



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:53 PM BST

PDB ID : 4V73  
EMDB ID: : EMD-2473  
Title : E. coli 70S-fMetVal-tRNAVal-tRNA<sup>f</sup>Met complex in hybrid pre-translocation state (pre5a)  
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

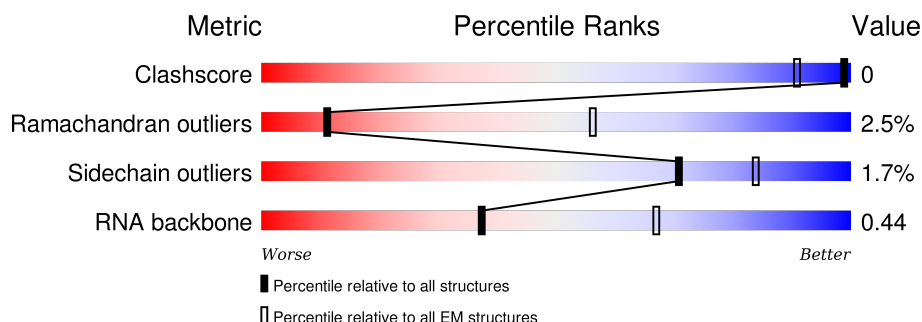
# 1 Overall quality at a glance ⓘ

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.













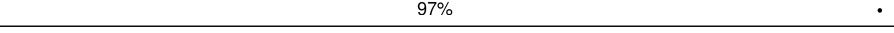
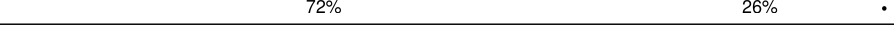
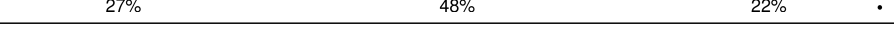


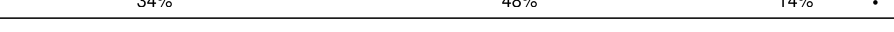


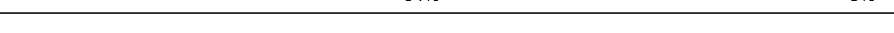






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	93% 7%
2	AC	208	90% 10%
3	AD	206	89% 10%
4	AE	152	92% 8%
5	AF	101	84% 14% •
6	AG	152	90% 9% •
7	AH	130	92% 8% •
8	AI	128	86% 13% •













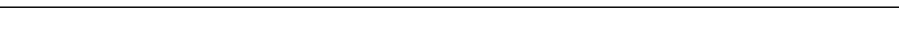



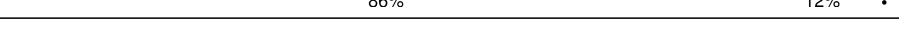




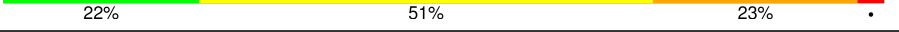
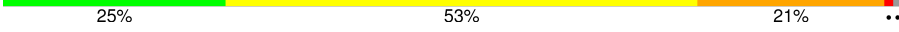
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Mol	Chain	Length	Quality of chain
9	AJ	100	 86% 13% .
10	AK	118	 92% 8%
11	AL	124	 82% 16% ..
12	AM	115	 85% 14% .
13	AN	101	 84% 13% ...
14	AO	89	 83% 16% .
15	AP	81	 86% 14%
16	AQ	82	 91% 6% .
17	AR	57	 86% 14%
18	AS	81	 88% 12%
19	AT	86	 97% .
20	AU	53	 72% 26% .
21	AA	1533	 27% 48% 22% .
22	A1	76	 32% 45% 22% .
23	A2	15	 27% 27% 47%
24	A3	77	 34% 48% 14% .
25	BC	273	 87% 12% .
26	BD	209	 90% 10%
27	BE	201	 94% 5% .
28	BF	179	 90% 9% .
29	BG	177	 91% 8% ..
30	BH	149	 93% 6% .
31	BI	142	 94% 5% .
32	BJ	142	 92% 8%
33	BK	123	 89% 11%

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Mol	Chain	Length	Quality of chain
34	BL	144	 85% 14% .
35	BM	136	 90% 8% .
36	BN	121	 83% 17%
37	BO	117	 91% 9% .
38	BP	115	 83% 15% ..
39	BQ	118	 86% 12% ..
40	BR	103	 89% 11%
41	BS	110	 90% 9% .
42	BT	94	 88% 11% .
43	BU	104	 88% 11% .
44	BV	94	 91% 9%
45	BW	80	 83% 18%
46	BX	79	 85% 13% .
47	BY	63	 89% 10% .
48	BZ	59	 88% 8% ..
49	B0	57	 86% 12% .
50	B1	52	 88% 12%
51	B2	46	 78% 22%
52	B3	65	 88% 11% .
53	B4	38	 87% 13%
54	BA	2903	 22% 51% 23% .
55	BB	118	 25% 53% 21% ..
56	B5	234	 91% 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		

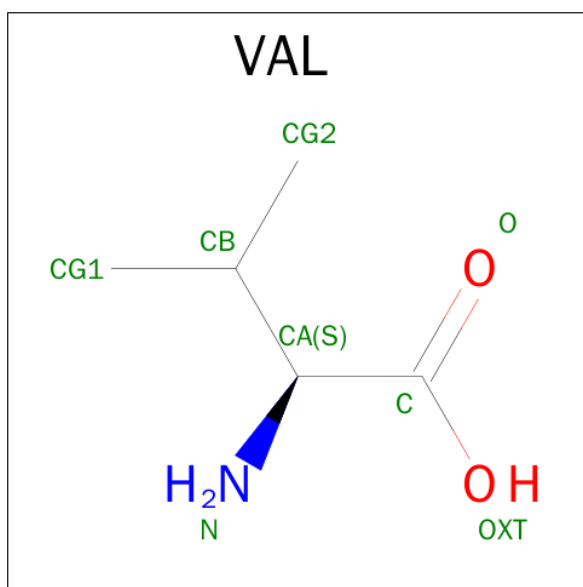
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

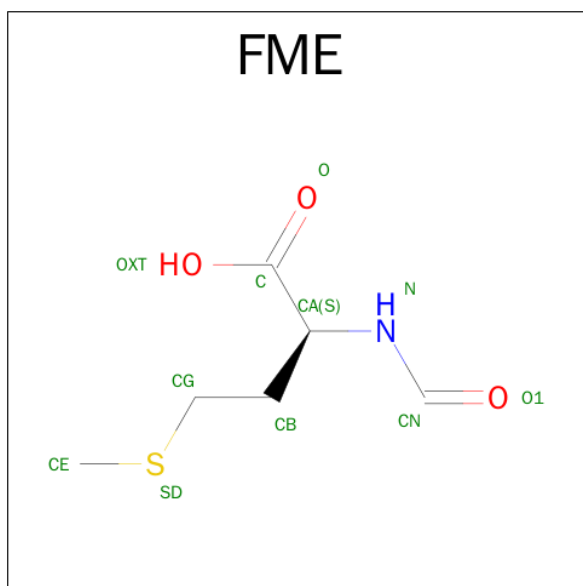
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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).



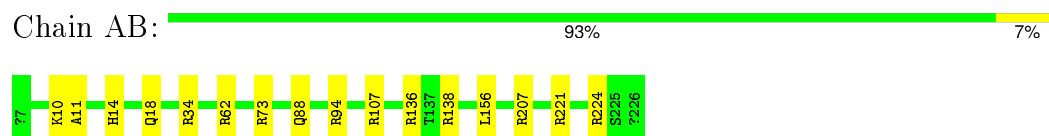
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	



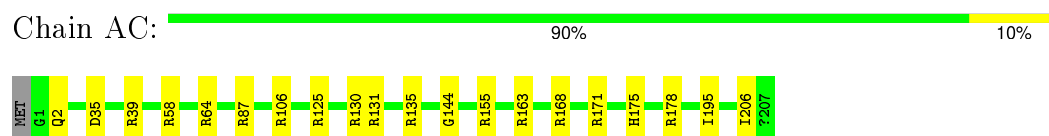
### 3 Residue-property plots

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.

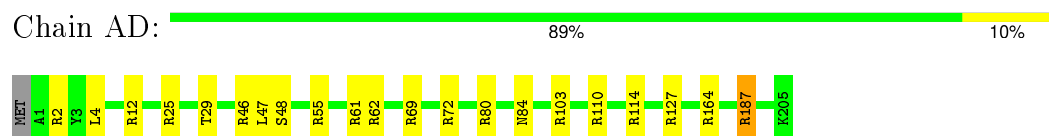
- Molecule 1: 30S ribosomal protein S2



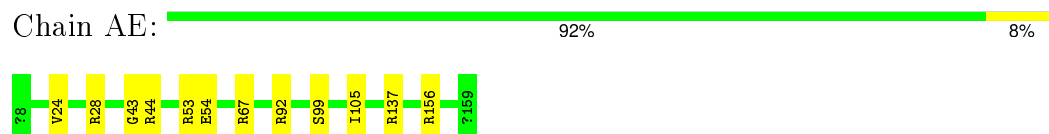
- Molecule 2: 30S ribosomal protein S3



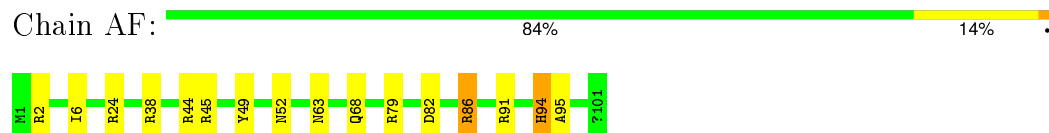
- Molecule 3: 30S ribosomal protein S4



- 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% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 86% 13%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 86% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 92% 8%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 82% 16%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%




- Molecule 13: 30S ribosomal protein S14

Chain AN: 84% 13%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  83% 16%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  86% 14%




- Molecule 16: 30S ribosomal protein S17

Chain AQ:  91% 6%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  86% 14%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  88% 12%



- Molecule 19: 30S ribosomal protein S20

Chain AT:  97%



- Molecule 20: 30S ribosomal protein S21

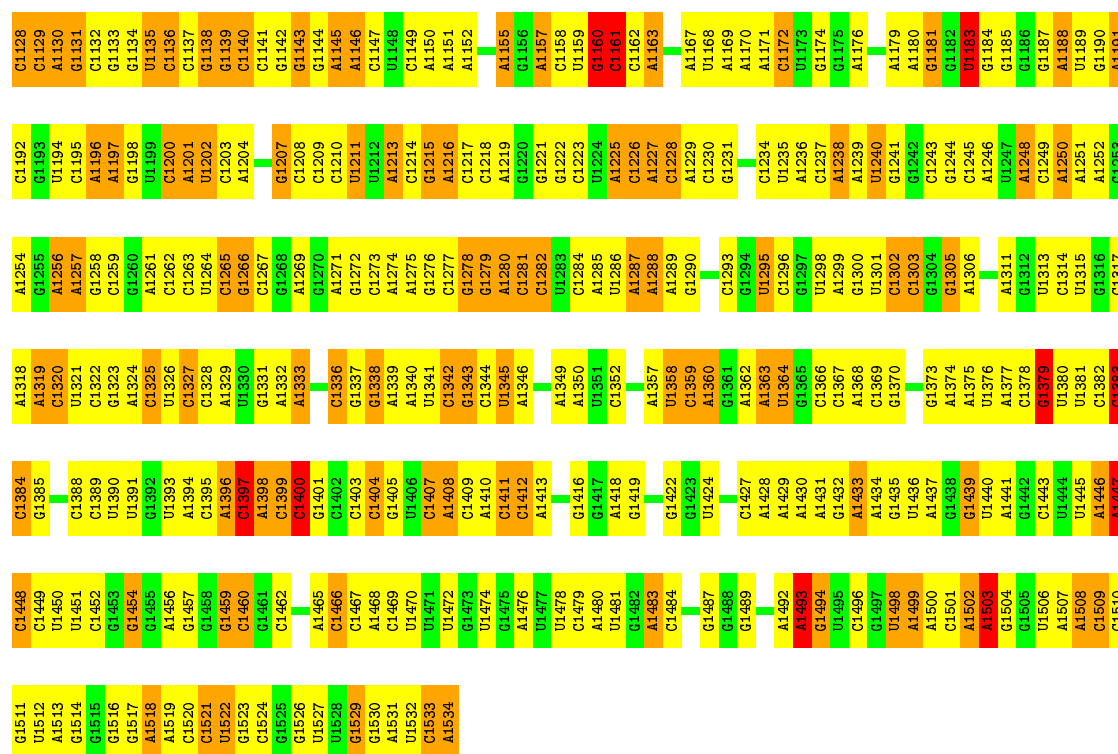
Chain AU:  72% 26%



- Molecule 21: 16S ribosomal RNA

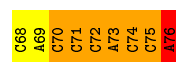
Chain AA:  27% 48% 22%



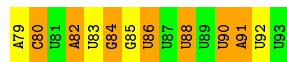
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 32% 45% 22% .



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

Chain A2: 27% 27% 47%



• Molecule 24: tRNA-fMet

Chain A3: 34% 48% 14% .



• Molecule 25: 50S ribosomal protein L2

Chain BC: 87% 12% .



- Molecule 26: 50S ribosomal protein L3

Chain BD: 90% 10%



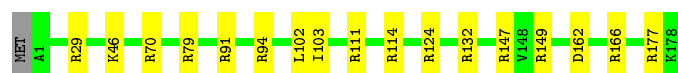
- Molecule 27: 50S ribosomal protein L4

Chain BE: 94% 5%



- Molecule 28: 50S ribosomal protein L5

Chain BF: 90% 9%



- Molecule 29: 50S ribosomal protein L6

Chain BG: 91% 8%



- Molecule 30: 50S ribosomal protein L9

Chain BH: 93% 6%



- Molecule 31: 50S ribosomal protein L11

Chain BI: 94% 5%



- Molecule 32: 50S ribosomal protein L13

Chain BJ: 92% 8%



- Molecule 33: 50S ribosomal protein L14

Chain BK: 89% 11%



- Molecule 34: 50S ribosomal protein L15

Chain BL: 85% 14%



- Molecule 35: 50S ribosomal protein L16

Chain BM: 90% 8%



- Molecule 36: 50S ribosomal protein L17

Chain BN: 83% 17%



- Molecule 37: 50S ribosomal protein L18

Chain BO: 91% 9%



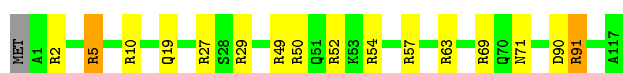
- Molecule 38: 50S ribosomal protein L19

Chain BP: 83% 15%



- Molecule 39: 50S ribosomal protein L20

Chain BQ: 86% 12%



- Molecule 40: 50S ribosomal protein L21

Chain BR:  89% 11%



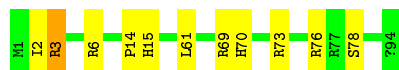
- Molecule 41: 50S ribosomal protein L22

Chain BS:  90% 9%



- Molecule 42: 50S ribosomal protein L23

Chain BT:  88% 11%



- Molecule 43: 50S ribosomal protein L24

Chain BU:  88% 11%




- Molecule 44: 50S ribosomal protein L25

Chain BV:  91% 9%




- Molecule 45: 50S ribosomal protein L27

Chain BW:  83% 18%



- Molecule 46: 50S ribosomal protein L28

Chain BX:  85% 13%




- Molecule 47: 50S ribosomal protein L29



Chain BY:  89% 10%




- Molecule 48: 50S ribosomal protein L30

Chain BZ:  88% 8%



- Molecule 49: 50S ribosomal protein L32

Chain B0:  86% 12%




- Molecule 50: 50S ribosomal protein L33

Chain B1:  88% 12%




- Molecule 51: 50S ribosomal protein L34

Chain B2:  78% 22%




- Molecule 52: 50S ribosomal protein L35

Chain B3:  88% 11%

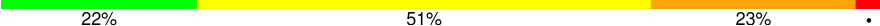


- Molecule 53: 50S ribosomal protein L36

Chain B4:  87% 13%

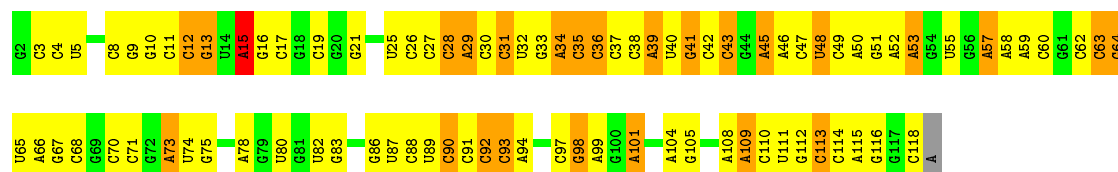
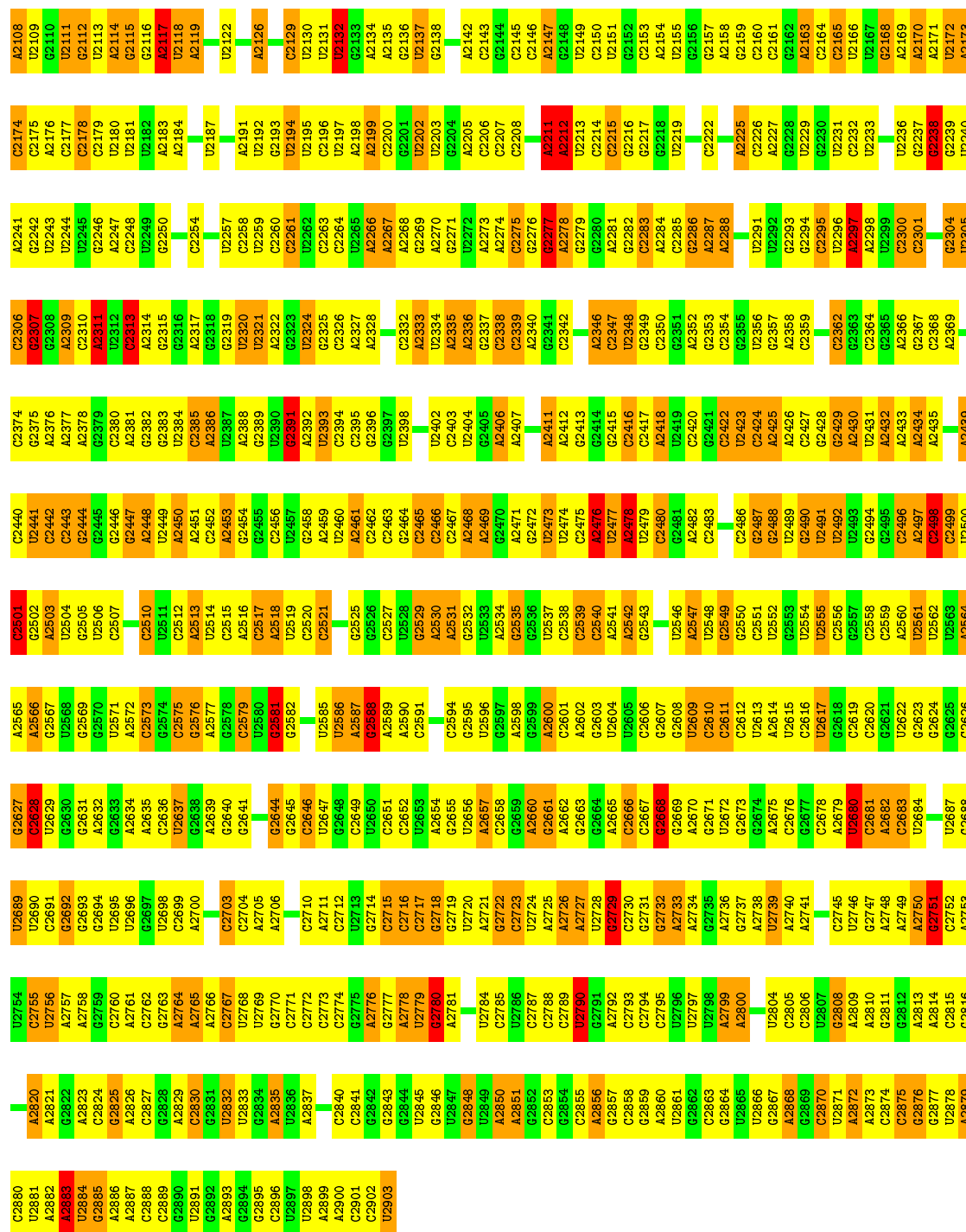


- Molecule 54: 23S ribosomal RNA

Chain BA:  22% 51% 23%

G1036	G971	A905	G775	G712	G649	G585	G518	G452	G386	C318	C253	U193	A126	A64	G1
A1039	A972	C908	G776	G713	C650	A586	U519	A463	U387	G319	G254	U194	A127	U65	G2
A1040	A973	A909		U714	G651	C587		A454	G388	A320	A255	A195	C128	C66	A5
G1041	G974	A910	A781	A715	U652	U588	A522	C455	G389	U321	A256	A196	C129	U67	A6
G1042	A975	A911	A782	A716	U653	U589	C523	C456	U390	A322	C257	A197	C130	G68	A7
C1043	G976	A912	A783	C717	A654	A590	G524	A457	A391	C323	G258	C198	A131	C69	A8
C1044		C912	G784	A718	A655	U591	U525	C458	U392	A324		A199	G132	G70	A9
C1045	A979	U913	G785	C719	G656	A592	A526	U459	C393		A282	U200	U133	A71	
C1046	A980	C915	C786	U720	U657	U593	C527	A460	C394		G263	C201	G134	U72	A10
A1047	A981	C916	C787	A721	U658	U594	A528	C461	U395	A330	A265	U202		A73	A11
G1047	A982	G916	A788	A722	G659	C595	A529	C462	G396	C331	A266	A203	U137	A74	U12
A1048	A983	A917	A789	G723	C660	U596	G530	U459	U397	A332	G266	A204	U138	G75	A13
C1049	A984	A918	U790	U724	A661	G597	C531	U464	C398	G333	C267	G205	U139	C76	A14
A1050	C985	U919	C791	G725	G662	U598	A532	G465		C334	C268	U206	C140	G77	G15
G1051	C986	A920	A792	G726	G663	A599	G533	A466	A401	C335	C269	A207	G141	U78	C16
C1052	C987	C921	A793	A727		G600		G467	A402	C336	A270	C208	A142	C79	G17
A1053	A988	C922	A794	G728	A666	C601	A538	C468	U403	G337	A271	C209	C143	G80	U18
C1054	G989	G923	C795	G729	A667	A602	G539	G469	A404	G338	A272	C210	A144	G81	A19
G1055	A990	G924	C796	A730	A668	A603	C540	A470	U405	U339	G273	C211	C145	U82	C20
G1056	C991	A925		C731	G669	G604	A541	A471		A340	C274	G212	A146	A83	A21
A1057	C992	G926	A800	C732	A670	G605	C542	A472	G411	C341	C275	A213		A84	C22
G1058	G993	A927	G801	G733	C671	U606	G543	G473	C412	A342	U276	G214	U148	U87	U25
G1059	C994	A928	A802	A734	C672	U607	C544		C413	G343	G277	G215	A149	G88	G26
C1060	C995		U803	A735	G673		C545	A477	C414	A344	A278	A216	U150	G89	G27
U1061	A996	U931	A804	C736	G674	A609	U546	A478	C415	A345	A279	A217	U151	A89	
G1062	G997	U932	G805	C737	A675	C610	A547	A479	U416	A346	U280	A218	A152	U90	A28
G1063	C998	A933	C806	G738	A676	C611	G548	A480	C417	A347	C281	A219	U153	A91	U29
C1064	U999	U934	U807	A739	A677	G612	G549	C481	C418	A348	A282	G220	U154		G30
U1065	A1000	C935	G808	C740	C678	A613	C550	A482	U419		G283	A221	A155	A94	C31
G1066	A1001	A936		U741	C679	A614		A483	C420	C351	U284	A222	A156	A95	C32
A1067		C937	U811	A742	C680	U615	U554	C484	C421	A352	G285	A223	C157	C96	
G1068	C1005		C812	A743	G681	A616	G555	C485	A422	C353	U286	U224	U158	C97	G33
A1069	C1006	A941	U813	U744	G682		A556	C486	A423	G354	G287	C225	G159	G98	G35
A1070	A1007	G942	C814	G745	U683	G620	C557	C487	G424	U355	U288	A226	A160	U99	G36
G1071	A1008	A943	C815	U746	G684	A621	U558		G425	G356	G289	A227	A161	U100	C37
C1072	A1009	C944	C816	U747	A685	G622	G559	C490	C426	C357		C228	U162	A101	A38
A1073	A1010	A945	C817	G748	U686	G623	C560	C491	U427	U358	A294	C229	C163	U102	G39
G1074	C1011	C946	C818	A749		C624		A492	A428	G359	G295	G230	C164	U40	U40
C1075	U1012	A947	A819	A750	A689	G625	A563	A493	A429	U360	U296	A231	A165	A104	C41
G1076	C1013	C948	A820	A751	G690	A626	C564		A430	G361	G297	G232	U166	C105	A42
U1015	A1014	G949	A821	C692	C691	A627	C565	A496	U431	A362	G298	A233	A167	C106	G43
C1077	U1015	C951	G822	A753	C692		U566	A497	A432	G363	A299	U234	G168	G107	A44
A1078	G1016	C952	C823		A693	A631	U567		C433	C364	A300	U235		G108	A44
C1079	U1019	G953	U824	A756	U694	A632	U568	G500	U434	U365	G301	G236	A172	G45	G45
A1080	U1081	G954	A825	G757	G695	A633	U569	A501	C435	C366	C302	C237	A173	C47	
U1082	A1020		U826	C758	G696	A634	C570	A502	U436	G367	G303	C238	U174	G48	
U1083	A1021	C957	U827		G697	C635	U571	A503	C437	A368	G175	C239	G175	U112	A49
A1084	G1022	U958	U828	A761	C698	G636	A572	A504	G438	U369	A176	C240	A176	U113	U50
A1085	U1023	C959	A829	U762	A699	A637	U573	A505	A439	G370	U306	A241	G177	U114	G51
A1086	G1024	A959	G830	G763	G700	G638	A574	G506	C440	A371	G307	G242	G178	C115	A52
G1087	U1025		G831	A764	G701	U639	A575	A507		G372	G308	U243	C179	C116	A53
A1088	G1026	C961	U832	C765	U702	C640	U576	A508	A443	U373	A309	G245	G180	G117	G54
A1089	A1027		A833	U766	G703	U641	G577	C509	C444	A374	A310	G246	A181	G118	G55
A1090	C964	C964	G834		G704	U642	G578	C510	C445	A311	A182	C246	A182	A119	A56
C1091	A1029	C965	A835	A769	A705	A643	G579		G446	C378	G183	G247	C184	U120	C57
C1092	G1030	G966	G836	U770	A706	A644	U580	A513	U447	A382	G312	G248	C184	G121	G58
G1093	G1031	U967	C837	G771		C645	C581	A514	U448	A383	G313	C249		G122	
U1094	A1032	C968	C838	C772	U709	U646	A582	A515	G449	C384	G315	G250	A190	G123	G61
A1095	U1033	G969	U839	U773	U710	G647	G583	A516	G450	A384	G316	A251	A191	G124	U62
A1096			C840	G774	G711	G648	C584	C517	U451	C385	G317	G252	C192	A125	A63

C2047	A1987	C1925	U1864	G1799	A1672	C1605	U1542	G1478	U1409	C1349	A1287	A1226	G1160	U1097
C2050	G1988	U1926	U1865	C1800	G1673	C1606	G1543	G1479	U1412	C1350	G1288	G1227	C1161	A1093
A2051	G1989	A1927	U1866	A1801	G1674	C1607	A1544	U1480	U1413	C1351	C1289	G1228	G1162	G1099
A2052	C1990	A1928	A1866	A1802	G1675	A1608	A1545	U1481	C1413	U1352	C1290	C1229	G1163	C1100
G2053	G1992	G1930	G1867	C1804	A1676	A1609	C1547	G1482	C1414	A1353	G1291	U1230	C1164	U1101
A2054	U1993	U1931	C1868	C1803	A1677	A1610	A1548	G1483	U1415	A1354	C1292	U1231	A1165	C1102
C2055	A1998	A1806	G1869	A1805	A1678	C1611	A1549	U1484	G1416	G1355	C1293	G1232	G1166	A1103
G2056	G1995	A1932	C1870	C1806	A1679	G1612	A1549	U1484	C1417	G1356	U1294	C1233	C1167	A1104
C2057	C1996	G1933	A1871	G1807	U1680	G1613	C1550	C1488	G1418	G1357	C1295	U1234	G1168	U1105
A2058	C1996	A1934	A1872	A1808	G1681	A1614	A1551	C1489	A1419	G1358	G1296	G1235	G1169	G1106
G2059	C1997	G1935	G1873	A1809	A1682	C1615	A1552	A1490	A1420	A1359	C1297	G1236	C1170	C1107
A2063	A1998	A1936	C1874	A1810	U1685	A1616	A1553	G1491	A1492	G1360	C1298	A1237	G1171	U1108
A2060	G1999	A1937	G1875	G1811	C1686	C1617	U1563	G1492	G1424	G1361	G1299	G1238	G1172	C1109
G2061	C2000	A1938	A1876	U1812	C1687	A1618	C1556	C1493	G1425	C1362	G1300	G1239	U1173	G1110
A2062	C2001	U1939	G1877	G1813	U1688	U1619	C1557	C1494	G1426	C1363	A1301	U1240	U1174	A1111
C2063	G2002	G1940	A1878	G1814	U1689	U1620	C1558	A1495	A1427	G1364	A1302	A1241	G1175	G1112
C2064	A2003	C1941	G1752	A1815	A1690	A1625	U1559	A1496	C1428	A1365	G1303	U1242	U1176	U1113
C2065	G2004	C1942	G1753	C1816	A1691	A1626	G1560	U1497	G1429	A1366	A1304	C1243	G1177	C1114
C2066	A2005	U1943	A1754	G1817	C1691	G1627	C1561	C1498	G1430	A1367	C1305	A1244	C1178	G1115
C2067	C2006	U1944	A1755	U1818	A1692	G1628	U1562	C1499	A1431	G1368	C1306	G1245	G1179	G1116
G2068	U2007	U1883	U1883	A1819	U1693	G1629	U1563	G1500	G1432	G1369	A1307	A1246	U1180	C1117
G2069	C2008	G1884	A1884	U1820	G1694	A1630	C1564	G1501	A1433	C1370	A1308	A1247	U1181	C1118
A2070	A2009	A1885	A1885	A1821	G1695	G1631	C1565	A1502	A1434	C1371	A1247	U1182	G1182	
C2071	G2010	U1886	U1886	C1822	A1759	A1632	A1566	A1503	G1437	U1372	G1311	G1250	G1185	G1121
C2072	U2011	G1823	C1827	G1823	G1696	G1633	G1567	A1504	A1437	A1373	U1312	C1251	G1186	C1122
C2073	G2012	G1824	G1888	G1824	A1698	A1634	G1568	A1505	U1438	G1374	U1313	G1252	G1187	C1123
U2074	A2013	A1890	A1889	G1825	A1762	U1635	A1569	U1506	A1439	U1375	C1314	A1253	G1188	G1124
U2075	C2014	A1952	A1890	G1826	G1699	U1636	U1570	C1507	U1440	C1376	C1315	A1254	G1125	G1125
U2076	A2015	G1954	G1891	G1827	G1764	A1637	A1571	A1508	U1441	G1377	U1316	U1255	A1189	A1126
A2077	U2016	U1965	C1892	G1828	U1765	G1638	A1572	A1509	U1442	A1378	G1317	G1256	A1190	A1127
C2078	U2017	U1956	C1893	A1829	G1766	C1639	G1573	G1510	U1445	U1379	U1318	C1257	G1191	G1128
U2079	G2018	C1957	C1894	C1830	G1767	A1640	A1574	G1511	G1446	G1380	C1319	U1258	A1129	A1129
A2080	A2019	C1958	C1895	G1831	A1705	A1641	C1575	C1381	C1446	G1381	C1320	G1259	A1194	U1130
C2081	C2020	G1959	A1896	A1832	C1706	G1642	U1576	U1513	C1447	G1382	A1321	A1260	G1195	G1131
G2082	U2021	A1960	C1837	G1833	G1707	G1643	C1577	G1514	G1451	A1383	C1322	C1261	C1196	U1132
C2084	C2022	C1961	U1834	U1834	U1708	C1644	U1578	A1515	G1452	A1384	C1323	A1262	A1133	A1133
U2085	C2023	G1962	A1900	G1835	G1710	G1645	A1579	C1518	A1463	C1385	G1324	U1263	G1200	A1134
U2086	G2024	U1963	A1901	C1836	A1714	C1646	A1580	C1518	A1463	C1386		A1264		C1135
C2087	C2025	G1964	C1902	C1837	A1711	U1647	G1581	G1519	C1454	A1387	A1327	A1265	U1203	G1138
A2088	G2026	C1965	G1903	U1837	U1712	U1648	C1582	U1522	G1455	G1388	A1328	G1266	A1204	G1139
C2089	C2027	A1966	C1904	G1842	A1713	G1649	A1583	U1523	U1458	U1329	U1329	U1267	A1205	G1140
A2090	U2028	C1967	G1905	C1843	U1714	A1650	U1584	G1524	U1469	A1330	A1330	A1268	G1206	C1140
C2091	G2029	G1968	G1906	C1844	G1715	G1651	C1585	A1524	U1469	U1391	A1269	A1269	C1207	U1141
C2091	A2030	A1969	G1907	C1844	U1716	A1652	A1586	A1525	U1460	A1392	G1332	C1270	C1208	A1142
U2092	C2031	C1970	C1908	G1845	A1717	G1653	G1587	C1526	C1461	A1393	G1333	G1271	U1209	A1143
G2093	G2032	U1971	C1909	G1846	A1784	A1654	U1590	A1528	C1462	U1394	A1334	A1272	G1210	A1144
A2094	A2033	G1972	G1910	A1847	U1720	A1655	A1591	G1527	C1463	C1395	C1335	U1273	C1211	C1145
A2095	C2034	U1911	G1911	C1848	G1721	C1656	G1529	G1529	U1464	U1396	A1336	A1274	C1212	C1146
C2096	G2035	A1912	A1912	G1849	A1722	U1657	C1592	G1530	G1465	U1397	G1337	A1275	A1213	A1147
A2097	C2036	C1913	A1913	C1850	G1723	C1658	A1593	C1531	U1466	C1398	G1338	A1276	A1214	
U2098	A2037	C1914	C1914	U1851	G1724	G1659	U1594	A1532	U1467	C1399	G1339	G1277	G1215	C1150
U2099	G2038	A1978	U1915	A1852	U1725	C1595	C1595	C1533	U1468	U1400	U1340	C1278	G1216	A1151
G2100	U2039	U1979	A1916	A1853	C1726	A1596	A1596	U1534	A1469	G1401	G1279	G1217	U1217	C1152
A2101	C2040	G1980	U1917	A1854	C1727	A1665	A1597	A1534	U1470	U1402	A1342	G1280	C1153	C1153
G2102	U2041	A1981	A1918	C1793	C1728	G1666	U1598	C1536	G1471	A1403	G1343	G1281	G1220	G1154
C2103	A2042	A1919	U1919	U1856	U1729	G1667	U1599	G1537	C1472	C1404	U1344	U1282	C1221	A1155
C2104	C2043	G1983	C1920	G1857	C1730	A1668	C1600	G1538	C1475	U1405	C1345	G1283	U1222	A1156
U2105	C2044	G1984	U1923	A1858	C1731	A1669	A1603	U1539	G1476	U1406	G1346	A1284	G1223	G1157
U2106	C2045	C1985	G1797	U1859	C1732	C1670	A1671	G1540	U1477	A1407	A1347	A1285	U1224	C1158
G2107	C2046	C1986	U1798	G1860	U1671		C1604	C1541	A1477	G1408	C1348	A1286	G1225	U1159



● Molecule 56: 50S ribosomal protein L1

Chain B5: 

91%

5%

5%



## 4 Experimental information

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	AB	0.72	0/1736	1.05	13/2340 (0.6%)
10	AK	0.76	0/894	1.14	8/1207 (0.7%)
11	AL	0.77	0/969	1.28	13/1300 (1.0%)
12	AM	0.75	0/884	1.29	16/1181 (1.4%)
13	AN	0.76	0/817	1.24	12/1088 (1.1%)
14	AO	0.75	0/722	1.17	10/964 (1.0%)
15	AP	0.79	0/648	1.28	12/870 (1.4%)
16	AQ	0.70	0/658	1.15	6/883 (0.7%)
17	AR	0.82	0/463	1.19	6/623 (1.0%)
18	AS	0.76	0/653	1.18	9/879 (1.0%)
19	AT	0.68	0/672	0.97	3/890 (0.3%)
2	AC	0.74	0/1651	1.07	13/2225 (0.6%)
20	AU	0.86	0/431	1.43	7/572 (1.2%)
21	AA	1.52	1/36759 (0.0%)	2.22	1955/57346 (3.4%)
22	A1	1.55	0/1668	2.27	88/2595 (3.4%)
23	A2	1.50	0/343	2.33	19/531 (3.6%)
24	A3	1.55	0/1722	2.18	90/2685 (3.4%)
25	BC	0.75	0/2121	1.29	30/2852 (1.1%)
26	BD	0.68	0/1586	1.13	9/2134 (0.4%)
27	BE	0.68	0/1571	1.15	10/2113 (0.5%)
28	BF	0.75	0/1444	1.21	16/1937 (0.8%)
29	BG	0.69	0/1343	1.10	9/1816 (0.5%)
3	AD	0.77	0/1665	1.13	16/2227 (0.7%)
30	BH	0.66	0/1122	1.10	7/1515 (0.5%)
31	BI	0.68	0/1046	1.08	5/1410 (0.4%)
32	BJ	0.74	0/1152	1.17	12/1551 (0.8%)
33	BK	0.71	0/947	1.23	11/1268 (0.9%)
34	BL	0.74	0/1054	1.33	11/1403 (0.8%)
35	BM	0.75	0/1093	1.28	12/1460 (0.8%)
36	BN	0.76	0/973	1.31	13/1301 (1.0%)
37	BO	0.73	0/902	1.24	10/1209 (0.8%)
38	BP	0.76	0/929	1.33	13/1242 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.80	0/960	1.31	12/1278 (0.9%)
4	AE	0.71	0/1119	1.06	7/1506 (0.5%)
40	BR	0.73	0/829	1.10	5/1107 (0.5%)
41	BS	0.65	0/864	1.15	6/1156 (0.5%)
42	BT	0.67	0/744	1.19	6/994 (0.6%)
43	BU	0.69	0/787	1.12	6/1051 (0.6%)
44	BV	0.73	0/766	1.16	6/1025 (0.6%)
45	BW	0.77	0/604	1.27	8/799 (1.0%)
46	BX	0.76	0/635	1.22	6/848 (0.7%)
47	BY	0.67	0/510	1.17	6/677 (0.9%)
48	BZ	0.69	0/453	1.20	3/605 (0.5%)
49	B0	0.75	0/450	1.24	5/599 (0.8%)
5	AF	0.74	0/835	1.14	8/1128 (0.7%)
50	B1	0.73	0/417	1.16	3/556 (0.5%)
51	B2	0.80	0/380	1.50	10/498 (2.0%)
52	B3	0.75	0/513	1.23	6/676 (0.9%)
53	B4	0.69	0/303	1.32	5/397 (1.3%)
54	BA	1.40	0/69796	2.21	4028/108888 (3.7%)
55	BB	1.41	0/2800	2.20	152/4367 (3.5%)
56	B5	0.66	0/1673	1.07	10/2255 (0.4%)
6	AG	0.76	0/1188	1.24	14/1593 (0.9%)
7	AH	0.72	0/989	1.07	6/1326 (0.5%)
8	AI	0.81	0/1035	1.27	14/1377 (1.0%)
9	AJ	0.72	0/797	1.12	9/1079 (0.8%)
All	All	1.28	1/160085 (0.0%)	1.99	6805/239402 (2.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	AK	0	1
21	AA	0	358
22	A1	0	15
23	A2	0	5
24	A3	0	9
26	BD	0	1
41	BS	0	1
50	B1	0	1
54	BA	0	709
55	BB	0	21
All	All	0	1121



All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	348	G	C4'-O4'	-5.47	1.38	1.45

All (6805) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	76	A	N1-C6-N6	-15.19	109.49	118.60
54	BA	1714	U	O4'-C1'-N1	14.33	119.66	108.20
54	BA	546	U	O4'-C1'-N1	13.75	119.20	108.20
54	BA	218	A	N1-C6-N6	-12.03	111.39	118.60
21	AA	152	A	N1-C6-N6	-11.78	111.53	118.60
54	BA	142	A	N1-C6-N6	-11.77	111.54	118.60
54	BA	330	A	O4'-C1'-N9	11.77	117.61	108.20
21	AA	344	A	N1-C6-N6	-11.70	111.58	118.60
21	AA	1362	A	N1-C6-N6	-11.56	111.67	118.60
21	AA	1391	U	C1'-O4'-C4'	-11.48	100.72	109.90
54	BA	988	A	N1-C6-N6	-11.41	111.75	118.60
54	BA	196	A	N1-C6-N6	-11.40	111.76	118.60
54	BA	2473	U	O4'-C1'-N1	11.40	117.32	108.20
21	AA	1248	A	N1-C6-N6	-11.39	111.77	118.60
54	BA	1155	A	N1-C6-N6	-11.32	111.81	118.60
54	BA	1434	A	N1-C6-N6	-11.30	111.82	118.60
21	AA	1274	A	N1-C6-N6	-11.29	111.83	118.60
21	AA	397	A	N1-C6-N6	-11.27	111.84	118.60
54	BA	793	A	N1-C6-N6	-11.24	111.86	118.60
21	AA	171	A	N1-C6-N6	-11.24	111.86	118.60
21	AA	1396	A	N1-C6-N6	-11.22	111.87	118.60
54	BA	1786	A	N1-C6-N6	-11.22	111.87	118.60
21	AA	780	A	N1-C6-N6	-11.21	111.88	118.60
54	BA	1069	A	O4'-C1'-N9	11.20	117.16	108.20
21	AA	1254	A	N1-C6-N6	-11.18	111.89	118.60
54	BA	2814	A	N1-C6-N6	-11.17	111.90	118.60
54	BA	1532	A	N1-C6-N6	-11.16	111.90	118.60
21	AA	665	A	N1-C6-N6	-11.15	111.91	118.60
21	AA	563	A	N1-C6-N6	-11.13	111.92	118.60
54	BA	1272	A	N1-C6-N6	-11.11	111.93	118.60
54	BA	1226	A	N1-C6-N6	-11.09	111.95	118.60
21	AA	7	A	N1-C6-N6	-11.09	111.95	118.60
32	BJ	95	ARG	NE-CZ-NH2	11.07	125.83	120.30
54	BA	1890	A	N1-C6-N6	-11.06	111.96	118.60
55	BB	78	A	N1-C6-N6	-11.06	111.96	118.60
21	AA	179	A	N1-C6-N6	-11.04	111.98	118.60
54	BA	204	A	N1-C6-N6	-11.03	111.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	927	A	N1-C6-N6	-10.99	112.01	118.60
54	BA	602	A	N1-C6-N6	-10.98	112.01	118.60
21	AA	983	A	N1-C6-N6	-10.98	112.01	118.60
54	BA	1009	A	N1-C6-N6	-10.97	112.02	118.60
22	A1	73	A	N1-C6-N6	-10.97	112.02	118.60
54	BA	2886	A	N1-C6-N6	-10.97	112.02	118.60
54	BA	2418	A	N1-C6-N6	-10.95	112.03	118.60
54	BA	84	A	N1-C6-N6	-10.94	112.04	118.60
21	AA	845	A	N1-C6-N6	-10.92	112.05	118.60
21	AA	1246	A	N1-C6-N6	-10.91	112.05	118.60
21	AA	675	A	N1-C6-N6	-10.90	112.06	118.60
54	BA	38	A	N1-C6-N6	-10.90	112.06	118.60
54	BA	2632	A	N1-C6-N6	-10.90	112.06	118.60
35	BM	51	ARG	NE-CZ-NH1	10.88	125.74	120.30
54	BA	654	A	N1-C6-N6	-10.84	112.09	118.60
54	BA	1383	A	N1-C6-N6	-10.83	112.10	118.60
54	BA	2435	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	1129	A	N1-C6-N6	-10.79	112.13	118.60
54	BA	613	A	N1-C6-N6	-10.76	112.14	118.60
54	BA	1535	A	N1-C6-N6	-10.76	112.14	118.60
21	AA	574	A	N1-C6-N6	-10.75	112.15	118.60
54	BA	181	A	N1-C6-N6	-10.74	112.16	118.60
21	AA	1441	A	N1-C6-N6	-10.73	112.16	118.60
54	BA	119	A	N1-C6-N6	-10.71	112.17	118.60
21	AA	5	U	O4'-C1'-N1	10.71	116.76	108.20
21	AA	573	A	N1-C6-N6	-10.70	112.18	118.60
54	BA	1758	U	O4'-C1'-N1	10.70	116.76	108.20
54	BA	2147	A	N1-C6-N6	-10.69	112.19	118.60
21	AA	1216	A	N1-C6-N6	-10.68	112.19	118.60
21	AA	1429	A	N1-C6-N6	-10.68	112.19	118.60
21	AA	1500	A	N1-C6-N6	-10.67	112.20	118.60
54	BA	2082	A	N1-C6-N6	-10.66	112.20	118.60
21	AA	448	A	N1-C6-N6	-10.66	112.20	118.60
54	BA	513	A	N1-C6-N6	-10.66	112.21	118.60
54	BA	2513	A	N1-C6-N6	-10.65	112.21	118.60
21	AA	653	U	O4'-C1'-N1	10.64	116.72	108.20
54	BA	1084	A	O4'-C1'-N9	10.64	116.71	108.20
21	AA	101	A	N1-C6-N6	-10.63	112.22	118.60
21	AA	1280	A	N1-C6-N6	-10.63	112.22	118.60
54	BA	1308	A	N1-C6-N6	-10.62	112.23	118.60
21	AA	1287	A	N1-C6-N6	-10.62	112.23	118.60
21	AA	435	A	N1-C6-N6	-10.57	112.26	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1095	A	N1-C6-N6	-10.57	112.26	118.60
54	BA	207	A	N1-C6-N6	-10.56	112.26	118.60
54	BA	2883	A	N1-C6-N6	-10.55	112.27	118.60
21	AA	704	A	N1-C6-N6	-10.55	112.27	118.60
21	AA	77	A	N1-C6-N6	-10.54	112.28	118.60
54	BA	1352	U	O4'-C1'-N1	10.54	116.63	108.20
54	BA	900	A	N1-C6-N6	-10.54	112.28	118.60
55	BB	15	A	N1-C6-N6	-10.53	112.28	118.60
54	BA	2132	U	O4'-C1'-N1	10.51	116.61	108.20
54	BA	1269	A	N1-C6-N6	-10.51	112.30	118.60
21	AA	393	A	N1-C6-N6	-10.51	112.30	118.60
54	BA	262	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	443	A	N1-C6-N6	-10.49	112.30	118.60
54	BA	1086	A	N1-C6-N6	-10.49	112.31	118.60
54	BA	1713	A	N1-C6-N6	-10.48	112.31	118.60
54	BA	515	A	N1-C6-N6	-10.48	112.31	118.60
54	BA	1304	A	N1-C6-N6	-10.47	112.32	118.60
16	AQ	62	GLU	OE1-CD-OE2	-10.46	110.75	123.30
21	AA	532	A	N1-C6-N6	-10.44	112.34	118.60
21	AA	1152	A	N1-C6-N6	-10.43	112.34	118.60
54	BA	1262	A	N1-C6-N6	-10.41	112.35	118.60
21	AA	681	A	N1-C6-N6	-10.41	112.35	118.60
54	BA	2212	A	O4'-C1'-N9	10.41	116.53	108.20
54	BA	2882	A	N1-C6-N6	-10.41	112.36	118.60
54	BA	603	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	196	A	O4'-C1'-N9	10.39	116.52	108.20
54	BA	490	C	N3-C2-O2	-10.39	114.63	121.90
22	A1	69	A	N1-C6-N6	-10.38	112.38	118.60
54	BA	2386	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	2587	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	1322	A	N1-C6-N6	-10.34	112.40	118.60
21	AA	914	A	N1-C6-N6	-10.33	112.40	118.60
21	AA	452	A	N1-C6-N6	-10.32	112.41	118.60
42	BT	6	ARG	NE-CZ-NH2	10.32	125.46	120.30
54	BA	111	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	1784	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	975	A	N1-C6-N6	-10.31	112.41	118.60
21	AA	192	A	N1-C6-N6	-10.31	112.42	118.60
54	BA	309	A	N1-C6-N6	-10.30	112.42	118.60
54	BA	1204	A	O4'-C1'-N9	10.30	116.44	108.20
21	AA	228	A	N1-C6-N6	-10.29	112.43	118.60
21	AA	958	A	N1-C6-N6	-10.29	112.43	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2738	A	N1-C6-N6	-10.28	112.43	118.60
21	AA	1350	A	N1-C6-N6	-10.28	112.43	118.60
54	BA	2170	A	N1-C6-N6	-10.28	112.43	118.60
54	BA	1847	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	2070	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	1614	A	N1-C6-N6	-10.24	112.46	118.60
54	BA	821	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	408	A	N1-C6-N6	-10.22	112.47	118.60
54	BA	781	A	N1-C6-N6	-10.22	112.47	118.60
21	AA	1130	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	2267	A	N1-C6-N6	-10.21	112.48	118.60
21	AA	975	A	N1-C6-N6	-10.20	112.48	118.60
55	BB	13	G	O4'-C1'-N9	10.20	116.36	108.20
21	AA	747	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	2900	A	N1-C6-N6	-10.18	112.50	118.60
54	BA	2097	A	N1-C6-N6	-10.17	112.50	118.60
21	AA	938	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	1054	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	959	A	N1-C6-N6	-10.14	112.52	118.60
21	AA	1055	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	2134	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	280	U	O4'-C1'-N1	10.13	116.30	108.20
54	BA	1821	A	N1-C6-N6	-10.13	112.52	118.60
39	BQ	50	ARG	NE-CZ-NH2	10.13	125.36	120.30
21	AA	831	A	N1-C6-N6	-10.12	112.53	118.60
21	AA	389	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	643	A	N1-C6-N6	-10.11	112.53	118.60
21	AA	1428	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	294	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	2009	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	2176	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	479	A	N1-C6-N6	-10.08	112.55	118.60
21	AA	250	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	2129	C	O4'-C1'-N1	10.07	116.26	108.20
21	AA	1171	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	2826	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	347	A	N1-C6-N6	-10.06	112.57	118.60
54	BA	1901	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	1036	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	2451	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	2169	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	1254	A	N1-C6-N6	-10.02	112.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1284	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	161	A	N1-C6-N6	-9.99	112.61	118.60
21	AA	964	A	N1-C6-N6	-9.99	112.60	118.60
54	BA	1583	A	N1-C6-N6	-9.99	112.61	118.60
54	BA	102	U	O4'-C1'-N1	9.97	116.18	108.20
7	AH	14	ARG	NE-CZ-NH1	9.96	125.28	120.30
21	AA	1179	A	N1-C6-N6	-9.96	112.63	118.60
54	BA	2542	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	1635	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	1073	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	2241	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	143	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	282	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	1150	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	1447	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	139	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	1044	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	1067	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	1981	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	373	A	N1-C6-N6	-9.91	112.65	118.60
21	AA	51	A	N1-C6-N6	-9.91	112.65	118.60
54	BA	866	A	N1-C6-N6	-9.91	112.65	118.60
21	AA	1035	A	N1-C6-N6	-9.91	112.66	118.60
54	BA	1664	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	2135	A	N1-C6-N6	-9.89	112.67	118.60
54	BA	820	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	886	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	73	A	N1-C6-N6	-9.86	112.69	118.60
21	AA	1377	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	621	A	N1-C6-N6	-9.85	112.69	118.60
21	AA	1019	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	753	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	371	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	788	A	N1-C6-N6	-9.82	112.70	118.60
54	BA	2142	A	N1-C6-N6	-9.82	112.71	118.60
54	BA	1606	C	O4'-C1'-N1	9.82	116.06	108.20
54	BA	2158	A	N1-C6-N6	-9.82	112.71	118.60
54	BA	1885	A	N1-C6-N6	-9.81	112.71	118.60
21	AA	131	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	2541	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	1084	A	N1-C6-N6	-9.79	112.73	118.60
54	BA	1453	A	N1-C6-N6	-9.79	112.73	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	845	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	165	A	N1-C6-N6	-9.78	112.73	118.60
21	AA	901	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	63	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	538	A	N1-C6-N6	-9.77	112.73	118.60
54	BA	2682	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	181	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	465	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	1142	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	532	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	1938	A	N1-C6-N6	-9.74	112.75	118.60
54	BA	2054	A	N1-C6-N6	-9.74	112.75	118.60
54	BA	905	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2060	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	91	A	O4'-C1'-N9	9.72	115.98	108.20
54	BA	497	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	1494	A	N1-C6-N6	-9.72	112.77	118.60
24	A3	45	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	2450	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	759	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	919	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	199	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	1363	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	74	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1505	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	2825	G	O4'-C1'-N9	9.70	115.96	108.20
21	AA	1311	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	2076	U	O4'-C1'-N1	9.69	115.95	108.20
21	AA	356	A	N1-C6-N6	-9.69	112.79	118.60
21	AA	1394	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	1373	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	2288	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	241	A	N1-C6-N6	-9.68	112.80	118.60
54	BA	348	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	507	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	1089	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	1679	A	N1-C6-N6	-9.66	112.80	118.60
55	BB	35	C	N3-C2-O2	-9.65	115.14	121.90
21	AA	768	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	766	A	N1-C6-N6	-9.64	112.81	118.60
51	B2	34	ARG	NE-CZ-NH1	9.64	125.12	120.30
54	BA	323	C	N3-C2-O2	-9.64	115.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	861	A	N1-C6-N6	-9.64	112.81	118.60
21	AA	1102	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	2740	A	N1-C6-N6	-9.63	112.82	118.60
21	AA	1368	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	727	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	1866	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1545	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	1299	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2835	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	739	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	1327	A	N1-C6-N6	-9.61	112.83	118.60
2	AC	131	ARG	NE-CZ-NH1	9.60	125.10	120.30
21	AA	499	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	101	A	N1-C6-N6	-9.59	112.84	118.60
21	AA	65	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	539	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	1324	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	978	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	1434	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	920	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	2850	A	N1-C6-N6	-9.57	112.86	118.60
21	AA	415	A	N1-C6-N6	-9.57	112.86	118.60
22	A1	6	A	N1-C6-N6	-9.56	112.86	118.60
21	AA	431	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	21	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	1451	C	O4'-C1'-N1	9.55	115.84	108.20
21	AA	55	A	N1-C6-N6	-9.54	112.87	118.60
21	AA	546	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	761	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	1054	C	N3-C2-O2	-9.52	115.23	121.90
21	AA	149	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	590	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2872	A	N1-C6-N6	-9.52	112.89	118.60
21	AA	977	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2439	A	O4'-C1'-N9	9.51	115.81	108.20
21	AA	1022	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	1395	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	1274	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	2031	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	825	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	1413	A	N1-C6-N6	-9.49	112.91	118.60
55	BB	115	A	N1-C6-N6	-9.48	112.91	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	520	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	630	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1029	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1937	A	O4'-C1'-N9	9.47	115.77	108.20
54	BA	2820	A	N1-C6-N6	-9.46	112.92	118.60
21	AA	547	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	1230	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	2376	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	1237	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	892	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	1531	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	354	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	802	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	2336	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	1608	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1090	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1609	A	O4'-C1'-N9	9.42	115.74	108.20
54	BA	979	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	1829	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	60	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	547	A	O4'-C1'-N9	9.41	115.73	108.20
5	AF	2	ARG	NE-CZ-NH1	9.41	125.00	120.30
54	BA	844	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	2482	A	N1-C6-N6	-9.41	112.96	118.60
21	AA	994	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	1403	A	N1-C6-N6	-9.40	112.96	118.60
38	BP	100	ARG	NE-CZ-NH1	9.40	125.00	120.30
54	BA	575	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	2566	A	N1-C6-N6	-9.39	112.96	118.60
54	BA	1427	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	197	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	1815	A	N1-C6-N6	-9.38	112.97	118.60
48	BZ	29	ARG	NE-CZ-NH1	9.38	124.99	120.30
54	BA	405	U	O4'-C1'-N1	9.37	115.70	108.20
21	AA	649	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1040	A	N1-C6-N6	-9.37	112.98	118.60
55	BB	52	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	666	A	N1-C6-N6	-9.36	112.99	118.60
54	BA	2530	A	N1-C6-N6	-9.36	112.99	118.60
54	BA	1096	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	1536	C	N3-C2-O2	-9.35	115.35	121.90
54	BA	2750	A	N1-C6-N6	-9.35	112.99	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	BS	92	ARG	NE-CZ-NH2	9.34	124.97	120.30
54	BA	310	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1630	A	N1-C6-N6	-9.34	113.00	118.60
21	AA	694	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	2666	C	O4'-C1'-N1	9.34	115.67	108.20
22	A1	41	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	592	A	N1-C6-N6	-9.34	113.00	118.60
21	AA	195	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	872	A	C1'-O4'-C4'	-9.32	102.45	109.90
54	BA	627	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	2564	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	849	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	504	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	1515	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	2020	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	1534	A	C5-C6-N1	9.29	122.34	117.70
54	BA	1848	A	N1-C6-N6	-9.29	113.03	118.60
55	BB	29	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	1785	A	C5-C6-N1	9.28	122.34	117.70
24	A3	1	C	N3-C2-O2	-9.28	115.41	121.90
54	BA	2059	A	N1-C6-N6	-9.28	113.03	118.60
55	BB	50	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	382	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	583	A	N1-C6-N6	-9.27	113.03	118.60
54	BA	1126	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1128	G	O4'-C1'-N9	9.27	115.62	108.20
21	AA	622	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	1180	A	N1-C6-N6	-9.27	113.04	118.60
23	A2	82	A	N1-C6-N6	-9.27	113.04	118.60
28	BF	111	ARG	NE-CZ-NH1	9.26	124.93	120.30
24	A3	38	A	N1-C6-N6	-9.26	113.05	118.60
54	BA	2453	A	N1-C6-N6	-9.26	113.05	118.60
21	AA	336	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	655	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	794	A	N1-C6-N6	-9.25	113.05	118.60
55	BB	109	A	N1-C6-N6	-9.25	113.05	118.60
24	A3	60	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	1746	A	N1-C6-N6	-9.24	113.06	118.60
21	AA	716	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	1943	U	O4'-C1'-N1	9.23	115.59	108.20
45	BW	76	ARG	NE-CZ-NH1	9.23	124.92	120.30
21	AA	1340	A	N1-C6-N6	-9.23	113.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1225	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1027	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	2434	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	661	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	6	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	1853	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	144	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	253	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	1021	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	1227	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	1251	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	439	A	N1-C6-N6	-9.20	113.08	118.60
15	AP	56	ARG	NE-CZ-NH1	9.20	124.90	120.30
54	BA	346	A	N1-C6-N6	-9.19	113.08	118.60
30	BH	123	ARG	NE-CZ-NH1	9.19	124.89	120.30
54	BA	676	A	N1-C6-N6	-9.19	113.09	118.60
23	A2	79	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	637	A	N1-C6-N6	-9.18	113.09	118.60
21	AA	753	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1759	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1854	A	N1-C6-N6	-9.18	113.09	118.60
28	BF	91	ARG	NE-CZ-NH1	9.17	124.89	120.30
54	BA	1098	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	510	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	620	G	O4'-C1'-N9	9.16	115.53	108.20
54	BA	2317	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	673	A	N1-C6-N6	-9.16	113.11	118.60
21	AA	1201	A	N1-C6-N6	-9.16	113.11	118.60
55	BB	59	A	N1-C6-N6	-9.16	113.11	118.60
55	BB	45	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	10	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	205	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	1319	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	1398	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1103	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	1214	C	N3-C2-O2	-9.14	115.50	121.90
54	BA	160	A	N1-C6-N6	-9.14	113.11	118.60
54	BA	478	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	478	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	2273	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	2274	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	560	A	N1-C6-N6	-9.13	113.12	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2765	A	N1-C6-N6	-9.12	113.12	118.60
54	BA	1165	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	1031	C	N3-C2-O2	-9.12	115.52	121.90
54	BA	173	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2154	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2448	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	262	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	1805	A	N1-C6-N6	-9.11	113.13	118.60
21	AA	1145	A	N1-C6-N6	-9.11	113.14	118.60
55	BB	94	A	N1-C6-N6	-9.11	113.14	118.60
33	BK	64	ARG	NE-CZ-NH1	9.11	124.85	120.30
51	B2	28	ARG	NE-CZ-NH1	9.11	124.85	120.30
22	A1	73	A	P-O3'-C3'	9.11	130.63	119.70
54	BA	1014	A	N1-C6-N6	-9.11	113.14	118.60
21	AA	109	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	1678	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2600	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	675	A	N1-C6-N6	-9.10	113.14	118.60
11	AL	30	ARG	NE-CZ-NH1	9.10	124.85	120.30
21	AA	466	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	2893	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	743	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	49	A	O4'-C1'-N9	9.08	115.47	108.20
54	BA	2468	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	626	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	72	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	1359	A	N1-C6-N6	-9.06	113.16	118.60
3	AD	12	ARG	NE-CZ-NH1	9.06	124.83	120.30
54	BA	1509	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	345	A	N1-C6-N6	-9.06	113.17	118.60
21	AA	729	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	906	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1640	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	1042	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	764	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1169	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	1105	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1000	A	N1-C6-N6	-9.04	113.17	118.60
21	AA	374	A	N1-C6-N6	-9.04	113.17	118.60
39	BQ	57	ARG	NE-CZ-NH1	9.04	124.82	120.30
54	BA	2314	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	514	A	N1-C6-N6	-9.03	113.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	928	A	N1-C6-N6	-9.03	113.19	118.60
54	BA	2602	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	1937	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	223	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2062	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	95	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	749	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	161	A	N1-C6-N6	-9.01	113.19	118.60
21	AA	353	A	N1-C6-N6	-9.01	113.20	118.60
54	BA	1496	A	N1-C6-N6	-9.01	113.20	118.60
54	BA	1384	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	327	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	1433	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	127	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	889	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	631	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	274	A	N1-C6-N6	-8.99	113.20	118.60
54	BA	2287	A	N1-C6-N6	-8.99	113.20	118.60
21	AA	1219	A	N1-C6-N6	-8.99	113.20	118.60
55	BB	39	A	N1-C6-N6	-8.99	113.20	118.60
54	BA	213	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	529	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	1314	C	N3-C2-O2	-8.98	115.61	121.90
21	AA	1391	U	O4'-C1'-N1	8.98	115.39	108.20
54	BA	789	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	1092	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	307	C	N3-C2-O2	-8.97	115.62	121.90
54	BA	2184	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	1446	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	265	A	N1-C6-N6	-8.97	113.22	118.60
25	BC	100	ARG	NE-CZ-NH1	8.97	124.78	120.30
54	BA	104	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1302	A	N1-C6-N6	-8.97	113.22	118.60
8	AI	105	ARG	NE-CZ-NH1	8.96	124.78	120.30
54	BA	2461	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	501	C	N3-C2-O2	-8.96	115.63	121.90
21	AA	1257	A	N1-C6-N6	-8.96	113.23	118.60
33	BK	98	ARG	NE-CZ-NH1	8.95	124.78	120.30
54	BA	1603	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	300	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	2108	A	N1-C6-N6	-8.95	113.23	118.60
14	AO	53	ARG	NE-CZ-NH1	8.94	124.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	366	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	1014	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	1711	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	695	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	430	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	2191	A	N1-C6-N6	-8.93	113.25	118.60
21	AA	155	A	N1-C6-N6	-8.92	113.25	118.60
21	AA	554	A	N1-C6-N6	-8.92	113.25	118.60
21	AA	1176	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	699	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	219	A	N1-C6-N6	-8.92	113.25	118.60
6	AG	3	ARG	NE-CZ-NH1	8.92	124.76	120.30
21	AA	1502	A	N1-C6-N6	-8.91	113.25	118.60
21	AA	1269	A	N1-C6-N6	-8.91	113.25	118.60
25	BC	86	ARG	NE-CZ-NH1	8.91	124.75	120.30
54	BA	2077	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1127	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	199	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	913	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1428	C	N3-C2-O2	-8.90	115.67	121.90
54	BA	2335	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1007	C	N3-C2-O2	-8.89	115.67	121.90
54	BA	2764	A	N1-C6-N6	-8.89	113.26	118.60
54	BA	1610	A	O4'-C1'-N9	8.89	115.31	108.20
54	BA	1652	A	N1-C6-N6	-8.89	113.27	118.60
55	BB	53	A	C5-C6-N1	8.89	122.14	117.70
54	BA	609	A	N1-C6-N6	-8.89	113.27	118.60
54	BA	2019	A	C5-C6-N1	8.89	122.14	117.70
54	BA	460	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	961	U	O4'-C1'-N1	8.88	115.31	108.20
54	BA	2753	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	754	C	N3-C2-O2	-8.88	115.69	121.90
56	B5	9	ARG	NE-CZ-NH1	8.88	124.74	120.30
54	BA	2516	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	99	U	O4'-C1'-N1	8.87	115.30	108.20
54	BA	1570	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	607	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	2077	A	C5-C6-N1	8.87	122.13	117.70
55	BB	89	U	O4'-C1'-N1	8.87	115.29	108.20
44	BV	79	ARG	NE-CZ-NH1	8.87	124.73	120.30
54	BA	689	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	2095	A	N1-C6-N6	-8.87	113.28	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2666	C	N3-C2-O2	-8.86	115.69	121.90
34	BL	48	ARG	NE-CZ-NH1	8.86	124.73	120.30
54	BA	2646	C	N3-C2-O2	-8.86	115.70	121.90
54	BA	911	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	2572	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	949	A	N1-C6-N6	-8.86	113.29	118.60
21	AA	749	A	N1-C6-N6	-8.85	113.29	118.60
24	A3	39	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	1461	C	N3-C2-O2	-8.84	115.71	121.90
54	BA	1508	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	2333	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	943	A	C5-C6-N1	8.84	122.12	117.70
54	BA	2088	A	N1-C6-N6	-8.84	113.30	118.60
38	BP	108	ARG	NE-CZ-NH2	8.83	124.72	120.30
21	AA	1197	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	340	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	1641	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	2813	A	N1-C6-N6	-8.83	113.30	118.60
21	AA	182	A	N1-C6-N6	-8.83	113.30	118.60
31	BI	64	ARG	NE-CZ-NH1	8.83	124.71	120.30
54	BA	1593	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	384	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	1803	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	2503	A	O4'-C1'-N9	8.82	115.25	108.20
21	AA	461	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	1626	A	N1-C6-N6	-8.82	113.31	118.60
55	BB	34	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	677	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	81	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1387	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	1256	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	977	A	C5-C6-N1	8.79	122.10	117.70
21	AA	1188	A	N1-C6-N6	-8.79	113.33	118.60
39	BQ	27	ARG	NE-CZ-NH1	8.79	124.69	120.30
54	BA	2090	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2700	A	N1-C6-N6	-8.78	113.33	118.60
28	BF	149	ARG	NE-CZ-NH1	8.78	124.69	120.30
54	BA	2837	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	482	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	282	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1470	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	941	A	N1-C6-N6	-8.77	113.34	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1919	A	N1-C6-N6	-8.76	113.34	118.60
10	AK	127	ARG	NE-CZ-NH1	8.76	124.68	120.30
14	AO	71	ARG	NE-CZ-NH1	8.76	124.68	120.30
21	AA	53	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	706	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	116	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	1081	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	1093	A	N1-C6-N6	-8.75	113.35	118.60
22	A1	2	G	O4'-C1'-N9	8.75	115.20	108.20
54	BA	931	U	O4'-C1'-N1	8.75	115.20	108.20
54	BA	49	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	2281	A	N1-C6-N6	-8.74	113.36	118.60
21	AA	1167	A	C5-C6-N1	8.74	122.07	117.70
21	AA	1170	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	2309	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	126	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	162	A	N1-C6-N6	-8.72	113.36	118.60
54	BA	899	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	2799	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	1349	A	N1-C6-N6	-8.71	113.38	118.60
21	AA	509	A	N1-C6-N6	-8.70	113.38	118.60
21	AA	1082	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	1987	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	2800	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	1705	A	N1-C6-N6	-8.69	113.38	118.60
54	BA	1268	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	687	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	1357	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	234	C	O4'-C1'-N1	8.69	115.15	108.20
21	AA	279	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	1167	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	825	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	644	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1791	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1970	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	349	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1872	A	N1-C6-N6	-8.67	113.39	118.60
54	BA	1789	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	1155	A	N1-C6-N6	-8.66	113.40	118.60
21	AA	1465	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	1755	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	969	A	N1-C6-N6	-8.65	113.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	9	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	802	A	N1-C6-N6	-8.65	113.41	118.60
35	BM	59	ARG	NE-CZ-NH1	8.65	124.62	120.30
54	BA	156	A	N1-C6-N6	-8.65	113.41	118.60
13	AN	81	ARG	NE-CZ-NH1	8.64	124.62	120.30
54	BA	613	A	O4'-C1'-N9	8.64	115.11	108.20
21	AA	1333	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	2614	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	794	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	865	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	873	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	412	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	750	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	1275	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	2426	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	777	A	N1-C6-N6	-8.62	113.42	118.60
54	BA	878	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	896	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	221	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	782	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	298	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	323	C	N1-C2-O2	8.61	124.07	118.90
21	AA	300	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	1936	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	2799	A	O4'-C1'-N9	8.61	115.09	108.20
21	AA	172	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	227	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	2503	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	2758	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	790	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	2471	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	432	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	244	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	782	A	N1-C6-N6	-8.59	113.44	118.60
26	BD	128	ARG	NE-CZ-NH1	8.59	124.60	120.30
21	AA	608	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	1410	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	225	C	O4'-C1'-N1	8.59	115.07	108.20
21	AA	151	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	2358	A	N1-C6-N6	-8.58	113.45	118.60
4	AE	92	ARG	NE-CZ-NH1	8.58	124.59	120.30
50	B1	5	ARG	NE-CZ-NH1	8.58	124.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1668	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	2899	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	1088	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2298	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2328	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	572	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	415	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	814	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2741	A	N1-C6-N6	-8.56	113.46	118.60
7	AH	116	ARG	NE-CZ-NH1	8.56	124.58	120.30
54	BA	1665	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	981	A	C5-C6-N1	8.56	121.98	117.70
54	BA	1553	A	N1-C6-N6	-8.56	113.47	118.60
54	BA	1632	A	N1-C6-N6	-8.56	113.47	118.60
21	AA	1168	U	O4'-C1'-N1	8.55	115.04	108.20
54	BA	1028	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	172	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	1353	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	152	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	547	A	N1-C6-N6	-8.52	113.49	118.60
6	AG	4	ARG	NE-CZ-NH1	8.52	124.56	120.30
21	AA	223	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	1277	C	N3-C2-O2	-8.52	115.94	121.90
54	BA	1586	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	995	C	N3-C2-O2	-8.51	115.94	121.90
54	BA	311	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1616	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	98	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	528	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1265	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	1329	A	N1-C6-N6	-8.51	113.50	118.60
21	AA	251	G	O4'-C1'-N9	8.51	115.00	108.20
21	AA	1204	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	457	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	689	A	C5-C6-N1	8.50	121.95	117.70
54	BA	2114	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	2887	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	167	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	174	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1285	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	2119	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1569	A	N1-C6-N6	-8.49	113.50	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	66	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	1117	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	1783	A	C5-C6-N1	8.49	121.94	117.70
54	BA	1889	A	N1-C6-N6	-8.49	113.51	118.60
8	AI	40	ARG	NE-CZ-NH1	8.49	124.54	120.30
12	AM	112	ARG	NE-CZ-NH1	8.48	124.54	120.30
54	BA	734	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1392	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1745	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	2425	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1069	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1502	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1264	A	N1-C6-N6	-8.48	113.52	118.60
21	AA	459	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	1347	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	2705	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	655	A	N1-C6-N6	-8.47	113.52	118.60
11	AL	120	ARG	NE-CZ-NH2	8.46	124.53	120.30
21	AA	345	C	N3-C2-O2	-8.46	115.97	121.90
54	BA	1213	A	C5-C6-N1	8.46	121.93	117.70
54	BA	64	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	2423	U	O4'-C1'-N1	8.46	114.97	108.20
24	A3	22	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1544	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	2868	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	1525	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	1101	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	750	A	C5-C6-N1	8.45	121.92	117.70
54	BA	1288	G	O4'-C1'-N9	8.45	114.96	108.20
54	BA	1367	A	C5-C6-N1	8.45	121.92	117.70
54	BA	563	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	2005	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	2727	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	2340	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	2734	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	160	A	N1-C6-N6	-8.43	113.54	118.60
38	BP	92	ARG	NE-CZ-NH1	8.43	124.52	120.30
21	AA	1430	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	1077	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	322	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	2411	A	N1-C6-N6	-8.43	113.55	118.60
21	AA	1151	A	N1-C6-N6	-8.42	113.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	640	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	1205	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	1238	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	1433	A	C5-C6-N1	8.41	121.91	117.70
54	BA	1854	A	C5-C6-N1	8.41	121.91	117.70
54	BA	429	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	535	A	C5-C6-N1	8.41	121.91	117.70
54	BA	1552	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	2388	A	N1-C6-N6	-8.41	113.55	118.60
36	BN	71	ARG	NE-CZ-NH1	8.41	124.50	120.30
54	BA	330	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	990	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	1048	A	N1-C6-N6	-8.41	113.56	118.60
21	AA	1016	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	26	A	N1-C6-N6	-8.40	113.56	118.60
30	BH	27	ARG	NE-CZ-NH1	8.39	124.50	120.30
27	BE	44	ARG	NE-CZ-NH1	8.39	124.50	120.30
54	BA	1080	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	497	A	C5-C6-N1	8.39	121.89	117.70
21	AA	1200	C	N3-C2-O2	-8.39	116.03	121.90
54	BA	910	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	2055	C	O4'-C1'-N1	8.39	114.91	108.20
21	AA	1163	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	490	C	N1-C2-O2	8.38	123.93	118.90
54	BA	2058	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	452	A	C5-C6-N1	8.38	121.89	117.70
54	BA	2711	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	784	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1431	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	1257	A	C5-C6-N1	8.37	121.89	117.70
54	BA	2378	A	N1-C6-N6	-8.37	113.58	118.60
38	BP	61	ARG	NE-CZ-NH1	8.37	124.48	120.30
54	BA	1932	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1912	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	2080	A	N1-C6-N6	-8.37	113.58	118.60
6	AG	9	ARG	NE-CZ-NH1	8.36	124.48	120.30
21	AA	456	A	N1-C6-N6	-8.36	113.58	118.60
21	AA	1110	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	1567	G	O4'-C1'-N9	8.36	114.89	108.20
21	AA	576	C	N3-C2-O2	-8.36	116.05	121.90
54	BA	1070	A	C5-C6-N1	8.36	121.88	117.70
54	BA	1597	A	N1-C6-N6	-8.36	113.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1615	C	N3-C2-O2	-8.35	116.05	121.90
55	BB	36	C	N3-C2-O2	-8.35	116.05	121.90
12	AM	92	ARG	NE-CZ-NH1	8.35	124.47	120.30
54	BA	1420	A	C5-C6-N1	8.35	121.87	117.70
21	AA	1289	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	792	A	N1-C6-N6	-8.35	113.59	118.60
14	AO	57	ARG	NE-CZ-NH1	8.34	124.47	120.30
54	BA	270	A	C5-C6-N1	8.34	121.87	117.70
21	AA	1492	A	N1-C6-N6	-8.34	113.59	118.60
55	BB	66	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	1699	G	O4'-C1'-N9	8.34	114.87	108.20
21	AA	1493	A	C5-C6-N1	8.34	121.87	117.70
21	AA	338	A	N1-C6-N6	-8.33	113.60	118.60
20	AU	32	ARG	NE-CZ-NH1	8.33	124.47	120.30
21	AA	559	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1057	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1266	G	O4'-C1'-N9	8.33	114.87	108.20
54	BA	94	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	586	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1459	G	O4'-C1'-N9	8.33	114.86	108.20
21	AA	181	A	C5-C6-N1	8.33	121.86	117.70
21	AA	441	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	2163	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	164	G	O4'-C1'-N9	8.32	114.86	108.20
21	AA	246	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	706	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	219	A	C5-C6-N1	8.32	121.86	117.70
54	BA	1810	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	1321	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	1050	A	C5-C6-N1	8.32	121.86	117.70
54	BA	1253	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	535	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	1437	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	50	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	526	A	N1-C6-N6	-8.30	113.62	118.60
21	AA	665	A	C5-C6-N1	8.30	121.85	117.70
32	BJ	37	ARG	NE-CZ-NH1	8.30	124.45	120.30
54	BA	352	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	2021	C	N3-C2-O2	-8.30	116.09	121.90
54	BA	2198	A	N1-C6-N6	-8.30	113.62	118.60
21	AA	807	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1254	A	C5-C6-N1	8.29	121.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1871	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	118	A	C5-C6-N1	8.28	121.84	117.70
54	BA	1918	A	N1-C6-N6	-8.28	113.63	118.60
21	AA	152	A	C5-C6-N1	8.28	121.84	117.70
21	AA	1480	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	1650	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	2602	A	C5-C6-N1	8.27	121.83	117.70
21	AA	1447	A	C5-C6-N1	8.27	121.83	117.70
21	AA	1518	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	1531	A	C5-C6-N1	8.27	121.83	117.70
54	BA	1618	A	C5-C6-N1	8.27	121.83	117.70
54	BA	2055	C	N3-C2-O2	-8.27	116.11	121.90
12	AM	2	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	1434	A	C5-C6-N1	8.26	121.83	117.70
56	B5	134	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	2327	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	1596	A	N1-C6-N6	-8.26	113.65	118.60
54	BA	2114	A	C5-C6-N1	8.26	121.83	117.70
54	BA	2660	A	N1-C6-N6	-8.26	113.65	118.60
54	BA	404	A	N1-C6-N6	-8.25	113.65	118.60
24	A3	44	A	N1-C6-N6	-8.25	113.65	118.60
3	AD	127	ARG	NE-CZ-NH1	8.25	124.42	120.30
28	BF	94	ARG	NE-CZ-NH1	8.25	124.42	120.30
54	BA	2126	A	N1-C6-N6	-8.24	113.65	118.60
21	AA	320	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1499	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	103	A	N1-C6-N6	-8.24	113.65	118.60
54	BA	1609	A	N1-C6-N6	-8.24	113.65	118.60
54	BA	1342	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	1757	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1080	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1227	A	C5-C6-N1	8.24	121.82	117.70
25	BC	216	ARG	NE-CZ-NH1	8.24	124.42	120.30
54	BA	1040	A	C5-C6-N1	8.24	121.82	117.70
54	BA	668	A	N1-C6-N6	-8.23	113.66	118.60
18	AS	2	ARG	NE-CZ-NH1	8.23	124.42	120.30
21	AA	946	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	255	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2736	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	579	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	696	A	N1-C6-N6	-8.23	113.66	118.60
1	AB	94	ARG	NE-CZ-NH1	8.23	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AL	85	ARG	NE-CZ-NH1	8.23	124.41	120.30
21	AA	1213	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	118	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	522	A	C5-C6-N1	8.22	121.81	117.70
21	AA	87	C	N3-C2-O2	-8.22	116.15	121.90
21	AA	395	C	N3-C2-O2	-8.22	116.15	121.90
21	AA	1275	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1819	A	C5-C6-N1	8.22	121.81	117.70
21	AA	236	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	742	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	981	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	1046	A	O4'-C1'-N9	8.21	114.77	108.20
21	AA	596	A	C5-C6-N1	8.21	121.80	117.70
21	AA	648	A	N1-C6-N6	-8.21	113.68	118.60
21	AA	1080	A	C5-C6-N1	8.21	121.80	117.70
54	BA	1214	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1773	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	767	A	C5-C6-N1	8.19	121.80	117.70
54	BA	735	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2171	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	364	A	N1-C6-N6	-8.18	113.69	118.60
36	BN	17	ARG	NE-CZ-NH1	8.18	124.39	120.30
54	BA	1144	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1286	A	C5-C6-N1	8.18	121.79	117.70
54	BA	2565	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	16	A	C5-C6-N1	8.18	121.79	117.70
54	BA	983	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1143	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	629	A	C5-C6-N1	8.17	121.79	117.70
21	AA	8	A	C5-C6-N1	8.17	121.78	117.70
37	BO	81	ARG	NE-CZ-NH1	8.17	124.39	120.30
54	BA	2778	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2061	G	O4'-C1'-N9	8.16	114.73	108.20
21	AA	635	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	1456	A	N1-C6-N6	-8.16	113.70	118.60
44	BV	18	ARG	NE-CZ-NH1	8.16	124.38	120.30
11	AL	53	ARG	NE-CZ-NH1	8.16	124.38	120.30
54	BA	1086	A	C5-C6-N1	8.16	121.78	117.70
21	AA	189	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	2740	A	C5-C6-N1	8.15	121.78	117.70
54	BA	1088	A	C5-C6-N1	8.15	121.78	117.70
54	BA	53	A	N1-C6-N6	-8.15	113.71	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BO	25	ARG	NE-CZ-NH1	8.15	124.37	120.30
54	BA	751	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	996	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	1032	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	614	A	N1-C6-N6	-8.13	113.72	118.60
5	AF	91	ARG	NE-CZ-NH1	8.13	124.36	120.30
21	AA	1239	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	1012	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	1214	C	O4'-C1'-N1	8.13	114.70	108.20
13	AN	24	ARG	NE-CZ-NH1	8.12	124.36	120.30
54	BA	91	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	715	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1654	A	C5-C6-N1	8.12	121.76	117.70
54	BA	1783	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	2469	A	N1-C6-N6	-8.12	113.73	118.60
55	BB	58	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	501	C	N1-C2-O2	8.12	123.77	118.90
54	BA	896	A	C5-C6-N1	8.12	121.76	117.70
54	BA	973	A	C5-C6-N1	8.12	121.76	117.70
54	BA	429	A	C5-C6-N1	8.11	121.76	117.70
21	AA	353	A	C5-C6-N1	8.11	121.76	117.70
21	AA	344	A	C5-C6-N1	8.11	121.75	117.70
21	AA	371	A	C5-C6-N1	8.11	121.75	117.70
54	BA	1809	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2792	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	522	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	2733	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	815	A	N1-C6-N6	-8.10	113.74	118.60
1	AB	34	ARG	NE-CZ-NH1	8.09	124.35	120.30
21	AA	1183	U	N3-C2-O2	-8.09	116.54	122.20
54	BA	146	A	N1-C6-N6	-8.09	113.75	118.60
21	AA	1519	A	C5-C6-N1	8.09	121.74	117.70
54	BA	1580	A	N1-C6-N6	-8.09	113.75	118.60
21	AA	465	A	C5-C6-N1	8.09	121.74	117.70
21	AA	1299	A	C5-C6-N1	8.09	121.74	117.70
54	BA	1020	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	1808	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2266	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	372	G	O4'-C1'-N9	8.08	114.67	108.20
54	BA	742	A	C5-C6-N1	8.08	121.74	117.70
54	BA	1156	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	1490	A	N1-C6-N6	-8.08	113.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1899	A	C5-C6-N1	8.08	121.74	117.70
54	BA	423	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	2129	C	N3-C2-O2	-8.08	116.24	121.90
54	BA	2725	A	N1-C6-N6	-8.08	113.75	118.60
33	BK	31	ARG	NE-CZ-NH1	8.08	124.34	120.30
54	BA	508	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	1069	A	C5-C6-N1	8.07	121.74	117.70
54	BA	2369	A	N1-C6-N6	-8.07	113.75	118.60
54	BA	2105	U	O4'-C1'-N1	8.07	114.66	108.20
47	BY	23	ARG	NE-CZ-NH1	8.07	124.34	120.30
54	BA	1314	C	N1-C2-O2	8.07	123.74	118.90
21	AA	915	A	N1-C6-N6	-8.07	113.76	118.60
38	BP	71	ARG	NE-CZ-NH1	8.07	124.33	120.30
54	BA	1672	A	C5-C6-N1	8.07	121.73	117.70
37	BO	16	ARG	NE-CZ-NH1	8.06	124.33	120.30
54	BA	119	A	C5-C6-N1	8.06	121.73	117.70
54	BA	265	A	C5-C6-N1	8.06	121.73	117.70
54	BA	730	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	2270	A	C5-C6-N1	8.06	121.73	117.70
15	AP	31	ARG	NE-CZ-NH1	8.06	124.33	120.30
21	AA	238	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	515	A	C5-C6-N1	8.05	121.73	117.70
21	AA	243	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	670	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	2003	A	C5-C6-N1	8.05	121.72	117.70
54	BA	1497	U	O4'-C1'-N1	8.04	114.64	108.20
54	BA	2311	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	2297	A	C5-C6-N1	8.04	121.72	117.70
54	BA	2589	A	N1-C6-N6	-8.04	113.77	118.60
55	BB	29	A	C5-C6-N1	8.05	121.72	117.70
21	AA	382	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	1004	A	N1-C6-N6	-8.04	113.77	118.60
27	BE	170	ARG	NE-CZ-NH1	8.04	124.32	120.30
54	BA	756	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	44	A	C5-C6-N1	8.04	121.72	117.70
21	AA	1287	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1367	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	1548	A	N1-C6-N6	-8.04	113.78	118.60
22	A1	38	A	C5-C6-N1	8.03	121.72	117.70
22	A1	38	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	1528	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	1928	A	N1-C6-N6	-8.03	113.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	95	C	N3-C2-O2	-8.03	116.28	121.90
54	BA	422	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	1378	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	1433	A	N1-C6-N6	-8.03	113.78	118.60
23	A2	91	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	877	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	1913	A	N1-C6-N6	-8.03	113.78	118.60
34	BL	47	ARG	NE-CZ-NH1	8.03	124.31	120.30
54	BA	1439	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	1021	A	C5-C6-N1	8.02	121.71	117.70
25	BC	174	ARG	NE-CZ-NH2	-8.02	116.29	120.30
54	BA	721	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	1579	A	C5-C6-N1	8.01	121.71	117.70
54	BA	2381	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	2426	A	C5-C6-N1	8.01	121.71	117.70
54	BA	1385	A	N1-C6-N6	-8.01	113.79	118.60
21	AA	262	A	C5-C6-N1	8.01	121.70	117.70
54	BA	1050	A	N1-C6-N6	-8.01	113.80	118.60
24	A3	36	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	1392	A	C5-C6-N1	8.01	121.70	117.70
55	BB	108	A	N1-C6-N6	-8.01	113.80	118.60
25	BC	155	ARG	NE-CZ-NH1	8.00	124.30	120.30
10	AK	126	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	1780	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1469	A	C5-C6-N1	8.00	121.70	117.70
54	BA	391	A	C5-C6-N1	7.99	121.70	117.70
54	BA	204	A	C5-C6-N1	7.99	121.70	117.70
54	BA	2033	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	2281	A	C5-C6-N1	7.99	121.69	117.70
12	AM	106	ARG	C-N-CA	7.99	141.67	121.70
54	BA	449	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	1204	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	2590	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	26	A	C5-C6-N1	7.99	121.69	117.70
54	BA	1304	A	C4-C5-C6	-7.99	113.01	117.00
54	BA	2726	A	C5-C6-N1	7.99	121.69	117.70
54	BA	2306	C	N3-C2-O2	-7.98	116.31	121.90
21	AA	621	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	195	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	1784	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1870	C	N3-C2-O2	-7.98	116.31	121.90
54	BA	401	A	N1-C6-N6	-7.98	113.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1419	A	C5-C6-N1	7.98	121.69	117.70
54	BA	2547	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	1111	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	1451	C	N3-C2-O2	-7.98	116.32	121.90
54	BA	1700	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	676	A	C5-C6-N1	7.97	121.69	117.70
54	BA	342	A	C5-C6-N1	7.97	121.69	117.70
21	AA	1145	A	C5-C6-N1	7.97	121.69	117.70
54	BA	574	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	2632	A	C4-C5-C6	-7.97	113.01	117.00
54	BA	1085	A	C5-C6-N1	7.97	121.68	117.70
54	BA	2662	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	990	A	C5-C6-N1	7.97	121.68	117.70
54	BA	2435	A	C5-C6-N1	7.97	121.68	117.70
44	BV	93	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	1477	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	1871	A	O4'-C1'-N9	7.96	114.57	108.20
54	BA	1084	A	C5-C6-N1	7.96	121.68	117.70
56	B5	162	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	2749	A	N1-C6-N6	-7.96	113.82	118.60
21	AA	873	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1735	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1495	A	N1-C6-N6	-7.96	113.83	118.60
21	AA	1287	A	C4-C5-C6	-7.96	113.02	117.00
54	BA	2706	A	N1-C6-N6	-7.96	113.83	118.60
25	BC	68	ARG	NE-CZ-NH1	7.95	124.28	120.30
21	AA	547	A	C5-C6-N1	7.95	121.67	117.70
21	AA	120	A	C5-C6-N1	7.95	121.67	117.70
11	AL	82	ARG	NE-CZ-NH1	7.95	124.27	120.30
21	AA	119	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	878	A	N1-C6-N6	-7.95	113.83	118.60
8	AI	124	PRO	CA-N-CD	-7.95	100.38	111.50
54	BA	344	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	513	A	C5-C6-N1	7.95	121.67	117.70
7	AH	83	ARG	NE-CZ-NH1	7.94	124.27	120.30
21	AA	1431	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	1008	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	74	A	C5-C6-N1	7.94	121.67	117.70
21	AA	1429	A	C4-C5-C6	-7.94	113.03	117.00
54	BA	833	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	2135	A	C5-C6-N1	7.94	121.67	117.70
21	AA	1288	A	N1-C6-N6	-7.93	113.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2750	A	C5-C6-N1	7.93	121.67	117.70
21	AA	412	A	C5-C6-N1	7.93	121.67	117.70
54	BA	983	A	C5-C6-N1	7.93	121.67	117.70
54	BA	1625	C	N3-C2-O2	-7.93	116.35	121.90
21	AA	280	C	N3-C2-O2	-7.93	116.35	121.90
21	AA	1196	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1028	A	C5-C6-N1	7.93	121.66	117.70
21	AA	1274	A	C5-C6-N1	7.93	121.66	117.70
54	BA	270	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1385	A	C5-C6-N1	7.93	121.66	117.70
21	AA	152	A	C4-C5-C6	-7.92	113.04	117.00
25	BC	79	ARG	NE-CZ-NH1	7.92	124.26	120.30
54	BA	428	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	608	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1189	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	162	A	C5-C6-N1	7.92	121.66	117.70
54	BA	504	A	C5-C6-N1	7.92	121.66	117.70
21	AA	968	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1654	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	19	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	71	A	C5-C6-N1	7.92	121.66	117.70
11	AL	113	ARG	NE-CZ-NH1	7.92	124.26	120.30
54	BA	1073	A	O4'-C1'-N9	7.92	114.53	108.20
16	AQ	5	ARG	NE-CZ-NH1	7.92	124.26	120.30
21	AA	451	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	943	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	959	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	1095	A	C5-C6-N1	7.91	121.66	117.70
21	AA	1346	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	1626	A	C5-C6-N1	7.91	121.66	117.70
21	AA	574	A	C5-C6-N1	7.91	121.65	117.70
21	AA	1503	A	C5-C6-N1	7.91	121.65	117.70
54	BA	1460	U	O4'-C1'-N1	7.91	114.53	108.20
21	AA	363	A	C5-C6-N1	7.91	121.65	117.70
54	BA	139	U	O4'-C1'-N1	7.91	114.53	108.20
21	AA	197	A	N1-C6-N6	-7.91	113.86	118.60
47	BY	47	ARG	NE-CZ-NH1	7.91	124.25	120.30
54	BA	1755	A	C5-C6-N1	7.91	121.65	117.70
15	AP	5	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	1522	A	N1-C6-N6	-7.90	113.86	118.60
22	A1	76	A	C5-C6-N6	7.90	130.02	123.70
31	BI	133	ARG	NE-CZ-NH1	7.90	124.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	502	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	1129	A	C5-C6-N1	7.90	121.65	117.70
54	BA	1610	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	2587	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2776	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1005	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2577	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1441	A	C5-C6-N1	7.89	121.65	117.70
54	BA	432	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	1773	A	C5-C6-N1	7.89	121.65	117.70
54	BA	2126	A	O4'-C1'-N9	7.89	114.52	108.20
15	AP	28	ARG	NE-CZ-NH1	7.89	124.25	120.30
54	BA	368	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	867	C	N3-C2-O2	-7.89	116.38	121.90
54	BA	793	A	C5-C6-N1	7.89	121.65	117.70
21	AA	1375	A	N1-C6-N6	-7.89	113.87	118.60
41	BS	25	ARG	NE-CZ-NH1	7.89	124.24	120.30
54	BA	2856	A	N1-C6-N6	-7.89	113.87	118.60
54	BA	278	A	C5-C6-N1	7.88	121.64	117.70
54	BA	845	A	C5-C6-N1	7.88	121.64	117.70
21	AA	415	A	C5-C6-N1	7.88	121.64	117.70
21	AA	461	A	C5-C6-N1	7.88	121.64	117.70
55	BB	104	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	2829	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	1690	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	2297	A	N1-C6-N6	-7.87	113.88	118.60
7	AH	113	ARG	NE-CZ-NH1	7.87	124.23	120.30
54	BA	800	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	1169	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	309	A	C5-C6-N1	7.87	121.63	117.70
54	BA	1070	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	1211	C	N3-C2-O2	-7.87	116.39	121.90
54	BA	2322	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	2418	A	C4-C5-C6	-7.87	113.07	117.00
54	BA	2497	A	C5-C6-N1	7.87	121.63	117.70
21	AA	764	C	N3-C2-O2	-7.86	116.39	121.90
54	BA	2311	A	C5-C6-N1	7.86	121.63	117.70
54	BA	727	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2518	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	2284	A	N1-C6-N6	-7.86	113.89	118.60
21	AA	519	C	N3-C2-O2	-7.86	116.40	121.90
21	AA	629	A	N1-C6-N6	-7.86	113.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	35	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2094	A	N1-C6-N6	-7.86	113.89	118.60
21	AA	1396	A	C4-C5-C6	-7.86	113.07	117.00
25	BC	174	ARG	NE-CZ-NH1	7.86	124.23	120.30
54	BA	1700	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1762	A	N1-C6-N6	-7.85	113.89	118.60
21	AA	78	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2212	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	1535	A	C5-C6-N1	7.85	121.62	117.70
54	BA	2518	A	O4'-C1'-N9	7.85	114.48	108.20
54	BA	505	A	N1-C6-N6	-7.85	113.89	118.60
22	A1	47	U	C1'-O4'-C4'	-7.85	103.62	109.90
54	BA	2761	A	C5-C6-N1	7.85	121.62	117.70
54	BA	2781	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	2062	A	C5-C6-N1	7.84	121.62	117.70
21	AA	373	A	C5-C6-N1	7.84	121.62	117.70
21	AA	665	A	C4-C5-C6	-7.83	113.08	117.00
21	AA	1004	A	C5-C6-N1	7.83	121.62	117.70
54	BA	1978	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	513	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	89	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	2037	A	C5-C6-N1	7.83	121.61	117.70
21	AA	238	A	C5-C6-N1	7.83	121.61	117.70
3	AD	114	ARG	NE-CZ-NH1	7.83	124.21	120.30
54	BA	1847	A	C5-C6-N1	7.83	121.61	117.70
21	AA	65	A	C5-C6-N1	7.82	121.61	117.70
21	AA	935	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	2513	A	C5-C6-N1	7.82	121.61	117.70
21	AA	71	A	N1-C6-N6	-7.82	113.91	118.60
22	A1	73	A	C5-C6-N1	7.82	121.61	117.70
54	BA	195	A	C5-C6-N1	7.82	121.61	117.70
54	BA	2037	A	N1-C6-N6	-7.82	113.91	118.60
16	AQ	10	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	2823	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	2063	C	N3-C2-O2	-7.81	116.43	121.90
54	BA	2147	A	C5-C6-N1	7.81	121.61	117.70
54	BA	2407	A	N1-C6-N6	-7.81	113.91	118.60
21	AA	129	A	N1-C6-N6	-7.81	113.91	118.60
21	AA	130	A	C5-C6-N1	7.81	121.61	117.70
54	BA	572	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	1365	A	N1-C6-N6	-7.81	113.91	118.60
21	AA	279	A	C5-C6-N1	7.81	121.61	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	820	A	C5-C6-N1	7.81	121.60	117.70
54	BA	1669	A	N1-C6-N6	-7.81	113.92	118.60
21	AA	8	A	N1-C6-N6	-7.81	113.92	118.60
43	BU	5	ARG	NE-CZ-NH1	7.81	124.20	120.30
54	BA	1552	A	O4'-C1'-N9	7.81	114.45	108.20
21	AA	533	A	N1-C6-N6	-7.81	113.92	118.60
21	AA	50	A	C5-C6-N1	7.80	121.60	117.70
54	BA	19	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	1534	U	O4'-C1'-N1	7.80	114.44	108.20
54	BA	1387	A	C5-C6-N1	7.80	121.60	117.70
54	BA	2288	A	C5-C6-N1	7.80	121.60	117.70
54	BA	2366	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	414	A	N1-C6-N6	-7.79	113.92	118.60
21	AA	523	A	N1-C6-N6	-7.79	113.92	118.60
55	BB	80	U	O4'-C1'-N1	7.79	114.44	108.20
21	AA	1398	A	C5-C6-N1	7.79	121.60	117.70
54	BA	5	A	N1-C6-N6	-7.79	113.92	118.60
54	BA	1057	A	C5-C6-N1	7.79	121.60	117.70
54	BA	1635	A	C5-C6-N1	7.79	121.60	117.70
54	BA	2475	C	N3-C2-O2	-7.79	116.45	121.90
21	AA	702	A	C5-C6-N1	7.79	121.59	117.70
54	BA	2432	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	509	A	C5-C6-N1	7.79	121.59	117.70
54	BA	52	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	241	A	C5-C6-N1	7.79	121.59	117.70
54	BA	582	A	N1-C6-N6	-7.79	113.93	118.60
4	AE	137	ARG	NE-CZ-NH1	7.78	124.19	120.30
54	BA	507	A	C5-C6-N1	7.78	121.59	117.70
54	BA	972	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	1134	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1246	A	C4-C5-C6	-7.78	113.11	117.00
54	BA	2799	A	C5-C6-N1	7.78	121.59	117.70
54	BA	342	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	742	A	C4-C5-C6	-7.78	113.11	117.00
54	BA	1669	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2406	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	1246	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	393	A	C4-C5-C6	-7.78	113.11	117.00
21	AA	1507	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	752	A	N1-C6-N6	-7.78	113.94	118.60
54	BA	299	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	1545	A	C5-C6-N1	7.77	121.59	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	447	A	C5-C6-N1	7.77	121.59	117.70
4	AE	156	ARG	NE-CZ-NH1	7.77	124.19	120.30
21	AA	560	A	C5-C6-N1	7.77	121.58	117.70
54	BA	38	A	C4-C5-C6	-7.77	113.11	117.00
54	BA	1247	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	676	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	199	A	C5-C6-N1	7.77	121.58	117.70
21	AA	595	A	C5-C6-N1	7.76	121.58	117.70
36	BN	103	ARG	NE-CZ-NH1	7.76	124.18	120.30
21	AA	120	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	1456	A	C5-C6-N1	7.75	121.58	117.70
54	BA	1689	A	C5-C6-N1	7.75	121.58	117.70
21	AA	1339	A	N1-C6-N6	-7.75	113.95	118.60
6	AG	94	ARG	NE-CZ-NH1	7.75	124.17	120.30
54	BA	1077	A	C5-C6-N1	7.75	121.58	117.70
21	AA	151	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1236	A	C5-C6-N1	7.75	121.57	117.70
54	BA	176	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2723	C	N3-C2-O2	-7.75	116.48	121.90
54	BA	603	A	C5-C6-N1	7.75	121.57	117.70
54	BA	2749	A	C5-C6-N1	7.75	121.57	117.70
22	A1	73	A	C4-C5-C6	-7.74	113.13	117.00
54	BA	1553	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1598	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1265	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1900	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	2700	A	C5-C6-N1	7.74	121.57	117.70
21	AA	313	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	1987	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1689	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	1000	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	2542	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2670	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	608	A	C5-C6-N1	7.73	121.57	117.70
54	BA	761	A	C5-C6-N1	7.73	121.57	117.70
21	AA	718	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	526	A	C5-C6-N1	7.73	121.56	117.70
54	BA	2835	A	C5-C6-N1	7.73	121.56	117.70
21	AA	937	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	169	C	N3-C2-O2	-7.72	116.50	121.90
54	BA	532	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1749	A	N1-C6-N6	-7.72	113.97	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1998	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	1794	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	288	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	412	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	718	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	907	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	705	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	2880	C	N3-C2-O2	-7.71	116.50	121.90
21	AA	501	C	O4'-C1'-N1	7.71	114.37	108.20
21	AA	523	A	C5-C6-N1	7.71	121.56	117.70
21	AA	767	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	1067	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	73	C	N3-C2-O2	-7.71	116.50	121.90
21	AA	228	A	C4-C5-C6	-7.71	113.15	117.00
21	AA	715	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	1285	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	1434	A	O4'-C1'-N9	7.71	114.37	108.20
54	BA	2587	A	C4-C5-C6	-7.71	113.15	117.00
54	BA	1213	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	1551	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	2268	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	2758	A	C5-C6-N1	7.71	121.55	117.70
55	BB	70	C	N3-C2-O2	-7.71	116.51	121.90
28	BF	177	ARG	NE-CZ-NH1	7.71	124.15	120.30
54	BA	802	A	C5-C6-N1	7.71	121.55	117.70
21	AA	248	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	332	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2430	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1073	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1327	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1919	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1928	A	C5-C6-N1	7.70	121.55	117.70
54	BA	453	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1802	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	197	A	C5-C6-N1	7.70	121.55	117.70
21	AA	468	A	C5-C6-N1	7.70	121.55	117.70
21	AA	746	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	804	A	C5-C6-N1	7.69	121.55	117.70
21	AA	1204	A	C5-C6-N1	7.69	121.55	117.70
40	BR	68	ARG	NE-CZ-NH1	7.69	124.15	120.30
54	BA	1404	C	N3-C2-O2	-7.69	116.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1377	A	C5-C6-N1	7.69	121.54	117.70
35	BM	114	ARG	NE-CZ-NH1	7.69	124.14	120.30
54	BA	101	A	C5-C6-N1	7.69	121.54	117.70
54	BA	616	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	1275	A	C5-C6-N1	7.69	121.54	117.70
54	BA	1801	A	N1-C6-N6	-7.69	113.99	118.60
46	BX	56	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	1072	C	N3-C2-O2	-7.68	116.52	121.90
21	AA	306	A	C5-C6-N1	7.68	121.54	117.70
21	AA	315	A	C5-C6-N1	7.68	121.54	117.70
54	BA	310	A	C5-C6-N1	7.68	121.54	117.70
22	A1	14	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	1677	A	N1-C6-N6	-7.68	114.00	118.60
54	BA	2667	C	N3-C2-O2	-7.68	116.53	121.90
54	BA	527	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	980	A	C5-C6-N1	7.67	121.54	117.70
54	BA	2646	C	N1-C2-O2	7.67	123.50	118.90
21	AA	595	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1216	A	O4'-C1'-N9	7.67	114.34	108.20
24	A3	58	A	N1-C6-N6	-7.67	114.00	118.60
52	B3	39	ARG	NE-CZ-NH1	7.67	124.14	120.30
21	AA	1418	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	909	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	1336	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	1678	A	C5-C6-N1	7.67	121.53	117.70
54	BA	2336	A	C5-C6-N1	7.67	121.53	117.70
54	BA	2733	A	C5-C6-N1	7.67	121.53	117.70
6	AG	118	ARG	NE-CZ-NH1	7.67	124.13	120.30
54	BA	985	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	2117	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2766	A	C5-C6-N1	7.67	121.53	117.70
21	AA	16	A	N1-C6-N6	-7.67	114.00	118.60
16	AQ	61	ARG	NE-CZ-NH1	7.66	124.13	120.30
54	BA	654	A	C5-C6-N1	7.66	121.53	117.70
54	BA	1900	A	C5-C6-N1	7.66	121.53	117.70
25	BC	176	ARG	NE-CZ-NH1	7.66	124.13	120.30
54	BA	563	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2729	G	O4'-C1'-N9	7.66	114.33	108.20
21	AA	815	A	C5-C6-N1	7.66	121.53	117.70
54	BA	1591	A	C5-C6-N1	7.66	121.53	117.70
54	BA	294	A	C5-C6-N1	7.66	121.53	117.70
21	AA	1028	C	N3-C2-O2	-7.66	116.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	222	A	N1-C6-N6	-7.66	114.01	118.60
21	AA	432	A	C5-C6-N1	7.65	121.53	117.70
21	AA	1152	A	C5-C6-N1	7.65	121.53	117.70
22	A1	60	C	N3-C2-O2	-7.65	116.54	121.90
54	BA	2030	A	C5-C6-N1	7.65	121.53	117.70
21	AA	845	A	C5-C6-N1	7.65	121.53	117.70
54	BA	793	A	C4-C5-C6	-7.65	113.17	117.00
54	BA	2273	A	C5-C6-N1	7.65	121.53	117.70
54	BA	2886	A	C5-C6-N1	7.65	121.53	117.70
21	AA	532	A	C5-C6-N1	7.65	121.52	117.70
21	AA	1197	A	C5-C6-N1	7.65	121.52	117.70
54	BA	1008	A	C5-C6-N1	7.65	121.52	117.70
6	AG	137	ARG	NE-CZ-NH1	7.64	124.12	120.30
21	AA	321	A	N1-C6-N6	-7.64	114.01	118.60
54	BA	627	A	C5-C6-N1	7.64	121.52	117.70
54	BA	1786	A	C5-C6-N1	7.64	121.52	117.70
12	AM	106	ARG	NE-CZ-NH1	7.64	124.12	120.30
54	BA	272	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	947	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2009	A	C4-C5-C6	-7.64	113.18	117.00
54	BA	2853	C	O4'-C1'-N1	7.64	114.31	108.20
21	AA	1054	C	N1-C2-O2	7.64	123.48	118.90
54	BA	1965	C	N3-C2-O2	-7.64	116.55	121.90
54	BA	1801	A	C5-C6-N1	7.64	121.52	117.70
21	AA	383	A	C5-C6-N1	7.64	121.52	117.70
54	BA	982	C	N3-C2-O2	-7.64	116.56	121.90
54	BA	2238	G	O4'-C1'-N9	7.64	114.31	108.20
21	AA	1336	C	N3-C2-O2	-7.63	116.56	121.90
22	A1	66	A	C5-C6-N1	7.63	121.52	117.70
54	BA	275	C	N3-C2-O2	-7.63	116.56	121.90
54	BA	718	A	C5-C6-N1	7.63	121.52	117.70
54	BA	1655	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	2748	A	C5-C6-N1	7.63	121.52	117.70
54	BA	1858	A	C5-C6-N1	7.63	121.52	117.70
54	BA	2858	C	N3-C2-O2	-7.63	116.56	121.90
51	B2	34	ARG	NE-CZ-NH2	-7.63	116.48	120.30
54	BA	639	U	O4'-C1'-N1	7.63	114.30	108.20
54	BA	233	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	819	A	N1-C6-N6	-7.62	114.03	118.60
22	A1	21	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2099	U	N3-C2-O2	-7.62	116.86	122.20
4	AE	28	ARG	NE-CZ-NH1	7.62	124.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	655	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1111	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	324	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	1346	A	C5-C6-N1	7.62	121.51	117.70
24	A3	77	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1598	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2287	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1260	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1268	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1877	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2411	A	C5-C6-N1	7.62	121.51	117.70
21	AA	864	A	C5-C6-N1	7.61	121.51	117.70
35	BM	40	ARG	NE-CZ-NH1	7.61	124.11	120.30
35	BM	55	ARG	NE-CZ-NH2	7.61	124.11	120.30
54	BA	1916	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	2820	A	C5-C6-N1	7.61	121.51	117.70
21	AA	964	A	C5-C6-N1	7.61	121.51	117.70
21	AA	975	A	C5-C6-N1	7.61	121.50	117.70
54	BA	140	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	1365	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1877	A	C5-C6-N1	7.61	121.50	117.70
54	BA	2030	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	414	A	C5-C6-N1	7.61	121.50	117.70
54	BA	207	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1322	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1606	C	N3-C2-O2	-7.61	116.58	121.90
54	BA	2539	C	N3-C2-O2	-7.61	116.58	121.90
28	BF	70	ARG	NE-CZ-NH1	7.60	124.10	120.30
21	AA	1239	A	C5-C6-N1	7.60	121.50	117.70
22	A1	3	G	C5'-C4'-O4'	7.60	118.22	109.10
54	BA	404	A	C5-C6-N1	7.60	121.50	117.70
54	BA	458	G	O4'-C1'-N9	7.60	114.28	108.20
54	BA	959	A	C5-C6-N1	7.60	121.50	117.70
54	BA	1732	C	N3-C2-O2	-7.60	116.58	121.90
6	AG	91	ARG	NE-CZ-NH1	7.60	124.10	120.30
21	AA	48	C	N3-C2-O2	-7.59	116.58	121.90
54	BA	272	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1009	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1632	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1677	A	C5-C6-N1	7.59	121.50	117.70
54	BA	2284	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1890	A	C5-C6-N1	7.59	121.50	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	348	A	C5-C6-N1	7.59	121.50	117.70
54	BA	849	A	C5-C6-N1	7.59	121.50	117.70
21	AA	642	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	63	A	C5-C6-N1	7.59	121.49	117.70
21	AA	574	A	C4-C5-C6	-7.59	113.21	117.00
22	A1	58	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	863	A	C5-C6-N1	7.59	121.49	117.70
54	BA	1469	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	2868	A	C5-C6-N1	7.59	121.49	117.70
54	BA	91	A	C5-C6-N1	7.58	121.49	117.70
54	BA	788	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1276	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	1616	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2887	A	C5-C6-N1	7.58	121.49	117.70
34	BL	132	ARG	NE-CZ-NH1	7.58	124.09	120.30
54	BA	1952	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1032	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1134	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	1427	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2482	A	C5-C6-N1	7.58	121.49	117.70
54	BA	331	C	N3-C2-O2	-7.58	116.59	121.90
54	BA	455	C	N3-C2-O2	-7.58	116.59	121.90
54	BA	1342	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2059	A	C5-C6-N1	7.58	121.49	117.70
21	AA	511	C	N3-C2-O2	-7.58	116.60	121.90
54	BA	2134	A	C5-C6-N1	7.58	121.49	117.70
54	BA	391	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	866	A	C5-C6-N1	7.57	121.49	117.70
55	BB	73	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	1938	A	C5-C6-N1	7.57	121.49	117.70
53	B4	36	ARG	NE-CZ-NH1	7.57	124.08	120.30
54	BA	1244	A	N1-C6-N6	-7.57	114.06	118.60
21	AA	81	A	C5-C6-N1	7.57	121.48	117.70
21	AA	974	A	N1-C6-N6	-7.57	114.06	118.60
21	AA	234	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	602	A	C4-C5-C6	-7.56	113.22	117.00
21	AA	389	A	C5-C6-N1	7.56	121.48	117.70
21	AA	1082	A	C5-C6-N1	7.56	121.48	117.70
21	AA	1467	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	10	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	2765	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2873	A	N1-C6-N6	-7.56	114.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1762	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2809	A	N1-C6-N6	-7.56	114.06	118.60
21	AA	1501	C	N3-C2-O2	-7.56	116.61	121.90
24	A3	73	A	N1-C6-N6	-7.56	114.07	118.60
21	AA	382	A	C5-C6-N1	7.56	121.48	117.70
54	BA	73	A	C5-C6-N1	7.56	121.48	117.70
21	AA	913	A	C5-C6-N1	7.55	121.48	117.70
28	BF	124	ARG	NE-CZ-NH1	7.55	124.08	120.30
54	BA	2129	C	N1-C2-O2	7.55	123.43	118.90
54	BA	2635	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	510	A	C5-C6-N1	7.55	121.48	117.70
54	BA	503	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2247	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1446	A	C5-C6-N1	7.55	121.47	117.70
54	BA	176	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	439	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	1147	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1572	A	C5-C6-N1	7.54	121.47	117.70
54	BA	2388	A	C5-C6-N1	7.54	121.47	117.70
24	A3	77	A	N1-C6-N6	-7.54	114.08	118.60
27	BE	114	ARG	NE-CZ-NH1	7.54	124.07	120.30
54	BA	362	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	2126	A	C5-C6-N1	7.54	121.47	117.70
55	BB	45	A	C5-C6-N1	7.54	121.47	117.70
21	AA	28	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	2163	A	O4'-C1'-N9	7.54	114.23	108.20
54	BA	1552	A	C5-C6-N1	7.53	121.47	117.70
27	BE	79	ARG	NE-CZ-NH1	7.53	124.07	120.30
21	AA	780	A	C5-C6-N1	7.53	121.47	117.70
54	BA	56	A	C5-C6-N1	7.53	121.47	117.70
54	BA	587	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	1048	A	C5-C6-N1	7.53	121.47	117.70
54	BA	2184	A	C5-C6-N1	7.53	121.47	117.70
21	AA	607	A	C5-C6-N1	7.53	121.47	117.70
21	AA	1333	A	C5-C6-N1	7.53	121.47	117.70
54	BA	1912	A	C5-C6-N1	7.53	121.46	117.70
54	BA	2748	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	227	A	C5-C6-N1	7.53	121.46	117.70
54	BA	2031	A	C5-C6-N1	7.53	121.46	117.70
54	BA	2307	G	O4'-C1'-N9	7.53	114.22	108.20
54	BA	28	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1021	A	N1-C6-N6	-7.52	114.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1366	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2169	A	C5-C6-N1	7.52	121.46	117.70
55	BB	78	A	C4-C5-C6	-7.52	113.24	117.00
10	AK	92	ARG	NE-CZ-NH1	7.52	124.06	120.30
21	AA	728	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1130	A	C4-C5-C6	-7.52	113.24	117.00
54	BA	1625	C	O4'-C1'-N1	7.52	114.22	108.20
54	BA	2654	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2205	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2559	C	O4'-C1'-N1	7.52	114.22	108.20
11	AL	98	ARG	NE-CZ-NH1	7.52	124.06	120.30
21	AA	1238	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1360	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2809	A	C5-C6-N1	7.51	121.46	117.70
54	BA	432	A	C5-C6-N1	7.51	121.46	117.70
21	AA	106	C	N3-C2-O2	-7.51	116.64	121.90
21	AA	282	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2241	A	C4-C5-C6	-7.51	113.25	117.00
33	BK	105	ARG	NE-CZ-NH1	7.50	124.05	120.30
34	BL	60	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	226	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	1528	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2726	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	819	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1701	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	2309	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2882	A	C4-C5-C6	-7.50	113.25	117.00
21	AA	768	A	C4-C5-C6	-7.50	113.25	117.00
21	AA	787	A	C5-C6-N1	7.50	121.45	117.70
54	BA	599	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	1284	A	C5-C6-N1	7.50	121.45	117.70
21	AA	366	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2332	C	N3-C2-O2	-7.50	116.65	121.90
54	BA	2458	G	O4'-C1'-N9	7.50	114.20	108.20
54	BA	222	A	C5-C6-N1	7.49	121.45	117.70
54	BA	1439	A	O4'-C1'-N9	7.49	114.19	108.20
21	AA	172	A	C5-C6-N1	7.49	121.45	117.70
54	BA	262	A	C5-C6-N1	7.49	121.45	117.70
54	BA	299	A	C5-C6-N1	7.49	121.45	117.70
2	AC	135	ARG	NE-CZ-NH1	7.49	124.05	120.30
21	AA	129	A	C5-C6-N1	7.49	121.44	117.70
22	A1	23	A	N1-C6-N6	-7.49	114.11	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BN	8	ARG	NE-CZ-NH1	7.49	124.05	120.30
54	BA	1981	A	C5-C6-N1	7.49	121.44	117.70
54	BA	2268	A	C5-C6-N1	7.49	121.45	117.70
54	BA	2721	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	2077	A	C4-C5-C6	-7.49	113.26	117.00
56	B5	164	ARG	NE-CZ-NH1	7.49	124.04	120.30
21	AA	130	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	2565	A	C5-C6-N1	7.49	121.44	117.70
21	AA	655	A	C5-C6-N1	7.48	121.44	117.70
21	AA	906	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2814	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2346	A	C5-C6-N1	7.48	121.44	117.70
22	A1	26	A	C5-C6-N1	7.48	121.44	117.70
21	AA	139	A	C5-C6-N1	7.48	121.44	117.70
21	AA	915	A	C5-C6-N1	7.48	121.44	117.70
6	AG	52	ARG	NE-CZ-NH1	7.48	124.04	120.30
21	AA	1158	C	N1-C2-O2	7.48	123.39	118.90
54	BA	1393	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	1609	A	C5-C6-N1	7.48	121.44	117.70
54	BA	1739	A	N1-C6-N6	-7.48	114.11	118.60
21	AA	1191	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	1871	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2717	C	N3-C2-O2	-7.47	116.67	121.90
21	AA	1319	A	C5-C6-N1	7.47	121.44	117.70
53	B4	12	ARG	NE-CZ-NH1	7.47	124.03	120.30
54	BA	508	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1321	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1755	A	C4-C5-C6	-7.47	113.27	117.00
54	BA	2173	A	N1-C6-N6	-7.47	114.12	118.60
13	AN	85	ARG	NE-CZ-NH1	7.46	124.03	120.30
21	AA	1196	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1250	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1513	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	2778	A	C5-C6-N1	7.46	121.43	117.70
21	AA	572	A	C5-C6-N1	7.46	121.43	117.70
21	AA	704	A	C5-C6-N1	7.46	121.43	117.70
21	AA	759	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1048	A	C4-C5-C6	-7.46	113.27	117.00
21	AA	889	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1566	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2665	A	N1-C6-N6	-7.46	114.12	118.60
21	AA	149	A	C5-C6-N1	7.46	121.43	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2654	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1031	C	N1-C2-O2	7.45	123.37	118.90
54	BA	1899	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	288	A	C5-C6-N1	7.45	121.42	117.70
39	BQ	49	ARG	NE-CZ-NH1	7.45	124.03	120.30
21	AA	182	A	C5-C6-N1	7.45	121.42	117.70
21	AA	1150	A	C5-C6-N1	7.45	121.42	117.70
21	AA	1324	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1549	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	2317	A	C5-C6-N1	7.45	121.42	117.70
21	AA	190	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	539	A	C5-C6-N1	7.45	121.42	117.70
22	A1	9	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1320	C	N3-C2-O2	-7.45	116.69	121.90
1	AB	136	ARG	NE-CZ-NH2	-7.44	116.58	120.30
21	AA	109	A	C5-C6-N1	7.44	121.42	117.70
21	AA	345	C	C1'-O4'-C4'	-7.44	103.94	109.90
21	AA	1188	A	C5-C6-N1	7.44	121.42	117.70
21	AA	1311	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	1085	A	N1-C6-N6	-7.44	114.13	118.60
21	AA	712	A	C5-C6-N1	7.44	121.42	117.70
21	AA	794	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2019	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	2573	C	N3-C2-O2	-7.44	116.69	121.90
21	AA	44	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	156	A	C5-C6-N1	7.44	121.42	117.70
54	BA	345	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2183	A	N1-C6-N6	-7.44	114.14	118.60
21	AA	938	A	C5-C6-N1	7.44	121.42	117.70
21	AA	23	C	N3-C2-O2	-7.43	116.70	121.90
21	AA	982	U	P-O3'-C3'	7.43	128.62	119.70
21	AA	1430	A	C5-C6-N1	7.43	121.42	117.70
54	BA	203	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	2097	A	C4-C5-C6	-7.43	113.28	117.00
21	AA	189	A	C5-C6-N1	7.43	121.42	117.70
21	AA	243	A	C4-C5-C6	-7.43	113.28	117.00
21	AA	1012	A	C5-C6-N1	7.43	121.42	117.70
54	BA	177	G	O4'-C1'-N9	7.43	114.15	108.20
54	BA	2790	U	O4'-C1'-N1	7.43	114.15	108.20
54	BA	218	A	C5-C6-N1	7.43	121.42	117.70
54	BA	1143	A	C5-C6-N1	7.43	121.41	117.70
54	BA	2636	C	N3-C2-O2	-7.43	116.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2070	A	C4-C5-C6	-7.43	113.29	117.00
21	AA	937	A	C5-C6-N1	7.42	121.41	117.70
24	A3	44	A	C5-C6-N1	7.42	121.41	117.70
54	BA	26	G	O4'-C1'-N9	7.42	114.14	108.20
54	BA	529	A	C5-C6-N1	7.42	121.41	117.70
54	BA	13	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	1289	A	C5-C6-N1	7.42	121.41	117.70
54	BA	56	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	1744	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	1966	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	397	A	C5-C6-N1	7.42	121.41	117.70
21	AA	621	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1158	C	N3-C2-O2	-7.42	116.71	121.90
54	BA	1453	A	C5-C6-N1	7.42	121.41	117.70
54	BA	2147	A	C4-C5-C6	-7.42	113.29	117.00
21	AA	573	A	C4-C5-C6	-7.41	113.29	117.00
54	BA	1614	A	C5-C6-N1	7.41	121.41	117.70
21	AA	1383	C	N3-C2-O2	-7.41	116.71	121.90
54	BA	362	A	C5-C6-N1	7.41	121.41	117.70
54	BA	504	A	O4'-C1'-N9	7.41	114.13	108.20
54	BA	608	A	C5-C6-N1	7.41	121.41	117.70
54	BA	792	A	C5-C6-N1	7.41	121.41	117.70
8	AI	122	ARG	NE-CZ-NH1	7.41	124.00	120.30
13	AN	13	ARG	NE-CZ-NH1	7.41	124.00	120.30
21	AA	1508	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	322	A	C5-C6-N1	7.41	121.40	117.70
54	BA	781	A	C5-C6-N1	7.40	121.40	117.70
21	AA	792	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1350	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	643	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1156	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2635	A	C5-C6-N1	7.40	121.40	117.70
21	AA	784	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1336	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2870	C	O4'-C1'-N1	7.40	114.12	108.20
54	BA	384	A	C5-C6-N1	7.40	121.40	117.70
21	AA	747	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2660	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2706	A	C5-C6-N1	7.40	121.40	117.70
21	AA	716	A	C5-C6-N1	7.39	121.40	117.70
21	AA	841	C	N3-C2-O2	-7.39	116.72	121.90
55	BB	15	A	C5-C6-N1	7.39	121.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	482	A	C5-C6-N1	7.39	121.40	117.70
54	BA	925	A	C5-C6-N1	7.39	121.40	117.70
54	BA	2725	A	C5-C6-N1	7.39	121.40	117.70
21	AA	663	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	1717	A	N1-C6-N6	-7.39	114.17	118.60
21	AA	753	A	C5-C6-N1	7.39	121.39	117.70
21	AA	1256	A	C5-C6-N1	7.39	121.39	117.70
21	AA	1427	C	N3-C2-O2	-7.39	116.73	121.90
42	BT	3	ARG	NE-CZ-NH1	7.39	123.99	120.30
54	BA	531	C	N3-C2-O2	-7.39	116.73	121.90
54	BA	783	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	1194	A	N1-C6-N6	-7.39	114.17	118.60
55	BB	39	A	C5-C6-N1	7.39	121.39	117.70
21	AA	466	A	C5-C6-N1	7.39	121.39	117.70
21	AA	663	A	C5-C6-N1	7.39	121.39	117.70
54	BA	346	A	C5-C6-N1	7.39	121.39	117.70
54	BA	538	A	C5-C6-N1	7.39	121.39	117.70
54	BA	374	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	2512	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	1722	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	164	C	N3-C2-O2	-7.38	116.73	121.90
21	AA	609	A	N1-C6-N6	-7.38	114.17	118.60
21	AA	1413	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	1439	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1858	A	N1-C6-N6	-7.38	114.17	118.60
21	AA	430	A	N1-C6-N6	-7.38	114.17	118.60
21	AA	712	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	556	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	722	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	1548	A	C5-C6-N1	7.38	121.39	117.70
21	AA	1170	A	C5-C6-N1	7.37	121.39	117.70
21	AA	1360	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1490	A	C5-C6-N1	7.37	121.39	117.70
21	AA	284	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	320	A	C5-C6-N1	7.37	121.39	117.70
54	BA	783	A	C5-C6-N1	7.37	121.39	117.70
54	BA	637	A	C5-C6-N1	7.37	121.39	117.70
54	BA	804	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	250	G	O4'-C1'-N9	7.37	114.09	108.20
21	AA	918	A	N1-C6-N6	-7.37	114.18	118.60
21	AA	1261	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	2030	A	O4'-C1'-N9	7.37	114.09	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	573	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1151	A	C5-C6-N1	7.36	121.38	117.70
54	BA	685	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	1383	A	O4'-C1'-N9	7.36	114.09	108.20
21	AA	59	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1493	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	223	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1393	A	C5-C6-N1	7.36	121.38	117.70
21	AA	33	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	74	A	N1-C6-N6	-7.36	114.18	118.60
21	AA	236	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1157	A	C5-C6-N1	7.36	121.38	117.70
24	A3	59	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1000	A	C5-C6-N1	7.36	121.38	117.70
21	AA	349	A	C5-C6-N1	7.36	121.38	117.70
39	BQ	29	ARG	NE-CZ-NH1	7.36	123.98	120.30
54	BA	335	C	N3-C2-O2	-7.35	116.75	121.90
54	BA	547	A	C5-C6-N1	7.35	121.38	117.70
47	BY	48	ARG	NE-CZ-NH1	7.35	123.98	120.30
54	BA	2376	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2670	A	C5-C6-N1	7.35	121.38	117.70
54	BA	972	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2560	A	C5-C6-N1	7.35	121.38	117.70
21	AA	356	A	C5-C6-N1	7.35	121.38	117.70
54	BA	1785	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	768	A	C5-C6-N1	7.34	121.37	117.70
21	AA	1092	A	C5-C6-N1	7.34	121.37	117.70
23	A2	82	A	C5-C6-N1	7.34	121.37	117.70
54	BA	483	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2065	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	1952	A	N1-C6-N6	-7.34	114.19	118.60
54	BA	1359	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1597	A	C5-C6-N1	7.34	121.37	117.70
21	AA	560	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	1796	U	O4'-C1'-N1	7.34	114.07	108.20
54	BA	1990	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2503	A	C5-C6-N1	7.34	121.37	117.70
21	AA	487	A	N1-C6-N6	-7.34	114.20	118.60
26	BD	179	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	1960	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2546	U	O4'-C1'-N1	7.34	114.07	108.20
54	BA	1504	A	C5-C6-N1	7.34	121.37	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2867	G	O4'-C1'-N9	7.34	114.07	108.20
54	BA	2042	A	C5-C6-N1	7.33	121.37	117.70
21	AA	866	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	1254	A	C4-C5-C6	-7.33	113.33	117.00
21	AA	790	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2850	A	C5-C6-N1	7.33	121.36	117.70
21	AA	602	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	814	A	C5-C6-N1	7.33	121.36	117.70
54	BA	156	A	C4-C5-C6	-7.33	113.34	117.00
54	BA	2705	A	C5-C6-N1	7.33	121.36	117.70
21	AA	1513	A	C5-C6-N1	7.32	121.36	117.70
53	B4	19	ARG	NE-CZ-NH1	7.32	123.96	120.30
54	BA	218	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	412	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2158	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2882	A	C5-C6-N1	7.32	121.36	117.70
21	AA	1404	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	119	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	928	A	C5-C6-N1	7.32	121.36	117.70
21	AA	1531	A	C4-C5-C6	-7.32	113.34	117.00
8	AI	121	ARG	NE-CZ-NH1	7.32	123.96	120.30
21	AA	460	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2761	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	957	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	1205	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2422	C	N3-C2-O2	-7.32	116.78	121.90
21	AA	611	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	718	A	C5-C6-N1	7.31	121.36	117.70
21	AA	1352	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	251	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2071	A	N1-C6-N6	-7.31	114.21	118.60
21	AA	1338	G	C1'-O4'-C4'	-7.31	104.05	109.90
29	BG	169	ARG	NE-CZ-NH1	7.31	123.96	120.30
54	BA	2764	A	C5-C6-N1	7.31	121.36	117.70
21	AA	923	A	C5-C6-N1	7.31	121.36	117.70
21	AA	1252	A	C5-C6-N1	7.31	121.35	117.70
54	BA	1615	C	N1-C2-O2	7.31	123.29	118.90
54	BA	2377	A	N1-C6-N6	-7.31	114.21	118.60
54	BA	2541	A	C4-C5-C6	-7.31	113.35	117.00
54	BA	2657	A	N1-C6-N6	-7.31	114.21	118.60
54	BA	1133	A	N1-C6-N6	-7.31	114.22	118.60
54	BA	2386	A	C5-C6-N1	7.31	121.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	66	A	C4-C5-C6	-7.31	113.35	117.00
54	BA	1301	A	C5-C6-N1	7.31	121.35	117.70
54	BA	2025	C	N3-C2-O2	-7.31	116.79	121.90
1	AB	136	ARG	NE-CZ-NH1	7.30	123.95	120.30
21	AA	72	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1269	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2267	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2434	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	2757	A	C5-C6-N1	7.30	121.35	117.70
1	AB	62	ARG	NE-CZ-NH1	7.30	123.95	120.30
54	BA	1936	A	C5-C6-N1	7.30	121.35	117.70
21	AA	862	C	N3-C2-O2	-7.30	116.79	121.90
22	A1	76	A	C6-C5-N7	7.30	137.41	132.30
54	BA	509	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	2019	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	988	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	309	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1428	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	514	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1496	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2872	A	C5-C6-N1	7.30	121.35	117.70
21	AA	994	A	C5-C6-N1	7.29	121.35	117.70
21	AA	1510	C	N3-C2-O2	-7.29	116.79	121.90
54	BA	2078	C	N3-C2-O2	-7.29	116.79	121.90
32	BJ	35	ARG	NE-CZ-NH1	7.29	123.95	120.30
54	BA	1668	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1698	A	C5-C6-N1	7.29	121.35	117.70
54	BA	550	C	N3-C2-O2	-7.29	116.80	121.90
21	AA	1431	A	C5-C6-N1	7.29	121.34	117.70
52	B3	41	ARG	NE-CZ-NH1	7.29	123.94	120.30
54	BA	1274	A	C5-C6-N1	7.29	121.34	117.70
21	AA	60	A	C5-C6-N1	7.29	121.34	117.70
54	BA	936	A	C5-C6-N1	7.29	121.34	117.70
21	AA	320	A	C4-C5-C6	-7.29	113.36	117.00
21	AA	1147	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	1378	A	C5-C6-N1	7.29	121.34	117.70
54	BA	2346	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	2815	C	N3-C2-O2	-7.29	116.80	121.90
4	AE	44	ARG	NE-CZ-NH1	7.28	123.94	120.30
21	AA	478	A	C5-C6-N1	7.28	121.34	117.70
21	AA	600	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	1318	A	N1-C6-N6	-7.28	114.23	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	470	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1529	G	O4'-C1'-N9	7.28	114.03	108.20
21	AA	67	C	N3-C2-O2	-7.28	116.80	121.90
21	AA	243	A	C5-C6-N1	7.28	121.34	117.70
21	AA	766	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1204	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	1213	A	C5-C6-N1	7.28	121.34	117.70
21	AA	983	A	C5-C6-N1	7.28	121.34	117.70
54	BA	980	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	2856	A	C5-C6-N1	7.28	121.34	117.70
21	AA	33	A	C5-C6-N1	7.28	121.34	117.70
37	BO	111	ARG	NE-CZ-NH1	7.28	123.94	120.30
54	BA	278	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	2564	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1219	A	C5-C6-N1	7.27	121.34	117.70
54	BA	2883	A	C5-C6-N1	7.27	121.34	117.70
21	AA	78	A	C5-C6-N1	7.27	121.34	117.70
25	BC	269	ARG	NE-CZ-NH1	7.27	123.94	120.30
38	BP	52	ARG	NE-CZ-NH1	7.27	123.94	120.30
54	BA	428	A	C5-C6-N1	7.27	121.34	117.70
54	BA	2366	A	C5-C6-N1	7.27	121.34	117.70
21	AA	53	A	C4-C5-C6	-7.27	113.36	117.00
24	A3	36	A	C5-C6-N1	7.27	121.33	117.70
54	BA	888	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	909	A	C5-C6-N1	7.27	121.33	117.70
15	AP	25	ARG	NE-CZ-NH1	7.27	123.94	120.30
21	AA	313	A	C5-C6-N1	7.27	121.33	117.70
21	AA	622	A	C5-C6-N1	7.27	121.33	117.70
54	BA	311	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1015	U	O4'-C1'-N1	7.27	114.02	108.20
54	BA	1089	A	C5-C6-N1	7.27	121.33	117.70
54	BA	2556	C	N3-C2-O2	-7.27	116.81	121.90
21	AA	1396	A	C5-C6-N1	7.27	121.33	117.70
21	AA	1492	A	C5-C6-N1	7.27	121.33	117.70
21	AA	7	A	C5-C6-N1	7.26	121.33	117.70
21	AA	1169	A	C5-C6-N1	7.26	121.33	117.70
21	AA	1246	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2497	A	N1-C6-N6	-7.26	114.24	118.60
21	AA	694	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	1757	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2572	A	C5-C6-N1	7.26	121.33	117.70
54	BA	279	A	N1-C6-N6	-7.26	114.24	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1746	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1953	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2094	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2566	A	C5-C6-N1	7.26	121.33	117.70
21	AA	109	A	C1'-O4'-C4'	-7.26	104.09	109.90
38	BP	112	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	817	C	N3-C2-O2	-7.26	116.82	121.90
21	AA	1350	A	C5-C6-N1	7.26	121.33	117.70
31	BI	102	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	1809	A	C5-C6-N1	7.26	121.33	117.70
54	BA	462	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	270	A	C5-C6-N1	7.25	121.33	117.70
21	AA	563	A	C5-C6-N1	7.25	121.33	117.70
45	BW	38	ARG	NE-CZ-NH1	7.25	123.93	120.30
24	A3	11	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	2851	A	C5-C6-N1	7.25	121.33	117.70
21	AA	171	A	C5-C6-N1	7.25	121.33	117.70
21	AA	182	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	1730	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	728	A	N1-C6-N6	-7.25	114.25	118.60
46	BX	10	ARG	NE-CZ-NH1	7.25	123.92	120.30
54	BA	1165	A	C5-C6-N1	7.25	121.32	117.70
21	AA	1046	A	N1-C6-N6	-7.25	114.25	118.60
21	AA	958	A	C5-C6-N1	7.25	121.32	117.70
54	BA	44	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1175	A	C5-C6-N1	7.24	121.32	117.70
55	BB	91	C	O4'-C1'-N1	7.24	114.00	108.20
54	BA	1502	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1611	C	N3-C2-O2	-7.24	116.83	121.90
21	AA	819	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	483	A	N1-C6-N6	-7.24	114.25	118.60
54	BA	1590	A	N1-C6-N6	-7.24	114.26	118.60
21	AA	629	A	C4-C5-C6	-7.24	113.38	117.00
28	BF	29	ARG	NE-CZ-NH1	7.24	123.92	120.30
54	BA	829	A	N1-C6-N6	-7.24	114.26	118.60
21	AA	1280	A	C5-C6-N1	7.24	121.32	117.70
54	BA	354	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1383	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2150	C	N3-C2-O2	-7.24	116.83	121.90
21	AA	32	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2434	A	C5-C6-N1	7.24	121.32	117.70
21	AA	325	A	C5-C6-N1	7.23	121.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	702	A	N1-C6-N6	-7.23	114.26	118.60
21	AA	1132	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	668	A	C5-C6-N1	7.23	121.32	117.70
55	BB	108	A	C5-C6-N1	7.23	121.32	117.70
21	AA	223	A	C5-C6-N1	7.23	121.32	117.70
54	BA	1754	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	1885	A	C5-C6-N1	7.23	121.32	117.70
54	BA	2448	A	C5-C6-N1	7.23	121.32	117.70
24	A3	39	A	C5-C6-N1	7.23	121.31	117.70
54	BA	449	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1961	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	126	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1784	A	C4-C5-C6	-7.23	113.39	117.00
54	BA	2406	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2589	A	C5-C6-N1	7.23	121.31	117.70
54	BA	633	A	C5-C6-N1	7.23	121.31	117.70
21	AA	968	A	O4'-C1'-N9	7.22	113.98	108.20
21	AA	1136	C	N3-C2-O2	-7.22	116.84	121.90
54	BA	1301	A	N1-C6-N6	-7.22	114.27	118.60
21	AA	435	A	C4-C5-C6	-7.22	113.39	117.00
21	AA	781	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	457	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	845	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	2170	A	C5-C6-N1	7.22	121.31	117.70
54	BA	104	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1006	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	595	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	1260	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2476	A	C5-C6-N1	7.22	121.31	117.70
21	AA	190	A	C5-C6-N1	7.22	121.31	117.70
21	AA	193	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	2174	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	1303	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	181	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2358	A	C5-C6-N1	7.21	121.31	117.70
54	BA	324	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2051	A	C5-C6-N1	7.21	121.31	117.70
55	BB	115	A	C5-C6-N1	7.21	121.31	117.70
3	AD	80	ARG	NE-CZ-NH1	7.21	123.91	120.30
21	AA	1261	A	C5-C6-N1	7.21	121.30	117.70
34	BL	2	ARG	NE-CZ-NH2	7.21	123.90	120.30
54	BA	221	A	C5-C6-N1	7.21	121.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	BS	110	ARG	NE-CZ-NH1	7.21	123.90	120.30
21	AA	706	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1022	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1434	A	C5-C6-N1	7.20	121.30	117.70
54	BA	272	A	O4'-C1'-N9	7.20	113.96	108.20
54	BA	2541	A	C5-C6-N1	7.20	121.30	117.70
55	BB	59	A	C5-C6-N1	7.20	121.30	117.70
23	A2	79	A	C5-C6-N1	7.20	121.30	117.70
21	AA	575	G	P-O3'-C3'	7.20	128.34	119.70
54	BA	371	A	C5-C6-N1	7.20	121.30	117.70
21	AA	719	C	N3-C2-O2	-7.20	116.86	121.90
25	BC	132	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	1977	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	677	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2212	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2634	A	N1-C6-N6	-7.20	114.28	118.60
9	AJ	37	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	1428	C	N1-C2-O2	7.20	123.22	118.90
21	AA	704	A	C4-C5-C6	-7.19	113.40	117.00
21	AA	1413	A	C5-C6-N1	7.19	121.30	117.70
54	BA	190	A	N1-C6-N6	-7.19	114.28	118.60
54	BA	1327	A	C4-C5-C6	-7.19	113.40	117.00
54	BA	2194	U	O4'-C1'-N1	7.19	113.95	108.20
54	BA	877	A	C5-C6-N1	7.19	121.30	117.70
54	BA	131	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	454	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	743	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	1800	C	N3-C2-O2	-7.19	116.87	121.90
54	BA	1915	U	O4'-C1'-N1	7.19	113.95	108.20
21	AA	1524	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	227	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1044	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	2177	C	N3-C2-O2	-7.18	116.87	121.90
21	AA	325	A	N1-C6-N6	-7.18	114.29	118.60
21	AA	1395	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	2163	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1014	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1428	A	C5-C6-N1	7.18	121.29	117.70
2	AC	155	ARG	NE-CZ-NH1	7.18	123.89	120.30
9	AJ	45	ARG	NE-CZ-NH1	7.18	123.89	120.30
21	AA	539	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	602	A	C5-C6-N1	7.18	121.29	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	681	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	2060	A	C5-C6-N1	7.18	121.29	117.70
7	AH	87	ARG	NE-CZ-NH2	7.18	123.89	120.30
54	BA	1978	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2610	C	N3-C2-O2	-7.18	116.88	121.90
21	AA	1357	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1441	A	C4-C5-C6	-7.18	113.41	117.00
26	BD	83	ARG	NE-CZ-NH1	7.18	123.89	120.30
54	BA	1169	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1241	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2752	C	N3-C2-O2	-7.18	116.88	121.90
21	AA	754	C	N1-C2-O2	7.17	123.20	118.90
54	BA	472	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1204	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1226	A	C5-C6-N1	7.17	121.29	117.70
21	AA	451	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1042	A	C5-C6-N1	7.17	121.28	117.70
21	AA	1191	A	C5-C6-N1	7.17	121.28	117.70
54	BA	430	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2676	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	547	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	38	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1544	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2198	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2614	A	C5-C6-N1	7.17	121.28	117.70
21	AA	452	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	83	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	226	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1637	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2451	A	C5-C6-N1	7.17	121.28	117.70
21	AA	1410	A	C5-C6-N1	7.17	121.28	117.70
54	BA	231	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	344	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1067	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1382	G	O4'-C1'-N9	7.17	113.93	108.20
54	BA	1470	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2712	C	N3-C2-O2	-7.17	116.88	121.90
55	BB	88	C	N3-C2-O2	-7.17	116.89	121.90
21	AA	1044	A	C5-C6-N1	7.16	121.28	117.70
21	AA	817	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	294	A	C4-C5-C6	-7.16	113.42	117.00
54	BA	947	A	N1-C6-N6	-7.16	114.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2171	A	C5-C6-N1	7.16	121.28	117.70
54	BA	1348	C	O4'-C1'-N1	7.16	113.93	108.20
55	BB	11	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	84	A	C5-C6-N1	7.16	121.28	117.70
21	AA	51	A	C5-C6-N1	7.16	121.28	117.70
24	A3	58	A	C5-C6-N1	7.16	121.28	117.70
43	BU	6	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	1147	A	N1-C6-N6	-7.16	114.31	118.60
21	AA	460	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	1036	A	C5-C6-N1	7.15	121.28	117.70
54	BA	347	A	C5-C6-N1	7.15	121.28	117.70
21	AA	371	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	1353	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2278	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2823	A	C5-C6-N1	7.15	121.28	117.70
21	AA	487	A	C5-C6-N1	7.15	121.28	117.70
54	BA	480	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	2829	A	C5-C6-N1	7.15	121.28	117.70
54	BA	743	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1151	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1641	A	C5-C6-N1	7.15	121.27	117.70
21	AA	545	C	N3-C2-O2	-7.15	116.90	121.90
21	AA	687	A	C5-C6-N1	7.15	121.27	117.70
54	BA	716	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	975	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1503	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	559	A	C5-C6-N1	7.14	121.27	117.70
21	AA	795	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	311	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1001	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	1771	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	2835	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	1203	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	355	U	O4'-C1'-N1	7.14	113.91	108.20
54	BA	1788	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	181	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1822	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	2639	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2738	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1608	A	C5-C6-N1	7.13	121.27	117.70
22	A1	74	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	644	A	C5-C6-N1	7.13	121.27	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	196	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	990	C	N3-C2-O2	-7.13	116.91	121.90
21	AA	1443	C	N3-C2-O2	-7.13	116.91	121.90
36	BN	12	ARG	NE-CZ-NH1	7.13	123.86	120.30
54	BA	671	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	1609	A	C1'-O4'-C4'	-7.13	104.20	109.90
21	AA	263	A	C5-C6-N1	7.13	121.26	117.70
54	BA	2013	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	2173	A	C5-C6-N1	7.13	121.26	117.70
21	AA	1332	A	N1-C6-N6	-7.12	114.33	118.60
21	AA	1508	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2821	A	C5-C6-N1	7.12	121.26	117.70
34	BL	33	ARG	NE-CZ-NH1	7.12	123.86	120.30
54	BA	13	A	C5-C6-N1	7.12	121.26	117.70
54	BA	466	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2352	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2598	A	C5-C6-N1	7.12	121.26	117.70
24	A3	38	A	C5-C6-N1	7.12	121.26	117.70
54	BA	735	A	C5-C6-N1	7.12	121.26	117.70
54	BA	782	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2600	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	472	A	N1-C6-N6	-7.12	114.33	118.60
21	AA	900	A	C5-C6-N1	7.12	121.26	117.70
54	BA	893	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	431	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1395	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2227	A	C5-C6-N1	7.12	121.26	117.70
18	AS	35	ARG	NE-CZ-NH1	7.12	123.86	120.30
21	AA	648	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1408	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	1808	A	C5-C6-N1	7.12	121.26	117.70
54	BA	127	A	C5-C6-N1	7.11	121.26	117.70
54	BA	587	C	O4'-C1'-N1	7.11	113.89	108.20
21	AA	441	A	C5-C6-N1	7.11	121.26	117.70
21	AA	1500	A	C4-C5-C6	-7.11	113.44	117.00
54	BA	249	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	944	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	2403	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	2459	A	C5-C6-N1	7.11	121.26	117.70
54	BA	1493	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	1876	A	N1-C6-N6	-7.11	114.33	118.60
22	A1	23	A	C5-C6-N1	7.11	121.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	411	A	N1-C6-N6	-7.11	114.34	118.60
54	BA	347	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	765	C	N3-C2-O2	-7.11	116.93	121.90
54	BA	1039	A	C5-C6-N1	7.11	121.25	117.70
21	AA	777	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1005	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	1419	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	1225	A	C5-C6-N1	7.10	121.25	117.70
54	BA	917	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	872	A	O4'-C1'-N9	7.10	113.88	108.20
21	AA	306	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	695	A	C5-C6-N1	7.10	121.25	117.70
22	A1	16	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	1111	A	C5-C6-N1	7.10	121.25	117.70
24	A3	49	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	2191	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1272	A	C5-C6-N1	7.10	121.25	117.70
9	AJ	89	ARG	NE-CZ-NH1	7.09	123.85	120.30
21	AA	1336	C	N1-C2-O2	7.09	123.16	118.90
54	BA	575	A	C5-C6-N1	7.09	121.25	117.70
54	BA	160	A	C5-C6-N1	7.09	121.25	117.70
54	BA	477	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2666	C	N1-C2-O2	7.09	123.16	118.90
21	AA	80	A	N1-C6-N6	-7.09	114.34	118.60
21	AA	1248	A	C5-C6-N1	7.09	121.25	117.70
37	BO	102	ARG	NE-CZ-NH2	-7.09	116.75	120.30
54	BA	2328	A	C5-C6-N1	7.09	121.25	117.70
21	AA	1226	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	1452	C	N3-C2-O2	-7.09	116.94	121.90
22	A1	70	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	53	A	C5-C6-N1	7.09	121.24	117.70
54	BA	131	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1322	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	1575	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	1306	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	95	A	C5-C6-N1	7.09	121.24	117.70
54	BA	936	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	1129	A	O4'-C1'-N9	7.09	113.87	108.20
54	BA	2675	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	2058	A	C5-C6-N1	7.09	121.24	117.70
54	BA	752	A	C5-C6-N1	7.08	121.24	117.70
21	AA	596	A	N1-C6-N6	-7.08	114.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	21	A	C5-C6-N1	7.08	121.24	117.70
54	BA	262	A	C4-C5-C6	-7.08	113.46	117.00
24	A3	22	A	C5-C6-N1	7.08	121.24	117.70
43	BU	21	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	163	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	151	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	493	A	C5-C6-N1	7.08	121.24	117.70
25	BC	211	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	21	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	209	C	O4'-C1'-N1	7.08	113.86	108.20
54	BA	789	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2498	C	N3-C2-O2	-7.08	116.95	121.90
21	AA	1251	A	C4-C5-C6	-7.08	113.46	117.00
24	A3	35	C	N3-C2-O2	-7.08	116.95	121.90
35	BM	44	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	1914	C	N3-C2-O2	-7.08	116.95	121.90
21	AA	327	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	1363	A	C5-C6-N1	7.08	121.24	117.70
21	AA	1460	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	892	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1571	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1593	A	C5-C6-N1	7.08	121.24	117.70
21	AA	909	A	C5-C6-N1	7.07	121.24	117.70
21	AA	1483	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	1638	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	1137	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	353	A	O4'-C1'-N9	7.07	113.86	108.20
21	AA	1418	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1033	U	O4'-C1'-N1	7.07	113.86	108.20
54	BA	2478	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	1259	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1749	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2374	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	995	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1335	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	47	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	949	A	C5-C6-N1	7.07	121.23	117.70
54	BA	94	A	C5-C6-N1	7.07	121.23	117.70
54	BA	513	A	C4-C5-C6	-7.07	113.47	117.00
21	AA	495	A	N1-C6-N6	-7.06	114.36	118.60
21	AA	1468	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1403	A	C5-C6-N1	7.06	121.23	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2225	A	N1-C6-N6	-7.06	114.36	118.60
24	A3	14	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	457	A	C5-C6-N1	7.06	121.23	117.70
21	AA	576	C	N1-C2-O2	7.06	123.14	118.90
54	BA	1938	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2516	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	1257	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	217	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	927	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	1431	A	C5-C6-N1	7.05	121.23	117.70
21	AA	1466	C	N3-C2-O2	-7.05	116.96	121.90
54	BA	1508	A	C5-C6-N1	7.05	121.23	117.70
21	AA	692	U	N3-C2-O2	-7.05	117.26	122.20
21	AA	1163	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1413	A	C4-C5-C6	-7.05	113.47	117.00
33	BK	49	ARG	NE-CZ-NH1	7.05	123.83	120.30
6	AG	142	ARG	NE-CZ-NH1	7.05	123.83	120.30
21	AA	1035	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1318	A	C5-C6-N1	7.05	121.22	117.70
54	BA	439	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2101	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2887	A	C4-C5-C6	-7.05	113.48	117.00
21	AA	1499	A	C5-C6-N1	7.05	121.22	117.70
26	BD	13	ARG	NE-CZ-NH1	7.05	123.82	120.30
54	BA	251	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	1287	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1812	U	O4'-C1'-N1	7.05	113.84	108.20
54	BA	2734	A	C4-C5-C6	-7.05	113.48	117.00
54	BA	1302	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2518	A	C5-C6-N1	7.04	121.22	117.70
21	AA	71	A	C5-C6-N1	7.04	121.22	117.70
24	A3	44	A	C4-C5-C6	-7.04	113.48	117.00
48	BZ	15	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	749	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	1098	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2151	U	O4'-C1'-N1	7.04	113.83	108.20
49	B0	12	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	602	A	C5-C6-N1	7.04	121.22	117.70
5	AF	79	ARG	NE-CZ-NH1	7.04	123.82	120.30
21	AA	1271	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1739	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2335	A	C5-C6-N1	7.04	121.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2711	A	C5-C6-N1	7.04	121.22	117.70
21	AA	579	A	C5-C6-N1	7.04	121.22	117.70
21	AA	765	G	O4'-C1'-N9	7.04	113.83	108.20
21	AA	974	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1502	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1009	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	2092	U	O4'-C1'-N1	7.04	113.83	108.20
21	AA	1408	A	C5-C6-N1	7.03	121.22	117.70
30	BH	51	ARG	NE-CZ-NH1	7.03	123.82	120.30
54	BA	1993	U	O4'-C1'-N1	7.03	113.83	108.20
21	AA	5	U	C1'-O4'-C4'	-7.03	104.28	109.90
54	BA	1046	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1307	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1354	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1433	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1634	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1916	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2103	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	2082	A	C5-C6-N1	7.03	121.22	117.70
21	AA	816	A	C5-C6-N1	7.03	121.21	117.70
21	AA	1155	A	C5-C6-N1	7.03	121.21	117.70
54	BA	621	A	C5-C6-N1	7.03	121.21	117.70
54	BA	821	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	2530	A	C5-C6-N1	7.03	121.21	117.70
14	AO	16	ARG	NE-CZ-NH1	7.02	123.81	120.30
21	AA	1096	C	N3-C2-O2	-7.02	116.98	121.90
8	AI	10	ARG	NE-CZ-NH1	7.02	123.81	120.30
21	AA	187	G	C1'-O4'-C4'	-7.02	104.28	109.90
21	AA	860	A	C5-C6-N1	7.02	121.21	117.70
54	BA	574	A	C5-C6-N1	7.02	121.21	117.70
54	BA	610	C	O4'-C1'-N1	7.02	113.82	108.20
54	BA	1618	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	2309	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	751	A	C1'-O4'-C4'	-7.02	104.28	109.90
54	BA	2054	A	C5-C6-N1	7.02	121.21	117.70
45	BW	54	ARG	NE-CZ-NH2	7.02	123.81	120.30
54	BA	466	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1400	C	N3-C2-O2	-7.02	116.99	121.90
24	A3	16	C	N3-C2-O2	-7.02	116.99	121.90
21	AA	946	A	C5-C6-N1	7.01	121.21	117.70
21	AA	1032	G	O4'-C1'-N9	7.01	113.81	108.20
54	BA	460	A	C5-C6-N1	7.01	121.21	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	503	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	933	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	1551	A	C5-C6-N1	7.01	121.21	117.70
54	BA	435	C	O4'-C1'-N1	7.01	113.81	108.20
54	BA	1454	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	549	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	1045	C	N3-C2-O2	-7.01	116.99	121.90
22	A1	47	U	O4'-C1'-N1	7.01	113.81	108.20
54	BA	2145	C	N3-C2-O2	-7.01	116.99	121.90
22	A1	75	C	N3-C4-N4	-7.01	113.09	118.00
54	BA	901	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	2146	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	2183	A	C5-C6-N1	7.01	121.20	117.70
54	BA	878	A	C5-C6-N1	7.01	121.20	117.70
54	BA	1745	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2738	A	C5-C6-N1	7.01	121.20	117.70
54	BA	1133	A	C5-C6-N1	7.00	121.20	117.70
21	AA	694	A	C5-C6-N1	7.00	121.20	117.70
54	BA	693	A	C5-C6-N1	7.00	121.20	117.70
21	AA	83	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	179	A	C5-C6-N1	7.00	121.20	117.70
21	AA	819	A	C5-C6-N1	7.00	121.20	117.70
21	AA	1146	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	1969	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	2158	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	2478	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2851	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	98	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1532	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1583	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	750	C	N3-C2-O2	-6.99	117.00	121.90
21	AA	1262	C	N3-C2-O2	-6.99	117.00	121.90
54	BA	1505	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	1735	A	N1-C6-N6	-6.99	114.40	118.60
54	BA	2776	A	C5-C6-N1	6.99	121.20	117.70
45	BW	19	ARG	NE-CZ-NH1	6.99	123.80	120.30
54	BA	844	A	C5-C6-N1	6.99	121.20	117.70
21	AA	250	A	C5-C6-N1	6.99	121.19	117.70
54	BA	415	A	C5-C6-N1	6.99	121.19	117.70
21	AA	793	U	C1'-O4'-C4'	-6.99	104.31	109.90
21	AA	1082	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	480	A	C5-C6-N1	6.99	121.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2327	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1786	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	2006	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	2169	A	O4'-C1'-N9	6.99	113.79	108.20
54	BA	1522	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1966	A	C5-C6-N1	6.99	121.19	117.70
21	AA	1293	C	N3-C2-O2	-6.98	117.01	121.90
55	BB	115	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	673	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	1117	A	C5-C6-N1	6.98	121.19	117.70
21	AA	1329	A	C5-C6-N1	6.98	121.19	117.70
49	B0	16	ARG	NE-CZ-NH1	6.98	123.79	120.30
54	BA	900	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1014	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	2612	C	N3-C2-O2	-6.98	117.01	121.90
21	AA	872	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	423	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1752	C	N3-C2-O2	-6.98	117.02	121.90
21	AA	192	A	C5-C6-N1	6.98	121.19	117.70
21	AA	274	A	C5-C6-N1	6.98	121.19	117.70
54	BA	744	U	O4'-C1'-N1	6.98	113.78	108.20
54	BA	1583	A	C5-C6-N1	6.98	121.19	117.70
39	BQ	91	ARG	NE-CZ-NH1	6.98	123.79	120.30
54	BA	1987	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	336	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	386	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	749	A	C5-C6-N1	6.97	121.19	117.70
21	AA	1465	A	C5-C6-N1	6.97	121.19	117.70
54	BA	204	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	1500	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1214	A	C5-C6-N1	6.97	121.19	117.70
55	BB	35	C	N1-C2-O2	6.97	123.08	118.90
21	AA	949	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	892	A	C5-C6-N1	6.97	121.19	117.70
54	BA	270	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	900	A	C5-C6-N1	6.97	121.18	117.70
55	BB	78	A	C5-C6-N1	6.97	121.18	117.70
21	AA	900	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	913	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	332	A	O4'-C1'-N9	6.97	113.77	108.20
21	AA	653	U	N3-C2-O2	-6.96	117.33	122.20
21	AA	155	A	C5-C6-N1	6.96	121.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1367	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	101	A	C5-C6-N1	6.96	121.18	117.70
21	AA	675	A	C5-C6-N1	6.96	121.18	117.70
21	AA	936	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	1347	A	C5-C6-N1	6.96	121.18	117.70
21	AA	781	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1110	A	C5-C6-N1	6.96	121.18	117.70
25	BC	51	ARG	NE-CZ-NH1	6.96	123.78	120.30
54	BA	216	A	N1-C6-N6	-6.96	114.42	118.60
55	BB	90	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	327	A	C5-C6-N1	6.96	121.18	117.70
54	BA	613	A	C5-C6-N1	6.96	121.18	117.70
54	BA	689	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1549	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1942	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	2473	U	N3-C2-O2	-6.96	117.33	122.20
21	AA	364	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1468	A	N1-C6-N6	-6.96	114.43	118.60
54	BA	1821	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	1311	A	C5-C6-N1	6.95	121.18	117.70
54	BA	2758	A	C4-C5-C6	-6.95	113.52	117.00
21	AA	199	A	C5-C6-N1	6.95	121.18	117.70
54	BA	2013	A	C5-C6-N1	6.95	121.18	117.70
21	AA	80	A	C5-C6-N1	6.95	121.17	117.70
33	BK	30	ARG	NE-CZ-NH1	6.95	123.78	120.30
40	BR	79	ARG	NE-CZ-NH1	6.95	123.78	120.30
46	BX	26	ARG	NE-CZ-NH1	6.95	123.78	120.30
54	BA	590	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1446	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	2347	C	O4'-C1'-N1	6.95	113.76	108.20
13	AN	61	ARG	NE-CZ-NH1	6.95	123.78	120.30
21	AA	28	A	C5-C6-N1	6.95	121.17	117.70
21	AA	1059	C	N3-C2-O2	-6.95	117.04	121.90
21	AA	1179	A	C5-C6-N1	6.95	121.17	117.70
22	A1	58	A	C5-C6-N1	6.95	121.17	117.70
54	BA	21	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1947	C	N3-C2-O2	-6.95	117.04	121.90
21	AA	303	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	1328	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	2211	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2430	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	2468	A	C5-C6-N1	6.95	121.17	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	103	A	C5-C6-N1	6.94	121.17	117.70
54	BA	632	A	N1-C6-N6	-6.94	114.43	118.60
21	AA	475	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	934	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	851	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	1241	A	N1-C6-N6	-6.94	114.44	118.60
54	BA	1384	A	C5-C6-N1	6.94	121.17	117.70
21	AA	1126	U	N3-C2-O2	-6.94	117.34	122.20
54	BA	1027	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1050	A	C4-C5-C6	-6.94	113.53	117.00
21	AA	729	A	C5-C6-N1	6.94	121.17	117.70
54	BA	155	A	N1-C6-N6	-6.94	114.44	118.60
54	BA	2432	A	C5-C6-N1	6.94	121.17	117.70
21	AA	1518	A	C5-C6-N1	6.94	121.17	117.70
24	A3	74	A	N1-C6-N6	-6.94	114.44	118.60
54	BA	2476	A	N1-C6-N6	-6.94	114.44	118.60
21	AA	422	C	N3-C2-O2	-6.94	117.05	121.90
24	A3	60	A	C5-C6-N1	6.94	121.17	117.70
39	BQ	10	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	821	A	C5-C6-N1	6.94	121.17	117.70
55	BB	50	A	C4-C5-C6	-6.94	113.53	117.00
34	BL	59	ARG	NE-CZ-NH1	6.93	123.77	120.30
54	BA	470	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	705	A	C5-C6-N1	6.93	121.17	117.70
54	BA	988	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1508	A	O4'-C1'-N9	6.93	113.75	108.20
54	BA	1793	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	228	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1248	A	C4-C5-C6	-6.93	113.53	117.00
47	BY	29	ARG	NE-CZ-NH1	6.93	123.77	120.30
54	BA	2893	A	C5-C6-N1	6.93	121.17	117.70
55	BB	57	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1357	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	661	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1151	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	946	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	582	A	O4'-C1'-N9	6.93	113.74	108.20
54	BA	2020	A	C5-C6-N1	6.93	121.16	117.70
54	BA	2700	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	111	A	C5-C6-N1	6.93	121.16	117.70
54	BA	2033	A	O4'-C1'-N9	6.93	113.74	108.20
54	BA	2902	C	N3-C2-O2	-6.93	117.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	99	A	C5-C6-N1	6.93	121.16	117.70
21	AA	160	A	C5-C6-N1	6.92	121.16	117.70
21	AA	782	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1537	G	O4'-C1'-N9	6.92	113.74	108.20
54	BA	2516	A	C5-C6-N1	6.92	121.16	117.70
21	AA	572	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	675	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	964	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1413	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	2393	U	O4'-C1'-N1	6.92	113.74	108.20
54	BA	1150	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	313	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	1271	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	172	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1046	A	N1-C6-N6	-6.92	114.45	118.60
21	AA	264	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	817	C	C1'-O4'-C4'	-6.92	104.37	109.90
54	BA	1175	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	1349	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	1650	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2439	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2679	A	C5-C6-N1	6.92	121.16	117.70
21	AA	7	A	C4-C5-C6	-6.91	113.54	117.00
27	BE	21	ARG	NE-CZ-NH1	6.91	123.76	120.30
54	BA	1045	C	O4'-C1'-N1	6.91	113.73	108.20
54	BA	2392	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	2745	C	N3-C2-O2	-6.91	117.06	121.90
55	BB	50	A	C5-C6-N1	6.91	121.16	117.70
54	BA	2134	A	C4-C5-C6	-6.91	113.54	117.00
54	BA	256	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	2176	A	C5-C6-N1	6.91	121.16	117.70
54	BA	2453	A	C5-C6-N1	6.91	121.16	117.70
17	AR	60	ARG	NE-CZ-NH1	6.91	123.75	120.30
21	AA	205	A	C5-C6-N1	6.91	121.15	117.70
21	AA	613	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	829	A	C5-C6-N1	6.91	121.15	117.70
21	AA	935	A	C5-C6-N1	6.91	121.15	117.70
24	A3	75	C	N3-C2-O2	-6.91	117.07	121.90
54	BA	2059	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2888	C	N3-C2-O2	-6.91	117.07	121.90
21	AA	10	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	979	A	C5-C6-N1	6.90	121.15	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1579	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	1708	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	176	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	645	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	1307	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	1970	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1012	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	1457	G	N1-C6-O6	-6.90	115.76	119.90
54	BA	2762	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	1646	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	178	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	339	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	182	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1617	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2724	U	O4'-C1'-N1	6.90	113.72	108.20
21	AA	872	A	C5-C6-N1	6.90	121.15	117.70
36	BN	96	ARG	NE-CZ-NH1	6.90	123.75	120.30
54	BA	453	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1794	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1339	A	C5-C6-N1	6.89	121.15	117.70
54	BA	2108	A	C5-C6-N1	6.89	121.15	117.70
24	A3	17	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	6	A	C5-C6-N1	6.89	121.15	117.70
54	BA	229	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	2386	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	231	A	C5-C6-N1	6.89	121.14	117.70
54	BA	2879	A	C5-C6-N1	6.89	121.14	117.70
21	AA	246	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1143	G	N1-C6-O6	-6.89	115.77	119.90
21	AA	681	A	C5-C6-N1	6.89	121.14	117.70
54	BA	1640	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1021	A	C5-C6-N1	6.89	121.14	117.70
54	BA	544	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1913	A	C5-C6-N1	6.89	121.14	117.70
54	BA	2412	A	N1-C6-N6	-6.89	114.47	118.60
54	BA	2774	C	N3-C2-O2	-6.89	117.08	121.90
55	BB	34	A	C5-C6-N1	6.89	121.14	117.70
1	AB	221	ARG	NE-CZ-NH1	6.88	123.74	120.30
21	AA	210	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	860	A	N1-C6-N6	-6.88	114.47	118.60
54	BA	896	A	O4'-C1'-N9	6.88	113.71	108.20
54	BA	1610	A	C5-C6-N1	6.88	121.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2720	U	O4'-C1'-N1	6.88	113.71	108.20
54	BA	968	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	411	A	C5-C6-N1	6.88	121.14	117.70
21	AA	743	A	C5-C6-N1	6.88	121.14	117.70
21	AA	865	A	C5-C6-N1	6.88	121.14	117.70
21	AA	181	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1069	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	2314	A	C5-C6-N1	6.88	121.14	117.70
21	AA	1101	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2119	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2837	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	179	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	397	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1214	C	N1-C2-O2	6.88	123.03	118.90
25	BC	202	ARG	NE-CZ-NH1	6.88	123.74	120.30
54	BA	1503	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2254	C	N3-C2-O2	-6.88	117.09	121.90
54	BA	2588	G	O4'-C1'-N9	6.88	113.70	108.20
54	BA	921	C	N3-C2-O2	-6.88	117.09	121.90
21	AA	279	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	1067	A	C5-C6-N1	6.87	121.14	117.70
26	BD	77	ARG	NE-CZ-NH1	6.87	123.74	120.30
54	BA	99	U	N3-C2-O2	-6.87	117.39	122.20
54	BA	590	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	1155	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	1854	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	938	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	740	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	2860	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	928	A	C4-C5-C6	-6.87	113.57	117.00
22	A1	6	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	443	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	1169	A	C5-C6-N1	6.87	121.13	117.70
54	BA	592	A	C5-C6-N1	6.87	121.13	117.70
54	BA	2074	U	O4'-C1'-N1	6.87	113.69	108.20
54	BA	2439	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	2873	A	C5-C6-N1	6.87	121.13	117.70
55	BB	101	A	N1-C6-N6	-6.87	114.48	118.60
21	AA	1288	A	C5-C6-N1	6.86	121.13	117.70
21	AA	1433	A	C4-C5-C6	-6.86	113.57	117.00
38	BP	50	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	105	C	N3-C2-O2	-6.86	117.10	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2665	A	C5-C6-N1	6.86	121.13	117.70
21	AA	493	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	2800	A	C5-C6-N1	6.86	121.13	117.70
21	AA	116	A	C5-C6-N1	6.86	121.13	117.70
21	AA	1152	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	1251	A	C5-C6-N1	6.86	121.13	117.70
54	BA	340	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1960	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	2632	A	C5-C6-N1	6.86	121.13	117.70
20	AU	33	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	519	U	O4'-C1'-N1	6.86	113.69	108.20
54	BA	941	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1881	C	N3-C2-O2	-6.86	117.10	121.90
55	BB	59	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	363	A	N1-C6-N6	-6.85	114.49	118.60
54	BA	2866	U	O4'-C1'-N1	6.85	113.68	108.20
21	AA	459	A	C5-C6-N1	6.85	121.13	117.70
54	BA	228	C	O4'-C1'-N1	6.85	113.68	108.20
54	BA	1237	A	C5-C6-N1	6.85	121.13	117.70
54	BA	1744	A	C5-C6-N1	6.85	121.13	117.70
21	AA	186	C	N3-C2-O2	-6.85	117.11	121.90
54	BA	1566	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	195	A	C5-C6-N1	6.85	121.12	117.70
21	AA	448	A	C5-C6-N1	6.85	121.12	117.70
21	AA	816	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	1130	A	C5-C6-N1	6.85	121.12	117.70
21	AA	1274	A	C4-C5-C6	-6.85	113.58	117.00
25	BC	12	ARG	NE-CZ-NH1	6.85	123.72	120.30
54	BA	125	A	C5-C6-N1	6.85	121.12	117.70
54	BA	984	A	N1-C6-N6	-6.85	114.49	118.60
54	BA	2199	A	C5-C6-N1	6.85	121.12	117.70
54	BA	144	A	C5-C6-N1	6.85	121.12	117.70
54	BA	1054	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1285	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1477	A	C5-C6-N1	6.84	121.12	117.70
21	AA	810	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	2721	A	C5-C6-N1	6.84	121.12	117.70
54	BA	603	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1101	U	O4'-C1'-N1	6.84	113.67	108.20
54	BA	1821	A	C5-C6-N1	6.84	121.12	117.70
21	AA	499	A	C4-C5-C6	-6.84	113.58	117.00
23	A2	91	A	C5-C6-N1	6.84	121.12	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	142	A	C5-C6-N1	6.84	121.12	117.70
54	BA	481	G	O4'-C1'-N9	6.84	113.67	108.20
21	AA	74	A	C4-C5-C6	-6.84	113.58	117.00
21	AA	1507	A	C5-C6-N1	6.84	121.12	117.70
54	BA	237	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	522	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1127	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1258	U	O4'-C1'-N1	6.84	113.67	108.20
54	BA	1585	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	2450	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2459	A	N1-C6-N6	-6.84	114.50	118.60
54	BA	2466	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1194	A	C5-C6-N1	6.83	121.12	117.70
21	AA	498	A	C5-C6-N1	6.83	121.12	117.70
22	A1	41	A	C5-C6-N1	6.83	121.12	117.70
42	BT	6	ARG	NE-CZ-NH1	-6.83	116.88	120.30
54	BA	241	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	734	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2462	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	256	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2590	A	C5-C6-N1	6.83	121.12	117.70
21	AA	845	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	510	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	172	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	2734	A	C5-C6-N1	6.83	121.11	117.70
54	BA	208	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	946	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1100	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1284	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	1308	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	1848	A	C5-C6-N1	6.83	121.11	117.70
54	BA	1996	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	215	C	N3-C2-O2	-6.82	117.12	121.90
21	AA	277	C	N3-C2-O2	-6.82	117.12	121.90
21	AA	1245	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	2531	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1096	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2352	A	N1-C6-N6	-6.82	114.51	118.60
21	AA	640	A	C5-C6-N1	6.82	121.11	117.70
21	AA	892	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	856	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	1264	A	C5-C6-N1	6.82	121.11	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1918	A	C5-C6-N1	6.82	121.11	117.70
21	AA	32	A	N1-C6-N6	-6.82	114.51	118.60
21	AA	932	C	N3-C2-O2	-6.82	117.13	121.90
25	BC	220	ARG	NE-CZ-NH1	6.82	123.71	120.30
44	BV	9	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	927	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1936	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	2211	A	O4'-C1'-N9	6.82	113.65	108.20
21	AA	931	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	5	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	368	A	C5-C6-N1	6.82	121.11	117.70
54	BA	564	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	1142	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2830	C	O4'-C1'-N1	6.82	113.65	108.20
22	A1	56	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	920	A	C5-C6-N1	6.81	121.11	117.70
21	AA	499	A	C5-C6-N1	6.81	121.11	117.70
21	AA	715	A	C5-C6-N1	6.81	121.11	117.70
21	AA	808	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	87	U	O4'-C1'-N1	6.81	113.65	108.20
54	BA	2071	A	C5-C6-N1	6.81	121.11	117.70
54	BA	2427	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	156	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	250	A	C4-C5-C6	-6.81	113.59	117.00
21	AA	1044	A	C4-C5-C6	-6.81	113.59	117.00
25	BC	13	ARG	NE-CZ-NH1	6.81	123.70	120.30
54	BA	945	A	N1-C6-N6	-6.81	114.51	118.60
54	BA	1969	A	C5-C6-N1	6.81	121.11	117.70
21	AA	583	A	C5-C6-N1	6.81	121.10	117.70
54	BA	196	A	C5-C6-N1	6.81	121.10	117.70
54	BA	2300	C	N3-C2-O2	-6.81	117.14	121.90
55	BB	29	A	C4-C5-C6	-6.81	113.60	117.00
12	AM	69	ARG	NE-CZ-NH1	6.80	123.70	120.30
21	AA	372	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	1036	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	1404	C	N1-C2-O2	6.80	122.98	118.90
54	BA	1679	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1879	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	784	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	56	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	171	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	1230	A	C5-C6-N1	6.80	121.10	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2109	U	O4'-C1'-N1	6.80	113.64	108.20
54	BA	2227	A	N1-C6-N6	-6.80	114.52	118.60
21	AA	546	A	C4-C5-C6	-6.80	113.60	117.00
22	A1	14	A	C5-C6-N1	6.80	121.10	117.70
39	BQ	5	ARG	NE-CZ-NH1	6.80	123.70	120.30
54	BA	2196	C	N3-C2-O2	-6.80	117.14	121.90
55	BB	46	A	C5-C6-N1	6.80	121.10	117.70
24	A3	45	A	C5-C6-N1	6.80	121.10	117.70
54	BA	71	A	N1-C6-N6	-6.80	114.52	118.60
54	BA	2005	A	C5-C6-N1	6.80	121.10	117.70
21	AA	322	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	2394	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	55	A	C5-C6-N1	6.79	121.10	117.70
21	AA	546	A	C5-C6-N1	6.79	121.10	117.70
21	AA	696	A	C5-C6-N1	6.79	121.10	117.70
21	AA	985	C	N3-C2-O2	-6.79	117.14	121.90
21	AA	143	A	C5-C6-N1	6.79	121.10	117.70
21	AA	1105	A	C5-C6-N1	6.79	121.10	117.70
54	BA	833	A	C5-C6-N1	6.79	121.10	117.70
54	BA	1126	A	C5-C6-N1	6.79	121.10	117.70
54	BA	1499	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	1827	U	O4'-C1'-N1	6.79	113.64	108.20
54	BA	2142	A	C4-C5-C6	-6.79	113.60	117.00
55	BB	101	A	C5-C6-N1	6.79	121.10	117.70
24	A3	45	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	14	A	C5-C6-N1	6.79	121.10	117.70
54	BA	104	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	161	A	C5-C6-N1	6.79	121.09	117.70
54	BA	282	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	572	A	C5-C6-N1	6.79	121.10	117.70
54	BA	751	A	C5-C6-N1	6.79	121.10	117.70
54	BA	830	G	N3-C2-N2	-6.79	115.15	119.90
54	BA	2900	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	1363	A	O4'-C1'-N9	6.79	113.63	108.20
51	B2	39	ARG	NE-CZ-NH1	6.79	123.69	120.30
54	BA	1469	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	1672	A	N1-C6-N6	-6.79	114.53	118.60
21	AA	746	A	C5-C6-N1	6.79	121.09	117.70
54	BA	2317	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	298	A	C5-C6-N1	6.78	121.09	117.70
21	AA	959	A	C5-C6-N1	6.78	121.09	117.70
54	BA	172	A	C4-C5-C6	-6.78	113.61	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2814	A	C4-C5-C6	-6.78	113.61	117.00
1	AB	73	ARG	NE-CZ-NH1	6.78	123.69	120.30
21	AA	996	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	528	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1741	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	2274	A	C5-C6-N1	6.78	121.09	117.70
21	AA	912	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	614	A	C5-C6-N1	6.78	121.09	117.70
25	BC	268	ARG	NE-CZ-NH1	6.78	123.69	120.30
54	BA	981	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	1230	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1254	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	1489	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	1523	U	O4'-C1'-N1	6.78	113.62	108.20
54	BA	199	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	515	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	1287	A	N1-C6-N6	-6.77	114.54	118.60
54	BA	2084	C	N3-C2-O2	-6.77	117.16	121.90
5	AF	24	ARG	NE-CZ-NH1	6.77	123.69	120.30
21	AA	797	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	1325	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	1253	A	C5-C6-N1	6.77	121.09	117.70
21	AA	183	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	1349	A	C5-C6-N1	6.77	121.08	117.70
54	BA	415	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	1293	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	2060	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	167	A	N1-C6-N6	-6.77	114.54	118.60
54	BA	716	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2886	A	O4'-C1'-N9	6.77	113.61	108.20
55	BB	94	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1476	U	O4'-C1'-N1	6.77	113.61	108.20
21	AA	663	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	443	A	C5-C6-N1	6.76	121.08	117.70
54	BA	2008	C	N3-C2-O2	-6.76	117.16	121.90
54	BA	1376	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2433	A	N1-C6-N6	-6.76	114.54	118.60
21	AA	324	G	N1-C6-O6	-6.76	115.84	119.90
21	AA	1000	A	C5-C6-N1	6.76	121.08	117.70
49	B0	39	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	2369	A	C5-C6-N1	6.76	121.08	117.70
54	BA	892	A	N1-C6-N6	-6.76	114.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1490	A	O4'-C1'-N9	6.76	113.61	108.20
54	BA	1665	A	C5-C6-N1	6.76	121.08	117.70
54	BA	2733	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	743	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	1035	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	1180	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1229	A	N1-C6-N6	-6.76	114.55	118.60
54	BA	1433	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	766	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	1362	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	1533	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	300	A	C5-C6-N1	6.75	121.08	117.70
54	BA	721	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1713	A	C5-C6-N1	6.75	121.08	117.70
21	AA	131	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	907	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1590	A	C5-C6-N1	6.75	121.08	117.70
21	AA	612	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	813	U	O4'-C1'-N1	6.75	113.60	108.20
21	AA	914	A	C5-C6-N1	6.75	121.07	117.70
54	BA	675	A	C5-C6-N1	6.75	121.07	117.70
54	BA	1664	A	C5-C6-N1	6.75	121.07	117.70
54	BA	2111	U	O4'-C1'-N1	6.75	113.60	108.20
54	BA	2564	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	432	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	702	U	O4'-C1'-N1	6.75	113.60	108.20
54	BA	1054	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	2772	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	890	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	196	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1344	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1319	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	2698	U	O4'-C1'-N1	6.74	113.59	108.20
25	BC	166	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	1178	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	300	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1320	C	N3-C2-O2	-6.74	117.18	121.90
24	A3	14	A	C5-C6-N1	6.74	121.07	117.70
54	BA	730	A	C5-C6-N1	6.74	121.07	117.70
54	BA	984	A	C5-C6-N1	6.74	121.07	117.70
21	AA	634	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	968	A	C5-C6-N1	6.74	121.07	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1332	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1403	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1957	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	2781	A	C5-C6-N1	6.74	121.07	117.70
54	BA	28	A	N1-C6-N6	-6.74	114.56	118.60
54	BA	820	A	C4-C5-C6	-6.74	113.63	117.00
13	AN	69	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	348	A	C4-C5-C6	-6.74	113.63	117.00
3	AD	61	ARG	NE-CZ-NH1	6.73	123.67	120.30
21	AA	253	A	C5-C6-N1	6.73	121.07	117.70
24	A3	63	C	N3-C2-O2	-6.73	117.19	121.90
37	BO	102	ARG	NE-CZ-NH1	6.73	123.67	120.30
21	AA	1216	A	C5-C6-N1	6.73	121.07	117.70
35	BM	16	ARG	NE-CZ-NH2	6.73	123.67	120.30
10	AK	121	ARG	NE-CZ-NH2	6.73	123.67	120.30
21	AA	802	A	C5-C6-N1	6.73	121.06	117.70
54	BA	795	C	N3-C2-O2	-6.73	117.19	121.90
6	AG	101	ARG	NE-CZ-NH1	6.73	123.66	120.30
21	AA	1412	C	N3-C2-O2	-6.73	117.19	121.90
24	A3	72	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	961	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2362	C	O4'-C1'-N1	6.73	113.58	108.20
54	BA	1306	C	O4'-C1'-N1	6.73	113.58	108.20
55	BB	46	A	N1-C6-N6	-6.73	114.56	118.60
22	A1	70	C	P-O3'-C3'	6.72	127.77	119.70
54	BA	125	A	N1-C6-N6	-6.72	114.56	118.60
54	BA	722	A	C5-C6-N1	6.72	121.06	117.70
55	BB	52	A	C5-C6-N1	6.72	121.06	117.70
21	AA	355	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	649	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	780	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	906	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	626	A	C5-C6-N1	6.72	121.06	117.70
54	BA	723	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	374	A	C5-C6-N1	6.72	121.06	117.70
21	AA	995	C	N1-C2-O2	6.72	122.93	118.90
54	BA	2009	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2628	C	N3-C2-O2	-6.72	117.20	121.90
19	AT	17	ARG	NE-CZ-NH1	6.72	123.66	120.30
21	AA	648	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	157	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	277	G	O4'-C1'-N9	6.72	113.58	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1477	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	767	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	1093	A	C5-C6-N1	6.72	121.06	117.70
54	BA	805	G	N3-C2-N2	-6.72	115.20	119.90
54	BA	861	A	C5-C6-N1	6.72	121.06	117.70
54	BA	1021	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1134	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2715	C	N3-C2-O2	-6.72	117.20	121.90
55	BB	12	C	N3-C2-O2	-6.72	117.20	121.90
21	AA	320	A	C5-C6-N1	6.71	121.06	117.70
54	BA	305	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	2095	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	167	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1475	G	P-O3'-C3'	6.71	127.76	119.70
54	BA	1981	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2800	A	C4-C5-C6	-6.71	113.64	117.00
21	AA	739	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	1398	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	753	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1308	A	C5-C6-N1	6.71	121.06	117.70
21	AA	270	A	N1-C6-N6	-6.71	114.57	118.60
54	BA	899	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1370	C	O4'-C1'-N1	6.71	113.57	108.20
32	BJ	99	ARG	NE-CZ-NH1	6.71	123.65	120.30
54	BA	316	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1020	A	C5-C6-N1	6.71	121.05	117.70
54	BA	2175	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	2651	C	N3-C2-O2	-6.71	117.20	121.90
55	BB	99	A	N1-C6-N6	-6.71	114.58	118.60
21	AA	58	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	1328	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	430	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	599	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2340	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1698	A	N1-C6-N6	-6.70	114.58	118.60
21	AA	1250	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	1609	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	311	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	1389	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	11	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1505	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1727	C	N3-C2-O2	-6.70	117.21	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2425	A	C5-C6-N1	6.70	121.05	117.70
21	AA	194	C	N3-C2-O2	-6.70	117.21	121.90
2	AC	178	ARG	NE-CZ-NH1	6.69	123.65	120.30
21	AA	263	A	N1-C6-N6	-6.69	114.58	118.60
24	A3	74	A	C5-C6-N1	6.69	121.05	117.70
54	BA	933	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1354	A	N1-C6-N6	-6.69	114.58	118.60
21	AA	55	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	430	A	C5-C6-N1	6.69	121.05	117.70
21	AA	746	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	118	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	191	A	N1-C6-N6	-6.69	114.59	118.60
54	BA	1650	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	354	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	161	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	905	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1711	A	C5-C6-N1	6.68	121.04	117.70
54	BA	5	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2469	A	C5-C6-N1	6.68	121.04	117.70
21	AA	139	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	501	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1399	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	747	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1029	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2860	A	C5-C6-N1	6.68	121.04	117.70
21	AA	924	C	N3-C2-O2	-6.68	117.23	121.90
54	BA	22	C	N3-C2-O2	-6.68	117.23	121.90
54	BA	353	C	N3-C2-O2	-6.68	117.23	121.90
54	BA	371	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	668	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	677	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1142	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1243	C	N3-C2-O2	-6.68	117.23	121.90
27	BE	170	ARG	NE-CZ-NH2	-6.67	116.96	120.30
54	BA	527	C	N1-C2-O2	6.67	122.90	118.90
55	BB	68	C	O4'-C1'-N1	6.67	113.54	108.20
21	AA	110	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	206	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	825	A	C5-C6-N1	6.67	121.03	117.70
54	BA	19	A	C5-C6-N1	6.67	121.04	117.70
55	BB	36	C	N1-C2-O2	6.67	122.90	118.90
44	BV	19	ARG	NE-CZ-NH1	6.67	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	76	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	149	A	C5-C6-N1	6.67	121.03	117.70
54	BA	715	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2114	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	2154	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	879	C	N3-C2-O2	-6.67	117.23	121.90
34	BL	41	ARG	NE-CZ-NH1	6.67	123.63	120.30
54	BA	718	A	O4'-C1'-N9	6.67	113.53	108.20
54	BA	1155	A	C5-C6-N1	6.67	121.03	117.70
54	BA	709	U	O4'-C1'-N1	6.67	113.53	108.20
54	BA	866	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	2135	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	2471	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	2843	G	O4'-C1'-N9	6.67	113.53	108.20
21	AA	34	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1367	C	N3-C2-O2	-6.66	117.23	121.90
54	BA	752	A	O4'-C1'-N9	6.66	113.53	108.20
54	BA	814	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1595	C	N3-C2-O2	-6.66	117.23	121.90
54	BA	2611	C	O4'-C1'-N1	6.66	113.53	108.20
21	AA	349	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	541	A	C5-C6-N1	6.66	121.03	117.70
21	AA	649	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1890	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2082	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	223	A	C4-C5-C6	-6.66	113.67	117.00
55	BB	66	A	C5-C6-N1	6.66	121.03	117.70
21	AA	502	A	N1-C6-N6	-6.66	114.61	118.60
54	BA	634	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	787	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	609	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1328	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1974	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1927	A	C5-C6-N1	6.65	121.03	117.70
54	BA	2448	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	152	A	C6-C5-N7	6.65	136.96	132.30
21	AA	720	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	1407	C	N3-C2-O2	-6.65	117.24	121.90
22	A1	66	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	918	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1494	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	1918	A	C4-C5-C6	-6.65	113.67	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2606	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	2675	A	C5-C6-N1	6.65	121.03	117.70
21	AA	889	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	1201	A	C5-C6-N1	6.65	121.03	117.70
54	BA	825	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1565	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	1577	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	1691	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	2042	A	N1-C6-N6	-6.65	114.61	118.60
54	BA	2785	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	84	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	142	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	2899	A	C5-C6-N1	6.65	121.03	117.70
21	AA	246	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	749	A	C5-C6-N1	6.65	121.02	117.70
54	BA	1791	A	C5-C6-N1	6.65	121.02	117.70
54	BA	2310	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	393	A	C5-C6-N1	6.64	121.02	117.70
21	AA	787	A	N1-C6-N6	-6.64	114.61	118.60
54	BA	1509	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1759	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2295	C	O4'-C1'-N1	6.64	113.52	108.20
21	AA	823	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	1101	A	P-O3'-C3'	6.64	127.67	119.70
21	AA	1483	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1234	U	O4'-C1'-N1	6.64	113.51	108.20
54	BA	2101	A	N1-C6-N6	-6.64	114.61	118.60
21	AA	53	A	C5-C6-N1	6.64	121.02	117.70
54	BA	739	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2281	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2362	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1143	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2142	A	C5-C6-N1	6.64	121.02	117.70
21	AA	770	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	1103	C	N3-C2-O2	-6.64	117.25	121.90
41	BS	88	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	364	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	873	C	O4'-C1'-N1	6.64	113.51	108.20
54	BA	1247	A	C5-C6-N1	6.64	121.02	117.70
2	AC	130	ARG	NE-CZ-NH2	6.64	123.62	120.30
21	AA	356	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	758	C	N3-C2-O2	-6.64	117.25	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	101	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	925	A	N1-C6-N6	-6.64	114.62	118.60
54	BA	1289	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2534	A	N1-C6-N6	-6.63	114.62	118.60
13	AN	53	ARG	NE-CZ-NH1	6.63	123.61	120.30
21	AA	162	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	309	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	96	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1260	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	1110	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	948	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	1016	A	C5-C6-N1	6.63	121.01	117.70
22	A1	41	A	C4-C5-C6	-6.63	113.69	117.00
36	BN	30	ARG	NE-CZ-NH1	6.63	123.61	120.30
54	BA	477	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	1899	A	C4-C5-C6	-6.63	113.69	117.00
16	AQ	76	ARG	NE-CZ-NH1	6.63	123.61	120.30
21	AA	59	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	1303	C	N1-C2-O2	6.63	122.88	118.90
21	AA	1476	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	2634	A	C5-C6-N1	6.63	121.01	117.70
21	AA	19	A	C5-C6-N1	6.62	121.01	117.70
21	AA	77	A	C5-C6-N1	6.62	121.01	117.70
43	BU	93	ARG	NE-CZ-NH1	6.62	123.61	120.30
54	BA	905	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	238	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	244	A	C5-C6-N1	6.62	121.01	117.70
54	BA	486	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	922	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	943	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	960	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1413	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2679	A	N1-C6-N6	-6.62	114.63	118.60
54	BA	2180	U	O4'-C1'-N1	6.62	113.50	108.20
21	AA	66	A	N1-C6-N6	-6.62	114.63	118.60
21	AA	520	A	C5-C6-N1	6.62	121.01	117.70
23	A2	82	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	255	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1039	A	N1-C6-N6	-6.62	114.63	118.60
20	AU	20	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	1285	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1100	C	N3-C2-O2	-6.62	117.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1676	A	N1-C6-N6	-6.62	114.63	118.60
21	AA	329	A	C5-C6-N1	6.61	121.01	117.70
21	AA	1046	A	C5-C6-N1	6.61	121.01	117.70
54	BA	637	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	1810	A	C5-C6-N1	6.61	121.01	117.70
54	BA	1934	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	2176	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	2456	C	O4'-C1'-N1	6.61	113.49	108.20
54	BA	2810	A	C5-C6-N1	6.61	121.01	117.70
54	BA	722	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	2424	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	1019	A	C4-C5-C6	-6.61	113.69	117.00
21	AA	1267	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	239	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1795	C	N3-C2-O2	-6.61	117.27	121.90
3	AD	72	ARG	NE-CZ-NH1	6.61	123.60	120.30
54	BA	1551	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	1603	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	1829	A	C5-C6-N1	6.61	121.00	117.70
54	BA	2212	A	C1'-O4'-C4'	-6.61	104.61	109.90
54	BA	840	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	1040	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	1462	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	1515	A	C5-C6-N1	6.61	121.00	117.70
54	BA	2298	A	C5-C6-N1	6.61	121.00	117.70
35	BM	6	ARG	NE-CZ-NH1	6.60	123.60	120.30
54	BA	1866	A	C5-C6-N1	6.60	121.00	117.70
21	AA	756	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	796	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1591	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	1592	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1665	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	2871	U	O4'-C1'-N1	6.60	113.48	108.20
21	AA	253	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	345	C	N1-C2-O2	6.60	122.86	118.90
54	BA	737	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1526	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	2461	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1172	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1789	A	C5-C6-N1	6.60	121.00	117.70
54	BA	2810	A	N1-C6-N6	-6.60	114.64	118.60
21	AA	383	A	N1-C6-N6	-6.60	114.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	495	A	C5-C6-N1	6.60	121.00	117.70
55	BB	58	A	C5-C6-N1	6.60	121.00	117.70
21	AA	370	C	N3-C2-O2	-6.60	117.28	121.90
25	BC	181	ARG	NE-CZ-NH1	6.60	123.60	120.30
21	AA	321	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	644	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1246	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	2073	C	N3-C2-O2	-6.59	117.28	121.90
5	AF	38	ARG	NE-CZ-NH1	6.59	123.60	120.30
54	BA	996	A	C5-C6-N1	6.59	121.00	117.70
54	BA	2314	A	C4-C5-C6	-6.59	113.70	117.00
47	BY	7	ARG	NE-CZ-NH1	6.59	123.59	120.30
54	BA	582	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	806	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	1356	G	O4'-C1'-N9	6.59	113.47	108.20
21	AA	1092	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	505	A	C5-C6-N1	6.59	121.00	117.70
54	BA	601	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1580	A	C5-C6-N1	6.59	120.99	117.70
54	BA	2870	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	775	G	O4'-C1'-N9	6.59	113.47	108.20
54	BA	2515	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	64	A	C5-C6-N1	6.59	120.99	117.70
54	BA	279	A	C5-C6-N1	6.59	120.99	117.70
54	BA	1076	C	N3-C2-O2	-6.59	117.29	121.90
22	A1	69	A	C5-C6-N1	6.58	120.99	117.70
21	AA	233	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	1368	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1805	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2821	A	N1-C6-N6	-6.58	114.65	118.60
26	BD	33	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	1533	C	N3-C2-O2	-6.58	117.29	121.90
24	A3	76	C	N3-C2-O2	-6.58	117.30	121.90
36	BN	86	ARG	NE-CZ-NH1	6.58	123.59	120.30
48	BZ	10	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	945	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2517	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	666	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1103	A	C5-C6-N1	6.58	120.99	117.70
55	BB	58	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1480	A	C5-C6-N1	6.57	120.99	117.70
54	BA	264	C	N3-C2-O2	-6.57	117.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	719	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	800	A	C5-C6-N1	6.57	120.99	117.70
54	BA	1001	A	C5-C6-N1	6.57	120.99	117.70
54	BA	1220	G	O4'-C1'-N9	6.57	113.46	108.20
54	BA	1986	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1570	A	C5-C6-N1	6.57	120.98	117.70
21	AA	25	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2035	G	O4'-C1'-N9	6.57	113.45	108.20
54	BA	2072	C	O4'-C1'-N1	6.57	113.45	108.20
21	AA	1197	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	756	A	C5-C6-N1	6.57	120.98	117.70
54	BA	1504	A	N1-C6-N6	-6.57	114.66	118.60
54	BA	2682	A	C5-C6-N1	6.57	120.98	117.70
21	AA	998	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	217	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2378	A	C5-C6-N1	6.57	120.98	117.70
21	AA	161	A	C5-C6-N1	6.56	120.98	117.70
21	AA	708	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	1219	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	1375	A	C5-C6-N1	6.56	120.98	117.70
54	BA	973	A	N1-C6-N6	-6.56	114.66	118.60
54	BA	1233	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1480	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1525	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2322	A	C5-C6-N1	6.56	120.98	117.70
21	AA	962	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	889	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	685	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2091	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	342	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	1626	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2117	A	C5-C6-N1	6.56	120.98	117.70
21	AA	1051	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	975	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	1196	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1265	A	O4'-C1'-N9	6.56	113.45	108.20
54	BA	1635	A	C4-C5-C6	-6.56	113.72	117.00
11	AL	49	ARG	NE-CZ-NH1	6.56	123.58	120.30
21	AA	432	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	440	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1746	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	582	A	C5-C6-N1	6.55	120.97	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2052	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	2358	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	2725	A	C4-C5-C6	-6.55	113.72	117.00
5	AF	45	ARG	NE-CZ-NH1	6.55	123.57	120.30
54	BA	10	A	C5-C6-N1	6.55	120.97	117.70
54	BA	211	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2267	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	2326	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	402	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	1305	C	N3-C2-O2	-6.55	117.32	121.90
21	AA	729	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	1340	A	C5-C6-N1	6.54	120.97	117.70
54	BA	478	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1634	A	N1-C6-N6	-6.54	114.67	118.60
54	BA	2112	G	O4'-C1'-N9	6.54	113.44	108.20
21	AA	510	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	1229	A	C5-C6-N1	6.54	120.97	117.70
54	BA	461	C	O4'-C1'-N1	6.54	113.43	108.20
54	BA	1828	G	O4'-C1'-N9	6.54	113.43	108.20
54	BA	2369	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	314	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	624	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	980	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	1394	A	C5-C6-N1	6.54	120.97	117.70
54	BA	401	A	C5-C6-N1	6.54	120.97	117.70
54	BA	937	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1463	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	131	A	C5-C6-N1	6.54	120.97	117.70
54	BA	788	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1385	A	O4'-C1'-N9	6.54	113.43	108.20
54	BA	1614	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	909	A	N1-C6-N6	-6.54	114.68	118.60
21	AA	994	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	449	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	676	A	C5-C6-N1	6.54	120.97	117.70
54	BA	83	A	C5-C6-N1	6.53	120.97	117.70
54	BA	1262	A	C5-C6-N1	6.53	120.97	117.70
21	AA	26	A	C4-C5-C6	-6.53	113.73	117.00
21	AA	396	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	441	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	556	A	C5-C6-N1	6.53	120.97	117.70
54	BA	1146	C	N3-C2-O2	-6.53	117.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2900	A	C5-C6-N1	6.53	120.97	117.70
21	AA	1362	A	C5-C6-N1	6.53	120.96	117.70
21	AA	1479	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	622	A	C4-C5-C6	-6.53	113.74	117.00
21	AA	1011	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1209	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1298	U	O4'-C1'-N1	6.53	113.42	108.20
54	BA	64	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1593	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1916	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	2332	C	N1-C2-O2	6.53	122.82	118.90
21	AA	1114	C	N3-C2-O2	-6.53	117.33	121.90
22	A1	35	A	N1-C6-N6	-6.53	114.69	118.60
54	BA	1010	A	C5-C6-N1	6.53	120.96	117.70
54	BA	2336	A	O4'-C1'-N9	6.53	113.42	108.20
54	BA	2600	A	C5-C6-N1	6.53	120.96	117.70
55	BB	45	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1775	U	O4'-C1'-N1	6.52	113.42	108.20
54	BA	435	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	1323	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	1352	U	N3-C2-O2	-6.52	117.64	122.20
54	BA	1630	A	C5-C6-N1	6.52	120.96	117.70
21	AA	1447	A	O4'-C1'-N9	6.52	113.42	108.20
54	BA	1244	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1532	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	1140	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	2161	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	2270	A	N1-C6-N6	-6.52	114.69	118.60
54	BA	2418	A	C5-C6-N1	6.52	120.96	117.70
54	BA	2547	A	C4-C5-C6	-6.52	113.74	117.00
9	AJ	5	ARG	NE-CZ-NH1	6.52	123.56	120.30
21	AA	188	C	N3-C2-O2	-6.52	117.34	121.90
24	A3	42	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	146	A	C5-C6-N1	6.52	120.96	117.70
54	BA	920	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1574	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	2071	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	136	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	111	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	461	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	1188	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	1706	C	N3-C2-O2	-6.51	117.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1155	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	1411	C	N3-C2-O2	-6.51	117.34	121.90
22	A1	36	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	344	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	517	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1366	A	C5-C6-N1	6.51	120.95	117.70
54	BA	2081	U	O4'-C1'-N1	6.51	113.41	108.20
21	AA	316	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	838	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1654	A	C4-C5-C6	-6.51	113.75	117.00
21	AA	600	A	C5-C6-N1	6.50	120.95	117.70
54	BA	20	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	1281	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	314	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1363	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2088	A	C5-C6-N1	6.50	120.95	117.70
21	AA	553	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	762	U	P-O3'-C3'	6.50	127.50	119.70
54	BA	1865	U	O4'-C1'-N1	6.50	113.40	108.20
21	AA	192	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	556	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1284	A	C4-C5-C6	-6.50	113.75	117.00
55	BB	8	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	1081	A	C4-C5-C6	-6.50	113.75	117.00
22	A1	25	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	79	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	197	A	C5-C6-N1	6.50	120.95	117.70
54	BA	304	U	O4'-C1'-N1	6.50	113.40	108.20
54	BA	1819	A	N1-C6-N6	-6.50	114.70	118.60
21	AA	970	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	482	A	C5-C6-N1	6.50	120.95	117.70
54	BA	611	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1596	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1909	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2657	A	C5-C6-N1	6.50	120.95	117.70
21	AA	1236	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1977	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	381	C	N3-C2-O2	-6.49	117.35	121.90
54	BA	63	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	382	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1265	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1717	A	C5-C6-N1	6.49	120.95	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1853	A	C5-C6-N1	6.49	120.95	117.70
54	BA	2551	C	N3-C2-O2	-6.49	117.35	121.90
54	BA	2398	U	O4'-C1'-N1	6.49	113.39	108.20
21	AA	1465	A	C4-C5-C6	-6.49	113.75	117.00
25	BC	176	ARG	NE-CZ-NH2	-6.49	117.06	120.30
54	BA	1960	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	344	A	C4-C5-C6	-6.49	113.76	117.00
21	AA	578	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	616	A	C5-C6-N1	6.49	120.94	117.70
54	BA	678	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1221	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	16	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	320	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	2736	A	C5-C6-N1	6.49	120.94	117.70
21	AA	60	A	P-O3'-C3'	6.49	127.48	119.70
54	BA	300	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	1007	C	N1-C2-O2	6.49	122.79	118.90
55	BB	15	A	O4'-C1'-N9	6.49	113.39	108.20
21	AA	98	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	459	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	460	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1690	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2755	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	873	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	635	C	O4'-C1'-N1	6.48	113.39	108.20
54	BA	910	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1833	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	2003	A	N1-C6-N6	-6.48	114.71	118.60
21	AA	59	A	N1-C6-N6	-6.48	114.71	118.60
54	BA	1700	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	631	A	C5-C6-N1	6.48	120.94	117.70
54	BA	908	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1509	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1672	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2741	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	980	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	426	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1940	U	O4'-C1'-N1	6.47	113.38	108.20
21	AA	630	A	C5-C6-N1	6.47	120.94	117.70
21	AA	1519	A	N1-C6-N6	-6.47	114.72	118.60
24	A3	52	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	456	A	C5-C6-N1	6.47	120.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	19	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	106	C	N1-C2-O2	6.47	122.78	118.90
54	BA	812	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1022	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	689	C	N3-C2-O2	-6.47	117.37	121.90
23	A2	79	A	O4'-C1'-N9	6.47	113.37	108.20
54	BA	271	G	P-O3'-C3'	6.47	127.46	119.70
54	BA	1045	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	103	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	791	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2011	U	O4'-C1'-N1	6.46	113.37	108.20
54	BA	2090	A	C5-C6-N1	6.46	120.93	117.70
21	AA	712	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	870	U	O4'-C1'-N1	6.46	113.37	108.20
21	AA	831	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1200	C	N1-C2-O2	6.46	122.78	118.90
55	BB	3	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1670	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	436	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1081	U	O4'-C1'-N1	6.46	113.37	108.20
54	BA	2183	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	731	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	998	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1014	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2014	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2417	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1162	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	130	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	311	A	O4'-C1'-N9	6.46	113.36	108.20
54	BA	487	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	523	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1924	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2014	A	N1-C6-N6	-6.46	114.73	118.60
55	BB	53	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	751	A	O4'-C1'-N9	6.45	113.36	108.20
54	BA	1261	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	1428	C	C1'-O4'-C4'	-6.45	104.74	109.90
54	BA	1460	U	N3-C2-O2	-6.45	117.68	122.20
21	AA	498	A	N1-C6-N6	-6.45	114.73	118.60
54	BA	911	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	1988	G	N3-C2-N2	-6.45	115.38	119.90
54	BA	2215	C	N3-C2-O2	-6.45	117.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	175	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	940	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1364	U	N3-C2-O2	-6.45	117.69	122.20
24	A3	13	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	1977	A	C5-C6-N1	6.45	120.92	117.70
54	BA	2273	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	2691	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	608	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	635	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1974	C	O4'-C1'-N1	6.45	113.36	108.20
54	BA	2045	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	119	A	C5-C6-N1	6.45	120.92	117.70
21	AA	1183	U	O4'-C1'-N1	6.45	113.36	108.20
21	AA	1377	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	1038	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	334	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1943	U	N3-C2-O2	-6.45	117.69	122.20
54	BA	2879	A	N1-C6-N6	-6.45	114.73	118.60
21	AA	1337	G	O4'-C1'-N9	6.44	113.36	108.20
54	BA	2381	A	C5-C6-N1	6.44	120.92	117.70
21	AA	274	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	606	U	O4'-C1'-N1	6.44	113.35	108.20
54	BA	1704	C	O4'-C1'-N1	6.44	113.36	108.20
54	BA	2794	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	1376	U	O4'-C1'-N1	6.44	113.35	108.20
54	BA	42	A	C5-C6-N1	6.44	120.92	117.70
54	BA	2889	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	1254	A	C5-C6-N1	6.44	120.92	117.70
54	BA	52	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1855	U	O4'-C1'-N1	6.44	113.35	108.20
21	AA	815	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	1374	A	N1-C6-N6	-6.44	114.74	118.60
54	BA	106	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	1937	A	C5-C6-N1	6.44	120.92	117.70
54	BA	2565	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	1394	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	650	C	N3-C2-O2	-6.43	117.39	121.90
54	BA	1607	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1908	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1927	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	2377	A	C5-C6-N1	6.43	120.92	117.70
21	AA	335	C	N3-C2-O2	-6.43	117.40	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	B2	35	ARG	NE-CZ-NH1	6.43	123.52	120.30
54	BA	310	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1637	A	C5-C6-N1	6.43	120.92	117.70
54	BA	1874	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2392	A	C5-C6-N1	6.43	120.92	117.70
54	BA	16	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	692	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1894	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2446	G	O4'-C1'-N9	6.43	113.34	108.20
54	BA	2471	A	C5-C6-N1	6.43	120.92	117.70
54	BA	2513	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	207	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	1004	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	329	G	N1-C6-O6	-6.43	116.04	119.90
54	BA	2339	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	607	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	1150	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	1403	C	N3-C2-O2	-6.43	117.40	121.90
24	A3	24	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1496	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	2662	A	C5-C6-N1	6.43	120.91	117.70
21	AA	282	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1518	A	C4-C5-C6	-6.42	113.79	117.00
29	BG	68	ARG	NE-CZ-NH1	6.42	123.51	120.30
54	BA	2340	A	C4-C5-C6	-6.42	113.79	117.00
14	AO	87	ARG	NE-CZ-NH1	6.42	123.51	120.30
15	AP	35	ARG	NE-CZ-NH1	6.42	123.51	120.30
21	AA	143	A	C4-C5-C6	-6.42	113.79	117.00
22	A1	72	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	908	A	C5-C6-N1	6.42	120.91	117.70
32	BJ	69	ARG	NE-CZ-NH1	6.42	123.51	120.30
34	BL	126	ARG	NE-CZ-NH1	6.42	123.51	120.30
54	BA	299	A	C4-C5-C6	-6.42	113.79	117.00
18	AS	31	ARG	NE-CZ-NH2	-6.42	117.09	120.30
21	AA	1296	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	626	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1269	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2614	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	461	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1080	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2826	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	262	A	C4-C5-C6	-6.42	113.79	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AL	11	ARG	NE-CZ-NH1	6.41	123.51	120.30
21	AA	753	A	C4-C5-C6	-6.41	113.79	117.00
21	AA	969	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	912	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1278	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1461	C	N1-C2-O2	6.41	122.75	118.90
21	AA	1342	C	P-O3'-C3'	6.41	127.39	119.70
54	BA	205	G	O4'-C1'-N9	6.41	113.33	108.20
54	BA	1785	A	C6-N1-C2	-6.41	114.75	118.60
21	AA	978	A	C5-C6-N1	6.41	120.91	117.70
54	BA	1872	A	C5-C6-N1	6.41	120.90	117.70
17	AR	42	ARG	NE-CZ-NH1	6.41	123.50	120.30
21	AA	1210	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	2537	U	O4'-C1'-N1	6.41	113.33	108.20
21	AA	533	A	C5-C6-N1	6.41	120.90	117.70
21	AA	866	C	N1-C2-O2	6.41	122.74	118.90
25	BC	261	ARG	NE-CZ-NH1	6.41	123.50	120.30
54	BA	207	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	586	A	C5-C6-N1	6.41	120.90	117.70
54	BA	794	A	C5-C6-N1	6.41	120.90	117.70
54	BA	1836	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	2178	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	2208	C	N3-C2-O2	-6.41	117.42	121.90
21	AA	52	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	983	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	160	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	1171	A	C5-C6-N1	6.40	120.90	117.70
24	A3	47	G	O4'-C1'-N9	6.40	113.32	108.20
54	BA	1472	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	968	C	O4'-C1'-N1	6.40	113.32	108.20
54	BA	2154	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2274	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	2620	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2753	A	C4-C5-C6	-6.40	113.80	117.00
18	AS	3	SER	C-N-CA	6.40	137.70	121.70
21	AA	507	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	146	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	987	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1262	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	908	A	N1-C6-N6	-6.40	114.76	118.60
54	BA	277	G	N3-C2-N2	-6.40	115.42	119.90
54	BA	1713	A	P-O3'-C3'	6.40	127.38	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	392	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	627	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	267	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	366	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	479	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	2723	C	N1-C2-O2	6.39	122.74	118.90
9	AJ	16	ARG	NE-CZ-NH1	6.39	123.50	120.30
22	A1	69	A	C4-C5-C6	-6.39	113.81	117.00
21	AA	266	G	O4'-C1'-N9	6.39	113.31	108.20
21	AA	1171	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	165	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	436	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1905	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1929	G	O4'-C1'-N9	6.39	113.31	108.20
54	BA	1966	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	2070	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2482	A	C4-C5-C6	-6.39	113.81	117.00
22	A1	48	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1814	G	N1-C6-O6	-6.39	116.07	119.90
54	BA	2826	A	C5-C6-N1	6.39	120.89	117.70
21	AA	535	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	761	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	825	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1100	C	O4'-C1'-N1	6.38	113.31	108.20
54	BA	1391	U	O4'-C1'-N1	6.38	113.31	108.20
55	BB	108	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	197	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	777	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	945	G	N3-C4-C5	-6.38	125.41	128.60
54	BA	2703	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	1089	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2097	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2115	G	O4'-C1'-N9	6.38	113.30	108.20
54	BA	1787	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	2058	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2601	C	O4'-C1'-N1	6.38	113.30	108.20
54	BA	2820	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	251	G	P-O3'-C3'	6.38	127.35	119.70
21	AA	330	C	N3-C2-O2	-6.38	117.44	121.90
34	BL	21	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BA	844	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	1434	A	C4-C5-C6	-6.38	113.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1005	C	O4'-C1'-N1	6.38	113.30	108.20
54	BA	1431	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	486	U	O4'-C1'-N1	6.37	113.30	108.20
21	AA	1109	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1064	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1090	A	C5-C6-N1	6.37	120.89	117.70
54	BA	1144	A	C5-C6-N1	6.37	120.89	117.70
21	AA	72	A	C4-C5-C6	-6.37	113.81	117.00
22	A1	60	C	N1-C2-O2	6.37	122.72	118.90
54	BA	1161	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	190	A	C5-C6-N1	6.37	120.89	117.70
54	BA	238	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2806	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2225	A	C5-C6-N1	6.37	120.88	117.70
54	BA	2394	C	O4'-C1'-N1	6.37	113.29	108.20
54	BA	2412	A	C5-C6-N1	6.37	120.89	117.70
30	BH	97	ARG	NE-CZ-NH1	6.37	123.48	120.30
8	AI	11	ARG	NE-CZ-NH1	6.37	123.48	120.30
21	AA	44	A	C4-C5-C6	-6.37	113.82	117.00
21	AA	328	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	915	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1213	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	1586	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	1859	U	O4'-C1'-N1	6.37	113.29	108.20
54	BA	1920	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2507	C	N3-C2-O2	-6.37	117.44	121.90
55	BB	42	C	N3-C2-O2	-6.37	117.44	121.90
55	BB	104	A	C5-C6-N1	6.37	120.88	117.70
21	AA	901	A	C5-C6-N1	6.36	120.88	117.70
21	AA	958	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	184	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1147	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1582	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2080	A	C5-C6-N1	6.36	120.88	117.70
54	BA	706	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1039	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1901	A	C5-C6-N1	6.36	120.88	117.70
21	AA	74	A	C5-C6-N1	6.36	120.88	117.70
21	AA	526	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	1333	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	69	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	540	C	N3-C2-O2	-6.36	117.45	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1962	C	O4'-C1'-N1	6.36	113.29	108.20
54	BA	2211	A	N1-C6-N6	-6.36	114.78	118.60
54	BA	2520	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1686	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1794	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	996	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1569	A	C5-C6-N1	6.36	120.88	117.70
54	BA	2095	A	C5-C6-N1	6.36	120.88	117.70
54	BA	2527	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	509	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	557	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2287	A	O4'-C1'-N9	6.36	113.28	108.20
55	BB	39	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	1359	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	1780	A	C5-C6-N1	6.35	120.88	117.70
54	BA	1211	C	N1-C2-O2	6.35	122.71	118.90
54	BA	1772	A	C5-C6-N1	6.35	120.88	117.70
54	BA	2451	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	1314	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	698	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	781	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	910	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	196	A	C1'-O4'-C4'	-6.35	104.82	109.90
54	BA	361	G	O4'-C1'-N9	6.35	113.28	108.20
54	BA	886	A	C5-C6-N1	6.35	120.88	117.70
54	BA	1774	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	1838	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2376	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	132	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	826	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	945	G	C5-C6-N1	6.35	114.67	111.50
54	BA	281	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	1092	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	1298	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1398	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1606	C	N1-C2-O2	6.34	122.71	118.90
54	BA	2311	A	O4'-C1'-N9	6.34	113.28	108.20
54	BA	2619	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2766	A	N1-C6-N6	-6.34	114.79	118.60
54	BA	2442	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1772	A	N1-C6-N6	-6.34	114.80	118.60
55	BB	43	C	N3-C2-O2	-6.34	117.46	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	92	C	N3-C2-O2	-6.34	117.46	121.90
3	AD	55	ARG	NE-CZ-NH1	6.34	123.47	120.30
21	AA	1167	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1641	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	903	C	N3-C2-O2	-6.34	117.46	121.90
12	AM	89	ARG	NE-CZ-NH1	6.34	123.47	120.30
41	BS	99	ARG	NE-CZ-NH1	6.34	123.47	120.30
54	BA	225	C	N3-C2-O2	-6.34	117.47	121.90
54	BA	1768	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1962	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1998	A	C5-C6-N1	6.34	120.87	117.70
54	BA	2041	U	O4'-C1'-N1	6.34	113.27	108.20
21	AA	1484	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1787	A	C5-C6-N1	6.33	120.87	117.70
21	AA	880	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	925	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	1027	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	2581	G	O4'-C1'-N9	6.33	113.27	108.20
21	AA	692	U	C2-N1-C1'	6.33	125.30	117.70
21	AA	1456	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	922	C	O4'-C1'-N1	6.33	113.26	108.20
55	BB	109	A	C5-C6-N1	6.33	120.86	117.70
3	AD	69	ARG	NE-CZ-NH1	6.33	123.46	120.30
54	BA	2084	C	O4'-C1'-N1	6.33	113.26	108.20
21	AA	1329	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	714	G	N3-C2-N2	-6.33	115.47	119.90
54	BA	661	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	909	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	2015	A	C5-C6-N1	6.33	120.86	117.70
54	BA	2043	C	N3-C2-O2	-6.33	117.47	121.90
24	A3	62	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	404	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	540	C	O4'-C1'-N1	6.32	113.26	108.20
54	BA	2781	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1658	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	49	A	C5-C6-N1	6.32	120.86	117.70
54	BA	352	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	2746	U	O4'-C1'-N1	6.32	113.25	108.20
21	AA	839	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	899	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1420	A	N1-C6-N6	-6.32	114.81	118.60
54	BA	1705	A	C4-C5-C6	-6.32	113.84	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1324	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	1480	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	538	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1762	A	C4-C5-C6	-6.31	113.84	117.00
55	BB	27	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	117	G	N1-C6-O6	-6.31	116.11	119.90
24	A3	42	C	N1-C2-O2	6.31	122.69	118.90
54	BA	66	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	391	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	471	A	C5-C6-N1	6.31	120.86	117.70
54	BA	1313	U	O4'-C1'-N1	6.31	113.25	108.20
54	BA	1625	C	N1-C2-O2	6.31	122.69	118.90
21	AA	1102	A	C5-C6-N1	6.31	120.86	117.70
54	BA	1313	U	N3-C2-O2	-6.31	117.78	122.20
21	AA	1236	A	N1-C6-N6	-6.31	114.81	118.60
22	A1	62	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2644	G	C3'-C2'-C1'	6.31	106.55	101.50
21	AA	1179	A	C4-C5-C6	-6.31	113.85	117.00
21	AA	1345	U	O4'-C1'-N1	6.31	113.25	108.20
54	BA	1932	A	C5-C6-N1	6.31	120.85	117.70
54	BA	2875	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	899	C	N3-C2-O2	-6.30	117.49	121.90
51	B2	33	ARG	NE-CZ-NH1	6.30	123.45	120.30
54	BA	549	G	N3-C2-N2	-6.30	115.49	119.90
54	BA	806	C	O4'-C1'-N1	6.30	113.24	108.20
54	BA	1304	A	C5-C6-N1	6.30	120.85	117.70
54	BA	1468	U	O4'-C1'-N1	6.30	113.24	108.20
54	BA	2313	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2191	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	77	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	167	A	C5-C6-N1	6.30	120.85	117.70
21	AA	1168	U	N3-C2-O2	-6.30	117.79	122.20
54	BA	764	A	C5-C6-N1	6.30	120.85	117.70
54	BA	2461	A	C4-C5-C6	-6.30	113.85	117.00
12	AM	70	ARG	NE-CZ-NH1	6.30	123.45	120.30
22	A1	60	C	C1'-O4'-C4'	-6.30	104.86	109.90
54	BA	507	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1655	A	C5-C6-N1	6.30	120.85	117.70
21	AA	857	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1306	A	C5-C6-N1	6.30	120.85	117.70
21	AA	290	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	435	A	C5-C6-N1	6.30	120.85	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	794	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1049	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2805	C	O4'-C1'-N1	6.30	113.24	108.20
21	AA	1248	A	O4'-C1'-N9	6.29	113.24	108.20
23	A2	80	C	N3-C4-C5	6.29	124.42	121.90
21	AA	40	C	N3-C2-O2	-6.29	117.49	121.90
21	AA	673	A	C5-C6-N1	6.29	120.85	117.70
21	AA	679	C	N3-C2-O2	-6.29	117.50	121.90
24	A3	68	C	N3-C2-O2	-6.29	117.49	121.90
55	BB	28	C	N3-C2-O2	-6.29	117.50	121.90
55	BB	57	A	N1-C6-N6	-6.29	114.82	118.60
21	AA	582	C	O4'-C1'-N1	6.29	113.23	108.20
21	AA	1227	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	1603	A	C5-C6-N1	6.29	120.85	117.70
54	BA	2727	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	1327	C	N3-C2-O2	-6.29	117.50	121.90
17	AR	52	ARG	NE-CZ-NH1	6.29	123.44	120.30
21	AA	155	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	270	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	502	A	C5-C6-N1	6.29	120.84	117.70
54	BA	2538	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	236	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	265	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	876	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1941	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2496	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2687	U	O4'-C1'-N1	6.29	113.23	108.20
21	AA	1001	C	N3-C2-O2	-6.28	117.50	121.90
22	A1	27	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1095	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	492	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	374	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1512	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1652	A	C5-C6-N1	6.28	120.84	117.70
21	AA	1397	C	N3-C2-O2	-6.28	117.50	121.90
30	BH	116	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	144	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	948	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	779	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1368	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	149	A	N1-C6-N6	-6.28	114.83	118.60
54	BA	918	A	N1-C6-N6	-6.28	114.83	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1350	C	N3-C2-O2	-6.28	117.51	121.90
55	BB	97	C	N3-C2-O2	-6.28	117.51	121.90
21	AA	984	C	N3-C2-O2	-6.28	117.51	121.90
21	AA	1097	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	917	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1564	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	2328	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	1437	A	C5-C6-N1	6.27	120.84	117.70
54	BA	2266	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	2591	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	819	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	1238	A	C4-C5-C6	-6.27	113.86	117.00
25	BC	12	ARG	NE-CZ-NH2	-6.27	117.16	120.30
54	BA	44	A	N1-C6-N6	-6.27	114.84	118.60
54	BA	1272	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	1848	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	1151	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	1160	G	O4'-C1'-N9	6.27	113.21	108.20
21	AA	1374	A	C5-C6-N1	6.27	120.83	117.70
22	A1	71	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	321	U	N3-C2-O2	-6.27	117.81	122.20
54	BA	1075	C	O4'-C1'-N1	6.27	113.21	108.20
54	BA	1257	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	129	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	651	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	959	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	219	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	571	U	O4'-C1'-N1	6.26	113.21	108.20
54	BA	2263	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	542	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	877	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1321	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1847	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	680	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	915	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1541	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2433	A	C5-C6-N1	6.26	120.83	117.70
55	BB	109	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	655	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	864	A	N1-C6-N6	-6.26	114.84	118.60
34	BL	47	ARG	NE-CZ-NH2	-6.26	117.17	120.30
37	BO	9	ARG	NE-CZ-NH1	6.26	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	632	A	C5-C6-N1	6.26	120.83	117.70
54	BA	655	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	861	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1164	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1507	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1596	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2851	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	408	A	C5-C6-N1	6.25	120.83	117.70
24	A3	67	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	1711	A	C4-C5-C6	-6.25	113.87	117.00
21	AA	1534	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	560	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	936	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	2000	C	N3-C2-O2	-6.25	117.52	121.90
11	AL	55	ARG	NE-CZ-NH1	6.25	123.43	120.30
54	BA	420	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	471	A	N1-C6-N6	-6.25	114.85	118.60
21	AA	602	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1211	C	O4'-C1'-N1	6.25	113.20	108.20
54	BA	1704	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	2080	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	554	A	C5-C6-N1	6.25	120.82	117.70
21	AA	1424	U	O4'-C1'-N1	6.25	113.20	108.20
54	BA	528	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1550	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1562	U	O4'-C1'-N1	6.25	113.20	108.20
54	BA	1847	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	1928	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2381	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	236	A	C4-C5-C6	-6.25	113.88	117.00
22	A1	23	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1402	U	O4'-C1'-N1	6.25	113.20	108.20
54	BA	1165	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	109	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	532	A	O4'-C1'-N9	6.24	113.19	108.20
54	BA	543	G	N1-C6-O6	-6.24	116.16	119.90
54	BA	634	C	O4'-C1'-N1	6.24	113.19	108.20
54	BA	1030	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	271	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1387	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2327	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	36	C	N3-C2-O2	-6.24	117.53	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	126	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	224	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	2283	C	O4'-C1'-N1	6.24	113.19	108.20
21	AA	1239	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1366	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	109	A	O4'-C1'-N9	6.24	113.19	108.20
21	AA	696	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	670	A	P-O3'-C3'	6.24	127.18	119.70
54	BA	2378	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	149	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	303	A	C5-C6-N1	6.23	120.82	117.70
54	BA	1336	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	1731	G	O4'-C1'-N9	6.23	113.19	108.20
54	BA	2577	A	C5-C6-N1	6.23	120.82	117.70
54	BA	2795	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1230	C	O4'-C1'-N1	6.23	113.18	108.20
21	AA	1476	A	C5-C6-N1	6.23	120.81	117.70
54	BA	352	A	C5-C6-N1	6.23	120.81	117.70
54	BA	478	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	867	C	N1-C2-O2	6.23	122.64	118.90
54	BA	1495	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	2054	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2342	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2616	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2837	A	C5-C6-N1	6.23	120.81	117.70
21	AA	1198	G	N3-C2-N2	-6.23	115.54	119.90
21	AA	1378	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1290	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2767	C	N3-C2-O2	-6.23	117.54	121.90
22	A1	28	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	947	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	2103	C	O4'-C1'-N1	6.23	113.18	108.20
55	BB	110	C	N3-C2-O2	-6.23	117.54	121.90
1	AB	221	ARG	NE-CZ-NH2	-6.23	117.19	120.30
54	BA	2534	A	C5-C6-N1	6.23	120.81	117.70
21	AA	167	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	2539	C	N1-C2-O2	6.22	122.63	118.90
21	AA	342	C	N3-C2-O2	-6.22	117.54	121.90
21	AA	1098	C	N3-C2-O2	-6.22	117.54	121.90
21	AA	1101	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1211	U	O4'-C1'-N1	6.22	113.18	108.20
22	A1	68	C	N3-C2-O2	-6.22	117.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	382	A	C5-C6-N1	6.22	120.81	117.70
54	BA	479	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1226	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1919	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	2416	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2658	C	N3-C2-O2	-6.22	117.54	121.90
2	AC	58	ARG	NE-CZ-NH1	6.22	123.41	120.30
21	AA	864	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	414	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	51	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	621	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1117	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	456	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1366	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1102	C	O4'-C1'-N1	6.22	113.17	108.20
21	AA	658	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	1503	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	996	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	2143	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2333	A	C5-C6-N1	6.22	120.81	117.70
21	AA	1382	C	C1'-O4'-C4'	-6.21	104.93	109.90
21	AA	1449	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2447	G	N3-C2-N2	-6.21	115.55	119.90
21	AA	582	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1801	A	C4-C5-C6	-6.21	113.89	117.00
55	BB	73	A	C5-C6-N1	6.21	120.81	117.70
24	A3	73	A	C5-C6-N1	6.21	120.81	117.70
54	BA	1608	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2020	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2261	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2779	U	O4'-C1'-N1	6.21	113.17	108.20
20	AU	34	ARG	NE-CZ-NH1	6.21	123.41	120.30
21	AA	489	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	1488	C	O4'-C1'-N1	6.21	113.17	108.20
54	BA	1612	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2646	C	O4'-C1'-N1	6.21	113.17	108.20
21	AA	1218	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1228	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1369	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1429	A	C5-C6-N1	6.21	120.80	117.70
54	BA	1268	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1937	A	C4-C5-C6	-6.21	113.90	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	65	A	C4-C5-C6	-6.20	113.90	117.00
27	BE	67	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	BA	61	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	282	A	C5-C6-N1	6.20	120.80	117.70
54	BA	739	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1127	A	C4-C5-C6	-6.20	113.90	117.00
55	BB	15	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	329	A	N1-C6-N6	-6.20	114.88	118.60
54	BA	1722	A	C5-C6-N1	6.20	120.80	117.70
54	BA	1748	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	693	A	N1-C6-N6	-6.20	114.88	118.60
54	BA	1383	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1889	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2626	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	336	A	C5-C6-N1	6.20	120.80	117.70
21	AA	1230	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	816	C	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1856	U	O4'-C1'-N1	6.20	113.16	108.20
21	AA	1081	A	C5-C6-N1	6.20	120.80	117.70
54	BA	1181	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	2359	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1158	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1437	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1676	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1877	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2088	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	923	A	N1-C6-N6	-6.19	114.88	118.60
54	BA	2207	C	N3-C2-O2	-6.19	117.56	121.90
21	AA	373	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	935	C	N3-C2-O2	-6.19	117.56	121.90
54	BA	1295	C	N3-C2-O2	-6.19	117.56	121.90
54	BA	2480	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	2635	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	145	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1032	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	1080	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	1414	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1553	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	2456	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1447	A	C4-C5-C6	-6.19	113.91	117.00
28	BF	79	ARG	NE-CZ-NH1	6.19	123.39	120.30
36	BN	90	ARG	NE-CZ-NH1	6.19	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BH	50	ARG	NE-CZ-NH1	6.19	123.39	120.30
54	BA	485	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	526	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	2863	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1494	A	C5-C6-N1	6.19	120.79	117.70
54	BA	2715	C	O4'-C1'-N1	6.19	113.15	108.20
54	BA	911	A	C5-C6-N1	6.18	120.79	117.70
54	BA	1135	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1270	C	N3-C2-O2	-6.18	117.57	121.90
55	BB	34	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	1180	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2258	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	2706	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2901	C	N3-C2-O2	-6.18	117.57	121.90
22	A1	9	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	257	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	792	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2880	C	N1-C2-O2	6.18	122.61	118.90
21	AA	174	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	371	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	1005	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	1339	A	C4-C5-C6	-6.18	113.91	117.00
22	A1	31	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1832	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	2547	A	C5-C6-N1	6.18	120.79	117.70
54	BA	758	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	484	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	2771	C	N3-C2-O2	-6.18	117.58	121.90
26	BD	184	ARG	NE-CZ-NH1	6.17	123.39	120.30
30	BH	27	ARG	NE-CZ-NH2	-6.17	117.21	120.30
54	BA	233	A	C5-C6-N1	6.17	120.79	117.70
54	BA	429	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	1246	A	C5-C6-N1	6.17	120.79	117.70
54	BA	1557	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1895	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	468	A	N1-C6-N6	-6.17	114.90	118.60
54	BA	1212	G	N3-C2-N2	-6.17	115.58	119.90
54	BA	592	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	1447	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	643	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	1094	G	O4'-C1'-N9	6.17	113.14	108.20
21	AA	1275	A	C5-C6-N1	6.17	120.78	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BJ	99	ARG	NE-CZ-NH2	-6.17	117.22	120.30
54	BA	1200	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1785	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	2813	A	C5-C6-N1	6.17	120.78	117.70
54	BA	541	A	N1-C6-N6	-6.17	114.90	118.60
54	BA	1470	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	2753	A	C5-C6-N1	6.17	120.78	117.70
54	BA	2297	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	1346	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	71	A	O4'-C1'-N9	6.16	113.13	108.20
54	BA	213	A	C5-C6-N1	6.16	120.78	117.70
54	BA	405	U	N3-C2-O2	-6.16	117.89	122.20
54	BA	992	C	N3-C2-O2	-6.16	117.59	121.90
2	AC	87	ARG	NE-CZ-NH1	6.16	123.38	120.30
21	AA	408	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	514	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	192	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2764	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	2025	C	O4'-C1'-N1	6.16	113.13	108.20
54	BA	2750	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	478	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	1345	U	N3-C2-O2	-6.16	117.89	122.20
54	BA	2510	C	O4'-C1'-N1	6.16	113.12	108.20
21	AA	1263	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	10	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	173	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1630	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	2751	G	O4'-C1'-N9	6.16	113.12	108.20
54	BA	2829	A	C4-C5-C6	-6.16	113.92	117.00
22	A1	21	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1362	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1958	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2296	U	O4'-C1'-N1	6.15	113.12	108.20
54	BA	152	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	332	A	N1-C6-N6	-6.15	114.91	118.60
54	BA	684	G	N3-C2-N2	-6.15	115.59	119.90
54	BA	2827	C	O4'-C1'-N1	6.15	113.12	108.20
21	AA	878	A	C5-C6-N1	6.15	120.78	117.70
21	AA	1200	C	N3-C4-C5	6.15	124.36	121.90
21	AA	1223	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	1508	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	89	A	C5-C6-N1	6.15	120.78	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1546	G	O4'-C1'-N9	6.15	113.12	108.20
54	BA	1844	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1111	A	C5-C6-N1	6.15	120.78	117.70
21	AA	177	G	N3-C4-C5	-6.15	125.53	128.60
21	AA	298	A	C4-C5-C6	-6.15	113.93	117.00
21	AA	401	C	N3-C2-O2	-6.15	117.60	121.90
53	B4	24	ARG	NE-CZ-NH1	6.15	123.37	120.30
54	BA	859	G	O4'-C1'-N9	6.15	113.12	108.20
54	BA	2052	A	C5-C6-N1	6.15	120.77	117.70
21	AA	95	C	N1-C2-O2	6.14	122.59	118.90
22	A1	38	A	C4-C5-C6	-6.14	113.93	117.00
22	A1	51	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2089	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2266	A	C5-C6-N1	6.14	120.77	117.70
54	BA	2740	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	978	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1121	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2248	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	609	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1768	C	O4'-C1'-N1	6.14	113.11	108.20
54	BA	1780	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1462	C	N3-C2-O2	-6.14	117.60	121.90
24	A3	26	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	460	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	632	A	O4'-C1'-N9	6.14	113.11	108.20
54	BA	2205	A	C5-C6-N1	6.14	120.77	117.70
55	BB	49	C	O4'-C1'-N1	6.14	113.11	108.20
21	AA	1129	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	231	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1000	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1136	C	O4'-C1'-N1	6.14	113.11	108.20
54	BA	195	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	652	U	O4'-C1'-N1	6.14	113.11	108.20
54	BA	1370	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2094	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	213	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	254	G	N1-C6-O6	-6.13	116.22	119.90
8	AI	121	ARG	NE-CZ-NH2	-6.13	117.23	120.30
22	A1	26	A	N1-C6-N6	-6.13	114.92	118.60
21	AA	177	G	O4'-C1'-N9	6.13	113.10	108.20
21	AA	443	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	1217	C	N3-C2-O2	-6.13	117.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	706	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	1783	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	195	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	315	A	N1-C6-N6	-6.13	114.92	118.60
21	AA	332	G	N3-C2-N2	-6.13	115.61	119.90
21	AA	1080	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	849	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	1067	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	1885	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2475	C	N1-C2-O2	6.13	122.58	118.90
54	BA	2741	A	C5-C6-N1	6.13	120.76	117.70
21	AA	794	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	147	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1357	C	O4'-C1'-N1	6.13	113.10	108.20
54	BA	1434	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2521	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2705	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	721	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2435	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	1105	A	C4-C5-C6	-6.12	113.94	117.00
27	BE	88	ARG	NE-CZ-NH1	6.12	123.36	120.30
54	BA	427	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	504	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1417	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	2055	C	N3-C4-N4	-6.12	113.71	118.00
54	BA	2423	U	N3-C2-O2	-6.12	117.91	122.20
54	BA	2530	A	C4-C5-C6	-6.12	113.94	117.00
5	AF	86	ARG	NE-CZ-NH1	6.12	123.36	120.30
50	B1	5	ARG	NE-CZ-NH2	-6.12	117.24	120.30
54	BA	42	A	N1-C6-N6	-6.12	114.93	118.60
54	BA	2305	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	2407	A	C5-C6-N1	6.12	120.76	117.70
54	BA	1735	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2883	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	120	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	1319	A	C4-C5-C6	-6.12	113.94	117.00
52	B3	12	ARG	NE-CZ-NH1	6.12	123.36	120.30
54	BA	502	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2247	A	N1-C6-N6	-6.12	114.93	118.60
21	AA	918	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	691	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1077	A	C4-C5-C6	-6.12	113.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AM	97	ARG	NE-CZ-NH2	6.12	123.36	120.30
21	AA	738	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	128	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	673	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1761	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2468	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2899	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	312	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	736	C	O4'-C1'-N1	6.11	113.09	108.20
54	BA	1427	A	C4-C5-C6	-6.11	113.94	117.00
21	AA	635	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	318	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1994	C	N3-C2-O2	-6.11	117.62	121.90
2	AC	163	ARG	NE-CZ-NH1	6.11	123.36	120.30
21	AA	637	C	N3-C2-O2	-6.11	117.62	121.90
24	A3	40	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1297	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	497	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	2129	C	C1'-O4'-C4'	-6.11	105.01	109.90
21	AA	267	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	1317	C	N3-C2-O2	-6.11	117.62	121.90
22	A1	26	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	946	C	N1-C2-O2	6.11	122.56	118.90
54	BA	2788	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2824	C	N3-C2-O2	-6.11	117.62	121.90
55	BB	17	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	1384	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	2031	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	2047	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	2789	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	2792	A	C5-C6-N1	6.11	120.75	117.70
21	AA	706	A	C4-C5-C6	-6.10	113.95	117.00
7	AH	79	ARG	NE-CZ-NH1	6.10	123.35	120.30
21	AA	519	C	N1-C2-O2	6.10	122.56	118.90
21	AA	620	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1430	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	253	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1096	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2726	A	O4'-C1'-N9	6.10	113.08	108.20
21	AA	831	A	C5-C6-N1	6.10	120.75	117.70
21	AA	1237	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1528	A	C4-C5-C6	-6.10	113.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1754	A	C5-C6-N1	6.10	120.75	117.70
21	AA	308	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	338	A	C5-C6-N1	6.10	120.75	117.70
21	AA	422	C	N3-C4-C5	6.10	124.34	121.90
54	BA	1498	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	385	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1195	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1590	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1600	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1868	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	833	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1678	A	C4-C5-C6	-6.10	113.95	117.00
55	BB	68	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1525	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	2062	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	2627	G	N1-C6-O6	-6.09	116.24	119.90
21	AA	883	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	116	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	1850	G	O4'-C1'-N9	6.09	113.07	108.20
21	AA	222	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	94	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	991	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	1159	U	O4'-C1'-N1	6.09	113.07	108.20
54	BA	1502	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	2335	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	2681	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	1055	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	477	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	1428	C	O4'-C1'-N1	6.09	113.07	108.20
54	BA	1488	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2322	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	1276	A	C5-C6-N1	6.08	120.74	117.70
54	BA	2237	G	N3-C2-N2	-6.08	115.64	119.90
42	BT	69	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	610	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	1408	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	951	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	1675	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	1893	C	O4'-C1'-N1	6.08	113.07	108.20
54	BA	2805	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	732	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	221	A	C4-C5-C6	-6.08	113.96	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2037	A	C4-C5-C6	-6.08	113.96	117.00
2	AC	39	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	717	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	1117	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2229	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	2463	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	2498	C	C3'-C2'-C1'	6.08	106.36	101.50
54	BA	1876	A	C5-C6-N1	6.08	120.74	117.70
21	AA	532	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	736	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	999	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	1410	A	C4-C5-C6	-6.08	113.96	117.00
36	BN	22	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	431	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	1152	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	1653	G	N1-C6-O6	-6.08	116.25	119.90
54	BA	2284	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	982	C	N1-C2-O2	6.07	122.54	118.90
54	BA	1669	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	78	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	1027	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	43	G	N1-C6-O6	-6.07	116.26	119.90
21	AA	1176	A	C5-C6-N1	6.07	120.73	117.70
54	BA	384	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	983	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	1264	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	1306	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2426	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	402	A	C5-C6-N1	6.07	120.73	117.70
54	BA	1895	C	O4'-C1'-N1	6.07	113.06	108.20
21	AA	734	G	N3-C2-N2	-6.07	115.65	119.90
54	BA	1005	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	618	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	759	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	2391	G	C1'-O4'-C4'	-6.07	105.05	109.90
54	BA	2577	A	C4-C5-C6	-6.07	113.97	117.00
55	BB	52	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	882	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	1055	A	C5-C6-N1	6.06	120.73	117.70
22	A1	48	C	N1-C2-O2	6.06	122.54	118.90
54	BA	1314	C	N1-C1'-C2'	6.06	121.88	114.00
54	BA	2531	A	N1-C6-N6	-6.06	114.96	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2649	C	N3-C2-O2	-6.06	117.66	121.90
22	A1	32	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1806	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	426	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	360	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	422	A	C5-C6-N1	6.06	120.73	117.70
54	BA	1170	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2135	A	O4'-C1'-N9	6.06	113.05	108.20
54	BA	2856	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	948	C	O4'-C1'-N1	6.06	113.05	108.20
54	BA	1301	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1802	A	C5-C6-N1	6.06	120.73	117.70
54	BA	1901	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2045	C	O4'-C1'-N1	6.06	113.05	108.20
54	BA	1069	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	599	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	165	A	C5-C6-N1	6.05	120.73	117.70
54	BA	1330	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	1679	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2364	C	N3-C2-O2	-6.05	117.66	121.90
46	BX	44	ARG	NE-CZ-NH1	6.05	123.33	120.30
54	BA	621	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2050	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	2611	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	1375	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	11	C	O4'-C1'-N1	6.05	113.04	108.20
54	BA	1656	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	2784	U	O4'-C1'-N1	6.05	113.04	108.20
54	BA	599	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	782	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2510	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	900	A	C4-C5-C6	-6.05	113.98	117.00
21	AA	1394	A	C3'-C2'-C1'	6.05	106.34	101.50
21	AA	1399	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	466	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	786	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1029	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1304	A	C6-C5-N7	6.05	136.53	132.30
54	BA	1772	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	2893	A	C4-C5-C6	-6.05	113.98	117.00
21	AA	431	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1250	A	C4-C5-C6	-6.04	113.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	8	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	345	C	O4'-C1'-N1	6.04	113.03	108.20
21	AA	502	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1248	A	C1'-O4'-C4'	-6.04	105.06	109.90
24	A3	22	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1586	A	C5-C6-N1	6.04	120.72	117.70
54	BA	1902	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	553	A	C5-C6-N1	6.04	120.72	117.70
21	AA	716	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	234	U	O4'-C1'-N1	6.04	113.03	108.20
54	BA	2874	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	530	G	N3-C4-C5	-6.04	125.58	128.60
21	AA	1128	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1053	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1887	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2468	A	O4'-C1'-N9	6.04	113.03	108.20
21	AA	10	A	C5-C6-N1	6.04	120.72	117.70
54	BA	223	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1536	C	N1-C2-O2	6.04	122.52	118.90
55	BB	91	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	586	C	N3-C2-O2	-6.04	117.68	121.90
54	BA	2319	G	N3-C2-N2	-6.04	115.68	119.90
11	AL	109	ARG	NE-CZ-NH1	6.03	123.32	120.30
54	BA	8	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	886	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2347	C	N3-C2-O2	-6.03	117.68	121.90
22	A1	3	G	C1'-O4'-C4'	-6.03	105.08	109.90
54	BA	1266	G	N3-C4-C5	-6.03	125.58	128.60
54	BA	2003	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2766	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	1249	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	1439	G	N3-C2-N2	-6.03	115.68	119.90
54	BA	6	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	130	C	O4'-C1'-N1	6.03	113.02	108.20
54	BA	958	U	O4'-C1'-N1	6.02	113.02	108.20
21	AA	73	C	N1-C2-O2	6.02	122.51	118.90
21	AA	807	A	C5-C6-N1	6.02	120.71	117.70
22	A1	18	G	O4'-C1'-N9	6.02	113.02	108.20
54	BA	675	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1965	C	N1-C2-O2	6.02	122.51	118.90
54	BA	2483	C	N3-C2-O2	-6.02	117.68	121.90
54	BA	2498	C	O4'-C1'-N1	6.02	113.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1816	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	2776	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	972	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	302	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	480	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2601	C	N3-C2-O2	-6.02	117.69	121.90
55	BB	37	C	N3-C2-O2	-6.02	117.69	121.90
32	BJ	120	ARG	NE-CZ-NH1	6.02	123.31	120.30
54	BA	1495	A	C5-C6-N1	6.02	120.71	117.70
21	AA	400	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	37	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	398	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	640	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2460	U	O4'-C1'-N1	6.01	113.01	108.20
29	BG	34	ARG	NE-CZ-NH1	6.01	123.31	120.30
54	BA	1978	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	2055	C	N1-C2-O2	6.01	122.51	118.90
54	BA	2232	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	73	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	394	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1312	U	P-O3'-C3'	6.01	126.92	119.70
54	BA	2153	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2346	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	96	U	O4'-C1'-N1	6.01	113.01	108.20
21	AA	456	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	967	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2792	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2033	A	C5-C6-N1	6.01	120.70	117.70
54	BA	2542	A	C4-C5-C6	-6.01	114.00	117.00
55	BB	118	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	614	C	N3-C2-O2	-6.01	117.70	121.90
54	BA	914	G	O4'-C1'-N9	6.01	113.01	108.20
54	BA	1466	U	O4'-C1'-N1	6.01	113.00	108.20
21	AA	1169	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1173	U	O4'-C1'-N1	6.00	113.00	108.20
54	BA	1548	A	C4-C5-C6	-6.00	114.00	117.00
14	AO	52	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	160	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	625	G	C4'-C3'-C2'	-6.00	96.60	102.60
54	BA	1393	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1713	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2301	C	N3-C2-O2	-6.00	117.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	554	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	609	A	C5-C6-N1	6.00	120.70	117.70
21	AA	1145	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	1201	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	873	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1079	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	935	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	271	G	O4'-C1'-N9	6.00	113.00	108.20
54	BA	357	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	554	U	O4'-C1'-N1	6.00	113.00	108.20
54	BA	1167	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1359	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1815	A	C5-C6-N1	6.00	120.70	117.70
21	AA	379	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1149	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1243	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	785	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	2287	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2845	U	O4'-C1'-N1	6.00	113.00	108.20
21	AA	1431	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	337	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	676	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	835	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	2275	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	580	C	N3-C2-O2	-6.00	117.70	121.90
40	BR	90	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	152	A	C5-C6-N1	6.00	120.70	117.70
54	BA	670	A	C5-C6-N1	6.00	120.70	117.70
54	BA	1215	G	O4'-C1'-N9	6.00	113.00	108.20
54	BA	2195	U	O4'-C1'-N1	6.00	113.00	108.20
2	AC	125	ARG	NE-CZ-NH1	5.99	123.30	120.30
9	AJ	48	ARG	NE-CZ-NH1	5.99	123.30	120.30
21	AA	544	G	N1-C6-O6	-5.99	116.30	119.90
21	AA	583	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	267	C	O4'-C1'-N1	5.99	113.00	108.20
54	BA	1685	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	1728	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	1991	U	O4'-C1'-N1	5.99	113.00	108.20
54	BA	296	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	1666	G	O4'-C1'-N9	5.99	112.99	108.20
21	AA	63	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	930	C	N3-C2-O2	-5.99	117.71	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1026	G	N3-C2-N2	-5.99	115.71	119.90
21	AA	482	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	1286	U	N3-C2-O2	-5.99	118.01	122.20
54	BA	41	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1349	C	N1-C2-O2	5.99	122.49	118.90
54	BA	1363	C	O4'-C1'-N1	5.99	112.99	108.20
21	AA	1217	C	C1'-O4'-C4'	-5.99	105.11	109.90
54	BA	2006	C	N1-C2-O2	5.99	122.49	118.90
54	BA	2738	A	O4'-C1'-N9	5.99	112.99	108.20
21	AA	1466	C	N1-C2-O2	5.99	122.49	118.90
54	BA	1315	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2540	C	N3-C2-O2	-5.99	117.71	121.90
55	BB	25	U	O4'-C1'-N1	5.99	112.99	108.20
55	BB	31	C	N3-C2-O2	-5.99	117.71	121.90
55	BB	38	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1269	A	C5-C6-N1	5.98	120.69	117.70
54	BA	1999	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	1146	A	C5-C6-N1	5.98	120.69	117.70
54	BA	1843	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	306	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	452	A	O4'-C1'-N9	5.98	112.98	108.20
21	AA	726	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	53	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1302	A	C4-C5-C6	-5.98	114.01	117.00
55	BB	71	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	288	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	752	A	P-O3'-C3'	5.98	126.88	119.70
54	BA	1229	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	1668	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2699	C	N3-C2-O2	-5.98	117.71	121.90
10	AK	68	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	710	G	C1'-O4'-C4'	-5.98	105.12	109.90
54	BA	95	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	305	C	N1-C2-O2	5.98	122.49	118.90
54	BA	1676	A	C5-C6-N1	5.98	120.69	117.70
54	BA	1853	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2730	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	2799	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	173	A	C5-C6-N1	5.98	120.69	117.70
54	BA	1118	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	1344	U	O4'-C1'-N1	5.98	112.98	108.20
54	BA	1789	A	C4-C5-C6	-5.98	114.01	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	31	ARG	NE-CZ-NH1	5.97	123.29	120.30
21	AA	108	G	N1-C6-O6	-5.97	116.31	119.90
54	BA	1933	G	O4'-C1'-N9	5.97	112.98	108.20
54	BA	2465	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1805	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	2652	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	600	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	1113	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1098	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	1395	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2009	A	C6-C5-N7	5.97	136.48	132.30
21	AA	225	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2469	A	C4-C5-C6	-5.97	114.02	117.00
55	BB	63	C	P-O3'-C3'	5.97	126.86	119.70
54	BA	97	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	309	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	340	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	481	G	N1-C6-O6	-5.97	116.32	119.90
54	BA	482	A	N1-C6-N6	-5.97	115.02	118.60
54	BA	2171	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2598	A	N1-C6-N6	-5.97	115.02	118.60
21	AA	1227	A	C1'-O4'-C4'	-5.96	105.13	109.90
24	A3	59	A	N1-C6-N6	-5.96	115.02	118.60
31	BI	126	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	2368	C	O4'-C1'-N1	5.96	112.97	108.20
54	BA	2710	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	1114	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2600	A	C5'-C4'-C3'	5.96	125.54	116.00
21	AA	1289	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	587	C	N1-C2-O2	5.96	122.48	118.90
54	BA	1392	A	C4-C5-C6	-5.96	114.02	117.00
25	BC	42	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	1274	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	217	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	635	A	C5-C6-N1	5.96	120.68	117.70
54	BA	166	U	O4'-C1'-N1	5.96	112.97	108.20
54	BA	197	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1300	G	P-O3'-C3'	5.96	126.85	119.70
21	AA	212	G	O4'-C1'-N9	5.96	112.97	108.20
21	AA	749	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	860	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	1240	U	C1'-O4'-C4'	-5.96	105.14	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	979	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1382	G	N3-C4-C5	-5.96	125.62	128.60
54	BA	584	C	O4'-C1'-N1	5.96	112.96	108.20
21	AA	261	U	N3-C2-O2	-5.95	118.03	122.20
21	AA	764	C	N1-C2-O2	5.95	122.47	118.90
54	BA	1239	G	N1-C6-O6	-5.95	116.33	119.90
54	BA	1513	U	O4'-C1'-N1	5.95	112.96	108.20
21	AA	790	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	671	C	N1-C2-O2	5.95	122.47	118.90
17	AR	72	ARG	NE-CZ-NH1	5.95	123.28	120.30
21	AA	327	A	C1'-O4'-C4'	-5.95	105.14	109.90
54	BA	32	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	699	A	C5-C6-N1	5.95	120.67	117.70
54	BA	959	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	986	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	2773	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	66	A	C5-C6-N1	5.95	120.67	117.70
21	AA	248	C	N1-C2-O2	5.95	122.47	118.90
21	AA	1234	C	N3-C2-O2	-5.95	117.73	121.90
45	BW	24	ARG	NE-CZ-NH1	5.95	123.27	120.30
54	BA	1758	U	N3-C2-O2	-5.95	118.03	122.20
21	AA	405	U	O4'-C1'-N1	5.95	112.96	108.20
21	AA	640	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1052	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1341	G	N3-C2-N2	-5.95	115.74	119.90
13	AN	41	ARG	NE-CZ-NH1	5.95	123.27	120.30
54	BA	666	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1453	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2104	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2418	A	C6-C5-N7	5.94	136.46	132.30
36	BN	69	ARG	NE-CZ-NH1	5.94	123.27	120.30
45	BW	40	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	908	C	N1-C2-O2	5.94	122.46	118.90
21	AA	1031	C	O4'-C1'-N1	5.94	112.95	108.20
36	BN	118	ARG	NE-CZ-NH1	5.94	123.27	120.30
39	BQ	52	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	857	G	O4'-C1'-N9	5.94	112.95	108.20
54	BA	1342	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1892	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	805	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	974	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	368	A	C4-C5-C6	-5.94	114.03	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1287	A	O4'-C1'-N9	5.93	112.95	108.20
55	BB	26	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	71	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	234	C	C4'-C3'-C2'	-5.93	96.67	102.60
21	AA	536	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	702	A	O4'-C1'-N9	5.93	112.95	108.20
21	AA	1467	C	N1-C2-O2	5.93	122.46	118.90
54	BA	1028	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2169	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2306	C	N1-C2-O2	5.93	122.46	118.90
21	AA	285	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	990	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2354	C	N3-C2-O2	-5.93	117.75	121.90
13	AN	75	ARG	NE-CZ-NH1	5.93	123.26	120.30
21	AA	95	C	O4'-C1'-N1	5.93	112.94	108.20
21	AA	230	G	N3-C2-N2	-5.93	115.75	119.90
54	BA	734	A	C4-C5-C6	-5.93	114.04	117.00
21	AA	169	C	N1-C2-O2	5.92	122.45	118.90
21	AA	299	G	O4'-C1'-N9	5.92	112.94	108.20
21	AA	796	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1291	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	2051	A	N1-C6-N6	-5.92	115.05	118.60
54	BA	1749	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	161	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1070	A	C4-C5-C6	-5.92	114.04	117.00
55	BB	114	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	34	C	O4'-C1'-N1	5.92	112.94	108.20
21	AA	271	C	N1-C2-O2	5.92	122.45	118.90
21	AA	596	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	1265	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	563	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1328	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1420	A	O4'-C1'-N9	5.92	112.93	108.20
21	AA	199	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1837	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	1496	C	N3-C2-O2	-5.92	117.76	121.90
49	B0	9	ARG	NE-CZ-NH2	5.92	123.26	120.30
54	BA	2617	U	O4'-C1'-N1	5.92	112.93	108.20
55	BB	94	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	1058	G	N1-C6-O6	-5.91	116.35	119.90
24	A3	70	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	393	C	N3-C2-O2	-5.91	117.76	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	572	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	1276	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	1547	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	413	C	N3-C2-O2	-5.91	117.76	121.90
14	AO	62	ARG	NE-CZ-NH1	5.91	123.25	120.30
54	BA	1386	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1701	A	C5-C6-N1	5.91	120.66	117.70
55	BB	3	C	O4'-C1'-N1	5.91	112.93	108.20
55	BB	19	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	914	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	1014	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	1102	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	193	U	O4'-C1'-N1	5.91	112.93	108.20
54	BA	490	C	O4'-C1'-N1	5.91	112.93	108.20
54	BA	1549	A	C4-C5-C6	-5.91	114.05	117.00
6	AG	77	ARG	NE-CZ-NH1	5.91	123.25	120.30
8	AI	44	ARG	NE-CZ-NH1	5.91	123.25	120.30
21	AA	1192	C	N3-C2-O2	-5.91	117.77	121.90
21	AA	1469	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	421	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	815	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	878	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	174	A	C5-C6-N1	5.91	120.65	117.70
21	AA	960	U	N3-C2-O2	-5.91	118.07	122.20
21	AA	1277	C	N1-C2-O2	5.91	122.44	118.90
24	A3	29	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	47	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	322	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	654	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	732	C	O4'-C1'-N1	5.91	112.92	108.20
54	BA	2285	C	N3-C2-O2	-5.91	117.77	121.90
21	AA	153	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	657	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	1520	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	835	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	660	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1126	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	2097	A	C6-C5-N7	5.90	136.43	132.30
54	BA	2214	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1509	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	817	C	O4'-C1'-N1	5.90	112.92	108.20
55	BB	55	U	O4'-C1'-N1	5.90	112.92	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2205	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	448	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	897	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1109	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	2072	C	N3-C2-O2	-5.90	117.77	121.90
55	BB	13	G	N3-C2-N2	-5.90	115.77	119.90
21	AA	1280	A	C1'-O4'-C4'	-5.90	105.18	109.90
54	BA	584	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	825	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	1556	C	N3-C2-O2	-5.89	117.77	121.90
21	AA	228	A	C6-C5-N7	5.89	136.43	132.30
54	BA	802	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	1208	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2170	A	C3'-C2'-C1'	5.89	106.21	101.50
54	BA	2270	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	609	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	1241	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	2336	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	389	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	179	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2187	U	O4'-C1'-N1	5.89	112.91	108.20
54	BA	902	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	569	C	N3-C2-O2	-5.89	117.78	121.90
24	A3	60	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	115	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2017	U	C3'-C2'-C1'	5.89	106.21	101.50
54	BA	2202	U	O4'-C1'-N1	5.89	112.91	108.20
54	BA	2558	C	O4'-C1'-N1	5.89	112.91	108.20
21	AA	1133	G	N1-C6-O6	-5.88	116.37	119.90
54	BA	417	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1378	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2039	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	2614	A	O4'-C1'-N9	5.88	112.91	108.20
21	AA	338	A	C4-C5-C6	-5.88	114.06	117.00
24	A3	11	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1301	A	C1'-O4'-C4'	-5.88	105.19	109.90
8	AI	118	ARG	NE-CZ-NH1	5.88	123.24	120.30
21	AA	1161	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1448	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	183	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	865	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1285	A	C4-C5-C6	-5.88	114.06	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2477	U	O4'-C1'-N1	5.88	112.91	108.20
21	AA	1067	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	403	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	2179	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	735	C	N3-C2-O2	-5.88	117.79	121.90
24	A3	39	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1803	A	C5-C6-N1	5.88	120.64	117.70
54	BA	2108	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2222	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	1351	C	N3-C2-O2	-5.87	117.79	121.90
14	AO	63	ARG	NE-CZ-NH1	5.87	123.23	120.30
54	BA	2751	G	N3-C4-C5	-5.87	125.66	128.60
54	BA	2841	C	N3-C2-O2	-5.87	117.79	121.90
18	AS	77	ARG	NE-CZ-NH1	5.87	123.23	120.30
21	AA	1114	C	O4'-C1'-N1	5.87	112.90	108.20
54	BA	2288	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	854	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	811	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2231	U	O4'-C1'-N1	5.87	112.89	108.20
54	BA	2411	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	2872	A	C4-C5-C6	-5.87	114.07	117.00
21	AA	522	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1395	C	N1-C2-O2	5.87	122.42	118.90
54	BA	330	A	C5-C6-N1	5.87	120.63	117.70
54	BA	462	C	N1-C2-O2	5.87	122.42	118.90
54	BA	2793	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1618	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	2660	A	O4'-C1'-N9	5.86	112.89	108.20
54	BA	2692	G	O4'-C1'-N9	5.86	112.89	108.20
21	AA	518	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	750	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1205	A	C4-C5-C6	-5.86	114.07	117.00
55	BB	46	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	504	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	1176	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1229	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1399	C	P-O3'-C3'	5.86	126.73	119.70
28	BF	111	ARG	NE-CZ-NH2	-5.86	117.37	120.30
10	AK	52	ARG	NE-CZ-NH1	5.86	123.23	120.30
54	BA	125	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	2896	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	382	A	C4-C5-C6	-5.86	114.07	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1507	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1804	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2366	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1331	G	N1-C6-O6	-5.86	116.39	119.90
54	BA	2291	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2670	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	129	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	613	A	C4-C5-C6	-5.85	114.07	117.00
17	AR	62	ARG	NE-CZ-NH1	5.85	123.22	120.30
21	AA	419	C	N3-C2-O2	-5.85	117.81	121.90
21	AA	1037	C	O4'-C1'-N1	5.85	112.88	108.20
21	AA	1191	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	345	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	660	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	2067	G	O4'-C1'-N9	5.85	112.88	108.20
54	BA	1983	G	N3-C2-N2	-5.85	115.81	119.90
21	AA	48	C	N1-C2-O2	5.85	122.41	118.90
35	BM	81	ARG	NE-CZ-NH2	5.85	123.22	120.30
54	BA	428	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1356	G	N3-C2-N2	-5.85	115.81	119.90
38	BP	97	TYR	CB-CG-CD2	-5.84	117.49	121.00
54	BA	57	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1629	U	O4'-C1'-N1	5.84	112.88	108.20
54	BA	2757	A	N1-C6-N6	-5.84	115.09	118.60
54	BA	2861	U	O4'-C1'-N1	5.84	112.88	108.20
54	BA	1214	A	O4'-C1'-N9	5.84	112.88	108.20
21	AA	924	C	N1-C2-O2	5.84	122.40	118.90
54	BA	362	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	972	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1088	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	2765	A	C4-C5-C6	-5.84	114.08	117.00
10	AK	105	ARG	NE-CZ-NH1	5.84	123.22	120.30
18	AS	54	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	AA	95	C	C3'-C2'-C1'	5.84	106.17	101.50
21	AA	166	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	1006	C	N1-C2-O2	5.84	122.40	118.90
20	AU	16	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	AA	848	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2561	U	O4'-C1'-N1	5.84	112.87	108.20
55	BB	4	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	632	U	O4'-C1'-N1	5.84	112.87	108.20
35	BM	50	ARG	NE-CZ-NH1	5.84	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	191	A	C5-C6-N1	5.84	120.62	117.70
54	BA	246	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	343	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1566	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1802	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	2350	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	286	C	N3-C2-O2	-5.83	117.81	121.90
21	AA	676	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	1288	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	848	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1953	A	N1-C6-N6	-5.83	115.10	118.60
54	BA	2422	C	N1-C2-O2	5.83	122.40	118.90
21	AA	99	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	689	C	O4'-C1'-N1	5.83	112.87	108.20
21	AA	1107	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	945	A	O4'-C1'-N9	5.83	112.86	108.20
54	BA	1764	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	418	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1504	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	2598	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	823	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1997	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	336	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2840	C	N3-C2-O2	-5.83	117.82	121.90
55	BB	104	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	33	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	341	C	N3-C2-O2	-5.82	117.82	121.90
54	BA	454	A	C5-C6-N1	5.82	120.61	117.70
54	BA	898	C	N3-C2-O2	-5.82	117.82	121.90
54	BA	1000	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1247	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2711	A	C4-C5-C6	-5.82	114.09	117.00
22	A1	73	A	C6-C5-N7	5.82	136.38	132.30
21	AA	130	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	68	G	N1-C6-O6	-5.82	116.41	119.90
21	AA	876	C	N3-C2-O2	-5.82	117.83	121.90
22	A1	56	C	N1-C2-O2	5.82	122.39	118.90
54	BA	2494	G	N3-C2-N2	-5.82	115.83	119.90
55	BB	30	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	177	G	C5-C6-N1	5.82	114.41	111.50
21	AA	353	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2036	C	N3-C2-O2	-5.82	117.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	975	A	O4'-C1'-N9	5.81	112.85	108.20
21	AA	1340	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	1591	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	470	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	505	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	648	G	O4'-C1'-N9	5.81	112.85	108.20
54	BA	2404	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	716	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1604	C	N3-C2-O2	-5.81	117.83	121.90
4	AE	53	ARG	NE-CZ-NH1	5.81	123.20	120.30
21	AA	686	U	O4'-C1'-N1	5.81	112.85	108.20
21	AA	996	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	921	C	N1-C2-O2	5.81	122.39	118.90
54	BA	1008	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1141	U	N3-C2-O2	-5.81	118.13	122.20
54	BA	2589	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2727	A	C5-C6-N1	5.81	120.60	117.70
21	AA	1216	A	C4-C5-C6	-5.81	114.10	117.00
24	A3	49	C	N1-C2-O2	5.81	122.39	118.90
54	BA	45	G	O4'-C1'-N9	5.81	112.85	108.20
54	BA	2015	A	N1-C6-N6	-5.81	115.11	118.60
37	BO	15	ARG	NE-CZ-NH1	5.80	123.20	120.30
21	AA	465	A	C1'-O4'-C4'	-5.80	105.26	109.90
54	BA	1047	G	N1-C6-O6	-5.80	116.42	119.90
54	BA	1726	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	54	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	490	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	1522	U	O4'-C1'-N1	5.80	112.84	108.20
54	BA	155	A	C5-C6-N1	5.80	120.60	117.70
54	BA	715	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2170	A	C4-C5-C6	-5.80	114.10	117.00
15	AP	70	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	140	C	N1-C2-O2	5.80	122.38	118.90
54	BA	182	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	251	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1705	A	C5-C6-N1	5.80	120.60	117.70
54	BA	2726	A	C4-C5-C6	-5.80	114.10	117.00
55	BB	92	C	O4'-C1'-N1	5.80	112.84	108.20
21	AA	295	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	307	C	N1-C2-O2	5.80	122.38	118.90
21	AA	363	A	C4-C5-C6	-5.80	114.10	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	274	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	2858	C	N1-C2-O2	5.80	122.38	118.90
54	BA	1773	A	C4-C5-C6	-5.79	114.10	117.00
21	AA	519	C	O4'-C1'-N1	5.79	112.84	108.20
21	AA	630	A	C4-C5-C6	-5.79	114.10	117.00
32	BJ	13	ARG	NE-CZ-NH1	5.79	123.20	120.30
54	BA	772	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	430	A	C4-C5-C6	-5.79	114.10	117.00
22	A1	65	C	N3-C2-O2	-5.79	117.85	121.90
29	BG	2	ARG	NE-CZ-NH1	5.79	123.20	120.30
54	BA	1085	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	1102	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1427	A	P-O3'-C3'	5.79	126.65	119.70
21	AA	300	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	528	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	647	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1347	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2539	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2813	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	347	G	P-O3'-C3'	5.79	126.64	119.70
54	BA	1699	G	C1'-O4'-C4'	-5.79	105.27	109.90
54	BA	158	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1203	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1459	G	N3-C4-C5	-5.79	125.71	128.60
54	BA	2164	C	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2458	G	N3-C4-C5	-5.78	125.71	128.60
54	BA	19	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	209	C	N3-C2-O2	-5.78	117.86	121.90
21	AA	919	A	C5-C6-N1	5.78	120.59	117.70
21	AA	1299	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1597	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1880	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	2163	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2902	C	N1-C2-O2	5.78	122.37	118.90
21	AA	116	A	C4-C5-C6	-5.78	114.11	117.00
45	BW	10	ARG	NE-CZ-NH2	5.78	123.19	120.30
54	BA	423	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1150	C	O4'-C1'-N1	5.78	112.82	108.20
44	BV	21	ARG	NE-CZ-NH1	5.77	123.19	120.30
54	BA	1122	G	N3-C2-N2	-5.77	115.86	119.90
54	BA	1153	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1720	U	O4'-C1'-N1	5.77	112.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2119	A	C4-C5-C6	-5.77	114.11	117.00
21	AA	101	A	C4-C5-C6	-5.77	114.11	117.00
21	AA	737	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	453	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	1275	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	1384	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	2654	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	43	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	266	G	N3-C4-C5	-5.77	125.72	128.60
21	AA	1360	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	965	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1043	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	132	C	C1'-O4'-C4'	-5.77	105.29	109.90
21	AA	919	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	1378	C	O4'-C1'-N1	5.77	112.81	108.20
50	B1	43	ARG	NE-CZ-NH1	5.77	123.18	120.30
54	BA	2283	C	C4'-C3'-C2'	-5.77	96.83	102.60
54	BA	2388	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	2662	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	730	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1943	U	C3'-C2'-C1'	5.76	106.11	101.50
54	BA	1644	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	1226	C	N1-C2-O2	5.76	122.36	118.90
54	BA	1531	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2761	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	234	C	C1'-O4'-C4'	-5.76	105.29	109.90
21	AA	1019	A	C5-C6-N1	5.76	120.58	117.70
54	BA	624	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	727	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1133	A	O4'-C1'-N9	5.76	112.81	108.20
54	BA	1385	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1637	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1985	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2260	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	496	A	C1'-O4'-C4'	-5.76	105.29	109.90
21	AA	868	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	1141	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	1019	U	N3-C2-O2	-5.76	118.17	122.20
21	AA	1120	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	260	G	N1-C6-O6	-5.75	116.45	119.90
54	BA	804	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	937	A	C4-C5-C6	-5.75	114.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	182	A	N1-C6-N6	-5.75	115.15	118.60
54	BA	244	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	612	G	N1-C6-O6	-5.75	116.45	119.90
21	AA	187	G	O4'-C1'-N9	5.75	112.80	108.20
21	AA	23	C	N1-C2-O2	5.75	122.35	118.90
22	A1	11	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	846	U	N3-C2-O2	-5.75	118.18	122.20
21	AA	221	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	318	G	N1-C6-O6	-5.75	116.45	119.90
21	AA	1513	A	C4-C5-C6	-5.75	114.13	117.00
52	B3	44	ARG	NE-CZ-NH1	5.75	123.17	120.30
54	BA	203	A	C5-C6-N1	5.75	120.57	117.70
54	BA	1677	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	1690	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	2326	C	O4'-C1'-N1	5.75	112.80	108.20
21	AA	321	A	C5-C6-N1	5.75	120.57	117.70
21	AA	381	C	N1-C2-O2	5.75	122.35	118.90
21	AA	1256	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	303	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	525	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1527	G	N1-C6-O6	-5.74	116.45	119.90
21	AA	719	C	N1-C2-O2	5.74	122.34	118.90
54	BA	657	U	O4'-C1'-N1	5.74	112.79	108.20
21	AA	1440	U	N3-C2-O2	-5.74	118.18	122.20
55	BB	113	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	2005	A	C4-C5-C6	-5.74	114.13	117.00
55	BB	93	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	1367	C	N1-C2-O2	5.74	122.34	118.90
21	AA	1064	G	N3-C2-N2	-5.74	115.89	119.90
54	BA	776	G	N1-C6-O6	-5.74	116.46	119.90
54	BA	2855	C	N3-C2-O2	-5.74	117.89	121.90
54	BA	1210	G	N1-C6-O6	-5.73	116.46	119.90
54	BA	1451	C	N1-C2-O2	5.73	122.34	118.90
54	BA	1616	A	C4-C5-C6	-5.73	114.13	117.00
54	BA	2506	U	O4'-C1'-N1	5.73	112.79	108.20
6	AG	137	ARG	NE-CZ-NH2	-5.73	117.43	120.30
21	AA	559	A	C4-C5-C6	-5.73	114.13	117.00
26	BD	46	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	1575	C	N1-C2-O2	5.73	122.34	118.90
21	AA	782	A	C4-C5-C6	-5.73	114.14	117.00
21	AA	1112	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1526	C	O4'-C1'-N1	5.73	112.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1332	G	O4'-C1'-N9	5.73	112.78	108.20
1	AB	207	ARG	NE-CZ-NH1	5.73	123.16	120.30
21	AA	211	G	N1-C6-O6	-5.73	116.46	119.90
21	AA	687	A	C4-C5-C6	-5.73	114.14	117.00
21	AA	1412	C	N1-C2-O2	5.73	122.34	118.90
22	A1	6	A	C5-C6-N1	5.73	120.56	117.70
54	BA	242	G	O4'-C1'-N9	5.73	112.78	108.20
54	BA	492	A	C5-C6-N1	5.73	120.56	117.70
54	BA	892	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1362	C	O4'-C1'-N1	5.73	112.78	108.20
54	BA	1967	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2386	A	O4'-C1'-N9	5.73	112.78	108.20
54	BA	2716	C	N3-C2-O2	-5.73	117.89	121.90
23	A2	88	U	N3-C2-O2	-5.72	118.19	122.20
54	BA	1754	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2496	C	O4'-C1'-N1	5.72	112.78	108.20
54	BA	2425	A	C4-C5-C6	-5.72	114.14	117.00
55	BB	33	G	N3-C2-N2	-5.72	115.90	119.90
21	AA	795	C	N1-C2-O2	5.72	122.33	118.90
21	AA	1519	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	492	A	N1-C6-N6	-5.72	115.17	118.60
54	BA	623	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	1609	A	C5'-C4'-O4'	5.72	115.96	109.10
54	BA	1889	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2166	U	O4'-C1'-N1	5.72	112.77	108.20
21	AA	81	A	C4-C5-C6	-5.71	114.14	117.00
21	AA	164	G	N1-C6-O6	-5.71	116.47	119.90
21	AA	840	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1503	A	C4-C5-C6	-5.71	114.14	117.00
33	BK	98	ARG	NE-CZ-NH2	-5.71	117.44	120.30
54	BA	7	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1241	A	O4'-C1'-N9	5.71	112.77	108.20
54	BA	1791	A	C4-C5-C6	-5.71	114.14	117.00
24	A3	58	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	38	A	C6-C5-N7	5.71	136.30	132.30
54	BA	465	G	N3-C2-N2	-5.71	115.90	119.90
42	BT	73	ARG	NE-CZ-NH2	5.71	123.16	120.30
54	BA	787	C	N1-C2-O2	5.71	122.33	118.90
54	BA	984	A	O4'-C1'-N9	5.71	112.77	108.20
54	BA	1409	U	O4'-C1'-N1	5.71	112.77	108.20
54	BA	2278	A	N1-C6-N6	-5.71	115.17	118.60
21	AA	849	G	N1-C6-O6	-5.71	116.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1217	C	N1-C2-O2	5.71	122.33	118.90
21	AA	783	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1409	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	1144	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2044	C	O4'-C1'-N1	5.71	112.77	108.20
21	AA	364	A	C4-C5-C6	-5.71	114.15	117.00
21	AA	529	G	N1-C6-O6	-5.71	116.48	119.90
21	AA	1342	C	C5'-C4'-C3'	-5.71	106.87	116.00
54	BA	233	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	249	C	P-O3'-C3'	5.71	126.55	119.70
54	BA	1353	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	1518	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	2385	C	N3-C2-O2	-5.71	117.91	121.90
21	AA	1534	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	1071	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	1468	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2382	G	C5'-C4'-O4'	5.70	115.94	109.10
21	AA	1302	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	1893	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	1494	G	N1-C6-O6	-5.70	116.48	119.90
24	A3	9	G	N3-C4-C5	-5.70	125.75	128.60
54	BA	2215	C	O4'-C1'-N1	5.70	112.76	108.20
55	BB	78	A	C6-C5-N7	5.69	136.29	132.30
21	AA	901	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	192	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	2137	U	O4'-C1'-N1	5.69	112.75	108.20
54	BA	2200	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	2443	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	2809	A	C4-C5-C6	-5.69	114.15	117.00
21	AA	816	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	632	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2356	U	C5'-C4'-O4'	5.69	115.93	109.10
21	AA	1322	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	269	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	2063	C	N1-C2-O2	5.69	122.31	118.90
54	BA	2206	C	N3-C2-O2	-5.69	117.92	121.90
15	AP	28	ARG	NE-CZ-NH2	-5.69	117.46	120.30
54	BA	896	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1133	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1286	A	N1-C6-N6	-5.69	115.19	118.60
54	BA	1800	C	N1-C2-O2	5.69	122.31	118.90
54	BA	1803	A	C4-C5-C6	-5.69	114.16	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2736	A	C4-C5-C6	-5.69	114.16	117.00
21	AA	1280	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	275	C	N1-C2-O2	5.68	122.31	118.90
54	BA	1464	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	1732	C	N1-C2-O2	5.68	122.31	118.90
54	BA	1757	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	2184	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	1446	A	O4'-C1'-N9	5.68	112.75	108.20
24	A3	38	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1632	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	2150	C	N1-C2-O2	5.68	122.31	118.90
54	BA	2241	A	C5-C6-N1	5.68	120.54	117.70
54	BA	137	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1605	C	O4'-C1'-N1	5.68	112.75	108.20
21	AA	309	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	553	A	C4-C5-C6	-5.68	114.16	117.00
22	A1	47	U	N3-C2-O2	-5.68	118.22	122.20
54	BA	1311	G	O4'-C1'-N9	5.68	112.74	108.20
55	BB	5	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	2655	G	O4'-C1'-N9	5.68	112.74	108.20
15	AP	25	ARG	NE-CZ-NH2	-5.68	117.46	120.30
21	AA	806	C	N3-C2-O2	-5.68	117.93	121.90
21	AA	814	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	860	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	950	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	1338	G	C5'-C4'-O4'	5.68	115.91	109.10
54	BA	2247	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	107	G	C5-C6-N1	5.67	114.34	111.50
54	BA	1354	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1595	C	N1-C2-O2	5.67	122.30	118.90
54	BA	2695	U	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2848	G	O4'-C1'-N9	5.67	112.74	108.20
3	AD	62	ARG	NE-CZ-NH1	5.67	123.14	120.30
21	AA	1450	U	N3-C2-O2	-5.67	118.23	122.20
21	AA	465	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	37	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	439	A	C6-C5-N7	5.67	136.27	132.30
54	BA	2538	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2776	A	P-O3'-C3'	5.67	126.51	119.70
54	BA	31	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	96	C	N1-C2-O2	5.67	122.30	118.90
54	BA	546	U	N3-C2-O2	-5.67	118.23	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	B5	53	ARG	NE-CZ-NH1	5.67	123.14	120.30
14	AO	83	ARG	NE-CZ-NH1	5.67	123.13	120.30
21	AA	412	A	C4-C5-C6	-5.67	114.17	117.00
47	BY	52	ARG	NE-CZ-NH1	5.67	123.13	120.30
54	BA	669	G	O4'-C1'-N9	5.67	112.74	108.20
54	BA	2168	G	O4'-C1'-N9	5.67	112.73	108.20
54	BA	2241	A	C6-C5-N7	5.67	136.27	132.30
54	BA	332	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	1572	A	N1-C6-N6	-5.67	115.20	118.60
54	BA	2560	A	N1-C6-N6	-5.67	115.20	118.60
21	AA	1388	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	1492	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	1011	G	N1-C6-O6	-5.67	116.50	119.90
9	AJ	62	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	897	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1151	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	352	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	469	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1824	G	N1-C6-O6	-5.66	116.50	119.90
21	AA	1437	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	918	A	C5-C6-N1	5.66	120.53	117.70
54	BA	34	U	O4'-C1'-N1	5.66	112.72	108.20
54	BA	789	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2676	C	N1-C2-O2	5.66	122.29	118.90
21	AA	1252	A	N1-C6-N6	-5.65	115.21	118.60
54	BA	1478	G	O4'-C1'-N9	5.65	112.72	108.20
54	BA	2559	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	67	C	N1-C2-O2	5.65	122.29	118.90
21	AA	1275	A	C4-C5-C6	-5.65	114.17	117.00
21	AA	1282	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	1287	A	C6-C5-N7	5.65	136.26	132.30
24	A3	18	U	N3-C2-O2	-5.65	118.24	122.20
54	BA	556	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1952	A	C3'-C2'-C1'	5.65	106.02	101.50
54	BA	2352	A	C4-C5-C6	-5.65	114.17	117.00
21	AA	642	A	C5-C6-N1	5.65	120.53	117.70
21	AA	896	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	1196	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	2566	A	C4-C5-C6	-5.65	114.17	117.00
21	AA	163	C	N3-C2-O2	-5.65	117.95	121.90
21	AA	1207	G	N1-C6-O6	-5.65	116.51	119.90
21	AA	1419	G	N1-C6-O6	-5.65	116.51	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	792	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	334	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	743	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	1955	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	2444	G	N1-C6-O6	-5.65	116.51	119.90
21	AA	208	U	N3-C2-O2	-5.64	118.25	122.20
21	AA	844	G	N1-C6-O6	-5.64	116.51	119.90
54	BA	210	C	N3-C2-O2	-5.64	117.95	121.90
33	BK	17	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	1576	U	O4'-C1'-N1	5.64	112.71	108.20
54	BA	1808	A	O4'-C1'-N9	5.64	112.72	108.20
54	BA	2268	A	C4-C5-C6	-5.64	114.18	117.00
39	BQ	69	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	102	U	N3-C2-O2	-5.64	118.25	122.20
21	AA	114	U	O4'-C1'-N1	5.64	112.71	108.20
21	AA	411	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	962	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	643	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1489	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	2704	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	1046	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	342	C	N3-C4-C5	5.63	124.15	121.90
21	AA	422	C	N1-C2-O2	5.63	122.28	118.90
54	BA	196	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	757	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	1103	A	C4-C5-C6	-5.63	114.18	117.00
25	BC	62	ARG	NE-CZ-NH1	5.63	123.12	120.30
54	BA	547	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	2440	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	2868	A	C4-C5-C6	-5.63	114.18	117.00
5	AF	44	ARG	NE-CZ-NH1	5.63	123.12	120.30
21	AA	503	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	994	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	1815	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	2748	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	150	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	447	A	N1-C6-N6	-5.63	115.22	118.60
54	BA	2590	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	265	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	563	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	923	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	943	U	O4'-C1'-N1	5.63	112.70	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2631	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	2636	C	O4'-C1'-N1	5.63	112.70	108.20
54	BA	1351	C	O4'-C1'-N1	5.63	112.70	108.20
54	BA	1972	G	O4'-C1'-N9	5.63	112.70	108.20
54	BA	1990	C	N1-C2-O2	5.63	122.28	118.90
21	AA	69	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	1075	U	O4'-C1'-N1	5.62	112.70	108.20
21	AA	1128	C	N1-C2-O2	5.62	122.27	118.90
21	AA	1427	C	N1-C2-O2	5.62	122.28	118.90
54	BA	378	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	444	C	N3-C2-O2	-5.62	117.96	121.90
21	AA	579	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	957	C	N3-C4-N4	-5.62	114.07	118.00
54	BA	1075	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1714	U	N3-C2-O2	-5.62	118.27	122.20
3	AD	110	ARG	NE-CZ-NH1	5.62	123.11	120.30
21	AA	492	C	C3'-C2'-C1'	5.62	105.99	101.50
22	A1	14	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1870	C	N1-C2-O2	5.62	122.27	118.90
54	BA	2137	U	N3-C2-O2	-5.62	118.27	122.20
54	BA	2519	U	O4'-C1'-N1	5.62	112.69	108.20
22	A1	76	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2596	U	O4'-C1'-N1	5.62	112.69	108.20
21	AA	1352	C	N1-C2-O2	5.62	122.27	118.90
32	BJ	120	ARG	NE-CZ-NH2	-5.62	117.49	120.30
54	BA	1253	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1287	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1646	C	O4'-C1'-N1	5.62	112.69	108.20
13	AN	9	ARG	NE-CZ-NH1	5.61	123.11	120.30
21	AA	890	G	O4'-C1'-N9	5.61	112.69	108.20
28	BF	70	ARG	NE-CZ-NH2	-5.61	117.49	120.30
40	BR	21	ARG	NE-CZ-NH1	5.61	123.11	120.30
54	BA	198	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	565	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1244	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	1545	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	1674	G	C3'-C2'-C1'	5.61	105.99	101.50
54	BA	1725	U	C5'-C4'-O4'	5.61	115.84	109.10
54	BA	1991	U	N3-C2-O2	-5.61	118.27	122.20
54	BA	2030	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	2066	C	N3-C2-O2	-5.61	117.97	121.90
12	AM	100	ARG	NE-CZ-NH1	5.61	123.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	988	A	C6-C5-N7	5.61	136.23	132.30
54	BA	1431	A	O4'-C1'-N9	5.61	112.69	108.20
54	BA	1745	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	2501	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	1157	A	C4-C5-C6	-5.61	114.20	117.00
46	BX	73	ARG	NE-CZ-NH1	5.61	123.11	120.30
54	BA	1395	A	O4'-C1'-N9	5.61	112.69	108.20
21	AA	756	C	N1-C2-O2	5.61	122.26	118.90
21	AA	1404	C	N1-C2-O2	5.61	122.27	118.90
54	BA	78	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1010	A	N1-C6-N6	-5.61	115.24	118.60
54	BA	1057	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	2704	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	2780	G	O4'-C1'-N9	5.61	112.69	108.20
54	BA	735	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	1652	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	1452	C	N1-C2-O2	5.60	122.26	118.90
54	BA	1298	C	N1-C2-O2	5.60	122.26	118.90
54	BA	1499	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2778	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	47	C	N1-C2-O2	5.60	122.26	118.90
21	AA	623	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	181	A	C6-C5-N7	5.60	136.22	132.30
54	BA	679	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1086	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1191	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	1764	C	C3'-C2'-C1'	5.60	105.98	101.50
54	BA	2065	C	N1-C2-O2	5.60	122.26	118.90
54	BA	2810	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	91	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	726	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	752	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	800	A	C4-C5-C6	-5.60	114.20	117.00
18	AS	80	ARG	NE-CZ-NH1	5.60	123.10	120.30
54	BA	2453	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	2787	C	N3-C2-O2	-5.60	117.98	121.90
11	AL	13	ARG	NE-CZ-NH1	5.59	123.10	120.30
54	BA	614	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	2021	C	N1-C2-O2	5.59	122.26	118.90
54	BA	2696	U	O4'-C1'-N1	5.59	112.68	108.20
54	BA	2790	U	N3-C2-O2	-5.59	118.28	122.20
54	BA	2637	U	O4'-C1'-N1	5.59	112.67	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AM	106	ARG	CA-C-N	5.59	129.50	117.20
24	A3	47	G	C1'-O4'-C4'	-5.59	105.43	109.90
28	BF	132	ARG	NE-CZ-NH1	5.59	123.09	120.30
54	BA	216	A	C5-C6-N1	5.59	120.50	117.70
54	BA	746	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	1262	A	O4'-C1'-N9	5.59	112.67	108.20
54	BA	2420	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2627	G	O4'-C1'-N9	5.59	112.67	108.20
55	BB	83	G	N1-C6-O6	-5.59	116.55	119.90
21	AA	5	U	N3-C2-O2	-5.59	118.29	122.20
21	AA	882	C	O4'-C1'-N1	5.59	112.67	108.20
54	BA	793	A	C6-C5-N7	5.59	136.21	132.30
54	BA	2579	C	N3-C2-O2	-5.59	117.99	121.90
22	A1	30	C	N3-C2-O2	-5.59	117.99	121.90
38	BP	87	ARG	NE-CZ-NH1	5.59	123.09	120.30
54	BA	2760	C	N3-C2-O2	-5.59	117.99	121.90
28	BF	149	ARG	NE-CZ-NH2	-5.58	117.51	120.30
54	BA	89	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	694	U	O4'-C1'-N1	5.58	112.67	108.20
54	BA	1054	A	O4'-C1'-N9	5.58	112.67	108.20
54	BA	2678	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	595	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	1344	C	N1-C2-O2	5.58	122.25	118.90
54	BA	403	U	O4'-C1'-N1	5.58	112.67	108.20
54	BA	791	C	O4'-C1'-N1	5.58	112.67	108.20
54	BA	1129	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1372	U	O4'-C1'-N1	5.58	112.67	108.20
54	BA	1552	A	C2-N3-C4	5.58	113.39	110.60
54	BA	1558	C	N3-C2-O2	-5.58	117.99	121.90
22	A1	61	C	N3-C4-C5	5.58	124.13	121.90
54	BA	1896	G	N1-C6-O6	-5.58	116.55	119.90
15	AP	51	ARG	NE-CZ-NH1	5.58	123.09	120.30
21	AA	1493	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	927	A	C6-C5-N7	5.58	136.21	132.30
54	BA	2427	C	O4'-C1'-N1	5.58	112.66	108.20
20	AU	46	ARG	NE-CZ-NH1	5.57	123.09	120.30
21	AA	578	C	N3-C4-N4	-5.57	114.10	118.00
54	BA	138	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	1686	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	2657	A	C4-C5-C6	-5.57	114.21	117.00
21	AA	938	A	O4'-C1'-N9	5.57	112.66	108.20
54	BA	2090	A	C4-C5-C6	-5.57	114.22	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2886	A	C4-C5-C6	-5.57	114.21	117.00
21	AA	200	G	O4'-C1'-N9	5.57	112.65	108.20
21	AA	610	U	N3-C2-O2	-5.57	118.30	122.20
21	AA	728	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	888	C	O4'-C1'-N1	5.57	112.65	108.20
54	BA	1959	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	2512	C	O4'-C1'-N1	5.57	112.65	108.20
54	BA	2745	C	N1-C2-O2	5.57	122.24	118.90
55	BB	60	C	N3-C2-O2	-5.57	118.00	121.90
6	AG	101	ARG	CD-NE-CZ	5.57	131.39	123.60
17	AR	56	ARG	NE-CZ-NH1	5.57	123.08	120.30
21	AA	1111	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	633	A	N1-C6-N6	-5.56	115.26	118.60
55	BB	62	C	N3-C2-O2	-5.56	118.00	121.90
54	BA	765	C	N1-C2-O2	5.56	122.24	118.90
54	BA	837	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1508	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1513	U	N3-C2-O2	-5.56	118.31	122.20
54	BA	2860	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	277	G	N3-C4-C5	-5.56	125.82	128.60
54	BA	581	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1322	A	C6-C5-N7	5.56	136.19	132.30
54	BA	2808	G	O4'-C1'-N9	5.56	112.65	108.20
54	BA	2853	C	N3-C2-O2	-5.56	118.01	121.90
21	AA	335	C	C5'-C4'-C3'	-5.56	107.11	116.00
24	A3	71	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	615	U	O4'-C1'-N1	5.56	112.65	108.20
54	BA	2867	G	N3-C4-C5	-5.56	125.82	128.60
21	AA	1042	A	C4-C5-C6	-5.56	114.22	117.00
23	A2	91	A	O4'-C1'-N9	5.56	112.65	108.20
54	BA	732	C	N3-C2-O2	-5.56	118.01	121.90
39	BQ	54	ARG	NE-CZ-NH1	5.56	123.08	120.30
54	BA	667	U	O4'-C1'-N1	5.56	112.64	108.20
54	BA	1214	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1373	A	C4-C5-C6	-5.55	114.22	117.00
55	BB	51	G	C1'-O4'-C4'	-5.55	105.46	109.90
54	BA	968	C	N1-C2-O2	5.55	122.23	118.90
54	BA	2632	A	C6-C5-N7	5.55	136.19	132.30
21	AA	325	A	C4-C5-C6	-5.55	114.22	117.00
21	AA	1039	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	18	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	816	C	N3-C2-O2	-5.55	118.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1090	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	2022	U	O4'-C1'-N1	5.55	112.64	108.20
21	AA	463	U	N3-C2-O2	-5.55	118.32	122.20
21	AA	722	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	973	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1989	G	N3-C2-N2	-5.55	116.02	119.90
22	A1	35	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	532	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	1666	G	N1-C6-O6	-5.54	116.57	119.90
54	BA	1912	A	C4-C5-C6	-5.54	114.23	117.00
8	AI	17	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	1208	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	124	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	1925	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2476	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	498	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	893	C	N1-C2-O2	5.54	122.22	118.90
54	BA	2503	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2738	A	C6-C5-N7	5.54	136.18	132.30
21	AA	1018	G	O4'-C1'-N9	5.54	112.63	108.20
54	BA	22	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1405	U	O4'-C1'-N1	5.54	112.63	108.20
54	BA	280	U	N3-C2-O2	-5.54	118.32	122.20
54	BA	1140	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	109	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	178	C	N1-C2-O2	5.54	122.22	118.90
21	AA	414	A	C4-C5-C6	-5.54	114.23	117.00
22	A1	20	G	O4'-C1'-N9	5.54	112.63	108.20
24	A3	7	G	O4'-C1'-N9	5.54	112.63	108.20
54	BA	336	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	791	C	C1'-O4'-C4'	-5.54	105.47	109.90
54	BA	1708	C	N1-C2-O2	5.54	122.22	118.90
21	AA	1279	G	N3-C4-C5	-5.53	125.83	128.60
54	BA	910	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	2518	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	251	G	N3-C4-C5	-5.53	125.83	128.60
21	AA	631	C	N3-C2-O2	-5.53	118.03	121.90
15	AP	14	ARG	NE-CZ-NH2	-5.53	117.53	120.30
21	AA	737	C	O4'-C1'-N1	5.53	112.62	108.20
21	AA	793	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	672	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	736	C	N3-C2-O2	-5.53	118.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2198	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	402	G	N1-C6-O6	-5.53	116.58	119.90
21	AA	1021	A	C4-C5-C6	-5.53	114.24	117.00
24	A3	36	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	38	A	O4'-C1'-N9	5.53	112.62	108.20
54	BA	1084	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1196	C	N1-C2-O2	5.53	122.22	118.90
1	AB	138	ARG	NE-CZ-NH1	5.53	123.06	120.30
21	AA	705	G	N1-C6-O6	-5.53	116.58	119.90
21	AA	865	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	1020	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	1237	A	C4-C5-C6	-5.53	114.24	117.00
56	B5	134	ARG	NE-CZ-NH2	-5.53	117.54	120.30
21	AA	1269	A	C4-C5-C6	-5.53	114.24	117.00
21	AA	1446	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	1072	C	N1-C2-O2	5.53	122.22	118.90
54	BA	1369	G	N1-C6-O6	-5.53	116.58	119.90
21	AA	1136	C	N1-C2-O2	5.52	122.21	118.90
28	BF	114	ARG	NE-CZ-NH1	5.52	123.06	120.30
54	BA	1189	A	C5-C6-N1	5.52	120.46	117.70
54	BA	2374	C	C5'-C4'-O4'	5.52	115.73	109.10
21	AA	87	C	N1-C2-O2	5.52	122.21	118.90
54	BA	176	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	830	G	O4'-C1'-N9	5.52	112.62	108.20
54	BA	888	C	N1-C2-O2	5.52	122.21	118.90
21	AA	1396	A	C6-C5-N7	5.52	136.16	132.30
21	AA	427	U	N3-C2-O2	-5.52	118.34	122.20
21	AA	912	C	N1-C2-O2	5.52	122.21	118.90
37	BO	13	ARG	NE-CZ-NH1	5.52	123.06	120.30
54	BA	1698	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2558	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	2682	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	83	C	N1-C2-O2	5.52	122.21	118.90
21	AA	418	C	N3-C2-O2	-5.52	118.04	121.90
21	AA	1379	G	N1-C6-O6	-5.52	116.59	119.90
54	BA	364	C	N1-C2-O2	5.52	122.21	118.90
54	BA	2420	C	O4'-C1'-N1	5.52	112.61	108.20
21	AA	802	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	516	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	1742	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	2435	A	O4'-C1'-N9	5.52	112.61	108.20
21	AA	961	U	N3-C2-O2	-5.51	118.34	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	863	A	N1-C6-N6	-5.51	115.29	118.60
54	BA	1866	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	1888	G	N3-C4-C5	-5.51	125.84	128.60
54	BA	2609	U	N1-C2-N3	5.51	118.21	114.90
39	BQ	63	ARG	NE-CZ-NH1	5.51	123.06	120.30
21	AA	107	G	N1-C6-O6	-5.51	116.59	119.90
54	BA	751	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	1685	C	O4'-C1'-N1	5.51	112.61	108.20
54	BA	2667	C	N1-C2-O2	5.51	122.21	118.90
21	AA	193	C	N1-C2-O2	5.51	122.20	118.90
21	AA	513	C	N1-C2-O2	5.51	122.21	118.90
21	AA	833	G	O4'-C1'-N9	5.51	112.61	108.20
54	BA	323	C	O4'-C1'-N1	5.51	112.61	108.20
55	BB	49	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	2042	A	C4-C5-C6	-5.51	114.25	117.00
1	AB	107	ARG	NE-CZ-NH1	5.51	123.05	120.30
21	AA	210	C	N1-C2-O2	5.51	122.20	118.90
21	AA	334	C	N3-C2-O2	-5.51	118.05	121.90
21	AA	881	G	O4'-C1'-N9	5.51	112.61	108.20
21	AA	1172	C	N3-C2-O2	-5.51	118.05	121.90
54	BA	13	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	821	A	O4'-C1'-N9	5.51	112.61	108.20
54	BA	2338	C	N3-C2-O2	-5.51	118.05	121.90
21	AA	483	C	N3-C2-O2	-5.50	118.05	121.90
37	BO	33	ARG	NE-CZ-NH2	5.50	123.05	120.30
54	BA	1195	G	C4'-C3'-C2'	-5.50	97.09	102.60
21	AA	212	G	C1'-O4'-C4'	-5.50	105.50	109.90
21	AA	415	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	155	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	503	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	753	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1156	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	2480	C	O4'-C1'-N1	5.50	112.60	108.20
45	BW	53	GLY	C-N-CA	5.50	135.45	121.70
54	BA	1979	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	2815	C	N1-C2-O2	5.50	122.20	118.90
21	AA	1170	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1437	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1717	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	2683	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	383	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	646	U	O4'-C1'-N1	5.50	112.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	385	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	857	G	N3-C2-N2	-5.50	116.05	119.90
54	BA	2875	C	N1-C2-O2	5.50	122.20	118.90
21	AA	979	C	N3-C2-O2	-5.49	118.06	121.90
26	BD	59	ARG	NE-CZ-NH1	5.49	123.05	120.30
54	BA	412	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	568	U	O4'-C1'-N1	5.49	112.60	108.20
13	AN	59	ARG	NE-CZ-NH1	5.49	123.05	120.30
21	AA	365	U	O4'-C1'-N1	5.49	112.59	108.20
23	A2	79	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	113	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	346	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	1073	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	2193	G	O4'-C1'-N9	5.49	112.59	108.20
54	BA	573	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	1307	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	1598	A	C4-C5-C6	-5.49	114.26	117.00
21	AA	572	A	C1'-O4'-C4'	-5.48	105.52	109.90
54	BA	237	C	N1-C2-O2	5.48	122.19	118.90
54	BA	595	C	N1-C2-O2	5.48	122.19	118.90
54	BA	2122	U	O4'-C1'-N1	5.48	112.59	108.20
54	BA	2555	U	O4'-C1'-N1	5.48	112.59	108.20
54	BA	2581	G	N1-C6-O6	-5.48	116.61	119.90
21	AA	613	C	N1-C2-O2	5.48	122.19	118.90
21	AA	1119	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	164	C	N1-C2-O2	5.48	122.19	118.90
54	BA	1348	C	N3-C2-O2	-5.48	118.06	121.90
55	BB	101	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2264	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	457	G	N1-C6-O6	-5.48	116.61	119.90
21	AA	834	U	O4'-C1'-N1	5.48	112.58	108.20
21	AA	1072	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	1998	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2070	A	C6-C5-N7	5.48	136.13	132.30
54	BA	2295	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	964	C	N3-C2-O2	-5.48	118.07	121.90
54	BA	1446	C	N1-C2-O2	5.48	122.19	118.90
21	AA	215	C	N1-C2-O2	5.47	122.18	118.90
24	A3	16	C	N1-C2-O2	5.47	122.18	118.90
54	BA	1419	A	C4-C5-C6	-5.47	114.26	117.00
55	BB	70	C	N1-C2-O2	5.47	122.18	118.90
21	AA	284	C	N1-C2-O2	5.47	122.18	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	523	A	C4-C5-C6	-5.47	114.26	117.00
54	BA	331	C	N1-C2-O2	5.47	122.18	118.90
54	BA	2441	U	O4'-C1'-N1	5.47	112.58	108.20
21	AA	82	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	480	A	C5'-C4'-C3'	-5.47	107.25	116.00
54	BA	1188	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	1900	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	79	C	N1-C2-O2	5.47	122.18	118.90
54	BA	395	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	745	G	N1-C6-O6	-5.47	116.62	119.90
55	BB	105	G	N3-C2-N2	-5.47	116.07	119.90
54	BA	1481	U	N3-C2-O2	-5.47	118.37	122.20
54	BA	2576	G	N3-C2-N2	-5.47	116.07	119.90
21	AA	272	C	O4'-C1'-N1	5.47	112.57	108.20
21	AA	1411	C	O4'-C1'-N1	5.47	112.57	108.20
51	B2	28	ARG	NH1-CZ-NH2	-5.47	113.39	119.40
54	BA	1106	G	O4'-C1'-N9	5.47	112.57	108.20
21	AA	702	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	1209	C	N1-C2-O2	5.46	122.18	118.90
54	BA	1732	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	341	C	N3-C2-O2	-5.46	118.08	121.90
55	BB	12	C	N1-C2-O2	5.46	122.18	118.90
55	BB	21	G	O4'-C1'-N9	5.46	112.57	108.20
36	BN	45	ARG	NE-CZ-NH1	5.46	123.03	120.30
38	BP	38	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	510	C	N1-C2-O2	5.46	122.18	118.90
54	BA	960	A	N1-C6-N6	-5.46	115.32	118.60
35	BM	51	ARG	NE-CZ-NH2	-5.46	117.57	120.30
54	BA	1123	C	N3-C2-O2	-5.46	118.08	121.90
24	A3	66	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	1874	C	O4'-C1'-N1	5.46	112.56	108.20
54	BA	2619	C	O4'-C1'-N1	5.46	112.56	108.20
32	BJ	34	ARG	NE-CZ-NH1	5.46	123.03	120.30
21	AA	211	G	N3-C4-C5	-5.45	125.87	128.60
54	BA	2073	C	N1-C2-O2	5.45	122.17	118.90
54	BA	1932	A	C4-C5-C6	-5.45	114.27	117.00
3	AD	164	ARG	NE-CZ-NH1	5.45	123.03	120.30
21	AA	1271	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	819	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2729	G	C1'-O4'-C4'	-5.45	105.54	109.90
18	AS	31	ARG	NE-CZ-NH1	5.45	123.02	120.30
54	BA	334	C	N1-C2-O2	5.45	122.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	445	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	1810	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2311	A	C4-C5-C6	-5.45	114.28	117.00
29	BG	151	ARG	NE-CZ-NH1	5.45	123.02	120.30
54	BA	2338	C	O4'-C1'-N1	5.45	112.56	108.20
8	AI	32	ARG	NE-CZ-NH1	5.44	123.02	120.30
21	AA	63	C	N1-C2-O2	5.44	122.17	118.90
21	AA	342	C	N1-C2-O2	5.44	122.17	118.90
25	BC	188	ARG	NE-CZ-NH1	5.44	123.02	120.30
25	BC	213	ARG	NE-CZ-NH1	5.44	123.02	120.30
54	BA	541	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1638	C	N1-C2-O2	5.44	122.17	118.90
21	AA	1314	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	1116	G	N1-C6-O6	-5.44	116.64	119.90
21	AA	186	C	N1-C2-O2	5.44	122.16	118.90
21	AA	533	A	C4-C5-C6	-5.44	114.28	117.00
22	A1	33	U	N3-C2-O2	-5.44	118.39	122.20
49	B0	51	ARG	NE-CZ-NH1	5.44	123.02	120.30
54	BA	2078	C	N1-C2-O2	5.44	122.16	118.90
15	AP	14	ARG	NE-CZ-NH1	5.44	123.02	120.30
25	BC	101	ARG	NE-CZ-NH1	5.44	123.02	120.30
54	BA	330	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	659	G	N3-C2-N2	-5.44	116.09	119.90
54	BA	2278	A	C4-C5-C6	-5.44	114.28	117.00
24	A3	41	C	N3-C2-O2	-5.44	118.09	121.90
10	AK	126	ARG	NE-CZ-NH2	-5.43	117.58	120.30
21	AA	893	C	N3-C2-O2	-5.43	118.10	121.90
56	B5	12	ARG	NE-CZ-NH1	5.43	123.02	120.30
54	BA	608	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	2000	C	O4'-C1'-N1	5.43	112.55	108.20
54	BA	2321	U	N3-C2-O2	-5.43	118.40	122.20
56	B5	74	ARG	NE-CZ-NH1	5.43	123.02	120.30
21	AA	496	A	C5-C6-N1	5.43	120.41	117.70
21	AA	824	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	1298	U	N3-C2-O2	-5.43	118.40	122.20
54	BA	424	G	C4'-C3'-C2'	-5.43	97.17	102.60
54	BA	2096	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	108	G	N3-C2-N2	-5.43	116.10	119.90
54	BA	1689	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	1104	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	1633	G	N3-C2-N2	-5.42	116.10	119.90
54	BA	1952	A	C4-C5-C6	-5.42	114.29	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2045	C	N1-C2-O2	5.42	122.15	118.90
54	BA	2283	C	N3-C2-O2	-5.42	118.10	121.90
21	AA	993	G	N3-C4-C5	-5.42	125.89	128.60
54	BA	2636	C	N1-C2-O2	5.42	122.15	118.90
21	AA	1285	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1071	G	N3-C2-N2	-5.42	116.11	119.90
54	BA	2875	C	O4'-C1'-N1	5.42	112.54	108.20
55	BB	89	U	N3-C2-O2	-5.42	118.41	122.20
21	AA	396	C	N1-C2-O2	5.42	122.15	118.90
21	AA	792	A	N1-C6-N6	-5.42	115.35	118.60
21	AA	1524	C	N1-C2-O2	5.42	122.15	118.90
54	BA	1605	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	2001	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	2174	C	N1-C2-O2	5.42	122.15	118.90
54	BA	1667	G	O4'-C1'-N9	5.42	112.53	108.20
55	BB	41	G	O4'-C1'-N9	5.42	112.53	108.20
21	AA	235	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	1259	C	N1-C2-O2	5.42	122.15	118.90
54	BA	1572	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	18	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	817	C	N1-C2-O2	5.41	122.15	118.90
54	BA	805	G	N1-C6-O6	-5.41	116.65	119.90
54	BA	1376	C	N1-C2-O2	5.41	122.15	118.90
54	BA	1515	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	2433	A	C4-C5-C6	-5.41	114.29	117.00
21	AA	1311	A	C6-C5-N7	5.41	136.09	132.30
24	A3	47	G	N1-C6-O6	-5.41	116.65	119.90
54	BA	386	G	O4'-C1'-N9	5.41	112.53	108.20
12	AM	78	ARG	NE-CZ-NH1	5.41	123.01	120.30
54	BA	1454	C	N1-C2-O2	5.41	122.15	118.90
54	BA	1567	G	C1'-O4'-C4'	-5.41	105.57	109.90
54	BA	1760	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	1793	C	N1-C2-O2	5.41	122.15	118.90
13	AN	100	SER	C-N-CA	5.41	135.22	121.70
21	AA	1146	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	90	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	941	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	960	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	366	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	493	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1732	C	N3-C4-N4	-5.41	114.22	118.00
54	BA	2499	C	N3-C2-O2	-5.41	118.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2609	U	O4'-C1'-N1	5.41	112.53	108.20
21	AA	695	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	1093	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	1279	G	N1-C6-O6	-5.41	116.66	119.90
21	AA	1202	U	O4'-C1'-N1	5.40	112.52	108.20
24	A3	25	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2717	C	N1-C2-O2	5.40	122.14	118.90
21	AA	588	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	107	G	N3-C4-C5	-5.40	125.90	128.60
54	BA	1308	A	C6-C5-N7	5.40	136.08	132.30
54	BA	1639	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	2679	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	135	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	511	C	N1-C2-O2	5.40	122.14	118.90
21	AA	1279	G	C5-C6-N1	5.40	114.20	111.50
54	BA	472	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2380	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	1857	G	N1-C6-O6	-5.40	116.66	119.90
21	AA	1163	A	C4-C5-C6	-5.40	114.30	117.00
33	BK	18	ARG	NE-CZ-NH1	5.40	123.00	120.30
43	BU	85	ARG	NE-CZ-NH1	5.40	123.00	120.30
54	BA	1534	U	N3-C2-O2	-5.40	118.42	122.20
54	BA	1766	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	2147	A	C6-C5-N7	5.40	136.08	132.30
54	BA	2855	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	1483	A	C4-C5-C6	-5.40	114.30	117.00
4	AE	67	ARG	NE-CZ-NH1	5.39	123.00	120.30
21	AA	520	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	151	C	N3-C2-O2	-5.39	118.12	121.90
21	AA	549	C	N1-C2-O2	5.39	122.14	118.90
23	A2	85	G	N1-C6-O6	-5.39	116.66	119.90
54	BA	398	C	N1-C2-O2	5.39	122.14	118.90
54	BA	1169	A	C6-C5-N7	5.39	136.07	132.30
54	BA	1722	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	1121	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1373	A	C5-C6-N1	5.39	120.39	117.70
54	BA	1519	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	1550	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	2342	C	O4'-C1'-N1	5.39	112.51	108.20
21	AA	190	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	723	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1113	U	O4'-C1'-N1	5.39	112.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1951	U	N3-C2-O2	-5.39	118.43	122.20
54	BA	2082	A	O4'-C1'-N9	5.39	112.51	108.20
54	BA	457	A	C6-C5-N7	5.39	136.07	132.30
54	BA	2023	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	2085	U	O4'-C1'-N1	5.39	112.51	108.20
21	AA	346	G	N3-C4-C5	-5.39	125.91	128.60
21	AA	466	A	O4'-C1'-N9	5.39	112.51	108.20
21	AA	564	C	N3-C2-O2	-5.39	118.13	121.90
21	AA	578	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	738	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	783	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	1559	U	N3-C2-O2	-5.39	118.43	122.20
54	BA	2846	G	N1-C6-O6	-5.39	116.67	119.90
21	AA	1429	A	C6-C5-N7	5.38	136.07	132.30
22	A1	20	G	N3-C4-C5	-5.38	125.91	128.60
54	BA	985	C	N1-C2-O2	5.38	122.13	118.90
54	BA	1013	C	N3-C2-O2	-5.38	118.13	121.90
54	BA	2827	C	N3-C2-O2	-5.38	118.13	121.90
55	BB	48	U	O4'-C1'-N1	5.38	112.51	108.20
54	BA	1585	C	N3-C4-C5	5.38	124.05	121.90
54	BA	2863	C	N1-C2-O2	5.38	122.13	118.90
55	BB	82	U	O4'-C1'-N1	5.38	112.51	108.20
21	AA	50	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	1016	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	1510	C	N1-C2-O2	5.38	122.13	118.90
22	A1	58	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1036	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1349	C	C3'-C2'-C1'	5.38	105.81	101.50
54	BA	1570	A	O4'-C1'-N9	5.38	112.50	108.20
54	BA	2644	G	O4'-C1'-N9	5.38	112.51	108.20
21	AA	395	C	N1-C2-O2	5.38	122.13	118.90
54	BA	1497	U	C1'-O4'-C4'	-5.38	105.60	109.90
54	BA	838	C	N1-C2-O2	5.38	122.13	118.90
54	BA	1145	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	2651	C	O4'-C1'-N1	5.38	112.50	108.20
54	BA	1914	C	N1-C2-O2	5.38	122.13	118.90
54	BA	2496	C	N1-C2-O2	5.38	122.13	118.90
21	AA	502	A	C5-C6-N1	5.38	120.39	117.70
21	AA	597	G	N1-C6-O6	-5.38	116.67	119.90
21	AA	681	A	C6-C5-N7	5.38	136.06	132.30
21	AA	1342	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	456	C	O4'-C1'-N1	5.38	112.50	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2248	C	N1-C2-O2	5.38	122.12	118.90
8	AI	98	ARG	NE-CZ-NH1	5.37	122.99	120.30
21	AA	90	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	903	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	1138	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	1479	C	N1-C2-O2	5.37	122.12	118.90
54	BA	524	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	650	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	876	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	2145	C	N3-C4-C5	5.37	124.05	121.90
54	BA	2388	A	C1'-O4'-C4'	-5.37	105.60	109.90
54	BA	2639	A	N1-C6-N6	-5.37	115.38	118.60
54	BA	2896	C	O4'-C1'-N1	5.37	112.50	108.20
55	BB	17	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	143	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	948	C	N1-C2-O2	5.37	122.12	118.90
54	BA	1345	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1681	G	O4'-C1'-N9	5.37	112.50	108.20
54	BA	2160	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1420	A	C4-C5-C6	-5.37	114.31	117.00
56	B5	7	ARG	NE-CZ-NH1	5.37	122.98	120.30
21	AA	862	C	N1-C2-O2	5.37	122.12	118.90
21	AA	1066	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1574	C	N1-C2-O2	5.37	122.12	118.90
21	AA	211	G	O4'-C1'-N9	5.37	112.49	108.20
21	AA	545	C	N1-C2-O2	5.37	122.12	118.90
21	AA	894	G	C5-C6-N1	5.37	114.18	111.50
54	BA	731	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2029	G	C5-C6-N1	5.37	114.18	111.50
54	BA	2486	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	2556	C	N1-C2-O2	5.37	122.12	118.90
54	BA	1237	A	O4'-C1'-N9	5.36	112.49	108.20
54	BA	1305	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1735	A	O4'-C1'-N9	5.36	112.49	108.20
54	BA	2083	G	N3-C2-N2	-5.36	116.15	119.90
21	AA	316	C	N1-C2-O2	5.36	122.12	118.90
3	AD	25	ARG	NE-CZ-NH1	5.36	122.98	120.30
21	AA	532	A	O4'-C1'-N9	5.36	112.49	108.20
21	AA	1364	U	O4'-C1'-N1	5.36	112.49	108.20
51	B2	14	ARG	NE-CZ-NH1	5.36	122.98	120.30
54	BA	508	A	O4'-C1'-N9	5.36	112.49	108.20
54	BA	596	U	O4'-C1'-N1	5.36	112.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1205	A	O4'-C1'-N9	5.36	112.49	108.20
54	BA	1208	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2472	G	C5-C6-N1	5.36	114.18	111.50
54	BA	2490	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	1507	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2680	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2850	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	768	A	C6-C5-N7	5.36	136.05	132.30
21	AA	819	A	C1'-O4'-C4'	-5.36	105.61	109.90
24	A3	11	A	C5-C6-N1	5.36	120.38	117.70
33	BK	78	ARG	NE-CZ-NH1	5.36	122.98	120.30
54	BA	240	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	2226	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	2732	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	2749	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	80	G	O4'-C1'-N9	5.36	112.48	108.20
54	BA	2525	G	N1-C6-O6	-5.36	116.69	119.90
54	BA	1251	C	N3-C2-O2	-5.35	118.15	121.90
54	BA	1503	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	351	C	N3-C2-O2	-5.35	118.15	121.90
54	BA	2354	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2374	C	N1-C2-O2	5.35	122.11	118.90
54	BA	2756	U	C5-C6-N1	-5.35	120.03	122.70
18	AS	36	ARG	NE-CZ-NH1	5.35	122.97	120.30
21	AA	28	A	C4-C5-C6	-5.35	114.33	117.00
21	AA	879	C	N1-C2-O2	5.35	122.11	118.90
21	AA	971	G	N1-C6-O6	-5.35	116.69	119.90
21	AA	1147	C	N1-C2-O2	5.35	122.11	118.90
32	BJ	27	ARG	NE-CZ-NH1	5.35	122.97	120.30
54	BA	2146	C	N1-C2-O2	5.35	122.11	118.90
54	BA	2562	U	O4'-C1'-N1	5.35	112.48	108.20
21	AA	132	C	N3-C4-N4	-5.35	114.26	118.00
54	BA	1829	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	2194	U	C1'-O4'-C4'	-5.35	105.62	109.90
54	BA	2199	A	N1-C6-N6	-5.35	115.39	118.60
55	BB	97	C	O4'-C1'-N1	5.35	112.48	108.20
21	AA	1225	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	2177	C	N1-C2-O2	5.35	122.11	118.90
21	AA	148	G	N1-C6-O6	-5.34	116.69	119.90
21	AA	196	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	977	A	C4-C5-C6	-5.34	114.33	117.00
38	BP	102	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	701	G	N3-C2-N2	-5.34	116.16	119.90
54	BA	1089	A	C1'-O4'-C4'	-5.34	105.62	109.90
24	A3	43	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	2285	C	O4'-C1'-N1	5.34	112.47	108.20
21	AA	214	C	N3-C2-O2	-5.34	118.16	121.90
52	B3	12	ARG	NE-CZ-NH2	-5.34	117.63	120.30
54	BA	1311	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	1864	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2277	G	C5'-C4'-C3'	-5.34	107.45	116.00
54	BA	2532	G	N3-C2-N2	-5.34	116.16	119.90
54	BA	2691	C	O4'-C1'-N1	5.34	112.47	108.20
55	BB	63	C	O4'-C1'-N1	5.34	112.47	108.20
2	AC	106	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BA	2236	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2885	G	N1-C6-O6	-5.34	116.70	119.90
21	AA	1237	C	N1-C2-O2	5.34	122.10	118.90
21	AA	1318	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	1086	A	O4'-C1'-N9	5.34	112.47	108.20
21	AA	744	C	N3-C2-O2	-5.34	118.16	121.90
21	AA	779	C	O4'-C1'-N1	5.34	112.47	108.20
21	AA	807	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	1349	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	705	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2061	G	C1'-O4'-C4'	-5.34	105.63	109.90
54	BA	1128	G	C1'-O4'-C4'	-5.33	105.63	109.90
54	BA	2359	C	O4'-C1'-N1	5.33	112.47	108.20
21	AA	1063	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	1536	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	1664	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	80	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	176	C	N1-C2-O2	5.33	122.10	118.90
21	AA	715	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	907	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	49	A	P-O3'-C3'	5.33	126.10	119.70
54	BA	1357	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	686	U	N3-C2-O2	-5.33	118.47	122.20
21	AA	953	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	1313	U	C3'-C2'-C1'	5.33	105.76	101.50
21	AA	926	G	C3'-C2'-C1'	5.33	105.76	101.50
54	BA	1606	C	C1'-O4'-C4'	-5.33	105.64	109.90
54	BA	1709	U	O4'-C1'-N1	5.33	112.46	108.20
21	AA	475	C	N1-C2-O2	5.32	122.09	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	218	A	C6-C5-N7	5.32	136.03	132.30
54	BA	710	U	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1822	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1923	U	O4'-C1'-N1	5.32	112.46	108.20
21	AA	975	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	615	U	N3-C2-O2	-5.32	118.47	122.20
54	BA	762	U	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1537	G	N3-C4-C5	-5.32	125.94	128.60
54	BA	2535	G	N3-C2-N2	-5.32	116.17	119.90
21	AA	926	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	1580	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	2450	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	462	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	492	C	N1-C2-O2	5.32	122.09	118.90
22	A1	18	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	589	U	O4'-C1'-N1	5.32	112.45	108.20
54	BA	1211	C	N3-C4-N4	-5.32	114.28	118.00
54	BA	1988	G	O4'-C1'-N9	5.32	112.45	108.20
54	BA	2459	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	2712	C	O4'-C1'-N1	5.32	112.45	108.20
21	AA	660	C	N1-C2-O2	5.31	122.09	118.90
54	BA	1881	C	N1-C2-O2	5.31	122.09	118.90
54	BA	1953	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	2541	A	C6-C5-N7	5.31	136.02	132.30
11	AL	8	ARG	NE-CZ-NH1	5.31	122.96	120.30
54	BA	1128	G	C5'-C4'-O4'	5.31	115.47	109.10
54	BA	1592	C	O4'-C1'-N1	5.31	112.45	108.20
54	BA	2035	G	N3-C4-C5	-5.31	125.94	128.60
54	BA	2407	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	2463	C	C4'-C3'-C2'	-5.31	97.29	102.60
29	BG	162	ARG	NE-CZ-NH1	5.31	122.95	120.30
54	BA	544	C	N1-C2-O2	5.31	122.09	118.90
54	BA	1585	C	N1-C2-O2	5.31	122.08	118.90
54	BA	1917	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	2500	U	N3-C2-O2	-5.31	118.48	122.20
21	AA	496	A	N1-C6-N6	-5.31	115.42	118.60
21	AA	1418	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	2067	G	N1-C6-O6	-5.31	116.72	119.90
21	AA	386	C	N1-C2-O2	5.31	122.08	118.90
43	BU	81	ARG	NE-CZ-NH1	5.31	122.95	120.30
54	BA	1583	A	C6-C5-N7	5.31	136.01	132.30
54	BA	1947	C	N1-C2-O2	5.31	122.08	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1974	C	N1-C2-O2	5.31	122.08	118.90
21	AA	842	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	1523	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	1739	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	2430	A	C3'-C2'-C1'	5.30	105.74	101.50
54	BA	131	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	2339	C	O4'-C1'-N1	5.30	112.44	108.20
55	BB	63	C	N3-C2-O2	-5.30	118.19	121.90
21	AA	1278	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	1511	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	501	A	N1-C6-N6	-5.30	115.42	118.60
54	BA	1189	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1261	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1399	C	O4'-C1'-N1	5.30	112.44	108.20
55	BB	108	A	O4'-C1'-N9	5.30	112.44	108.20
54	BA	2225	A	C4-C5-C6	-5.30	114.35	117.00
12	AM	108	ARG	NE-CZ-NH1	5.30	122.95	120.30
54	BA	20	C	N1-C2-O2	5.30	122.08	118.90
54	BA	2586	U	C4'-C3'-C2'	-5.30	97.30	102.60
21	AA	212	G	N1-C6-O6	-5.29	116.72	119.90
21	AA	269	C	N3-C2-O2	-5.29	118.19	121.90
54	BA	876	C	N1-C2-O2	5.29	122.08	118.90
54	BA	1024	G	N1-C6-O6	-5.29	116.72	119.90
54	BA	200	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1337	G	N1-C6-O6	-5.29	116.72	119.90
54	BA	1872	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	2665	A	C4-C5-C6	-5.29	114.35	117.00
21	AA	1201	A	O4'-C1'-N9	5.29	112.43	108.20
54	BA	422	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	1579	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	1896	G	O4'-C1'-N9	5.29	112.43	108.20
54	BA	2244	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2668	G	N3-C4-C5	-5.29	125.95	128.60
54	BA	2715	C	N1-C2-O2	5.29	122.08	118.90
21	AA	1138	G	C5-C6-N1	5.29	114.14	111.50
24	A3	74	A	O4'-C1'-N9	5.29	112.43	108.20
54	BA	105	C	N1-C2-O2	5.29	122.07	118.90
54	BA	1764	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2756	U	C3'-C2'-C1'	-5.29	97.27	101.50
54	BA	130	C	N1-C2-O2	5.29	122.07	118.90
23	A2	86	U	C5-C6-N1	-5.29	120.06	122.70
54	BA	433	C	N3-C2-O2	-5.29	118.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	902	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2013	A	C4-C5-C6	-5.29	114.36	117.00
16	AQ	64	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	AA	872	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1278	G	N3-C2-N2	-5.28	116.20	119.90
41	BS	18	ARG	NE-CZ-NH2	5.28	122.94	120.30
54	BA	817	C	N3-C4-N4	-5.28	114.30	118.00
54	BA	1811	G	O4'-C1'-N9	5.28	112.43	108.20
54	BA	2033	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1217	C	O4'-C1'-N1	5.28	112.43	108.20
54	BA	11	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2192	U	O4'-C1'-N1	5.28	112.43	108.20
54	BA	2549	G	C5'-C4'-C3'	-5.28	107.55	116.00
21	AA	179	A	C6-C5-N7	5.28	136.00	132.30
21	AA	1246	A	C6-C5-N7	5.28	136.00	132.30
21	AA	1262	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	421	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	698	C	N1-C2-O2	5.28	122.07	118.90
54	BA	1078	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2628	C	N1-C2-O2	5.28	122.07	118.90
54	BA	1186	G	O4'-C1'-N9	5.28	112.42	108.20
40	BR	80	ARG	NE-CZ-NH1	5.28	122.94	120.30
54	BA	28	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	427	U	N3-C2-O2	-5.28	118.51	122.20
1	AB	136	ARG	CD-NE-CZ	5.28	130.99	123.60
21	AA	1454	G	N1-C6-O6	-5.28	116.73	119.90
29	BG	54	ARG	NE-CZ-NH1	5.28	122.94	120.30
53	B4	4	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	AA	1201	A	P-O3'-C3'	5.27	126.03	119.70
54	BA	853	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	1108	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	1240	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2087	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	2826	A	C6-C5-N7	5.27	135.99	132.30
21	AA	1053	G	N3-C2-N2	-5.27	116.21	119.90
54	BA	40	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	217	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	931	U	N3-C2-O2	-5.27	118.51	122.20
3	AD	48	SER	C-N-CA	5.27	134.87	121.70
54	BA	2044	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	2406	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	2529	G	C3'-C2'-C1'	5.27	105.72	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	798	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	201	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	2093	G	O4'-C1'-N9	5.27	112.41	108.20
54	BA	883	G	N3-C4-C5	-5.27	125.97	128.60
54	BA	2813	A	O4'-C1'-N9	5.27	112.41	108.20
55	BB	57	A	C4-C5-C6	-5.27	114.37	117.00
21	AA	1338	G	N3-C2-N2	-5.26	116.21	119.90
54	BA	1288	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	1771	C	N1-C2-O2	5.26	122.06	118.90
54	BA	2534	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2672	U	O4'-C1'-N1	5.26	112.41	108.20
22	A1	16	C	N1-C2-O2	5.26	122.06	118.90
54	BA	242	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	1374	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	1382	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	112	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	95	A	O4'-C1'-N9	5.26	112.41	108.20
55	BB	111	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	985	C	N1-C2-O2	5.26	122.06	118.90
54	BA	1825	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	1094	G	N1-C6-O6	-5.26	116.75	119.90
42	BT	76	ARG	NE-CZ-NH1	5.26	122.93	120.30
54	BA	1985	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	2573	C	N1-C2-O2	5.26	122.05	118.90
54	BA	2594	C	N3-C2-O2	-5.26	118.22	121.90
55	BB	35	C	N3-C4-N4	-5.26	114.32	118.00
54	BA	455	C	N1-C2-O2	5.25	122.05	118.90
54	BA	1740	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	415	A	C2-N3-C4	5.25	113.23	110.60
24	A3	7	G	N1-C6-O6	-5.25	116.75	119.90
24	A3	35	C	N1-C2-O2	5.25	122.05	118.90
54	BA	693	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	1577	C	N1-C2-O2	5.25	122.05	118.90
54	BA	1727	C	N1-C2-O2	5.25	122.05	118.90
54	BA	601	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	756	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	784	G	N3-C4-C5	-5.25	125.97	128.60
54	BA	836	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	1481	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1760	C	O4'-C4'-C3'	5.25	110.30	106.10
54	BA	1779	U	N3-C2-O2	-5.25	118.52	122.20
21	AA	328	C	N1-C2-O2	5.25	122.05	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	205	A	C4-C5-C6	-5.25	114.38	117.00
21	AA	624	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2064	C	N3-C2-O2	-5.25	118.23	121.90
24	A3	73	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	1196	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1759	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	2339	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2497	A	C4-C5-C6	-5.25	114.38	117.00
21	AA	234	C	P-O3'-C3'	5.25	125.99	119.70
21	AA	1521	C	N3-C2-O2	-5.25	118.23	121.90
54	BA	1190	G	N3-C2-N2	-5.25	116.23	119.90
54	BA	2107	G	N3-C2-N2	-5.25	116.23	119.90
54	BA	2258	C	N1-C2-O2	5.25	122.05	118.90
21	AA	429	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	632	U	C1'-O4'-C4'	-5.24	105.71	109.90
21	AA	1362	A	C6-C5-N7	5.24	135.97	132.30
54	BA	54	G	O4'-C1'-N9	5.24	112.39	108.20
54	BA	701	G	O4'-C1'-N9	5.24	112.39	108.20
54	BA	2634	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	333	G	N1-C6-O6	-5.24	116.75	119.90
54	BA	1379	U	O4'-C1'-N1	5.24	112.39	108.20
21	AA	1036	A	C6-C5-N7	5.24	135.97	132.30
54	BA	361	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	424	G	O4'-C1'-N9	5.24	112.39	108.20
54	BA	1880	U	C3'-C2'-C1'	5.24	105.69	101.50
54	BA	2734	A	C6-C5-N7	5.24	135.97	132.30
54	BA	2898	U	C4'-C3'-C2'	-5.24	97.36	102.60
19	AT	28	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BA	82	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1236	G	N3-C2-N2	-5.24	116.23	119.90
54	BA	1288	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	2100	G	N3-C2-N2	-5.24	116.23	119.90
54	BA	2660	A	C4-C5-C6	-5.24	114.38	117.00
55	BB	11	C	N1-C2-O2	5.24	122.04	118.90
54	BA	1111	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1251	C	N3-C4-C5	5.24	124.00	121.90
54	BA	2227	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	194	C	N1-C2-O2	5.24	122.04	118.90
21	AA	610	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	33	C	N3-C4-C5	5.24	123.99	121.90
54	BA	335	C	N1-C2-O2	5.24	122.04	118.90
54	BA	2498	C	N1-C2-O2	5.24	122.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2572	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	2825	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	2575	C	N3-C4-C5	5.23	123.99	121.90
21	AA	711	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	249	C	N1-C2-O2	5.23	122.04	118.90
54	BA	2305	U	N3-C2-O2	-5.23	118.54	122.20
2	AC	171	ARG	NE-CZ-NH1	5.23	122.92	120.30
21	AA	1213	A	C4-C5-C6	-5.23	114.38	117.00
54	BA	984	A	C4-C5-C6	-5.23	114.38	117.00
54	BA	1048	A	C6-C5-N7	5.23	135.96	132.30
54	BA	1890	A	C6-C5-N7	5.23	135.96	132.30
21	AA	1196	A	O4'-C1'-N9	5.23	112.38	108.20
54	BA	1187	G	N3-C4-C5	-5.23	125.99	128.60
21	AA	1293	C	N1-C2-O2	5.23	122.04	118.90
54	BA	846	U	O4'-C1'-N1	5.23	112.38	108.20
54	BA	2145	C	N1-C2-O2	5.23	122.04	118.90
54	BA	2723	C	C5'-C4'-O4'	5.23	115.37	109.10
55	BB	73	A	C4-C5-C6	-5.23	114.39	117.00
55	BB	88	C	N1-C2-O2	5.23	122.04	118.90
28	BF	166	ARG	NE-CZ-NH1	5.23	122.91	120.30
54	BA	2132	U	N3-C2-O2	-5.23	118.54	122.20
21	AA	117	G	O4'-C1'-N9	5.22	112.38	108.20
21	AA	487	A	C4-C5-C6	-5.22	114.39	117.00
46	BX	71	ARG	NE-CZ-NH1	5.22	122.91	120.30
54	BA	867	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	1317	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	1561	C	N3-C2-O2	-5.22	118.24	121.90
54	BA	2368	C	N3-C2-O2	-5.22	118.24	121.90
21	AA	1445	U	N3-C2-O2	-5.22	118.54	122.20
54	BA	226	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	1335	C	N1-C2-O2	5.22	122.03	118.90
55	BB	53	A	N1-C6-N6	-5.22	115.47	118.60
54	BA	101	A	O4'-C1'-N9	5.22	112.38	108.20
54	BA	2824	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	1481	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	1204	A	C1'-O4'-C4'	-5.22	105.72	109.90
54	BA	1439	A	C2-N3-C4	5.22	113.21	110.60
54	BA	394	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	1233	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2694	G	C5-C6-N1	5.22	114.11	111.50
54	BA	2821	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	366	A	P-O3'-C3'	5.22	125.96	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	675	A	C6-C5-N7	5.22	135.95	132.30
54	BA	885	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	1293	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2442	C	N1-C2-O2	5.22	122.03	118.90
21	AA	117	G	C5-C6-N1	5.21	114.11	111.50
21	AA	718	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	279	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	1158	C	C5'-C4'-O4'	5.21	115.36	109.10
54	BA	119	A	O4'-C1'-N9	5.21	112.37	108.20
21	AA	305	G	O4'-C1'-N9	5.21	112.37	108.20
54	BA	1625	C	N3-C4-N4	-5.21	114.35	118.00
54	BA	1398	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1816	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2045	C	N3-C4-N4	-5.21	114.35	118.00
54	BA	2785	C	O4'-C1'-N1	5.21	112.37	108.20
21	AA	236	A	C3'-C2'-C1'	5.21	105.67	101.50
54	BA	1114	C	N1-C2-O2	5.21	122.02	118.90
54	BA	1594	U	C5-C6-N1	-5.21	120.10	122.70
54	BA	1631	G	C5-C6-N1	5.21	114.10	111.50
54	BA	2467	C	N3-C2-O2	-5.21	118.26	121.90
54	BA	2332	C	N3-C4-N4	-5.21	114.36	118.00
2	AC	64	ARG	NE-CZ-NH1	5.20	122.90	120.30
21	AA	1008	U	O4'-C1'-N1	5.20	112.36	108.20
21	AA	1115	U	O4'-C1'-N1	5.20	112.36	108.20
21	AA	1276	G	N7-C8-N9	5.20	115.70	113.10
54	BA	2326	C	N1-C2-O2	5.20	122.02	118.90
54	BA	2652	C	O4'-C1'-N1	5.20	112.36	108.20
56	B5	60	ARG	NE-CZ-NH2	5.20	122.90	120.30
20	AU	17	ARG	NE-CZ-NH2	5.20	122.90	120.30
21	AA	1381	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	2051	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	729	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	1177	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	2416	C	N1-C2-O2	5.20	122.02	118.90
54	BA	649	G	N3-C2-N2	-5.20	116.26	119.90
6	AG	110	ARG	NE-CZ-NH1	5.20	122.90	120.30
24	A3	13	C	N3-C4-N4	-5.20	114.36	118.00
54	BA	57	C	C4'-C3'-C2'	-5.20	97.41	102.60
54	BA	83	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	96	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	919	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1043	C	N1-C2-O2	5.20	122.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1387	A	O4'-C1'-N9	5.20	112.36	108.20
12	AM	86	ARG	NE-CZ-NH1	5.19	122.90	120.30
21	AA	61	G	C5-C6-N1	5.19	114.10	111.50
21	AA	1129	C	C3'-C2'-C1'	5.19	105.65	101.50
21	AA	1261	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	1744	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	1982	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	205	G	N1-C6-O6	-5.19	116.79	119.90
21	AA	581	G	N1-C6-O6	-5.19	116.79	119.90
21	AA	653	U	C3'-C2'-C1'	5.19	105.65	101.50
21	AA	1028	C	N1-C2-O2	5.19	122.01	118.90
21	AA	1054	C	N3-C4-C5	5.19	123.97	121.90
27	BE	162	ARG	NE-CZ-NH1	5.19	122.89	120.30
54	BA	316	C	N1-C2-O2	5.19	122.01	118.90
54	BA	479	A	C6-C5-N7	5.19	135.93	132.30
54	BA	1578	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	1942	C	N1-C2-O2	5.19	122.01	118.90
55	BB	105	G	O4'-C1'-N9	5.19	112.35	108.20
21	AA	373	A	O4'-C1'-N9	5.19	112.35	108.20
21	AA	1157	A	N1-C6-N6	-5.19	115.49	118.60
21	AA	1373	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	1959	G	C5'-C4'-O4'	5.19	115.32	109.10
55	BB	4	C	O4'-C1'-N1	5.19	112.35	108.20
3	AD	103	ARG	NE-CZ-NH1	5.18	122.89	120.30
21	AA	949	A	C6-C5-N7	5.18	135.93	132.30
38	BP	88	ARG	NE-CZ-NH1	5.18	122.89	120.30
54	BA	2515	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	2752	C	N1-C2-O2	5.18	122.01	118.90
21	AA	393	A	C6-C5-N7	5.18	135.93	132.30
21	AA	567	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	523	C	N1-C2-O2	5.18	122.01	118.90
54	BA	1005	C	C3'-C2'-C1'	5.18	105.65	101.50
54	BA	1297	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	1983	G	C5-C6-N1	5.18	114.09	111.50
55	BB	99	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	658	C	N3-C4-C5	5.18	123.97	121.90
51	B2	41	ARG	NE-CZ-NH1	5.18	122.89	120.30
54	BA	2772	C	N1-C2-O2	5.18	122.01	118.90
21	AA	412	A	O4'-C1'-N9	5.18	112.34	108.20
21	AA	440	C	N3-C2-O2	-5.18	118.27	121.90
21	AA	466	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	750	C	N1-C2-O2	5.18	122.01	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1306	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	1313	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	192	C	N3-C4-C5	5.18	123.97	121.90
54	BA	836	G	C5-C6-N1	5.18	114.09	111.50
21	AA	315	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	750	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	71	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	175	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1350	A	C6-C5-N7	5.18	135.92	132.30
54	BA	568	U	C5-C6-N1	-5.18	120.11	122.70
54	BA	1455	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	1469	A	C6-C5-N7	5.18	135.92	132.30
55	BB	110	C	O4'-C1'-N1	5.18	112.34	108.20
21	AA	1147	C	O4'-C1'-N1	5.17	112.34	108.20
21	AA	833	G	N3-C2-N2	-5.17	116.28	119.90
32	BJ	116	ARG	NE-CZ-NH1	5.17	122.89	120.30
54	BA	1653	G	O4'-C1'-N9	5.17	112.34	108.20
21	AA	1499	A	C4-C5-C6	-5.17	114.42	117.00
24	A3	59	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	278	A	O4'-C1'-N9	5.17	112.34	108.20
54	BA	560	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1570	A	C4-C5-C6	-5.17	114.42	117.00
21	AA	691	G	C5-C6-N1	5.17	114.08	111.50
21	AA	743	A	C6-C5-N7	5.17	135.92	132.30
21	AA	1441	A	C6-C5-N7	5.17	135.92	132.30
22	A1	56	C	C3'-C2'-C1'	5.17	105.64	101.50
54	BA	514	A	O4'-C1'-N9	5.17	112.33	108.20
54	BA	2069	G	C5-C6-N1	5.17	114.08	111.50
54	BA	2487	G	O4'-C1'-N9	5.17	112.33	108.20
55	BB	47	C	O4'-C1'-N1	5.17	112.33	108.20
21	AA	614	C	O4'-C1'-N1	5.17	112.33	108.20
21	AA	835	U	O4'-C1'-N1	5.17	112.33	108.20
21	AA	1273	C	N3-C2-O2	-5.17	118.28	121.90
21	AA	1363	A	C4-C5-C6	-5.17	114.42	117.00
24	A3	1	C	C6-N1-C2	-5.17	118.23	120.30
54	BA	1204	A	C4-C5-C6	-5.17	114.42	117.00
54	BA	2130	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	2428	G	P-O3'-C3'	5.17	125.90	119.70
54	BA	2586	U	C2'-C3'-O3'	5.17	121.97	113.70
21	AA	234	C	N1-C2-O2	5.17	122.00	118.90
52	B3	7	ARG	NE-CZ-NH1	5.17	122.88	120.30
54	BA	2246	G	C5-C6-N1	5.17	114.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	42	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	107	G	N7-C8-N9	5.16	115.68	113.10
54	BA	1314	C	C6-N1-C2	-5.16	118.23	120.30
54	BA	2483	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	119	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	963	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	338	G	N3-C4-C5	-5.16	126.02	128.60
54	BA	414	C	N1-C2-O2	5.16	122.00	118.90
54	BA	203	A	O4'-C1'-N9	5.16	112.33	108.20
54	BA	229	C	N1-C2-O2	5.16	122.00	118.90
54	BA	680	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	401	C	N1-C2-O2	5.16	121.99	118.90
24	A3	69	C	N3-C2-O2	-5.16	118.29	121.90
54	BA	1538	G	N1-C6-O6	-5.16	116.81	119.90
21	AA	968	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	1134	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	1779	U	O4'-C1'-N1	5.16	112.32	108.20
55	BB	26	C	N1-C2-O2	5.16	121.99	118.90
24	A3	13	C	N1-C2-O2	5.15	121.99	118.90
54	BA	211	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	468	G	O4'-C1'-N9	5.15	112.32	108.20
21	AA	496	A	O4'-C1'-N9	5.15	112.32	108.20
21	AA	574	A	C6-C5-N7	5.15	135.91	132.30
35	BM	81	ARG	NE-CZ-NH1	-5.15	117.72	120.30
54	BA	1111	A	O4'-C1'-N9	5.15	112.32	108.20
54	BA	1209	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2348	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	191	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	324	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	1067	A	O4'-C1'-N9	5.15	112.32	108.20
21	AA	31	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1852	U	N3-C2-O2	-5.15	118.60	122.20
55	BB	87	U	N3-C2-O2	-5.15	118.60	122.20
21	AA	450	G	O4'-C1'-N9	5.15	112.32	108.20
54	BA	1158	C	N1-C2-O2	5.15	121.99	118.90
54	BA	2059	A	C6-C5-N7	5.15	135.90	132.30
54	BA	2566	A	O4'-C1'-N9	5.15	112.32	108.20
21	AA	948	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	1175	A	O4'-C1'-N9	5.14	112.32	108.20
54	BA	1913	A	C4-C5-C6	-5.14	114.43	117.00
21	AA	990	C	N1-C2-O2	5.14	121.98	118.90
54	BA	33	C	O4'-C1'-N1	5.14	112.31	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	464	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	597	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	2101	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	904	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	2772	C	O4'-C1'-N1	5.14	112.31	108.20
21	AA	682	G	C5'-C4'-C3'	-5.14	107.78	116.00
21	AA	787	A	C4-C5-C6	-5.14	114.43	117.00
21	AA	1278	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	74	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	903	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	957	C	N1-C2-O2	5.14	121.98	118.90
54	BA	2769	U	O4'-C1'-N1	5.14	112.31	108.20
25	BC	132	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
54	BA	774	G	N3-C4-C5	-5.14	126.03	128.60
54	BA	1015	U	C3'-C2'-C1'	5.14	105.61	101.50
54	BA	2211	A	C4-C5-C6	-5.14	114.43	117.00
24	A3	57	C	N3-C2-O2	-5.14	118.31	121.90
12	AM	111	PRO	C-N-CA	5.13	134.54	121.70
21	AA	183	C	C1'-O4'-C4'	-5.13	105.79	109.90
21	AA	346	G	C8-N9-C4	-5.13	104.35	106.40
22	A1	76	A	C5-C6-N1	5.13	120.27	117.70
54	BA	1741	C	O4'-C1'-N1	5.13	112.31	108.20
54	BA	1830	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	1845	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2395	C	N3-C2-O2	-5.13	118.31	121.90
21	AA	280	C	N1-C2-O2	5.13	121.98	118.90
54	BA	1403	A	C6-C5-N7	5.13	135.89	132.30
54	BA	1842	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	251	G	C5'-C4'-C3'	-5.13	107.79	116.00
21	AA	844	G	O4'-C1'-N9	5.13	112.31	108.20
21	AA	987	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	119	A	C6-C5-N7	5.13	135.89	132.30
54	BA	320	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	993	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1258	U	C5-C6-N1	-5.13	120.13	122.70
54	BA	1767	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1857	G	N3-C4-C5	-5.13	126.03	128.60
55	BB	115	A	C6-C5-N7	5.13	135.89	132.30
21	AA	931	C	N1-C2-O2	5.13	121.98	118.90
54	BA	366	C	N1-C2-O2	5.13	121.98	118.90
54	BA	869	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	900	A	C6-C5-N7	5.13	135.89	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1640	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	1290	G	N3-C2-N2	-5.13	116.31	119.90
54	BA	564	C	O4'-C1'-N1	5.13	112.30	108.20
54	BA	1611	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2307	G	N3-C4-C5	-5.13	126.04	128.60
54	BA	2429	G	N3-C2-N2	-5.13	116.31	119.90
22	A1	36	C	N1-C2-O2	5.13	121.98	118.90
54	BA	1068	G	O4'-C1'-N9	5.13	112.30	108.20
54	BA	1694	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	148	U	N3-C2-O2	-5.12	118.61	122.20
54	BA	695	G	C5-C6-N1	5.12	114.06	111.50
54	BA	2837	A	C6-C5-N7	5.12	135.89	132.30
21	AA	198	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	468	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1748	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1787	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	1030	U	C1'-O4'-C4'	-5.12	105.80	109.90
21	AA	1252	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	1295	U	N3-C2-O2	-5.12	118.61	122.20
24	A3	41	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	157	C	N1-C2-O2	5.12	121.97	118.90
54	BA	435	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1289	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1933	G	C8-N9-C4	-5.12	104.35	106.40
54	BA	2675	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2763	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2816	G	N3-C2-N2	-5.12	116.31	119.90
54	BA	252	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	514	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1945	G	C5-C6-N1	5.12	114.06	111.50
54	BA	540	C	N1-C2-O2	5.12	121.97	118.90
54	BA	766	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	832	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1886	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	2882	A	C6-C5-N7	5.12	135.88	132.30
54	BA	239	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	1172	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	1535	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2412	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2795	C	N1-C2-O2	5.12	121.97	118.90
21	AA	367	U	N3-C2-O2	-5.11	118.62	122.20
21	AA	755	G	N3-C2-N2	-5.11	116.32	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	880	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	289	G	O4'-C1'-N9	5.11	112.29	108.20
54	BA	647	G	O4'-C1'-N9	5.11	112.29	108.20
54	BA	1097	U	N3-C2-O2	-5.11	118.62	122.20
54	BA	1243	C	N1-C2-O2	5.11	121.97	118.90
54	BA	1269	A	C6-C5-N7	5.11	135.88	132.30
54	BA	1497	U	O4'-C1'-C2'	-5.11	100.69	105.80
54	BA	2300	C	N1-C2-O2	5.11	121.97	118.90
12	AM	89	ARG	NE-CZ-NH2	-5.11	117.74	120.30
54	BA	1510	G	C5'-C4'-O4'	5.11	115.23	109.10
54	BA	2279	G	C4'-C3'-C2'	-5.11	97.49	102.60
1	AB	224	ARG	NE-CZ-NH1	5.11	122.86	120.30
54	BA	163	C	N1-C2-O2	5.11	121.97	118.90
54	BA	2052	A	C4-C5-C6	-5.11	114.44	117.00
21	AA	388	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	1301	A	O4'-C1'-C2'	-5.11	100.69	105.80
54	BA	2029	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	2233	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	544	G	O4'-C1'-N9	5.11	112.29	108.20
54	BA	140	C	N3-C4-N4	-5.11	114.43	118.00
54	BA	513	A	C6-C5-N7	5.11	135.87	132.30
54	BA	1294	U	O4'-C1'-N1	5.11	112.28	108.20
54	BA	1447	C	C4'-C3'-C2'	-5.11	97.49	102.60
21	AA	690	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	277	G	C5-C6-N1	5.10	114.05	111.50
3	AD	187	ARG	NE-CZ-NH1	5.10	122.85	120.30
24	A3	3	C	N3-C2-O2	-5.10	118.33	121.90
54	BA	529	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2337	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	2501	C	C3'-C2'-C1'	5.10	105.58	101.50
51	B2	19	ARG	NE-CZ-NH1	5.10	122.85	120.30
54	BA	1236	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	1864	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	2102	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	2833	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	216	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	303	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	1465	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	1505	A	C6-C5-N7	5.10	135.87	132.30
54	BA	1809	A	C4-C5-C6	-5.10	114.45	117.00
21	AA	1150	A	C6-C5-N7	5.10	135.87	132.30
54	BA	1194	A	C4-C5-C6	-5.10	114.45	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2384	U	O4'-C1'-N1	5.10	112.28	108.20
14	AO	88	ARG	NE-CZ-NH1	5.09	122.85	120.30
21	AA	843	U	N3-C2-O2	-5.09	118.63	122.20
54	BA	61	C	O4'-C1'-N1	5.09	112.28	108.20
54	BA	2025	C	N1-C2-O2	5.09	121.96	118.90
54	BA	2149	U	O4'-C1'-N1	5.09	112.28	108.20
21	AA	1200	C	N3-C4-N4	-5.09	114.44	118.00
54	BA	814	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1312	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	2250	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	2823	A	C4-C5-C6	-5.09	114.45	117.00
21	AA	423	G	N3-C4-C5	-5.09	126.06	128.60
21	AA	883	C	N1-C2-O2	5.09	121.95	118.90
54	BA	633	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	995	C	N1-C2-O2	5.09	121.95	118.90
54	BA	2396	G	N1-C6-O6	-5.09	116.85	119.90
21	AA	846	G	O4'-C1'-N9	5.09	112.27	108.20
23	A2	90	U	C5-C6-N1	-5.09	120.16	122.70
54	BA	1843	C	N1-C2-O2	5.09	121.95	118.90
21	AA	758	C	N1-C2-O2	5.09	121.95	118.90
21	AA	869	G	N1-C6-O6	-5.09	116.85	119.90
54	BA	401	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	1097	U	O4'-C1'-C2'	-5.09	100.71	105.80
54	BA	2091	C	N1-C2-O2	5.09	121.95	118.90
54	BA	2304	G	O4'-C1'-N9	5.09	112.27	108.20
54	BA	2424	C	N1-C2-O2	5.09	121.95	118.90
54	BA	2881	U	C3'-C2'-C1'	5.09	105.57	101.50
21	AA	505	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	148	U	O4'-C1'-N1	5.08	112.27	108.20
54	BA	1706	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2589	A	C3'-C2'-C1'	5.08	105.57	101.50
24	A3	17	C	N1-C2-O2	5.08	121.95	118.90
31	BI	133	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
54	BA	2066	C	O4'-C1'-N1	5.08	112.27	108.20
54	BA	2092	U	N3-C2-O2	-5.08	118.64	122.20
21	AA	882	C	N3-C4-N4	-5.08	114.44	118.00
21	AA	1132	C	N1-C2-O2	5.08	121.95	118.90
54	BA	80	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	764	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	826	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	1818	U	O4'-C1'-N1	5.08	112.27	108.20
54	BA	2658	C	O4'-C1'-N1	5.08	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	634	C	N3-C4-C5	5.08	123.93	121.90
54	BA	904	G	C5-C6-N1	5.08	114.04	111.50
54	BA	2806	C	O4'-C1'-N1	5.08	112.26	108.20
21	AA	362	G	N3-C4-C5	-5.08	126.06	128.60
21	AA	555	U	O4'-C1'-N1	5.08	112.26	108.20
21	AA	817	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1614	A	O4'-C1'-N9	5.08	112.26	108.20
54	BA	1798	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	2117	A	C3'-C2'-C1'	5.08	105.56	101.50
55	BB	19	C	C5'-C4'-O4'	5.08	115.19	109.10
21	AA	58	C	N1-C2-O2	5.08	121.95	118.90
21	AA	686	U	C1'-O4'-C4'	-5.08	105.84	109.90
21	AA	1332	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	1399	C	C3'-C2'-C1'	5.08	105.56	101.50
54	BA	1691	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1905	C	N1-C2-O2	5.08	121.95	118.90
21	AA	1131	G	C5-C6-N1	5.08	114.04	111.50
24	A3	75	C	C5'-C4'-C3'	-5.08	107.88	116.00
54	BA	331	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	828	U	N3-C2-O2	-5.08	118.65	122.20
54	BA	2604	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	2770	G	N3-C2-N2	-5.08	116.35	119.90
55	BB	28	C	O4'-C1'-N1	5.08	112.26	108.20
21	AA	232	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1054	A	C6-C5-N7	5.07	135.85	132.30
54	BA	1412	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	2111	U	C5-C6-N1	-5.07	120.16	122.70
54	BA	229	C	N3-C4-C5	5.07	123.93	121.90
21	AA	970	C	N1-C2-O2	5.07	121.94	118.90
54	BA	228	C	N3-C2-O2	-5.07	118.35	121.90
54	BA	2609	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	2719	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	808	C	N1-C2-O2	5.07	121.94	118.90
21	AA	1098	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1001	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	1123	C	O4'-C1'-N1	5.07	112.26	108.20
21	AA	415	A	O4'-C1'-N9	5.07	112.25	108.20
21	AA	1358	U	C5-C6-N1	-5.07	120.17	122.70
55	BB	86	G	N1-C6-O6	-5.07	116.86	119.90
8	AI	79	ARG	NE-CZ-NH1	5.07	122.83	120.30
21	AA	611	C	N1-C2-O2	5.07	121.94	118.90
24	A3	14	A	C4-C5-C6	-5.07	114.47	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BK	108	ARG	NE-CZ-NH1	5.07	122.83	120.30
54	BA	156	A	C6-C5-N7	5.07	135.85	132.30
54	BA	433	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1093	G	C5-C6-N1	5.07	114.03	111.50
54	BA	1647	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	2001	C	N3-C2-O2	-5.07	118.36	121.90
54	BA	2755	C	N1-C2-O2	5.07	121.94	118.90
21	AA	1487	G	N3-C2-N2	-5.06	116.36	119.90
54	BA	1524	G	C5-C6-N1	5.06	114.03	111.50
54	BA	2655	G	C3'-C2'-C1'	-5.06	97.45	101.50
21	AA	458	U	C5-C6-N1	-5.06	120.17	122.70
21	AA	717	U	O4'-C1'-N1	5.06	112.25	108.20
21	AA	1278	G	N3-C4-C5	-5.06	126.07	128.60
54	BA	496	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	650	C	N1-C2-O2	5.06	121.94	118.90
54	BA	669	G	C3'-C2'-C1'	5.06	105.55	101.50
54	BA	1439	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	360	G	C5-C6-N1	5.06	114.03	111.50
54	BA	2641	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	2752	C	O4'-C1'-N1	5.06	112.25	108.20
21	AA	184	G	N3-C4-C5	-5.06	126.07	128.60
54	BA	2015	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	173	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	191	G	N3-C4-C5	-5.05	126.07	128.60
25	BC	237	ARG	NE-CZ-NH1	5.05	122.83	120.30
54	BA	669	G	N3-C4-C5	-5.05	126.07	128.60
54	BA	706	A	C6-C5-N7	5.05	135.84	132.30
54	BA	1288	G	C1'-O4'-C4'	-5.05	105.86	109.90
54	BA	1798	U	C5-C6-N1	-5.05	120.17	122.70
54	BA	1956	U	N3-C2-O2	-5.05	118.66	122.20
21	AA	204	G	C5-C6-N1	5.05	114.03	111.50
21	AA	377	G	N3-C4-C5	-5.05	126.07	128.60
21	AA	699	C	N3-C2-O2	-5.05	118.36	121.90
21	AA	889	A	C6-C5-N7	5.05	135.84	132.30
24	A3	75	C	N3-C4-N4	-5.05	114.46	118.00
54	BA	1752	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1393	U	N3-C2-O2	-5.05	118.67	122.20
21	AA	1531	A	C6-C5-N7	5.05	135.84	132.30
23	A2	84	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	550	C	N1-C2-O2	5.05	121.93	118.90
54	BA	717	C	N1-C2-O2	5.05	121.93	118.90
54	BA	487	C	N3-C4-C5	5.05	123.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1527	G	O4'-C1'-N9	5.05	112.24	108.20
55	BB	98	G	C5-C6-N1	5.05	114.02	111.50
21	AA	110	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1027	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1313	U	N3-C2-O2	-5.05	118.67	122.20
24	A3	1	C	N1-C2-O2	5.05	121.93	118.90
54	BA	127	A	C4-C5-C6	-5.05	114.48	117.00
54	BA	1225	G	O4'-C1'-N9	5.05	112.24	108.20
54	BA	2875	C	C1'-O4'-C4'	-5.05	105.86	109.90
21	AA	339	C	O4'-C1'-N1	5.04	112.24	108.20
21	AA	790	A	C3'-C2'-C1'	5.04	105.54	101.50
21	AA	1407	C	N1-C2-O2	5.04	121.93	118.90
27	BE	61	ARG	NE-CZ-NH1	5.04	122.82	120.30
54	BA	1166	G	C5-C6-N1	5.04	114.02	111.50
54	BA	1871	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	2333	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	561	U	N3-C2-O2	-5.04	118.67	122.20
21	AA	724	G	N1-C6-O6	-5.04	116.87	119.90
24	A3	77	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	590	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1207	C	N3-C2-O2	-5.04	118.37	121.90
55	BB	66	A	C6-C5-N7	5.04	135.83	132.30
21	AA	453	G	N3-C4-C5	-5.04	126.08	128.60
22	A1	60	C	N3-C4-N4	-5.04	114.47	118.00
54	BA	1732	C	N3-C4-C5	5.04	123.92	121.90
54	BA	1933	G	N3-C4-C5	-5.04	126.08	128.60
9	AJ	68	ARG	NE-CZ-NH1	5.04	122.82	120.30
54	BA	1790	C	N3-C2-O2	-5.04	118.37	121.90
54	BA	2503	A	P-O3'-C3'	5.04	125.75	119.70
21	AA	434	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	571	U	N3-C2-O2	-5.04	118.67	122.20
21	AA	856	C	N1-C2-O2	5.04	121.92	118.90
54	BA	285	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	443	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1876	A	C4-C5-C6	-5.04	114.48	117.00
29	BG	68	ARG	NE-CZ-NH2	-5.04	117.78	120.30
54	BA	485	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	828	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	893	C	O4'-C1'-N1	5.04	112.23	108.20
55	BB	58	A	C6-C5-N7	5.04	135.83	132.30
21	AA	290	C	N1-C2-O2	5.04	121.92	118.90
54	BA	452	G	C5'-C4'-O4'	5.04	115.14	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	681	G	C5-C6-N1	5.04	114.02	111.50
54	BA	855	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	1906	G	O4'-C1'-N9	5.04	112.23	108.20
21	AA	1126	U	O4'-C1'-N1	5.03	112.23	108.20
54	BA	1060	U	O4'-C1'-N1	5.03	112.23	108.20
54	BA	1139	G	C5-C6-N1	5.03	114.02	111.50
54	BA	1812	U	C4'-C3'-C2'	-5.03	97.57	102.60
54	BA	2513	A	O4'-C1'-N9	5.03	112.23	108.20
54	BA	2626	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2723	C	O4'-C1'-N1	5.03	112.23	108.20
54	BA	2737	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	2879	A	C4-C5-C6	-5.03	114.48	117.00
21	AA	638	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	236	C	O4'-C1'-N1	5.03	112.23	108.20
54	BA	651	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	1967	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2591	C	N3-C4-C5	5.03	123.91	121.90
19	AT	24	ARG	NE-CZ-NH1	5.03	122.81	120.30
21	AA	374	A	C4-C5-C6	-5.03	114.48	117.00
21	AA	874	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	398	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1230	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1938	A	O4'-C1'-N9	5.03	112.22	108.20
21	AA	593	U	O4'-C1'-N1	5.03	112.22	108.20
21	AA	841	C	N1-C2-O2	5.03	121.92	118.90
54	BA	48	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	222	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	272	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	946	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1319	C	N1-C2-O2	5.03	121.92	118.90
54	BA	1679	A	C4'-C3'-C2'	-5.03	97.57	102.60
54	BA	1858	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	2554	U	O4'-C1'-N1	5.03	112.22	108.20
21	AA	32	A	C4-C5-C6	-5.03	114.49	117.00
21	AA	1113	C	N1-C2-O2	5.03	121.92	118.90
54	BA	249	C	N3-C4-C5	5.03	123.91	121.90
54	BA	1702	G	N1-C6-O6	-5.03	116.89	119.90
54	BA	2199	A	O4'-C1'-N9	5.03	112.22	108.20
21	AA	699	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1401	G	N3-C2-N2	-5.02	116.38	119.90
54	BA	2023	C	N3-C2-O2	-5.02	118.38	121.90
21	AA	314	C	N1-C2-O2	5.02	121.91	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	739	C	N1-C2-O2	5.02	121.91	118.90
54	BA	457	A	C3'-C2'-C1'	-5.02	97.48	101.50
54	BA	487	C	N1-C2-O2	5.02	121.91	118.90
54	BA	998	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1442	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1706	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	2403	C	N1-C2-O2	5.02	121.91	118.90
3	AD	46	ARG	NE-CZ-NH1	5.02	122.81	120.30
21	AA	881	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	547	A	N9-C1'-C2'	-5.02	106.48	112.00
54	BA	2644	G	O4'-C4'-C3'	5.02	110.12	106.10
54	BA	2671	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2739	U	O4'-C1'-N1	5.02	112.22	108.20
55	BB	65	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	31	G	O4'-C1'-N9	5.02	112.22	108.20
21	AA	569	C	N3-C4-C5	5.02	123.91	121.90
21	AA	1278	G	C3'-C2'-C1'	5.02	105.52	101.50
54	BA	41	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	103	A	C6-C5-N7	5.02	135.81	132.30
54	BA	507	A	O4'-C1'-N9	5.02	112.22	108.20
54	BA	2238	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2767	C	N1-C2-O2	5.02	121.91	118.90
21	AA	13	U	O4'-C4'-C3'	5.02	110.11	106.10
23	A2	82	A	C5'-C4'-C3'	-5.02	107.97	116.00
54	BA	803	U	N1-C2-N3	5.02	117.91	114.90
54	BA	829	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	1992	G	N3-C2-N2	-5.02	116.39	119.90
54	BA	2018	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2722	G	O4'-C1'-N9	5.02	112.21	108.20
54	BA	250	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	1923	U	C4'-C3'-C2'	-5.02	97.58	102.60
54	BA	2219	U	O4'-C1'-N1	5.02	112.21	108.20
55	BB	50	A	O4'-C1'-N9	5.02	112.21	108.20
21	AA	1198	G	N9-C4-C5	5.01	107.41	105.40
54	BA	294	A	C6-C5-N7	5.01	135.81	132.30
54	BA	723	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1821	A	C6-C5-N7	5.01	135.81	132.30
21	AA	559	A	O4'-C1'-N9	5.01	112.21	108.20
54	BA	121	G	C3'-C2'-C1'	5.01	105.51	101.50
54	BA	1026	G	O4'-C1'-N9	5.01	112.21	108.20
54	BA	634	C	N1-C2-O2	5.01	121.91	118.90
54	BA	673	C	N1-C2-O2	5.01	121.91	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1297	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1640	A	C5'-C4'-O4'	5.01	115.11	109.10
54	BA	2287	A	C2-N3-C4	5.01	113.11	110.60
54	BA	2494	G	C5-C6-N1	5.01	114.01	111.50
54	BA	2619	C	N1-C2-O2	5.01	121.91	118.90
21	AA	839	C	N1-C2-O2	5.01	121.91	118.90
23	A2	80	C	C5'-C4'-C3'	-5.01	107.98	116.00
28	BF	147	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	177	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	446	G	O4'-C4'-C3'	5.01	110.11	106.10
54	BA	1389	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	139	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	1065	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	1532	A	C6-C5-N7	5.01	135.81	132.30
54	BA	2324	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	1284	C	C6-N1-C2	-5.01	118.30	120.30
23	A2	84	G	N3-C2-N2	-5.01	116.39	119.90
29	BG	148	ARG	NE-CZ-NH1	5.01	122.80	120.30
54	BA	190	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	1272	A	C6-C5-N7	5.01	135.80	132.30
54	BA	1817	G	N3-C2-N2	-5.01	116.40	119.90
54	BA	2342	C	C4'-C3'-C2'	-5.01	97.59	102.60
54	BA	2607	G	C8-N9-C4	-5.01	104.40	106.40
54	BA	2888	C	N1-C2-O2	5.01	121.90	118.90
21	AA	171	A	C6-C5-N7	5.00	135.80	132.30
21	AA	752	G	O4'-C1'-N9	5.00	112.20	108.20
21	AA	1046	A	C4-C5-C6	-5.00	114.50	117.00
54	BA	1124	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	1493	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	1051	C	N1-C2-O2	5.00	121.90	118.90
24	A3	59	A	C1'-O4'-C4'	-5.00	105.90	109.90
54	BA	1	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	558	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	901	C	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1808	A	C4-C5-C6	-5.00	114.50	117.00
54	BA	1973	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	2903	U	N3-C2-O2	-5.00	118.70	122.20
21	AA	495	A	C4-C5-C6	-5.00	114.50	117.00
21	AA	945	G	N3-C4-N9	5.00	129.00	126.00
54	BA	33	C	N3-C2-O2	-5.00	118.40	121.90
54	BA	193	U	N3-C2-O2	-5.00	118.70	122.20
54	BA	331	C	N3-C4-C5	5.00	123.90	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
54	BA	1145	C	C5'-C4'-O4'	5.00	115.10	109.10
54	BA	1180	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1217	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1257	C	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1295	C	N1-C2-O2	5.00	121.90	118.90
54	BA	2730	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (1121) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	10	G	Sidechain
22	A1	16	C	Sidechain
22	A1	18	G	Sidechain
22	A1	2	G	Sidechain
22	A1	21	A	Sidechain
22	A1	24	G	Sidechain
22	A1	27	C	Sidechain
22	A1	45	G	Sidechain
22	A1	52	G	Sidechain
22	A1	61	C	Sidechain
22	A1	64	U	Sidechain
22	A1	67	U	Sidechain
22	A1	72	C	Sidechain
22	A1	76	A	Sidechain
22	A1	9	A	Sidechain
23	A2	80	C	Sidechain
23	A2	86	U	Sidechain
23	A2	88	U	Sidechain
23	A2	90	U	Sidechain
23	A2	91	A	Sidechain
24	A3	1	C	Sidechain
24	A3	2	G	Sidechain
24	A3	34	U	Sidechain
24	A3	44	A	Sidechain
24	A3	58	A	Sidechain
24	A3	60	A	Sidechain
24	A3	69	C	Sidechain
24	A3	72	C	Sidechain
24	A3	73	A	Sidechain
21	AA	10	A	Sidechain
21	AA	1010	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1012	A	Sidechain
21	AA	1013	G	Sidechain
21	AA	1014	A	Sidechain
21	AA	1018	G	Sidechain
21	AA	1025	U	Sidechain
21	AA	1027	C	Sidechain
21	AA	1029	U	Sidechain
21	AA	1033	G	Sidechain
21	AA	1036	A	Sidechain
21	AA	1043	G	Sidechain
21	AA	1045	C	Sidechain
21	AA	1046	A	Sidechain
21	AA	105	G	Sidechain
21	AA	1066	C	Sidechain
21	AA	1077	G	Sidechain
21	AA	108	G	Sidechain
21	AA	109	A	Sidechain
21	AA	1092	A	Sidechain
21	AA	1093	A	Sidechain
21	AA	1095	U	Sidechain
21	AA	1097	C	Sidechain
21	AA	1100	C	Sidechain
21	AA	1107	C	Sidechain
21	AA	1110	A	Sidechain
21	AA	1115	U	Sidechain
21	AA	1120	C	Sidechain
21	AA	1124	G	Sidechain
21	AA	1125	U	Sidechain
21	AA	1128	C	Sidechain
21	AA	1131	G	Sidechain
21	AA	1135	U	Sidechain
21	AA	1139	G	Sidechain
21	AA	114	U	Sidechain
21	AA	1142	G	Sidechain
21	AA	1144	G	Sidechain
21	AA	1145	A	Sidechain
21	AA	1155	A	Sidechain
21	AA	1157	A	Sidechain
21	AA	116	A	Sidechain
21	AA	1160	G	Sidechain
21	AA	1161	C	Sidechain
21	AA	1163	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	117	G	Sidechain
21	AA	1172	C	Sidechain
21	AA	1174	G	Sidechain
21	AA	1181	G	Sidechain
21	AA	1183	U	Sidechain
21	AA	1185	G	Sidechain
21	AA	1187	G	Sidechain
21	AA	1194	U	Sidechain
21	AA	12	U	Sidechain
21	AA	1200	C	Sidechain
21	AA	1207	G	Sidechain
21	AA	1211	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1215	G	Sidechain
21	AA	1216	A	Sidechain
21	AA	1221	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1228	C	Sidechain
21	AA	1235	U	Sidechain
21	AA	124	C	Sidechain
21	AA	1244	G	Sidechain
21	AA	1248	A	Sidechain
21	AA	1250	A	Sidechain
21	AA	1258	G	Sidechain
21	AA	126	G	Sidechain
21	AA	1264	U	Sidechain
21	AA	1265	C	Sidechain
21	AA	1266	G	Sidechain
21	AA	1272	G	Sidechain
21	AA	1278	G	Sidechain
21	AA	1288	A	Sidechain
21	AA	1295	U	Sidechain
21	AA	13	U	Sidechain
21	AA	1301	U	Sidechain
21	AA	1305	G	Sidechain
21	AA	131	A	Sidechain
21	AA	1315	U	Sidechain
21	AA	1325	C	Sidechain
21	AA	1326	U	Sidechain
21	AA	1327	C	Sidechain
21	AA	133	U	Sidechain
21	AA	1331	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1333	A	Sidechain
21	AA	1336	C	Sidechain
21	AA	1338	G	Sidechain
21	AA	134	G	Sidechain
21	AA	1343	G	Sidechain
21	AA	1345	U	Sidechain
21	AA	135	C	Sidechain
21	AA	1358	U	Sidechain
21	AA	1359	C	Sidechain
21	AA	1364	U	Sidechain
21	AA	1370	G	Sidechain
21	AA	1379	G	Sidechain
21	AA	1383	C	Sidechain
21	AA	1385	G	Sidechain
21	AA	139	A	Sidechain
21	AA	1396	A	Sidechain
21	AA	1397	C	Sidechain
21	AA	1400	C	Sidechain
21	AA	1404	C	Sidechain
21	AA	1405	G	Sidechain
21	AA	1408	A	Sidechain
21	AA	1411	C	Sidechain
21	AA	1412	C	Sidechain
21	AA	1416	G	Sidechain
21	AA	1422	G	Sidechain
21	AA	143	A	Sidechain
21	AA	1435	G	Sidechain
21	AA	1436	U	Sidechain
21	AA	1439	G	Sidechain
21	AA	1447	A	Sidechain
21	AA	1448	C	Sidechain
21	AA	1451	U	Sidechain
21	AA	1459	G	Sidechain
21	AA	146	G	Sidechain
21	AA	1460	C	Sidechain
21	AA	1466	C	Sidechain
21	AA	1470	U	Sidechain
21	AA	1472	U	Sidechain
21	AA	1474	U	Sidechain
21	AA	1478	U	Sidechain
21	AA	1483	A	Sidechain
21	AA	1489	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1493	A	Sidechain
21	AA	1498	U	Sidechain
21	AA	1502	A	Sidechain
21	AA	1503	A	Sidechain
21	AA	1508	A	Sidechain
21	AA	1509	C	Sidechain
21	AA	1512	U	Sidechain
21	AA	1514	G	Sidechain
21	AA	1516	G	Sidechain
21	AA	1517	G	Sidechain
21	AA	1518	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1521	C	Sidechain
21	AA	1522	U	Sidechain
21	AA	1526	G	Sidechain
21	AA	1527	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1532	U	Sidechain
21	AA	1533	C	Sidechain
21	AA	1534	A	Sidechain
21	AA	159	G	Sidechain
21	AA	164	G	Sidechain
21	AA	165	G	Sidechain
21	AA	168	G	Sidechain
21	AA	171	A	Sidechain
21	AA	179	A	Sidechain
21	AA	184	G	Sidechain
21	AA	186	C	Sidechain
21	AA	189	A	Sidechain
21	AA	19	A	Sidechain
21	AA	197	A	Sidechain
21	AA	200	G	Sidechain
21	AA	202	G	Sidechain
21	AA	215	C	Sidechain
21	AA	227	G	Sidechain
21	AA	234	C	Sidechain
21	AA	236	A	Sidechain
21	AA	237	G	Sidechain
21	AA	246	A	Sidechain
21	AA	249	U	Sidechain
21	AA	251	G	Sidechain
21	AA	252	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	254	G	Sidechain
21	AA	26	A	Sidechain
21	AA	261	U	Sidechain
21	AA	267	C	Sidechain
21	AA	269	C	Sidechain
21	AA	27	G	Sidechain
21	AA	270	A	Sidechain
21	AA	271	C	Sidechain
21	AA	272	C	Sidechain
21	AA	274	A	Sidechain
21	AA	280	C	Sidechain
21	AA	282	A	Sidechain
21	AA	297	G	Sidechain
21	AA	299	G	Sidechain
21	AA	301	G	Sidechain
21	AA	305	G	Sidechain
21	AA	309	A	Sidechain
21	AA	324	G	Sidechain
21	AA	325	A	Sidechain
21	AA	346	G	Sidechain
21	AA	347	G	Sidechain
21	AA	348	G	Sidechain
21	AA	349	A	Sidechain
21	AA	352	C	Sidechain
21	AA	353	A	Sidechain
21	AA	354	G	Sidechain
21	AA	359	G	Sidechain
21	AA	372	C	Sidechain
21	AA	377	G	Sidechain
21	AA	380	G	Sidechain
21	AA	390	U	Sidechain
21	AA	393	A	Sidechain
21	AA	395	C	Sidechain
21	AA	396	C	Sidechain
21	AA	400	C	Sidechain
21	AA	403	C	Sidechain
21	AA	404	G	Sidechain
21	AA	408	A	Sidechain
21	AA	409	U	Sidechain
21	AA	430	A	Sidechain
21	AA	446	G	Sidechain
21	AA	450	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	452	A	Sidechain
21	AA	464	U	Sidechain
21	AA	474	G	Sidechain
21	AA	485	U	Sidechain
21	AA	494	G	Sidechain
21	AA	496	A	Sidechain
21	AA	497	G	Sidechain
21	AA	499	A	Sidechain
21	AA	5	U	Sidechain
21	AA	501	C	Sidechain
21	AA	505	G	Sidechain
21	AA	506	G	Sidechain
21	AA	51	A	Sidechain
21	AA	514	C	Sidechain
21	AA	515	G	Sidechain
21	AA	517	G	Sidechain
21	AA	519	C	Sidechain
21	AA	522	C	Sidechain
21	AA	523	A	Sidechain
21	AA	525	C	Sidechain
21	AA	527	G	Sidechain
21	AA	529	G	Sidechain
21	AA	533	A	Sidechain
21	AA	535	A	Sidechain
21	AA	539	A	Sidechain
21	AA	540	G	Sidechain
21	AA	562	U	Sidechain
21	AA	565	U	Sidechain
21	AA	566	G	Sidechain
21	AA	571	U	Sidechain
21	AA	581	G	Sidechain
21	AA	582	C	Sidechain
21	AA	583	A	Sidechain
21	AA	589	U	Sidechain
21	AA	590	U	Sidechain
21	AA	6	G	Sidechain
21	AA	60	A	Sidechain
21	AA	600	A	Sidechain
21	AA	601	G	Sidechain
21	AA	608	A	Sidechain
21	AA	610	U	Sidechain
21	AA	616	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	618	C	Sidechain
21	AA	619	U	Sidechain
21	AA	63	C	Sidechain
21	AA	632	U	Sidechain
21	AA	637	C	Sidechain
21	AA	641	U	Sidechain
21	AA	650	G	Sidechain
21	AA	658	C	Sidechain
21	AA	66	A	Sidechain
21	AA	664	G	Sidechain
21	AA	667	G	Sidechain
21	AA	671	G	Sidechain
21	AA	676	A	Sidechain
21	AA	677	U	Sidechain
21	AA	678	U	Sidechain
21	AA	681	A	Sidechain
21	AA	686	U	Sidechain
21	AA	688	G	Sidechain
21	AA	691	G	Sidechain
21	AA	693	G	Sidechain
21	AA	701	U	Sidechain
21	AA	705	G	Sidechain
21	AA	708	C	Sidechain
21	AA	710	G	Sidechain
21	AA	714	G	Sidechain
21	AA	718	A	Sidechain
21	AA	721	G	Sidechain
21	AA	722	G	Sidechain
21	AA	724	G	Sidechain
21	AA	725	G	Sidechain
21	AA	727	G	Sidechain
21	AA	728	A	Sidechain
21	AA	741	G	Sidechain
21	AA	743	A	Sidechain
21	AA	744	C	Sidechain
21	AA	752	G	Sidechain
21	AA	759	A	Sidechain
21	AA	76	G	Sidechain
21	AA	763	G	Sidechain
21	AA	768	A	Sidechain
21	AA	778	G	Sidechain
21	AA	789	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	79	G	Sidechain
21	AA	791	G	Sidechain
21	AA	794	A	Sidechain
21	AA	8	A	Sidechain
21	AA	80	A	Sidechain
21	AA	808	C	Sidechain
21	AA	815	A	Sidechain
21	AA	816	A	Sidechain
21	AA	820	U	Sidechain
21	AA	823	C	Sidechain
21	AA	824	G	Sidechain
21	AA	826	C	Sidechain
21	AA	83	C	Sidechain
21	AA	833	G	Sidechain
21	AA	838	G	Sidechain
21	AA	84	U	Sidechain
21	AA	843	U	Sidechain
21	AA	847	G	Sidechain
21	AA	855	U	Sidechain
21	AA	857	C	Sidechain
21	AA	86	G	Sidechain
21	AA	862	C	Sidechain
21	AA	865	A	Sidechain
21	AA	869	G	Sidechain
21	AA	888	G	Sidechain
21	AA	889	A	Sidechain
21	AA	891	U	Sidechain
21	AA	892	A	Sidechain
21	AA	895	G	Sidechain
21	AA	90	C	Sidechain
21	AA	900	A	Sidechain
21	AA	903	G	Sidechain
21	AA	906	A	Sidechain
21	AA	91	U	Sidechain
21	AA	916	U	Sidechain
21	AA	920	U	Sidechain
21	AA	922	G	Sidechain
21	AA	925	G	Sidechain
21	AA	93	U	Sidechain
21	AA	931	C	Sidechain
21	AA	932	C	Sidechain
21	AA	939	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	946	A	Sidechain
21	AA	947	G	Sidechain
21	AA	951	G	Sidechain
21	AA	952	U	Sidechain
21	AA	955	U	Sidechain
21	AA	961	U	Sidechain
21	AA	962	C	Sidechain
21	AA	963	G	Sidechain
21	AA	966	G	Sidechain
21	AA	969	A	Sidechain
21	AA	977	A	Sidechain
21	AA	979	C	Sidechain
21	AA	982	U	Sidechain
21	AA	983	A	Sidechain
21	AA	984	C	Sidechain
21	AA	986	U	Sidechain
21	AA	987	G	Sidechain
21	AA	991	U	Sidechain
21	AA	995	C	Sidechain
21	AA	997	U	Sidechain
10	AK	115	ILE	Peptide
50	B1	48	TYR	Sidechain
54	BA	10	A	Sidechain
54	BA	1000	A	Sidechain
54	BA	1005	C	Sidechain
54	BA	1012	U	Sidechain
54	BA	1013	C	Sidechain
54	BA	1014	A	Sidechain
54	BA	1016	G	Sidechain
54	BA	102	U	Sidechain
54	BA	1025	G	Sidechain
54	BA	1031	G	Sidechain
54	BA	1036	G	Sidechain
54	BA	1042	G	Sidechain
54	BA	105	C	Sidechain
54	BA	1055	G	Sidechain
54	BA	1061	U	Sidechain
54	BA	1062	G	Sidechain
54	BA	1071	G	Sidechain
54	BA	1074	G	Sidechain
54	BA	1075	C	Sidechain
54	BA	1076	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1078	U	Sidechain
54	BA	1079	C	Sidechain
54	BA	1080	A	Sidechain
54	BA	1082	U	Sidechain
54	BA	1083	U	Sidechain
54	BA	1087	G	Sidechain
54	BA	1091	G	Sidechain
54	BA	1094	U	Sidechain
54	BA	1096	A	Sidechain
54	BA	1098	A	Sidechain
54	BA	11	C	Sidechain
54	BA	1106	G	Sidechain
54	BA	1107	G	Sidechain
54	BA	1116	G	Sidechain
54	BA	1121	C	Sidechain
54	BA	1133	A	Sidechain
54	BA	1135	C	Sidechain
54	BA	1138	G	Sidechain
54	BA	1139	G	Sidechain
54	BA	114	U	Sidechain
54	BA	1142	A	Sidechain
54	BA	115	C	Sidechain
54	BA	1153	C	Sidechain
54	BA	1158	C	Sidechain
54	BA	1160	G	Sidechain
54	BA	1162	G	Sidechain
54	BA	1170	C	Sidechain
54	BA	1181	U	Sidechain
54	BA	1182	G	Sidechain
54	BA	1186	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1200	C	Sidechain
54	BA	1209	U	Sidechain
54	BA	1212	G	Sidechain
54	BA	1220	G	Sidechain
54	BA	1221	C	Sidechain
54	BA	1223	G	Sidechain
54	BA	1229	C	Sidechain
54	BA	1236	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	124	G	Sidechain
54	BA	1241	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1244	A	Sidechain
54	BA	1250	G	Sidechain
54	BA	1257	C	Sidechain
54	BA	1259	G	Sidechain
54	BA	1265	A	Sidechain
54	BA	1266	G	Sidechain
54	BA	1267	U	Sidechain
54	BA	1271	G	Sidechain
54	BA	1272	A	Sidechain
54	BA	1275	A	Sidechain
54	BA	1277	G	Sidechain
54	BA	1279	G	Sidechain
54	BA	1280	G	Sidechain
54	BA	1285	A	Sidechain
54	BA	129	C	Sidechain
54	BA	1296	G	Sidechain
54	BA	1300	G	Sidechain
54	BA	1305	C	Sidechain
54	BA	1311	G	Sidechain
54	BA	1315	C	Sidechain
54	BA	1316	U	Sidechain
54	BA	1319	C	Sidechain
54	BA	132	G	Sidechain
54	BA	1324	G	Sidechain
54	BA	1329	U	Sidechain
54	BA	1330	C	Sidechain
54	BA	1332	G	Sidechain
54	BA	1334	G	Sidechain
54	BA	134	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1343	G	Sidechain
54	BA	1346	G	Sidechain
54	BA	1355	G	Sidechain
54	BA	1356	G	Sidechain
54	BA	1361	G	Sidechain
54	BA	1364	G	Sidechain
54	BA	1367	A	Sidechain
54	BA	1374	G	Sidechain
54	BA	1381	G	Sidechain
54	BA	1387	A	Sidechain
54	BA	1396	U	Sidechain
54	BA	1398	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	14	A	Sidechain
54	BA	1400	U	Sidechain
54	BA	1402	U	Sidechain
54	BA	1403	A	Sidechain
54	BA	1404	C	Sidechain
54	BA	1407	G	Sidechain
54	BA	141	G	Sidechain
54	BA	1417	C	Sidechain
54	BA	1424	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1426	G	Sidechain
54	BA	1427	A	Sidechain
54	BA	143	C	Sidechain
54	BA	1430	G	Sidechain
54	BA	1439	A	Sidechain
54	BA	1442	U	Sidechain
54	BA	1445	G	Sidechain
54	BA	1446	C	Sidechain
54	BA	1460	U	Sidechain
54	BA	1465	G	Sidechain
54	BA	1468	U	Sidechain
54	BA	1471	G	Sidechain
54	BA	1477	A	Sidechain
54	BA	1479	G	Sidechain
54	BA	1484	U	Sidechain
54	BA	1488	C	Sidechain
54	BA	1492	G	Sidechain
54	BA	1493	C	Sidechain
54	BA	1494	A	Sidechain
54	BA	1495	A	Sidechain
54	BA	1498	C	Sidechain
54	BA	1500	G	Sidechain
54	BA	1508	A	Sidechain
54	BA	1512	C	Sidechain
54	BA	1513	U	Sidechain
54	BA	152	A	Sidechain
54	BA	1524	G	Sidechain
54	BA	1529	G	Sidechain
54	BA	153	U	Sidechain
54	BA	1542	U	Sidechain
54	BA	1546	G	Sidechain
54	BA	1548	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1551	A	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1567	G	Sidechain
54	BA	1575	C	Sidechain
54	BA	1580	A	Sidechain
54	BA	1585	C	Sidechain
54	BA	1587	G	Sidechain
54	BA	1593	A	Sidechain
54	BA	1594	U	Sidechain
54	BA	1599	U	Sidechain
54	BA	1606	C	Sidechain
54	BA	1607	C	Sidechain
54	BA	1610	A	Sidechain
54	BA	1618	A	Sidechain
54	BA	1628	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1642	G	Sidechain
54	BA	1646	C	Sidechain
54	BA	1657	U	Sidechain
54	BA	1659	G	Sidechain
54	BA	1669	A	Sidechain
54	BA	1671	U	Sidechain
54	BA	1672	A	Sidechain
54	BA	1678	A	Sidechain
54	BA	168	G	Sidechain
54	BA	1681	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1687	G	Sidechain
54	BA	1692	U	Sidechain
54	BA	1695	G	Sidechain
54	BA	1698	A	Sidechain
54	BA	17	G	Sidechain
54	BA	1705	A	Sidechain
54	BA	1706	C	Sidechain
54	BA	1707	G	Sidechain
54	BA	1708	C	Sidechain
54	BA	1709	U	Sidechain
54	BA	1717	A	Sidechain
54	BA	1723	G	Sidechain
54	BA	1724	G	Sidechain
54	BA	1727	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1729	U	Sidechain
54	BA	1731	G	Sidechain
54	BA	1732	C	Sidechain
54	BA	1736	U	Sidechain
54	BA	1738	G	Sidechain
54	BA	174	U	Sidechain
54	BA	1748	C	Sidechain
54	BA	1749	A	Sidechain
54	BA	1752	C	Sidechain
54	BA	1753	G	Sidechain
54	BA	1757	A	Sidechain
54	BA	1760	C	Sidechain
54	BA	1765	U	Sidechain
54	BA	177	G	Sidechain
54	BA	1772	A	Sidechain
54	BA	1774	C	Sidechain
54	BA	1779	U	Sidechain
54	BA	178	G	Sidechain
54	BA	1781	U	Sidechain
54	BA	1784	A	Sidechain
54	BA	1788	C	Sidechain
54	BA	1790	C	Sidechain
54	BA	1802	A	Sidechain
54	BA	1805	A	Sidechain
54	BA	1808	A	Sidechain
54	BA	1811	G	Sidechain
54	BA	1812	U	Sidechain
54	BA	1817	G	Sidechain
54	BA	1818	U	Sidechain
54	BA	1820	U	Sidechain
54	BA	1824	G	Sidechain
54	BA	1828	G	Sidechain
54	BA	183	C	Sidechain
54	BA	1830	C	Sidechain
54	BA	1831	G	Sidechain
54	BA	1833	C	Sidechain
54	BA	1834	U	Sidechain
54	BA	1842	G	Sidechain
54	BA	1845	G	Sidechain
54	BA	1849	G	Sidechain
54	BA	1860	G	Sidechain
54	BA	1865	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1869	G	Sidechain
54	BA	1870	C	Sidechain
54	BA	1878	G	Sidechain
54	BA	1882	U	Sidechain
54	BA	1885	A	Sidechain
54	BA	1893	C	Sidechain
54	BA	1903	G	Sidechain
54	BA	1904	G	Sidechain
54	BA	1906	G	Sidechain
54	BA	1908	C	Sidechain
54	BA	1909	C	Sidechain
54	BA	1910	G	Sidechain
54	BA	1912	A	Sidechain
54	BA	1916	A	Sidechain
54	BA	1918	A	Sidechain
54	BA	1925	C	Sidechain
54	BA	1927	A	Sidechain
54	BA	1928	A	Sidechain
54	BA	1931	U	Sidechain
54	BA	1933	G	Sidechain
54	BA	1937	A	Sidechain
54	BA	1938	A	Sidechain
54	BA	1941	C	Sidechain
54	BA	1943	U	Sidechain
54	BA	1945	G	Sidechain
54	BA	1946	U	Sidechain
54	BA	195	A	Sidechain
54	BA	1950	G	Sidechain
54	BA	1956	U	Sidechain
54	BA	1957	C	Sidechain
54	BA	1958	C	Sidechain
54	BA	1959	G	Sidechain
54	BA	1962	C	Sidechain
54	BA	1964	G	Sidechain
54	BA	1969	A	Sidechain
54	BA	1973	G	Sidechain
54	BA	1974	C	Sidechain
54	BA	1978	A	Sidechain
54	BA	1983	G	Sidechain
54	BA	1984	G	Sidechain
54	BA	1989	G	Sidechain
54	BA	1996	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2	G	Sidechain
54	BA	2001	C	Sidechain
54	BA	2003	A	Sidechain
54	BA	2007	U	Sidechain
54	BA	2009	A	Sidechain
54	BA	2013	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2020	A	Sidechain
54	BA	2022	U	Sidechain
54	BA	2025	C	Sidechain
54	BA	2027	G	Sidechain
54	BA	2029	G	Sidechain
54	BA	2031	A	Sidechain
54	BA	2034	U	Sidechain
54	BA	2037	A	Sidechain
54	BA	2040	G	Sidechain
54	BA	2041	U	Sidechain
54	BA	2043	C	Sidechain
54	BA	2044	C	Sidechain
54	BA	2046	G	Sidechain
54	BA	2057	G	Sidechain
54	BA	2059	A	Sidechain
54	BA	206	U	Sidechain
54	BA	2061	G	Sidechain
54	BA	2064	C	Sidechain
54	BA	2065	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	207	A	Sidechain
54	BA	2080	A	Sidechain
54	BA	2083	G	Sidechain
54	BA	209	C	Sidechain
54	BA	2093	G	Sidechain
54	BA	2103	C	Sidechain
54	BA	2108	A	Sidechain
54	BA	2111	U	Sidechain
54	BA	2115	G	Sidechain
54	BA	2117	A	Sidechain
54	BA	2118	U	Sidechain
54	BA	2132	U	Sidechain
54	BA	2136	G	Sidechain
54	BA	2147	A	Sidechain
54	BA	215	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2155	U	Sidechain
54	BA	2163	A	Sidechain
54	BA	2165	C	Sidechain
54	BA	2168	G	Sidechain
54	BA	2170	A	Sidechain
54	BA	2172	U	Sidechain
54	BA	2178	C	Sidechain
54	BA	219	A	Sidechain
54	BA	2197	U	Sidechain
54	BA	2199	A	Sidechain
54	BA	2202	U	Sidechain
54	BA	221	A	Sidechain
54	BA	2211	A	Sidechain
54	BA	2212	A	Sidechain
54	BA	2213	U	Sidechain
54	BA	2215	C	Sidechain
54	BA	2217	G	Sidechain
54	BA	2238	G	Sidechain
54	BA	2240	U	Sidechain
54	BA	2242	G	Sidechain
54	BA	2243	U	Sidechain
54	BA	2257	U	Sidechain
54	BA	2259	U	Sidechain
54	BA	2266	A	Sidechain
54	BA	2267	A	Sidechain
54	BA	227	A	Sidechain
54	BA	2271	G	Sidechain
54	BA	2276	G	Sidechain
54	BA	2277	G	Sidechain
54	BA	2278	A	Sidechain
54	BA	2286	G	Sidechain
54	BA	2287	A	Sidechain
54	BA	2293	G	Sidechain
54	BA	2294	G	Sidechain
54	BA	2295	C	Sidechain
54	BA	2297	A	Sidechain
54	BA	2300	C	Sidechain
54	BA	2301	C	Sidechain
54	BA	2304	G	Sidechain
54	BA	2311	A	Sidechain
54	BA	2313	C	Sidechain
54	BA	2315	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2320	U	Sidechain
54	BA	2324	U	Sidechain
54	BA	233	A	Sidechain
54	BA	2336	A	Sidechain
54	BA	2338	C	Sidechain
54	BA	2339	C	Sidechain
54	BA	2348	U	Sidechain
54	BA	2349	G	Sidechain
54	BA	2357	G	Sidechain
54	BA	2362	C	Sidechain
54	BA	2375	G	Sidechain
54	BA	2389	G	Sidechain
54	BA	2391	G	Sidechain
54	BA	2393	U	Sidechain
54	BA	2411	A	Sidechain
54	BA	2413	G	Sidechain
54	BA	2415	G	Sidechain
54	BA	2416	C	Sidechain
54	BA	2418	A	Sidechain
54	BA	2422	C	Sidechain
54	BA	2424	C	Sidechain
54	BA	2431	U	Sidechain
54	BA	2434	A	Sidechain
54	BA	244	A	Sidechain
54	BA	2442	C	Sidechain
54	BA	2443	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2447	G	Sidechain
54	BA	2450	A	Sidechain
54	BA	2452	C	Sidechain
54	BA	2453	A	Sidechain
54	BA	2454	G	Sidechain
54	BA	2461	A	Sidechain
54	BA	2464	G	Sidechain
54	BA	2465	C	Sidechain
54	BA	2466	C	Sidechain
54	BA	2468	A	Sidechain
54	BA	2469	A	Sidechain
54	BA	247	G	Sidechain
54	BA	2476	A	Sidechain
54	BA	2477	U	Sidechain
54	BA	2478	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2479	U	Sidechain
54	BA	2487	G	Sidechain
54	BA	2488	G	Sidechain
54	BA	249	C	Sidechain
54	BA	2490	G	Sidechain
54	BA	2491	U	Sidechain
54	BA	2492	U	Sidechain
54	BA	2496	C	Sidechain
54	BA	2498	C	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2501	C	Sidechain
54	BA	2510	C	Sidechain
54	BA	2514	U	Sidechain
54	BA	2517	C	Sidechain
54	BA	2521	C	Sidechain
54	BA	2530	A	Sidechain
54	BA	2535	G	Sidechain
54	BA	2539	C	Sidechain
54	BA	2548	U	Sidechain
54	BA	2549	G	Sidechain
54	BA	2550	G	Sidechain
54	BA	2552	U	Sidechain
54	BA	2555	U	Sidechain
54	BA	2561	U	Sidechain
54	BA	2564	A	Sidechain
54	BA	2566	A	Sidechain
54	BA	257	C	Sidechain
54	BA	2571	U	Sidechain
54	BA	2575	C	Sidechain
54	BA	2579	C	Sidechain
54	BA	258	G	Sidechain
54	BA	2581	G	Sidechain
54	BA	2588	G	Sidechain
54	BA	2595	G	Sidechain
54	BA	2608	G	Sidechain
54	BA	2613	U	Sidechain
54	BA	2615	U	Sidechain
54	BA	2617	U	Sidechain
54	BA	262	A	Sidechain
54	BA	2622	U	Sidechain
54	BA	2623	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2624	G	Sidechain
54	BA	2627	G	Sidechain
54	BA	2628	C	Sidechain
54	BA	2637	U	Sidechain
54	BA	264	C	Sidechain
54	BA	2640	G	Sidechain
54	BA	2646	C	Sidechain
54	BA	2647	U	Sidechain
54	BA	265	A	Sidechain
54	BA	2656	U	Sidechain
54	BA	2657	A	Sidechain
54	BA	2661	G	Sidechain
54	BA	2666	C	Sidechain
54	BA	2668	G	Sidechain
54	BA	2669	G	Sidechain
54	BA	2673	G	Sidechain
54	BA	268	C	Sidechain
54	BA	2680	U	Sidechain
54	BA	2682	A	Sidechain
54	BA	2684	U	Sidechain
54	BA	2688	G	Sidechain
54	BA	2689	U	Sidechain
54	BA	269	C	Sidechain
54	BA	2692	G	Sidechain
54	BA	2693	G	Sidechain
54	BA	27	G	Sidechain
54	BA	2703	C	Sidechain
54	BA	2715	C	Sidechain
54	BA	2716	C	Sidechain
54	BA	2717	C	Sidechain
54	BA	2718	G	Sidechain
54	BA	272	A	Sidechain
54	BA	2722	G	Sidechain
54	BA	2723	C	Sidechain
54	BA	2727	A	Sidechain
54	BA	2728	U	Sidechain
54	BA	2729	G	Sidechain
54	BA	2731	G	Sidechain
54	BA	2739	U	Sidechain
54	BA	2747	G	Sidechain
54	BA	2751	G	Sidechain
54	BA	2755	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2764	A	Sidechain
54	BA	2765	A	Sidechain
54	BA	2767	C	Sidechain
54	BA	2768	U	Sidechain
54	BA	277	G	Sidechain
54	BA	2779	U	Sidechain
54	BA	2780	G	Sidechain
54	BA	2790	U	Sidechain
54	BA	2797	U	Sidechain
54	BA	2804	U	Sidechain
54	BA	2808	G	Sidechain
54	BA	2811	G	Sidechain
54	BA	2825	G	Sidechain
54	BA	283	G	Sidechain
54	BA	2830	C	Sidechain
54	BA	2832	U	Sidechain
54	BA	2835	A	Sidechain
54	BA	2848	G	Sidechain
54	BA	285	G	Sidechain
54	BA	2851	A	Sidechain
54	BA	2856	A	Sidechain
54	BA	2857	G	Sidechain
54	BA	2859	G	Sidechain
54	BA	2864	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	287	G	Sidechain
54	BA	2870	C	Sidechain
54	BA	2876	G	Sidechain
54	BA	2877	G	Sidechain
54	BA	2878	U	Sidechain
54	BA	2879	A	Sidechain
54	BA	2883	A	Sidechain
54	BA	2884	U	Sidechain
54	BA	2885	G	Sidechain
54	BA	2891	U	Sidechain
54	BA	29	U	Sidechain
54	BA	2903	U	Sidechain
54	BA	297	G	Sidechain
54	BA	307	G	Sidechain
54	BA	313	G	Sidechain
54	BA	314	C	Sidechain
54	BA	319	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	322	A	Sidechain
54	BA	329	G	Sidechain
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	337	C	Sidechain
54	BA	339	U	Sidechain
54	BA	34	U	Sidechain
54	BA	340	A	Sidechain
54	BA	356	G	Sidechain
54	BA	358	U	Sidechain
54	BA	361	G	Sidechain
54	BA	362	A	Sidechain
54	BA	364	C	Sidechain
54	BA	367	G	Sidechain
54	BA	374	A	Sidechain
54	BA	378	C	Sidechain
54	BA	385	C	Sidechain
54	BA	386	G	Sidechain
54	BA	389	G	Sidechain
54	BA	39	G	Sidechain
54	BA	391	A	Sidechain
54	BA	392	U	Sidechain
54	BA	393	C	Sidechain
54	BA	394	C	Sidechain
54	BA	395	U	Sidechain
54	BA	401	A	Sidechain
54	BA	403	U	Sidechain
54	BA	405	U	Sidechain
54	BA	417	C	Sidechain
54	BA	418	C	Sidechain
54	BA	419	U	Sidechain
54	BA	423	A	Sidechain
54	BA	425	G	Sidechain
54	BA	426	C	Sidechain
54	BA	43	G	Sidechain
54	BA	430	A	Sidechain
54	BA	437	U	Sidechain
54	BA	443	A	Sidechain
54	BA	446	G	Sidechain
54	BA	448	U	Sidechain
54	BA	453	A	Sidechain
54	BA	455	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	457	A	Sidechain
54	BA	458	G	Sidechain
54	BA	460	A	Sidechain
54	BA	461	C	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	477	A	Sidechain
54	BA	48	G	Sidechain
54	BA	480	A	Sidechain
54	BA	481	G	Sidechain
54	BA	49	A	Sidechain
54	BA	493	G	Sidechain
54	BA	497	A	Sidechain
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain
54	BA	502	A	Sidechain
54	BA	516	C	Sidechain
54	BA	518	G	Sidechain
54	BA	52	A	Sidechain
54	BA	524	G	Sidechain
54	BA	529	A	Sidechain
54	BA	533	G	Sidechain
54	BA	538	A	Sidechain
54	BA	541	A	Sidechain
54	BA	545	U	Sidechain
54	BA	547	A	Sidechain
54	BA	56	A	Sidechain
54	BA	568	U	Sidechain
54	BA	569	U	Sidechain
54	BA	577	G	Sidechain
54	BA	578	G	Sidechain
54	BA	579	G	Sidechain
54	BA	58	G	Sidechain
54	BA	580	U	Sidechain
54	BA	581	C	Sidechain
54	BA	594	U	Sidechain
54	BA	597	G	Sidechain
54	BA	599	A	Sidechain
54	BA	600	G	Sidechain
54	BA	602	A	Sidechain
54	BA	605	G	Sidechain
54	BA	608	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	61	C	Sidechain
54	BA	611	C	Sidechain
54	BA	613	A	Sidechain
54	BA	616	A	Sidechain
54	BA	622	G	Sidechain
54	BA	623	C	Sidechain
54	BA	631	A	Sidechain
54	BA	632	A	Sidechain
54	BA	635	C	Sidechain
54	BA	640	C	Sidechain
54	BA	641	U	Sidechain
54	BA	644	A	Sidechain
54	BA	654	A	Sidechain
54	BA	662	G	Sidechain
54	BA	663	G	Sidechain
54	BA	666	A	Sidechain
54	BA	667	U	Sidechain
54	BA	672	C	Sidechain
54	BA	677	A	Sidechain
54	BA	679	C	Sidechain
54	BA	680	C	Sidechain
54	BA	683	U	Sidechain
54	BA	686	U	Sidechain
54	BA	69	C	Sidechain
54	BA	697	G	Sidechain
54	BA	704	G	Sidechain
54	BA	712	G	Sidechain
54	BA	714	U	Sidechain
54	BA	718	A	Sidechain
54	BA	72	U	Sidechain
54	BA	723	C	Sidechain
54	BA	724	U	Sidechain
54	BA	725	G	Sidechain
54	BA	734	A	Sidechain
54	BA	739	A	Sidechain
54	BA	74	A	Sidechain
54	BA	748	G	Sidechain
54	BA	750	A	Sidechain
54	BA	751	A	Sidechain
54	BA	753	A	Sidechain
54	BA	766	U	Sidechain
54	BA	769	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	77	G	Sidechain
54	BA	771	G	Sidechain
54	BA	772	C	Sidechain
54	BA	775	G	Sidechain
54	BA	784	G	Sidechain
54	BA	788	A	Sidechain
54	BA	79	C	Sidechain
54	BA	790	U	Sidechain
54	BA	800	A	Sidechain
54	BA	802	A	Sidechain
54	BA	805	G	Sidechain
54	BA	808	G	Sidechain
54	BA	81	G	Sidechain
54	BA	817	C	Sidechain
54	BA	826	U	Sidechain
54	BA	836	G	Sidechain
54	BA	840	C	Sidechain
54	BA	851	C	Sidechain
54	BA	852	U	Sidechain
54	BA	857	G	Sidechain
54	BA	862	G	Sidechain
54	BA	864	G	Sidechain
54	BA	865	C	Sidechain
54	BA	868	U	Sidechain
54	BA	869	G	Sidechain
54	BA	874	G	Sidechain
54	BA	876	C	Sidechain
54	BA	879	G	Sidechain
54	BA	881	G	Sidechain
54	BA	885	C	Sidechain
54	BA	887	U	Sidechain
54	BA	89	A	Sidechain
54	BA	891	G	Sidechain
54	BA	892	A	Sidechain
54	BA	893	C	Sidechain
54	BA	896	A	Sidechain
54	BA	912	C	Sidechain
54	BA	920	A	Sidechain
54	BA	921	C	Sidechain
54	BA	923	G	Sidechain
54	BA	924	G	Sidechain
54	BA	934	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	942	G	Sidechain
54	BA	945	A	Sidechain
54	BA	95	A	Sidechain
54	BA	950	G	Sidechain
54	BA	953	G	Sidechain
54	BA	954	G	Sidechain
54	BA	959	A	Sidechain
54	BA	961	C	Sidechain
54	BA	966	G	Sidechain
54	BA	97	C	Sidechain
54	BA	970	U	Sidechain
54	BA	974	G	Sidechain
54	BA	976	G	Sidechain
54	BA	982	C	Sidechain
54	BA	984	A	Sidechain
54	BA	989	G	Sidechain
54	BA	993	G	Sidechain
55	BB	10	G	Sidechain
55	BB	101	A	Sidechain
55	BB	112	G	Sidechain
55	BB	113	C	Sidechain
55	BB	116	G	Sidechain
55	BB	15	A	Sidechain
55	BB	28	C	Sidechain
55	BB	29	A	Sidechain
55	BB	31	C	Sidechain
55	BB	32	U	Sidechain
55	BB	39	A	Sidechain
55	BB	40	U	Sidechain
55	BB	41	G	Sidechain
55	BB	43	C	Sidechain
55	BB	48	U	Sidechain
55	BB	57	A	Sidechain
55	BB	64	G	Sidechain
55	BB	75	G	Sidechain
55	BB	92	C	Sidechain
55	BB	93	C	Sidechain
55	BB	98	G	Sidechain
26	BD	124	ARG	Sidechain
41	BS	86	MET	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	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	3	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	1	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16522	2	0
22	A1	1627	0	832	1	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	1	0
25	BC	2083	0	2157	1	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	1	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	1	0
35	BM	1074	0	1157	1	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31345	6	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99665	15	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 (15) 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)
30:BH:143:ILE:H	30:BH:143:ILE:HD13	1.72	0.54
24:A3:72:C:C5	24:A3:73:A:C8	2.98	0.51
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.33	0.47
35:BM:80:VAL:H	35:BM:81:ARG:HA	1.81	0.46
22:A1:76:A:H62	54:BA:2600:A:H3'	1.82	0.44
54:BA:308:G:H21	54:BA:329:G:N2	2.15	0.43
54:BA:2306:C:H3'	54:BA:2307:G:H5''	2.01	0.43
54:BA:1771:C:H2'	54:BA:1772:A:C8	2.53	0.42
21:AA:979:C:N4	21:AA:1360:A:H62	2.16	0.42
54:BA:1025:G:C5	54:BA:1135:C:H1'	2.55	0.41
5:AF:94:HIS:CG	5:AF:95:ALA:N	2.89	0.41
11:AL:115:LYS:HE3	11:AL:116:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AF:49:TYR:CE1	21:AA:674:G:H5''	2.55	0.41
25:BC:14:HIS:CE1	54:BA:1830:C:H5'	2.56	0.40
34:BL:25:SER:CB	34:BL:26:GLY:CA	2.99	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%)	202 (93%)	13 (6%)	3 (1%)	14	58
2	AC	205/208 (99%)	189 (92%)	13 (6%)	3 (2%)	13	57
3	AD	203/206 (98%)	192 (95%)	6 (3%)	5 (2%)	7	46
4	AE	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	6	45
5	AF	99/101 (98%)	85 (86%)	8 (8%)	6 (6%)	2	26
6	AG	150/152 (99%)	139 (93%)	9 (6%)	2 (1%)	15	60
7	AH	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
8	AI	126/128 (98%)	112 (89%)	10 (8%)	4 (3%)	5	41
9	AJ	98/100 (98%)	90 (92%)	4 (4%)	4 (4%)	3	35
10	AK	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
11	AL	121/124 (98%)	109 (90%)	7 (6%)	5 (4%)	3	35
12	AM	112/115 (97%)	93 (83%)	17 (15%)	2 (2%)	11	53
13	AN	98/101 (97%)	85 (87%)	9 (9%)	4 (4%)	3	35
14	AO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	8	48
15	AP	79/81 (98%)	67 (85%)	10 (13%)	2 (2%)	7	46
16	AQ	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	15	60
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	11	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AS	79/81 (98%)	74 (94%)	4 (5%)	1 (1%)	15	60
19	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	AU	51/53 (96%)	34 (67%)	9 (18%)	8 (16%)	0	5
25	BC	270/273 (99%)	245 (91%)	21 (8%)	4 (2%)	13	57
26	BD	207/209 (99%)	182 (88%)	17 (8%)	8 (4%)	4	36
27	BE	199/201 (99%)	183 (92%)	11 (6%)	5 (2%)	7	46
28	BF	176/179 (98%)	156 (89%)	17 (10%)	3 (2%)	11	55
29	BG	174/177 (98%)	156 (90%)	14 (8%)	4 (2%)	8	48
30	BH	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	26	71
31	BI	139/142 (98%)	125 (90%)	11 (8%)	3 (2%)	8	49
32	BJ	140/142 (99%)	130 (93%)	10 (7%)	0	100	100
33	BK	121/123 (98%)	109 (90%)	9 (7%)	3 (2%)	7	46
34	BL	141/144 (98%)	124 (88%)	10 (7%)	7 (5%)	3	31
35	BM	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	13	57
36	BN	119/121 (98%)	101 (85%)	13 (11%)	5 (4%)	3	34
37	BO	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
38	BP	112/115 (97%)	98 (88%)	9 (8%)	5 (4%)	3	33
39	BQ	115/118 (98%)	103 (90%)	8 (7%)	4 (4%)	4	39
40	BR	101/103 (98%)	95 (94%)	3 (3%)	3 (3%)	5	42
41	BS	108/110 (98%)	95 (88%)	11 (10%)	2 (2%)	10	52
42	BT	92/94 (98%)	73 (79%)	12 (13%)	7 (8%)	1	20
43	BU	101/104 (97%)	85 (84%)	11 (11%)	5 (5%)	3	31
44	BV	92/94 (98%)	89 (97%)	2 (2%)	1 (1%)	17	63
45	BW	78/80 (98%)	58 (74%)	17 (22%)	3 (4%)	4	37
46	BX	75/79 (95%)	60 (80%)	11 (15%)	4 (5%)	2	29
47	BY	61/63 (97%)	57 (93%)	2 (3%)	2 (3%)	5	40
48	BZ	56/59 (95%)	49 (88%)	6 (11%)	1 (2%)	11	53
49	B0	54/57 (95%)	50 (93%)	3 (6%)	1 (2%)	10	52
50	B1	50/52 (96%)	43 (86%)	5 (10%)	2 (4%)	4	35
51	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8	48
52	B3	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	12	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
56	B5	221/234 (94%)	210 (95%)	11 (5%)	0	100	100
All	All	5876/6008 (98%)	5290 (90%)	442 (8%)	144 (2%)	11	46

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AF	86	ARG
8	AI	124	PRO
12	AM	42	VAL
13	AN	56	SER
17	AR	20	ILE
20	AU	17	ARG
20	AU	24	LYS
26	BD	2	ILE
26	BD	51	THR
26	BD	119	ALA
27	BE	61	ARG
30	BH	9	VAL
33	BK	103	VAL
36	BN	47	VAL
38	BP	31	VAL
43	BU	70	ALA
52	B3	3	ILE
5	AF	63	ASN
9	AJ	75	ASP
11	AL	17	LYS
11	AL	78	VAL
13	AN	99	ALA
15	AP	17	TYR
16	AQ	35	LYS
20	AU	22	CYS
20	AU	30	GLU
25	BC	153	LEU
25	BC	197	ALA
26	BD	118	PHE
27	BE	43	THR
27	BE	90	GLN
28	BF	103	ILE
31	BI	10	LEU
34	BL	27	LEU

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Mol	Chain	Res	Type
34	BL	34	GLY
36	BN	10	LEU
38	BP	110	LYS
40	BR	24	LYS
40	BR	53	PHE
42	BT	2	ILE
42	BT	3	ARG
42	BT	70	HIS
43	BU	43	LYS
43	BU	45	GLN
44	BV	71	LYS
46	BX	24	THR
47	BY	7	ARG
48	BZ	9	THR
49	B0	5	ASN
50	B1	6	GLU
51	B2	44	VAL
1	AB	10	LYS
3	AD	4	LEU
3	AD	47	LEU
3	AD	187	ARG
4	AE	43	GLY
4	AE	54	GLU
4	AE	105	ILE
5	AF	52	ASN
5	AF	82	ASP
6	AG	147	ASN
8	AI	55	ASP
9	AJ	41	PRO
9	AJ	57	VAL
9	AJ	58	ASN
11	AL	33	CYS
11	AL	112	ALA
13	AN	100	SER
15	AP	79	ASN
20	AU	15	LEU
26	BD	15	PHE
26	BD	136	ASN
26	BD	138	LEU
33	BK	111	LYS
34	BL	99	ASN
36	BN	32	GLU

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Mol	Chain	Res	Type
39	BQ	91	ARG
41	BS	41	LYS
41	BS	92	ARG
42	BT	61	LEU
45	BW	23	LYS
46	BX	27	ARG
46	BX	75	GLU
1	AB	18	GLN
3	AD	84	ASN
5	AF	6	ILE
5	AF	94	HIS
6	AG	43	TYR
8	AI	41	GLU
8	AI	114	LYS
14	AO	43	ALA
20	AU	25	ALA
25	BC	144	GLU
28	BF	46	LYS
29	BG	9	VAL
31	BI	132	ALA
31	BI	135	MET
33	BK	119	ALA
35	BM	21	ALA
36	BN	93	GLY
38	BP	74	GLN
38	BP	113	LEU
39	BQ	90	ASP
40	BR	28	ALA
42	BT	14	PRO
42	BT	15	HIS
42	BT	78	SER
43	BU	12	VAL
45	BW	8	SER
45	BW	26	GLY
46	BX	43	LYS
47	BY	9	LYS
50	B1	50	GLU
1	AB	11	ALA
3	AD	29	THR
4	AE	24	VAL
11	AL	11	ARG
13	AN	58	SER

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Mol	Chain	Res	Type
26	BD	34	VAL
27	BE	79	ARG
29	BG	22	VAL
29	BG	164	ALA
34	BL	19	LEU
34	BL	36	LYS
38	BP	112	ARG
2	AC	144	GLY
14	AO	74	VAL
18	AS	39	ILE
20	AU	27	VAL
20	AU	48	LYS
28	BF	102	LEU
29	BG	112	VAL
36	BN	105	GLY
39	BQ	2	ARG
39	BQ	5	ARG
43	BU	101	THR
34	BL	11	GLY
2	AC	195	ILE
25	BC	123	ILE
27	BE	31	VAL
34	BL	101	ILE
35	BM	80	VAL
2	AC	206	ILE
12	AM	8	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	177 (98%)	3 (2%)	68	87
2	AC	170/171 (99%)	166 (98%)	4 (2%)	57	82
3	AD	172/173 (99%)	171 (99%)	1 (1%)	90	95
4	AE	113/113 (100%)	112 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AF	87/87 (100%)	86 (99%)	1 (1%)	80	91
6	AG	123/123 (100%)	121 (98%)	2 (2%)	70	88
7	AH	104/105 (99%)	100 (96%)	4 (4%)	40	73
8	AI	105/105 (100%)	103 (98%)	2 (2%)	65	86
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%)	101 (98%)	2 (2%)	65	86
12	AM	91/92 (99%)	90 (99%)	1 (1%)	80	91
13	AN	83/84 (99%)	81 (98%)	2 (2%)	57	82
14	AO	76/77 (99%)	74 (97%)	2 (3%)	54	80
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	52	79
17	AR	48/48 (100%)	47 (98%)	1 (2%)	61	84
18	AS	70/70 (100%)	69 (99%)	1 (1%)	74	89
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	42 (96%)	2 (4%)	34	69
25	BC	216/217 (100%)	211 (98%)	5 (2%)	58	83
26	BD	164/164 (100%)	162 (99%)	2 (1%)	78	90
27	BE	165/165 (100%)	164 (99%)	1 (1%)	90	95
28	BF	149/150 (99%)	148 (99%)	1 (1%)	88	94
29	BG	137/138 (99%)	133 (97%)	4 (3%)	50	78
30	BH	114/114 (100%)	111 (97%)	3 (3%)	54	80
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	68	87
33	BK	103/103 (100%)	102 (99%)	1 (1%)	82	92
34	BL	102/103 (99%)	101 (99%)	1 (1%)	82	92
35	BM	109/109 (100%)	106 (97%)	3 (3%)	51	78
36	BN	100/100 (100%)	97 (97%)	3 (3%)	48	77
37	BO	86/87 (99%)	85 (99%)	1 (1%)	78	90
38	BP	99/100 (99%)	98 (99%)	1 (1%)	82	92
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BR	84/84 (100%)	81 (96%)	3 (4%)	42	74
41	BS	93/93 (100%)	90 (97%)	3 (3%)	46	76
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	83 (100%)	0	100	100
44	BV	78/78 (100%)	77 (99%)	1 (1%)	76	89
45	BW	59/59 (100%)	56 (95%)	3 (5%)	29	66
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	45 (94%)	3 (6%)	22	59
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%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	171 (99%)	2 (1%)	78	90
All	All	4842/4870 (99%)	4759 (98%)	83 (2%)	71	87

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	14	HIS
1	AB	88	GLN
1	AB	156	LEU
2	AC	2	GLN
2	AC	35	ASP
2	AC	168	ARG
2	AC	175	HIS
3	AD	2	ARG
4	AE	99	SER
5	AF	68	GLN
6	AG	3	ARG
6	AG	78	ARG
7	AH	3	GLN
7	AH	20	ASN
7	AH	100	ILE
7	AH	112	ASP
8	AI	59	LYS

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Mol	Chain	Res	Type
8	AI	129	ARG
9	AJ	48	ARG
9	AJ	87	LEU
10	AK	60	PHE
11	AL	28	GLN
11	AL	71	HIS
12	AM	90	HIS
13	AN	59	ARG
13	AN	100	SER
14	AO	45	HIS
14	AO	73	ASP
16	AQ	62	GLU
16	AQ	64	ARG
17	AR	71	ASP
18	AS	65	MET
20	AU	8	ASN
20	AU	17	ARG
25	BC	36	ASN
25	BC	51	ARG
25	BC	62	ARG
25	BC	212	TRP
25	BC	218	THR
26	BD	126	ASN
26	BD	176	ASP
27	BE	163	ASN
28	BF	162	ASP
29	BG	34	ARG
29	BG	105	SER
29	BG	115	GLN
29	BG	176	LYS
30	BH	29	PHE
30	BH	137	GLU
30	BH	143	ILE
32	BJ	1	MET
32	BJ	49	ASP
33	BK	107	LEU
34	BL	76	GLU
35	BM	1	MET
35	BM	6	ARG
35	BM	97	GLN
36	BN	1	MET
36	BN	59	SER

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Mol	Chain	Res	Type
36	BN	70	THR
37	BO	95	SER
38	BP	75	THR
39	BQ	19	GLN
39	BQ	71	ASN
40	BR	22	LEU
40	BR	39	LEU
40	BR	41	ILE
41	BS	12	SER
41	BS	82	MET
41	BS	108	SER
44	BV	12	GLN
45	BW	36	ILE
45	BW	39	GLN
45	BW	59	PHE
48	BZ	9	THR
48	BZ	39	ASP
48	BZ	40	THR
49	B0	45	ASP
50	B1	35	LEU
51	B2	16	HIS
52	B3	61	LEU
56	B5	40	GLU
56	B5	129	GLN

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

Mol	Chain	Res	Type
19	AT	69	ASN
34	BL	35	HIS
36	BN	107	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	255 (16%)	88 (5%)
22	A1	73/76 (96%)	12 (16%)	7 (9%)
23	A2	14/15 (93%)	4 (28%)	1 (7%)
24	A3	76/77 (98%)	11 (14%)	4 (5%)
54	BA	2902/2903 (99%)	485 (16%)	125 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	BB	116/118 (98%)	14 (12%)	5 (4%)
All	All	4711/4722 (99%)	781 (16%)	230 (4%)

All (781) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	16	A
21	AA	26	A
21	AA	27	G
21	AA	32	A
21	AA	33	A
21	AA	36	C
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	50	A
21	AA	52	C
21	AA	61	G
21	AA	64	G
21	AA	65	A
21	AA	72	A
21	AA	80	A
21	AA	81	A
21	AA	84	U
21	AA	86	G
21	AA	89	U
21	AA	90	C
21	AA	94	G
21	AA	95	C
21	AA	96	U
21	AA	109	A
21	AA	110	C
21	AA	121	U
21	AA	125	U
21	AA	131	A
21	AA	134	G
21	AA	163	C
21	AA	165	G

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Mol	Chain	Res	Type
21	AA	182	A
21	AA	187	G
21	AA	188	C
21	AA	191	G
21	AA	198	G
21	AA	201	G
21	AA	210	C
21	AA	235	C
21	AA	236	A
21	AA	237	G
21	AA	238	A
21	AA	239	U
21	AA	244	U
21	AA	245	U
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	272	C
21	AA	280	C
21	AA	282	A
21	AA	289	G
21	AA	301	G
21	AA	310	G
21	AA	317	U
21	AA	328	C
21	AA	329	A
21	AA	330	C
21	AA	343	U
21	AA	344	A
21	AA	347	G
21	AA	348	G
21	AA	349	A
21	AA	351	G
21	AA	352	C
21	AA	354	G
21	AA	356	A
21	AA	361	G
21	AA	366	A
21	AA	367	U
21	AA	381	C
21	AA	397	A
21	AA	406	G

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Mol	Chain	Res	Type
21	AA	413	G
21	AA	414	A
21	AA	415	A
21	AA	421	U
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	452	A
21	AA	453	G
21	AA	461	A
21	AA	462	G
21	AA	463	U
21	AA	465	A
21	AA	466	A
21	AA	467	U
21	AA	468	A
21	AA	484	G
21	AA	492	C
21	AA	493	A
21	AA	511	C
21	AA	524	G
21	AA	525	C
21	AA	527	G
21	AA	529	G
21	AA	532	A
21	AA	547	A
21	AA	559	A
21	AA	564	C
21	AA	566	G
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	577	G
21	AA	588	G
21	AA	611	C
21	AA	612	C
21	AA	619	U
21	AA	620	C
21	AA	653	U
21	AA	665	A
21	AA	675	A

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Mol	Chain	Res	Type
21	AA	700	G
21	AA	718	A
21	AA	719	C
21	AA	721	G
21	AA	724	G
21	AA	728	A
21	AA	729	A
21	AA	731	G
21	AA	734	G
21	AA	735	C
21	AA	755	G
21	AA	756	C
21	AA	765	G
21	AA	777	A
21	AA	791	G
21	AA	794	A
21	AA	812	G
21	AA	817	C
21	AA	818	G
21	AA	819	A
21	AA	821	G
21	AA	827	U
21	AA	828	U
21	AA	829	G
21	AA	841	C
21	AA	842	U
21	AA	843	U
21	AA	844	G
21	AA	845	A
21	AA	846	G
21	AA	914	A
21	AA	927	G
21	AA	930	C
21	AA	932	C
21	AA	934	C
21	AA	939	G
21	AA	940	C
21	AA	942	G
21	AA	945	G
21	AA	946	A
21	AA	960	U
21	AA	962	C

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Mol	Chain	Res	Type
21	AA	966	G
21	AA	968	A
21	AA	969	A
21	AA	970	C
21	AA	971	G
21	AA	976	G
21	AA	977	A
21	AA	980	C
21	AA	983	A
21	AA	984	C
21	AA	993	G
21	AA	994	A
21	AA	1004	A
21	AA	1025	U
21	AA	1026	G
21	AA	1031	C
21	AA	1032	G
21	AA	1045	C
21	AA	1054	C
21	AA	1056	U
21	AA	1065	U
21	AA	1094	G
21	AA	1101	A
21	AA	1102	A
21	AA	1129	C
21	AA	1130	A
21	AA	1135	U
21	AA	1136	C
21	AA	1138	G
21	AA	1139	G
21	AA	1140	C
21	AA	1143	G
21	AA	1146	A
21	AA	1159	U
21	AA	1160	G
21	AA	1161	C
21	AA	1181	G
21	AA	1183	U
21	AA	1184	G
21	AA	1188	A
21	AA	1189	U
21	AA	1191	A

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Mol	Chain	Res	Type
21	AA	1196	A
21	AA	1197	A
21	AA	1201	A
21	AA	1202	U
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1238	A
21	AA	1240	U
21	AA	1241	G
21	AA	1256	A
21	AA	1257	A
21	AA	1266	G
21	AA	1279	G
21	AA	1280	A
21	AA	1281	C
21	AA	1282	C
21	AA	1287	A
21	AA	1300	G
21	AA	1302	C
21	AA	1303	C
21	AA	1305	G
21	AA	1320	C
21	AA	1321	U
21	AA	1323	G
21	AA	1341	U
21	AA	1343	G
21	AA	1363	A
21	AA	1379	G
21	AA	1380	U
21	AA	1383	C
21	AA	1384	C
21	AA	1390	U
21	AA	1397	C
21	AA	1398	A
21	AA	1399	C
21	AA	1400	C
21	AA	1401	G
21	AA	1432	G
21	AA	1433	A
21	AA	1446	A
21	AA	1447	A

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Mol	Chain	Res	Type
21	AA	1454	G
21	AA	1494	G
21	AA	1499	A
21	AA	1503	A
21	AA	1504	G
21	AA	1506	U
21	AA	1523	G
21	AA	1529	G
21	AA	1530	G
22	A1	3	G
22	A1	17	U
22	A1	43	G
22	A1	44	G
22	A1	46	7MG
22	A1	48	C
22	A1	60	C
22	A1	71	C
22	A1	73	A
22	A1	74	C
22	A1	75	C
22	A1	76	A
23	A2	82	A
23	A2	83	U
23	A2	84	G
23	A2	92	U
24	A3	2	G
24	A3	9	G
24	A3	10	G
24	A3	18	U
24	A3	22	A
24	A3	36	A
24	A3	48	U
24	A3	49	C
24	A3	60	A
24	A3	72	C
24	A3	73	A
54	BA	10	A
54	BA	11	C
54	BA	15	G
54	BA	20	C
54	BA	27	G
54	BA	34	U

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Mol	Chain	Res	Type
54	BA	35	G
54	BA	45	G
54	BA	50	U
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	91	A
54	BA	98	G
54	BA	100	U
54	BA	101	A
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	126	A
54	BA	127	A
54	BA	128	C
54	BA	142	A
54	BA	196	A
54	BA	197	A
54	BA	200	U
54	BA	204	A
54	BA	216	A
54	BA	222	A
54	BA	224	U
54	BA	248	G
54	BA	250	G
54	BA	265	A
54	BA	266	G
54	BA	271	G
54	BA	272	A
54	BA	273	G
54	BA	278	A
54	BA	283	G
54	BA	299	A
54	BA	302	C
54	BA	316	C
54	BA	330	A
54	BA	332	A
54	BA	335	C
54	BA	370	G

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Mol	Chain	Res	Type
54	BA	372	G
54	BA	373	U
54	BA	374	A
54	BA	385	C
54	BA	386	G
54	BA	387	U
54	BA	389	G
54	BA	392	U
54	BA	396	G
54	BA	404	A
54	BA	411	G
54	BA	428	A
54	BA	429	A
54	BA	430	A
54	BA	436	C
54	BA	447	A
54	BA	448	U
54	BA	451	U
54	BA	453	A
54	BA	454	A
54	BA	457	A
54	BA	458	G
54	BA	473	G
54	BA	481	G
54	BA	482	A
54	BA	490	C
54	BA	503	A
54	BA	504	A
54	BA	506	G
54	BA	508	A
54	BA	518	G
54	BA	527	C
54	BA	529	A
54	BA	532	A
54	BA	533	G
54	BA	548	G
54	BA	563	A
54	BA	566	U
54	BA	571	U
54	BA	575	A
54	BA	586	A
54	BA	588	U

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Mol	Chain	Res	Type
54	BA	614	A
54	BA	627	A
54	BA	637	A
54	BA	644	A
54	BA	645	C
54	BA	653	U
54	BA	662	G
54	BA	663	G
54	BA	670	A
54	BA	671	C
54	BA	686	U
54	BA	716	A
54	BA	719	C
54	BA	727	A
54	BA	728	G
54	BA	730	A
54	BA	747	U
54	BA	750	A
54	BA	751	A
54	BA	753	A
54	BA	762	U
54	BA	763	G
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	785	G
54	BA	789	A
54	BA	790	U
54	BA	791	C
54	BA	792	A
54	BA	805	G
54	BA	811	U
54	BA	824	U
54	BA	827	U
54	BA	828	U
54	BA	836	G
54	BA	846	U
54	BA	848	C
54	BA	856	G
54	BA	858	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	BA	866	A
54	BA	889	C
54	BA	890	C
54	BA	891	G
54	BA	892	A
54	BA	896	A
54	BA	897	C
54	BA	910	A
54	BA	914	G
54	BA	931	U
54	BA	932	U
54	BA	934	U
54	BA	941	A
54	BA	946	C
54	BA	959	A
54	BA	961	C
54	BA	974	G
54	BA	981	A
54	BA	983	A
54	BA	994	C
54	BA	995	C
54	BA	996	A
54	BA	1006	C
54	BA	1008	A
54	BA	1012	U
54	BA	1013	C
54	BA	1022	G
54	BA	1024	G
54	BA	1025	G
54	BA	1026	G
54	BA	1028	A
54	BA	1033	U
54	BA	1044	C
54	BA	1045	C
54	BA	1046	A
54	BA	1055	G
54	BA	1058	U
54	BA	1067	A
54	BA	1068	G
54	BA	1069	A
54	BA	1070	A
54	BA	1071	G

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Mol	Chain	Res	Type
54	BA	1072	C
54	BA	1073	A
54	BA	1076	C
54	BA	1087	G
54	BA	1088	A
54	BA	1090	A
54	BA	1097	U
54	BA	1098	A
54	BA	1112	G
54	BA	1124	G
54	BA	1126	A
54	BA	1128	G
54	BA	1129	A
54	BA	1130	U
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1139	G
54	BA	1144	A
54	BA	1175	A
54	BA	1176	U
54	BA	1185	G
54	BA	1188	U
54	BA	1190	G
54	BA	1204	A
54	BA	1210	G
54	BA	1211	C
54	BA	1227	G
54	BA	1237	A
54	BA	1242	U
54	BA	1250	G
54	BA	1251	C
54	BA	1252	G
54	BA	1253	A
54	BA	1256	G
54	BA	1266	G
54	BA	1272	A
54	BA	1275	A
54	BA	1276	A
54	BA	1287	A
54	BA	1288	G
54	BA	1291	C

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Mol	Chain	Res	Type
54	BA	1292	G
54	BA	1300	G
54	BA	1301	A
54	BA	1302	A
54	BA	1313	U
54	BA	1314	C
54	BA	1315	C
54	BA	1329	U
54	BA	1332	G
54	BA	1341	G
54	BA	1349	C
54	BA	1350	C
54	BA	1361	G
54	BA	1365	A
54	BA	1366	A
54	BA	1368	G
54	BA	1378	A
54	BA	1379	U
54	BA	1382	G
54	BA	1383	A
54	BA	1384	A
54	BA	1388	G
54	BA	1392	A
54	BA	1400	U
54	BA	1402	U
54	BA	1416	G
54	BA	1417	C
54	BA	1420	A
54	BA	1428	C
54	BA	1439	A
54	BA	1440	U
54	BA	1451	C
54	BA	1452	G
54	BA	1454	C
54	BA	1455	G
54	BA	1458	U
54	BA	1459	G
54	BA	1460	U
54	BA	1476	U
54	BA	1482	G
54	BA	1490	A
54	BA	1493	C

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Mol	Chain	Res	Type
54	BA	1508	A
54	BA	1509	A
54	BA	1512	C
54	BA	1523	U
54	BA	1528	A
54	BA	1532	A
54	BA	1535	A
54	BA	1536	C
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1541	C
54	BA	1566	A
54	BA	1568	G
54	BA	1569	A
54	BA	1599	U
54	BA	1608	A
54	BA	1610	A
54	BA	1611	C
54	BA	1614	A
54	BA	1617	C
54	BA	1618	A
54	BA	1619	G
54	BA	1627	G
54	BA	1630	A
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1651	G
54	BA	1654	A
54	BA	1656	C
54	BA	1668	A
54	BA	1669	A
54	BA	1670	C
54	BA	1674	G
54	BA	1675	C
54	BA	1696	G
54	BA	1699	G
54	BA	1700	A
54	BA	1712	U
54	BA	1714	U
54	BA	1715	G

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Mol	Chain	Res	Type
54	BA	1730	C
54	BA	1758	U
54	BA	1763	G
54	BA	1764	C
54	BA	1773	A
54	BA	1780	A
54	BA	1782	U
54	BA	1789	A
54	BA	1800	C
54	BA	1807	G
54	BA	1808	A
54	BA	1809	A
54	BA	1814	G
54	BA	1815	A
54	BA	1816	C
54	BA	1820	U
54	BA	1821	A
54	BA	1829	A
54	BA	1830	C
54	BA	1877	A
54	BA	1884	G
54	BA	1900	A
54	BA	1913	A
54	BA	1914	C
54	BA	1926	U
54	BA	1937	A
54	BA	1940	U
54	BA	1945	G
54	BA	1946	U
54	BA	1952	A
54	BA	1955	U
54	BA	1963	U
54	BA	1967	C
54	BA	1971	U
54	BA	1972	G
54	BA	1982	U
54	BA	1983	G
54	BA	1993	U
54	BA	1997	C
54	BA	2023	C
54	BA	2026	U
54	BA	2030	A

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Mol	Chain	Res	Type
54	BA	2031	A
54	BA	2032	G
54	BA	2034	U
54	BA	2043	C
54	BA	2055	C
54	BA	2059	A
54	BA	2061	G
54	BA	2062	A
54	BA	2063	C
54	BA	2093	G
54	BA	2094	A
54	BA	2112	G
54	BA	2113	U
54	BA	2114	A
54	BA	2116	G
54	BA	2117	A
54	BA	2118	U
54	BA	2119	A
54	BA	2126	A
54	BA	2129	C
54	BA	2131	U
54	BA	2132	U
54	BA	2137	U
54	BA	2138	G
54	BA	2157	G
54	BA	2159	G
54	BA	2165	C
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2181	U
54	BA	2194	U
54	BA	2203	U
54	BA	2211	A
54	BA	2212	A
54	BA	2216	G
54	BA	2225	A
54	BA	2238	G
54	BA	2239	G
54	BA	2261	C
54	BA	2269	G
54	BA	2275	C

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Mol	Chain	Res	Type
54	BA	2277	G
54	BA	2283	C
54	BA	2297	A
54	BA	2305	U
54	BA	2307	G
54	BA	2309	A
54	BA	2311	A
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2333	A
54	BA	2334	U
54	BA	2335	A
54	BA	2347	C
54	BA	2353	G
54	BA	2367	G
54	BA	2383	G
54	BA	2385	C
54	BA	2386	A
54	BA	2402	U
54	BA	2406	A
54	BA	2423	U
54	BA	2425	A
54	BA	2429	G
54	BA	2430	A
54	BA	2432	A
54	BA	2441	U
54	BA	2448	A
54	BA	2449	U
54	BA	2473	U
54	BA	2474	U
54	BA	2476	A
54	BA	2478	A
54	BA	2480	C
54	BA	2488	G
54	BA	2489	U
54	BA	2491	U
54	BA	2492	U
54	BA	2498	C
54	BA	2499	C
54	BA	2501	C

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Mol	Chain	Res	Type
54	BA	2502	G
54	BA	2503	A
54	BA	2504	U
54	BA	2505	G
54	BA	2513	A
54	BA	2518	A
54	BA	2529	G
54	BA	2531	A
54	BA	2540	C
54	BA	2542	A
54	BA	2543	G
54	BA	2547	A
54	BA	2567	G
54	BA	2573	C
54	BA	2576	G
54	BA	2581	G
54	BA	2582	G
54	BA	2585	U
54	BA	2587	A
54	BA	2588	G
54	BA	2603	G
54	BA	2609	U
54	BA	2610	C
54	BA	2611	C
54	BA	2628	C
54	BA	2629	U
54	BA	2645	G
54	BA	2660	A
54	BA	2661	G
54	BA	2663	G
54	BA	2668	G
54	BA	2681	C
54	BA	2683	C
54	BA	2689	U
54	BA	2690	U
54	BA	2714	G
54	BA	2718	G
54	BA	2726	A
54	BA	2729	G
54	BA	2732	G
54	BA	2733	A
54	BA	2750	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	BA	2751	G
54	BA	2756	U
54	BA	2776	A
54	BA	2777	G
54	BA	2778	A
54	BA	2780	G
54	BA	2799	A
54	BA	2800	A
54	BA	2820	A
54	BA	2832	U
54	BA	2850	A
54	BA	2872	A
54	BA	2875	C
54	BA	2876	G
54	BA	2883	A
54	BA	2884	U
54	BA	2895	G
55	BB	9	G
55	BB	12	C
55	BB	13	G
55	BB	15	A
55	BB	16	G
55	BB	35	C
55	BB	36	C
55	BB	45	A
55	BB	53	A
55	BB	64	G
55	BB	67	G
55	BB	74	U
55	BB	90	C
55	BB	109	A

All (230) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	AA	5	U
21	AA	26	A
21	AA	32	A
21	AA	51	A
21	AA	60	A
21	AA	64	G
21	AA	80	A

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Mol	Chain	Res	Type
21	AA	89	U
21	AA	94	G
21	AA	95	C
21	AA	109	A
21	AA	133	U
21	AA	184	G
21	AA	205	A
21	AA	209	U
21	AA	236	A
21	AA	238	A
21	AA	244	U
21	AA	246	A
21	AA	251	G
21	AA	307	C
21	AA	309	A
21	AA	316	C
21	AA	329	A
21	AA	343	U
21	AA	344	A
21	AA	345	C
21	AA	347	G
21	AA	366	A
21	AA	452	A
21	AA	465	A
21	AA	492	C
21	AA	524	G
21	AA	563	A
21	AA	575	G
21	AA	611	C
21	AA	619	U
21	AA	674	G
21	AA	718	A
21	AA	728	A
21	AA	733	G
21	AA	734	G
21	AA	755	G
21	AA	790	A
21	AA	817	C
21	AA	818	G
21	AA	827	U
21	AA	841	C
21	AA	843	U

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Mol	Chain	Res	Type
21	AA	844	G
21	AA	845	A
21	AA	884	U
21	AA	945	G
21	AA	970	C
21	AA	975	A
21	AA	982	U
21	AA	983	A
21	AA	991	U
21	AA	994	A
21	AA	1025	U
21	AA	1044	A
21	AA	1049	U
21	AA	1101	A
21	AA	1126	U
21	AA	1129	C
21	AA	1159	U
21	AA	1181	G
21	AA	1188	A
21	AA	1190	G
21	AA	1196	A
21	AA	1201	A
21	AA	1215	G
21	AA	1227	A
21	AA	1231	G
21	AA	1238	A
21	AA	1280	A
21	AA	1300	G
21	AA	1319	A
21	AA	1342	C
21	AA	1379	G
21	AA	1383	C
21	AA	1399	C
21	AA	1407	C
21	AA	1446	A
21	AA	1447	A
21	AA	1459	G
21	AA	1493	A
21	AA	1498	U
22	A1	3	G
22	A1	17	U
22	A1	43	G

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Mol	Chain	Res	Type
22	A1	47	U
22	A1	60	C
22	A1	70	C
22	A1	73	A
23	A2	83	U
24	A3	10	G
24	A3	16	C
24	A3	48	U
24	A3	61	U
54	BA	49	A
54	BA	118	A
54	BA	121	G
54	BA	126	A
54	BA	249	C
54	BA	271	G
54	BA	272	A
54	BA	278	A
54	BA	384	A
54	BA	428	A
54	BA	446	G
54	BA	448	U
54	BA	453	A
54	BA	481	G
54	BA	482	A
54	BA	503	A
54	BA	506	G
54	BA	509	C
54	BA	532	A
54	BA	603	A
54	BA	670	A
54	BA	749	A
54	BA	750	A
54	BA	762	U
54	BA	784	G
54	BA	789	A
54	BA	791	C
54	BA	827	U
54	BA	847	U
54	BA	890	C
54	BA	896	A
54	BA	909	A
54	BA	911	A

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Mol	Chain	Res	Type
54	BA	931	U
54	BA	933	A
54	BA	981	A
54	BA	994	C
54	BA	1005	C
54	BA	1033	U
54	BA	1068	G
54	BA	1070	A
54	BA	1072	C
54	BA	1097	U
54	BA	1128	G
54	BA	1129	A
54	BA	1132	U
54	BA	1187	G
54	BA	1232	G
54	BA	1282	U
54	BA	1287	A
54	BA	1288	G
54	BA	1300	G
54	BA	1301	A
54	BA	1312	U
54	BA	1313	U
54	BA	1314	C
54	BA	1329	U
54	BA	1349	C
54	BA	1385	A
54	BA	1396	U
54	BA	1427	A
54	BA	1428	C
54	BA	1451	C
54	BA	1460	U
54	BA	1475	G
54	BA	1508	A
54	BA	1511	G
54	BA	1534	U
54	BA	1536	C
54	BA	1598	A
54	BA	1610	A
54	BA	1617	C
54	BA	1618	A
54	BA	1655	A
54	BA	1668	A

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Mol	Chain	Res	Type
54	BA	1674	G
54	BA	1699	G
54	BA	1713	A
54	BA	1760	C
54	BA	1808	A
54	BA	1813	G
54	BA	1820	U
54	BA	1912	A
54	BA	1913	A
54	BA	1936	A
54	BA	1945	G
54	BA	1951	U
54	BA	1952	A
54	BA	1963	U
54	BA	2021	C
54	BA	2030	A
54	BA	2062	A
54	BA	2092	U
54	BA	2113	U
54	BA	2117	A
54	BA	2126	A
54	BA	2211	A
54	BA	2282	G
54	BA	2286	G
54	BA	2288	A
54	BA	2321	U
54	BA	2346	A
54	BA	2391	G
54	BA	2429	G
54	BA	2430	A
54	BA	2439	A
54	BA	2473	U
54	BA	2489	U
54	BA	2497	A
54	BA	2501	C
54	BA	2503	A
54	BA	2504	U
54	BA	2518	A
54	BA	2542	A
54	BA	2569	G
54	BA	2581	G
54	BA	2586	U

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Mol	Chain	Res	Type
54	BA	2609	U
54	BA	2644	G
54	BA	2680	U
54	BA	2689	U
54	BA	2732	G
54	BA	2776	A
54	BA	2790	U
54	BA	2875	C
55	BB	15	A
55	BB	34	A
55	BB	35	C
55	BB	63	C
55	BB	73	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CM0	A1	34	22	15,26,27	1.83	3 (20%)	18,37,40	3.38	3 (16%)
22	6MZ	A1	37	22	17,25,26	0.82	0	15,36,39	1.32	1 (6%)
22	7MG	A1	46	22	20,26,27	2.20	4 (20%)	23,39,42	2.24	2 (8%)
22	5MU	A1	54	22	13,22,23	1.06	1 (7%)	16,32,35	4.60	2 (12%)
22	PSU	A1	55	22	15,21,22	1.07	1 (6%)	16,30,33	3.46	5 (31%)
22	4SU	A1	7	22	12,21,22	0.94	0	15,30,33	2.22	3 (20%)
24	H2U	A3	21	24	17,21,22	1.46	2 (11%)	23,30,33	1.45	4 (17%)
24	OMC	A3	33	24	15,22,23	1.03	0	20,31,34	0.74	0
24	5MU	A3	55	24	13,22,23	1.15	1 (7%)	16,32,35	4.57	2 (12%)
24	PSU	A3	56	24	15,21,22	1.08	1 (6%)	16,30,33	3.71	5 (31%)
24	4SU	A3	8	24	12,21,22	1.25	2 (16%)	15,30,33	2.22	2 (13%)

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

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.11	1.33	1.45
22	A1	34	CM0	O5-C5	-5.53	1.26	1.37
24	A3	21	H2U	C4-N3	-3.69	1.31	1.37
24	A3	21	H2U	C2-N3	-3.35	1.31	1.38
22	A1	46	7MG	C8-N7	-2.76	1.30	1.43
22	A1	46	7MG	C4-N3	2.11	1.37	1.34
22	A1	55	PSU	C4-N3	2.14	1.36	1.33
24	A3	8	4SU	O4'-C1'	2.29	1.44	1.41
24	A3	8	4SU	C6-N1	2.35	1.38	1.35
24	A3	56	PSU	C4-N3	2.44	1.37	1.33
22	A1	34	CM0	C4-N3	2.49	1.37	1.33
22	A1	54	5MU	C4-N3	2.53	1.37	1.33
24	A3	55	5MU	C4-N3	2.75	1.38	1.33
22	A1	46	7MG	C6-N1	2.82	1.38	1.33
22	A1	34	CM0	C4-C5	2.87	1.48	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-12.58	114.79	125.35
24	A3	55	5MU	C5-C4-N3	-12.39	114.95	125.35
24	A3	8	4SU	C5-C4-N3	-7.72	115.37	123.56
22	A1	7	4SU	C5-C4-N3	-7.43	115.68	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	C5-C6-N1	-6.98	113.00	123.39
24	A3	56	PSU	C4'-O4'-C1'	-4.67	104.73	109.54
22	A1	55	PSU	C5-C6-N1	-3.44	119.58	124.38
22	A1	55	PSU	C5-C1'-C2'	-3.33	109.78	115.44
22	A1	55	PSU	C4'-O4'-C1'	-3.29	106.15	109.54
24	A3	56	PSU	C5-C6-N1	-2.99	120.22	124.38
24	A3	56	PSU	C5-C1'-C2'	-2.75	110.76	115.44
22	A1	7	4SU	C4'-O4'-C1'	-2.41	107.09	109.64
24	A3	21	H2U	O2-C2-N3	-2.35	116.84	121.44
24	A3	8	4SU	C4'-O4'-C1'	-2.19	107.32	109.64
22	A1	34	CM0	O5-C7-C8	2.11	112.37	108.01
22	A1	7	4SU	O4'-C4'-C3'	2.13	109.48	105.16
24	A3	21	H2U	C5-C6-N1	2.53	113.53	110.76
24	A3	21	H2U	C5-C4-N3	2.74	119.51	116.62
22	A1	37	6MZ	C2-N1-C6	3.42	118.93	116.47
22	A1	34	CM0	C7-O5-C5	3.63	124.50	117.83
22	A1	55	PSU	O4'-C1'-C2'	3.75	108.75	104.69
24	A3	21	H2U	N3-C2-N1	3.92	120.27	116.64
24	A3	56	PSU	O4'-C1'-C2'	4.09	109.11	104.69
22	A1	46	7MG	C6-N1-C2	7.39	124.54	115.88
22	A1	55	PSU	C4-N3-C2	11.75	124.96	115.16
24	A3	56	PSU	C4-N3-C2	12.59	125.66	115.16
24	A3	55	5MU	C4-N3-C2	12.86	125.89	115.16
22	A1	54	5MU	C4-N3-C2	13.02	126.02	115.16
22	A1	34	CM0	C4-N3-C2	13.20	126.17	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	VAL	A1	101	58,22	5,6,7	0.68	0	5,7,9	1.29	1 (20%)
58	FME	BA	3001	57	8,9,10	0.83	0	5,9,11	1.23	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	-	0/6/9/11	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	-2.57	118.68	125.69
58	BA	3001	FME	O-C-CA	-2.53	118.78	125.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.