



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 12:51 pm GMT

PDB ID : 4V78
EMDB ID: : EMD-2475
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post3a)
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on : 2013-10-14
Resolution : 20.00 Å(reported)
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

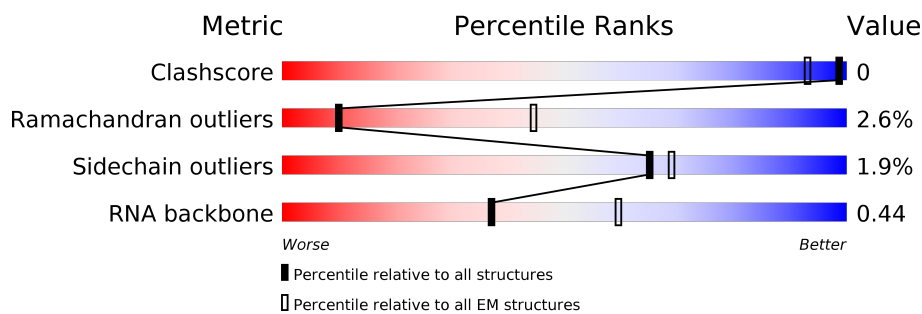
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 Å.

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














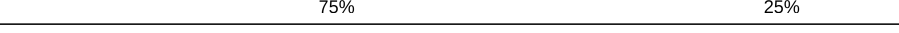
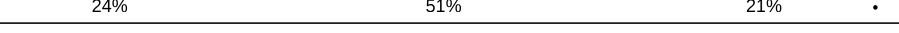
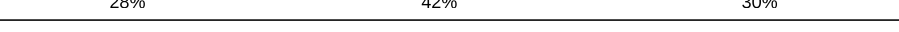

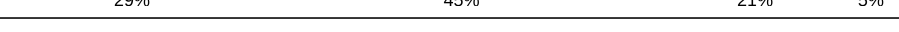



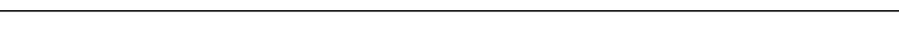
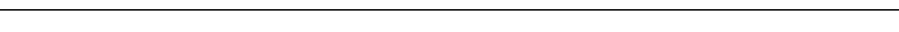

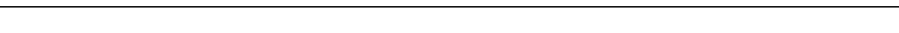
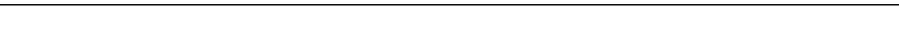

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

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











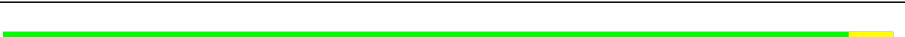


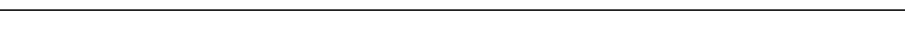







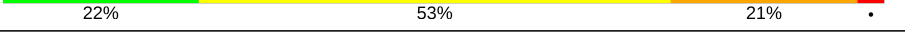
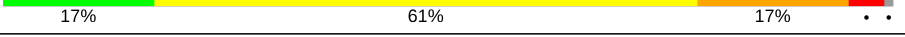
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Mol	Chain	Length	Quality of chain
9	AJ	100	 86% 13% .
10	AK	118	 92% 7% .
11	AL	124	 85% 15% .
12	AM	115	 90% 10% .
13	AN	101	 87% 10% ..
14	AO	89	 88% 11% .
15	AP	81	 78% 22%
16	AQ	82	 90% 9% .
17	AR	57	 84% 16%
18	AS	81	 90% 9% .
19	AT	86	 86% 13% .
20	AU	53	 75% 25%
21	AA	1533	 24% 51% 21% .
22	A1	76	 28% 42% 30%
23	A2	15	 13% 47% 27% 13%
24	A3	77	 29% 45% 21% 5%
25	BC	273	 89% 9% .
26	BD	209	 90% 9%
27	BE	201	 89% 10%
28	BF	179	 89% 10% ..
29	BG	177	 89% 10% .
30	BH	149	 95% 5%
31	BI	142	 95% . .
32	BJ	142	 90% 10%
33	BK	123	 89% 11%

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

2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

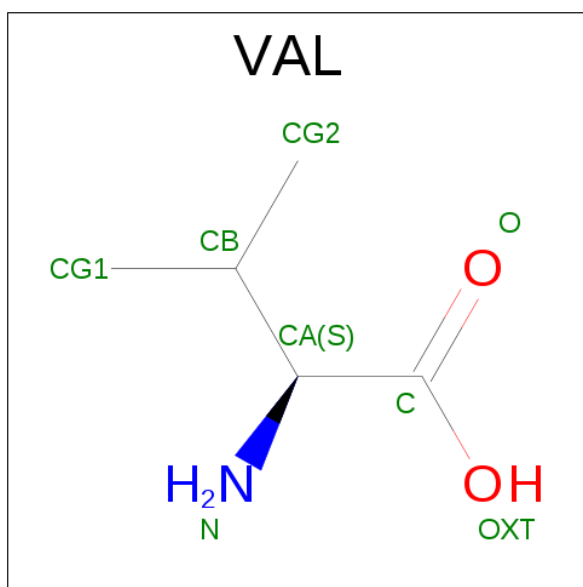
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

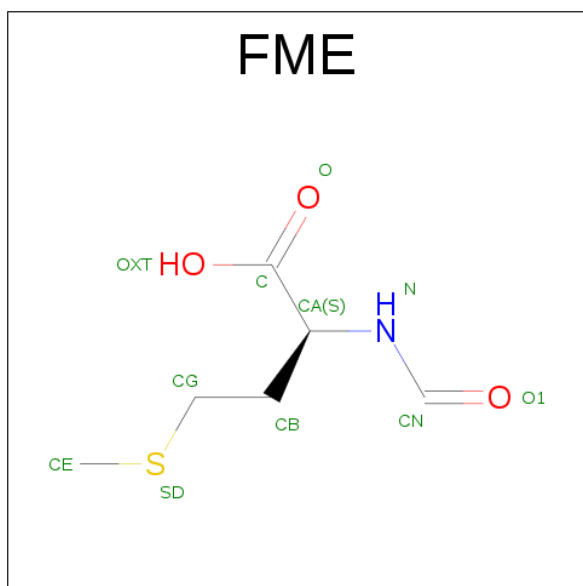
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C₅H₁₁NO₂).



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: C₆H₁₁NO₃S).

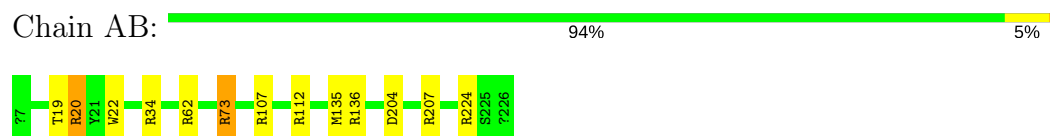


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

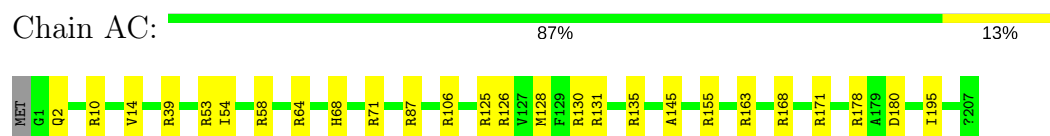
3 Residue-property plots

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

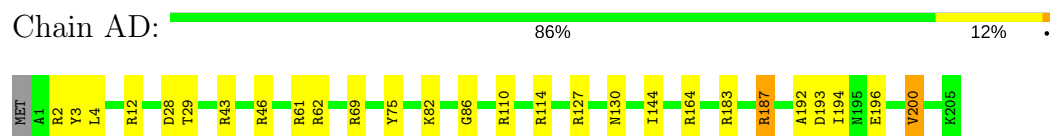
- Molecule 1: 30S ribosomal protein S2



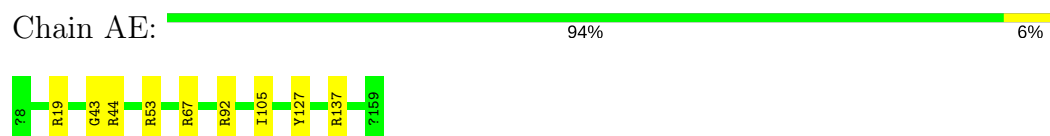
- Molecule 2: 30S ribosomal protein S3



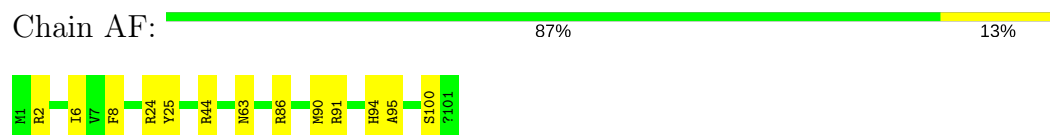
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 92% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 84% 16%



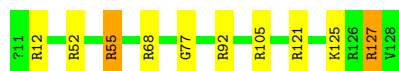
- Molecule 9: 30S ribosomal protein S10

Chain AJ: 86% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 92% 7%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 85% 15%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 90% 10%

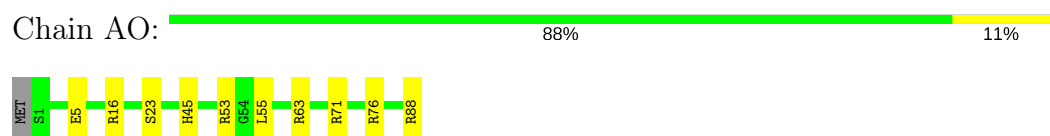


- Molecule 13: 30S ribosomal protein S14

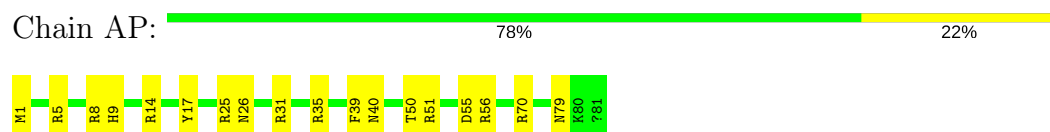
Chain AN: 87% 10%



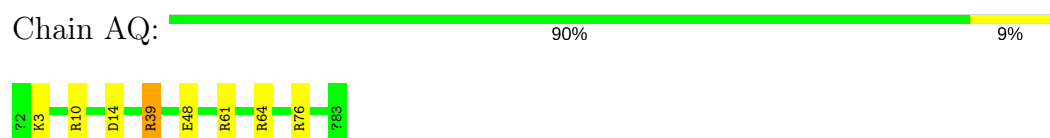
- Molecule 14: 30S ribosomal protein S15



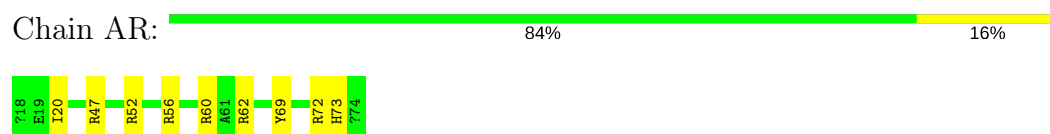
- Molecule 15: 30S ribosomal protein S16



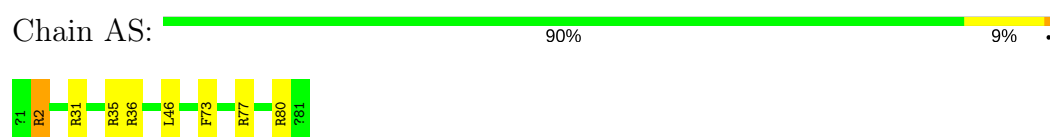
- Molecule 16: 30S ribosomal protein S17



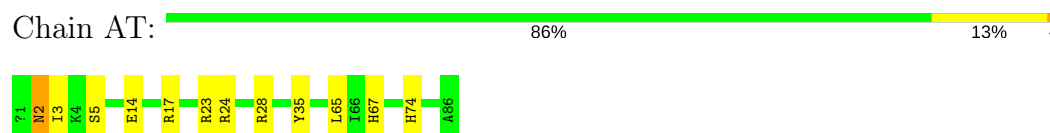
- Molecule 17: 30S ribosomal protein S18



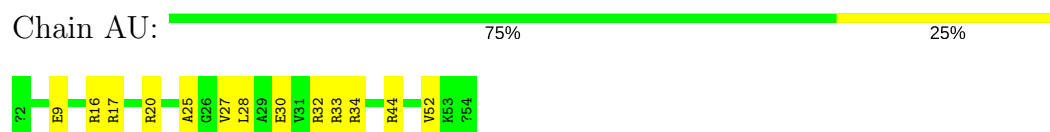
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



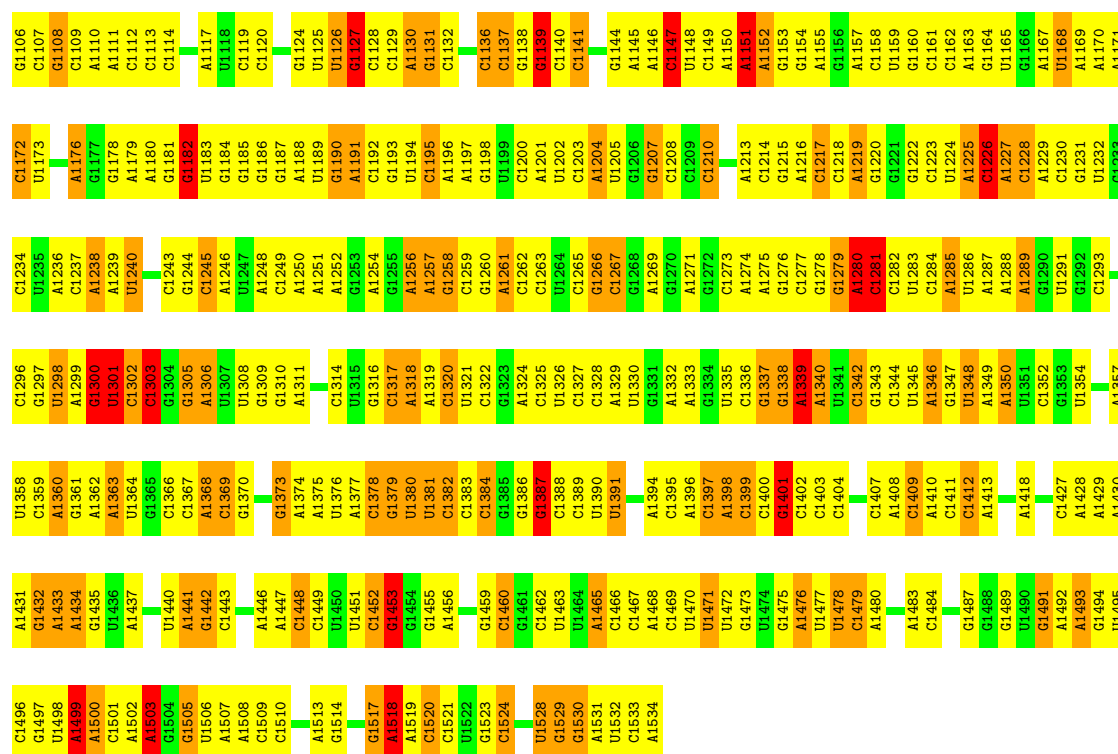
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA

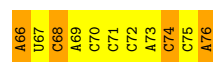
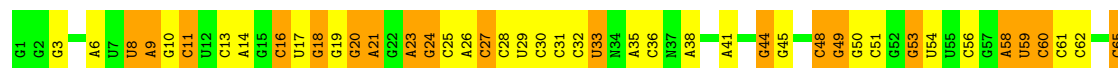


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U1040	G976	U911	G847	G778	A712	G643	C578	G515	A452	G391	G324		A197	C135	A65	A
G1041	A977	C912	G848	C779	G713	G646	C580	U516	G455	C392	A325		G198	U	A66	U
A1042	A978	A913	G849	A780	G714	G647	C581	C519	A456	A393	G326		G199	G6	C67	
G1043	C979	A914	U850	A781	A715	A648	C582	C519		C395	A327		G200	G68	G69	
A1044	C980	A915	G851	A782	A716	A649	C583	A520	A459	G396	C328		G201	G69	U70	
G1045	G981		G852	C783	U717	A649	A584	G521	A460	C397	A329		G202	A8		
A1046	U982	A918	C853	A784	C718	G650	G585	G521	A461	U398	C330		A205	A8		
G1047	A983	U919		G785	A719	C651	G586	C522	A462	U399			C206	G9	A71	
G1048	C984	U920	C856	G786	C720	G652	C587	G524	A463	G399	C334		C207	A10	A72	
U1049	C985	U921	C857	A787	G721	A655	G588	G524	U464	C400	C335		U208	G11	A73	
G1050		G922	G858		G722	G656	G589	C526	U465	C401	C336		U209	U13		
C1051	A923	A923	C859	A790	U723	U662	U595	G527	A466	C403	G337		C210	U14	A77	
U1052	C924	G925	A860	G791	G724	G661	U596	G528	A467	G404	A338		G211	U15	A78	
C1053	G925	G926	C861	A792	G725	C660	U597	G529	U468	U405	C339		G212	A16	A79	
G1054	U991	U921	C862	U793	C726	G662	A600	C530	A469	G406	U340		G213	U17	A80	
A1055	U992	G927	G863	C794	G727	U663	G601	U531	C470	U407	C341		C214	C18	A81	
U1056	G933	G928	A864	C795	A728	A663	G597	G532	U471	U408	C342		C215	A19	A82	
G1057	A994	G929	A865	C796	A729	G664	U598	A533	U472	U409	U343		U216	U20	A83	
C1058	C995	C930	C866	C797	G730	G665	C599	A534	U473	G410	U344		C217	G21	U84	
U1059	A996	C931	G867		G731	U666	A602	G537	C477	A414	C345		A223	G22	U85	
G1060	U997	C932	C868	G800	G732	G667	G603	C536	U478	A415	A346		C222	U24	C87	
G1061	C998	G933	C869	U801	C733	G668	U603	C537	A479	A416	C347		A223	G25	C90	
U1062	A999	C934	U870	A802	G734	G669	U604	G538	C478	A417	A348		C224	A26	U91	
C1063	C1000	A935	U871		C735	G670		A539	U479	G418	G350		G225	G27	U92	
G1064	C1001	C936	A872	C805	C736		A607	G542	U479	G419	C351		G226	A28	U93	
U1065		A937	A873	C806	C737	A673	A608	U543	U479	G420	C352		G227	U29	C99	
C1066	A1004	A938	C874	A807	C738	G674	G609	U544	A482	C418	C353		A228	G31	U94	
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G1071	U1009		C879	G812	C743	C679	C614	G548	A487	G423	C358		C233	G35	U99	
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		U950	C881	A814	G745	A681	G616		C489	U425	G362		G235	U37	A101	
U1078	A1013	G948	C883	A815	A746	A682	G617	A553	C490	G426	A363		A236	G38	G102	
G1079	A1014	A949	U884	C817	A747	A687	C618	A554	C491	U427	A364		G237	G39	C106	
A1080	G1015	U951	C885	G818	A749	G688	U619	U555	C492	G428	A365		A238	C40	G107	
A1081	A1016	G951	C886	A819	C750	C889	C620	C556	A493	U429	U366		G239	C41	G108	
U1082				U820	U751	U692	A621	G557	C494	A431	U367		U240	C43	G109	
G1083	A1019	G954	A889	G821	G752	G693	A622	G558	A495	A432	U368		A243	C44	G110	
U1084	G1020		C890	U822	A753	A694	C623	A559	C496	G433	U369		U244	A44	G111	
U1085	A1021	A958	U891	C823	C754	A695	U625	U561	A498	U434	C370		U245		G112	
U1086	A1022	A959	A892	G824	G756	A696	G626	U562	A499	A435	A306		U246			
	U1023	U960	C893	A825	C758	A697	G627	U563	A500	C436	A307		A247		G115	
A1092	G1024	U961	C896	C826	A759	G698	G628	C564	C501	U437	A371		A248		G116	
G1094	U1025	C962	C897	U827	G760	G699	A629	C565	A502	U438	A372		G249		G117	
U1095	C1027	A964	C898	G829	G761	G700	A630	G566	C503	U439	A373		C248		A51	
C1096	C1028	U965	C899	G830		U701	C631	G567	C504	C440	A374		U249		C52	
G1097	U1029	G966	A900	A831	C764	A702	C632	G568	C505	A441	C379		A250		A119	
C1098	U1030	C967	A901		G765	G703	G633	G569	U506	G442	G380		G251		A120	
G1099	C1031	A968	G902	C839	A766	A704	C634	C570	C507	C443	C381		U252		C54	
C1100	G1032	A969	G903	C840	A767	G705	A635	U571	U508	G444	A382		C124		G125	
A1101		C970	C841	C841	A768	A706	A636	U572	A509	G445	A383		U125		A59	
A1102	A1035	G971	U842	U842	G769	U707	C637	A573	A510		A384		G254		A60	
C1103	A1036	C972	U843	U843	C770	U708		A574	C511	A448	A385		U256		A61	
G1104	C1037	G973	G844	G844	C771	U709	A640	G575	C512	G449	C386		G257		A62	
A1105	C1038	A974	A909	A845	G776	G710	U641	C576	C513	G450	A389		G258		U62	
													G259		C63	



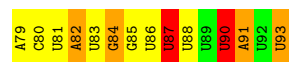
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 28% 42% 30%



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

Chain A2: 13% 47% 27% 13%



• Molecule 24: tRNA-fMet

Chain A3: 29% 45% 21% 5%



• Molecule 25: 50S ribosomal protein L2

Chain BC: 89% 9%



- Molecule 26: 50S ribosomal protein L3

Chain BD: 90% 9%



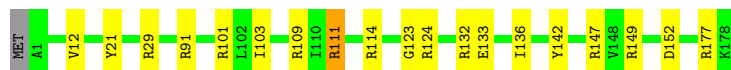
- Molecule 27: 50S ribosomal protein L4

Chain BE: 89% 10%



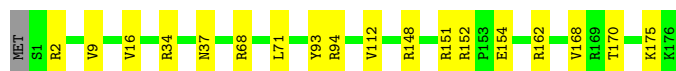
- Molecule 28: 50S ribosomal protein L5

Chain BF: 89% 10% ..



- Molecule 29: 50S ribosomal protein L6

Chain BG: 89% 10% .



- Molecule 30: 50S ribosomal protein L9

Chain BH: 95% 5%



- Molecule 31: 50S ribosomal protein L11

Chain BI: 95% . .

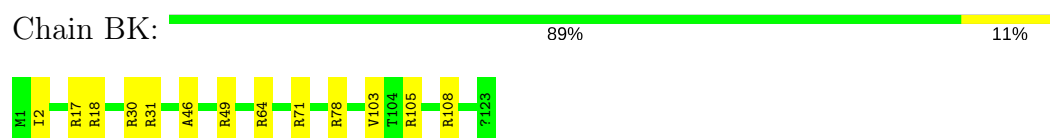


- Molecule 32: 50S ribosomal protein L13

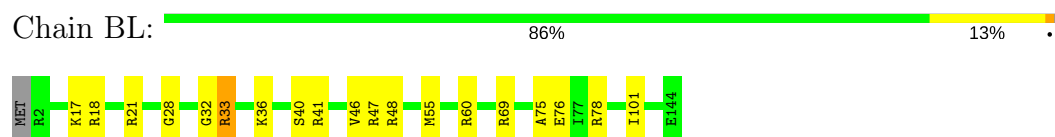
Chain BJ: 90% 10%



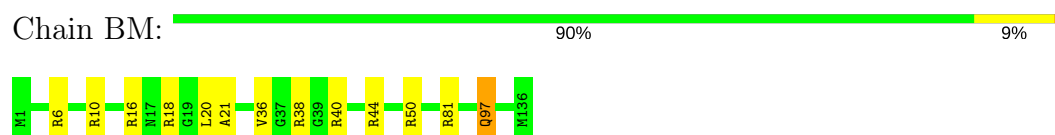
- Molecule 33: 50S ribosomal protein L14



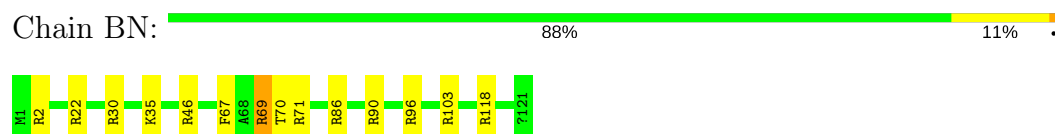
- Molecule 34: 50S ribosomal protein L15



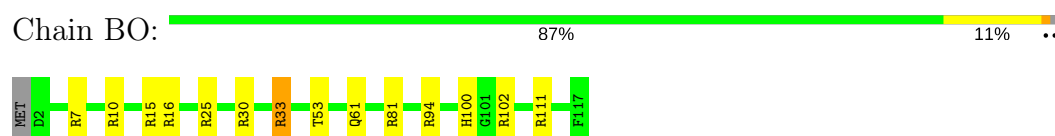
- Molecule 35: 50S ribosomal protein L16



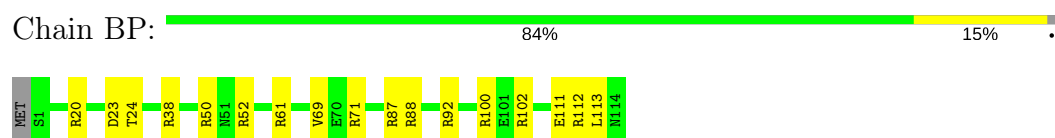
- Molecule 36: 50S ribosomal protein L17



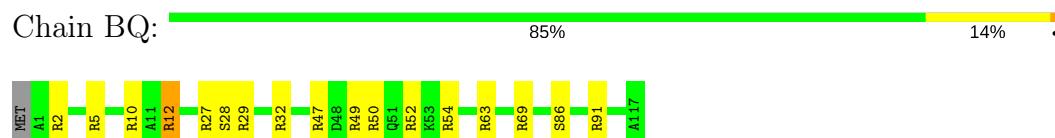
- Molecule 37: 50S ribosomal protein L18



- Molecule 38: 50S ribosomal protein L19



- Molecule 39: 50S ribosomal protein L20



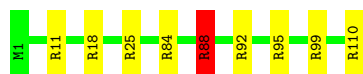
- Molecule 40: 50S ribosomal protein L21

Chain BR:  92% 8%



- Molecule 41: 50S ribosomal protein L22

Chain BS:  92% 7%




- Molecule 42: 50S ribosomal protein L23

Chain BT:  91% 7%



- Molecule 43: 50S ribosomal protein L24

Chain BU:  88% 12%



- Molecule 44: 50S ribosomal protein L25

Chain BV:  95% 5%



- Molecule 45: 50S ribosomal protein L27

Chain BW:  89% 10%



- Molecule 46: 50S ribosomal protein L28

Chain BX:  86% 11%



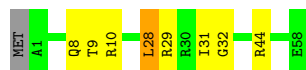
- Molecule 47: 50S ribosomal protein L29

Chain BY:  92% 8%



- Molecule 48: 50S ribosomal protein L30

Chain BZ: 85% 12% . .



- Molecule 49: 50S ribosomal protein L32

Chain B0: 77% 21% .



- Molecule 50: 50S ribosomal protein L33

Chain B1: 87% 13%



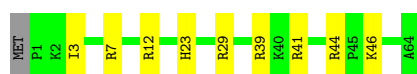
- Molecule 51: 50S ribosomal protein L34

Chain B2: 78% 22%



- Molecule 52: 50S ribosomal protein L35

Chain B3: 85% 14% .



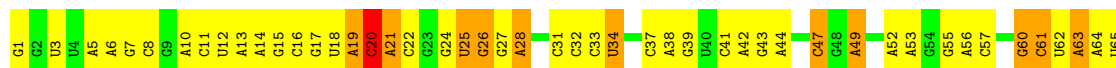
- Molecule 53: 50S ribosomal protein L36

Chain B4: 87% 13%



- Molecule 54: 23S ribosomal RNA

Chain BA: 22% 53% 21% .






A2095	G2035	G1972	G1845	A1784	G1723	G1595	C1533	A1469	A1403	G1339	A1274	U1209	A1146
C2096	C2036	G1973	G1846	A1785	G1726	A1596	U1534	A1470	C1404	U1340	A1275	G1210	A1147
A2097	A2037	G1974	A1847	A1786	C1727	A1597	A1535	G1471		A1342	A1276	G1211	U1148
U2098	G2038	G1975	A1848	A1787	G1728	A1598	C1536	C1472	U1409	A1343	G1277	G1212	G1149
U2099	U2039	G1976	G1849	C1788	C1729	U1599	G1537	G1473	G1410	G1343	C1278	A1213	C1150
G2100	G2040	A1977	G1850	A1789	G1730	C1600	G1538	U1474	U1411	U1344	G1279	A1214	A1151
A2101	U2041	A1978	U1851	C1790	G1731	G1601	U1539	G1475	U1412	C1345		G1215	C1152
G2102	A2042	U1979	U1852	A1791	G1732	A1602	G1540	U1476	A1413	G1346	A1284		C1153
G2103	C2043	G1980	A1853	G1792	G1733	U1603	C1541	A1477	A1414	A1347	A1285	G1218	G1154
C2104	C2044	A1981	A1854	C1793	G1734	C1604	U1542	G1478	U1415	A1348	A1286	U1219	A1155
	C2045	U1982		A1794	G1735	G1605	G1543	G1479	G1416	A1287	A1287	U1220	A1156
A2108	G2046	G1983	G1857	C1795	A1735	C1606	A1544	A1480	C1417	C1350	G1288	C1221	G1157
U2109	C2047	G1984	A1858	U1796	U1736	C1607	U1545	U1481	G1418	C1351	G1289	U1222	C1158
	G2048	C1985	U1859	G1797	G1737	A1608	G1546	G1482	A1419	U1352	C1290		U1159
U2113	G2049	C1986	G1860	U1798	G1738	A1609	C1547		A1420	A1353	C1291	G1226	G1160
A2114	C2050	A1987	G1861	G1799	A1739	A1610	A1548	U1485	G1421	A1354	G1292	G1227	C1161
G2115	A2051			A1800	G1740	C1611	A1549		G1422	G1355	C1293	G1228	G1162
A2117	G1929	G1990	U1864	A1801	C1741	A1612	C1550	C1488	G1423	G1356	U1294	C1229	G1163
G2063	G1930	U1991	A1865	A1802	U1742	G1613	A1551	C1489	G1424	C1357	A1230	A1230	C1164
A2054	U1931	G1992	A1866	A1803	G1743	A1614	A1552	A1490	G1425	G1358	G1296	U1231	A1165
A2119	A1932	U1993	G1867	C1804	U1744	C1615	A1553	G1491	G1426	A1359		U1232	G1166
G2065	C1994	G1994	C1868	A1805	A1745	G1616	U1554	G1492	C1427	C1362	G1298	U1233	C1167
G2056	G1933	U1995	G1869	C1806	A1746	U1617	G1555	C1493	C1428	G1300	G1235	U1234	G1168
G2057	C1934	C1996	C1870	G1807	U1747	A1618	C1556	A1494		G1363	A1169	G1235	A1169
A2058	G1935	C1997	A1871	A1808	C1748	C1685	C1557	A1495	A1431	G1364	A1301	G1236	G1170
A2059	A1936	C1997	C1872	A1809	A1749	C1686	C1558	A1496	G1432	A1365	A1302	A1237	G1171
A2060	A1937	A1998	A1873	A1810	G1750	G1687	C1559	U1497	A1433	A1366	G1303		U1172
G2061	C1938	C1999	C1874	G1811	U1751	U1688	G1560	A1504	A1434	A1367	A1304	U1240	U1173
A2126	A2062	C2000	A1880	C1812	G1752	A1689	C1561	U1506	G1435	C1368	C1305	A1241	U1174
G2127	C2063	C2001	G1875	G1813	C1753	A1690	U1562	G1500	G1436	G1369	C1306	U1242	A1175
C2129	C2064	G2002	A1876	G1814	G1754	C1691	U1563	G1501	G1437	C1370	A1307	G1243	U1176
G2120	C2065	A2003	A1877	A1815	A1755	U1692	C1564	A1502	U1438	G1371	A1308	A1244	G1177
G2121	C2066	G2004	G1878	C1816	G1756	U1693	C1565	A1503	U1439	U1372		G1245	C1178
U2122	G2067	A2005	A1880	C1817	A1757	G1694	A1566	A1504	U1442	A1373		A1246	U1179
	C2068	C2006	C1881	U1817	U1758	G1695	G1567	A1505	U1443	U1312	U1312	A1247	U1180
A2134	G2069	U2007	C1882	A1818	A1759	G1696	A1568	U1506	G1443	U1313	U1313	U1248	U1181
A2135	A2070	C2008	C1883	A1819	C1760	G1697	A1569	C1507	G1444	C1314	U1249	U1249	G1182
G2136	C1947		G1884	U1820	G1761	A1698	A1570	A1508	G1445	C1315		G1250	U1183
U2137	G1948	A2009	A1885	A1821	C1762	U1699	A1571	A1509	C1446	U1316		C1251	U1184
G2138	G1949		A1886	C1822	G1763	G1699	A1572	G1510	G1447			G1252	G1185
U2139	G1950	A2013	C1887	G1823	A1764	A1701	G1573	G1511	G1448			A1253	G1186
G2140	U1951	A2014	A1888	G1824	U1765		C1574	G1512		C1319	C1320	A1254	U1187
G2141	A1952	A2015	G1889	U1825	G1766	A1641	U1575	G1513	G1451	A1321	A1321		U1188
A2142	A1953	U2016	A1890	G1826	G1767	G1642	C1576	G1514	G1452	A1322		G1257	A1189
C2143	G1954	G2017	A1891	U1827	C1768	G1643	C1577	U1515	A1453	A1384	A1322	U1258	G1190
G2144	U1955	G2018	C1892	G1828	U1769	C1644	U1578	G1516	C1454	C1385	G1323	G1259	G1191
C2145	G1956	A2019	C1893	A1829	G1770	G1645	A1579	G1517	G1455	C1386	G1324	U1260	U1192
U2079	C1957	A2020	C1894	C1830	C1771	C1646	A1580	C1518	G1456	U1326	U1326	C1261	G1193
A2080	C1958	C2021	C1895	G1831	U1709	U1647	G1581		U1457	A1327	A1327	A1262	A1194
U2081	G1959	U2022	C1895	C1832	A1772	U1648	C1582	U1458	U1458	A1328		U1263	G1195
A2082	A1960	C2023		C1833	A1773	G1649	A1583	A1522	G1459	U1329		A1264	C1196
G2083	C1961	G2024	U1898	C1833	C1774	G1649	A1583	G1523	U1459	U1329		A1265	
C2084	C1962	C2025	A1899	C1836	U1775	A1650	U1584	G1524	G1460	A1330		G1266	C1200
U2085	U1963		A1900	C1837	U1776	G1651	U1585	A1525	C1461	G1331	G1267	U1201	U1201
U2086	G1964	A2021	A1901	C1838	G1777	G1715	A1586	A1526	C1462	G1332	U1267	A1268	
G2087	C1965	U2028	C1902	G1839	U1778	U1716	G1653	G1527	G1463	G1333	A1268	A1269	
A2088	A1966	G1903	G1904	G1840	U1779	A1717		A1528	G1463	G1334			A1204
C2089	C1967	G1904	C1905	U1841	A1780	A1655	A1590	G1529	G1465	C1335		G1270	A1205
A2090	G1968	A2031	G1906	G1842	U1781	C1656	A1591	G1530	U1466	A1336		G1271	G1206
C2091	G1969	U2092	G1907	C1843	U1782	A1657	A1592	G1531	U1467	G1337		A1272	C1207
U2092	A1969	G2032	A1970	C1843	A1783	C1658	A1593	A1532	U1468	U1402		U1273	C1208
G2093	G2157												
G2158													
G2159													
C2160													



Chain B5:

88%

7%

5%



4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

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

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

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

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

All (89) bond length outliers are listed below:

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

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

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

All (7075) bond angle outliers are listed below:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2651	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	2766	A	C5-C6-N1	6.35	120.88	117.70
21	AA	401	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	393	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	420	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	966	G	N1-C6-O6	-6.35	116.09	119.90
54	BA	1494	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	2225	A	C5-C6-N1	6.35	120.87	117.70
54	BA	2326	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2451	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	1507	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	1699	G	O4'-C1'-C2'	-6.35	99.45	105.80
21	AA	55	A	C5-C6-N1	6.34	120.87	117.70
21	AA	72	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	167	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	544	C	N1-C2-O2	6.34	122.71	118.90
54	BA	1084	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	1151	A	C5-C6-N1	6.34	120.87	117.70
54	BA	2362	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	167	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1528	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1934	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	368	U	C1'-O4'-C4'	-6.34	104.83	109.90
21	AA	179	A	C5-C6-N1	6.34	120.87	117.70
21	AA	826	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1563	U	O4'-C1'-N1	6.34	113.27	108.20
21	AA	443	C	N3-C2-O2	-6.33	117.47	121.90
25	BC	176	ARG	NE-CZ-NH1	6.33	123.47	120.30
26	BD	13	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	238	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	362	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	2392	A	C5-C6-N1	6.33	120.87	117.70
21	AA	408	A	C4-C5-C6	-6.33	113.83	117.00
21	AA	807	A	C4-C5-C6	-6.33	113.83	117.00
34	BL	78	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	271	G	O4'-C1'-N9	6.33	113.27	108.20
54	BA	673	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1477	A	C5-C6-N1	6.33	120.87	117.70
54	BA	2531	A	C5-C6-N1	6.33	120.87	117.70
54	BA	2745	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	753	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	23	C	N3-C2-O2	-6.33	117.47	121.90

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	64	A	C5-C6-N1	6.13	120.76	117.70
54	BA	835	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	925	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	60	G	N3-C2-N2	-6.13	115.61	119.90
54	BA	2432	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2823	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	1005	A	C5-C6-N1	6.12	120.76	117.70
54	BA	144	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	211	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	776	G	O4'-C1'-N9	6.12	113.10	108.20
21	AA	623	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	704	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	878	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1328	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1332	G	N3-C4-C5	-6.12	125.54	128.60
54	BA	1837	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	2301	C	N3-C2-O2	-6.12	117.61	121.90
24	A3	52	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1420	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1698	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2476	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2837	A	C5-C6-N1	6.12	120.76	117.70
54	BA	946	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1378	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2717	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2835	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1689	A	N1-C6-N6	-6.12	114.93	118.60
21	AA	324	G	N1-C6-O6	-6.12	116.23	119.90
21	AA	456	A	C5-C6-N1	6.12	120.76	117.70
21	AA	646	G	N1-C6-O6	-6.12	116.23	119.90
21	AA	792	A	O4'-C1'-N9	6.12	113.09	108.20
21	AA	1433	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	52	A	C5-C6-N1	6.12	120.76	117.70
54	BA	314	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1780	A	C4-C5-C6	-6.11	113.94	117.00
6	AG	91	ARG	NE-CZ-NH1	6.11	123.36	120.30
21	AA	1113	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1515	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	541	A	C5-C6-N1	6.11	120.75	117.70
54	BA	1744	A	C5-C6-N1	6.11	120.75	117.70
54	BA	2176	A	C4-C5-C6	-6.11	113.94	117.00
55	BB	29	A	N1-C6-N6	-6.11	114.94	118.60

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

All (1072) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	11	C	Sidechain

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Res	Type	Group
55	BB	57	A	Sidechain
55	BB	58	A	Sidechain
55	BB	59	A	Sidechain
55	BB	6	G	Sidechain
55	BB	63	C	Sidechain
55	BB	64	G	Sidechain
55	BB	66	A	Sidechain
55	BB	67	G	Sidechain
55	BB	68	C	Sidechain
55	BB	69	G	Sidechain
55	BB	7	G	Sidechain
55	BB	72	G	Sidechain
55	BB	84	G	Sidechain
55	BB	90	C	Sidechain
55	BB	95	U	Sidechain
55	BB	98	G	Sidechain
25	BC	102	TYR	Sidechain
26	BD	151	THR	Peptide
31	BI	140	GLU	Mainchain
35	BM	97	GLN	Peptide
36	BN	90	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	1	0
3	AD	1643	0	1710	1	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	1	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	1	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	1	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16457	2	0
22	A1	1627	0	832	1	0
23	A2	309	0	158	0	0
24	A3	1642	0	839	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31205	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BB	2504	0	1269	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99454	17	0

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

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BA:1068:G:H1'	54:BA:1069:A:C6	2.45	0.51
54:BA:1131:G:C5	54:BA:2025:C:H4'	2.50	0.46
22:A1:53:G:C8	22:A1:54:5MU:H72	2.50	0.46
18:AS:46:LEU:HD23	18:AS:46:LEU:H	1.81	0.46
3:AD:86:GLY:H	3:AD:200:VAL:HG23	1.81	0.45
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.82	0.45
8:AI:2:ACE:H1	8:AI:22:PRO:HG2	2.00	0.44
21:AA:477:C:H2'	21:AA:478:A:C8	2.53	0.43
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.37	0.43
21:AA:315:A:HO2'	21:AA:316:C:P	2.42	0.42
54:BA:1801:A:H3'	54:BA:1802:A:C5'	2.49	0.42
54:BA:1132:U:H2'	54:BA:1133:A:C8	2.55	0.42
54:BA:2233:U:H2'	54:BA:2234:G:C8	2.55	0.42
54:BA:1891:G:H2'	54:BA:1892:C:C6	2.55	0.41
2:AC:54:ILE:HG22	2:AC:68:HIS:H	1.86	0.41
54:BA:2014:A:H2'	54:BA:2015:A:C8	2.57	0.40
54:BA:2063:C:H2'	54:BA:2064:C:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	200 (92%)	15 (7%)	3 (1%)	13	54
2	AC	205/208 (99%)	188 (92%)	12 (6%)	5 (2%)	7	42
3	AD	203/206 (98%)	190 (94%)	7 (3%)	6 (3%)	5	37
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	9	46
5	AF	99/101 (98%)	83 (84%)	12 (12%)	4 (4%)	3	31
6	AG	150/152 (99%)	133 (89%)	14 (9%)	3 (2%)	9	46
7	AH	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
8	AI	126/128 (98%)	117 (93%)	6 (5%)	3 (2%)	7	42
9	AJ	98/100 (98%)	87 (89%)	6 (6%)	5 (5%)	2	26
10	AK	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	11	50
11	AL	121/124 (98%)	109 (90%)	8 (7%)	4 (3%)	4	35
12	AM	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
13	AN	98/101 (97%)	86 (88%)	9 (9%)	3 (3%)	5	37
14	AO	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	7	43
15	AP	79/81 (98%)	64 (81%)	9 (11%)	6 (8%)	1	18
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	14	56
17	AR	55/57 (96%)	51 (93%)	3 (6%)	1 (2%)	10	49
18	AS	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	14	56
19	AT	84/86 (98%)	75 (89%)	5 (6%)	4 (5%)	2	28
20	AU	51/53 (96%)	34 (67%)	13 (26%)	4 (8%)	1	18
25	BC	270/273 (99%)	241 (89%)	21 (8%)	8 (3%)	5	37
26	BD	207/209 (99%)	181 (87%)	18 (9%)	8 (4%)	3	31
27	BE	199/201 (99%)	172 (86%)	18 (9%)	9 (4%)	3	29
28	BF	176/179 (98%)	151 (86%)	20 (11%)	5 (3%)	6	39
29	BG	174/177 (98%)	151 (87%)	16 (9%)	7 (4%)	3	31
30	BH	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	13	54
31	BI	139/142 (98%)	128 (92%)	10 (7%)	1 (1%)	25	68
32	BJ	140/142 (99%)	123 (88%)	14 (10%)	3 (2%)	8	45
33	BK	121/123 (98%)	104 (86%)	13 (11%)	4 (3%)	4	35
34	BL	141/144 (98%)	110 (78%)	23 (16%)	8 (6%)	2	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BM	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	8	44
36	BN	119/121 (98%)	102 (86%)	16 (13%)	1 (1%)	22	67
37	BO	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
38	BP	112/115 (97%)	96 (86%)	12 (11%)	4 (4%)	4	33
39	BQ	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	20	63
40	BR	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
41	BS	108/110 (98%)	95 (88%)	12 (11%)	1 (1%)	20	63
42	BT	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	8	44
43	BU	101/104 (97%)	83 (82%)	13 (13%)	5 (5%)	2	27
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	63 (81%)	11 (14%)	4 (5%)	2	26
46	BX	75/79 (95%)	68 (91%)	5 (7%)	2 (3%)	6	40
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	50 (89%)	3 (5%)	3 (5%)	2	25
49	B0	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	4	33
50	B1	50/52 (96%)	42 (84%)	4 (8%)	4 (8%)	1	17
51	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	7	43
52	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	5	36
53	B4	36/38 (95%)	27 (75%)	8 (22%)	1 (3%)	6	39
56	B5	221/234 (94%)	207 (94%)	11 (5%)	3 (1%)	13	54
All	All	5876/6008 (98%)	5232 (89%)	490 (8%)	154 (3%)	10	40

All (154) Ramachandran outliers are listed below:

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

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

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

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

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Mol	Chain	Res	Type
50	B1	4	ILE
50	B1	37	LYS
51	B2	44	VAL
10	AK	77	GLY
25	BC	230	PRO
34	BL	55	MET
9	AJ	42	LEU
17	AR	20	ILE
29	BG	168	VAL
32	BJ	11	VAL
43	BU	56	GLY
48	BZ	32	GLY
50	B1	46	VAL
26	BD	93	GLY
29	BG	112	VAL
33	BK	71	ARG
27	BE	169	VAL
38	BP	69	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	178 (99%)	2 (1%)	78	89
2	AC	170/171 (99%)	169 (99%)	1 (1%)	89	94
3	AD	172/173 (99%)	167 (97%)	5 (3%)	48	73
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	86 (99%)	1 (1%)	78	89
6	AG	123/123 (100%)	121 (98%)	2 (2%)	68	85
7	AH	104/105 (99%)	101 (97%)	3 (3%)	48	73
8	AI	105/105 (100%)	101 (96%)	4 (4%)	38	67
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	56	79
10	AK	90/90 (100%)	89 (99%)	1 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	81 (98%)	2 (2%)	54	78
14	AO	76/77 (99%)	74 (97%)	2 (3%)	51	75
15	AP	65/65 (100%)	62 (95%)	3 (5%)	31	62
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	50	74
17	AR	48/48 (100%)	46 (96%)	2 (4%)	34	64
18	AS	70/70 (100%)	69 (99%)	1 (1%)	71	86
19	AT	65/65 (100%)	62 (95%)	3 (5%)	31	62
20	AU	44/44 (100%)	42 (96%)	2 (4%)	32	63
25	BC	216/217 (100%)	211 (98%)	5 (2%)	56	79
26	BD	164/164 (100%)	162 (99%)	2 (1%)	75	88
27	BE	165/165 (100%)	160 (97%)	5 (3%)	46	72
28	BF	149/150 (99%)	146 (98%)	3 (2%)	60	82
29	BG	137/138 (99%)	134 (98%)	3 (2%)	57	79
30	BH	114/114 (100%)	113 (99%)	1 (1%)	82	91
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	51	75
33	BK	103/103 (100%)	103 (100%)	0	100	100
34	BL	102/103 (99%)	100 (98%)	2 (2%)	60	82
35	BM	109/109 (100%)	108 (99%)	1 (1%)	82	91
36	BN	100/100 (100%)	97 (97%)	3 (3%)	46	72
37	BO	86/87 (99%)	82 (95%)	4 (5%)	30	62
38	BP	99/100 (99%)	95 (96%)	4 (4%)	36	65
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	57	79
40	BR	84/84 (100%)	83 (99%)	1 (1%)	75	88
41	BS	93/93 (100%)	92 (99%)	1 (1%)	78	89
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	54	78
44	BV	78/78 (100%)	77 (99%)	1 (1%)	73	87
45	BW	59/59 (100%)	58 (98%)	1 (2%)	66	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	46 (96%)	2 (4%)	34	64
49	B0	47/48 (98%)	43 (92%)	4 (8%)	12	42
50	B1	45/45 (100%)	44 (98%)	1 (2%)	57	79
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	50 (98%)	1 (2%)	60	82
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	171 (99%)	2 (1%)	75	88
All	All	4842/4870 (99%)	4750 (98%)	92 (2%)	65	82

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

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

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

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

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

Mol	Chain	Res	Type
2	AC	184	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	254 (16%)	0
22	A1	73/76 (96%)	10 (13%)	0
23	A2	14/15 (93%)	8 (57%)	0
24	A3	76/77 (98%)	15 (19%)	0
54	BA	2902/2903 (99%)	474 (16%)	0
55	BB	116/118 (98%)	18 (15%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4710/4722 (99%)	779 (16%)	0

All (779) RNA backbone outliers are listed below:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are no RNA pucker outliers to report.

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	16,26,27	1.79	3 (18%)	14,37,40	3.39	2 (14%)
22	6MZ	A1	37	22	18,25,26	1.12	2 (11%)	16,36,39	1.56	2 (12%)
22	7MG	A1	46	22	20,26,27	2.31	4 (20%)	22,39,42	1.92	2 (9%)
22	5MU	A1	54	22	14,22,23	1.13	1 (7%)	16,32,35	4.11	2 (12%)
22	PSU	A1	55	22	16,21,22	1.09	1 (6%)	20,30,33	5.37	7 (35%)
22	4SU	A1	7	22	14,21,22	1.13	1 (7%)	15,30,33	2.72	2 (13%)
24	H2U	A3	21	24	17,21,22	1.46	3 (17%)	21,30,33	1.28	4 (19%)
24	OMC	A3	33	24	15,22,23	1.21	1 (6%)	19,31,34	0.81	0
24	5MU	A3	55	24	14,22,23	1.18	1 (7%)	16,32,35	4.02	2 (12%)
24	PSU	A3	56	24	16,21,22	1.37	3 (18%)	20,30,33	5.17	7 (35%)
24	4SU	A3	8	24	14,21,22	1.12	0	15,30,33	2.88	3 (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
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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.64	1.32	1.45
22	A1	34	CM0	O5-C5	-5.44	1.26	1.37
24	A3	21	H2U	C4-N3	-3.53	1.32	1.37
24	A3	21	H2U	C2-N3	-3.41	1.31	1.38
22	A1	46	7MG	O5'-C5'	-3.00	1.40	1.44
22	A1	46	7MG	C8-N7	-2.80	1.31	1.43
24	A3	56	PSU	O5'-C5'	-2.75	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	37	6MZ	C8-N7	-2.55	1.29	1.34
24	A3	33	OMC	O5'-C5'	-2.29	1.41	1.44
24	A3	21	H2U	O5'-C5'	-2.24	1.41	1.44
24	A3	56	PSU	C6-C5	-2.21	1.35	1.38
22	A1	7	4SU	C2'-C1'	-2.18	1.50	1.53
22	A1	37	6MZ	O5'-C5'	-2.05	1.41	1.44
22	A1	46	7MG	C6-N1	2.16	1.37	1.33
24	A3	56	PSU	C4-N3	2.17	1.37	1.33
22	A1	55	PSU	C4-N3	2.47	1.37	1.33
22	A1	34	CM0	C4-C5	2.48	1.47	1.41
22	A1	34	CM0	C4-N3	2.52	1.37	1.33
22	A1	54	5MU	C4-N3	2.55	1.37	1.33
24	A3	55	5MU	C4-N3	2.67	1.37	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	55	PSU	N1-C2-N3	-15.74	117.08	128.40
24	A3	56	PSU	N1-C2-N3	-14.88	117.70	128.40
22	A1	55	PSU	C5-C4-N3	-12.52	115.16	125.43
24	A3	56	PSU	C5-C4-N3	-12.09	115.51	125.43
22	A1	54	5MU	C5-C4-N3	-9.68	114.56	125.24
24	A3	55	5MU	C5-C4-N3	-9.56	114.70	125.24
24	A3	8	4SU	C5-C4-N3	-7.00	114.89	123.73
22	A1	46	7MG	C5-C6-N1	-6.47	113.22	123.37
22	A1	7	4SU	C5-C4-N3	-6.43	115.60	123.73
24	A3	56	PSU	C5-C6-N1	-3.59	119.74	124.39
22	A1	55	PSU	C5-C1'-C2'	-3.29	109.88	115.55
22	A1	55	PSU	C5-C6-N1	-3.05	120.44	124.39
24	A3	56	PSU	C5-C1'-C2'	-2.67	110.93	115.55
24	A3	8	4SU	C4'-O4'-C1'	-2.30	107.32	109.77
22	A1	55	PSU	O4'-C1'-C2'	2.11	107.84	104.45
24	A3	21	H2U	C4-N3-C2	2.16	127.67	125.81
24	A3	21	H2U	C5-C4-N3	2.35	119.06	116.72
24	A3	21	H2U	C5-C6-N1	2.53	113.33	110.70
24	A3	56	PSU	O4'-C1'-C2'	2.58	108.60	104.45
24	A3	21	H2U	N3-C2-N1	2.81	119.53	116.73
22	A1	34	CM0	C7-O5-C5	3.16	124.11	117.75
22	A1	37	6MZ	C2-N1-C6	3.43	118.77	116.53
22	A1	55	PSU	C6-N1-C2	4.04	121.83	115.36
24	A3	56	PSU	C6-N1-C2	4.32	122.28	115.36
22	A1	37	6MZ	C9-N6-C6	4.42	126.64	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	C6-N1-C2	5.30	123.69	116.06
22	A1	7	4SU	C2-N3-C4	7.47	126.12	115.11
24	A3	8	4SU	C2-N3-C4	8.05	126.99	115.11
24	A3	56	PSU	C4-N3-C2	10.65	124.47	115.16
22	A1	55	PSU	C4-N3-C2	11.17	124.92	115.16
22	A1	34	CM0	C4-N3-C2	11.72	125.41	115.16
24	A3	55	5MU	C4-N3-C2	12.57	126.15	115.16
22	A1	54	5MU	C4-N3-C2	12.78	126.34	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [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	6,6,7	0.71	0	6,7,9	1.82	2 (33%)
58	FME	BA	3001	57	9,9,10	1.32	1 (11%)	7,9,11	1.05	1 (14%)

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	-	0/5/6/8	0/0/0/0
58	FME	BA	3001	57	-	1/6/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	3001	FME	CA-C	3.60	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
57	A1	101	VAL	O-C-CA	-3.89	116.07	125.15
58	BA	3001	FME	O-C-CA	-2.18	120.06	125.15
57	A1	101	VAL	C-CA-N	2.06	114.01	109.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.