22	119.90
54	BA	1431	A	C5-C6-N1	6.14	120.77	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2459	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	610	U	O4'-C1'-N1	6.13	113.11	108.20
21	AA	1480	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	445	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1890	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	2179	C	N3-C2-O2	-6.13	117.61	121.90
24	A3	1	C	N1-C2-O2	6.13	122.58	118.90
54	BA	2899	A	C4-C5-C6	-6.13	113.93	117.00
24	A3	67	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2825	G	N3-C4-C5	-6.13	125.53	128.60
21	AA	194	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	408	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	5	A	N1-C6-N6	-6.13	114.92	118.60
54	BA	839	U	O4'-C1'-N1	6.13	113.10	108.20
54	BA	898	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	108	G	N3-C4-C5	-6.13	125.54	128.60
22	A1	35	A	C5-C6-N1	6.13	120.76	117.70
25	BC	237	ARG	NE-CZ-NH1	6.13	123.36	120.30
34	BL	33	ARG	NE-CZ-NH1	6.13	123.36	120.30
21	AA	156	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	188	C	O4'-C1'-N1	6.13	113.10	108.20
21	AA	253	A	C5-C6-N1	6.13	120.76	117.70
54	BA	918	A	N1-C6-N6	-6.13	114.92	118.60
54	BA	1351	C	N3-C2-O2	-6.13	117.61	121.90
7	AH	76	ARG	NE-CZ-NH1	6.12	123.36	120.30
21	AA	418	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	1434	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	740	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	863	A	N1-C6-N6	-6.12	114.93	118.60
54	BA	1070	A	C1'-O4'-C4'	-6.12	105.00	109.90
1	AB	138	ARG	NE-CZ-NH1	6.12	123.36	120.30
6	AG	3	ARG	NE-CZ-NH2	6.12	123.36	120.30
21	AA	451	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	754	C	N1-C2-O2	6.12	122.57	118.90
21	AA	1325	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	365	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	538	A	C5-C6-N1	6.12	120.76	117.70
54	BA	2593	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	710	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	1375	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	2541	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	611	C	N3-C2-O2	-6.12	117.62	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	582	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	774	G	O4'-C1'-N9	6.12	113.09	108.20
54	BA	905	A	C5-C6-N1	6.12	120.76	117.70
54	BA	2335	A	C5-C6-N1	6.12	120.76	117.70
21	AA	339	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	197	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1213	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	63	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	1443	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	508	A	C3'-C2'-C1'	6.12	106.39	101.50
54	BA	1665	A	C5-C6-N1	6.12	120.76	117.70
54	BA	2088	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2103	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	496	A	C5-C6-N1	6.11	120.76	117.70
54	BA	934	U	C5'-C4'-O4'	6.11	116.44	109.10
29	BG	152	ARG	NE-CZ-NH1	6.11	123.36	120.30
54	BA	1796	U	O4'-C1'-N1	6.11	113.09	108.20
54	BA	2157	G	O4'-C1'-N9	6.11	113.09	108.20
54	BA	2286	G	C3'-C2'-C1'	6.11	106.39	101.50
24	A3	60	A	C6-C5-N7	6.11	136.58	132.30
54	BA	83	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	2297	A	C4-C5-C6	-6.11	113.94	117.00
21	AA	15	G	N3-C2-N2	-6.11	115.62	119.90
21	AA	1346	A	C4-C5-C6	-6.11	113.95	117.00
24	A3	66	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1641	A	C4-C5-C6	-6.11	113.95	117.00
21	AA	269	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	1131	G	N3-C2-N2	-6.11	115.62	119.90
54	BA	393	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1754	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	2070	A	C5-C6-N1	6.11	120.75	117.70
54	BA	2342	C	N1-C2-O2	6.11	122.56	118.90
21	AA	1019	A	N1-C6-N6	-6.10	114.94	118.60
48	BZ	10	ARG	NE-CZ-NH1	6.10	123.35	120.30
54	BA	1202	G	N1-C6-O6	-6.10	116.24	119.90
21	AA	284	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1180	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	1467	U	O4'-C1'-N1	6.10	113.08	108.20
21	AA	634	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1265	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	125	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	616	A	C4-C5-C6	-6.10	113.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	634	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	2176	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2723	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	2762	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1183	U	O4'-C1'-N1	6.10	113.08	108.20
21	AA	1389	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	564	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1298	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1999	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	2300	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1080	A	C4-C5-C6	-6.10	113.95	117.00
55	BB	35	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	20	C	N1-C2-O2	6.09	122.56	118.90
54	BA	2036	C	N3-C2-O2	-6.09	117.63	121.90
55	BB	104	A	C4-C5-C6	-6.09	113.95	117.00
22	A1	71	C	N3-C2-O2	-6.09	117.64	121.90
22	A1	73	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	747	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	1342	C	N3-C2-O2	-6.09	117.64	121.90
25	BC	68	ARG	NE-CZ-NH1	6.09	123.35	120.30
54	BA	418	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	687	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	468	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	985	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	1900	A	C4-C5-C6	-6.09	113.95	117.00
17	AR	47	ARG	NE-CZ-NH1	6.09	123.34	120.30
21	AA	886	G	N1-C6-O6	-6.09	116.25	119.90
54	BA	182	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	1526	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2295	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2727	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	647	C	N3-C2-O2	-6.09	117.64	121.90
24	A3	75	C	N1-C2-O2	6.09	122.55	118.90
54	BA	2675	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	1363	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1997	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	517	C	O4'-C1'-N1	6.08	113.07	108.20
54	BA	1575	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	752	G	O4'-C1'-N9	6.08	113.06	108.20
21	AA	1320	C	N1-C2-O2	6.08	122.55	118.90
54	BA	639	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	840	C	N3-C2-O2	-6.08	117.64	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2477	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	2478	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	586	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	1352	C	N1-C2-O2	6.08	122.55	118.90
54	BA	1354	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	689	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	973	A	C5-C6-N1	6.08	120.74	117.70
54	BA	2199	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2676	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	249	C	O4'-C1'-N1	6.08	113.06	108.20
54	BA	1556	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	509	A	C5-C6-N1	6.08	120.74	117.70
54	BA	946	C	N1-C2-O2	6.08	122.55	118.90
54	BA	1117	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	186	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1020	A	N1-C6-N6	-6.07	114.96	118.60
54	BA	1820	U	O4'-C1'-N1	6.07	113.06	108.20
54	BA	1825	U	O4'-C1'-N1	6.07	113.06	108.20
54	BA	14	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	719	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2096	C	N3-C2-O2	-6.07	117.65	121.90
2	AC	39	ARG	NE-CZ-NH1	6.07	123.34	120.30
21	AA	485	U	C3'-C2'-C1'	6.07	106.36	101.50
21	AA	908	A	N1-C6-N6	-6.07	114.96	118.60
54	BA	69	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	237	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	486	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	1183	U	N3-C2-O2	-6.07	117.95	122.20
54	BA	823	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	749	A	C4-C5-C6	-6.07	113.97	117.00
55	BB	57	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	919	A	C5-C6-N1	6.07	120.73	117.70
54	BA	353	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	575	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	2691	C	N3-C2-O2	-6.07	117.66	121.90
55	BB	60	C	O4'-C1'-N1	6.07	113.05	108.20
21	AA	977	A	C4-C5-C6	-6.06	113.97	117.00
24	A3	38	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	323	C	C1'-O4'-C4'	-6.06	105.05	109.90
54	BA	1595	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1315	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	160	A	C4-C5-C6	-6.06	113.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	990	C	N3-C2-O2	-6.06	117.66	121.90
22	A1	47	U	N3-C2-O2	-6.06	117.96	122.20
54	BA	343	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2810	A	N1-C6-N6	-6.06	114.96	118.60
21	AA	44	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	129	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2847	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	2200	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	595	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	833	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1169	A	N1-C6-N6	-6.05	114.97	118.60
54	BA	1924	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	313	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	143	C	O4'-C1'-N1	6.05	113.04	108.20
54	BA	1297	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	2750	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	611	C	N3-C2-O2	-6.05	117.66	121.90
15	AP	62	GLY	C-N-CA	6.05	136.82	121.70
54	BA	2143	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	596	A	C5-C6-N1	6.05	120.72	117.70
21	AA	923	A	N1-C6-N6	-6.05	114.97	118.60
54	BA	239	C	O4'-C1'-N1	6.04	113.04	108.20
21	AA	311	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	430	A	N1-C6-N6	-6.04	114.97	118.60
35	BM	6	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	815	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1151	A	C5-C6-N1	6.04	120.72	117.70
54	BA	2612	C	N3-C2-O2	-6.04	117.67	121.90
22	A1	9	A	C5-C6-N1	6.04	120.72	117.70
54	BA	305	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	447	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	626	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1953	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2381	A	C4-C5-C6	-6.04	113.98	117.00
56	B5	9	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	1967	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2652	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2738	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	282	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1005	A	C5-C6-N1	6.04	120.72	117.70
21	AA	1105	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2163	A	C4-C5-C6	-6.04	113.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1242	U	O4'-C1'-N1	6.04	113.03	108.20
21	AA	1408	A	C4-C5-C6	-6.04	113.98	117.00
36	BN	30	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	1121	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1243	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1580	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	513	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	1431	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2097	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2317	A	C4-C5-C6	-6.03	113.98	117.00
40	BR	68	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	1489	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2063	C	N1-C2-O2	6.03	122.52	118.90
22	A1	27	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	632	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	670	A	P-O3'-C3'	6.03	126.93	119.70
54	BA	865	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	920	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	80	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	389	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	1286	A	C4-C5-C6	-6.03	113.99	117.00
6	AG	2	ARG	NE-CZ-NH1	6.02	123.31	120.30
21	AA	465	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	1081	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2649	C	O4'-C1'-N1	6.02	113.02	108.20
55	BB	50	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	779	C	N3-C2-O2	-6.02	117.68	121.90
21	AA	999	C	N3-C2-O2	-6.02	117.68	121.90
21	AA	1216	A	C1'-O4'-C4'	-6.02	105.08	109.90
21	AA	1362	A	C4-C5-C6	-6.02	113.99	117.00
24	A3	76	C	O3'-P-O5'	-6.02	92.56	104.00
54	BA	2025	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1331	G	N1-C6-O6	-6.02	116.29	119.90
21	AA	790	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	1279	G	C1'-O4'-C4'	-6.02	105.08	109.90
54	BA	609	A	C5-C6-N1	6.02	120.71	117.70
54	BA	1129	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	190	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	892	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	1152	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	201	C	O4'-C1'-N1	6.01	113.01	108.20
21	AA	131	A	C4-C5-C6	-6.01	113.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	901	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	523	A	C5-C6-N1	6.01	120.71	117.70
54	BA	89	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	1000	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	1155	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	614	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	719	C	N1-C2-O2	6.01	122.51	118.90
21	AA	781	A	C5-C6-N1	6.01	120.70	117.70
21	AA	1012	A	C5-C6-N1	6.01	120.70	117.70
21	AA	1400	C	N1-C2-O2	6.01	122.50	118.90
54	BA	398	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2475	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	793	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	800	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	1937	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	214	C	N3-C2-O2	-6.01	117.70	121.90
21	AA	608	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	1262	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	1288	A	C5-C6-N1	6.01	120.70	117.70
21	AA	1499	A	N1-C6-N6	-6.01	115.00	118.60
54	BA	867	C	N3-C2-O2	-6.01	117.70	121.90
54	BA	2249	U	O4'-C1'-N1	6.01	113.00	108.20
54	BA	2611	C	N3-C2-O2	-6.01	117.70	121.90
54	BA	737	C	N3-C2-O2	-6.00	117.70	121.90
8	AI	112	ARG	NE-CZ-NH1	6.00	123.30	120.30
21	AA	396	C	O4'-C1'-N1	6.00	113.00	108.20
21	AA	1150	A	C5-C6-N1	6.00	120.70	117.70
51	B2	39	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	620	G	N3-C2-N2	-6.00	115.70	119.90
54	BA	866	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2456	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	2880	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2043	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2199	A	C5-C6-N1	6.00	120.70	117.70
54	BA	2480	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2577	A	O4'-C1'-N9	6.00	113.00	108.20
21	AA	1150	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	1452	C	C1'-O4'-C4'	-6.00	105.10	109.90
54	BA	1543	G	N3-C2-N2	-6.00	115.70	119.90
21	AA	501	C	N1-C2-O2	6.00	122.50	118.90
54	BA	2064	C	N3-C2-O2	-6.00	117.70	121.90
55	BB	45	A	C4-C5-C6	-6.00	114.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1357	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	876	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1127	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1653	G	O4'-C1'-N9	6.00	113.00	108.20
54	BA	1728	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	879	C	N3-C2-O2	-6.00	117.70	121.90
22	A1	60	C	N1-C2-O2	6.00	122.50	118.90
54	BA	743	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1359	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	490	C	N3-C2-O2	-5.99	117.70	121.90
21	AA	640	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	702	U	O4'-C1'-N1	5.99	113.00	108.20
54	BA	1194	A	C5-C6-N1	5.99	120.70	117.70
54	BA	1205	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1384	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1777	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	2690	U	N3-C2-O2	-5.99	118.00	122.20
55	BB	50	A	C5-C6-N1	5.99	120.70	117.70
21	AA	1319	A	C5-C6-N1	5.99	120.70	117.70
13	AN	69	ARG	NE-CZ-NH1	5.99	123.30	120.30
54	BA	1276	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	2376	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	423	A	O4'-C1'-N9	5.99	112.99	108.20
54	BA	635	C	N1-C2-O2	5.99	122.49	118.90
54	BA	1095	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1109	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2512	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	225	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	1314	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	970	C	N1-C2-O2	5.99	122.49	118.90
54	BA	328	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	528	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	2411	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	415	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1457	U	O4'-C1'-N1	5.98	112.99	108.20
54	BA	1952	A	C4-C5-C6	-5.98	114.01	117.00
13	AN	85	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	33	A	C5-C6-N1	5.98	120.69	117.70
21	AA	188	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	932	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	392	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	646	G	N1-C6-O6	-5.98	116.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	643	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	986	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	1167	C	N1-C2-O2	5.98	122.49	118.90
54	BA	1518	C	N3-C2-O2	-5.98	117.71	121.90
4	AE	28	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	737	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	1330	C	N3-C2-O2	-5.98	117.72	121.90
55	BB	77	U	O4'-C1'-N1	5.98	112.98	108.20
12	AM	69	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	987	G	O4'-C1'-N9	5.98	112.98	108.20
54	BA	885	C	O4'-C1'-N1	5.98	112.98	108.20
54	BA	2716	C	O4'-C1'-N1	5.98	112.98	108.20
26	BD	128	ARG	NE-CZ-NH1	5.98	123.29	120.30
54	BA	918	A	C5-C6-N1	5.98	120.69	117.70
54	BA	1305	C	N1-C2-O2	5.98	122.48	118.90
21	AA	52	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	67	C	C1'-O4'-C4'	-5.97	105.12	109.90
21	AA	175	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	1287	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	783	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	309	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	1456	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	1533	C	N1-C2-O2	5.97	122.48	118.90
22	A1	21	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	1102	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	267	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1493	C	O4'-C1'-N1	5.97	112.98	108.20
13	AN	65	ARG	NE-CZ-NH1	5.97	123.28	120.30
21	AA	972	C	C1'-O4'-C4'	-5.97	105.12	109.90
21	AA	1250	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	1382	C	N1-C2-O2	5.97	122.48	118.90
54	BA	1050	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	1365	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	1641	A	C5-C6-N1	5.97	120.68	117.70
54	BA	1779	U	C1'-O4'-C4'	-5.97	105.12	109.90
54	BA	2651	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2785	C	N3-C2-O2	-5.97	117.72	121.90
6	AG	52	ARG	NE-CZ-NH1	5.97	123.28	120.30
21	AA	866	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	584	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1507	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2241	A	C5-C6-N1	5.97	120.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	119	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	146	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	151	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	393	C	O4'-C1'-N1	5.97	112.97	108.20
54	BA	547	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	976	G	N7-C8-N9	5.97	116.08	113.10
54	BA	2347	C	O4'-C1'-N1	5.97	112.97	108.20
55	BB	4	C	N3-C2-O2	-5.97	117.72	121.90
7	AH	80	PRO	CA-C-N	5.96	128.13	116.20
21	AA	181	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	264	C	N1-C2-O2	5.96	122.48	118.90
21	AA	526	C	N3-C2-O2	-5.96	117.72	121.90
21	AA	649	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	560	C	O4'-C1'-N1	5.96	112.97	108.20
54	BA	2260	C	N3-C2-O2	-5.96	117.72	121.90
41	BS	99	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	314	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1496	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1637	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	1163	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	1446	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	708	C	N1-C2-O2	5.96	122.48	118.90
25	BC	257	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	482	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1509	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	216	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	919	U	O4'-C1'-N1	5.96	112.97	108.20
22	A1	41	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	478	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	1324	A	C5-C6-N1	5.95	120.68	117.70
21	AA	1388	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	99	U	N3-C2-O2	-5.95	118.03	122.20
54	BA	311	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	1168	U	N3-C2-O2	-5.95	118.03	122.20
21	AA	1531	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	302	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	404	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1335	C	N3-C2-O2	-5.95	117.73	121.90
55	BB	68	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	33	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	177	G	O4'-C1'-N9	5.95	112.96	108.20
21	AA	546	A	C6-C5-N7	5.95	136.46	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1397	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1217	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	1504	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	1204	A	C5-C6-N1	5.95	120.67	117.70
21	AA	415	A	O4'-C1'-N9	5.95	112.96	108.20
54	BA	878	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1090	A	C5-C6-N1	5.95	120.67	117.70
54	BA	1746	A	C5-C6-N1	5.95	120.67	117.70
54	BA	1768	C	N3-C2-O2	-5.95	117.74	121.90
55	BB	97	C	O4'-C1'-N1	5.95	112.96	108.20
24	A3	69	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2258	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	412	A	C4-C5-C6	-5.94	114.03	117.00
24	A3	15	G	N1-C6-O6	-5.94	116.34	119.90
54	BA	142	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	529	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1096	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2851	A	N1-C6-N6	-5.94	115.04	118.60
21	AA	366	A	C3'-C2'-C1'	5.94	106.25	101.50
21	AA	817	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	950	U	O4'-C1'-N1	5.94	112.95	108.20
21	AA	1287	A	C5-C6-N1	5.94	120.67	117.70
54	BA	155	A	C5-C6-N1	5.94	120.67	117.70
54	BA	1398	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1650	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2875	C	O4'-C1'-N1	5.94	112.95	108.20
5	AF	44	ARG	NE-CZ-NH1	5.94	123.27	120.30
21	AA	32	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	660	C	N3-C2-O2	-5.94	117.75	121.90
54	BA	394	C	N3-C2-O2	-5.94	117.75	121.90
49	B0	16	ARG	NE-CZ-NH1	5.93	123.27	120.30
54	BA	585	G	N1-C6-O6	-5.93	116.34	119.90
21	AA	1140	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	722	A	C4-C5-C6	-5.93	114.03	117.00
17	AR	52	ARG	NE-CZ-NH1	5.93	123.27	120.30
21	AA	1368	A	C4-C5-C6	-5.93	114.03	117.00
36	BN	30	ARG	NE-CZ-NH2	-5.93	117.33	120.30
54	BA	436	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	181	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1902	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	2774	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1201	A	C5-C6-N1	5.93	120.66	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1310	G	N3-C2-N2	-5.93	115.75	119.90
54	BA	2360	G	O4'-C1'-N9	5.93	112.94	108.20
1	AB	207	ARG	NE-CZ-NH1	5.93	123.26	120.30
54	BA	787	C	N1-C2-O2	5.93	122.46	118.90
54	BA	1054	A	C4-C5-C6	-5.93	114.04	117.00
54	BA	1221	C	N3-C2-O2	-5.93	117.75	121.90
55	BB	114	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	485	C	N3-C2-O2	-5.92	117.75	121.90
55	BB	116	G	N7-C8-N9	5.92	116.06	113.10
54	BA	613	A	O4'-C1'-N9	5.92	112.94	108.20
11	AL	55	ARG	NE-CZ-NH2	-5.92	117.34	120.30
21	AA	489	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	2089	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	2818	U	O4'-C1'-N1	5.92	112.94	108.20
21	AA	1179	A	C5-C6-N1	5.92	120.66	117.70
54	BA	1928	A	C5-C6-N1	5.92	120.66	117.70
21	AA	344	A	C4-C5-C6	-5.92	114.04	117.00
25	BC	13	ARG	NE-CZ-NH1	5.92	123.26	120.30
21	AA	1364	U	O4'-C1'-N1	5.92	112.93	108.20
54	BA	2829	A	C6-C5-N7	5.92	136.44	132.30
54	BA	1306	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	623	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	451	U	C1'-O4'-C4'	-5.91	105.17	109.90
54	BA	2071	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	2248	C	O4'-C1'-N1	5.91	112.93	108.20
21	AA	237	G	N1-C6-O6	-5.91	116.35	119.90
22	A1	32	C	N1-C2-O2	5.91	122.45	118.90
54	BA	272	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	492	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	1586	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	2081	U	O4'-C1'-N1	5.91	112.93	108.20
14	AO	87	ARG	NE-CZ-NH1	5.91	123.25	120.30
54	BA	1503	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	2015	A	O4'-C1'-N9	5.91	112.93	108.20
54	BA	2095	A	C5-C6-N1	5.91	120.66	117.70
21	AA	1071	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	5	A	C5-C6-N1	5.91	120.66	117.70
54	BA	156	A	C5-C6-N1	5.91	120.65	117.70
54	BA	2540	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2850	A	N1-C6-N6	-5.91	115.06	118.60
54	BA	531	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	685	A	C4-C5-C6	-5.91	114.05	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2752	C	O4'-C1'-N1	5.91	112.92	108.20
21	AA	1110	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1176	U	C1'-O4'-C4'	-5.90	105.18	109.90
54	BA	2496	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	91	A	O4'-C1'-N9	5.90	112.92	108.20
54	BA	1677	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1987	A	C5-C6-N1	5.90	120.65	117.70
54	BA	2352	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	2713	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	1204	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	458	G	O4'-C1'-N9	5.90	112.92	108.20
54	BA	1336	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	2681	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	479	A	C6-C5-N7	5.90	136.43	132.30
54	BA	1760	C	N1-C2-O2	5.90	122.44	118.90
54	BA	2328	A	C4-C5-C6	-5.90	114.05	117.00
20	AU	3	ILE	C-N-CA	5.89	136.44	121.70
21	AA	1019	A	C5-C6-N1	5.89	120.65	117.70
54	BA	37	C	O4'-C1'-N1	5.89	112.92	108.20
54	BA	2080	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	2667	C	C1'-O4'-C4'	-5.89	105.19	109.90
21	AA	681	A	C4-C5-C6	-5.89	114.05	117.00
21	AA	900	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	19	A	C5-C6-N1	5.89	120.65	117.70
54	BA	1208	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	385	C	N1-C2-O2	5.89	122.43	118.90
24	A3	72	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1103	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	1895	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	595	A	C5-C6-N1	5.89	120.64	117.70
54	BA	526	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	1158	C	N3-C4-C5	5.89	124.26	121.90
55	BB	91	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	222	C	N3-C2-O2	-5.89	117.78	121.90
27	BE	61	ARG	NE-CZ-NH1	5.89	123.24	120.30
54	BA	680	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1914	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	873	A	N1-C6-N6	-5.88	115.07	118.60
54	BA	331	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	897	C	O4'-C1'-N1	5.88	112.91	108.20
54	BA	2442	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	2683	C	O4'-C1'-N1	5.88	112.91	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2835	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1075	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1427	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	2713	U	N3-C2-O2	-5.88	118.08	122.20
21	AA	1251	A	C6-C5-N7	5.88	136.42	132.30
21	AA	1483	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1142	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2285	C	N3-C2-O2	-5.88	117.78	121.90
10	AK	126	ARG	C-N-CA	5.88	136.39	121.70
54	BA	734	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	895	U	O4'-C1'-N1	5.88	112.90	108.20
54	BA	2385	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	2620	C	N3-C2-O2	-5.88	117.79	121.90
21	AA	513	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	127	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	226	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	372	G	N3-C2-N2	-5.87	115.79	119.90
54	BA	466	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	1775	U	O4'-C1'-N1	5.87	112.90	108.20
54	BA	2173	A	C4-C5-C6	-5.87	114.06	117.00
8	AI	123	ARG	NE-CZ-NH1	5.87	123.24	120.30
23	A2	87	U	N3-C2-O2	-5.87	118.09	122.20
54	BA	1395	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2851	A	C5-C6-N1	5.87	120.64	117.70
31	BI	133	ARG	NE-CZ-NH1	5.87	123.23	120.30
54	BA	1462	C	O4'-C1'-N1	5.87	112.90	108.20
54	BA	1761	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	119	A	O4'-C1'-N9	5.87	112.89	108.20
54	BA	565	C	O4'-C1'-N1	5.87	112.89	108.20
54	BA	1302	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2061	G	N1-C6-O6	-5.87	116.38	119.90
54	BA	2114	A	C6-C5-N7	5.87	136.41	132.30
21	AA	1463	U	O4'-C1'-N1	5.87	112.89	108.20
54	BA	1493	C	N3-C4-N4	-5.87	113.89	118.00
54	BA	2207	C	N1-C2-O2	5.87	122.42	118.90
21	AA	231	U	O4'-C1'-N1	5.87	112.89	108.20
54	BA	1404	C	O4'-C1'-N1	5.87	112.89	108.20
54	BA	1604	C	N3-C2-O2	-5.87	117.79	121.90
2	AC	142	ARG	NE-CZ-NH1	5.86	123.23	120.30
21	AA	758	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	1399	C	C1'-O4'-C4'	-5.86	105.21	109.90
54	BA	1508	A	C4-C5-C6	-5.86	114.07	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2496	C	N1-C2-O2	5.86	122.42	118.90
54	BA	2633	G	O4'-C1'-N9	5.86	112.89	108.20
21	AA	25	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	352	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	650	G	N1-C6-O6	-5.86	116.38	119.90
37	BO	111	ARG	NE-CZ-NH1	5.86	123.23	120.30
54	BA	1313	U	N3-C2-O2	-5.86	118.10	122.20
54	BA	2146	C	N1-C2-O2	5.86	122.42	118.90
54	BA	2798	U	O4'-C1'-N1	5.86	112.89	108.20
21	AA	642	A	C5-C6-N1	5.86	120.63	117.70
21	AA	914	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	560	C	N1-C2-O2	5.86	122.42	118.90
54	BA	1788	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2617	U	O4'-C1'-N1	5.86	112.89	108.20
54	BA	2875	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	1181	G	C5'-C4'-C3'	-5.86	106.63	116.00
54	BA	1872	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	2628	C	N1-C2-O2	5.86	122.41	118.90
54	BA	126	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	470	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	581	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	1270	C	N3-C2-O2	-5.85	117.80	121.90
5	AF	25	TYR	CB-CG-CD2	-5.85	117.49	121.00
54	BA	424	G	O4'-C1'-N9	5.85	112.88	108.20
54	BA	1685	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	2883	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	2066	C	N3-C2-O2	-5.85	117.81	121.90
6	AG	4	ARG	NE-CZ-NH1	5.85	123.22	120.30
21	AA	172	A	C4-C5-C6	-5.85	114.08	117.00
21	AA	1238	A	C4-C5-C6	-5.85	114.08	117.00
22	A1	48	C	N1-C2-O2	5.85	122.41	118.90
39	BQ	12	ARG	NE-CZ-NH1	5.85	123.22	120.30
54	BA	2241	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	2577	A	C4-C5-C6	-5.85	114.08	117.00
3	AD	72	ARG	NE-CZ-NH1	5.85	123.22	120.30
21	AA	1234	C	N3-C2-O2	-5.85	117.81	121.90
4	AE	19	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	AA	1155	A	C6-C5-N7	5.84	136.39	132.30
28	BF	177	ARG	NE-CZ-NH1	5.84	123.22	120.30
54	BA	1072	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2177	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2448	A	C4-C5-C6	-5.84	114.08	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2773	C	O4'-C1'-N1	5.84	112.88	108.20
21	AA	948	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	1103	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	151	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	172	A	C5-C6-N1	5.84	120.62	117.70
54	BA	156	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1206	G	C5-C6-N1	5.84	114.42	111.50
54	BA	2863	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2864	G	N1-C6-O6	-5.84	116.40	119.90
54	BA	2558	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	918	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	3	U	O4'-C1'-N1	5.83	112.87	108.20
54	BA	914	G	C1'-O4'-C4'	-5.83	105.23	109.90
22	A1	76	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	508	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	1262	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	1269	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	2711	A	C4'-C3'-C2'	-5.83	96.77	102.60
54	BA	510	C	O4'-C1'-N1	5.83	112.86	108.20
54	BA	615	U	O4'-C1'-N1	5.83	112.87	108.20
21	AA	210	C	N1-C2-O2	5.83	122.40	118.90
21	AA	504	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	839	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	309	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	1030	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1490	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	2215	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2794	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	165	G	N1-C6-O6	-5.83	116.40	119.90
54	BA	1010	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	2372	U	O4'-C1'-N1	5.83	112.86	108.20
21	AA	77	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	1411	C	N1-C2-O2	5.83	122.40	118.90
54	BA	1342	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	862	C	N3-C2-O2	-5.82	117.82	121.90
25	BC	220	ARG	NE-CZ-NH2	-5.82	117.39	120.30
54	BA	945	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1395	A	C3'-C2'-C1'	5.82	106.16	101.50
54	BA	2639	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2732	G	N3-C4-C5	-5.82	125.69	128.60
21	AA	1467	C	N1-C2-O2	5.82	122.39	118.90
21	AA	1479	C	N3-C2-O2	-5.82	117.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1678	A	O4'-C1'-N9	5.82	112.86	108.20
54	BA	2533	U	O4'-C1'-N1	5.82	112.86	108.20
21	AA	1124	G	O4'-C1'-N9	5.82	112.86	108.20
21	AA	1502	A	O4'-C1'-N9	5.82	112.86	108.20
54	BA	96	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	238	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1088	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1821	A	C5-C6-N1	5.82	120.61	117.70
54	BA	2263	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	930	G	C5-C6-N1	5.82	114.41	111.50
21	AA	1404	C	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2000	C	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2084	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2264	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	241	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	896	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	56	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1569	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2761	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	1054	C	N1-C2-O2	5.81	122.39	118.90
54	BA	165	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	334	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	544	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1207	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1233	C	O4'-C1'-N1	5.81	112.85	108.20
54	BA	1407	G	O4'-C1'-N9	5.81	112.85	108.20
54	BA	2009	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2771	C	N1-C2-O2	5.81	122.39	118.90
55	BB	17	C	N3-C2-O2	-5.81	117.83	121.90
55	BB	30	C	N3-C2-O2	-5.81	117.83	121.90
55	BB	90	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1087	G	N1-C6-O6	-5.81	116.42	119.90
54	BA	2581	G	N1-C6-O6	-5.81	116.42	119.90
54	BA	1726	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	334	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	1005	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1135	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2732	G	C8-N9-C4	-5.80	104.08	106.40
21	AA	698	G	N1-C6-O6	-5.80	116.42	119.90
21	AA	1129	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	630	G	O4'-C1'-N9	5.80	112.84	108.20
54	BA	979	A	C4-C5-C6	-5.80	114.10	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1053	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	542	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1185	G	O4'-C1'-N9	5.80	112.84	108.20
46	BX	27	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	1308	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1340	U	N3-C2-O2	-5.80	118.14	122.20
54	BA	1803	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2153	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2313	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	2358	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	255	A	N1-C6-N6	-5.79	115.12	118.60
54	BA	1771	C	N1-C2-O2	5.79	122.38	118.90
54	BA	1073	A	O4'-C1'-N9	5.79	112.83	108.20
54	BA	1439	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	1563	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2695	U	O4'-C1'-N1	5.79	112.83	108.20
21	AA	153	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	854	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	753	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	1488	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	2050	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1152	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1574	C	N1-C2-O2	5.79	122.37	118.90
10	AK	52	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
54	BA	300	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	1408	G	N3-C2-N2	-5.79	115.85	119.90
54	BA	1664	A	N1-C6-N6	-5.79	115.13	118.60
54	BA	1985	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1986	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	760	G	N1-C6-O6	-5.79	116.43	119.90
54	BA	1446	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1977	A	N1-C6-N6	-5.79	115.13	118.60
21	AA	414	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	1014	A	C4-C5-C6	-5.79	114.11	117.00
26	BD	179	ARG	NE-CZ-NH1	5.79	123.19	120.30
54	BA	1390	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1393	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	1634	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2807	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	6	A	C6-C5-N7	5.78	136.35	132.30
54	BA	389	G	O4'-C1'-N9	5.78	112.83	108.20
54	BA	2430	A	O4'-C1'-N9	5.78	112.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	516	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	670	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1579	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1317	C	C1'-O4'-C4'	-5.78	105.28	109.90
27	BE	49	ARG	NE-CZ-NH1	5.78	123.19	120.30
54	BA	1898	U	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2099	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	2204	G	N3-C2-N2	-5.78	115.85	119.90
54	BA	2264	C	O4'-C1'-N1	5.78	112.83	108.20
24	A3	52	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	1508	A	C1'-O4'-C4'	-5.78	105.28	109.90
54	BA	1602	U	O4'-C1'-N1	5.78	112.82	108.20
21	AA	738	C	N3-C2-O2	-5.78	117.86	121.90
21	AA	1213	A	C4-C5-C6	-5.78	114.11	117.00
22	A1	20	G	N3-C4-C5	-5.78	125.71	128.60
54	BA	402	A	N1-C6-N6	-5.78	115.13	118.60
54	BA	1974	C	O4'-C1'-N1	5.78	112.82	108.20
54	BA	2003	A	C4-C5-C6	-5.78	114.11	117.00
38	BP	112	ARG	NE-CZ-NH1	5.78	123.19	120.30
54	BA	988	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1812	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	2751	G	N3-C4-C5	-5.78	125.71	128.60
54	BA	1206	G	N3-C2-N2	-5.77	115.86	119.90
55	BB	22	U	O4'-C1'-N1	5.77	112.82	108.20
54	BA	61	C	O4'-C1'-N1	5.77	112.82	108.20
54	BA	336	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1731	G	C5-C6-N1	5.77	114.39	111.50
54	BA	2183	A	C5-C6-N1	5.77	120.59	117.70
54	BA	2183	A	C4-C5-C6	-5.77	114.11	117.00
13	AN	13	ARG	NE-CZ-NH1	5.77	123.19	120.30
54	BA	565	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	699	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	1542	U	N3-C2-O2	-5.77	118.16	122.20
21	AA	236	A	C3'-C2'-C1'	5.77	106.12	101.50
21	AA	576	C	N1-C2-O2	5.77	122.36	118.90
54	BA	1723	G	N1-C6-O6	-5.77	116.44	119.90
54	BA	1947	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	2855	C	N3-C2-O2	-5.77	117.86	121.90
55	BB	94	A	C5-C6-N1	5.77	120.58	117.70
54	BA	689	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	1378	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	1987	A	C4-C5-C6	-5.77	114.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	19	C	N3-C2-O2	-5.77	117.86	121.90
6	AG	118	ARG	NE-CZ-NH1	5.77	123.18	120.30
14	AO	16	ARG	NE-CZ-NH1	5.77	123.18	120.30
33	BK	105	ARG	NE-CZ-NH1	5.77	123.18	120.30
54	BA	2595	G	O4'-C1'-N9	5.77	112.81	108.20
21	AA	556	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	1759	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1912	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2198	A	O4'-C1'-N9	5.76	112.81	108.20
54	BA	2443	C	N3-C2-O2	-5.76	117.86	121.90
24	A3	40	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	322	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	366	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	680	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	1446	A	O4'-C1'-N9	5.76	112.81	108.20
54	BA	1535	A	O4'-C1'-N9	5.76	112.81	108.20
54	BA	2018	G	N3-C2-N2	-5.76	115.87	119.90
54	BA	2042	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	983	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	158	U	O4'-C1'-N1	5.76	112.81	108.20
22	A1	15	G	N9-C4-C5	5.76	107.70	105.40
25	BC	268	ARG	NE-CZ-NH1	5.76	123.18	120.30
47	BY	7	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	782	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1345	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	1928	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	1209	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	1874	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	58	C	C5'-C4'-C3'	-5.75	106.79	116.00
21	AA	814	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	1096	C	N1-C2-O2	5.75	122.35	118.90
54	BA	351	C	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2208	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	897	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	1477	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2247	A	C5-C6-N1	5.75	120.58	117.70
4	AE	24	VAL	C-N-CA	5.75	136.07	121.70
21	AA	868	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	964	A	C4-C5-C6	-5.75	114.13	117.00
24	A3	41	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	730	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	1296	G	N1-C6-O6	-5.75	116.45	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2311	A	O4'-C1'-N9	5.75	112.80	108.20
54	BA	2626	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	238	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	1326	U	C1'-O4'-C4'	-5.75	105.30	109.90
54	BA	548	G	O4'-C1'-N9	5.75	112.80	108.20
54	BA	851	C	O4'-C1'-N1	5.75	112.80	108.20
54	BA	1328	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	2203	U	O4'-C1'-N1	5.75	112.80	108.20
22	A1	31	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	483	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	1296	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	327	G	N1-C6-O6	-5.74	116.45	119.90
54	BA	375	G	C5-C6-N1	5.74	114.37	111.50
54	BA	1758	U	N3-C2-O2	-5.74	118.18	122.20
21	AA	572	A	C1'-O4'-C4'	-5.74	105.31	109.90
54	BA	613	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1522	A	C4-C5-C6	-5.74	114.13	117.00
56	B5	122	ARG	NE-CZ-NH2	5.74	123.17	120.30
21	AA	910	C	N3-C2-O2	-5.74	117.89	121.90
21	AA	1060	U	N3-C2-O2	-5.74	118.19	122.20
54	BA	773	U	O4'-C1'-N1	5.74	112.79	108.20
21	AA	1498	U	N3-C2-O2	-5.73	118.19	122.20
14	AO	52	ARG	NE-CZ-NH1	5.73	123.17	120.30
21	AA	894	G	C5-C6-N1	5.73	114.37	111.50
30	BH	51	ARG	NE-CZ-NH1	5.73	123.17	120.30
46	BX	71	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	637	A	O4'-C1'-N9	5.73	112.79	108.20
54	BA	1550	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1617	C	O4'-C1'-N1	5.73	112.79	108.20
21	AA	1350	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	848	C	N1-C2-O2	5.73	122.34	118.90
54	BA	1558	C	N1-C2-O2	5.73	122.34	118.90
54	BA	1927	A	C3'-C2'-C1'	5.73	106.08	101.50
54	BA	1970	A	C4-C5-C6	-5.73	114.14	117.00
21	AA	532	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	989	G	N1-C6-O6	-5.73	116.46	119.90
54	BA	2307	G	N3-C4-C5	-5.73	125.74	128.60
21	AA	415	A	C4-C5-C6	-5.73	114.14	117.00
22	A1	61	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	746	A	C4-C5-C6	-5.73	114.14	117.00
36	BN	46	ARG	NE-CZ-NH2	-5.73	117.44	120.30
54	BA	394	C	O4'-C1'-N1	5.73	112.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1236	G	O4'-C1'-N9	5.73	112.78	108.20
21	AA	782	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	116	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	207	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	961	C	N1-C2-O2	5.72	122.33	118.90
21	AA	653	U	O4'-C1'-N1	5.72	112.78	108.20
24	A3	13	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	1254	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2346	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	332	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	609	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	981	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1096	A	C1'-O4'-C4'	-5.72	105.32	109.90
21	AA	539	A	C5-C6-N1	5.72	120.56	117.70
54	BA	1472	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	1157	G	N1-C6-O6	-5.72	116.47	119.90
54	BA	1528	A	C3'-C2'-C1'	5.72	106.07	101.50
54	BA	2311	A	C4-C5-C6	-5.72	114.14	117.00
20	AU	44	ARG	NE-CZ-NH1	5.71	123.16	120.30
21	AA	1113	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1303	C	N1-C2-O2	5.71	122.33	118.90
54	BA	597	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1746	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2425	A	O4'-C1'-N9	5.71	112.77	108.20
21	AA	783	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1098	C	N3-C2-O2	-5.71	117.90	121.90
22	A1	36	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	105	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	1349	C	N1-C2-O2	5.71	122.33	118.90
54	BA	1414	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	2766	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2717	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	85	U	C3'-C2'-C1'	5.71	106.07	101.50
21	AA	1367	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1410	A	C4-C5-C6	-5.71	114.14	117.00
21	AA	1494	G	O4'-C1'-N9	5.71	112.77	108.20
54	BA	948	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	1170	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	1894	C	N1-C2-O2	5.71	122.33	118.90
54	BA	2000	C	N3-C4-N4	-5.71	114.00	118.00
54	BA	2096	C	O4'-C1'-N1	5.71	112.77	108.20
21	AA	569	C	N3-C2-O2	-5.71	117.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	978	A	C4-C5-C6	-5.71	114.15	117.00
39	BQ	54	ARG	NE-CZ-NH1	5.71	123.15	120.30
54	BA	1057	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	1349	C	N3-C4-N4	-5.71	114.01	118.00
54	BA	2386	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	49	A	C5-C6-N1	5.71	120.55	117.70
54	BA	759	G	N3-C4-C5	-5.71	125.75	128.60
21	AA	169	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	178	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	315	G	O4'-C1'-N9	5.70	112.76	108.20
2	AC	58	ARG	NE-CZ-NH1	5.70	123.15	120.30
21	AA	285	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	2456	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	353	A	O4'-C1'-N9	5.70	112.76	108.20
21	AA	795	C	N1-C2-O2	5.70	122.32	118.90
21	AA	1092	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	1257	A	C4-C5-C6	-5.70	114.15	117.00
36	BN	22	ARG	NE-CZ-NH1	5.70	123.15	120.30
54	BA	400	G	N1-C6-O6	-5.70	116.48	119.90
54	BA	550	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	694	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	2465	C	N3-C2-O2	-5.70	117.91	121.90
55	BB	96	G	O4'-C1'-N9	5.70	112.76	108.20
12	AM	91	ARG	C-N-CA	5.70	135.95	121.70
21	AA	1243	C	N3-C2-O2	-5.70	117.91	121.90
9	AJ	62	ARG	NE-CZ-NH1	5.70	123.15	120.30
21	AA	1415	G	N3-C2-N2	-5.70	115.91	119.90
21	AA	374	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	518	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	118	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1076	C	C1'-O4'-C4'	-5.70	105.34	109.90
21	AA	145	G	N3-C2-N2	-5.69	115.91	119.90
54	BA	454	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	519	U	O4'-C1'-N1	5.69	112.75	108.20
54	BA	922	C	N3-C2-O2	-5.69	117.91	121.90
54	BA	2548	U	O4'-C1'-N1	5.69	112.75	108.20
16	AQ	61	ARG	NE-CZ-NH2	-5.69	117.45	120.30
54	BA	218	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	2380	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	2382	G	O4'-C1'-N9	5.69	112.75	108.20
54	BA	2704	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	957	C	N3-C2-O2	-5.69	117.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	93	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	996	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	2518	A	O4'-C1'-N9	5.69	112.75	108.20
21	AA	54	C	O4'-C1'-N1	5.68	112.75	108.20
21	AA	136	C	N1-C2-O2	5.68	122.31	118.90
21	AA	253	A	C4-C5-C6	-5.68	114.16	117.00
34	BL	47	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	633	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	853	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	2658	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	262	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	871	U	N3-C2-O2	-5.68	118.22	122.20
54	BA	1246	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1295	C	N3-C2-O2	-5.68	117.92	121.90
21	AA	1180	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	249	C	N1-C2-O2	5.68	122.31	118.90
54	BA	704	G	O4'-C1'-N9	5.68	112.74	108.20
21	AA	176	C	N3-C2-O2	-5.68	117.93	121.90
21	AA	1042	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	2028	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	2037	A	C4-C5-C6	-5.68	114.16	117.00
55	BB	102	G	O4'-C1'-N9	5.68	112.74	108.20
8	AI	84	ARG	NE-CZ-NH1	5.68	123.14	120.30
21	AA	314	C	N3-C2-O2	-5.68	117.93	121.90
21	AA	324	G	N3-C4-C5	-5.68	125.76	128.60
21	AA	906	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	164	C	N3-C2-O2	-5.68	117.93	121.90
21	AA	1179	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	1275	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	1437	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	253	C	N3-C2-O2	-5.67	117.93	121.90
55	BB	8	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	716	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	871	U	O4'-C1'-N1	5.67	112.74	108.20
54	BA	1755	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	2860	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	270	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	699	C	N3-C2-O2	-5.67	117.93	121.90
24	A3	36	A	C4-C5-C6	-5.67	114.16	117.00
51	B2	21	ARG	NE-CZ-NH1	5.67	123.14	120.30
54	BA	828	U	N3-C2-O2	-5.67	118.23	122.20
54	BA	1189	A	C4-C5-C6	-5.67	114.17	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	234	U	N1-C2-N3	5.67	118.30	114.90
54	BA	1912	A	C3'-C2'-C1'	5.67	106.03	101.50
54	BA	2430	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	2678	C	O4'-C1'-N1	5.67	112.73	108.20
21	AA	321	A	C6-C5-N7	5.67	136.26	132.30
54	BA	1725	U	O4'-C1'-N1	5.67	112.73	108.20
21	AA	753	A	C4-C5-C6	-5.66	114.17	117.00
38	BP	102	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	1762	A	C4-C5-C6	-5.66	114.17	117.00
55	BB	3	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	218	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1547	C	O4'-C1'-N1	5.66	112.73	108.20
21	AA	49	U	O4'-C1'-N1	5.66	112.73	108.20
21	AA	726	C	N1-C2-O2	5.66	122.30	118.90
54	BA	139	U	N3-C2-O2	-5.66	118.24	122.20
54	BA	1208	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	2195	U	O4'-C1'-N1	5.66	112.73	108.20
21	AA	1086	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1260	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	534	U	N3-C2-O2	-5.66	118.24	122.20
21	AA	425	G	N3-C2-N2	-5.66	115.94	119.90
32	BJ	34	ARG	NE-CZ-NH2	-5.66	117.47	120.30
54	BA	1241	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1542	U	O4'-C1'-N1	5.66	112.72	108.20
21	AA	1032	G	N3-C4-C5	-5.65	125.77	128.60
54	BA	2581	G	N3-C4-C5	-5.65	125.77	128.60
21	AA	466	A	C4-C5-C6	-5.65	114.17	117.00
22	A1	70	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	1750	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	2457	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	97	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	676	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	737	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	2769	U	O4'-C1'-N1	5.65	112.72	108.20
22	A1	35	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1887	C	O4'-C1'-N1	5.65	112.72	108.20
21	AA	1012	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	948	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1246	A	C5-C6-N1	5.65	120.52	117.70
54	BA	1355	G	O4'-C1'-N9	5.65	112.72	108.20
54	BA	1386	C	N3-C2-O2	-5.65	117.95	121.90
54	BA	2838	G	N1-C6-O6	-5.65	116.51	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1417	C	N1-C2-O2	5.65	122.29	118.90
21	AA	8	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	87	C	O4'-C1'-N1	5.64	112.72	108.20
21	AA	1339	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1014	A	C5-C6-N1	5.64	120.52	117.70
54	BA	2789	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	946	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1332	G	C5'-C4'-C3'	-5.64	106.97	116.00
54	BA	1486	U	C1'-O4'-C4'	-5.64	105.39	109.90
54	BA	1798	U	O4'-C1'-N1	5.64	112.71	108.20
54	BA	2820	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	592	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	1225	A	C1'-O4'-C4'	-5.64	105.39	109.90
27	BE	162	ARG	NE-CZ-NH2	-5.64	117.48	120.30
54	BA	372	G	O4'-C1'-N9	5.64	112.71	108.20
54	BA	490	C	N1-C2-O2	5.64	122.28	118.90
21	AA	327	A	N1-C6-N6	-5.64	115.22	118.60
54	BA	219	A	C6-C5-N7	5.64	136.25	132.30
54	BA	664	G	N1-C6-O6	-5.64	116.52	119.90
21	AA	422	C	N1-C2-O2	5.64	122.28	118.90
54	BA	324	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	421	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	693	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1810	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	843	U	N3-C2-O2	-5.63	118.25	122.20
21	AA	1448	C	N1-C2-O2	5.63	122.28	118.90
22	A1	72	C	N1-C2-O2	5.63	122.28	118.90
55	BB	110	C	N3-C2-O2	-5.63	117.95	121.90
21	AA	111	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	370	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	253	C	O4'-C1'-N1	5.63	112.71	108.20
6	AG	108	ARG	NE-CZ-NH1	5.63	123.12	120.30
54	BA	1967	C	O4'-C1'-N1	5.63	112.70	108.20
55	BB	27	C	N1-C2-O2	5.63	122.28	118.90
54	BA	544	C	C1'-O4'-C4'	-5.63	105.40	109.90
54	BA	1090	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	1853	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	182	A	C2-N3-C4	5.63	113.41	110.60
21	AA	1431	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	610	U	N3-C2-O2	-5.63	118.26	122.20
21	AA	959	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1521	C	N1-C2-O2	5.63	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	503	A	O4'-C1'-N9	5.63	112.70	108.20
21	AA	95	C	N1-C2-O2	5.62	122.28	118.90
54	BA	222	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	298	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2469	A	C4-C5-C6	-5.62	114.19	117.00
32	BJ	96	ARG	NE-CZ-NH2	-5.62	117.49	120.30
21	AA	1394	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1111	A	C4-C5-C6	-5.62	114.19	117.00
24	A3	42	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	899	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1362	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1534	U	N3-C2-O2	-5.62	118.27	122.20
54	BA	2275	C	N1-C2-O2	5.62	122.27	118.90
54	BA	892	A	P-O3'-C3'	5.62	126.44	119.70
54	BA	1527	G	N3-C2-N2	-5.62	115.97	119.90
55	BB	44	G	N1-C6-O6	-5.62	116.53	119.90
17	AR	72	ARG	C-N-CA	5.61	135.74	121.70
54	BA	1784	A	O4'-C1'-N9	5.61	112.69	108.20
54	BA	2516	A	C6-C5-N7	5.61	136.23	132.30
21	AA	352	C	N1-C2-O2	5.61	122.27	118.90
54	BA	1704	C	O4'-C1'-N1	5.61	112.69	108.20
21	AA	973	G	N1-C6-O6	-5.61	116.53	119.90
21	AA	1063	C	C6-N1-C2	-5.61	118.06	120.30
32	BJ	13	ARG	NE-CZ-NH1	5.61	123.11	120.30
54	BA	131	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	631	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	2425	A	P-O3'-C3'	5.61	126.43	119.70
55	BB	5	U	O4'-C1'-N1	5.61	112.69	108.20
21	AA	765	G	N3-C4-C5	-5.61	125.80	128.60
54	BA	427	U	O4'-C1'-N1	5.61	112.69	108.20
9	AJ	37	ARG	NE-CZ-NH1	5.61	123.10	120.30
21	AA	335	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	975	A	O4'-C1'-N9	5.61	112.69	108.20
21	AA	1236	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	25	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1304	A	O4'-C1'-N9	5.61	112.69	108.20
52	B3	41	ARG	NE-CZ-NH1	5.61	123.10	120.30
54	BA	379	G	N1-C6-O6	-5.61	116.54	119.90
54	BA	533	G	C8-N9-C4	-5.61	104.16	106.40
54	BA	2112	G	N3-C2-N2	-5.61	115.98	119.90
54	BA	2560	A	C6-C5-N7	5.61	136.22	132.30
54	BA	692	C	N3-C2-O2	-5.60	117.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1535	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1609	A	C4-C5-C6	-5.60	114.20	117.00
5	AF	86	ARG	NE-CZ-NH1	5.60	123.10	120.30
21	AA	183	C	N1-C2-O2	5.60	122.26	118.90
54	BA	2117	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	2768	U	C4'-C3'-C2'	-5.60	97.00	102.60
21	AA	665	A	C6-C5-N7	5.60	136.22	132.30
21	AA	670	G	N3-C2-N2	-5.60	115.98	119.90
54	BA	1790	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	2501	C	N1-C2-O2	5.60	122.26	118.90
6	AG	110	ARG	NE-CZ-NH1	5.60	123.10	120.30
21	AA	28	A	C6-C5-N7	5.60	136.22	132.30
21	AA	1496	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	756	A	N1-C6-N6	-5.60	115.24	118.60
54	BA	1137	G	O4'-C1'-N9	5.60	112.68	108.20
21	AA	715	A	C5-C6-N1	5.60	120.50	117.70
54	BA	832	U	O4'-C1'-N1	5.60	112.68	108.20
21	AA	1124	G	N3-C4-C5	-5.60	125.80	128.60
21	AA	1299	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1752	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	888	C	O4'-C1'-N1	5.59	112.68	108.20
54	BA	1385	A	C5-C6-N1	5.59	120.50	117.70
54	BA	2133	G	N1-C6-O6	-5.59	116.54	119.90
21	AA	883	C	N1-C2-O2	5.59	122.26	118.90
54	BA	679	C	N3-C2-O2	-5.59	117.98	121.90
54	BA	1165	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	1664	A	P-O3'-C3'	5.59	126.41	119.70
14	AO	83	ARG	NE-CZ-NH1	5.59	123.10	120.30
24	A3	57	C	N1-C2-O2	5.59	122.25	118.90
54	BA	1544	A	C6-C5-N7	5.59	136.21	132.30
54	BA	1708	C	O4'-C1'-N1	5.59	112.67	108.20
16	AQ	10	ARG	NE-CZ-NH1	5.59	123.09	120.30
20	AU	21	SER	C-N-CA	5.59	135.68	121.70
21	AA	1107	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2475	C	C6-N1-C2	-5.59	118.06	120.30
54	BA	61	C	N1-C2-O2	5.58	122.25	118.90
54	BA	1027	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1710	G	O4'-C1'-N9	5.58	112.67	108.20
54	BA	2776	A	O4'-C1'-N9	5.58	112.67	108.20
5	AF	45	ARG	NE-CZ-NH1	5.58	123.09	120.30
21	AA	221	C	N1-C2-O2	5.58	122.25	118.90
21	AA	1249	C	N3-C2-O2	-5.58	117.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	203	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1956	U	O4'-C1'-N1	5.58	112.67	108.20
54	BA	2388	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	304	U	O4'-C1'-N1	5.58	112.66	108.20
54	BA	1287	A	O4'-C1'-N9	5.58	112.66	108.20
21	AA	934	C	N1-C2-O2	5.58	122.25	118.90
21	AA	1403	C	N1-C2-O2	5.58	122.25	118.90
24	A3	60	A	C5-C6-N6	5.58	128.16	123.70
54	BA	278	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1032	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1040	A	C6-C5-N7	5.58	136.21	132.30
54	BA	2632	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	29	U	O4'-C1'-N1	5.57	112.66	108.20
21	AA	940	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	1038	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	1333	A	C4-C5-C6	-5.57	114.21	117.00
54	BA	884	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	1865	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	1394	U	O4'-C1'-N1	5.57	112.66	108.20
8	AI	121	ARG	NH1-CZ-NH2	-5.57	113.27	119.40
21	AA	228	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	1320	C	N1-C2-O2	5.57	122.24	118.90
54	BA	2058	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	2284	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	1170	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	1289	A	C6-C5-N7	5.57	136.20	132.30
54	BA	144	A	O4'-C1'-N9	5.57	112.66	108.20
54	BA	1233	C	N1-C2-O2	5.57	122.24	118.90
55	BB	27	C	O4'-C1'-N1	5.57	112.66	108.20
21	AA	246	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	819	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	294	A	C6-C5-N7	5.57	136.20	132.30
21	AA	166	U	O4'-C1'-N1	5.57	112.65	108.20
21	AA	420	U	C3'-C2'-C1'	5.57	105.95	101.50
54	BA	129	C	N1-C2-O2	5.57	122.24	118.90
54	BA	757	G	O4'-C1'-N9	5.57	112.65	108.20
54	BA	2113	U	O4'-C1'-N1	5.57	112.65	108.20
54	BA	2730	C	N3-C2-O2	-5.57	118.00	121.90
4	AE	149	PRO	CA-N-CD	-5.56	103.71	111.50
54	BA	366	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	964	C	N3-C2-O2	-5.56	118.00	121.90
21	AA	1257	A	O4'-C1'-N9	5.56	112.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	554	U	O4'-C1'-N1	5.56	112.65	108.20
54	BA	2447	G	C5-C6-N1	5.56	114.28	111.50
1	AB	206	ILE	CA-C-N	5.56	129.43	117.20
21	AA	718	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1528	A	O4'-C1'-N9	5.56	112.65	108.20
21	AA	389	A	C5-C6-N1	5.56	120.48	117.70
51	B2	12	ARG	NE-CZ-NH1	5.56	123.08	120.30
54	BA	458	G	C5-C6-N1	5.56	114.28	111.50
54	BA	2715	C	N3-C2-O2	-5.56	118.01	121.90
21	AA	10	A	C5-C6-N1	5.56	120.48	117.70
21	AA	81	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	953	G	O4'-C1'-N9	5.56	112.64	108.20
54	BA	1880	U	O4'-C1'-N1	5.56	112.65	108.20
54	BA	2045	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	2427	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	2778	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	2607	G	C5'-C4'-O4'	5.56	115.77	109.10
54	BA	557	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1974	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	2288	A	C4-C5-C6	-5.55	114.22	117.00
21	AA	1169	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	2884	U	O4'-C1'-N1	5.55	112.64	108.20
55	BB	117	G	O4'-C1'-N9	5.55	112.64	108.20
21	AA	198	G	N1-C6-O6	-5.55	116.57	119.90
21	AA	533	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	1786	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	860	U	O4'-C1'-N1	5.55	112.64	108.20
55	BB	42	C	N3-C2-O2	-5.55	118.02	121.90
21	AA	806	C	N3-C2-O2	-5.55	118.02	121.90
24	A3	62	C	N3-C2-O2	-5.55	118.02	121.90
32	BJ	13	ARG	NE-CZ-NH2	5.55	123.07	120.30
54	BA	366	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	424	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	540	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	684	G	C5'-C4'-C3'	-5.55	107.13	116.00
54	BA	2082	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	2538	C	N1-C2-O2	5.55	122.23	118.90
55	BB	37	C	N3-C4-N4	-5.55	114.12	118.00
21	AA	217	C	N1-C2-O2	5.54	122.23	118.90
21	AA	676	A	C4-C5-C6	-5.54	114.23	117.00
36	BN	64	ARG	NE-CZ-NH1	5.54	123.07	120.30
24	A3	49	C	N1-C2-O2	5.54	122.22	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	211	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	1727	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2287	A	C4-C5-C6	-5.54	114.23	117.00
55	BB	9	G	N1-C6-O6	-5.54	116.58	119.90
53	B4	36	ARG	NE-CZ-NH1	5.54	123.07	120.30
54	BA	2470	G	N1-C6-O6	-5.54	116.58	119.90
54	BA	196	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1351	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1397	U	N3-C2-O2	-5.54	118.32	122.20
55	BB	26	C	N1-C2-O2	5.54	122.22	118.90
55	BB	51	G	N1-C6-O6	-5.54	116.58	119.90
54	BA	761	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	1402	C	N1-C2-O2	5.54	122.22	118.90
27	BE	40	ARG	NE-CZ-NH2	5.54	123.07	120.30
54	BA	903	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	2420	C	N3-C2-O2	-5.54	118.03	121.90
54	BA	2568	U	O4'-C1'-N1	5.54	112.63	108.20
54	BA	2667	C	N1-C2-O2	5.54	122.22	118.90
21	AA	339	C	C5'-C4'-C3'	-5.53	107.15	116.00
54	BA	759	G	C5'-C4'-O4'	5.53	115.74	109.10
54	BA	987	C	N1-C2-O2	5.53	122.22	118.90
54	BA	1392	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	2015	A	C1'-O4'-C4'	-5.53	105.47	109.90
55	BB	56	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	53	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	751	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1088	A	O4'-C1'-N9	5.53	112.63	108.20
54	BA	1408	G	O4'-C1'-N9	5.53	112.63	108.20
21	AA	1311	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	440	C	N1-C2-O2	5.53	122.22	118.90
54	BA	804	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	835	C	O4'-C1'-N1	5.53	112.62	108.20
21	AA	417	G	C5-C6-N1	5.53	114.26	111.50
21	AA	1132	C	N1-C2-O2	5.53	122.22	118.90
22	A1	25	C	N1-C2-O2	5.53	122.22	118.90
54	BA	1463	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2591	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	148	G	N3-C2-N2	-5.53	116.03	119.90
21	AA	1271	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	2175	C	N1-C2-O2	5.53	122.22	118.90
54	BA	1237	A	C5-C6-N1	5.53	120.46	117.70
54	BA	1990	C	O4'-C1'-N1	5.53	112.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	55	U	O4'-C1'-N1	5.53	112.62	108.20
21	AA	297	G	N3-C2-N2	-5.52	116.03	119.90
54	BA	1086	A	O4'-C1'-N9	5.52	112.62	108.20
54	BA	1234	U	O4'-C1'-N1	5.52	112.62	108.20
21	AA	1239	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2211	A	O4'-C1'-N9	5.52	112.62	108.20
21	AA	1465	A	C4-C5-C6	-5.52	114.24	117.00
24	A3	61	U	C3'-C2'-C1'	5.52	105.92	101.50
54	BA	198	C	N1-C2-O2	5.52	122.21	118.90
54	BA	1121	C	O4'-C1'-N1	5.52	112.62	108.20
54	BA	1481	U	O4'-C1'-N1	5.52	112.62	108.20
54	BA	1887	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	1941	C	N3-C2-O2	-5.52	118.04	121.90
21	AA	520	A	C6-C5-N7	5.52	136.16	132.30
21	AA	870	U	N3-C2-O2	-5.52	118.34	122.20
54	BA	29	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	1353	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2598	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	1312	G	C5-C6-N1	5.52	114.26	111.50
23	A2	91	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	997	G	C5-C6-N1	5.52	114.26	111.50
54	BA	1288	G	N1-C6-O6	-5.52	116.59	119.90
24	A3	63	C	N1-C2-O2	5.51	122.21	118.90
54	BA	192	C	O4'-C1'-N1	5.51	112.61	108.20
54	BA	1958	C	C2-N3-C4	-5.51	117.14	119.90
21	AA	1281	C	N1-C2-O2	5.51	122.21	118.90
21	AA	1369	C	N1-C2-O2	5.51	122.21	118.90
54	BA	34	U	N3-C2-O2	-5.51	118.34	122.20
2	AC	126	ARG	NE-CZ-NH2	-5.51	117.55	120.30
21	AA	756	C	N1-C2-O2	5.51	122.21	118.90
54	BA	608	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	1175	A	C4-C5-C6	-5.51	114.25	117.00
21	AA	843	U	O4'-C1'-N1	5.51	112.61	108.20
41	BS	11	ARG	NE-CZ-NH1	5.51	123.05	120.30
54	BA	1215	G	N3-C2-N2	-5.51	116.04	119.90
21	AA	572	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	1609	A	C5'-C4'-O4'	5.51	115.71	109.10
8	AI	10	ARG	NE-CZ-NH1	5.51	123.05	120.30
54	BA	776	G	O4'-C1'-N9	5.51	112.61	108.20
14	AO	62	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	AA	68	G	N3-C2-N2	-5.50	116.05	119.90
21	AA	206	C	N3-C2-O2	-5.50	118.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1564	C	N1-C2-O2	5.50	122.20	118.90
54	BA	2863	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	236	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	607	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1453	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	279	A	C4-C5-C6	-5.50	114.25	117.00
34	BL	18	ARG	NE-CZ-NH2	-5.50	117.55	120.30
54	BA	2551	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	620	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	105	C	O4'-C1'-N1	5.50	112.60	108.20
55	BB	107	G	O4'-C1'-N9	5.50	112.60	108.20
2	AC	130	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	AA	167	A	C6-C5-N7	5.50	136.15	132.30
21	AA	462	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	1104	G	O4'-C1'-N9	5.50	112.60	108.20
32	BJ	96	ARG	NE-CZ-NH1	5.50	123.05	120.30
54	BA	213	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1093	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	1538	G	O4'-C1'-N9	5.50	112.60	108.20
54	BA	1794	A	C6-C5-N7	5.50	136.15	132.30
54	BA	2237	G	C5-C6-N1	5.50	114.25	111.50
54	BA	540	C	N1-C2-O2	5.50	122.20	118.90
54	BA	1919	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	1322	C	N1-C2-O2	5.49	122.20	118.90
21	AA	1428	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	1126	A	P-O3'-C3'	5.49	126.29	119.70
54	BA	1533	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	1959	G	N1-C6-O6	-5.49	116.60	119.90
54	BA	1286	A	O4'-C1'-N9	5.49	112.59	108.20
21	AA	770	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	1137	C	N1-C2-O2	5.49	122.19	118.90
54	BA	2733	A	C4-C5-C6	-5.49	114.25	117.00
55	BB	53	A	C4-C5-C6	-5.49	114.25	117.00
21	AA	149	A	C4-C5-C6	-5.49	114.26	117.00
21	AA	311	C	N1-C2-O2	5.49	122.19	118.90
54	BA	36	G	N3-C2-N2	-5.49	116.06	119.90
54	BA	41	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	2243	U	N1-C2-N3	5.49	118.19	114.90
21	AA	313	A	C6-C5-N7	5.49	136.14	132.30
21	AA	1329	A	C6-C5-N7	5.49	136.14	132.30
54	BA	645	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1830	C	C5'-C4'-O4'	5.49	115.68	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2055	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1021	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1349	C	N3-C4-C5	5.48	124.09	121.90
54	BA	559	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	943	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1181	U	O4'-C1'-N1	5.48	112.59	108.20
10	AK	97	ARG	NE-CZ-NH1	5.48	123.04	120.30
21	AA	446	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	1244	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1247	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2342	C	O4'-C1'-N1	5.48	112.58	108.20
21	AA	87	C	N1-C2-O2	5.48	122.19	118.90
54	BA	931	U	N3-C2-O2	-5.48	118.36	122.20
54	BA	1294	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2482	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	994	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	1211	U	C1'-O4'-C4'	-5.48	105.52	109.90
54	BA	254	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	729	G	N3-C2-N2	-5.48	116.07	119.90
54	BA	2299	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2472	G	C5-C6-N1	5.48	114.24	111.50
54	BA	1628	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	434	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	933	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	236	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	326	G	N1-C6-O6	-5.47	116.62	119.90
21	AA	872	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	1181	G	C3'-C2'-C1'	5.47	105.88	101.50
54	BA	873	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	1409	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	1646	C	N1-C2-O2	5.47	122.18	118.90
54	BA	2432	A	C4-C5-C6	-5.47	114.26	117.00
54	BA	2895	G	N1-C6-O6	-5.47	116.62	119.90
21	AA	924	C	N1-C2-O2	5.47	122.18	118.90
27	BE	69	ARG	NE-CZ-NH1	5.47	123.03	120.30
21	AA	796	C	N1-C2-O2	5.47	122.18	118.90
21	AA	1124	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	209	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	421	U	O4'-C1'-N1	5.47	112.57	108.20
54	BA	435	C	N1-C2-O2	5.47	122.18	118.90
54	BA	453	A	O4'-C1'-N9	5.47	112.57	108.20
54	BA	476	G	N1-C6-O6	-5.47	116.62	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	552	U	O4'-C1'-N1	5.47	112.57	108.20
54	BA	1592	C	N1-C2-O2	5.47	122.18	118.90
21	AA	199	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	1430	A	N1-C6-N6	-5.46	115.32	118.60
54	BA	2032	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	2486	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	2801	G	O4'-C1'-N9	5.46	112.57	108.20
21	AA	1359	C	N1-C2-O2	5.46	122.18	118.90
54	BA	1015	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1080	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1433	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	48	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	759	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1893	C	N1-C2-O2	5.46	122.18	118.90
54	BA	2513	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	1302	C	N1-C2-O2	5.46	122.18	118.90
21	AA	1366	C	N3-C2-O2	-5.46	118.08	121.90
42	BT	12	ARG	NE-CZ-NH1	5.46	123.03	120.30
51	B2	33	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	2716	C	N3-C2-O2	-5.46	118.08	121.90
55	BB	36	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	842	U	C3'-C2'-C1'	5.45	105.86	101.50
21	AA	1399	C	P-O3'-C3'	5.45	126.25	119.70
28	BF	114	ARG	NE-CZ-NH1	5.45	123.03	120.30
54	BA	2187	U	O4'-C1'-N1	5.45	112.56	108.20
55	BB	43	C	N3-C4-C5	5.45	124.08	121.90
54	BA	480	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	703	U	O4'-C1'-N1	5.45	112.56	108.20
54	BA	2174	C	N1-C2-O2	5.45	122.17	118.90
21	AA	1254	A	C5-C6-N1	5.45	120.42	117.70
22	A1	15	G	N3-C2-N2	-5.45	116.09	119.90
55	BB	115	A	O4'-C1'-N9	5.45	112.56	108.20
54	BA	2135	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2349	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	809	G	C5'-C4'-O4'	5.45	115.63	109.10
54	BA	1150	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	2357	G	N1-C6-O6	-5.45	116.63	119.90
21	AA	341	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	422	A	C4-C5-C6	-5.44	114.28	117.00
25	BC	174	ARG	NE-CZ-NH1	5.44	123.02	120.30
54	BA	2178	C	N1-C2-O2	5.44	122.17	118.90
54	BA	2250	G	C5-C6-N1	5.44	114.22	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2575	C	O4'-C1'-N1	5.44	112.56	108.20
21	AA	744	C	N1-C2-O2	5.44	122.17	118.90
21	AA	840	C	N1-C2-O2	5.44	122.16	118.90
54	BA	251	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1038	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	2130	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	2765	A	O4'-C1'-N9	5.44	112.55	108.20
54	BA	2008	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	2018	G	O4'-C4'-C3'	5.44	110.45	106.10
21	AA	374	A	N1-C6-N6	-5.44	115.34	118.60
21	AA	1230	C	N1-C2-O2	5.44	122.16	118.90
54	BA	118	A	C5'-C4'-O4'	5.44	115.62	109.10
54	BA	928	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1254	A	O4'-C1'-N9	5.44	112.55	108.20
54	BA	2360	G	N3-C2-N2	-5.44	116.09	119.90
54	BA	2594	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	2758	A	C4-C5-C6	-5.44	114.28	117.00
55	BB	8	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	2116	G	N3-C2-N2	-5.44	116.09	119.90
54	BA	315	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	988	G	N3-C4-C5	-5.43	125.88	128.60
54	BA	31	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	788	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	968	C	N1-C2-O2	5.43	122.16	118.90
54	BA	1683	U	O4'-C1'-N1	5.43	112.55	108.20
54	BA	1862	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1498	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	419	C	O4'-C1'-N1	5.43	112.54	108.20
54	BA	147	C	N1-C2-O2	5.43	122.16	118.90
54	BA	184	C	O4'-C1'-N1	5.43	112.54	108.20
54	BA	1996	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	431	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	1191	A	C6-C5-N7	5.43	136.10	132.30
54	BA	729	G	N3-C4-C5	-5.43	125.89	128.60
54	BA	316	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	318	C	O4'-C1'-N1	5.43	112.54	108.20
54	BA	501	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	514	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	610	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	1843	C	N1-C2-O2	5.43	122.16	118.90
54	BA	2023	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	2092	U	N3-C2-O2	-5.43	118.40	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2837	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	972	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	1770	G	C5-C6-N1	5.42	114.21	111.50
21	AA	1016	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1191	G	O4'-C1'-N9	5.42	112.54	108.20
21	AA	987	G	N9-C4-C5	5.42	107.57	105.40
24	A3	70	C	N1-C2-O2	5.42	122.15	118.90
54	BA	870	U	C5-C6-N1	-5.42	119.99	122.70
54	BA	2439	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2874	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	1795	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	327	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1551	A	C6-C5-N7	5.42	136.09	132.30
55	BB	4	C	O4'-C1'-N1	5.42	112.53	108.20
21	AA	1037	C	N1-C2-O2	5.42	122.15	118.90
22	A1	59	U	N3-C2-O2	-5.42	118.41	122.20
54	BA	621	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1506	U	O4'-C1'-N1	5.42	112.53	108.20
21	AA	1229	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1497	U	O4'-C1'-N1	5.42	112.53	108.20
54	BA	2406	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2225	A	O4'-C1'-N9	5.41	112.53	108.20
54	BA	2237	G	O4'-C4'-C3'	5.41	110.43	106.10
54	BA	2566	A	P-O3'-C3'	5.41	126.20	119.70
21	AA	255	G	C5'-C4'-C3'	-5.41	107.34	116.00
54	BA	1194	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	2759	G	C5'-C4'-O4'	5.41	115.59	109.10
21	AA	275	G	C5-C6-N1	5.41	114.20	111.50
21	AA	339	C	N1-C2-O2	5.41	122.15	118.90
21	AA	578	C	N1-C2-O2	5.41	122.15	118.90
21	AA	1326	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	310	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	841	G	N1-C6-O6	-5.41	116.65	119.90
54	BA	1729	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1764	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1802	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	2031	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	899	C	N1-C2-O2	5.41	122.15	118.90
21	AA	1374	A	C4-C5-C6	-5.41	114.30	117.00
24	A3	45	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	395	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1437	C	N3-C2-O2	-5.41	118.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1505	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1624	U	O4'-C1'-N1	5.41	112.53	108.20
21	AA	1168	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	160	A	O4'-C1'-N9	5.41	112.53	108.20
39	BQ	10	ARG	NE-CZ-NH1	5.41	123.00	120.30
54	BA	440	C	N3-C4-N4	-5.41	114.22	118.00
54	BA	1104	C	N1-C2-O2	5.41	122.14	118.90
21	AA	308	C	N1-C2-O2	5.40	122.14	118.90
21	AA	1451	U	P-O3'-C3'	5.40	126.19	119.70
54	BA	76	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	2853	C	N1-C2-O2	5.40	122.14	118.90
54	BA	439	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1528	A	C4-C5-C6	-5.40	114.30	117.00
56	B5	164	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	864	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	650	C	N1-C2-O2	5.40	122.14	118.90
54	BA	1111	A	O4'-C1'-N9	5.40	112.52	108.20
54	BA	2628	C	N3-C4-N4	-5.40	114.22	118.00
24	A3	1	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	36	C	N1-C2-O2	5.40	122.14	118.90
54	BA	635	C	C5'-C4'-O4'	5.40	115.58	109.10
54	BA	814	C	N1-C2-O2	5.40	122.14	118.90
54	BA	1151	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1611	C	N1-C2-O2	5.40	122.14	118.90
54	BA	1637	A	C5-C6-N1	5.40	120.40	117.70
54	BA	2544	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	2675	A	O4'-C1'-N9	5.40	112.52	108.20
54	BA	2721	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	448	A	C4-C5-C6	-5.40	114.30	117.00
28	BF	70	ARG	NE-CZ-NH1	5.40	123.00	120.30
54	BA	902	C	N1-C2-O2	5.40	122.14	118.90
21	AA	152	A	C6-C5-N7	5.39	136.08	132.30
21	AA	762	U	O4'-C1'-N1	5.39	112.52	108.20
21	AA	1162	C	N3-C2-O2	-5.39	118.12	121.90
21	AA	1504	G	N1-C6-O6	-5.39	116.66	119.90
24	A3	24	C	O4'-C1'-N1	5.39	112.52	108.20
54	BA	2019	A	C4-C5-C6	-5.39	114.30	117.00
21	AA	879	C	N1-C2-O2	5.39	122.14	118.90
54	BA	21	A	C6-C5-N7	5.39	136.07	132.30
54	BA	1690	A	C6-C5-N7	5.39	136.07	132.30
27	BE	44	ARG	NE-CZ-NH1	5.39	123.00	120.30
54	BA	444	C	O4'-C1'-N1	5.39	112.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1178	C	N1-C2-O2	5.39	122.13	118.90
54	BA	2554	U	C5'-C4'-O4'	5.39	115.57	109.10
54	BA	846	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	925	A	O4'-C1'-N9	5.39	112.51	108.20
54	BA	1008	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	2074	U	O4'-C1'-N1	5.39	112.51	108.20
21	AA	86	G	O4'-C1'-N9	5.39	112.51	108.20
54	BA	1290	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	1383	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	2044	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	2690	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1086	A	C1'-O4'-C4'	-5.39	105.59	109.90
54	BA	2466	C	N3-C2-O2	-5.39	118.13	121.90
21	AA	435	A	C6-C5-N7	5.38	136.07	132.30
24	A3	41	C	O4'-C1'-N1	5.38	112.51	108.20
54	BA	221	A	C3'-C2'-C1'	-5.38	97.19	101.50
54	BA	257	C	N1-C2-O2	5.38	122.13	118.90
54	BA	1122	G	N3-C4-C5	-5.38	125.91	128.60
54	BA	1376	C	N3-C2-O2	-5.38	118.13	121.90
54	BA	2827	C	C5'-C4'-O4'	5.38	115.56	109.10
54	BA	247	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1141	U	N3-C2-O2	-5.38	118.43	122.20
54	BA	1178	C	N3-C4-C5	5.38	124.05	121.90
21	AA	51	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	60	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	2628	C	O4'-C1'-N1	5.38	112.50	108.20
21	AA	514	C	N3-C2-O2	-5.38	118.13	121.90
21	AA	869	G	N3-C4-C5	-5.38	125.91	128.60
21	AA	904	U	O4'-C1'-N1	5.38	112.50	108.20
21	AA	1195	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	589	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	615	U	N3-C2-O2	-5.38	118.44	122.20
54	BA	756	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1930	G	N3-C2-N2	-5.38	116.13	119.90
21	AA	598	U	C1'-O4'-C4'	-5.38	105.60	109.90
52	B3	29	ARG	NE-CZ-NH2	-5.38	117.61	120.30
54	BA	698	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	1001	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1261	C	O4'-C1'-N1	5.38	112.50	108.20
54	BA	1917	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	2351	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	2474	U	C5-C6-N1	-5.38	120.01	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	398	C	O4'-C1'-N1	5.38	112.50	108.20
54	BA	1847	A	O4'-C1'-N9	5.38	112.50	108.20
21	AA	530	G	N3-C4-C5	-5.37	125.91	128.60
54	BA	246	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	341	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	384	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	654	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	2279	G	N3-C4-C5	-5.37	125.91	128.60
21	AA	6	G	N3-C4-C5	-5.37	125.91	128.60
54	BA	311	A	C3'-C2'-C1'	5.37	105.80	101.50
54	BA	2089	C	C3'-C2'-C1'	5.37	105.80	101.50
21	AA	766	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	2542	A	C4-C5-C6	-5.37	114.31	117.00
4	AE	53	ARG	NE-CZ-NH1	5.37	122.98	120.30
21	AA	647	C	C3'-C2'-C1'	5.37	105.79	101.50
47	BY	52	ARG	NE-CZ-NH1	5.37	122.98	120.30
54	BA	646	U	C4'-C3'-C2'	-5.37	97.23	102.60
54	BA	1512	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2706	A	C4-C5-C6	-5.37	114.32	117.00
34	BL	69	ARG	NE-CZ-NH1	5.37	122.98	120.30
54	BA	100	U	N3-C2-O2	-5.37	118.44	122.20
54	BA	1083	U	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2340	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	195	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	1303	C	C5'-C4'-C3'	-5.37	107.42	116.00
23	A2	92	U	N3-C2-O2	-5.37	118.44	122.20
54	BA	1011	G	O4'-C1'-N9	5.37	112.49	108.20
54	BA	1587	G	C5-C6-N1	5.37	114.18	111.50
54	BA	1773	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	515	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	1470	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1277	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	1529	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	1918	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	286	C	N1-C2-O2	5.36	122.12	118.90
21	AA	1052	U	C1'-O4'-C4'	-5.36	105.61	109.90
54	BA	732	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	789	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2447	G	N1-C6-O6	-5.36	116.68	119.90
55	BB	52	A	O4'-C4'-C3'	5.36	110.39	106.10
21	AA	542	G	N1-C6-O6	-5.36	116.69	119.90
54	BA	998	C	N1-C2-O2	5.36	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	550	G	N1-C6-O6	-5.36	116.69	119.90
21	AA	1191	A	C5-C6-N6	5.36	127.99	123.70
54	BA	103	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	490	C	C6-N1-C2	-5.36	118.16	120.30
54	BA	1229	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1695	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	1733	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	1934	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	2773	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	991	U	N3-C2-O2	-5.36	118.45	122.20
21	AA	1228	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	145	C	N1-C2-O2	5.36	122.11	118.90
54	BA	444	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	1434	A	O4'-C1'-N9	5.36	112.48	108.20
54	BA	417	C	N3-C2-O2	-5.35	118.15	121.90
54	BA	433	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	1326	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	1357	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	1905	C	N1-C2-O2	5.35	122.11	118.90
21	AA	272	C	N1-C2-O2	5.35	122.11	118.90
21	AA	1052	U	N3-C2-O2	-5.35	118.46	122.20
21	AA	1193	G	N3-C2-N2	-5.35	116.16	119.90
54	BA	158	U	C5-C6-N1	-5.35	120.03	122.70
54	BA	299	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	851	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	2226	C	N3-C4-C5	5.35	124.04	121.90
54	BA	2257	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2601	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	2871	U	N3-C2-O2	-5.35	118.45	122.20
55	BB	113	C	N1-C2-O2	5.35	122.11	118.90
54	BA	901	C	N1-C2-O2	5.35	122.11	118.90
54	BA	1076	C	N1-C2-O2	5.35	122.11	118.90
54	BA	1993	U	N3-C2-O2	-5.35	118.46	122.20
54	BA	995	C	N1-C2-O2	5.35	122.11	118.90
55	BB	116	G	N3-C4-C5	-5.34	125.93	128.60
21	AA	1013	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	817	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1039	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2494	G	N3-C4-C5	-5.34	125.93	128.60
54	BA	2689	U	C5-C6-N1	-5.34	120.03	122.70
55	BB	12	C	O4'-C1'-N1	5.34	112.47	108.20
21	AA	482	A	C4-C5-C6	-5.34	114.33	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1383	C	N3-C4-N4	-5.34	114.26	118.00
54	BA	175	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	1229	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1301	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	1739	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	1780	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2503	A	C1'-O4'-C4'	-5.34	105.63	109.90
21	AA	908	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	7	G	O4'-C1'-N9	5.34	112.47	108.20
21	AA	1284	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	2463	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	778	G	N1-C6-O6	-5.33	116.70	119.90
4	AE	104	ILE	C-N-CA	5.33	135.03	121.70
21	AA	1208	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	345	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	1703	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	2243	U	C4'-C3'-C2'	-5.33	97.27	102.60
54	BA	57	C	N1-C2-O2	5.33	122.10	118.90
54	BA	604	G	C5'-C4'-O4'	5.33	115.50	109.10
54	BA	908	C	N1-C2-O2	5.33	122.10	118.90
54	BA	1877	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	1484	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	320	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	795	C	N3-C4-C5	5.33	124.03	121.90
21	AA	979	C	N1-C2-O2	5.33	122.10	118.90
21	AA	1161	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	1221	C	O4'-C1'-N1	5.33	112.46	108.20
54	BA	2449	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	2646	C	C1'-O4'-C4'	-5.33	105.64	109.90
55	BB	88	C	N1-C2-O2	5.33	122.10	118.90
21	AA	345	C	N1-C2-O2	5.33	122.10	118.90
21	AA	717	U	N3-C2-O2	-5.33	118.47	122.20
21	AA	997	U	N3-C2-O2	-5.33	118.47	122.20
54	BA	503	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	1882	U	O4'-C1'-N1	5.33	112.46	108.20
21	AA	84	U	O4'-C1'-N1	5.33	112.46	108.20
21	AA	409	U	O4'-C1'-N1	5.33	112.46	108.20
21	AA	485	U	O4'-C1'-N1	5.33	112.46	108.20
24	A3	17	C	C3'-C2'-C1'	5.33	105.76	101.50
54	BA	2902	C	N1-C2-O2	5.33	122.09	118.90
21	AA	784	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	844	G	N3-C4-C5	-5.32	125.94	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1237	C	N1-C2-O2	5.32	122.09	118.90
54	BA	385	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	1960	A	C6-C5-N7	5.32	136.03	132.30
54	BA	2614	A	C6-C5-N7	5.32	136.03	132.30
21	AA	585	G	N3-C4-C5	-5.32	125.94	128.60
54	BA	695	G	C5'-C4'-O4'	5.32	115.49	109.10
54	BA	784	G	N1-C6-O6	-5.32	116.71	119.90
24	A3	12	G	N1-C6-O6	-5.32	116.71	119.90
37	BO	7	ARG	NE-CZ-NH2	-5.32	117.64	120.30
54	BA	486	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1575	C	N3-C4-N4	-5.32	114.28	118.00
54	BA	1874	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	2851	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	182	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	960	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	738	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	1598	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	1837	C	O4'-C1'-N1	5.32	112.45	108.20
54	BA	1976	U	O4'-C1'-N1	5.32	112.45	108.20
54	BA	2238	G	C3'-C2'-C1'	5.32	105.75	101.50
54	BA	2882	A	C6-C5-N7	5.32	136.02	132.30
55	BB	101	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	750	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1510	G	N3-C2-N2	-5.32	116.18	119.90
54	BA	1559	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	2774	C	O4'-C1'-N1	5.32	112.45	108.20
55	BB	49	C	N1-C2-O2	5.32	122.09	118.90
21	AA	380	G	O4'-C1'-N9	5.31	112.45	108.20
54	BA	1832	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	1960	A	O4'-C1'-N9	5.31	112.45	108.20
54	BA	264	C	O4'-C1'-N1	5.31	112.45	108.20
54	BA	2265	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1373	A	C4-C5-C6	-5.31	114.34	117.00
21	AA	923	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	1136	G	C5-C6-N1	5.31	114.16	111.50
54	BA	2077	A	C4-C5-C6	-5.31	114.35	117.00
21	AA	1525	G	N1-C6-O6	-5.31	116.72	119.90
21	AA	1530	G	O4'-C1'-N9	5.31	112.45	108.20
54	BA	735	A	N1-C6-N6	-5.31	115.42	118.60
54	BA	1468	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1654	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	1859	U	C5'-C4'-O4'	5.31	115.47	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	553	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	802	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	1805	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	2458	G	N3-C4-C5	-5.31	125.95	128.60
21	AA	320	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	620	C	N3-C2-O2	-5.30	118.19	121.90
21	AA	1335	U	C1'-O4'-C4'	-5.30	105.66	109.90
54	BA	572	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1706	C	N3-C2-O2	-5.30	118.19	121.90
21	AA	430	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	339	U	C5'-C4'-O4'	5.30	115.46	109.10
54	BA	970	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1982	U	N3-C2-O2	-5.30	118.49	122.20
55	BB	63	C	N1-C2-O2	5.30	122.08	118.90
21	AA	791	G	C1'-O4'-C4'	-5.30	105.66	109.90
54	BA	32	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1059	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	1867	G	N3-C4-C5	-5.30	125.95	128.60
54	BA	2501	C	C6-N1-C2	-5.30	118.18	120.30
21	AA	201	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	979	C	N3-C4-C5	5.30	124.02	121.90
24	A3	16	C	N1-C2-O2	5.29	122.08	118.90
24	A3	51	U	O4'-C1'-N1	5.29	112.44	108.20
54	BA	242	G	C5-C6-N1	5.29	114.15	111.50
54	BA	1278	C	N1-C2-O2	5.29	122.08	118.90
54	BA	401	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	758	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2137	U	N3-C2-O2	-5.29	118.49	122.20
54	BA	2821	A	C4-C5-C6	-5.29	114.35	117.00
21	AA	1526	G	N1-C6-O6	-5.29	116.72	119.90
54	BA	763	G	N1-C6-O6	-5.29	116.72	119.90
54	BA	1529	G	N3-C2-N2	-5.29	116.19	119.90
54	BA	558	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2831	G	N3-C2-N2	-5.29	116.20	119.90
21	AA	791	G	N1-C6-O6	-5.29	116.73	119.90
53	B4	4	ARG	NE-CZ-NH1	5.29	122.94	120.30
54	BA	976	G	C8-N9-C4	-5.29	104.28	106.40
54	BA	1293	C	N1-C2-O2	5.29	122.07	118.90
2	AC	53	ARG	NE-CZ-NH1	5.29	122.94	120.30
21	AA	58	C	N1-C2-O2	5.29	122.07	118.90
21	AA	744	C	N3-C4-N4	-5.29	114.30	118.00
54	BA	51	G	O4'-C1'-N9	5.29	112.43	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	786	C	O4'-C1'-N1	5.29	112.43	108.20
8	AI	79	ARG	NE-CZ-NH1	5.29	122.94	120.30
54	BA	479	A	C3'-C2'-C1'	-5.29	97.27	101.50
54	BA	1341	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	2622	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2814	A	C6-C5-N7	5.29	136.00	132.30
54	BA	2858	C	C3'-C2'-C1'	5.29	105.73	101.50
21	AA	100	G	N1-C6-O6	-5.28	116.73	119.90
21	AA	493	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	580	C	N1-C2-O2	5.28	122.07	118.90
21	AA	609	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1288	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1524	C	N3-C2-O2	-5.28	118.20	121.90
54	BA	167	A	N1-C6-N6	-5.28	115.43	118.60
54	BA	215	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	1024	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	1869	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	2267	A	C4-C5-C6	-5.28	114.36	117.00
12	AM	97	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	AA	916	U	N3-C2-O2	-5.28	118.50	122.20
21	AA	1263	C	N1-C2-O2	5.28	122.07	118.90
22	A1	30	C	N3-C2-O2	-5.28	118.20	121.90
22	A1	75	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2827	C	N3-C2-O2	-5.28	118.20	121.90
21	AA	1049	U	C1'-O4'-C4'	-5.28	105.68	109.90
21	AA	1189	U	N3-C2-O2	-5.28	118.51	122.20
54	BA	1347	A	C6-C5-N7	5.28	135.99	132.30
10	AK	126	ARG	CA-C-N	5.28	128.81	117.20
54	BA	209	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	731	C	N3-C2-O2	-5.28	118.21	121.90
54	BA	1560	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	340	A	C4-C5-C6	-5.27	114.36	117.00
21	AA	1324	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	1554	U	O4'-C1'-N1	5.27	112.42	108.20
21	AA	570	G	C8-N9-C4	-5.27	104.29	106.40
24	A3	7	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	629	G	C5-C6-N1	5.27	114.14	111.50
54	BA	1303	G	N1-C6-O6	-5.27	116.74	119.90
21	AA	106	C	N1-C2-O2	5.27	122.06	118.90
29	BG	93	TYR	CB-CG-CD2	-5.27	117.84	121.00
54	BA	1549	A	C4-C5-C6	-5.27	114.37	117.00
21	AA	805	C	N1-C2-O2	5.27	122.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	893	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	1122	G	C5-C6-N1	5.27	114.13	111.50
54	BA	1698	A	C4-C5-C6	-5.27	114.37	117.00
54	BA	2151	U	C5-C6-N1	-5.27	120.07	122.70
54	BA	2674	G	N1-C6-O6	-5.27	116.74	119.90
21	AA	371	A	C4-C5-C6	-5.27	114.37	117.00
22	A1	16	C	C3'-C2'-C1'	5.27	105.71	101.50
54	BA	1602	U	O4'-C4'-C3'	5.27	110.31	106.10
21	AA	315	A	C3'-C2'-C1'	5.26	105.71	101.50
22	A1	23	A	C4-C5-C6	-5.26	114.37	117.00
22	A1	69	A	C6-C5-N7	5.26	135.99	132.30
54	BA	752	A	O4'-C1'-N9	5.26	112.41	108.20
54	BA	1045	C	N1-C2-O2	5.26	122.06	118.90
54	BA	1233	C	N3-C4-C5	5.26	124.01	121.90
54	BA	2292	U	O4'-C1'-N1	5.26	112.41	108.20
12	AM	56	ARG	NE-CZ-NH2	-5.26	117.67	120.30
54	BA	921	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	84	U	N3-C2-O2	-5.26	118.52	122.20
21	AA	234	C	N1-C2-O2	5.26	122.06	118.90
54	BA	135	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	1251	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	1469	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1530	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	2219	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	411	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	705	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	1109	C	O4'-C1'-N1	5.26	112.41	108.20
6	AG	108	ARG	C-N-CA	5.26	134.84	121.70
54	BA	114	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	453	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2073	C	N1-C2-O2	5.26	122.05	118.90
21	AA	278	G	O4'-C1'-N9	5.25	112.40	108.20
21	AA	1031	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	790	U	C5-C6-N1	-5.25	120.07	122.70
21	AA	554	A	C6-C5-N7	5.25	135.98	132.30
54	BA	634	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2339	C	C1'-O4'-C4'	-5.25	105.70	109.90
56	B5	180	PHE	CB-CG-CD2	-5.25	117.12	120.80
21	AA	755	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	1077	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	1655	A	C4-C5-C6	-5.25	114.38	117.00
55	BB	52	A	C4-C5-C6	-5.25	114.38	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	873	C	N1-C2-O2	5.25	122.05	118.90
54	BA	1612	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1800	C	N3-C2-O2	-5.25	118.23	121.90
54	BA	2364	C	N1-C2-O2	5.25	122.05	118.90
54	BA	184	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2108	A	C6-C5-N7	5.25	135.97	132.30
54	BA	2501	C	O4'-C1'-C2'	-5.25	100.55	105.80
54	BA	2561	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2576	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	2087	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	483	C	N1-C2-O2	5.24	122.05	118.90
21	AA	1231	G	C5-C6-N1	5.24	114.12	111.50
28	BF	111	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BA	574	A	C1'-O4'-C4'	-5.24	105.71	109.90
54	BA	1691	C	N1-C2-O2	5.24	122.05	118.90
13	AN	24	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BA	1586	A	O4'-C1'-N9	5.24	112.39	108.20
54	BA	1822	C	C5'-C4'-O4'	5.24	115.39	109.10
54	BA	2160	C	N1-C2-O2	5.24	122.04	118.90
54	BA	33	C	N1-C2-O2	5.24	122.04	118.90
54	BA	709	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2468	A	C6-C5-N7	5.24	135.97	132.30
46	BX	44	ARG	NE-CZ-NH2	-5.24	117.68	120.30
54	BA	2810	A	C4'-C3'-C2'	-5.24	97.36	102.60
54	BA	2214	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2238	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	2624	G	C4'-C3'-C2'	-5.24	97.36	102.60
54	BA	2634	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	1029	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	505	A	O4'-C1'-N9	5.23	112.39	108.20
54	BA	992	C	O4'-C1'-N1	5.23	112.39	108.20
54	BA	1056	G	N3-C4-C5	-5.23	125.98	128.60
54	BA	1108	U	N1-C2-N3	5.23	118.04	114.90
54	BA	1648	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2467	C	N3-C2-O2	-5.23	118.24	121.90
21	AA	495	A	C4-C5-C6	-5.23	114.38	117.00
21	AA	1296	C	N1-C2-O2	5.23	122.04	118.90
54	BA	678	C	N1-C2-O2	5.23	122.04	118.90
54	BA	1992	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	2297	A	C6-C5-N7	5.23	135.96	132.30
21	AA	90	C	N1-C2-O2	5.23	122.04	118.90
21	AA	637	C	N1-C2-O2	5.23	122.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	321	U	O4'-C1'-N1	5.23	112.38	108.20
54	BA	1140	C	O4'-C1'-N1	5.23	112.38	108.20
54	BA	1291	C	N1-C2-O2	5.23	122.04	118.90
54	BA	2230	G	O4'-C1'-N9	5.23	112.38	108.20
54	BA	2787	C	N1-C2-O2	5.23	122.04	118.90
21	AA	830	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	1413	A	O4'-C1'-N9	5.23	112.38	108.20
54	BA	1744	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	2415	G	N3-C2-N2	-5.23	116.24	119.90
21	AA	1304	G	N3-C4-C5	-5.23	125.99	128.60
21	AA	931	C	N1-C2-O2	5.22	122.03	118.90
24	A3	54	G	N1-C6-O6	-5.22	116.77	119.90
37	BO	10	ARG	NE-CZ-NH2	5.22	122.91	120.30
54	BA	154	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	694	U	N3-C2-O2	-5.22	118.54	122.20
54	BA	1065	U	N3-C2-O2	-5.22	118.54	122.20
54	BA	1076	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	1118	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1358	G	N3-C4-C5	-5.22	125.99	128.60
12	AM	112	ARG	NE-CZ-NH2	-5.22	117.69	120.30
21	AA	1502	A	C4-C5-C6	-5.22	114.39	117.00
24	A3	65	G	N3-C2-N2	-5.22	116.25	119.90
54	BA	1869	G	C5-C6-N1	5.22	114.11	111.50
54	BA	2273	A	C5'-C4'-C3'	-5.22	107.64	116.00
54	BA	2301	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	2452	C	C2-N3-C4	-5.22	117.29	119.90
21	AA	1284	C	N1-C1'-C2'	-5.22	106.26	112.00
54	BA	885	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	1068	G	N3-C2-N2	-5.22	116.25	119.90
6	AG	142	ARG	NE-CZ-NH1	5.22	122.91	120.30
21	AA	38	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	40	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	1167	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	63	A	C6-C5-N7	5.22	135.95	132.30
54	BA	1748	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2409	G	C5-C6-N1	5.22	114.11	111.50
55	BB	98	G	N3-C4-C5	-5.22	125.99	128.60
54	BA	2573	C	O4'-C1'-N1	5.22	112.37	108.20
21	AA	1494	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	558	U	N3-C2-O2	-5.22	118.55	122.20
54	BA	1313	U	C3'-C2'-C1'	5.22	105.67	101.50
21	AA	128	G	N3-C2-N2	-5.21	116.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	322	C	N1-C2-O2	5.21	122.03	118.90
22	A1	65	C	N1-C2-O2	5.21	122.03	118.90
24	A3	75	C	C1'-O4'-C4'	-5.21	105.73	109.90
54	BA	47	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	234	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	511	U	N1-C2-N3	5.21	118.03	114.90
55	BB	85	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	2810	A	C4-C5-C6	-5.21	114.39	117.00
55	BB	97	C	N1-C2-O2	5.21	122.03	118.90
56	B5	134	ARG	NE-CZ-NH1	5.21	122.91	120.30
6	AG	91	ARG	NE-CZ-NH2	-5.21	117.69	120.30
21	AA	1032	G	O4'-C1'-N9	5.21	112.37	108.20
54	BA	255	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	1499	C	N3-C2-O2	-5.21	118.25	121.90
21	AA	298	A	C3'-C2'-C1'	5.21	105.67	101.50
54	BA	16	C	N1-C2-O2	5.21	122.03	118.90
54	BA	281	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	532	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	958	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	816	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2417	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2634	A	O4'-C1'-N9	5.21	112.37	108.20
21	AA	43	C	N3-C4-N4	-5.21	114.36	118.00
21	AA	1216	A	C3'-C2'-C1'	-5.21	97.33	101.50
21	AA	1282	C	N3-C2-O2	-5.21	118.26	121.90
54	BA	1080	A	C5-C6-N1	5.21	120.30	117.70
54	BA	1594	U	O4'-C1'-N1	5.21	112.36	108.20
54	BA	2540	C	O4'-C1'-N1	5.21	112.36	108.20
54	BA	2564	A	O4'-C1'-N9	5.21	112.37	108.20
54	BA	2709	G	C5-C6-N1	5.21	114.10	111.50
54	BA	601	C	N1-C2-O2	5.21	122.02	118.90
54	BA	2281	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1674	G	C3'-C2'-C1'	5.20	105.66	101.50
21	AA	1501	C	N3-C4-N4	-5.20	114.36	118.00
54	BA	292	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1053	C	N1-C2-O2	5.20	122.02	118.90
54	BA	1515	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	1718	G	C5-C6-N1	5.20	114.10	111.50
54	BA	1842	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	2342	C	C4'-C3'-C2'	-5.20	97.40	102.60
21	AA	337	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	876	C	N1-C2-O2	5.20	122.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	306	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	779	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	1084	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1108	U	C5-C6-N1	-5.20	120.10	122.70
2	AC	178	ARG	CD-NE-CZ	5.20	130.88	123.60
21	AA	1317	C	N1-C2-O2	5.20	122.02	118.90
54	BA	2879	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	1416	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	2842	G	O4'-C1'-N9	5.20	112.36	108.20
21	AA	883	C	O4'-C1'-N1	5.19	112.36	108.20
21	AA	1345	U	N3-C2-O2	-5.19	118.56	122.20
54	BA	938	G	N1-C6-O6	-5.19	116.78	119.90
54	BA	1838	C	N3-C2-O2	-5.19	118.26	121.90
54	BA	2395	C	N3-C4-C5	5.19	123.98	121.90
21	AA	526	C	O4'-C1'-N1	5.19	112.35	108.20
21	AA	1280	A	C3'-C2'-C1'	5.19	105.66	101.50
54	BA	2824	C	O4'-C1'-N1	5.19	112.36	108.20
21	AA	793	U	N3-C2-O2	-5.19	118.57	122.20
21	AA	1197	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	893	C	N1-C2-O2	5.19	122.01	118.90
54	BA	2535	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	2610	C	N1-C2-O2	5.19	122.01	118.90
54	BA	569	U	N3-C2-O2	-5.19	118.57	122.20
54	BA	2134	A	C4-C5-C6	-5.19	114.41	117.00
21	AA	520	A	C5-C6-N6	5.19	127.85	123.70
21	AA	559	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	916	G	N7-C8-N9	5.19	115.69	113.10
54	BA	919	U	N1-C2-N3	5.19	118.01	114.90
54	BA	1352	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	1565	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	2902	C	O4'-C1'-N1	5.19	112.35	108.20
21	AA	182	A	C5'-C4'-C3'	-5.19	107.70	116.00
21	AA	567	G	N3-C4-C5	-5.19	126.01	128.60
21	AA	1172	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	1128	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	1941	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	868	U	O4'-C1'-N1	5.18	112.35	108.20
54	BA	2010	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	2730	C	O4'-C1'-N1	5.18	112.35	108.20
21	AA	65	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	93	U	N3-C2-O2	-5.18	118.57	122.20
21	AA	492	C	N1-C2-O2	5.18	122.01	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1287	A	C6-C5-N7	5.18	135.93	132.30
21	AA	1338	G	N3-C2-N2	-5.18	116.27	119.90
54	BA	113	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	277	G	O4'-C1'-N9	5.18	112.35	108.20
54	BA	376	G	O4'-C1'-N9	5.18	112.35	108.20
54	BA	1896	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	48	C	N1-C2-O2	5.18	122.01	118.90
21	AA	166	U	C1'-O4'-C4'	-5.18	105.76	109.90
21	AA	447	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	723	C	N1-C2-O2	5.18	122.01	118.90
54	BA	2889	C	N1-C2-O2	5.18	122.01	118.90
55	BB	47	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	201	C	N1-C2-O2	5.18	122.01	118.90
54	BA	1669	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2145	C	N1-C2-O2	5.18	122.01	118.90
21	AA	250	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	1145	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	441	U	C5-C6-N1	-5.18	120.11	122.70
21	AA	978	A	O4'-C1'-N9	5.18	112.34	108.20
23	A2	93	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	168	G	N3-C4-C5	-5.18	126.01	128.60
54	BA	208	C	N1-C2-O2	5.18	122.01	118.90
54	BA	974	G	N1-C6-O6	-5.18	116.80	119.90
54	BA	1255	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	1272	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	1628	G	C3'-C2'-C1'	5.18	105.64	101.50
54	BA	2375	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	865	C	N1-C2-O2	5.17	122.00	118.90
54	BA	974	G	C5-C6-N1	5.17	114.09	111.50
21	AA	303	A	C6-C5-N7	5.17	135.92	132.30
21	AA	1019	A	C4-C5-C6	-5.17	114.41	117.00
21	AA	1508	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	922	C	O4'-C1'-N1	5.17	112.34	108.20
21	AA	88	U	C5-C6-N1	-5.17	120.11	122.70
21	AA	1011	C	N1-C2-O2	5.17	122.00	118.90
22	A1	29	U	O4'-C1'-N1	5.17	112.34	108.20
26	BD	77	ARG	NE-CZ-NH1	5.17	122.89	120.30
54	BA	1991	U	O4'-C1'-N1	5.17	112.34	108.20
54	BA	2090	A	C4-C5-C6	-5.17	114.42	117.00
54	BA	2424	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	2533	U	C5-C6-N1	-5.17	120.11	122.70
21	AA	292	G	N1-C6-O6	-5.17	116.80	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	729	A	C6-C5-N7	5.17	135.92	132.30
54	BA	141	G	N3-C4-C5	-5.17	126.02	128.60
54	BA	412	A	C6-C5-N7	5.17	135.92	132.30
54	BA	766	U	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1538	G	C5-C6-N1	5.17	114.08	111.50
21	AA	43	C	N3-C2-O2	-5.17	118.28	121.90
21	AA	1064	G	N3-C4-C5	-5.17	126.02	128.60
54	BA	102	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	403	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	1330	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1872	A	O4'-C1'-N9	5.17	112.33	108.20
54	BA	2020	A	C6-C5-N7	5.17	135.92	132.30
21	AA	1002	G	N1-C6-O6	-5.17	116.80	119.90
23	A2	87	U	O4'-C1'-N1	5.17	112.33	108.20
24	A3	2	G	N3-C4-C5	-5.17	126.02	128.60
54	BA	258	G	C5-C6-N1	5.17	114.08	111.50
54	BA	708	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	764	A	C4-C5-C6	-5.17	114.42	117.00
54	BA	1837	C	N1-C2-O2	5.17	122.00	118.90
54	BA	2585	U	N3-C2-O2	-5.17	118.58	122.20
55	BB	15	A	C4-C5-C6	-5.17	114.42	117.00
21	AA	934	C	N3-C4-N4	-5.17	114.39	118.00
54	BA	979	A	C5'-C4'-O4'	5.17	115.30	109.10
54	BA	2762	C	N1-C2-O2	5.17	122.00	118.90
21	AA	205	A	C6-C5-N7	5.16	135.91	132.30
21	AA	1046	A	C4-C5-C6	-5.16	114.42	117.00
25	BC	213	ARG	NE-CZ-NH2	-5.16	117.72	120.30
54	BA	136	G	N3-C2-N2	-5.16	116.29	119.90
54	BA	696	G	C5-C6-N1	5.16	114.08	111.50
54	BA	1101	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1250	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	1658	C	N3-C2-O2	-5.16	118.29	121.90
54	BA	2490	G	C5-C6-N1	5.16	114.08	111.50
54	BA	2701	U	O4'-C1'-N1	5.16	112.33	108.20
21	AA	662	U	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1529	G	C3'-C2'-C1'	5.16	105.63	101.50
54	BA	2848	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	2886	A	C2-N3-C4	5.16	113.18	110.60
24	A3	49	C	O4'-C1'-N1	5.16	112.33	108.20
33	BK	71	ARG	NE-CZ-NH1	5.16	122.88	120.30
35	BM	18	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BA	1265	A	C6-C5-N7	5.16	135.91	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2175	C	N3-C4-C5	5.16	123.96	121.90
21	AA	101	A	C6-C5-N7	5.16	135.91	132.30
21	AA	262	A	C6-C5-N7	5.16	135.91	132.30
21	AA	704	A	C6-C5-N7	5.16	135.91	132.30
21	AA	818	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	1308	A	C6-C5-N7	5.16	135.91	132.30
54	BA	1714	U	N3-C2-O2	-5.16	118.59	122.20
55	BB	94	A	C6-C5-N7	5.16	135.91	132.30
54	BA	1924	C	N1-C2-O2	5.16	121.99	118.90
54	BA	2634	A	N1-C6-N6	-5.16	115.51	118.60
13	AN	9	ARG	NE-CZ-NH1	5.16	122.88	120.30
21	AA	1328	C	N1-C2-O2	5.16	121.99	118.90
24	A3	17	C	N1-C2-O2	5.16	121.99	118.90
54	BA	1588	G	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	2327	A	C6-C5-N7	5.16	135.91	132.30
54	BA	2698	U	O4'-C1'-N1	5.16	112.32	108.20
21	AA	934	C	C1'-O4'-C4'	-5.15	105.78	109.90
54	BA	690	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	905	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	2225	A	C3'-C2'-C1'	5.15	105.62	101.50
54	BA	2840	C	O4'-C1'-N1	5.15	112.32	108.20
21	AA	596	A	C4-C5-C6	-5.15	114.42	117.00
21	AA	793	U	N1-C2-N3	5.15	117.99	114.90
21	AA	794	A	C6-C5-N7	5.15	135.91	132.30
21	AA	1051	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	2	G	N3-C4-C5	-5.15	126.03	128.60
54	BA	673	C	N1-C2-O2	5.15	121.99	118.90
54	BA	1778	U	N3-C2-O2	-5.15	118.59	122.20
54	BA	1784	A	C6-C5-N7	5.15	135.91	132.30
54	BA	2129	C	N1-C2-O2	5.15	121.99	118.90
54	BA	2790	U	O4'-C1'-C2'	-5.15	100.65	105.80
21	AA	536	C	N1-C2-O2	5.15	121.99	118.90
22	A1	75	C	C3'-C2'-C1'	5.15	105.62	101.50
37	BO	102	ARG	NE-CZ-NH1	5.15	122.87	120.30
54	BA	210	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	313	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	2048	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	2497	A	C4-C5-C6	-5.15	114.42	117.00
21	AA	365	U	O4'-C1'-N1	5.15	112.32	108.20
21	AA	630	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	1176	A	C6-C5-N7	5.15	135.90	132.30
21	AA	1520	C	N1-C2-O2	5.15	121.99	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B0	15	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
54	BA	846	U	N3-C2-O2	-5.15	118.60	122.20
54	BA	1085	A	C4-C5-C6	-5.15	114.43	117.00
35	BM	51	ARG	NE-CZ-NH1	5.15	122.87	120.30
54	BA	650	C	O4'-C1'-N1	5.15	112.32	108.20
21	AA	14	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	230	G	N3-C2-N2	-5.14	116.30	119.90
21	AA	730	G	C5-C6-N1	5.14	114.07	111.50
54	BA	1082	U	O4'-C1'-N1	5.14	112.31	108.20
21	AA	464	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	590	U	O4'-C1'-N1	5.14	112.31	108.20
21	AA	1268	G	N1-C6-O6	-5.14	116.81	119.90
22	A1	8	U	N3-C2-O2	-5.14	118.60	122.20
54	BA	1922	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	2830	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	2837	A	N1-C6-N6	-5.14	115.52	118.60
54	BA	408	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	512	G	O4'-C1'-N9	5.14	112.31	108.20
9	AJ	68	ARG	NE-CZ-NH1	5.14	122.87	120.30
21	AA	1177	G	N3-C2-N2	-5.14	116.30	119.90
54	BA	1667	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	2220	U	C5-C6-N1	-5.14	120.13	122.70
21	AA	275	G	N1-C6-O6	-5.14	116.82	119.90
21	AA	388	G	N3-C2-N2	-5.14	116.30	119.90
54	BA	1334	G	C5'-C4'-O4'	5.14	115.27	109.10
21	AA	277	C	N3-C2-O2	-5.14	118.31	121.90
21	AA	278	G	N3-C2-N2	-5.14	116.30	119.90
21	AA	531	U	N3-C2-O2	-5.14	118.61	122.20
21	AA	1226	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	1251	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	1686	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	1023	U	O4'-C1'-N1	5.13	112.31	108.20
54	BA	2070	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	2143	C	C4'-C3'-C2'	-5.13	97.47	102.60
21	AA	507	C	N1-C2-O2	5.13	121.98	118.90
21	AA	1310	G	O4'-C1'-N9	5.13	112.31	108.20
54	BA	51	G	C5-C6-N1	5.13	114.07	111.50
11	AL	53	ARG	NE-CZ-NH2	-5.13	117.73	120.30
54	BA	736	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	1410	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2227	A	C4-C5-C6	-5.13	114.43	117.00
19	AT	59	ARG	NE-CZ-NH2	-5.13	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	826	C	N1-C2-O2	5.13	121.98	118.90
54	BA	160	A	C6-C5-N7	5.13	135.89	132.30
21	AA	49	U	C1'-O4'-C4'	-5.13	105.80	109.90
21	AA	1072	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	1112	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2164	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2431	U	O4'-C1'-N1	5.13	112.30	108.20
54	BA	2501	C	O4'-C1'-N1	5.13	112.30	108.20
54	BA	210	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	2732	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	939	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	429	U	N3-C2-O2	-5.12	118.61	122.20
21	AA	702	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	170	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	2418	A	C6-C5-N7	5.12	135.89	132.30
54	BA	2873	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	1335	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	273	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1994	C	N3-C2-O2	-5.12	118.31	121.90
54	BA	2371	G	N1-C6-O6	-5.12	116.83	119.90
55	BB	28	C	N1-C2-O2	5.12	121.97	118.90
55	BB	41	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	831	A	C6-C5-N7	5.12	135.88	132.30
54	BA	353	C	N1-C2-O2	5.12	121.97	118.90
21	AA	307	C	N1-C2-O2	5.12	121.97	118.90
21	AA	814	A	C1'-O4'-C4'	-5.12	105.81	109.90
21	AA	1093	A	C6-C5-N7	5.12	135.88	132.30
21	AA	1184	G	C5-C6-N1	5.12	114.06	111.50
54	BA	717	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1289	C	C3'-C2'-C1'	5.12	105.60	101.50
54	BA	1982	U	C5'-C4'-O4'	5.12	115.24	109.10
21	AA	1360	A	C6-C5-N7	5.12	135.88	132.30
54	BA	42	A	C5-C6-N1	5.12	120.26	117.70
21	AA	355	C	N1-C2-O2	5.12	121.97	118.90
21	AA	1115	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	657	U	O4'-C1'-N1	5.12	112.29	108.20
54	BA	735	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	990	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1408	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1942	C	N1-C2-O2	5.12	121.97	118.90
54	BA	2182	U	O4'-C1'-N1	5.12	112.29	108.20
21	AA	68	G	N1-C6-O6	-5.11	116.83	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	277	G	N3-C4-C5	-5.11	126.04	128.60
54	BA	729	G	C5-C6-N1	5.11	114.06	111.50
54	BA	999	U	C5-C6-N1	-5.11	120.14	122.70
21	AA	200	G	N1-C6-O6	-5.11	116.83	119.90
21	AA	564	C	N3-C4-N4	-5.11	114.42	118.00
54	BA	989	G	O4'-C1'-N9	5.11	112.29	108.20
54	BA	1014	A	C6-C5-N7	5.11	135.88	132.30
54	BA	1742	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	2731	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	2845	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	85	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	285	C	O4'-C1'-N1	5.11	112.29	108.20
21	AA	1283	U	N1-C2-N3	5.11	117.97	114.90
54	BA	1980	G	O4'-C4'-C3'	5.11	110.19	106.10
21	AA	644	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	8	C	N1-C2-O2	5.11	121.97	118.90
21	AA	452	A	C6-C5-N7	5.11	135.88	132.30
21	AA	479	U	N3-C2-O2	-5.11	118.62	122.20
21	AA	1059	C	N1-C2-O2	5.11	121.97	118.90
22	A1	11	C	N1-C2-O2	5.11	121.96	118.90
54	BA	1217	U	N3-C2-O2	-5.11	118.62	122.20
54	BA	1666	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	2193	G	O4'-C1'-N9	5.11	112.29	108.20
21	AA	73	C	N3-C2-O2	-5.11	118.33	121.90
21	AA	561	U	O4'-C1'-N1	5.11	112.28	108.20
24	A3	59	A	C4-C5-C6	-5.11	114.45	117.00
52	B3	7	ARG	NE-CZ-NH1	5.11	122.85	120.30
54	BA	1020	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	2001	C	O4'-C1'-N1	5.11	112.28	108.20
54	BA	2423	U	N3-C2-O2	-5.11	118.63	122.20
54	BA	2607	G	N1-C6-O6	-5.11	116.84	119.90
54	BA	2824	C	N1-C2-O2	5.11	121.96	118.90
21	AA	761	G	N3-C4-C5	-5.10	126.05	128.60
21	AA	1102	A	C4-C5-C6	-5.10	114.45	117.00
21	AA	1273	C	N1-C2-O2	5.10	121.96	118.90
24	A3	74	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	461	C	N3-C2-O2	-5.10	118.33	121.90
54	BA	555	G	C3'-C2'-C1'	5.10	105.58	101.50
54	BA	1878	G	O4'-C1'-N9	5.10	112.28	108.20
16	AQ	76	ARG	NE-CZ-NH2	-5.10	117.75	120.30
21	AA	1395	C	N1-C2-O2	5.10	121.96	118.90
33	BK	105	ARG	NE-CZ-NH2	-5.10	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	106	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	191	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	425	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	1387	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	1348	C	N3-C4-C5	5.10	123.94	121.90
54	BA	1969	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2528	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	6	G	C8-N9-C4	-5.10	104.36	106.40
54	BA	1349	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	1473	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	1532	A	C6-C5-N7	5.10	135.87	132.30
54	BA	1552	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	1578	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2140	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	2901	C	N1-C2-O2	5.10	121.96	118.90
21	AA	473	U	C1'-O4'-C4'	-5.10	105.82	109.90
21	AA	591	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	873	A	C4-C5-C6	-5.10	114.45	117.00
21	AA	1066	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1312	G	N1-C6-O6	-5.10	116.84	119.90
41	BS	99	ARG	NE-CZ-NH2	-5.10	117.75	120.30
51	B2	14	ARG	NE-CZ-NH1	5.10	122.85	120.30
54	BA	247	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	2298	A	C4-C5-C6	-5.10	114.45	117.00
21	AA	47	C	N3-C4-C5	5.10	123.94	121.90
21	AA	1412	C	N1-C2-O2	5.10	121.96	118.90
54	BA	1419	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	1648	U	C5'-C4'-C3'	-5.10	107.85	116.00
54	BA	2589	A	C6-C5-N7	5.10	135.87	132.30
21	AA	503	C	O4'-C1'-N1	5.09	112.28	108.20
21	AA	1298	U	N3-C2-O2	-5.09	118.63	122.20
21	AA	1341	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1110	G	N3-C2-N2	-5.09	116.33	119.90
54	BA	1240	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1311	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	1357	C	N3-C2-O2	-5.09	118.33	121.90
55	BB	56	G	N3-C4-C5	-5.09	126.05	128.60
21	AA	469	C	N1-C2-O2	5.09	121.96	118.90
21	AA	706	A	C6-C5-N7	5.09	135.87	132.30
21	AA	1216	A	C6-C5-N7	5.09	135.87	132.30
27	BE	88	ARG	NE-CZ-NH1	5.09	122.85	120.30
32	BJ	13	ARG	NH1-CZ-NH2	-5.09	113.80	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	177	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	192	C	N3-C4-C5	5.09	123.94	121.90
54	BA	312	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	1219	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2752	C	N3-C2-O2	-5.09	118.33	121.90
21	AA	1460	C	N1-C2-O2	5.09	121.95	118.90
54	BA	497	A	C6-C5-N7	5.09	135.86	132.30
54	BA	1536	C	N1-C2-O2	5.09	121.95	118.90
54	BA	1647	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	2530	A	C6-C5-N7	5.09	135.87	132.30
54	BA	2602	A	C6-C5-N7	5.09	135.86	132.30
21	AA	336	A	O4'-C1'-N9	5.09	112.27	108.20
21	AA	344	A	O4'-C1'-N9	5.09	112.27	108.20
21	AA	817	C	N1-C2-O2	5.09	121.95	118.90
54	BA	413	C	N3-C2-O2	-5.09	118.34	121.90
54	BA	506	G	N1-C6-O6	-5.09	116.85	119.90
54	BA	1513	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1981	A	C3'-C2'-C1'	5.09	105.57	101.50
21	AA	1297	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	510	A	C6-C5-N7	5.09	135.86	132.30
21	AA	1280	A	C4-C5-C6	-5.09	114.46	117.00
21	AA	1417	G	C8-N9-C4	-5.09	104.37	106.40
54	BA	1836	C	N1-C2-O2	5.09	121.95	118.90
54	BA	2398	U	O4'-C1'-N1	5.09	112.27	108.20
21	AA	233	C	N3-C4-N4	-5.08	114.44	118.00
54	BA	402	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	993	G	O4'-C1'-N9	5.08	112.27	108.20
54	BA	1066	U	O4'-C1'-N1	5.08	112.27	108.20
54	BA	2000	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2793	C	N3-C2-O2	-5.08	118.34	121.90
55	BB	91	C	O4'-C1'-N1	5.08	112.27	108.20
21	AA	18	C	N1-C2-O2	5.08	121.95	118.90
21	AA	771	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	617	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	910	A	C6-C5-N7	5.08	135.86	132.30
54	BA	1523	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	1568	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2331	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	113	G	C5-C6-N1	5.08	114.04	111.50
38	BP	87	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
54	BA	350	G	N3-C2-N2	-5.08	116.34	119.90
54	BA	695	G	N3-C2-N2	-5.08	116.34	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2247	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	2808	G	O4'-C1'-N9	5.08	112.26	108.20
21	AA	130	A	C6-C5-N7	5.08	135.85	132.30
21	AA	1031	C	C2-N3-C4	-5.08	117.36	119.90
21	AA	1143	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	87	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	2007	U	O4'-C1'-N1	5.08	112.26	108.20
21	AA	1389	C	O4'-C1'-N1	5.08	112.26	108.20
25	BC	216	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
54	BA	107	G	O4'-C1'-N9	5.08	112.26	108.20
54	BA	1181	U	C5-C6-N1	-5.08	120.16	122.70
54	BA	1338	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1475	G	N1-C6-O6	-5.08	116.86	119.90
54	BA	1828	G	P-O3'-C3'	5.08	125.79	119.70
54	BA	2141	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	1396	A	C6-C5-N7	5.07	135.85	132.30
54	BA	93	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	1195	G	C8-N9-C4	-5.07	104.37	106.40
54	BA	1720	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	1816	C	N1-C2-O2	5.07	121.94	118.90
21	AA	925	G	N3-C2-N2	-5.07	116.35	119.90
54	BA	983	A	C5-C6-N6	5.07	127.76	123.70
54	BA	1425	G	C5-C6-N1	5.07	114.04	111.50
54	BA	2681	C	N1-C2-O2	5.07	121.94	118.90
54	BA	2795	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1314	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1758	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	1818	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	2156	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	2209	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1069	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	2103	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	2512	C	N1-C2-O2	5.07	121.94	118.90
13	AN	59	ARG	NE-CZ-NH1	5.07	122.83	120.30
21	AA	98	A	C4-C5-C6	-5.07	114.47	117.00
21	AA	1255	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	1277	C	N1-C2-O2	5.07	121.94	118.90
22	A1	30	C	C2-N3-C4	-5.07	117.37	119.90
30	BH	97	ARG	NE-CZ-NH2	-5.07	117.77	120.30
54	BA	741	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	907	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1011	G	N1-C6-O6	-5.07	116.86	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2872	A	C4-C5-C6	-5.07	114.47	117.00
21	AA	215	C	N1-C2-O2	5.07	121.94	118.90
21	AA	844	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	606	U	C5-C6-N1	-5.07	120.17	122.70
54	BA	853	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1012	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	1068	G	C5-C6-N1	5.07	114.03	111.50
54	BA	1217	U	C5-C6-N1	-5.07	120.17	122.70
54	BA	1526	C	N1-C2-O2	5.07	121.94	118.90
54	BA	2458	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2816	G	C3'-C2'-C1'	5.07	105.55	101.50
40	BR	78	ARG	NE-CZ-NH1	5.06	122.83	120.30
55	BB	2	G	C5-C6-N1	5.06	114.03	111.50
54	BA	10	A	C4-C5-C6	-5.06	114.47	117.00
9	AJ	16	ARG	NE-CZ-NH1	5.06	122.83	120.30
21	AA	1316	G	N3-C2-N2	-5.06	116.36	119.90
54	BA	1627	G	C5-C6-N1	5.06	114.03	111.50
54	BA	1644	C	N1-C2-O2	5.06	121.94	118.90
54	BA	2813	A	O4'-C1'-N9	5.06	112.25	108.20
55	BB	116	G	C8-N9-C4	-5.06	104.38	106.40
21	AA	1086	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	1981	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	2566	A	C6-C5-N7	5.06	135.84	132.30
54	BA	2646	C	N1-C2-O2	5.06	121.93	118.90
54	BA	264	C	N3-C4-C5	5.06	123.92	121.90
54	BA	337	C	C4'-C3'-C2'	-5.06	97.54	102.60
54	BA	808	G	N1-C6-O6	-5.06	116.87	119.90
54	BA	1011	G	C5-C6-N1	5.06	114.03	111.50
54	BA	2258	C	P-O3'-C3'	5.06	125.77	119.70
54	BA	2805	C	C3'-C2'-C1'	5.06	105.55	101.50
21	AA	274	A	C6-C5-N7	5.05	135.84	132.30
21	AA	773	G	N1-C6-O6	-5.05	116.87	119.90
39	BQ	32	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
54	BA	162	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	546	U	C1'-O4'-C4'	-5.05	105.86	109.90
54	BA	1114	C	N3-C2-O2	-5.05	118.36	121.90
54	BA	1146	C	N1-C2-O2	5.05	121.93	118.90
54	BA	2018	G	C3'-C2'-C1'	5.05	105.54	101.50
54	BA	2063	C	N3-C4-N4	-5.05	114.46	118.00
21	AA	1140	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	439	A	O4'-C1'-N9	5.05	112.24	108.20
54	BA	930	G	O4'-C1'-N9	5.05	112.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1717	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	2146	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2823	A	C4-C5-C6	-5.05	114.47	117.00
4	AE	68	ARG	NE-CZ-NH1	5.05	122.83	120.30
21	AA	1262	C	O4'-C1'-N1	5.05	112.24	108.20
21	AA	1445	U	N3-C2-O2	-5.05	118.66	122.20
54	BA	642	U	N3-C2-O2	-5.05	118.66	122.20
54	BA	775	G	N3-C4-C5	-5.05	126.08	128.60
2	AC	183	TYR	CB-CG-CD2	-5.05	117.97	121.00
21	AA	492	C	N3-C4-N4	-5.05	114.47	118.00
21	AA	897	C	N3-C2-O2	-5.05	118.36	121.90
21	AA	1120	C	N3-C2-O2	-5.05	118.36	121.90
21	AA	1297	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	704	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1612	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1884	G	N3-C4-C5	-5.05	126.08	128.60
54	BA	2083	G	O4'-C1'-N9	5.05	112.24	108.20
54	BA	1057	A	O4'-C1'-N9	5.05	112.24	108.20
54	BA	2748	A	C6-C5-N7	5.05	135.83	132.30
21	AA	71	A	C4-C5-C6	-5.05	114.48	117.00
21	AA	1196	A	N1-C6-N6	-5.05	115.57	118.60
21	AA	1400	C	O4'-C1'-N1	5.05	112.24	108.20
34	BL	32	GLY	C-N-CA	5.05	134.32	121.70
54	BA	1936	A	P-O3'-C3'	5.05	125.75	119.70
54	BA	2371	G	O4'-C1'-N9	5.05	112.24	108.20
54	BA	2751	G	C5-C6-N1	5.05	114.02	111.50
54	BA	536	G	N1-C6-O6	-5.04	116.87	119.90
54	BA	2248	C	N1-C2-O2	5.04	121.93	118.90
21	AA	545	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	1525	G	O4'-C1'-N9	5.04	112.23	108.20
28	BF	70	ARG	NE-CZ-NH2	-5.04	117.78	120.30
54	BA	2588	G	O4'-C1'-N9	5.04	112.23	108.20
55	BB	31	C	C6-N1-C2	-5.04	118.28	120.30
21	AA	693	G	C3'-C2'-C1'	5.04	105.53	101.50
21	AA	844	G	C5-C6-N1	5.04	114.02	111.50
54	BA	172	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	629	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2349	G	C5-C6-N1	5.04	114.02	111.50
54	BA	2896	C	N1-C2-O2	5.04	121.92	118.90
54	BA	141	G	C4'-C3'-C2'	-5.04	97.56	102.60
54	BA	1731	G	N1-C6-O6	-5.04	116.88	119.90
2	AC	135	ARG	NE-CZ-NH1	5.04	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	45	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
21	AA	8	A	C5'-C4'-C3'	-5.04	107.94	116.00
21	AA	395	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	582	C	N3-C2-O2	-5.04	118.37	121.90
21	AA	907	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	706	A	C6-C5-N7	5.04	135.83	132.30
54	BA	774	G	C5-C6-N1	5.04	114.02	111.50
54	BA	947	A	C6-C5-N7	5.04	135.83	132.30
54	BA	2140	G	C5-C6-N1	5.04	114.02	111.50
21	AA	1365	G	C5-C6-N1	5.04	114.02	111.50
54	BA	285	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	571	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	1299	G	N7-C8-N9	5.04	115.62	113.10
54	BA	2404	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	2556	C	N1-C2-O2	5.04	121.92	118.90
21	AA	22	G	N3-C2-N2	-5.04	116.38	119.90
21	AA	63	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	766	A	O4'-C1'-N9	5.04	112.23	108.20
54	BA	339	U	N1-C2-N3	5.04	117.92	114.90
54	BA	372	G	C8-N9-C4	-5.04	104.39	106.40
54	BA	1332	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	1643	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2274	A	C6-C5-N7	5.04	135.82	132.30
55	BB	89	U	N1-C2-N3	5.04	117.92	114.90
21	AA	81	A	C5'-C4'-C3'	-5.03	107.94	116.00
21	AA	599	C	O4'-C1'-N1	5.03	112.23	108.20
21	AA	801	U	O4'-C1'-N1	5.03	112.23	108.20
54	BA	322	A	C1'-O4'-C4'	-5.03	105.87	109.90
54	BA	1290	C	C3'-C2'-C1'	5.03	105.53	101.50
54	BA	1480	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2094	A	C6-C5-N7	5.03	135.82	132.30
54	BA	2111	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	2229	U	C4'-C3'-C2'	-5.03	97.57	102.60
54	BA	685	A	O4'-C1'-N9	5.03	112.22	108.20
54	BA	1985	C	N1-C2-O2	5.03	121.92	118.90
21	AA	354	G	N3-C4-C5	-5.03	126.08	128.60
21	AA	461	A	C4-C5-C6	-5.03	114.48	117.00
24	A3	50	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	178	G	C5-C6-N1	5.03	114.02	111.50
54	BA	1093	G	C3'-C2'-C1'	5.03	105.53	101.50
54	BA	1528	A	C1'-O4'-C4'	-5.03	105.88	109.90
54	BA	1839	G	N1-C6-O6	-5.03	116.88	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2115	G	N3-C2-N2	-5.03	116.38	119.90
54	BA	2179	C	O4'-C1'-N1	5.03	112.22	108.20
4	AE	24	VAL	CA-C-N	5.03	128.26	117.20
21	AA	1447	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	839	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	1645	G	C5-C6-N1	5.03	114.01	111.50
24	A3	14	A	C4-C5-C6	-5.03	114.49	117.00
42	BT	76	ARG	NE-CZ-NH2	-5.03	117.79	120.30
54	BA	421	C	N1-C2-O2	5.03	121.92	118.90
54	BA	478	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1531	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2344	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	2364	C	O4'-C1'-N1	5.03	112.22	108.20
21	AA	241	G	C5-C6-N1	5.03	114.01	111.50
21	AA	621	A	C6-C5-N7	5.03	135.82	132.30
21	AA	1460	C	N3-C4-N4	-5.03	114.48	118.00
24	A3	69	C	N1-C2-O2	5.03	121.92	118.90
54	BA	512	G	N1-C6-O6	-5.03	116.89	119.90
54	BA	1209	U	N1-C2-N3	5.03	117.92	114.90
54	BA	2273	A	C5'-C4'-O4'	5.03	115.13	109.10
54	BA	2353	G	C5-C6-N1	5.03	114.01	111.50
21	AA	114	U	O4'-C1'-N1	5.02	112.22	108.20
27	BE	40	ARG	NE-CZ-NH1	5.02	122.81	120.30
21	AA	72	A	C6-C5-N7	5.02	135.82	132.30
21	AA	249	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	265	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	325	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2723	C	N1-C2-O2	5.02	121.91	118.90
21	AA	208	U	C3'-C2'-C1'	5.02	105.52	101.50
21	AA	144	G	C5-C6-N1	5.02	114.01	111.50
21	AA	1192	C	N1-C2-O2	5.02	121.91	118.90
21	AA	1427	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	506	G	N3-C2-N2	-5.02	116.39	119.90
54	BA	1639	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1971	U	N3-C2-O2	-5.02	118.69	122.20
55	BB	92	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	115	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1112	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	1484	U	C5-C6-N1	-5.02	120.19	122.70
54	BA	1639	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1823	G	N3-C2-N2	-5.02	116.39	119.90
54	BA	1881	C	N1-C2-O2	5.02	121.91	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	737	C	O4'-C1'-N1	5.01	112.21	108.20
54	BA	173	A	C6-C5-N7	5.01	135.81	132.30
54	BA	543	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	886	A	C6-C5-N7	5.01	135.81	132.30
54	BA	1046	A	O4'-C1'-N9	5.01	112.21	108.20
54	BA	1608	A	C4-C5-C6	-5.01	114.49	117.00
54	BA	1851	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	2164	C	N3-C4-C5	5.01	123.91	121.90
12	AM	86	ARG	NE-CZ-NH2	-5.01	117.79	120.30
21	AA	909	A	C4-C5-C6	-5.01	114.49	117.00
54	BA	80	G	C5-C6-N1	5.01	114.01	111.50
54	BA	807	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	900	A	C4-C5-C6	-5.01	114.49	117.00
54	BA	1100	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1928	A	O4'-C1'-N9	5.01	112.21	108.20
21	AA	50	A	C6-C5-N7	5.01	135.81	132.30
21	AA	380	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	679	C	O4'-C1'-N1	5.01	112.21	108.20
54	BA	1859	U	C5-C6-N1	-5.01	120.19	122.70
54	BA	2473	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	2674	G	O4'-C1'-N9	5.01	112.21	108.20
54	BA	2816	G	N3-C4-C5	-5.01	126.09	128.60
55	BB	37	C	N3-C4-C5	5.01	123.91	121.90
21	AA	1049	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	534	U	C5-C6-N1	-5.01	120.19	122.70
54	BA	840	C	N1-C2-O2	5.01	121.91	118.90
54	BA	864	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	1885	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	2286	G	N3-C4-C5	-5.01	126.09	128.60
55	BB	36	C	N1-C2-O2	5.01	121.91	118.90
21	AA	570	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	935	A	C5-N7-C8	-5.01	101.40	103.90
54	BA	344	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	2440	C	O4'-C1'-N1	5.01	112.21	108.20
3	AD	62	ARG	NE-CZ-NH1	5.01	122.80	120.30
21	AA	693	G	N3-C4-C5	-5.01	126.10	128.60
21	AA	1039	G	N1-C6-O6	-5.01	116.90	119.90
54	BA	30	G	N1-C6-O6	-5.01	116.90	119.90
54	BA	719	C	N1-C2-O2	5.01	121.90	118.90
54	BA	1339	G	N1-C6-O6	-5.01	116.90	119.90
54	BA	1583	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	1691	C	O4'-C1'-N1	5.01	112.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1848	A	C4-C5-C6	-5.01	114.50	117.00
21	AA	564	C	C5'-C4'-C3'	-5.00	107.99	116.00
21	AA	1219	A	O4'-C1'-N9	5.00	112.20	108.20
54	BA	510	C	N1-C2-O2	5.00	121.90	118.90
54	BA	2755	C	N1-C2-O2	5.00	121.90	118.90
21	AA	1385	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	725	G	C5'-C4'-O4'	5.00	115.10	109.10
54	BA	1587	G	O4'-C1'-N9	5.00	112.20	108.20
21	AA	6	G	C5'-C4'-O4'	5.00	115.10	109.10
21	AA	417	G	N3-C4-C5	-5.00	126.10	128.60
21	AA	1028	C	O4'-C1'-N1	5.00	112.20	108.20
54	BA	870	U	N1-C2-N3	5.00	117.90	114.90
54	BA	881	G	C5-C6-N1	5.00	114.00	111.50
54	BA	898	C	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1014	A	O4'-C1'-N9	5.00	112.20	108.20
54	BA	1467	U	N3-C2-O2	-5.00	118.70	122.20
54	BA	1571	A	N1-C6-N6	-5.00	115.60	118.60
54	BA	1986	C	C4'-C3'-C2'	-5.00	97.60	102.60
54	BA	2368	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (1115) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	11	C	Sidechain
22	A1	17	U	Sidechain
22	A1	22	G	Sidechain
22	A1	24	G	Sidechain
22	A1	39	G	Sidechain
22	A1	42	G	Sidechain
22	A1	43	G	Sidechain
22	A1	44	G	Sidechain
22	A1	49	G	Sidechain
22	A1	57	G	Sidechain
22	A1	6	A	Sidechain
22	A1	61	C	Sidechain
22	A1	63	G	Sidechain
22	A1	66	A	Sidechain
22	A1	70	C	Sidechain
22	A1	74	C	Sidechain
23	A2	83	U	Sidechain
23	A2	85	G	Sidechain

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Mol	Chain	Res	Type	Group
23	A2	86	U	Sidechain
23	A2	92	U	Sidechain
23	A2	93	U	Sidechain
24	A3	12	G	Sidechain
24	A3	23	G	Sidechain
24	A3	28	U	Sidechain
24	A3	34	U	Sidechain
24	A3	37	U	Sidechain
24	A3	57	C	Sidechain
24	A3	60	A	Sidechain
24	A3	68	C	Sidechain
21	AA	100	G	Sidechain
21	AA	1000	A	Sidechain
21	AA	1001	C	Sidechain
21	AA	1002	G	Sidechain
21	AA	1007	U	Sidechain
21	AA	1008	U	Sidechain
21	AA	1010	U	Sidechain
21	AA	1013	G	Sidechain
21	AA	1017	U	Sidechain
21	AA	103	U	Sidechain
21	AA	1031	C	Sidechain
21	AA	1033	G	Sidechain
21	AA	1035	A	Sidechain
21	AA	1039	G	Sidechain
21	AA	1042	A	Sidechain
21	AA	1046	A	Sidechain
21	AA	1047	G	Sidechain
21	AA	1048	G	Sidechain
21	AA	1049	U	Sidechain
21	AA	105	G	Sidechain
21	AA	1053	G	Sidechain
21	AA	1054	C	Sidechain
21	AA	1065	U	Sidechain
21	AA	1068	G	Sidechain
21	AA	1073	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	108	G	Sidechain
21	AA	1083	U	Sidechain
21	AA	1084	G	Sidechain
21	AA	1091	U	Sidechain
21	AA	1092	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1093	A	Sidechain
21	AA	1094	G	Sidechain
21	AA	1095	U	Sidechain
21	AA	1100	C	Sidechain
21	AA	1104	G	Sidechain
21	AA	1107	C	Sidechain
21	AA	111	G	Sidechain
21	AA	112	G	Sidechain
21	AA	1120	C	Sidechain
21	AA	1131	G	Sidechain
21	AA	1135	U	Sidechain
21	AA	1137	C	Sidechain
21	AA	1139	G	Sidechain
21	AA	1144	G	Sidechain
21	AA	1149	C	Sidechain
21	AA	115	G	Sidechain
21	AA	1151	A	Sidechain
21	AA	1154	G	Sidechain
21	AA	1156	G	Sidechain
21	AA	1158	C	Sidechain
21	AA	1162	C	Sidechain
21	AA	1166	G	Sidechain
21	AA	1169	A	Sidechain
21	AA	117	G	Sidechain
21	AA	1186	G	Sidechain
21	AA	1198	G	Sidechain
21	AA	1200	C	Sidechain
21	AA	1202	U	Sidechain
21	AA	1205	U	Sidechain
21	AA	1211	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1215	G	Sidechain
21	AA	1216	A	Sidechain
21	AA	1217	C	Sidechain
21	AA	1220	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1226	C	Sidechain
21	AA	1230	C	Sidechain
21	AA	1233	G	Sidechain
21	AA	1234	C	Sidechain
21	AA	124	C	Sidechain
21	AA	1241	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1242	G	Sidechain
21	AA	1243	C	Sidechain
21	AA	1244	G	Sidechain
21	AA	1247	U	Sidechain
21	AA	1257	A	Sidechain
21	AA	1261	A	Sidechain
21	AA	1266	G	Sidechain
21	AA	1267	C	Sidechain
21	AA	127	G	Sidechain
21	AA	1274	A	Sidechain
21	AA	1275	A	Sidechain
21	AA	1276	G	Sidechain
21	AA	1282	C	Sidechain
21	AA	1283	U	Sidechain
21	AA	1284	C	Sidechain
21	AA	1289	A	Sidechain
21	AA	1292	G	Sidechain
21	AA	1293	C	Sidechain
21	AA	1297	G	Sidechain
21	AA	1302	C	Sidechain
21	AA	1304	G	Sidechain
21	AA	1306	A	Sidechain
21	AA	1307	U	Sidechain
21	AA	1308	U	Sidechain
21	AA	1312	G	Sidechain
21	AA	1317	C	Sidechain
21	AA	1318	A	Sidechain
21	AA	1319	A	Sidechain
21	AA	1323	G	Sidechain
21	AA	1330	U	Sidechain
21	AA	1333	A	Sidechain
21	AA	1335	U	Sidechain
21	AA	1336	C	Sidechain
21	AA	1337	G	Sidechain
21	AA	1349	A	Sidechain
21	AA	1357	A	Sidechain
21	AA	1358	U	Sidechain
21	AA	1362	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	1379	G	Sidechain
21	AA	138	G	Sidechain
21	AA	1381	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1383	C	Sidechain
21	AA	1388	C	Sidechain
21	AA	1393	U	Sidechain
21	AA	1397	C	Sidechain
21	AA	14	U	Sidechain
21	AA	1402	C	Sidechain
21	AA	1404	C	Sidechain
21	AA	1408	A	Sidechain
21	AA	1412	C	Sidechain
21	AA	1413	A	Sidechain
21	AA	1416	G	Sidechain
21	AA	1421	G	Sidechain
21	AA	1422	G	Sidechain
21	AA	1431	A	Sidechain
21	AA	1433	A	Sidechain
21	AA	1435	G	Sidechain
21	AA	1439	G	Sidechain
21	AA	1451	U	Sidechain
21	AA	1474	U	Sidechain
21	AA	1477	U	Sidechain
21	AA	1483	A	Sidechain
21	AA	149	A	Sidechain
21	AA	1495	U	Sidechain
21	AA	150	U	Sidechain
21	AA	1500	A	Sidechain
21	AA	1504	G	Sidechain
21	AA	1509	C	Sidechain
21	AA	1510	C	Sidechain
21	AA	1512	U	Sidechain
21	AA	1514	G	Sidechain
21	AA	1515	G	Sidechain
21	AA	1517	G	Sidechain
21	AA	1519	A	Sidechain
21	AA	153	C	Sidechain
21	AA	1531	A	Sidechain
21	AA	156	C	Sidechain
21	AA	157	U	Sidechain
21	AA	159	G	Sidechain
21	AA	165	G	Sidechain
21	AA	166	U	Sidechain
21	AA	181	A	Sidechain
21	AA	185	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	186	C	Sidechain
21	AA	187	G	Sidechain
21	AA	188	C	Sidechain
21	AA	190	A	Sidechain
21	AA	191	G	Sidechain
21	AA	193	C	Sidechain
21	AA	194	C	Sidechain
21	AA	195	A	Sidechain
21	AA	196	A	Sidechain
21	AA	197	A	Sidechain
21	AA	204	G	Sidechain
21	AA	205	A	Sidechain
21	AA	207	C	Sidechain
21	AA	212	G	Sidechain
21	AA	213	G	Sidechain
21	AA	222	C	Sidechain
21	AA	229	U	Sidechain
21	AA	236	A	Sidechain
21	AA	253	A	Sidechain
21	AA	255	G	Sidechain
21	AA	273	U	Sidechain
21	AA	277	C	Sidechain
21	AA	278	G	Sidechain
21	AA	286	C	Sidechain
21	AA	287	U	Sidechain
21	AA	288	A	Sidechain
21	AA	295	C	Sidechain
21	AA	297	G	Sidechain
21	AA	309	A	Sidechain
21	AA	310	G	Sidechain
21	AA	312	C	Sidechain
21	AA	324	G	Sidechain
21	AA	325	A	Sidechain
21	AA	328	C	Sidechain
21	AA	330	C	Sidechain
21	AA	331	G	Sidechain
21	AA	339	C	Sidechain
21	AA	340	U	Sidechain
21	AA	362	G	Sidechain
21	AA	364	A	Sidechain
21	AA	366	A	Sidechain
21	AA	37	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	373	A	Sidechain
21	AA	375	U	Sidechain
21	AA	39	G	Sidechain
21	AA	391	G	Sidechain
21	AA	395	C	Sidechain
21	AA	399	G	Sidechain
21	AA	401	C	Sidechain
21	AA	409	U	Sidechain
21	AA	416	G	Sidechain
21	AA	425	G	Sidechain
21	AA	426	U	Sidechain
21	AA	430	A	Sidechain
21	AA	431	A	Sidechain
21	AA	432	A	Sidechain
21	AA	433	G	Sidechain
21	AA	435	A	Sidechain
21	AA	438	U	Sidechain
21	AA	442	G	Sidechain
21	AA	453	G	Sidechain
21	AA	454	G	Sidechain
21	AA	464	U	Sidechain
21	AA	466	A	Sidechain
21	AA	467	U	Sidechain
21	AA	468	A	Sidechain
21	AA	479	U	Sidechain
21	AA	48	C	Sidechain
21	AA	482	A	Sidechain
21	AA	487	A	Sidechain
21	AA	491	G	Sidechain
21	AA	492	C	Sidechain
21	AA	496	A	Sidechain
21	AA	503	C	Sidechain
21	AA	512	U	Sidechain
21	AA	517	G	Sidechain
21	AA	523	A	Sidechain
21	AA	524	G	Sidechain
21	AA	527	G	Sidechain
21	AA	529	G	Sidechain
21	AA	532	A	Sidechain
21	AA	534	U	Sidechain
21	AA	536	C	Sidechain
21	AA	537	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	539	A	Sidechain
21	AA	547	A	Sidechain
21	AA	552	U	Sidechain
21	AA	560	A	Sidechain
21	AA	561	U	Sidechain
21	AA	564	C	Sidechain
21	AA	569	C	Sidechain
21	AA	573	A	Sidechain
21	AA	575	G	Sidechain
21	AA	576	C	Sidechain
21	AA	58	C	Sidechain
21	AA	580	C	Sidechain
21	AA	583	A	Sidechain
21	AA	588	G	Sidechain
21	AA	589	U	Sidechain
21	AA	59	A	Sidechain
21	AA	592	G	Sidechain
21	AA	596	A	Sidechain
21	AA	598	U	Sidechain
21	AA	6	G	Sidechain
21	AA	600	A	Sidechain
21	AA	606	G	Sidechain
21	AA	607	A	Sidechain
21	AA	609	A	Sidechain
21	AA	610	U	Sidechain
21	AA	614	C	Sidechain
21	AA	618	C	Sidechain
21	AA	65	A	Sidechain
21	AA	652	U	Sidechain
21	AA	656	G	Sidechain
21	AA	66	A	Sidechain
21	AA	666	G	Sidechain
21	AA	67	C	Sidechain
21	AA	673	A	Sidechain
21	AA	674	G	Sidechain
21	AA	677	U	Sidechain
21	AA	68	G	Sidechain
21	AA	682	G	Sidechain
21	AA	683	G	Sidechain
21	AA	687	A	Sidechain
21	AA	690	G	Sidechain
21	AA	697	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	698	G	Sidechain
21	AA	699	C	Sidechain
21	AA	704	A	Sidechain
21	AA	712	A	Sidechain
21	AA	718	A	Sidechain
21	AA	722	G	Sidechain
21	AA	73	C	Sidechain
21	AA	749	A	Sidechain
21	AA	751	U	Sidechain
21	AA	752	G	Sidechain
21	AA	754	C	Sidechain
21	AA	759	A	Sidechain
21	AA	765	G	Sidechain
21	AA	77	A	Sidechain
21	AA	775	G	Sidechain
21	AA	778	G	Sidechain
21	AA	780	A	Sidechain
21	AA	789	U	Sidechain
21	AA	790	A	Sidechain
21	AA	792	A	Sidechain
21	AA	802	A	Sidechain
21	AA	812	G	Sidechain
21	AA	816	A	Sidechain
21	AA	819	A	Sidechain
21	AA	821	G	Sidechain
21	AA	822	U	Sidechain
21	AA	826	C	Sidechain
21	AA	827	U	Sidechain
21	AA	828	U	Sidechain
21	AA	83	C	Sidechain
21	AA	836	G	Sidechain
21	AA	838	G	Sidechain
21	AA	842	U	Sidechain
21	AA	844	G	Sidechain
21	AA	845	A	Sidechain
21	AA	850	U	Sidechain
21	AA	855	U	Sidechain
21	AA	856	C	Sidechain
21	AA	858	G	Sidechain
21	AA	869	G	Sidechain
21	AA	870	U	Sidechain
21	AA	871	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	873	A	Sidechain
21	AA	874	G	Sidechain
21	AA	877	G	Sidechain
21	AA	88	U	Sidechain
21	AA	881	G	Sidechain
21	AA	892	A	Sidechain
21	AA	898	G	Sidechain
21	AA	90	C	Sidechain
21	AA	91	U	Sidechain
21	AA	914	A	Sidechain
21	AA	918	A	Sidechain
21	AA	919	A	Sidechain
21	AA	922	G	Sidechain
21	AA	924	C	Sidechain
21	AA	928	G	Sidechain
21	AA	937	A	Sidechain
21	AA	94	G	Sidechain
21	AA	940	C	Sidechain
21	AA	946	A	Sidechain
21	AA	948	C	Sidechain
21	AA	949	A	Sidechain
21	AA	951	G	Sidechain
21	AA	956	U	Sidechain
21	AA	958	A	Sidechain
21	AA	961	U	Sidechain
21	AA	962	C	Sidechain
21	AA	965	U	Sidechain
21	AA	970	C	Sidechain
21	AA	974	A	Sidechain
21	AA	975	A	Sidechain
21	AA	988	G	Sidechain
21	AA	99	C	Sidechain
21	AA	991	U	Sidechain
21	AA	998	C	Sidechain
3	AD	13	ARG	Sidechain
54	BA	1	G	Sidechain
54	BA	1000	A	Sidechain
54	BA	1002	G	Sidechain
54	BA	1006	C	Sidechain
54	BA	101	A	Sidechain
54	BA	1014	A	Sidechain
54	BA	1015	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1018	U	Sidechain
54	BA	1020	A	Sidechain
54	BA	1027	A	Sidechain
54	BA	1029	A	Sidechain
54	BA	1030	C	Sidechain
54	BA	1032	A	Sidechain
54	BA	1037	G	Sidechain
54	BA	1051	G	Sidechain
54	BA	1055	G	Sidechain
54	BA	1056	G	Sidechain
54	BA	106	C	Sidechain
54	BA	1063	G	Sidechain
54	BA	1069	A	Sidechain
54	BA	1075	C	Sidechain
54	BA	108	G	Sidechain
54	BA	1087	G	Sidechain
54	BA	1098	A	Sidechain
54	BA	1110	G	Sidechain
54	BA	1111	A	Sidechain
54	BA	1121	C	Sidechain
54	BA	1130	U	Sidechain
54	BA	1143	A	Sidechain
54	BA	1159	U	Sidechain
54	BA	1164	C	Sidechain
54	BA	1165	A	Sidechain
54	BA	1168	G	Sidechain
54	BA	117	G	Sidechain
54	BA	1171	G	Sidechain
54	BA	1175	A	Sidechain
54	BA	1182	G	Sidechain
54	BA	1186	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	119	A	Sidechain
54	BA	1190	G	Sidechain
54	BA	1198	U	Sidechain
54	BA	1202	G	Sidechain
54	BA	1206	G	Sidechain
54	BA	1210	G	Sidechain
54	BA	1212	G	Sidechain
54	BA	122	G	Sidechain
54	BA	1223	G	Sidechain
54	BA	1224	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1235	G	Sidechain
54	BA	1236	G	Sidechain
54	BA	1244	A	Sidechain
54	BA	1247	A	Sidechain
54	BA	1248	G	Sidechain
54	BA	1251	C	Sidechain
54	BA	1254	A	Sidechain
54	BA	1256	G	Sidechain
54	BA	1257	C	Sidechain
54	BA	1261	C	Sidechain
54	BA	1263	U	Sidechain
54	BA	1264	A	Sidechain
54	BA	1272	A	Sidechain
54	BA	1275	A	Sidechain
54	BA	1281	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	1287	A	Sidechain
54	BA	1292	G	Sidechain
54	BA	1294	U	Sidechain
54	BA	1307	A	Sidechain
54	BA	1320	C	Sidechain
54	BA	1323	C	Sidechain
54	BA	1327	A	Sidechain
54	BA	1330	C	Sidechain
54	BA	1339	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1342	A	Sidechain
54	BA	1343	G	Sidechain
54	BA	1344	U	Sidechain
54	BA	1345	C	Sidechain
54	BA	1347	A	Sidechain
54	BA	1349	C	Sidechain
54	BA	1354	A	Sidechain
54	BA	1356	G	Sidechain
54	BA	1359	A	Sidechain
54	BA	1364	G	Sidechain
54	BA	1366	A	Sidechain
54	BA	1369	G	Sidechain
54	BA	1375	U	Sidechain
54	BA	1376	C	Sidechain
54	BA	1385	A	Sidechain
54	BA	1387	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1390	U	Sidechain
54	BA	1392	A	Sidechain
54	BA	1395	A	Sidechain
54	BA	1399	C	Sidechain
54	BA	1413	A	Sidechain
54	BA	1421	G	Sidechain
54	BA	1422	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1427	A	Sidechain
54	BA	1430	G	Sidechain
54	BA	1433	A	Sidechain
54	BA	1434	A	Sidechain
54	BA	144	A	Sidechain
54	BA	1442	U	Sidechain
54	BA	1448	G	Sidechain
54	BA	1450	G	Sidechain
54	BA	1451	C	Sidechain
54	BA	1455	G	Sidechain
54	BA	1459	G	Sidechain
54	BA	1466	U	Sidechain
54	BA	1467	U	Sidechain
54	BA	1481	U	Sidechain
54	BA	1490	A	Sidechain
54	BA	1491	G	Sidechain
54	BA	1492	G	Sidechain
54	BA	1494	A	Sidechain
54	BA	15	G	Sidechain
54	BA	1502	A	Sidechain
54	BA	1517	G	Sidechain
54	BA	1519	G	Sidechain
54	BA	1525	A	Sidechain
54	BA	1526	C	Sidechain
54	BA	1532	A	Sidechain
54	BA	1533	C	Sidechain
54	BA	1534	U	Sidechain
54	BA	1540	G	Sidechain
54	BA	1546	G	Sidechain
54	BA	1550	C	Sidechain
54	BA	1551	A	Sidechain
54	BA	1552	A	Sidechain
54	BA	1556	C	Sidechain
54	BA	1561	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1569	A	Sidechain
54	BA	157	C	Sidechain
54	BA	1570	A	Sidechain
54	BA	1580	A	Sidechain
54	BA	1584	U	Sidechain
54	BA	1587	G	Sidechain
54	BA	1588	G	Sidechain
54	BA	1595	C	Sidechain
54	BA	1601	G	Sidechain
54	BA	1602	U	Sidechain
54	BA	1607	C	Sidechain
54	BA	1611	C	Sidechain
54	BA	1615	C	Sidechain
54	BA	1616	A	Sidechain
54	BA	1619	G	Sidechain
54	BA	1622	G	Sidechain
54	BA	1627	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1638	C	Sidechain
54	BA	1642	G	Sidechain
54	BA	1645	G	Sidechain
54	BA	1649	G	Sidechain
54	BA	1655	A	Sidechain
54	BA	1661	G	Sidechain
54	BA	1665	A	Sidechain
54	BA	1666	G	Sidechain
54	BA	1667	G	Sidechain
54	BA	1669	A	Sidechain
54	BA	1671	U	Sidechain
54	BA	1673	G	Sidechain
54	BA	1674	G	Sidechain
54	BA	1678	A	Sidechain
54	BA	1679	A	Sidechain
54	BA	168	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1693	U	Sidechain
54	BA	1697	G	Sidechain
54	BA	17	G	Sidechain
54	BA	1700	A	Sidechain
54	BA	1704	C	Sidechain
54	BA	1705	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1707	G	Sidechain
54	BA	1710	G	Sidechain
54	BA	1718	G	Sidechain
54	BA	1719	G	Sidechain
54	BA	1720	U	Sidechain
54	BA	1721	G	Sidechain
54	BA	1724	G	Sidechain
54	BA	1733	G	Sidechain
54	BA	1735	A	Sidechain
54	BA	1744	A	Sidechain
54	BA	1750	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1755	A	Sidechain
54	BA	1759	A	Sidechain
54	BA	1760	C	Sidechain
54	BA	1762	A	Sidechain
54	BA	1769	U	Sidechain
54	BA	177	G	Sidechain
54	BA	1780	A	Sidechain
54	BA	1787	A	Sidechain
54	BA	1790	C	Sidechain
54	BA	1796	U	Sidechain
54	BA	18	U	Sidechain
54	BA	180	G	Sidechain
54	BA	1806	C	Sidechain
54	BA	181	A	Sidechain
54	BA	182	A	Sidechain
54	BA	1820	U	Sidechain
54	BA	1827	U	Sidechain
54	BA	1830	C	Sidechain
54	BA	1831	G	Sidechain
54	BA	1840	G	Sidechain
54	BA	1841	U	Sidechain
54	BA	1842	G	Sidechain
54	BA	1845	G	Sidechain
54	BA	1852	U	Sidechain
54	BA	1855	U	Sidechain
54	BA	1859	U	Sidechain
54	BA	1864	U	Sidechain
54	BA	1869	G	Sidechain
54	BA	1876	A	Sidechain
54	BA	188	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1880	U	Sidechain
54	BA	1883	U	Sidechain
54	BA	1884	G	Sidechain
54	BA	1887	C	Sidechain
54	BA	1899	A	Sidechain
54	BA	190	A	Sidechain
54	BA	1902	C	Sidechain
54	BA	1904	G	Sidechain
54	BA	1907	G	Sidechain
54	BA	1909	C	Sidechain
54	BA	1920	C	Sidechain
54	BA	1922	G	Sidechain
54	BA	1931	U	Sidechain
54	BA	1932	A	Sidechain
54	BA	1936	A	Sidechain
54	BA	1938	A	Sidechain
54	BA	1949	G	Sidechain
54	BA	1952	A	Sidechain
54	BA	1957	C	Sidechain
54	BA	1958	C	Sidechain
54	BA	1959	G	Sidechain
54	BA	196	A	Sidechain
54	BA	1960	A	Sidechain
54	BA	1964	G	Sidechain
54	BA	1965	C	Sidechain
54	BA	1969	A	Sidechain
54	BA	1981	A	Sidechain
54	BA	1982	U	Sidechain
54	BA	1993	U	Sidechain
54	BA	200	U	Sidechain
54	BA	2007	U	Sidechain
54	BA	2008	C	Sidechain
54	BA	2013	A	Sidechain
54	BA	2015	A	Sidechain
54	BA	2016	U	Sidechain
54	BA	2018	G	Sidechain
54	BA	2022	U	Sidechain
54	BA	2023	C	Sidechain
54	BA	2025	C	Sidechain
54	BA	2028	U	Sidechain
54	BA	2029	G	Sidechain
54	BA	2036	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2037	A	Sidechain
54	BA	204	A	Sidechain
54	BA	2040	G	Sidechain
54	BA	2042	A	Sidechain
54	BA	2049	G	Sidechain
54	BA	2052	A	Sidechain
54	BA	2055	C	Sidechain
54	BA	206	U	Sidechain
54	BA	2060	A	Sidechain
54	BA	2062	A	Sidechain
54	BA	2064	C	Sidechain
54	BA	2065	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	2070	A	Sidechain
54	BA	2077	A	Sidechain
54	BA	2078	C	Sidechain
54	BA	2083	G	Sidechain
54	BA	2086	U	Sidechain
54	BA	2087	G	Sidechain
54	BA	209	C	Sidechain
54	BA	2090	A	Sidechain
54	BA	2091	C	Sidechain
54	BA	2092	U	Sidechain
54	BA	2098	U	Sidechain
54	BA	2099	U	Sidechain
54	BA	2102	G	Sidechain
54	BA	2104	C	Sidechain
54	BA	2112	G	Sidechain
54	BA	2114	A	Sidechain
54	BA	212	G	Sidechain
54	BA	2121	G	Sidechain
54	BA	2124	G	Sidechain
54	BA	2125	G	Sidechain
54	BA	2130	U	Sidechain
54	BA	2133	G	Sidechain
54	BA	2137	U	Sidechain
54	BA	2141	G	Sidechain
54	BA	2149	U	Sidechain
54	BA	2155	U	Sidechain
54	BA	2157	G	Sidechain
54	BA	2173	A	Sidechain
54	BA	2179	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	218	A	Sidechain
54	BA	2186	G	Sidechain
54	BA	2197	U	Sidechain
54	BA	2198	A	Sidechain
54	BA	2204	G	Sidechain
54	BA	2207	C	Sidechain
54	BA	2211	A	Sidechain
54	BA	2214	C	Sidechain
54	BA	2216	G	Sidechain
54	BA	2218	G	Sidechain
54	BA	2225	A	Sidechain
54	BA	2226	C	Sidechain
54	BA	2230	G	Sidechain
54	BA	2232	C	Sidechain
54	BA	2238	G	Sidechain
54	BA	2241	A	Sidechain
54	BA	2243	U	Sidechain
54	BA	2252	G	Sidechain
54	BA	2254	C	Sidechain
54	BA	2259	U	Sidechain
54	BA	226	A	Sidechain
54	BA	2260	C	Sidechain
54	BA	2269	G	Sidechain
54	BA	2271	G	Sidechain
54	BA	2273	A	Sidechain
54	BA	2274	A	Sidechain
54	BA	2282	G	Sidechain
54	BA	2283	C	Sidechain
54	BA	2286	G	Sidechain
54	BA	229	C	Sidechain
54	BA	2295	C	Sidechain
54	BA	230	G	Sidechain
54	BA	2300	C	Sidechain
54	BA	2306	C	Sidechain
54	BA	2307	G	Sidechain
54	BA	2308	G	Sidechain
54	BA	231	A	Sidechain
54	BA	2311	A	Sidechain
54	BA	2318	G	Sidechain
54	BA	2320	U	Sidechain
54	BA	2323	G	Sidechain
54	BA	2326	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2328	A	Sidechain
54	BA	2337	G	Sidechain
54	BA	234	U	Sidechain
54	BA	2341	G	Sidechain
54	BA	2342	C	Sidechain
54	BA	2349	G	Sidechain
54	BA	235	U	Sidechain
54	BA	2357	G	Sidechain
54	BA	2365	G	Sidechain
54	BA	2366	A	Sidechain
54	BA	2367	G	Sidechain
54	BA	2368	C	Sidechain
54	BA	2369	A	Sidechain
54	BA	2372	U	Sidechain
54	BA	2375	G	Sidechain
54	BA	238	C	Sidechain
54	BA	2387	U	Sidechain
54	BA	239	C	Sidechain
54	BA	2392	A	Sidechain
54	BA	2399	G	Sidechain
54	BA	24	G	Sidechain
54	BA	2400	G	Sidechain
54	BA	2409	G	Sidechain
54	BA	2410	G	Sidechain
54	BA	2411	A	Sidechain
54	BA	2413	G	Sidechain
54	BA	2418	A	Sidechain
54	BA	2420	C	Sidechain
54	BA	2421	G	Sidechain
54	BA	2426	A	Sidechain
54	BA	2427	C	Sidechain
54	BA	2428	G	Sidechain
54	BA	2430	A	Sidechain
54	BA	2432	A	Sidechain
54	BA	2434	A	Sidechain
54	BA	2436	G	Sidechain
54	BA	2437	G	Sidechain
54	BA	2440	C	Sidechain
54	BA	2443	C	Sidechain
54	BA	2446	G	Sidechain
54	BA	2454	G	Sidechain
54	BA	2460	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2462	C	Sidechain
54	BA	2466	C	Sidechain
54	BA	2473	U	Sidechain
54	BA	2475	C	Sidechain
54	BA	2478	A	Sidechain
54	BA	2485	G	Sidechain
54	BA	249	C	Sidechain
54	BA	2491	U	Sidechain
54	BA	2492	U	Sidechain
54	BA	2496	C	Sidechain
54	BA	2497	A	Sidechain
54	BA	2507	C	Sidechain
54	BA	2517	C	Sidechain
54	BA	2521	C	Sidechain
54	BA	2529	G	Sidechain
54	BA	2530	A	Sidechain
54	BA	2534	A	Sidechain
54	BA	2538	C	Sidechain
54	BA	2539	C	Sidechain
54	BA	2544	G	Sidechain
54	BA	2545	G	Sidechain
54	BA	2549	G	Sidechain
54	BA	2550	G	Sidechain
54	BA	2551	C	Sidechain
54	BA	2552	U	Sidechain
54	BA	2559	C	Sidechain
54	BA	256	A	Sidechain
54	BA	2560	A	Sidechain
54	BA	2564	A	Sidechain
54	BA	2565	A	Sidechain
54	BA	2571	U	Sidechain
54	BA	2572	A	Sidechain
54	BA	2575	C	Sidechain
54	BA	2576	G	Sidechain
54	BA	2579	C	Sidechain
54	BA	2580	U	Sidechain
54	BA	2581	G	Sidechain
54	BA	2585	U	Sidechain
54	BA	2587	A	Sidechain
54	BA	2595	G	Sidechain
54	BA	26	G	Sidechain
54	BA	2601	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2605	U	Sidechain
54	BA	2608	G	Sidechain
54	BA	2609	U	Sidechain
54	BA	2611	C	Sidechain
54	BA	2613	U	Sidechain
54	BA	2614	A	Sidechain
54	BA	262	A	Sidechain
54	BA	2623	G	Sidechain
54	BA	2626	C	Sidechain
54	BA	2631	G	Sidechain
54	BA	2638	G	Sidechain
54	BA	264	C	Sidechain
54	BA	2654	A	Sidechain
54	BA	2658	C	Sidechain
54	BA	2659	G	Sidechain
54	BA	266	G	Sidechain
54	BA	2661	G	Sidechain
54	BA	2663	G	Sidechain
54	BA	2670	A	Sidechain
54	BA	2683	C	Sidechain
54	BA	2686	G	Sidechain
54	BA	2689	U	Sidechain
54	BA	2690	U	Sidechain
54	BA	2694	G	Sidechain
54	BA	2696	U	Sidechain
54	BA	2701	U	Sidechain
54	BA	2710	C	Sidechain
54	BA	2712	C	Sidechain
54	BA	272	A	Sidechain
54	BA	2721	A	Sidechain
54	BA	2727	A	Sidechain
54	BA	2728	U	Sidechain
54	BA	2729	G	Sidechain
54	BA	273	G	Sidechain
54	BA	2732	G	Sidechain
54	BA	274	C	Sidechain
54	BA	2740	A	Sidechain
54	BA	2745	C	Sidechain
54	BA	2747	G	Sidechain
54	BA	2751	G	Sidechain
54	BA	2755	C	Sidechain
54	BA	2756	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	276	U	Sidechain
54	BA	2777	G	Sidechain
54	BA	2779	U	Sidechain
54	BA	2781	A	Sidechain
54	BA	2783	U	Sidechain
54	BA	2785	C	Sidechain
54	BA	2786	U	Sidechain
54	BA	2799	A	Sidechain
54	BA	2808	G	Sidechain
54	BA	281	C	Sidechain
54	BA	2815	C	Sidechain
54	BA	2817	U	Sidechain
54	BA	2819	G	Sidechain
54	BA	2825	G	Sidechain
54	BA	2827	C	Sidechain
54	BA	2831	G	Sidechain
54	BA	2832	U	Sidechain
54	BA	2833	U	Sidechain
54	BA	2836	U	Sidechain
54	BA	2853	C	Sidechain
54	BA	2856	A	Sidechain
54	BA	2859	G	Sidechain
54	BA	2860	A	Sidechain
54	BA	2862	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	287	G	Sidechain
54	BA	2873	A	Sidechain
54	BA	2877	G	Sidechain
54	BA	2878	U	Sidechain
54	BA	2879	A	Sidechain
54	BA	288	U	Sidechain
54	BA	2883	A	Sidechain
54	BA	2888	C	Sidechain
54	BA	2889	C	Sidechain
54	BA	2891	U	Sidechain
54	BA	2893	A	Sidechain
54	BA	2895	G	Sidechain
54	BA	2896	C	Sidechain
54	BA	291	G	Sidechain
54	BA	297	G	Sidechain
54	BA	301	G	Sidechain
54	BA	307	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	308	G	Sidechain
54	BA	310	A	Sidechain
54	BA	311	A	Sidechain
54	BA	313	G	Sidechain
54	BA	317	G	Sidechain
54	BA	319	G	Sidechain
54	BA	322	A	Sidechain
54	BA	33	C	Sidechain
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	342	A	Sidechain
54	BA	346	A	Sidechain
54	BA	350	G	Sidechain
54	BA	359	G	Sidechain
54	BA	360	U	Sidechain
54	BA	370	G	Sidechain
54	BA	372	G	Sidechain
54	BA	375	G	Sidechain
54	BA	383	C	Sidechain
54	BA	384	A	Sidechain
54	BA	389	G	Sidechain
54	BA	395	U	Sidechain
54	BA	401	A	Sidechain
54	BA	405	U	Sidechain
54	BA	411	G	Sidechain
54	BA	412	A	Sidechain
54	BA	416	U	Sidechain
54	BA	417	C	Sidechain
54	BA	418	C	Sidechain
54	BA	419	U	Sidechain
54	BA	42	A	Sidechain
54	BA	420	C	Sidechain
54	BA	43	G	Sidechain
54	BA	436	C	Sidechain
54	BA	446	G	Sidechain
54	BA	448	U	Sidechain
54	BA	452	G	Sidechain
54	BA	454	A	Sidechain
54	BA	457	A	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	471	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	474	G	Sidechain
54	BA	476	G	Sidechain
54	BA	479	A	Sidechain
54	BA	481	G	Sidechain
54	BA	484	C	Sidechain
54	BA	485	C	Sidechain
54	BA	486	C	Sidechain
54	BA	487	C	Sidechain
54	BA	489	G	Sidechain
54	BA	49	A	Sidechain
54	BA	490	C	Sidechain
54	BA	496	G	Sidechain
54	BA	498	G	Sidechain
54	BA	50	U	Sidechain
54	BA	500	G	Sidechain
54	BA	503	A	Sidechain
54	BA	505	A	Sidechain
54	BA	506	G	Sidechain
54	BA	509	C	Sidechain
54	BA	521	U	Sidechain
54	BA	522	A	Sidechain
54	BA	528	A	Sidechain
54	BA	530	G	Sidechain
54	BA	541	A	Sidechain
54	BA	544	C	Sidechain
54	BA	546	U	Sidechain
54	BA	550	C	Sidechain
54	BA	551	G	Sidechain
54	BA	555	G	Sidechain
54	BA	556	A	Sidechain
54	BA	559	G	Sidechain
54	BA	56	A	Sidechain
54	BA	562	U	Sidechain
54	BA	572	A	Sidechain
54	BA	575	A	Sidechain
54	BA	577	G	Sidechain
54	BA	58	G	Sidechain
54	BA	582	A	Sidechain
54	BA	585	G	Sidechain
54	BA	592	A	Sidechain
54	BA	595	C	Sidechain
54	BA	597	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	615	U	Sidechain
54	BA	617	G	Sidechain
54	BA	62	U	Sidechain
54	BA	621	A	Sidechain
54	BA	63	A	Sidechain
54	BA	630	G	Sidechain
54	BA	648	G	Sidechain
54	BA	654	A	Sidechain
54	BA	666	A	Sidechain
54	BA	671	C	Sidechain
54	BA	679	C	Sidechain
54	BA	680	C	Sidechain
54	BA	682	G	Sidechain
54	BA	683	U	Sidechain
54	BA	685	A	Sidechain
54	BA	686	U	Sidechain
54	BA	689	A	Sidechain
54	BA	690	G	Sidechain
54	BA	691	C	Sidechain
54	BA	697	G	Sidechain
54	BA	70	G	Sidechain
54	BA	700	G	Sidechain
54	BA	704	G	Sidechain
54	BA	710	U	Sidechain
54	BA	711	G	Sidechain
54	BA	714	U	Sidechain
54	BA	715	A	Sidechain
54	BA	716	A	Sidechain
54	BA	718	A	Sidechain
54	BA	719	C	Sidechain
54	BA	724	U	Sidechain
54	BA	726	G	Sidechain
54	BA	730	A	Sidechain
54	BA	733	G	Sidechain
54	BA	739	A	Sidechain
54	BA	753	A	Sidechain
54	BA	754	U	Sidechain
54	BA	76	C	Sidechain
54	BA	763	G	Sidechain
54	BA	791	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	792	A	Sidechain
54	BA	795	C	Sidechain
54	BA	800	A	Sidechain
54	BA	802	A	Sidechain
54	BA	810	U	Sidechain
54	BA	811	U	Sidechain
54	BA	812	C	Sidechain
54	BA	813	U	Sidechain
54	BA	821	A	Sidechain
54	BA	828	U	Sidechain
54	BA	829	A	Sidechain
54	BA	835	C	Sidechain
54	BA	839	U	Sidechain
54	BA	84	A	Sidechain
54	BA	85	G	Sidechain
54	BA	850	U	Sidechain
54	BA	852	U	Sidechain
54	BA	853	C	Sidechain
54	BA	854	C	Sidechain
54	BA	857	G	Sidechain
54	BA	858	G	Sidechain
54	BA	866	A	Sidechain
54	BA	871	U	Sidechain
54	BA	890	C	Sidechain
54	BA	893	C	Sidechain
54	BA	894	U	Sidechain
54	BA	895	U	Sidechain
54	BA	896	A	Sidechain
54	BA	905	A	Sidechain
54	BA	907	G	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	913	U	Sidechain
54	BA	914	G	Sidechain
54	BA	915	C	Sidechain
54	BA	92	U	Sidechain
54	BA	925	A	Sidechain
54	BA	932	U	Sidechain
54	BA	934	U	Sidechain
54	BA	936	A	Sidechain
54	BA	944	C	Sidechain
54	BA	949	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	95	A	Sidechain
54	BA	956	G	Sidechain
54	BA	957	C	Sidechain
54	BA	959	A	Sidechain
54	BA	97	C	Sidechain
54	BA	979	A	Sidechain
54	BA	982	C	Sidechain
54	BA	984	A	Sidechain
54	BA	986	C	Sidechain
54	BA	989	G	Sidechain
54	BA	990	A	Sidechain
54	BA	996	A	Sidechain
54	BA	998	C	Sidechain
55	BB	107	G	Sidechain
55	BB	109	A	Sidechain
55	BB	115	A	Sidechain
55	BB	117	G	Sidechain
55	BB	12	C	Sidechain
55	BB	13	G	Sidechain
55	BB	14	U	Sidechain
55	BB	27	C	Sidechain
55	BB	29	A	Sidechain
55	BB	31	C	Sidechain
55	BB	32	U	Sidechain
55	BB	33	G	Sidechain
55	BB	39	A	Sidechain
55	BB	40	U	Sidechain
55	BB	42	C	Sidechain
55	BB	48	U	Sidechain
55	BB	5	U	Sidechain
55	BB	50	A	Sidechain
55	BB	51	G	Sidechain
55	BB	54	G	Sidechain
55	BB	57	A	Sidechain
55	BB	68	C	Sidechain
55	BB	7	G	Sidechain
55	BB	73	A	Sidechain
55	BB	86	G	Sidechain
55	BB	87	U	Sidechain
55	BB	9	G	Sidechain
55	BB	90	C	Sidechain
55	BB	96	G	Sidechain

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Mol	Chain	Res	Type	Group
36	BN	4	ARG	Sidechain
37	BO	30	ARG	Peptide
38	BP	112	ARG	Sidechain
38	BP	38	ARG	Sidechain
46	BX	18	SER	Peptide

## 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	3	0
2	AC	1625	0	1699	1	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
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	1	0
20	AU	429	0	453	0	0
21	AA	32828	0	16514	4	0
22	A1	1627	0	830	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	1	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BG	1323	0	1374	1	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	1	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	1	0
41	BS	857	0	922	0	0
42	BT	739	0	807	1	0
43	BU	780	0	834	1	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	1	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	1	0
50	B1	413	0	444	2	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	31323	8	0
55	BB	2504	0	1271	2	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	99633	25	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 (25) 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)
2:AC:4:VAL:HG22	2:AC:5:HIS:H	1.60	0.65
1:AB:103:TRP:CZ2	1:AB:104:LYS:HE3	2.47	0.49
21:AA:483:C:H2'	21:AA:484:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BA:866:A:C8	54:BA:914:G:C8	3.02	0.47
50:B1:18:HIS:CG	50:B1:19:PHE:H	2.32	0.47
43:BU:3:LYS:HE3	43:BU:84:PHE:CZ	2.50	0.46
50:B1:36:LYS:HE2	50:B1:45:HIS:CG	2.50	0.46
29:BG:85:LYS:HE3	29:BG:163:TYR:CE2	2.51	0.46
55:BB:115:A:H2'	55:BB:116:G:C8	2.52	0.45
26:BD:175:LEU:HD23	26:BD:175:LEU:H	1.80	0.45
21:AA:715:A:H2'	21:AA:716:A:C8	2.53	0.44
40:BR:10:LYS:HE3	54:BA:994:C:H4'	1.98	0.44
42:BT:33:LYS:HE2	42:BT:80:TRP:CZ3	2.53	0.44
49:B0:38:LEU:H	49:B0:41:HIS:CD2	2.36	0.44
54:BA:250:G:H2'	54:BA:251:A:C8	2.53	0.43
1:AB:84:LEU:H	1:AB:84:LEU:HD23	1.85	0.42
21:AA:1001:C:H2'	21:AA:1002:G:C8	2.54	0.42
54:BA:1960:A:H2'	54:BA:1961:C:C6	2.55	0.42
19:AT:19:HIS:CE1	21:AA:1447:A:H1'	2.55	0.41
54:BA:77:G:H2'	54:BA:78:U:C6	2.56	0.41
54:BA:2243:U:H2'	54:BA:2244:U:C6	2.56	0.41
46:BX:61:LYS:HE3	54:BA:372:G:H5'	2.01	0.41
54:BA:1241:A:C2	54:BA:1242:U:H1'	2.56	0.41
1:AB:103:TRP:CH2	1:AB:104:LYS:HE3	2.56	0.40
35:BM:38:ARG:HH22	55:BB:90:C:P	2.44	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	195 (89%)	20 (9%)	3 (1%)	14	58
2	AC	205/208 (99%)	194 (95%)	7 (3%)	4 (2%)	9	51
3	AD	203/206 (98%)	189 (93%)	10 (5%)	4 (2%)	9	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AE	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	6	45
5	AF	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	5	42
6	AG	150/152 (99%)	131 (87%)	15 (10%)	4 (3%)	6	45
7	AH	127/130 (98%)	122 (96%)	3 (2%)	2 (2%)	12	56
8	AI	126/128 (98%)	118 (94%)	5 (4%)	3 (2%)	7	47
9	AJ	98/100 (98%)	88 (90%)	6 (6%)	4 (4%)	3	35
10	AK	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	21	67
11	AL	121/124 (98%)	107 (88%)	9 (7%)	5 (4%)	3	35
12	AM	112/115 (97%)	97 (87%)	12 (11%)	3 (3%)	6	45
13	AN	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	5	42
14	AO	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	AP	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	15	60
17	AR	55/57 (96%)	53 (96%)	2 (4%)	0	100	100
18	AS	79/81 (98%)	68 (86%)	9 (11%)	2 (2%)	7	46
19	AT	84/86 (98%)	77 (92%)	6 (7%)	1 (1%)	16	61
20	AU	51/53 (96%)	35 (69%)	13 (26%)	3 (6%)	2	27
25	BC	270/273 (99%)	244 (90%)	18 (7%)	8 (3%)	5	42
26	BD	207/209 (99%)	187 (90%)	12 (6%)	8 (4%)	4	36
27	BE	199/201 (99%)	177 (89%)	11 (6%)	11 (6%)	2	29
28	BF	176/179 (98%)	145 (82%)	24 (14%)	7 (4%)	4	35
29	BG	174/177 (98%)	157 (90%)	14 (8%)	3 (2%)	11	55
30	BH	147/149 (99%)	132 (90%)	12 (8%)	3 (2%)	9	51
31	BI	139/142 (98%)	126 (91%)	10 (7%)	3 (2%)	8	49
32	BJ	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
33	BK	121/123 (98%)	108 (89%)	9 (7%)	4 (3%)	5	40
34	BL	141/144 (98%)	112 (79%)	19 (14%)	10 (7%)	1	22
35	BM	134/136 (98%)	123 (92%)	7 (5%)	4 (3%)	5	42
36	BN	119/121 (98%)	104 (87%)	14 (12%)	1 (1%)	24	69
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	21	67
38	BP	112/115 (97%)	98 (88%)	11 (10%)	3 (3%)	6	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	BQ	115/118 (98%)	106 (92%)	6 (5%)	3 (3%)	7	45
40	BR	101/103 (98%)	90 (89%)	8 (8%)	3 (3%)	5	42
41	BS	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
42	BT	92/94 (98%)	70 (76%)	15 (16%)	7 (8%)	1	20
43	BU	101/104 (97%)	85 (84%)	10 (10%)	6 (6%)	2	27
44	BV	92/94 (98%)	86 (94%)	4 (4%)	2 (2%)	8	49
45	BW	78/80 (98%)	59 (76%)	14 (18%)	5 (6%)	2	25
46	BX	75/79 (95%)	64 (85%)	6 (8%)	5 (7%)	1	24
47	BY	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
48	BZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	4	38
49	B0	54/57 (95%)	49 (91%)	3 (6%)	2 (4%)	4	38
50	B1	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	9	51
51	B2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	8	48
52	B3	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	12	56
53	B4	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	6	44
56	B5	221/234 (94%)	205 (93%)	14 (6%)	2 (1%)	21	67
All	All	5876/6008 (98%)	5257 (90%)	462 (8%)	157 (3%)	10	45

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	4	VAL
3	AD	47	LEU
4	AE	105	ILE
4	AE	149	PRO
5	AF	61	LEU
6	AG	103	ILE
9	AJ	57	VAL
9	AJ	74	VAL
19	AT	4	LYS
26	BD	2	ILE
28	BF	73	VAL
34	BL	5	THR
34	BL	29	LYS
34	BL	101	ILE
38	BP	26	GLU

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Mol	Chain	Res	Type
42	BT	40	LYS
42	BT	63	VAL
43	BU	40	LEU
49	B0	2	VAL
51	B2	44	VAL
53	B4	16	ILE
1	AB	36	LYS
4	AE	24	VAL
5	AF	6	ILE
8	AI	126	PHE
9	AJ	77	VAL
11	AL	15	VAL
12	AM	42	VAL
13	AN	99	ALA
16	AQ	69	THR
20	AU	5	VAL
20	AU	37	TYR
25	BC	64	VAL
26	BD	75	ALA
26	BD	77	ARG
26	BD	119	ALA
26	BD	138	LEU
27	BE	43	THR
27	BE	55	SER
27	BE	70	SER
27	BE	149	ILE
27	BE	166	LYS
28	BF	12	VAL
29	BG	8	VAL
34	BL	30	THR
34	BL	32	GLY
34	BL	36	LYS
35	BM	134	THR
42	BT	70	HIS
42	BT	78	SER
43	BU	12	VAL
43	BU	96	LYS
45	BW	16	GLU
45	BW	74	LYS
46	BX	5	GLN
46	BX	33	HIS
1	AB	208	ALA

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Mol	Chain	Res	Type
2	AC	195	ILE
3	AD	203	TYR
4	AE	25	LYS
6	AG	4	ARG
8	AI	39	GLY
11	AL	78	VAL
11	AL	112	ALA
20	AU	32	ARG
25	BC	89	ASN
25	BC	153	LEU
25	BC	189	ALA
27	BE	147	LEU
27	BE	165	HIS
28	BF	176	PHE
29	BG	174	LYS
31	BI	18	ASN
33	BK	71	ARG
35	BM	36	VAL
39	BQ	91	ARG
40	BR	53	PHE
40	BR	86	GLN
40	BR	87	GLN
42	BT	66	LYS
45	BW	23	LYS
46	BX	52	ALA
46	BX	75	GLU
48	BZ	30	ARG
50	B1	6	GLU
2	AC	14	VAL
3	AD	28	ASP
3	AD	187	ARG
5	AF	92	THR
7	AH	2	MET
7	AH	69	ALA
8	AI	128	LYS
11	AL	33	CYS
18	AS	23	GLU
25	BC	144	GLU
26	BD	76	GLY
27	BE	160	ALA
28	BF	103	ILE
30	BH	75	LEU

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Mol	Chain	Res	Type
30	BH	121	VAL
31	BI	93	ASN
33	BK	25	LEU
33	BK	103	VAL
35	BM	82	MET
36	BN	47	VAL
39	BQ	86	SER
42	BT	61	LEU
42	BT	81	LYS
43	BU	19	GLY
46	BX	27	ARG
49	B0	5	ASN
56	B5	13	GLU
1	AB	18	GLN
10	AK	118	ASN
13	AN	38	ASP
18	AS	79	TYR
25	BC	123	ILE
25	BC	191	LEU
26	BD	112	THR
28	BF	119	LYS
29	BG	9	VAL
31	BI	13	ALA
33	BK	16	ALA
34	BL	55	MET
34	BL	66	PHE
34	BL	69	ARG
35	BM	20	LEU
39	BQ	21	LYS
43	BU	5	ARG
43	BU	16	LYS
44	BV	26	PHE
45	BW	44	PHE
6	AG	80	GLY
6	AG	133	ALA
12	AM	23	GLY
13	AN	39	GLU
27	BE	61	ARG
27	BE	71	GLY
28	BF	126	ASN
28	BF	175	PRO
34	BL	33	ARG

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Mol	Chain	Res	Type
38	BP	112	ARG
48	BZ	9	THR
25	BC	63	ILE
30	BH	61	VAL
45	BW	26	GLY
2	AC	206	ILE
11	AL	84	GLY
38	BP	63	ILE
12	AM	6	ILE
27	BE	148	ILE
37	BO	42	PRO
44	BV	83	LYS
26	BD	73	VAL
56	B5	91	GLY
9	AJ	42	LEU
52	B3	44	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	175 (97%)	5 (3%)	51	78
2	AC	170/171 (99%)	168 (99%)	2 (1%)	78	90
3	AD	172/173 (99%)	169 (98%)	3 (2%)	68	87
4	AE	113/113 (100%)	111 (98%)	2 (2%)	66	87
5	AF	87/87 (100%)	86 (99%)	1 (1%)	80	91
6	AG	123/123 (100%)	119 (97%)	4 (3%)	45	76
7	AH	104/105 (99%)	104 (100%)	0	100	100
8	AI	105/105 (100%)	104 (99%)	1 (1%)	82	92
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	58	83
10	AK	90/90 (100%)	89 (99%)	1 (1%)	80	91
11	AL	103/104 (99%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	82 (99%)	1 (1%)	78	90
14	AO	76/77 (99%)	74 (97%)	2 (3%)	54	80
15	AP	65/65 (100%)	64 (98%)	1 (2%)	72	88
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	64 (98%)	1 (2%)	72	88
20	AU	44/44 (100%)	43 (98%)	1 (2%)	58	83
25	BC	216/217 (100%)	211 (98%)	5 (2%)	58	83
26	BD	164/164 (100%)	163 (99%)	1 (1%)	90	95
27	BE	165/165 (100%)	158 (96%)	7 (4%)	36	70
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%)	113 (99%)	1 (1%)	84	93
31	BI	109/110 (99%)	107 (98%)	2 (2%)	66	87
32	BJ	116/116 (100%)	115 (99%)	1 (1%)	84	93
33	BK	103/103 (100%)	99 (96%)	4 (4%)	39	72
34	BL	102/103 (99%)	99 (97%)	3 (3%)	50	78
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%)	83 (96%)	3 (4%)	43	74
38	BP	99/100 (99%)	98 (99%)	1 (1%)	82	92
39	BQ	89/90 (99%)	89 (100%)	0	100	100
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	91 (98%)	2 (2%)	60	83
42	BT	80/80 (100%)	78 (98%)	2 (2%)	55	81
43	BU	83/84 (99%)	81 (98%)	2 (2%)	57	82
44	BV	78/78 (100%)	76 (97%)	2 (3%)	54	80
45	BW	59/59 (100%)	58 (98%)	1 (2%)	68	87
46	BX	67/68 (98%)	65 (97%)	2 (3%)	48	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	37 (97%)	1 (3%)	54	80
52	B3	51/52 (98%)	50 (98%)	1 (2%)	63	85
53	B4	34/34 (100%)	31 (91%)	3 (9%)	12	45
56	B5	173/181 (96%)	171 (99%)	2 (1%)	78	90
All	All	4842/4870 (99%)	4756 (98%)	86 (2%)	69	87

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	71	THR
1	AB	93	HIS
1	AB	103	TRP
1	AB	156	LEU
1	AB	219	THR
2	AC	19	SER
2	AC	128	MET
3	AD	119	HIS
3	AD	162	GLU
3	AD	196	GLU
4	AE	35	LEU
4	AE	119	VAL
5	AF	42	TRP
6	AG	3	ARG
6	AG	35	LYS
6	AG	57	GLU
6	AG	138	GLU
8	AI	56	MET
9	AJ	32	THR
9	AJ	75	ASP
10	AK	76	TYR
13	AN	73	PHE
14	AO	45	HIS
14	AO	68	TYR
15	AP	1	MET
19	AT	53	MET

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Mol	Chain	Res	Type
20	AU	18	PHE
25	BC	61	TYR
25	BC	62	ARG
25	BC	191	LEU
25	BC	200	MET
25	BC	238	ASN
26	BD	151	THR
27	BE	2	GLU
27	BE	69	ARG
27	BE	70	SER
27	BE	72	SER
27	BE	73	ILE
27	BE	77	ILE
27	BE	145	ASP
28	BF	113	PHE
28	BF	143	ASP
29	BG	25	ILE
29	BG	46	ASP
29	BG	71	LEU
29	BG	146	ASP
30	BH	137	GLU
31	BI	54	ILE
31	BI	124	MET
32	BJ	14	ASP
33	BK	23	LYS
33	BK	25	LEU
33	BK	37	ASP
33	BK	105	ARG
34	BL	86	GLU
34	BL	103	ILE
34	BL	109	LYS
35	BM	12	MET
35	BM	84	LYS
36	BN	97	ILE
37	BO	12	THR
37	BO	94	ARG
37	BO	100	HIS
38	BP	30	TRP
40	BR	1	MET
41	BS	57	ASN
41	BS	68	ASP
42	BT	50	LEU

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Mol	Chain	Res	Type
42	BT	93	LEU
43	BU	5	ARG
43	BU	44	HIS
44	BV	26	PHE
44	BV	80	HIS
45	BW	14	ASP
46	BX	24	THR
46	BX	37	PHE
47	BY	55	THR
49	B0	41	HIS
50	B1	42	VAL
51	B2	2	LYS
52	B3	1	PRO
53	B4	1	MET
53	B4	16	ILE
53	B4	36	ARG
56	B5	148	ASN
56	B5	165	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	AC	184	ASN
3	AD	163	GLN
19	AT	19	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	261 (17%)	92 (6%)
22	A1	73/76 (96%)	8 (10%)	4 (5%)
23	A2	14/15 (93%)	9 (64%)	2 (14%)
24	A3	76/77 (98%)	13 (17%)	6 (7%)
54	BA	2902/2903 (99%)	451 (15%)	127 (4%)
55	BB	116/118 (98%)	15 (12%)	4 (3%)
All	All	4711/4722 (99%)	757 (16%)	235 (4%)

All (757) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	25	C
21	AA	31	G
21	AA	32	A
21	AA	39	G
21	AA	43	C
21	AA	47	C
21	AA	48	C
21	AA	50	A
21	AA	51	A
21	AA	55	A
21	AA	58	C
21	AA	59	A
21	AA	83	C
21	AA	86	G
21	AA	87	C
21	AA	95	C
21	AA	98	A
21	AA	109	A
21	AA	110	C
21	AA	111	G
21	AA	120	A
21	AA	121	U
21	AA	125	U
21	AA	163	C
21	AA	173	U
21	AA	182	A
21	AA	189	A
21	AA	191	G
21	AA	198	G
21	AA	209	U
21	AA	212	G
21	AA	213	G
21	AA	235	C
21	AA	237	G
21	AA	240	G
21	AA	244	U
21	AA	247	G
21	AA	250	A

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Mol	Chain	Res	Type
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	267	C
21	AA	289	G
21	AA	299	G
21	AA	306	A
21	AA	315	A
21	AA	316	C
21	AA	328	C
21	AA	347	G
21	AA	351	G
21	AA	352	C
21	AA	354	G
21	AA	355	C
21	AA	367	U
21	AA	369	G
21	AA	372	C
21	AA	381	C
21	AA	384	G
21	AA	389	A
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	412	A
21	AA	415	A
21	AA	424	G
21	AA	429	U
21	AA	461	A
21	AA	462	G
21	AA	466	A
21	AA	467	U
21	AA	479	U
21	AA	482	A
21	AA	483	C
21	AA	484	G
21	AA	485	U
21	AA	486	U
21	AA	505	G
21	AA	511	C
21	AA	527	G
21	AA	532	A

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Mol	Chain	Res	Type
21	AA	533	A
21	AA	547	A
21	AA	559	A
21	AA	560	A
21	AA	564	C
21	AA	565	U
21	AA	566	G
21	AA	567	G
21	AA	569	C
21	AA	570	G
21	AA	572	A
21	AA	576	C
21	AA	577	G
21	AA	598	U
21	AA	622	A
21	AA	628	G
21	AA	633	G
21	AA	641	U
21	AA	642	A
21	AA	643	C
21	AA	649	A
21	AA	665	A
21	AA	674	G
21	AA	675	A
21	AA	685	G
21	AA	688	G
21	AA	700	G
21	AA	702	A
21	AA	718	A
21	AA	719	C
21	AA	729	A
21	AA	755	G
21	AA	756	C
21	AA	767	A
21	AA	777	A
21	AA	778	G
21	AA	779	C
21	AA	787	A
21	AA	793	U
21	AA	794	A
21	AA	803	G
21	AA	812	G

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Mol	Chain	Res	Type
21	AA	817	C
21	AA	819	A
21	AA	820	U
21	AA	821	G
21	AA	828	U
21	AA	842	U
21	AA	843	U
21	AA	846	G
21	AA	867	G
21	AA	873	A
21	AA	884	U
21	AA	885	G
21	AA	889	A
21	AA	914	A
21	AA	920	U
21	AA	927	G
21	AA	934	C
21	AA	940	C
21	AA	941	G
21	AA	948	C
21	AA	961	U
21	AA	966	G
21	AA	968	A
21	AA	969	A
21	AA	974	A
21	AA	975	A
21	AA	976	G
21	AA	977	A
21	AA	978	A
21	AA	979	C
21	AA	981	U
21	AA	983	A
21	AA	984	C
21	AA	990	C
21	AA	991	U
21	AA	992	U
21	AA	993	G
21	AA	995	C
21	AA	996	A
21	AA	1004	A
21	AA	1017	U
21	AA	1025	U

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Mol	Chain	Res	Type
21	AA	1026	G
21	AA	1030	U
21	AA	1032	G
21	AA	1037	C
21	AA	1050	G
21	AA	1051	C
21	AA	1054	C
21	AA	1055	A
21	AA	1056	U
21	AA	1065	U
21	AA	1073	U
21	AA	1094	G
21	AA	1101	A
21	AA	1102	A
21	AA	1124	G
21	AA	1125	U
21	AA	1126	U
21	AA	1129	C
21	AA	1136	C
21	AA	1139	G
21	AA	1182	G
21	AA	1189	U
21	AA	1191	A
21	AA	1195	C
21	AA	1196	A
21	AA	1202	U
21	AA	1203	C
21	AA	1211	U
21	AA	1212	U
21	AA	1217	C
21	AA	1222	G
21	AA	1227	A
21	AA	1238	A
21	AA	1256	A
21	AA	1258	G
21	AA	1268	G
21	AA	1274	A
21	AA	1280	A
21	AA	1281	C
21	AA	1285	A
21	AA	1286	U
21	AA	1298	U

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Mol	Chain	Res	Type
21	AA	1299	A
21	AA	1300	G
21	AA	1302	C
21	AA	1303	C
21	AA	1308	U
21	AA	1312	G
21	AA	1317	C
21	AA	1318	A
21	AA	1319	A
21	AA	1330	U
21	AA	1331	G
21	AA	1335	U
21	AA	1336	C
21	AA	1338	G
21	AA	1340	A
21	AA	1345	U
21	AA	1358	U
21	AA	1363	A
21	AA	1364	U
21	AA	1365	G
21	AA	1374	A
21	AA	1375	A
21	AA	1378	C
21	AA	1382	C
21	AA	1384	C
21	AA	1385	G
21	AA	1394	A
21	AA	1397	C
21	AA	1398	A
21	AA	1400	C
21	AA	1401	G
21	AA	1414	U
21	AA	1446	A
21	AA	1447	A
21	AA	1448	C
21	AA	1451	U
21	AA	1452	C
21	AA	1453	G
21	AA	1469	C
21	AA	1492	A
21	AA	1493	A
21	AA	1494	G

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Mol	Chain	Res	Type
21	AA	1502	A
21	AA	1503	A
21	AA	1506	U
21	AA	1507	A
21	AA	1520	C
21	AA	1529	G
21	AA	1530	G
21	AA	1534	A
22	A1	16	C
22	A1	18	G
22	A1	20	G
22	A1	46	7MG
22	A1	47	U
22	A1	48	C
22	A1	49	G
22	A1	75	C
23	A2	81	U
23	A2	82	A
23	A2	83	U
23	A2	84	G
23	A2	86	U
23	A2	87	U
23	A2	88	U
23	A2	92	U
23	A2	93	U
24	A3	16	C
24	A3	17	C
24	A3	18	U
24	A3	21	H2U
24	A3	22	A
24	A3	26	C
24	A3	48	U
24	A3	49	C
24	A3	61	U
24	A3	62	C
24	A3	73	A
24	A3	75	C
24	A3	77	A
54	BA	15	G
54	BA	33	C
54	BA	34	U
54	BA	45	G

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Mol	Chain	Res	Type
54	BA	46	G
54	BA	50	U
54	BA	51	G
54	BA	62	U
54	BA	71	A
54	BA	72	U
54	BA	74	A
54	BA	75	G
54	BA	84	A
54	BA	85	G
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	126	A
54	BA	128	C
54	BA	142	A
54	BA	143	C
54	BA	145	C
54	BA	146	A
54	BA	147	C
54	BA	161	A
54	BA	163	C
54	BA	164	C
54	BA	196	A
54	BA	199	A
54	BA	200	U
54	BA	204	A
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	245	G
54	BA	248	G
54	BA	249	C
54	BA	272	A
54	BA	273	G
54	BA	277	G
54	BA	278	A
54	BA	281	C
54	BA	294	A

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Mol	Chain	Res	Type
54	BA	295	G
54	BA	300	A
54	BA	301	G
54	BA	302	C
54	BA	316	C
54	BA	323	C
54	BA	324	A
54	BA	330	A
54	BA	331	C
54	BA	332	A
54	BA	335	C
54	BA	346	A
54	BA	347	A
54	BA	370	G
54	BA	374	A
54	BA	377	G
54	BA	383	C
54	BA	386	G
54	BA	387	U
54	BA	388	G
54	BA	404	A
54	BA	405	U
54	BA	411	G
54	BA	428	A
54	BA	435	C
54	BA	451	U
54	BA	453	A
54	BA	454	A
54	BA	457	A
54	BA	473	G
54	BA	478	A
54	BA	479	A
54	BA	484	C
54	BA	491	G
54	BA	504	A
54	BA	505	A
54	BA	508	A
54	BA	510	C
54	BA	512	G
54	BA	527	C
54	BA	528	A
54	BA	531	C

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Mol	Chain	Res	Type
54	BA	546	U
54	BA	547	A
54	BA	548	G
54	BA	549	G
54	BA	556	A
54	BA	562	U
54	BA	573	U
54	BA	575	A
54	BA	586	A
54	BA	603	A
54	BA	613	A
54	BA	614	A
54	BA	615	U
54	BA	616	A
54	BA	617	G
54	BA	627	A
54	BA	631	A
54	BA	632	A
54	BA	637	A
54	BA	644	A
54	BA	645	C
54	BA	646	U
54	BA	647	G
54	BA	653	U
54	BA	654	A
54	BA	671	C
54	BA	672	C
54	BA	686	U
54	BA	716	A
54	BA	719	C
54	BA	724	U
54	BA	727	A
54	BA	728	G
54	BA	730	A
54	BA	745	G
54	BA	747	U
54	BA	748	G
54	BA	750	A
54	BA	751	A
54	BA	764	A
54	BA	775	G
54	BA	776	G

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Mol	Chain	Res	Type
54	BA	782	A
54	BA	784	G
54	BA	785	G
54	BA	789	A
54	BA	791	C
54	BA	800	A
54	BA	805	G
54	BA	827	U
54	BA	830	G
54	BA	846	U
54	BA	860	U
54	BA	866	A
54	BA	867	C
54	BA	888	C
54	BA	889	C
54	BA	890	C
54	BA	893	C
54	BA	897	C
54	BA	905	A
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	934	U
54	BA	943	A
54	BA	945	A
54	BA	958	U
54	BA	961	C
54	BA	974	G
54	BA	982	C
54	BA	983	A
54	BA	987	C
54	BA	990	A
54	BA	996	A
54	BA	1005	C
54	BA	1006	C
54	BA	1011	G
54	BA	1012	U
54	BA	1013	C
54	BA	1024	G
54	BA	1025	G
54	BA	1026	G
54	BA	1057	A

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Mol	Chain	Res	Type
54	BA	1058	U
54	BA	1070	A
54	BA	1071	G
54	BA	1073	A
54	BA	1076	C
54	BA	1079	C
54	BA	1088	A
54	BA	1089	A
54	BA	1094	U
54	BA	1095	A
54	BA	1112	G
54	BA	1127	A
54	BA	1128	G
54	BA	1130	U
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1139	G
54	BA	1142	A
54	BA	1155	A
54	BA	1156	A
54	BA	1186	G
54	BA	1204	A
54	BA	1206	G
54	BA	1211	C
54	BA	1237	A
54	BA	1238	G
54	BA	1242	U
54	BA	1243	C
54	BA	1251	C
54	BA	1252	G
54	BA	1253	A
54	BA	1255	U
54	BA	1256	G
54	BA	1263	U
54	BA	1271	G
54	BA	1273	U
54	BA	1274	A
54	BA	1275	A
54	BA	1276	A
54	BA	1287	A
54	BA	1288	G

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Mol	Chain	Res	Type
54	BA	1290	C
54	BA	1292	G
54	BA	1301	A
54	BA	1304	A
54	BA	1311	G
54	BA	1312	U
54	BA	1314	C
54	BA	1324	G
54	BA	1325	U
54	BA	1332	G
54	BA	1334	G
54	BA	1341	G
54	BA	1360	G
54	BA	1365	A
54	BA	1368	G
54	BA	1379	U
54	BA	1383	A
54	BA	1385	A
54	BA	1388	G
54	BA	1416	G
54	BA	1427	A
54	BA	1428	C
54	BA	1435	G
54	BA	1440	U
54	BA	1452	G
54	BA	1454	C
54	BA	1455	G
54	BA	1458	U
54	BA	1460	U
54	BA	1475	G
54	BA	1482	G
54	BA	1486	U
54	BA	1493	C
54	BA	1508	A
54	BA	1523	U
54	BA	1536	C
54	BA	1538	G
54	BA	1560	G
54	BA	1569	A
54	BA	1585	C
54	BA	1598	A
54	BA	1607	C

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Mol	Chain	Res	Type
54	BA	1608	A
54	BA	1614	A
54	BA	1616	A
54	BA	1618	A
54	BA	1619	G
54	BA	1622	G
54	BA	1629	U
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1665	A
54	BA	1670	C
54	BA	1674	G
54	BA	1696	G
54	BA	1707	G
54	BA	1711	A
54	BA	1712	U
54	BA	1717	A
54	BA	1730	C
54	BA	1738	G
54	BA	1739	A
54	BA	1764	C
54	BA	1773	A
54	BA	1775	U
54	BA	1782	U
54	BA	1784	A
54	BA	1790	C
54	BA	1800	C
54	BA	1801	A
54	BA	1808	A
54	BA	1811	G
54	BA	1815	A
54	BA	1817	G
54	BA	1821	A
54	BA	1829	A
54	BA	1847	A
54	BA	1870	C
54	BA	1871	A
54	BA	1903	G
54	BA	1906	G
54	BA	1913	A
54	BA	1914	C

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Mol	Chain	Res	Type
54	BA	1919	A
54	BA	1937	A
54	BA	1938	A
54	BA	1939	U
54	BA	1940	U
54	BA	1955	U
54	BA	1963	U
54	BA	1965	C
54	BA	1969	A
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	2006	C
54	BA	2021	C
54	BA	2023	C
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2033	A
54	BA	2034	U
54	BA	2035	G
54	BA	2043	C
54	BA	2049	G
54	BA	2052	A
54	BA	2055	C
54	BA	2060	A
54	BA	2061	G
54	BA	2076	U
54	BA	2077	A
54	BA	2092	U
54	BA	2112	G
54	BA	2113	U
54	BA	2117	A
54	BA	2119	A
54	BA	2133	G
54	BA	2135	A
54	BA	2155	U
54	BA	2156	G
54	BA	2157	G

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Mol	Chain	Res	Type
54	BA	2159	G
54	BA	2160	C
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2194	U
54	BA	2198	A
54	BA	2203	U
54	BA	2208	C
54	BA	2211	A
54	BA	2212	A
54	BA	2213	U
54	BA	2225	A
54	BA	2232	C
54	BA	2233	U
54	BA	2238	G
54	BA	2239	G
54	BA	2245	U
54	BA	2250	G
54	BA	2259	U
54	BA	2262	U
54	BA	2283	C
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2310	C
54	BA	2320	U
54	BA	2325	G
54	BA	2333	A
54	BA	2334	U
54	BA	2335	A
54	BA	2339	C
54	BA	2345	G
54	BA	2346	A
54	BA	2347	C
54	BA	2353	G
54	BA	2383	G
54	BA	2385	C
54	BA	2403	C
54	BA	2407	A
54	BA	2418	A
54	BA	2422	C

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Mol	Chain	Res	Type
54	BA	2423	U
54	BA	2424	C
54	BA	2425	A
54	BA	2426	A
54	BA	2427	C
54	BA	2428	G
54	BA	2430	A
54	BA	2439	A
54	BA	2441	U
54	BA	2446	G
54	BA	2447	G
54	BA	2448	A
54	BA	2449	U
54	BA	2476	A
54	BA	2491	U
54	BA	2492	U
54	BA	2494	G
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2505	G
54	BA	2507	C
54	BA	2533	U
54	BA	2539	C
54	BA	2542	A
54	BA	2543	G
54	BA	2554	U
54	BA	2566	A
54	BA	2567	G
54	BA	2573	C
54	BA	2575	C
54	BA	2576	G
54	BA	2585	U
54	BA	2609	U
54	BA	2610	C
54	BA	2614	A
54	BA	2629	U
54	BA	2637	U
54	BA	2640	G
54	BA	2645	G
54	BA	2646	C
54	BA	2656	U

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Mol	Chain	Res	Type
54	BA	2660	A
54	BA	2661	G
54	BA	2665	A
54	BA	2668	G
54	BA	2669	G
54	BA	2684	U
54	BA	2689	U
54	BA	2690	U
54	BA	2712	C
54	BA	2726	A
54	BA	2746	U
54	BA	2756	U
54	BA	2765	A
54	BA	2766	A
54	BA	2778	A
54	BA	2797	U
54	BA	2799	A
54	BA	2800	A
54	BA	2817	U
54	BA	2823	A
54	BA	2850	A
54	BA	2858	C
54	BA	2859	G
54	BA	2868	A
54	BA	2884	U
54	BA	2886	A
54	BA	2895	G
55	BB	6	G
55	BB	7	G
55	BB	14	U
55	BB	15	A
55	BB	25	U
55	BB	36	C
55	BB	42	C
55	BB	45	A
55	BB	48	U
55	BB	51	G
55	BB	67	G
55	BB	86	G
55	BB	88	C
55	BB	90	C
55	BB	109	A

All (235) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	13	U
21	AA	30	U
21	AA	54	C
21	AA	64	G
21	AA	85	U
21	AA	110	C
21	AA	120	A
21	AA	130	A
21	AA	208	U
21	AA	236	A
21	AA	250	A
21	AA	251	G
21	AA	266	G
21	AA	315	A
21	AA	345	C
21	AA	354	G
21	AA	369	G
21	AA	420	U
21	AA	429	U
21	AA	461	A
21	AA	465	A
21	AA	466	A
21	AA	478	A
21	AA	482	A
21	AA	485	U
21	AA	505	G
21	AA	518	C
21	AA	532	A
21	AA	570	G
21	AA	575	G
21	AA	576	C
21	AA	611	C
21	AA	641	U
21	AA	642	A
21	AA	674	G
21	AA	701	U
21	AA	718	A
21	AA	719	C
21	AA	725	G

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Mol	Chain	Res	Type
21	AA	751	U
21	AA	755	G
21	AA	778	G
21	AA	820	U
21	AA	872	A
21	AA	884	U
21	AA	907	A
21	AA	919	A
21	AA	934	C
21	AA	960	U
21	AA	974	A
21	AA	977	A
21	AA	982	U
21	AA	983	A
21	AA	991	U
21	AA	1025	U
21	AA	1050	G
21	AA	1054	C
21	AA	1065	U
21	AA	1094	G
21	AA	1101	A
21	AA	1123	U
21	AA	1125	U
21	AA	1129	C
21	AA	1137	C
21	AA	1139	G
21	AA	1190	G
21	AA	1195	C
21	AA	1201	A
21	AA	1203	C
21	AA	1211	U
21	AA	1226	C
21	AA	1233	G
21	AA	1257	A
21	AA	1280	A
21	AA	1298	U
21	AA	1302	C
21	AA	1330	U
21	AA	1335	U
21	AA	1358	U
21	AA	1374	A
21	AA	1377	A

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Mol	Chain	Res	Type
21	AA	1382	C
21	AA	1384	C
21	AA	1397	C
21	AA	1399	C
21	AA	1445	U
21	AA	1452	C
21	AA	1492	A
21	AA	1504	G
22	A1	46	7MG
22	A1	48	C
22	A1	74	C
22	A1	75	C
23	A2	83	U
23	A2	86	U
24	A3	17	C
24	A3	19	G
24	A3	48	U
24	A3	61	U
24	A3	72	C
24	A3	75	C
54	BA	33	C
54	BA	34	U
54	BA	49	A
54	BA	70	G
54	BA	74	A
54	BA	83	A
54	BA	118	A
54	BA	143	C
54	BA	163	C
54	BA	177	G
54	BA	196	A
54	BA	199	A
54	BA	265	A
54	BA	272	A
54	BA	301	G
54	BA	323	C
54	BA	330	A
54	BA	332	A
54	BA	346	A
54	BA	376	G
54	BA	382	A
54	BA	387	U

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Mol	Chain	Res	Type
54	BA	457	A
54	BA	481	G
54	BA	490	C
54	BA	497	A
54	BA	527	C
54	BA	531	C
54	BA	547	A
54	BA	548	G
54	BA	574	A
54	BA	627	A
54	BA	631	A
54	BA	645	C
54	BA	670	A
54	BA	747	U
54	BA	750	A
54	BA	821	A
54	BA	892	A
54	BA	909	A
54	BA	914	G
54	BA	933	A
54	BA	981	A
54	BA	1057	A
54	BA	1070	A
54	BA	1093	G
54	BA	1096	A
54	BA	1126	A
54	BA	1205	A
54	BA	1209	U
54	BA	1210	G
54	BA	1242	U
54	BA	1272	A
54	BA	1275	A
54	BA	1286	A
54	BA	1289	C
54	BA	1313	U
54	BA	1320	C
54	BA	1324	G
54	BA	1378	A
54	BA	1397	U
54	BA	1420	A
54	BA	1427	A
54	BA	1451	C

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Mol	Chain	Res	Type
54	BA	1485	U
54	BA	1559	U
54	BA	1566	A
54	BA	1606	C
54	BA	1609	A
54	BA	1616	A
54	BA	1646	C
54	BA	1647	U
54	BA	1664	A
54	BA	1699	G
54	BA	1706	C
54	BA	1738	G
54	BA	1789	A
54	BA	1799	G
54	BA	1800	C
54	BA	1828	G
54	BA	1912	A
54	BA	1913	A
54	BA	1930	G
54	BA	1936	A
54	BA	1938	A
54	BA	1939	U
54	BA	1944	U
54	BA	1945	G
54	BA	1981	A
54	BA	2015	A
54	BA	2032	G
54	BA	2033	A
54	BA	2034	U
54	BA	2048	G
54	BA	2060	A
54	BA	2117	A
54	BA	2126	A
54	BA	2155	U
54	BA	2172	U
54	BA	2197	U
54	BA	2198	A
54	BA	2211	A
54	BA	2225	A
54	BA	2232	C
54	BA	2237	G
54	BA	2238	G

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Mol	Chain	Res	Type
54	BA	2258	C
54	BA	2286	G
54	BA	2307	G
54	BA	2345	G
54	BA	2422	C
54	BA	2423	U
54	BA	2425	A
54	BA	2429	G
54	BA	2430	A
54	BA	2489	U
54	BA	2501	C
54	BA	2542	A
54	BA	2566	A
54	BA	2585	U
54	BA	2602	A
54	BA	2636	C
54	BA	2646	C
54	BA	2690	U
54	BA	2782	G
54	BA	2797	U
54	BA	2885	G
55	BB	6	G
55	BB	14	U
55	BB	57	A
55	BB	88	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
22	CM0	A1	34	22	15,26,27	1.88	3 (20%)	18,37,40	3.18	3 (16%)
22	6MZ	A1	37	22	17,25,26	0.92	0	15,36,39	1.33	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	7MG	A1	46	22	20,26,27	2.18	4 (20%)	23,39,42	2.13	4 (17%)
22	5MU	A1	54	22	13,22,23	1.13	1 (7%)	16,32,35	4.71	2 (12%)
22	PSU	A1	55	22	15,21,22	1.13	1 (6%)	16,30,33	3.32	4 (25%)
22	4SU	A1	7	22	12,21,22	1.02	0	15,30,33	2.05	1 (6%)
24	H2U	A3	21	24	17,21,22	1.46	2 (11%)	23,30,33	1.45	2 (8%)
24	OMC	A3	33	24	15,22,23	1.04	0	20,31,34	0.62	0
24	5MU	A3	55	24	13,22,23	1.14	1 (7%)	16,32,35	4.66	2 (12%)
24	PSU	A3	56	24	15,21,22	1.14	1 (6%)	16,30,33	3.65	5 (31%)
24	4SU	A3	8	24	12,21,22	1.05	1 (8%)	15,30,33	2.29	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CM0	A1	34	22	-	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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.05	1.33	1.45
22	A1	34	CM0	O5-C5	-5.66	1.26	1.37
24	A3	21	H2U	C4-N3	-3.92	1.31	1.37
24	A3	21	H2U	C2-N3	-3.46	1.31	1.38
22	A1	46	7MG	C8-N7	-2.71	1.31	1.43
24	A3	56	PSU	C4-N3	2.13	1.36	1.33
22	A1	46	7MG	C1'-N9	2.13	1.49	1.44
22	A1	46	7MG	C6-N1	2.44	1.37	1.33
22	A1	54	5MU	C4-N3	2.45	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	8	4SU	C6-N1	2.51	1.39	1.35
22	A1	34	CM0	C4-C5	2.52	1.47	1.40
24	A3	55	5MU	C4-N3	2.52	1.37	1.33
22	A1	55	PSU	C4-N3	2.58	1.37	1.33
22	A1	34	CM0	C4-N3	2.81	1.38	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-12.63	114.75	125.35
24	A3	55	5MU	C5-C4-N3	-12.52	114.84	125.35
24	A3	8	4SU	C5-C4-N3	-8.25	114.81	123.56
22	A1	7	4SU	C5-C4-N3	-7.20	115.93	123.56
22	A1	46	7MG	C5-C6-N1	-6.73	113.38	123.39
24	A3	56	PSU	C5-C1'-C2'	-3.85	108.90	115.44
24	A3	56	PSU	C4'-O4'-C1'	-3.84	105.58	109.54
24	A3	56	PSU	C5-C6-N1	-2.87	120.38	124.38
22	A1	55	PSU	C5-C6-N1	-2.51	120.88	124.38
22	A1	55	PSU	C5-C1'-C2'	-2.48	111.22	115.44
24	A3	21	H2U	O2-C2-N3	-2.18	117.16	121.44
22	A1	46	7MG	C4'-O4'-C1'	-2.15	104.78	109.52
22	A1	37	6MZ	C4'-O4'-C1'	-2.14	107.37	109.64
22	A1	46	7MG	C8-N9-C1'	2.20	129.03	122.43
22	A1	34	CM0	O5-C7-C8	3.00	114.21	108.01
22	A1	37	6MZ	C2-N1-C6	3.15	118.74	116.47
22	A1	34	CM0	C7-O5-C5	3.22	123.75	117.83
22	A1	55	PSU	O4'-C1'-C2'	3.30	108.26	104.69
24	A3	56	PSU	O4'-C1'-C2'	3.48	108.45	104.69
24	A3	21	H2U	N3-C2-N1	4.66	120.96	116.64
22	A1	46	7MG	C6-N1-C2	6.30	123.26	115.88
22	A1	34	CM0	C4-N3-C2	12.06	125.22	115.16
22	A1	55	PSU	C4-N3-C2	12.17	125.31	115.16
24	A3	56	PSU	C4-N3-C2	12.42	125.52	115.16
24	A3	55	5MU	C4-N3-C2	13.22	126.19	115.16
22	A1	54	5MU	C4-N3-C2	13.51	126.43	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	1.14	1 (20%)
58	FME	BA	3001	57	8,9,10	0.63	0	5,9,11	1.33	1 (20%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-2.30	119.41	125.69
58	BA	3001	FME	O1-CN-N	-2.24	121.37	124.80

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.