



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:21 PM BST

PDB ID : 4V75
EMDB ID: : EMD-1721
Title : E. coli 70S-fMetVal-tRNAVal-tRNA^fMet complex in classic post-translocation state (post1)
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 : 12.00 Å(reported)
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

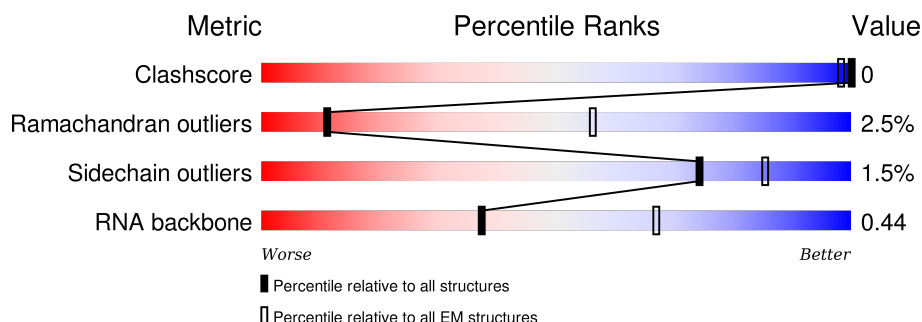
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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	97% .
2	AC	208	91% 8%
3	AD	206	89% 11%
4	AE	152	89% 11%
5	AF	101	87% 13%
6	AG	152	88% 11% .
7	AH	130	94% 5% .
8	AI	128	85% 15%

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

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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*P*AP*UP*U)-3'.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

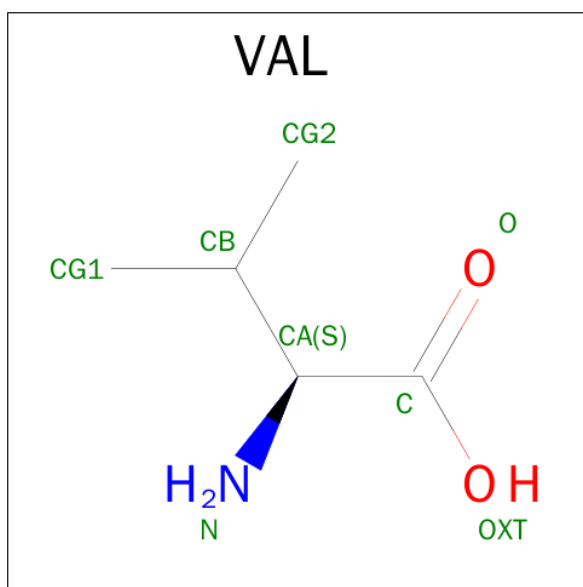
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

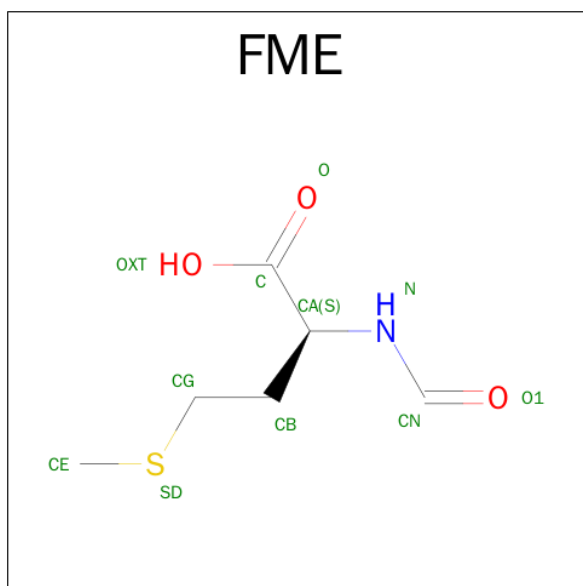
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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

- Molecule 1: 30S ribosomal protein S2

Category	Count
?7	1
R20	1
R62	1
R94	1
R112	1
T129	1
R221	1
R224	1
S225	1
?226	1

MET
G1
R10
V14
R39
R53
R71
R87
R106
R125
R126
R130
R142
R155
R163
R168
R171
R178
I195
Z207

ME1	A1	R2	Y3	R12	T29	A36	G41	A42	R43	R46	R55	R61	R62	R69	R72	R80	R103	R110	R114	R164	R183	R187	Y203	S204	Z205
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78	R19	R28	G43 R44	F47	R53 E54	R68	R92	I105 A106	R111	R137	S148 P149	R156	7159
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Category	Count
M1	1
R2	1
I6	1
R24	1
I36	1
L39	1
R44	1
R45	1
N52	1
N63	1
Q68	1
R86	1
M90	1
R91	1
?101	1

Chain AG: 88% 11%



- Molecule 7: 30S ribosomal protein S8

Chain AH: 94% 5%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 85% 15%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 87% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 91% 9%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 89% 10%



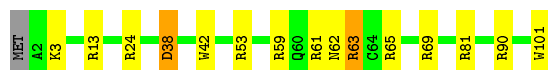
- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%




- Molecule 13: 30S ribosomal protein S14

Chain AN: 84% 13%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  85% 13%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  86% 14%



- Molecule 16: 30S ribosomal protein S17

Chain AQ:  89% 9%



- Molecule 17: 30S ribosomal protein S18

Chain AR:  89% 11%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  93% 7%




- Molecule 19: 30S ribosomal protein S20

Chain AT:  91% 9%



- Molecule 20: 30S ribosomal protein S21

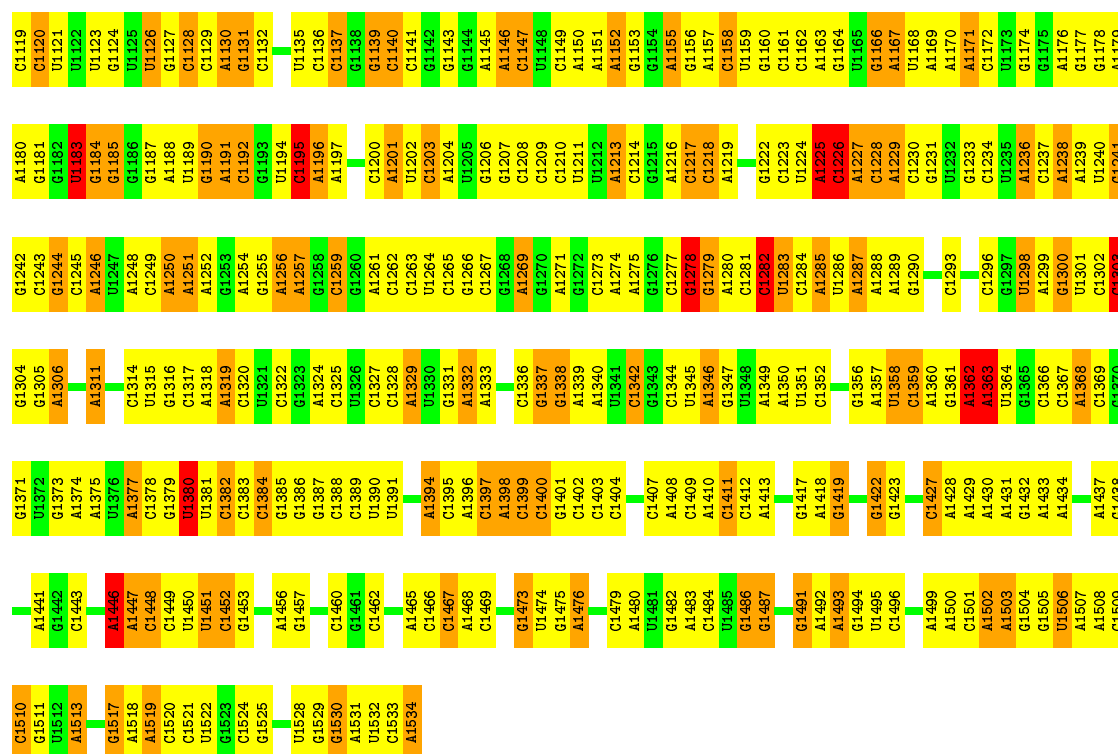
Chain AU:  79% 15% 6%



- Molecule 21: 16S ribosomal RNA

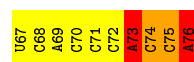
Chain AA:  26% 49% 22%





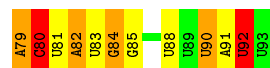
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 28% 54% 13% 5%



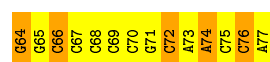
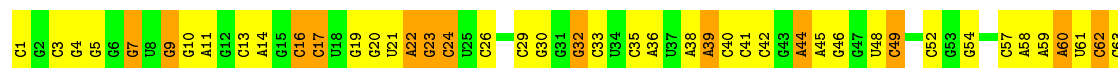
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

Chain A2: 27% 33% 27% 13%

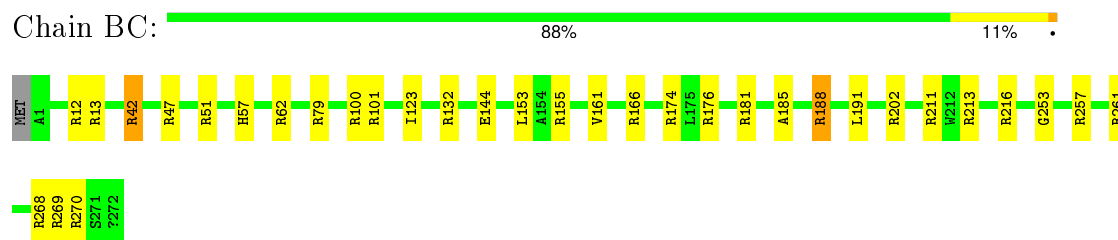


• Molecule 24: tRNA-fMet

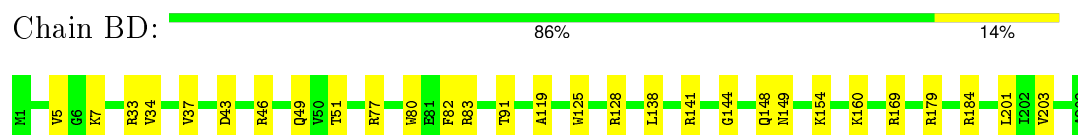
Chain A3: 25% 52% 23%



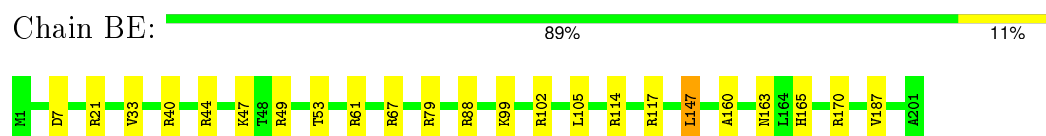
• Molecule 25: 50S ribosomal protein L2



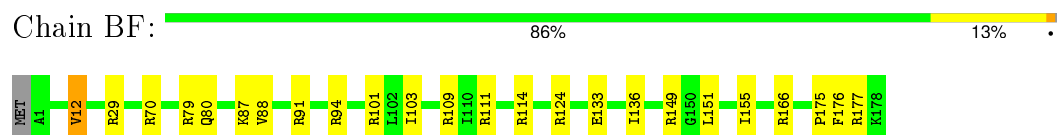
- Molecule 26: 50S ribosomal protein L3



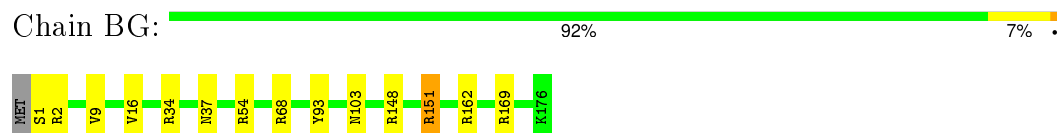
- Molecule 27: 50S ribosomal protein L4



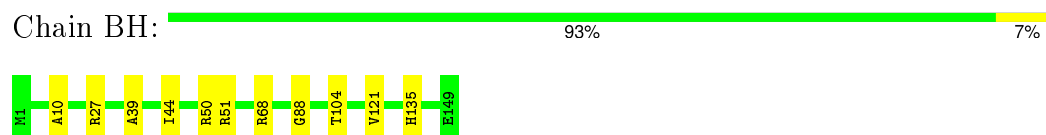
- Molecule 28: 50S ribosomal protein L5



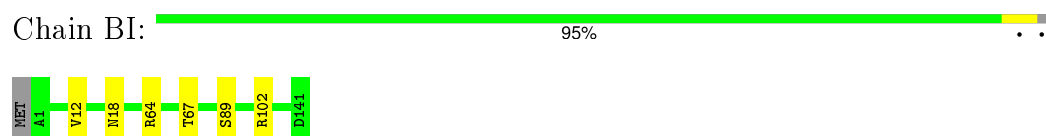
- Molecule 29: 50S ribosomal protein L6




- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L11



- Molecule 32: 50S ribosomal protein L13

Chain BJ:  92% 8%




- Molecule 33: 50S ribosomal protein L14

Chain BK:  88% 11%



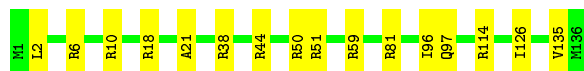
- Molecule 34: 50S ribosomal protein L15

Chain BL:  82% 17%




- Molecule 35: 50S ribosomal protein L16

Chain BM:  88% 12%



- Molecule 36: 50S ribosomal protein L17

Chain BN:  85% 15%




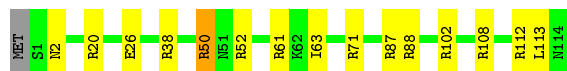
- Molecule 37: 50S ribosomal protein L18

Chain BO:  89% 10%



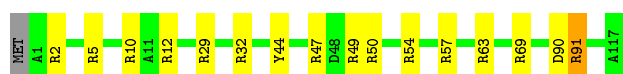
- Molecule 38: 50S ribosomal protein L19

Chain BP:  86% 12%



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  86% 13%



- Molecule 40: 50S ribosomal protein L21

Chain BR: 90% 10%



- Molecule 41: 50S ribosomal protein L22

Chain BS: 93% 7%



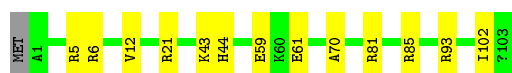
- Molecule 42: 50S ribosomal protein L23

Chain BT: 90% 10%



- Molecule 43: 50S ribosomal protein L24

Chain BU: 87% 13% •



- Molecule 44: 50S ribosomal protein L25

Chain BV: 90% 10%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 86% 11% •

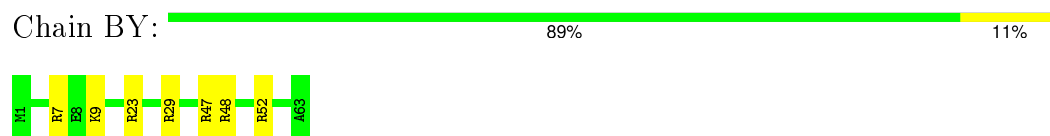


- Molecule 46: 50S ribosomal protein L28

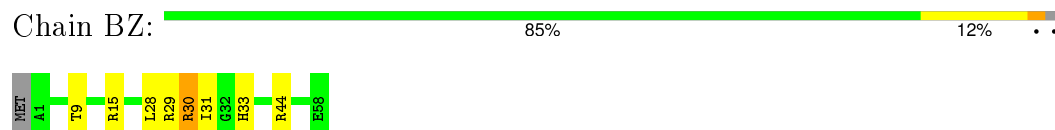
Chain BX: 82% 14% ••



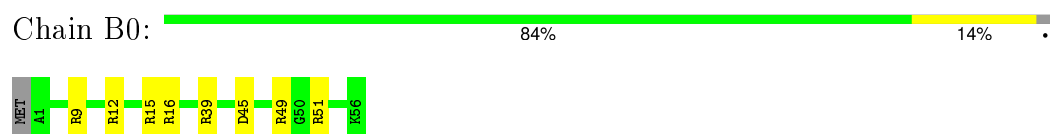
- Molecule 47: 50S ribosomal protein L29



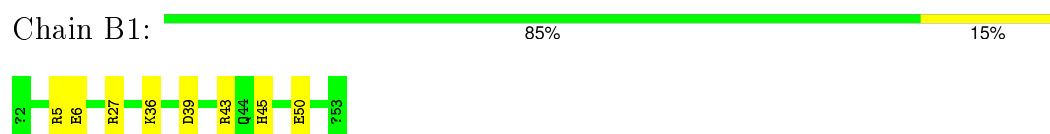
- Molecule 48: 50S ribosomal protein L30



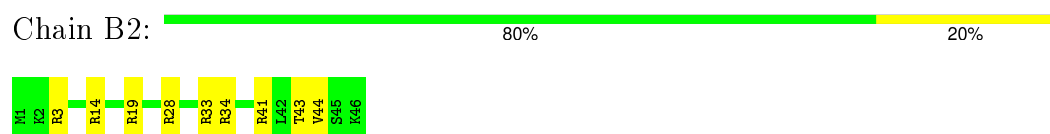
- Molecule 49: 50S ribosomal protein L32



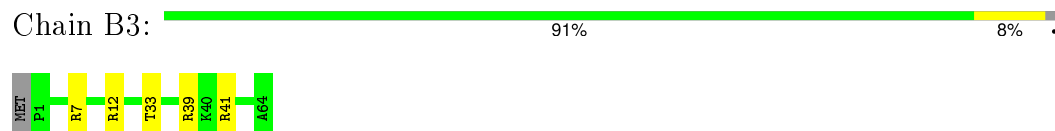
- Molecule 50: 50S ribosomal protein L33



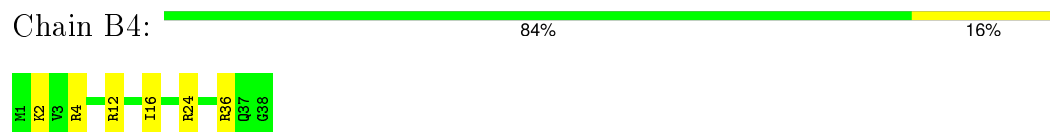
- Molecule 51: 50S ribosomal protein L34



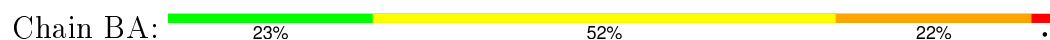
- Molecule 52: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L36

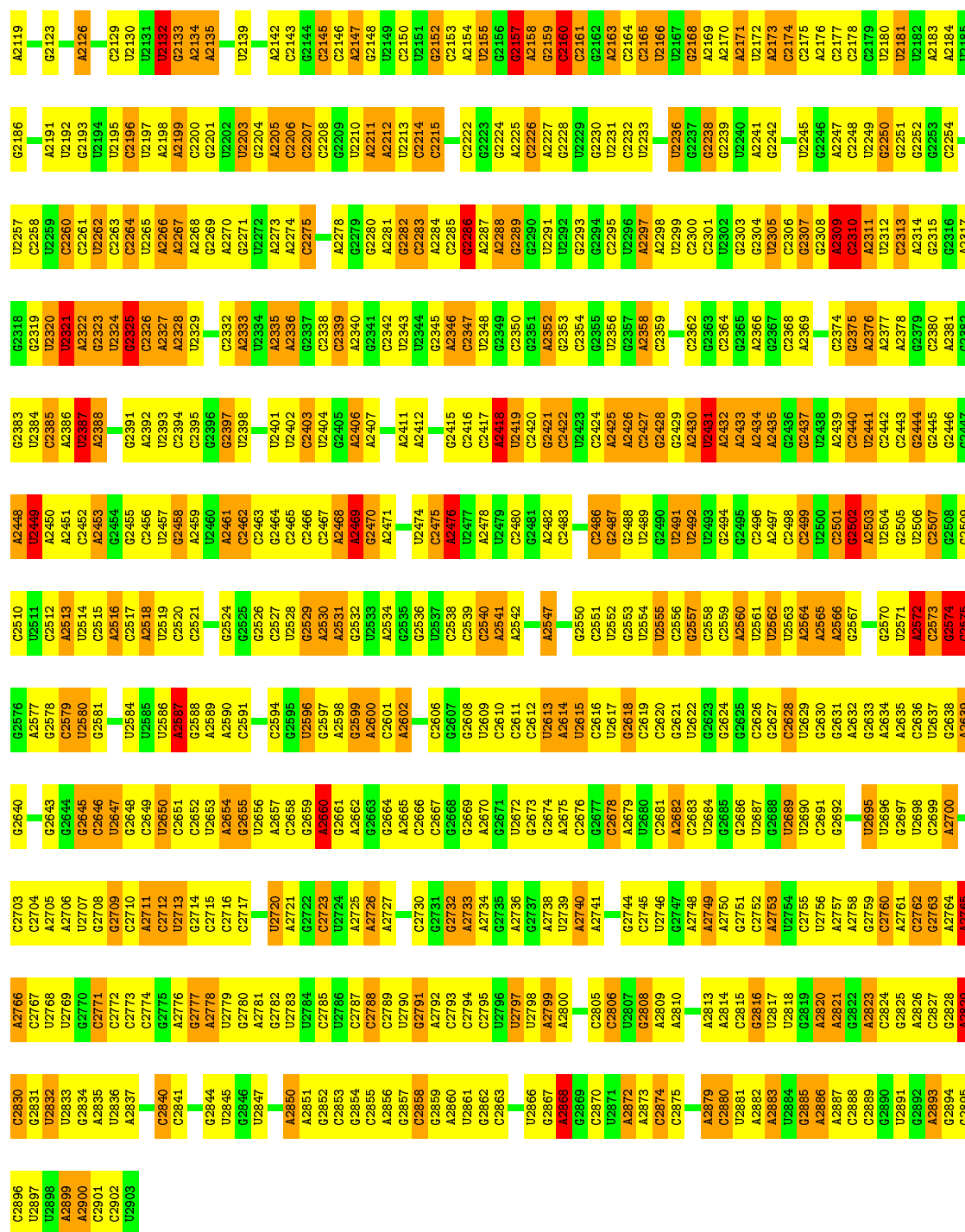


- Molecule 54: 23S ribosomal RNA



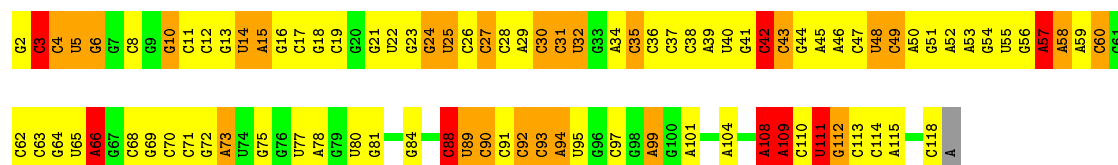
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G1036	A974	A910	A845	A781	A716	C545	A582	C516	A453	G388	A322	G258	A198	U72	A71	U3
G1037	G975	A911	A846	A782	C717	G647	A583	C517	A454	G389	C323	G259	A199	U73	U72	U4
A1038	A979	C912	U846	A783	C718		C584	G518	C455	U390	A324		U200	A73	A73	A5
A1040	A980	G913	U847	A784	C719	C650	A585	G519	C456	A391		A262	C201	A74	A74	A6
	A981	C915	C848	G785	U720		A586	G520	A457	U392	C327	C263	U202	C75	C75	A7
C1043	C982	G916	U850	C786	A721	U653	C587	U521	C458	C393	U328	C264	A203	C76	C76	A8
C1044	A983	A917	C851	A787	C722	A654	U588	A522	C459	C394	G329	A265	A204	G77	G77	A9
C1045	A984	A918	C852	A788	C723	A655	U589	G523	C460	U395	A330	C266	U205	C143	C143	A10
A1046	C985	U919	C853	A789	U724	A656	A590	G524	C461		C331	C267	U206	C144	C79	C11
G1047	C986	A920	C854	U790	G725	U657	U591	U525	C462	C398	A332	C268	A207	C145	U12	U12
A1048	C987	C921		U791	G726	U658	A592	A526	G463	C399	G333	C269	C208	A146	A13	A13
C1049	A988	C922	G858	C791	G727	U659	A593	C527	U464	G400	C334	A270	C209	C147	A84	A84
A1050	C989	G923	C859	A792	A727	G659	C595	A528	A465	A401	C335	G271	C210	U148	G85	G15
G1051	A990	A924	U860	A793	G728	C660	U596	A529	A466	A402	C336	A272	C211	U149	G86	C16
C1052	C991	G925	U861	A794	G729	A661	G597	G530		A403	G273		G212	U150	U87	
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G1056	C995		C865	G801	G733	U665	C601		G473	G406	A342	A278	A222	U154	A91	C22
A1057	A996	U931	A866	A802	A734	A666	A602	A538	G474	G411	C343	U279	A217	U155	U92	
G1058	G997	U932	C867	A803	C736	G668	A603	G540	G475	A412	A346	C282	A219	C157	A94	U25
C1059	C998	A933	U868	C737	G738	A670	U606	A541	A477	C413	A347	G283	A221	U158	A95	A28
U1060	U999	U934	G869	G805	G739	A671	U607	C542	A478	C414	A348	U284	A222	C96	C96	U29
U1061	A1000	C935	U870	C806	A739	C671	A608	G543	A479	A415	A349	G285	A223	A160	C97	G30
G1062	A1001	A936	U871	U807	C740	C672	A609	G544	A480	U416	U349	G286	A224	A161	G98	C31
G1063	G1002	C937	U872	G808	U741	C673	C610	U545	G481	C417	G350	U287	U225	U162	U99	C32
C1064	G1003		G874	G809	A742	G674	C611	U546	A482	C418	C351	G287	G225	C163	U100	C33
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U1066	G942	G942	C876	U811	U744	A677	A613	G548	C484	C420	C353	G289	A227	C165	U102	
A1067	A943	A943	A877	C812	U745	A678	A614	G549	C485	C421	A354	U290	C228	U166	A103	C37
G1068	C944	C944	A878	U813	U746	C678	U615	G550	C486	A422	C357	U292	C229	G168	A104	A38
A1069	A1008	A945		C814	U747	C679	A616		C487	A423		U293	G230	G169	C105	G39
A1070	A1009	A946	G883	C815	G748	C680	G617	U554	G488	G232	U294	G232	A231	U170	C106	U40
G1071	A1010	A947	C884	C816	A749			G555	G489	U427	A294	G233	A232	U171	G107	C51
C1072	G1011	C948	C885	C817	A750	U683	G620	A556	C490	U427	G295	A233	A233	A172	A42	A42
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G1074	C1013	C951	U887	A819	A752	A885	G622	U558	A492	A429	A299	U235	U235	A173	C109	A44
C1075	U1014	G952	C888	A820	A753	U686	C623	G559	G493	A430	A300	C236	C236	U174	A111	
C1076	U1015	G953	C889	A821	U754	C687	C624	G560	C494	U431	C364	G301	C237	G175	U112	
A1077	G1016	G954	C890	G822	U755	U688	G625	G561	G495	A432	C365	G302	C238	A176	U113	G48
U1078	G1017	U955	G891	C823	U756	A689	A626	U562	G496	C433	G367	G303	C239	G177	U114	A49
C1079	U1018	G956	A892	U824	G757	G690	A627	A563	C497	C434	A368	U304	C240	G178	C115	
A1080	U1019	C957	C893	A825	C758	C691	G628	C564		C435	U369	C305	A241	C179	C116	A52
U1081	A1020	U958	U894	U826	G759	C692	G629	C565	G500	C436	U370	U306	G242	G180	G117	A53
U1082	A1021	A959	U895	G760	G760	A693	G630	U566	A501	G370	A371	G307	U243	A118	A118	G54
U1083	G1022	A960	A896	U828	A761	U694	A631	U567	A502	G372	G372	G308	A244	A182	A119	G55
A1084	U1023	C961	C897	U829	U762	U694	A632	U568	A503	U373	A374	A309	G245	C183	U120	A56
A1085	G1024	G962	C898		G763	C698	A633		A504	U441	G374	A310	G246	C184	G121	C57
G1086	G1025	U963	A899	A764	A764	A699	C634	U571		G442	G375	A311	G247	G187	G122	
G1087	G1026	C964	A900	C765	C765		C635	A505	G442	G312	G376	G312	G248	A125	A125	C61
A1088	A1027	C965	C901	G834	U766	U702	G636	A506	C443	G313	C378	G313	C249	A126	U62	A63
A1089	A1028	G966	C902	C835	U767	G703	G637	A507	C444	G314	G379	G314	G250	A127	A127	A64
A1090	A1029	U967	C903	G836		G704	G638	A508	C445	G315	G379	G315	G251	A191	A191	A65
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C1092	G1031	G969	A905	C838	G773	A706	C640	C510	U447	G317	C383	G317	G253	C193	C129	A65
G1093	A1032	U970	U906	U839	G774	A707	U641	G511	U448	G318	A384	G318	G254	U194	C130	C66
U1094	U1033	G971	G907	C840	G775	U709	U642	G513	A513	G450	C385	G319	A255	A195	A131	

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G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548			
A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610						
C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678
A1679	A1680	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	A1690	A1691	A1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	A1700	A1701	A1702	A1703	A1704	A1705	A1706	A1707	A1708	A1709	A1710	A1711	A1712	A1713	A1714	A1715	A1716	A1717	A1718	A1719	A1720	A1721	A1722	A1723	A1724	A1725	A1726	A1727	A1728	A1729	A1730	A1731	A1732	A1733	A1734	A1735	A1736	A1737	A1738	A1739	A1740						
C1741	C1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803					
C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867				
C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930					
G1929	G1930	G1931	G1932	G1933	G1934	G1935	G1936	G1937	G1938	G1939	G1940	G1941	G1942	G1943	G1944	G1945	G1946	G1947	G1948	G1949	G1950	G1951	G1952	G1953	G1954	G1955	G1956	G1957	G1958	G1959	G1960	G1961	G1962	G1963	G1964	G1965	G1966	G1967	G1968	G1969	G1970	G1971	G1972	G1973	G1974	G1975	G1976	G1977	G1978	G1979	G1980	G1981	G1982	G1983	G1984	G1985	G1986	G1987	G1988	G1989	G1990						
C1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020	C2021	C2022	C2023	C2024	C2025	C2026	C2027	C2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041	C2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055					
G2056	G2057	A2058	A2059	G1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020	C2021	C2022	C2023	C2024	C2025	C2026	C2027	C2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041	C2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	

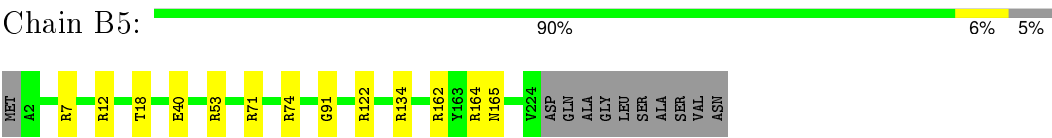


• Molecule 55: 5S ribosomal RNA

Chain BB: 20% 50% 22% 7%



- Molecule 56: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	13207	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	161000	Depositor
Image detector	4k CCD camera (TVIPS)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	AB	0.70	0/1736	0.99	6/2340 (0.3%)
10	AK	0.74	0/894	1.23	11/1207 (0.9%)
11	AL	0.74	0/969	1.22	13/1300 (1.0%)
12	AM	0.76	0/884	1.30	14/1181 (1.2%)
13	AN	0.78	0/817	1.25	11/1088 (1.0%)
14	AO	0.72	0/722	1.19	8/964 (0.8%)
15	AP	0.77	0/648	1.19	8/870 (0.9%)
16	AQ	0.70	0/658	1.14	7/883 (0.8%)
17	AR	0.81	0/463	1.22	5/623 (0.8%)
18	AS	0.74	0/653	1.08	5/879 (0.6%)
19	AT	0.69	0/672	1.12	8/890 (0.9%)
2	AC	0.73	0/1651	1.13	16/2225 (0.7%)
20	AU	0.83	0/431	1.51	9/572 (1.6%)
21	AA	1.53	0/36759	2.21	1951/57346 (3.4%)
22	A1	1.55	0/1668	2.23	94/2595 (3.6%)
23	A2	1.46	1/343 (0.3%)	2.24	14/531 (2.6%)
24	A3	1.52	0/1722	2.20	88/2685 (3.3%)
25	BC	0.74	0/2121	1.26	28/2852 (1.0%)
26	BD	0.69	0/1586	1.17	11/2134 (0.5%)
27	BE	0.67	0/1571	1.18	13/2113 (0.6%)
28	BF	0.75	0/1444	1.24	15/1937 (0.8%)
29	BG	0.69	0/1343	1.17	10/1816 (0.6%)
3	AD	0.75	0/1665	1.16	16/2227 (0.7%)
30	BH	0.65	0/1122	1.07	4/1515 (0.3%)
31	BI	0.66	0/1046	1.00	2/1410 (0.1%)
32	BJ	0.71	0/1152	1.14	8/1551 (0.5%)
33	BK	0.70	0/947	1.28	11/1268 (0.9%)
34	BL	0.73	0/1054	1.32	13/1403 (0.9%)
35	BM	0.74	0/1093	1.15	10/1460 (0.7%)
36	BN	0.77	0/973	1.27	14/1301 (1.1%)
37	BO	0.73	0/902	1.28	12/1209 (1.0%)
38	BP	0.76	0/929	1.28	12/1242 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.78	0/960	1.32	14/1278 (1.1%)
4	AE	0.69	0/1119	1.12	11/1506 (0.7%)
40	BR	0.73	0/829	1.16	8/1107 (0.7%)
41	BS	0.64	0/864	1.18	8/1156 (0.7%)
42	BT	0.64	0/744	1.21	7/994 (0.7%)
43	BU	0.69	0/787	1.17	7/1051 (0.7%)
44	BV	0.70	0/766	1.20	8/1025 (0.8%)
45	BW	0.73	0/604	1.28	9/799 (1.1%)
46	BX	0.76	0/635	1.31	10/848 (1.2%)
47	BY	0.67	0/510	1.24	6/677 (0.9%)
48	BZ	0.71	0/453	1.22	5/605 (0.8%)
49	B0	0.74	0/450	1.31	8/599 (1.3%)
5	AF	0.72	0/835	1.09	6/1128 (0.5%)
50	B1	0.74	0/417	1.16	3/556 (0.5%)
51	B2	0.81	0/380	1.48	8/498 (1.6%)
52	B3	0.72	0/513	1.18	4/676 (0.6%)
53	B4	0.67	0/303	1.29	4/397 (1.0%)
54	BA	1.41	1/69796 (0.0%)	2.21	4036/108888 (3.7%)
55	BB	1.41	0/2800	2.17	154/4367 (3.5%)
56	B5	0.64	0/1673	1.10	11/2255 (0.5%)
6	AG	0.74	0/1188	1.23	15/1593 (0.9%)
7	AH	0.70	0/989	1.00	5/1326 (0.4%)
8	AI	0.79	0/1035	1.28	19/1377 (1.4%)
9	AJ	0.71	0/797	1.18	10/1079 (0.9%)
All	All	1.28	2/160085 (0.0%)	1.99	6823/239402 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
21	AA	0	350
22	A1	0	14
23	A2	0	5
24	A3	0	16
25	BC	0	1
3	AD	0	2
38	BP	0	1
4	AE	0	1
54	BA	0	663
55	BB	0	31
All	All	0	1084

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A2	80	C	C4-N4	-5.22	1.29	1.33
54	BA	1314	C	C4-N4	-5.09	1.29	1.33

All (6823) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2740	A	O4'-C1'-N9	13.91	119.33	108.20
54	BA	1610	A	O4'-C1'-N9	13.75	119.20	108.20
54	BA	1584	U	O4'-C1'-N1	12.72	118.38	108.20
54	BA	280	U	O4'-C1'-N1	12.43	118.14	108.20
54	BA	1854	A	N1-C6-N6	-12.29	111.23	118.60
54	BA	2589	A	N1-C6-N6	-12.18	111.29	118.60
54	BA	2450	A	N1-C6-N6	-12.15	111.31	118.60
54	BA	1606	C	O4'-C1'-N1	12.12	117.90	108.20
21	AA	825	A	N1-C6-N6	-12.10	111.34	118.60
21	AA	935	A	N1-C6-N6	-12.02	111.39	118.60
54	BA	1384	A	N1-C6-N6	-11.94	111.43	118.60
54	BA	323	C	O4'-C1'-N1	11.90	117.72	108.20
22	A1	21	A	N1-C6-N6	-11.81	111.52	118.60
54	BA	2062	A	N1-C6-N6	-11.79	111.52	118.60
23	A2	79	A	N1-C6-N6	-11.75	111.55	118.60
54	BA	877	A	N1-C6-N6	-11.71	111.57	118.60
54	BA	103	A	N1-C6-N6	-11.67	111.60	118.60
54	BA	1155	A	N1-C6-N6	-11.60	111.64	118.60
54	BA	1427	A	N1-C6-N6	-11.54	111.68	118.60
54	BA	197	A	N1-C6-N6	-11.52	111.69	118.60
3	AD	12	ARG	NE-CZ-NH1	11.48	126.04	120.30
54	BA	99	U	O4'-C1'-N1	11.46	117.37	108.20
54	BA	1086	A	N1-C6-N6	-11.43	111.74	118.60
21	AA	499	A	N1-C6-N6	-11.40	111.76	118.60
54	BA	2009	A	N1-C6-N6	-11.38	111.77	118.60
21	AA	665	A	N1-C6-N6	-11.35	111.79	118.60
21	AA	716	A	N1-C6-N6	-11.34	111.80	118.60
54	BA	643	A	N1-C6-N6	-11.33	111.80	118.60
21	AA	1204	A	N1-C6-N6	-11.33	111.80	118.60
21	AA	194	C	N3-C2-O2	-11.31	113.98	121.90
54	BA	2600	A	N1-C6-N6	-11.27	111.84	118.60
21	AA	1080	A	N1-C6-N6	-11.19	111.89	118.60
21	AA	1250	A	N1-C6-N6	-11.18	111.89	118.60
54	BA	1780	A	N1-C6-N6	-11.17	111.90	118.60
22	A1	73	A	O4'-C1'-N9	11.16	117.13	108.20
54	BA	821	A	N1-C6-N6	-11.16	111.90	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1729	U	O4'-C1'-N1	11.14	117.11	108.20
54	BA	861	A	N1-C6-N6	-11.13	111.92	118.60
54	BA	1301	A	N1-C6-N6	-11.07	111.96	118.60
21	AA	968	A	N1-C6-N6	-11.07	111.96	118.60
54	BA	219	A	N1-C6-N6	-11.05	111.97	118.60
21	AA	279	A	N1-C6-N6	-11.03	111.98	118.60
54	BA	1810	A	N1-C6-N6	-11.03	111.98	118.60
54	BA	532	A	N1-C6-N6	-11.02	111.99	118.60
21	AA	1100	C	N3-C2-O2	-11.01	114.19	121.90
54	BA	1809	A	N1-C6-N6	-11.01	112.00	118.60
54	BA	2328	A	N1-C6-N6	-10.99	112.00	118.60
54	BA	2741	A	N1-C6-N6	-10.99	112.00	118.60
54	BA	149	A	N1-C6-N6	-10.98	112.01	118.60
21	AA	1252	A	N1-C6-N6	-10.98	112.01	118.60
21	AA	98	A	N1-C6-N6	-10.97	112.02	118.60
54	BA	2051	A	N1-C6-N6	-10.97	112.02	118.60
21	AA	547	A	N1-C6-N6	-10.96	112.02	118.60
54	BA	1630	A	N1-C6-N6	-10.96	112.02	118.60
54	BA	2727	A	N1-C6-N6	-10.96	112.02	118.60
54	BA	415	A	N1-C6-N6	-10.94	112.04	118.60
54	BA	2850	A	N1-C6-N6	-10.92	112.05	118.60
21	AA	199	A	N1-C6-N6	-10.92	112.05	118.60
43	BU	81	ARG	NE-CZ-NH1	10.91	125.76	120.30
54	BA	1392	A	N1-C6-N6	-10.89	112.06	118.60
54	BA	2572	A	O4'-C1'-N9	10.88	116.90	108.20
54	BA	1596	A	N1-C6-N6	-10.85	112.09	118.60
54	BA	217	A	N1-C6-N6	-10.83	112.10	118.60
54	BA	547	A	N1-C6-N6	-10.83	112.10	118.60
54	BA	1569	A	N1-C6-N6	-10.81	112.12	118.60
54	BA	1870	C	O4'-C1'-N1	10.80	116.84	108.20
21	AA	1431	A	N1-C6-N6	-10.79	112.12	118.60
54	BA	1247	A	N1-C6-N6	-10.77	112.14	118.60
54	BA	2434	A	N1-C6-N6	-10.75	112.15	118.60
54	BA	1679	A	N1-C6-N6	-10.74	112.16	118.60
21	AA	909	A	N1-C6-N6	-10.73	112.16	118.60
54	BA	38	A	N1-C6-N6	-10.73	112.16	118.60
21	AA	900	A	N1-C6-N6	-10.71	112.17	118.60
54	BA	1453	A	N1-C6-N6	-10.68	112.19	118.60
54	BA	2573	C	O4'-C1'-N1	10.68	116.74	108.20
54	BA	1395	A	N1-C6-N6	-10.67	112.20	118.60
54	BA	1699	G	O4'-C1'-N9	10.67	116.73	108.20
54	BA	2005	A	N1-C6-N6	-10.66	112.20	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1932	A	N1-C6-N6	-10.65	112.21	118.60
21	AA	194	C	N1-C2-O2	10.65	125.29	118.90
21	AA	914	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	2451	A	N1-C6-N6	-10.64	112.22	118.60
54	BA	1205	A	N1-C6-N6	-10.63	112.22	118.60
54	BA	1773	A	N1-C6-N6	-10.63	112.22	118.60
54	BA	1194	A	N1-C6-N6	-10.62	112.23	118.60
54	BA	1808	A	N1-C6-N6	-10.61	112.23	118.60
54	BA	1590	A	N1-C6-N6	-10.60	112.24	118.60
54	BA	2634	A	N1-C6-N6	-10.60	112.24	118.60
21	AA	1311	A	N1-C6-N6	-10.57	112.26	118.60
54	BA	1890	A	N1-C6-N6	-10.57	112.26	118.60
54	BA	119	A	N1-C6-N6	-10.56	112.26	118.60
21	AA	1105	A	N1-C6-N6	-10.55	112.27	118.60
21	AA	794	A	N1-C6-N6	-10.54	112.27	118.60
54	BA	2309	A	N1-C6-N6	-10.54	112.28	118.60
23	A2	91	A	N1-C6-N6	-10.54	112.28	118.60
55	BB	39	A	N1-C6-N6	-10.51	112.29	118.60
54	BA	1352	U	O4'-C1'-N1	10.51	116.61	108.20
54	BA	412	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	479	A	N1-C6-N6	-10.49	112.31	118.60
21	AA	915	A	N1-C6-N6	-10.48	112.31	118.60
54	BA	1914	C	N3-C2-O2	-10.48	114.57	121.90
54	BA	1755	A	N1-C6-N6	-10.47	112.31	118.60
21	AA	1398	A	N1-C6-N6	-10.46	112.32	118.60
54	BA	483	A	N1-C6-N6	-10.46	112.32	118.60
54	BA	2753	A	N1-C6-N6	-10.46	112.32	118.60
21	AA	74	A	N1-C6-N6	-10.46	112.32	118.60
54	BA	616	A	N1-C6-N6	-10.44	112.34	118.60
21	AA	553	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	1889	A	N1-C6-N6	-10.41	112.36	118.60
54	BA	1593	A	N1-C6-N6	-10.39	112.37	118.60
22	A1	6	A	N1-C6-N6	-10.38	112.37	118.60
54	BA	2587	A	N1-C6-N6	-10.37	112.38	118.60
21	AA	767	A	N1-C6-N6	-10.37	112.38	118.60
21	AA	1021	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	2336	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	2632	A	N1-C6-N6	-10.35	112.39	118.60
21	AA	1111	A	N1-C6-N6	-10.34	112.39	118.60
54	BA	1938	A	O4'-C1'-N9	10.34	116.47	108.20
54	BA	721	A	N1-C6-N6	-10.32	112.41	118.60
21	AA	766	A	N1-C6-N6	-10.31	112.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	298	A	N1-C6-N6	-10.30	112.42	118.60
54	BA	1758	U	O4'-C1'-N1	10.28	116.43	108.20
54	BA	1365	A	N1-C6-N6	-10.27	112.44	118.60
8	AI	94	ARG	NE-CZ-NH1	10.26	125.43	120.30
21	AA	937	A	N1-C6-N6	-10.26	112.45	118.60
54	BA	2628	C	O4'-C1'-N1	10.26	116.41	108.20
54	BA	2726	A	N1-C6-N6	-10.26	112.45	118.60
54	BA	1126	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	2766	A	N1-C6-N6	-10.24	112.46	118.60
55	BB	89	U	O4'-C1'-N1	10.23	116.39	108.20
54	BA	1866	A	N1-C6-N6	-10.23	112.46	118.60
54	BA	2860	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1410	A	N1-C6-N6	-10.20	112.48	118.60
21	AA	919	A	N1-C6-N6	-10.19	112.48	118.60
21	AA	1238	A	N1-C6-N6	-10.19	112.49	118.60
54	BA	1008	A	N1-C6-N6	-10.19	112.49	118.60
54	BA	2309	A	O4'-C1'-N9	10.19	116.35	108.20
21	AA	1287	A	N1-C6-N6	-10.18	112.49	118.60
21	AA	411	A	N1-C6-N6	-10.18	112.50	118.60
54	BA	1332	G	O4'-C1'-N9	10.16	116.33	108.20
54	BA	2225	A	N1-C6-N6	-10.16	112.50	118.60
21	AA	1500	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	622	A	N1-C6-N6	-10.15	112.51	118.60
54	BA	1672	A	N1-C6-N6	-10.15	112.51	118.60
54	BA	699	A	N1-C6-N6	-10.14	112.52	118.60
21	AA	65	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	1918	A	N1-C6-N6	-10.14	112.52	118.60
21	AA	321	A	N1-C6-N6	-10.13	112.52	118.60
21	AA	969	A	N1-C6-N6	-10.13	112.52	118.60
54	BA	430	A	N1-C6-N6	-10.12	112.53	118.60
54	BA	2541	A	N1-C6-N6	-10.11	112.54	118.60
21	AA	949	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	300	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	2516	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	1285	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	2530	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	2851	A	N1-C6-N6	-10.08	112.55	118.60
21	AA	1196	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	1803	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	637	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	1787	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	332	A	N1-C6-N6	-10.07	112.56	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2418	A	N1-C6-N6	-10.07	112.56	118.60
21	AA	197	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	1912	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	815	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	1260	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	1801	A	N1-C6-N6	-10.04	112.58	118.60
55	BB	108	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	182	A	N1-C6-N6	-10.02	112.59	118.60
25	BC	216	ARG	NE-CZ-NH1	10.01	125.31	120.30
54	BA	1496	A	N1-C6-N6	-10.01	112.59	118.60
44	BV	21	ARG	NE-CZ-NH2	9.99	125.29	120.30
21	AA	1396	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	28	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	213	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	746	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	607	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	1383	A	N1-C6-N6	-9.94	112.63	118.60
54	BA	1046	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	1084	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	2297	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	432	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	336	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	1340	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	1055	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	448	A	N1-C6-N6	-9.91	112.65	118.60
21	AA	196	A	N1-C6-N6	-9.91	112.65	118.60
21	AA	819	A	N1-C6-N6	-9.91	112.66	118.60
21	AA	913	A	N1-C6-N6	-9.91	112.66	118.60
54	BA	309	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1913	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	1130	A	N1-C6-N6	-9.89	112.66	118.60
54	BA	1029	A	N1-C6-N6	-9.89	112.67	118.60
12	AM	97	ARG	NE-CZ-NH1	9.89	125.25	120.30
54	BA	1805	A	N1-C6-N6	-9.89	112.67	118.60
21	AA	1430	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	1451	C	O4'-C1'-N1	9.87	116.10	108.20
21	AA	1531	A	N1-C6-N6	-9.87	112.68	118.60
47	BY	48	ARG	NE-CZ-NH1	9.87	125.23	120.30
54	BA	478	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	1495	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	1328	A	N1-C6-N6	-9.86	112.69	118.60
54	BA	1998	A	N1-C6-N6	-9.86	112.69	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	696	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	603	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	2376	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	429	A	N1-C6-N6	-9.85	112.69	118.60
10	AK	92	ARG	NE-CZ-NH1	9.84	125.22	120.30
54	BA	2856	A	N1-C6-N6	-9.84	112.70	118.60
21	AA	1150	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	626	A	N1-C6-N6	-9.82	112.70	118.60
1	AB	20	ARG	NE-CZ-NH1	9.82	125.21	120.30
21	AA	918	A	N1-C6-N6	-9.82	112.71	118.60
21	AA	831	A	N1-C6-N6	-9.81	112.71	118.60
21	AA	1169	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	1966	A	N1-C6-N6	-9.81	112.72	118.60
54	BA	988	A	N1-C6-N6	-9.81	112.72	118.60
39	BQ	63	ARG	NE-CZ-NH1	9.81	125.20	120.30
21	AA	1493	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	716	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	2800	A	N1-C6-N6	-9.81	112.72	118.60
21	AA	152	A	N1-C6-N6	-9.80	112.72	118.60
55	BB	15	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	1808	A	O4'-C1'-N9	9.79	116.04	108.20
54	BA	2572	A	N1-C6-N6	-9.79	112.72	118.60
54	BA	2705	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	2734	A	N1-C6-N6	-9.78	112.73	118.60
21	AA	181	A	N1-C6-N6	-9.78	112.73	118.60
55	BB	34	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	11	C	N3-C2-O2	-9.78	115.05	121.90
3	AD	114	ARG	NE-CZ-NH1	9.77	125.19	120.30
20	AU	6	ARG	NE-CZ-NH1	9.77	125.19	120.30
54	BA	847	U	O4'-C1'-N1	9.77	116.01	108.20
54	BA	1090	A	N1-C6-N6	-9.76	112.74	118.60
21	AA	554	A	N1-C6-N6	-9.76	112.75	118.60
54	BA	572	A	N1-C6-N6	-9.76	112.75	118.60
38	BP	88	ARG	NE-CZ-NH1	9.76	125.18	120.30
54	BA	241	A	N1-C6-N6	-9.76	112.75	118.60
54	BA	1953	A	N1-C6-N6	-9.76	112.75	118.60
21	AA	300	A	N1-C6-N6	-9.75	112.75	118.60
21	AA	1257	A	N1-C6-N6	-9.75	112.75	118.60
21	AA	414	A	N1-C6-N6	-9.74	112.75	118.60
54	BA	2426	A	N1-C6-N6	-9.74	112.75	118.60
21	AA	1319	A	N1-C6-N6	-9.74	112.75	118.60
54	BA	1598	A	N1-C6-N6	-9.74	112.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2392	A	N1-C6-N6	-9.74	112.75	118.60
21	AA	520	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	1276	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	2425	A	N1-C6-N6	-9.74	112.76	118.60
21	AA	1093	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2169	A	O4'-C1'-N9	9.72	115.98	108.20
54	BA	371	A	N1-C6-N6	-9.72	112.77	118.60
21	AA	642	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	1650	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	2422	C	N3-C2-O2	-9.71	115.10	121.90
54	BA	1272	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1508	A	O4'-C1'-N9	9.70	115.96	108.20
54	BA	2241	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	1289	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	2092	U	O4'-C1'-N1	9.70	115.96	108.20
27	BE	170	ARG	NE-CZ-NH1	9.69	125.14	120.30
54	BA	2497	A	N1-C6-N6	-9.67	112.80	118.60
21	AA	892	A	N1-C6-N6	-9.67	112.80	118.60
11	AL	35	ARG	NE-CZ-NH1	9.66	125.13	120.30
54	BA	146	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	2657	A	N1-C6-N6	-9.66	112.81	118.60
2	AC	171	ARG	NE-CZ-NH1	9.65	125.13	120.30
21	AA	1157	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	460	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	1256	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	461	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	340	A	N1-C6-N6	-9.65	112.81	118.60
48	BZ	15	ARG	NE-CZ-NH1	9.64	125.12	120.30
25	BC	270	ARG	NE-CZ-NH1	9.64	125.12	120.30
21	AA	59	A	N1-C6-N6	-9.64	112.82	118.60
54	BA	86	G	O4'-C1'-N9	9.63	115.90	108.20
54	BA	676	A	N1-C6-N6	-9.63	112.82	118.60
21	AA	1413	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	278	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2058	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	1191	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	1476	U	O4'-C1'-N1	9.61	115.89	108.20
54	BA	2169	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	1111	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	53	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1635	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	2266	A	N1-C6-N6	-9.56	112.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	865	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	1640	A	N1-C6-N6	-9.56	112.87	118.60
21	AA	309	A	N1-C6-N6	-9.55	112.87	118.60
24	A3	74	A	N1-C6-N6	-9.53	112.88	118.60
9	AJ	9	ARG	NE-CZ-NH1	9.53	125.06	120.30
21	AA	53	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2639	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	630	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	901	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	1253	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2764	A	N1-C6-N6	-9.51	112.89	118.60
2	AC	130	ARG	NE-CZ-NH1	9.51	125.05	120.30
21	AA	270	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	933	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	322	A	N1-C6-N6	-9.50	112.90	118.60
55	BB	66	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	1237	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	1169	A	N1-C6-N6	-9.49	112.90	118.60
54	BA	2307	G	O4'-C1'-N9	9.49	115.79	108.20
21	AA	466	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	1171	A	N1-C6-N6	-9.48	112.91	118.60
24	A3	22	A	N1-C6-N6	-9.48	112.92	118.60
54	BA	199	A	N1-C6-N6	-9.48	112.92	118.60
54	BA	1717	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	1214	C	N3-C2-O2	-9.47	115.27	121.90
54	BA	849	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	973	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	167	A	N1-C6-N6	-9.46	112.93	118.60
54	BA	1214	A	N1-C6-N6	-9.46	112.93	118.60
55	BB	94	A	N1-C6-N6	-9.46	112.93	118.60
15	AP	8	ARG	NE-CZ-NH1	9.45	125.03	120.30
22	A1	41	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1927	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	277	G	O4'-C1'-N9	9.45	115.76	108.20
54	BA	1494	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1900	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	33	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	2461	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	1393	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	397	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	294	A	N1-C6-N6	-9.43	112.94	118.60
6	AG	78	ARG	NE-CZ-NH1	9.42	125.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	78	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	313	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	1046	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	941	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	151	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	389	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	126	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	1784	A	C5-C6-N1	9.41	122.40	117.70
54	BA	2799	A	N1-C6-N6	-9.41	112.96	118.60
54	BA	1534	U	O4'-C1'-N1	9.40	115.72	108.20
21	AA	1219	A	N1-C6-N6	-9.39	112.96	118.60
54	BA	2191	A	N1-C6-N6	-9.39	112.96	118.60
54	BA	1783	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	502	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	2060	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	246	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	1545	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	2478	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	468	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	526	A	C5-C6-N1	9.38	122.39	117.70
54	BA	582	A	N1-C6-N6	-9.37	112.98	118.60
6	AG	94	ARG	NE-CZ-NH1	9.37	124.98	120.30
21	AA	1225	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	1302	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	1665	A	N1-C6-N6	-9.35	112.99	118.60
21	AA	1261	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	2565	A	N1-C6-N6	-9.34	113.00	118.60
21	AA	130	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	165	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	13	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	783	A	N1-C6-N6	-9.33	113.00	118.60
32	BJ	34	ARG	NE-CZ-NH1	9.33	124.97	120.30
21	AA	1468	A	N1-C6-N6	-9.32	113.01	118.60
22	A1	69	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	265	A	N1-C6-N6	-9.32	113.01	118.60
33	BK	49	ARG	NE-CZ-NH1	9.32	124.96	120.30
54	BA	1327	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	192	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	243	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	2358	A	N1-C6-N6	-9.31	113.02	118.60
55	BB	78	A	N1-C6-N6	-9.31	113.02	118.60
21	AA	695	A	N1-C6-N6	-9.30	113.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1749	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	2721	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	382	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1701	A	N1-C6-N6	-9.30	113.02	118.60
21	AA	747	A	N1-C6-N6	-9.30	113.02	118.60
21	AA	1054	C	N3-C2-O2	-9.29	115.39	121.90
54	BA	1785	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	633	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	1599	U	O4'-C1'-N1	9.29	115.63	108.20
21	AA	807	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	262	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2700	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	371	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	71	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1262	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	905	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	529	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	728	A	N1-C6-N6	-9.26	113.05	118.60
21	AA	274	A	N1-C6-N6	-9.26	113.05	118.60
54	BA	2825	G	O4'-C1'-N9	9.25	115.60	108.20
54	BA	101	A	N1-C6-N6	-9.25	113.05	118.60
56	B5	122	ARG	NE-CZ-NH1	9.25	124.92	120.30
54	BA	1213	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	1179	A	N1-C6-N6	-9.24	113.05	118.60
54	BA	627	A	N1-C6-N6	-9.24	113.05	118.60
54	BA	1265	A	N1-C6-N6	-9.24	113.05	118.60
54	BA	1284	A	N1-C6-N6	-9.24	113.05	118.60
21	AA	802	A	N1-C6-N6	-9.24	113.06	118.60
21	AA	1299	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	2055	C	O4'-C1'-N1	9.23	115.59	108.20
54	BA	2635	A	N1-C6-N6	-9.23	113.06	118.60
54	BA	1085	A	N1-C6-N6	-9.23	113.06	118.60
33	BK	64	ARG	NE-CZ-NH1	9.23	124.91	120.30
21	AA	441	A	N1-C6-N6	-9.22	113.06	118.60
21	AA	459	A	N1-C6-N6	-9.22	113.06	118.60
21	AA	681	A	N1-C6-N6	-9.22	113.07	118.60
34	BL	60	ARG	NE-CZ-NH1	9.22	124.91	120.30
54	BA	613	A	N1-C6-N6	-9.22	113.07	118.60
21	AA	1019	A	N1-C6-N6	-9.21	113.07	118.60
21	AA	190	A	N1-C6-N6	-9.21	113.07	118.60
21	AA	845	A	N1-C6-N6	-9.21	113.07	118.60
21	AA	325	A	N1-C6-N6	-9.20	113.08	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1204	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	1711	A	N1-C6-N6	-9.20	113.08	118.60
24	A3	36	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	655	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	1870	C	N3-C2-O2	-9.19	115.47	121.90
54	BA	2602	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	2369	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	889	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1014	A	N1-C6-N6	-9.18	113.09	118.60
21	AA	223	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	979	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1000	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	706	A	N1-C6-N6	-9.16	113.11	118.60
21	AA	1271	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	1508	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	1483	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	1080	A	N1-C6-N6	-9.16	113.11	118.60
21	AA	983	A	N1-C6-N6	-9.15	113.11	118.60
7	AH	113	ARG	NE-CZ-NH1	9.15	124.88	120.30
55	BB	52	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	541	A	N1-C6-N6	-9.14	113.11	118.60
54	BA	899	A	N1-C6-N6	-9.14	113.11	118.60
54	BA	1504	A	N1-C6-N6	-9.14	113.11	118.60
55	BB	46	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	5	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	1515	A	N1-C6-N6	-9.12	113.12	118.60
54	BA	2439	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	1786	A	N1-C6-N6	-9.12	113.13	118.60
24	A3	77	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2602	A	C5-C6-N1	9.12	122.26	117.70
54	BA	64	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	547	A	O4'-C1'-N9	9.12	115.49	108.20
21	AA	349	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	196	A	O4'-C1'-N9	9.11	115.49	108.20
21	AA	743	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	368	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	715	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2176	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	687	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	504	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	829	A	N1-C6-N6	-9.09	113.14	118.60
21	AA	408	A	N1-C6-N6	-9.09	113.15	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1304	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	515	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	528	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	1977	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	729	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	16	A	N1-C6-N6	-9.08	113.16	118.60
54	BA	1853	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	802	A	N1-C6-N6	-9.07	113.16	118.60
55	BB	15	A	O4'-C1'-N9	9.07	115.45	108.20
54	BA	344	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	8	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	1287	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	2560	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	718	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1127	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	1129	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	1431	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1522	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	89	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1549	A	N1-C6-N6	-9.05	113.17	118.60
55	BB	14	U	O4'-C1'-N1	9.05	115.44	108.20
21	AA	539	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	1537	G	O4'-C1'-N9	9.04	115.43	108.20
54	BA	1073	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	602	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1434	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	282	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	179	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2534	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2725	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	609	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	1265	A	C5-C6-N1	9.01	122.20	117.70
21	AA	1368	A	N1-C6-N6	-9.01	113.19	118.60
51	B2	34	ARG	NE-CZ-NH1	9.00	124.80	120.30
54	BA	1887	C	O4'-C1'-N1	9.00	115.40	108.20
54	BA	1579	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	2183	A	N1-C6-N6	-8.99	113.20	118.60
54	BA	1916	A	N1-C6-N6	-8.99	113.20	118.60
21	AA	1446	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	1374	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2471	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	860	A	N1-C6-N6	-8.97	113.22	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1264	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1937	A	N1-C6-N6	-8.97	113.22	118.60
14	AO	88	ARG	NE-CZ-NH1	8.96	124.78	120.30
27	BE	61	ARG	NE-CZ-NH1	8.96	124.78	120.30
54	BA	453	A	N1-C6-N6	-8.95	113.23	118.60
21	AA	582	C	N3-C2-O2	-8.95	115.63	121.90
54	BA	1847	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	751	A	N1-C6-N6	-8.94	113.23	118.60
21	AA	129	A	N1-C6-N6	-8.94	113.23	118.60
21	AA	563	A	N1-C6-N6	-8.94	113.23	118.60
22	A1	76	A	N1-C6-N6	-8.94	113.23	118.60
29	BG	151	ARG	NE-CZ-NH1	8.94	124.77	120.30
54	BA	91	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	800	A	N1-C6-N6	-8.94	113.24	118.60
55	BB	50	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	1176	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	613	A	O4'-C1'-N9	8.94	115.35	108.20
54	BA	1070	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1819	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	608	A	N1-C6-N6	-8.92	113.25	118.60
20	AU	33	ARG	NE-CZ-NH2	8.91	124.76	120.30
24	A3	73	A	N1-C6-N6	-8.91	113.25	118.60
39	BQ	54	ARG	NE-CZ-NH1	8.91	124.75	120.30
21	AA	1534	A	N1-C6-N6	-8.91	113.26	118.60
37	BO	81	ARG	NE-CZ-NH1	8.91	124.75	120.30
41	BS	8	ARG	NE-CZ-NH1	8.90	124.75	120.30
54	BA	1505	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2163	A	N1-C6-N6	-8.90	113.26	118.60
29	BG	148	ARG	NE-CZ-NH1	8.90	124.75	120.30
54	BA	1378	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	753	A	N1-C6-N6	-8.89	113.26	118.60
54	BA	1914	C	N1-C2-O2	8.89	124.24	118.90
21	AA	864	A	N1-C6-N6	-8.89	113.27	118.60
54	BA	2430	A	N1-C6-N6	-8.89	113.27	118.60
34	BL	18	ARG	NE-CZ-NH1	8.89	124.74	120.30
21	AA	1429	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	1744	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	1251	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	704	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	1246	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	50	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	936	A	N1-C6-N6	-8.87	113.28	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1156	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1069	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	1022	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	196	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	2873	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	1978	A	N1-C6-N6	-8.86	113.29	118.60
54	BA	2667	C	N3-C2-O2	-8.85	115.70	121.90
21	AA	629	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	2813	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	2227	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	702	A	N1-C6-N6	-8.84	113.30	118.60
21	AA	532	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	631	A	N1-C6-N6	-8.84	113.30	118.60
21	AA	1275	A	N1-C6-N6	-8.83	113.30	118.60
21	AA	493	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	677	A	N1-C6-N6	-8.83	113.30	118.60
55	BB	101	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	2468	A	N1-C6-N6	-8.82	113.31	118.60
24	A3	58	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	139	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	896	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	270	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1553	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1275	A	N1-C6-N6	-8.81	113.32	118.60
21	AA	253	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	1016	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	384	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	2071	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	2660	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	447	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	2052	A	C5-C6-N1	8.79	122.10	117.70
54	BA	2868	A	N1-C6-N6	-8.79	113.32	118.60
54	BA	734	A	N1-C6-N6	-8.79	113.32	118.60
54	BA	2412	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	2665	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	457	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	918	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1566	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	931	U	O4'-C1'-N1	8.78	115.23	108.20
21	AA	1329	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	111	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	1088	A	N1-C6-N6	-8.78	113.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	338	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	914	G	O4'-C1'-N9	8.78	115.22	108.20
54	BA	1320	C	N3-C2-O2	-8.78	115.76	121.90
21	AA	509	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	1397	C	N3-C2-O2	-8.77	115.76	121.90
21	AA	675	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	1364	U	O4'-C1'-N1	8.77	115.21	108.20
54	BA	42	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2453	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	712	A	N1-C6-N6	-8.76	113.34	118.60
22	A1	66	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	1413	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	2476	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	522	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	2430	A	C5-C6-N1	8.76	122.08	117.70
54	BA	2810	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	1614	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	26	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	1428	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	95	A	N1-C6-N6	-8.75	113.35	118.60
1	AB	62	ARG	NE-CZ-NH1	8.74	124.67	120.30
8	AI	48	ARG	NE-CZ-NH1	8.73	124.67	120.30
21	AA	431	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	1042	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	2814	A	N1-C6-N6	-8.73	113.36	118.60
55	BB	29	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	10	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	346	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1586	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	2266	A	C5-C6-N1	8.72	122.06	117.70
21	AA	1213	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	172	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	161	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	685	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	1490	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	2432	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	602	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	83	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	487	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	1772	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	1492	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	2503	A	N1-C6-N6	-8.71	113.38	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	331	C	N3-C2-O2	-8.71	115.81	121.90
54	BA	742	A	N1-C6-N6	-8.70	113.38	118.60
21	AA	171	A	N1-C6-N6	-8.69	113.38	118.60
21	AA	1146	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	1332	A	N1-C6-N6	-8.69	113.38	118.60
54	BA	2679	A	N1-C6-N6	-8.69	113.39	118.60
44	BV	19	ARG	NE-CZ-NH1	8.69	124.64	120.30
54	BA	614	A	O4'-C1'-N9	8.69	115.15	108.20
54	BA	1126	A	C5-C6-N1	8.69	122.04	117.70
54	BA	2829	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	983	A	C5-C6-N1	8.68	122.04	117.70
54	BA	1439	A	N1-C6-N6	-8.68	113.39	118.60
55	BB	73	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	1346	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	155	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	2287	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	919	A	C5-C6-N1	8.68	122.04	117.70
54	BA	205	G	O4'-C1'-N9	8.68	115.14	108.20
21	AA	363	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	964	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	1000	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	176	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1603	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1757	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	998	C	N3-C2-O2	-8.67	115.83	121.90
54	BA	1387	A	N1-C6-N6	-8.66	113.40	118.60
21	AA	1151	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	789	A	N1-C6-N6	-8.66	113.40	118.60
22	A1	59	U	O4'-C1'-N1	8.65	115.12	108.20
54	BA	722	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	1012	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	456	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	2883	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	975	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1943	U	O4'-C1'-N1	8.63	115.11	108.20
21	AA	609	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	2900	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	1970	A	N1-C6-N6	-8.63	113.42	118.60
4	AE	92	ARG	NE-CZ-NH1	8.63	124.61	120.30
54	BA	2031	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	2518	A	C5-C6-N1	8.63	122.01	117.70
21	AA	996	A	N1-C6-N6	-8.62	113.43	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	101	ARG	NE-CZ-NH1	8.62	124.61	120.30
54	BA	49	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	689	A	C5-C6-N1	8.62	122.01	117.70
24	A3	35	C	N3-C2-O2	-8.61	115.87	121.90
54	BA	1244	A	N1-C6-N6	-8.61	113.43	118.60
21	AA	499	A	C4-C5-C6	-8.61	112.70	117.00
21	AA	792	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	332	A	C5-C6-N1	8.60	122.00	117.70
54	BA	514	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	118	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	718	A	C5-C6-N1	8.60	122.00	117.70
37	BO	16	ARG	NE-CZ-NH1	8.59	124.59	120.30
3	AD	164	ARG	NE-CZ-NH1	8.58	124.59	120.30
54	BA	1001	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	1054	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	1652	A	N1-C6-N6	-8.57	113.46	118.60
34	BL	41	ARG	NE-CZ-NH1	8.57	124.58	120.30
54	BA	587	C	N3-C2-O2	-8.57	115.90	121.90
54	BA	1882	U	O4'-C1'-N1	8.57	115.05	108.20
21	AA	499	A	C5-C6-N1	8.56	121.98	117.70
39	BQ	10	ARG	NE-CZ-NH1	8.56	124.58	120.30
21	AA	51	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	131	A	N1-C6-N6	-8.56	113.46	118.60
36	BN	118	ARG	NE-CZ-NH1	8.56	124.58	120.30
21	AA	1288	A	N1-C6-N6	-8.55	113.47	118.60
42	BT	77	ARG	NE-CZ-NH1	8.55	124.58	120.30
54	BA	1147	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	119	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	1513	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	204	A	C5-C6-N1	8.54	121.97	117.70
54	BA	2126	A	O4'-C1'-N9	8.54	115.03	108.20
54	BA	527	C	N3-C2-O2	-8.54	115.92	121.90
54	BA	1204	A	O4'-C1'-N9	8.54	115.03	108.20
21	AA	498	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	814	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	2030	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	2750	A	N1-C6-N6	-8.53	113.48	118.60
38	BP	112	ARG	NE-CZ-NH1	8.53	124.57	120.30
54	BA	556	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	781	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	1268	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	1469	A	N1-C6-N6	-8.52	113.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	715	A	N1-C6-N6	-8.52	113.49	118.60
34	BL	123	ARG	NE-CZ-NH1	8.52	124.56	120.30
54	BA	526	A	N1-C6-N6	-8.51	113.49	118.60
28	BF	149	ARG	NE-CZ-NH1	8.51	124.56	120.30
54	BA	1713	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1618	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1745	A	N1-C6-N6	-8.51	113.50	118.60
21	AA	1004	A	N1-C6-N6	-8.51	113.50	118.60
21	AA	958	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	182	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1535	A	O4'-C1'-N9	8.50	115.00	108.20
54	BA	2820	A	C5-C6-N1	8.50	121.95	117.70
54	BA	2114	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	435	A	N1-C6-N6	-8.50	113.50	118.60
24	A3	44	A	N1-C6-N6	-8.50	113.50	118.60
6	AG	110	ARG	NE-CZ-NH1	8.49	124.55	120.30
37	BO	15	ARG	NE-CZ-NH1	8.49	124.55	120.30
21	AA	579	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	724	U	O4'-C1'-N1	8.49	114.99	108.20
54	BA	1246	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	1503	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1570	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	205	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1641	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1669	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1762	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	1919	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	2388	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	705	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	2573	C	N3-C2-O2	-8.46	115.98	121.90
21	AA	306	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	347	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	1678	A	N1-C6-N6	-8.45	113.53	118.60
3	AD	46	ARG	NE-CZ-NH1	8.45	124.52	120.30
54	BA	1420	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	673	A	N1-C6-N6	-8.44	113.53	118.60
21	AA	19	A	N1-C6-N6	-8.44	113.54	118.60
44	BV	9	ARG	NE-CZ-NH1	8.44	124.52	120.30
54	BA	1353	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	1730	C	N3-C2-O2	-8.43	116.00	121.90
54	BA	94	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	1175	A	O4'-C1'-N9	8.43	114.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1454	C	N3-C2-O2	-8.43	116.00	121.90
21	AA	344	A	N1-C6-N6	-8.43	113.55	118.60
54	BA	1347	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	1133	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	465	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	621	A	N1-C6-N6	-8.42	113.55	118.60
17	AR	52	ARG	NE-CZ-NH1	8.42	124.51	120.30
24	A3	39	A	N1-C6-N6	-8.42	113.55	118.60
6	AG	52	ARG	NE-CZ-NH1	8.41	124.51	120.30
22	A1	74	C	N3-C2-O2	-8.41	116.01	121.90
54	BA	231	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	55	A	N1-C6-N6	-8.41	113.56	118.60
21	AA	782	A	N1-C6-N6	-8.41	113.56	118.60
21	AA	906	A	N1-C6-N6	-8.41	113.56	118.60
21	AA	1044	A	N1-C6-N6	-8.41	113.56	118.60
21	AA	412	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2097	A	N1-C6-N6	-8.40	113.56	118.60
11	AL	11	ARG	NE-CZ-NH1	8.40	124.50	120.30
54	BA	590	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2682	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	1152	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	752	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	1953	A	C5-C6-N1	8.40	121.90	117.70
21	AA	1254	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2070	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	149	A	C5-C6-N1	8.39	121.89	117.70
54	BA	44	A	N1-C6-N6	-8.38	113.57	118.60
10	AK	36	ARG	NE-CZ-NH1	8.38	124.49	120.30
54	BA	1155	A	C5-C6-N1	8.38	121.89	117.70
52	B3	41	ARG	NE-CZ-NH1	8.38	124.49	120.30
54	BA	2426	A	C5-C6-N1	8.38	121.89	117.70
54	BA	160	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	666	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1151	A	N1-C6-N6	-8.38	113.58	118.60
21	AA	72	A	C5-C6-N1	8.37	121.89	117.70
24	A3	59	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	457	A	C5-C6-N1	8.37	121.88	117.70
13	AN	65	ARG	NE-CZ-NH1	8.37	124.48	120.30
54	BA	1010	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	892	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	1459	G	O4'-C1'-N9	8.36	114.89	108.20
54	BA	2590	A	N1-C6-N6	-8.36	113.58	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	250	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	567	U	O4'-C1'-N1	8.35	114.88	108.20
54	BA	222	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	840	C	O4'-C1'-N1	8.35	114.88	108.20
54	BA	1866	A	C5-C6-N1	8.35	121.87	117.70
21	AA	974	A	N1-C6-N6	-8.34	113.59	118.60
22	A1	47	U	O4'-C1'-N1	8.34	114.87	108.20
21	AA	195	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	1536	C	N3-C2-O2	-8.34	116.06	121.90
21	AA	189	A	C5-C6-N1	8.34	121.87	117.70
21	AA	383	A	N1-C6-N6	-8.34	113.60	118.60
24	A3	38	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	1759	A	N1-C6-N6	-8.34	113.60	118.60
10	AK	126	ARG	NE-CZ-NH2	-8.33	116.13	120.30
22	A1	73	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	644	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	131	A	C5-C6-N1	8.33	121.86	117.70
21	AA	1502	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1493	C	O4'-C1'-N1	8.33	114.86	108.20
46	BX	27	ARG	NE-CZ-NH1	8.33	124.46	120.30
54	BA	2288	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	2835	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	382	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	1322	C	N3-C2-O2	-8.32	116.08	121.90
54	BA	454	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	915	A	C5-C6-N1	8.32	121.86	117.70
54	BA	497	A	N1-C6-N6	-8.32	113.61	118.60
56	B5	164	ARG	NE-CZ-NH1	8.32	124.46	120.30
21	AA	1306	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	391	A	C5-C6-N1	8.32	121.86	117.70
21	AA	1145	A	C5-C6-N1	8.31	121.86	117.70
26	BD	169	ARG	NE-CZ-NH1	8.31	124.46	120.30
21	AA	1280	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	1269	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	1876	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2899	A	N1-C6-N6	-8.31	113.61	118.60
25	BC	211	ARG	NE-CZ-NH1	8.31	124.45	120.30
37	BO	13	ARG	NE-CZ-NH1	8.31	124.45	120.30
54	BA	435	C	N3-C2-O2	-8.31	116.09	121.90
54	BA	886	A	N1-C6-N6	-8.31	113.62	118.60
54	BA	2513	A	N1-C6-N6	-8.31	113.62	118.60
21	AA	1306	A	C5-C6-N1	8.30	121.85	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2879	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	1791	A	C5-C6-N1	8.30	121.85	117.70
54	BA	404	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	2430	A	O4'-C1'-N9	8.30	114.84	108.20
54	BA	2435	A	N1-C6-N6	-8.30	113.62	118.60
12	AM	100	ARG	NE-CZ-NH1	8.29	124.45	120.30
54	BA	320	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	1490	A	C5-C6-N1	8.29	121.85	117.70
54	BA	1241	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	2433	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	2758	A	N1-C6-N6	-8.29	113.63	118.60
21	AA	631	C	N3-C2-O2	-8.29	116.10	121.90
54	BA	1205	A	C5-C6-N1	8.28	121.84	117.70
54	BA	1552	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	371	A	C5-C6-N1	8.28	121.84	117.70
21	AA	795	C	N3-C2-O2	-8.28	116.11	121.90
54	BA	661	A	N1-C6-N6	-8.28	113.63	118.60
21	AA	1201	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	793	A	C5-C6-N1	8.27	121.84	117.70
54	BA	2670	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	780	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	52	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	911	A	N1-C6-N6	-8.27	113.64	118.60
28	BF	29	ARG	NE-CZ-NH1	8.27	124.43	120.30
54	BA	1532	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	482	A	N1-C6-N6	-8.27	113.64	118.60
20	AU	20	ARG	NE-CZ-NH1	8.26	124.43	120.30
21	AA	1299	A	C5-C6-N1	8.26	121.83	117.70
54	BA	782	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	2476	A	C5-C6-N1	8.26	121.83	117.70
9	AJ	62	ARG	NE-CZ-NH1	8.26	124.43	120.30
24	A3	60	A	N1-C6-N6	-8.26	113.64	118.60
28	BF	111	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	399	U	O4'-C1'-N1	8.26	114.81	108.20
54	BA	1678	A	C5-C6-N1	8.26	121.83	117.70
54	BA	2054	A	N1-C6-N6	-8.26	113.64	118.60
21	AA	1155	A	N1-C6-N6	-8.26	113.65	118.60
11	AL	30	ARG	NE-CZ-NH1	8.25	124.43	120.30
21	AA	160	A	N1-C6-N6	-8.25	113.65	118.60
42	BT	6	ARG	NE-CZ-NH1	8.25	124.43	120.30
54	BA	56	A	N1-C6-N6	-8.25	113.65	118.60
5	AF	24	ARG	NE-CZ-NH1	8.24	124.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	14	A	N1-C6-N6	-8.24	113.65	118.60
54	BA	1754	A	N1-C6-N6	-8.24	113.65	118.60
54	BA	2042	A	N1-C6-N6	-8.24	113.65	118.60
54	BA	2199	A	N1-C6-N6	-8.24	113.65	118.60
21	AA	189	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1004	A	C5-C6-N1	8.23	121.82	117.70
54	BA	910	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	127	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	727	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2267	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2411	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2654	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	451	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1717	A	C5-C6-N1	8.22	121.81	117.70
21	AA	109	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	423	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	2080	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1871	A	N1-C6-N6	-8.22	113.67	118.60
17	AR	47	ARG	NE-CZ-NH1	8.22	124.41	120.30
24	A3	3	C	N3-C2-O2	-8.22	116.15	121.90
54	BA	1780	A	C5-C6-N1	8.22	121.81	117.70
54	BA	1552	A	O4'-C1'-N9	8.22	114.77	108.20
54	BA	2158	A	C5-C6-N1	8.22	121.81	117.70
21	AA	183	C	N3-C2-O2	-8.21	116.15	121.90
54	BA	1089	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	753	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	1901	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	983	A	N1-C6-N6	-8.21	113.67	118.60
17	AR	72	ARG	NE-CZ-NH1	8.21	124.41	120.30
54	BA	2577	A	C5-C6-N1	8.21	121.81	117.70
54	BA	1690	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	546	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	596	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	1447	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1366	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	2887	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1936	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	2311	A	N1-C6-N6	-8.20	113.68	118.60
45	BW	54	ARG	NE-CZ-NH1	8.19	124.39	120.30
54	BA	1088	A	C5-C6-N1	8.19	121.80	117.70
54	BA	2792	A	N1-C6-N6	-8.19	113.68	118.60
54	BA	2634	A	C4-C5-C6	-8.19	112.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	449	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2450	A	C5-C6-N1	8.19	121.79	117.70
21	AA	1333	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2031	A	C5-C6-N1	8.18	121.79	117.70
21	AA	353	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	1282	C	N3-C2-O2	-8.18	116.17	121.90
54	BA	2314	A	N1-C6-N6	-8.18	113.69	118.60
34	BL	132	ARG	NE-CZ-NH1	8.18	124.39	120.30
54	BA	1367	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1664	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1544	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	675	A	N1-C6-N6	-8.17	113.70	118.60
25	BC	13	ARG	NE-CZ-NH1	8.17	124.39	120.30
54	BA	918	A	C5-C6-N1	8.17	121.79	117.70
54	BA	492	A	N1-C6-N6	-8.17	113.70	118.60
21	AA	336	A	C4-C5-C6	-8.17	112.92	117.00
54	BA	2882	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	1032	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	975	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	756	A	N1-C6-N6	-8.16	113.70	118.60
9	AJ	5	ARG	NE-CZ-NH1	8.16	124.38	120.30
21	AA	1318	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	761	A	N1-C6-N6	-8.16	113.71	118.60
10	AK	126	ARG	NE-CZ-NH1	8.15	124.38	120.30
54	BA	477	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1885	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1677	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	2407	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	2516	A	C5-C6-N1	8.15	121.78	117.70
54	BA	1630	A	C4-C5-C6	-8.15	112.93	117.00
21	AA	906	A	C5-C6-N1	8.15	121.77	117.70
54	BA	599	A	N1-C6-N6	-8.14	113.71	118.60
21	AA	465	A	C5-C6-N1	8.14	121.77	117.70
54	BA	391	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	1009	A	N1-C6-N6	-8.14	113.72	118.60
21	AA	1100	C	N1-C2-O2	8.14	123.78	118.90
54	BA	1021	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	2403	C	O4'-C1'-N1	8.14	114.71	108.20
33	BK	71	ARG	NE-CZ-NH1	8.14	124.37	120.30
54	BA	2628	C	N3-C2-O2	-8.14	116.20	121.90
55	BB	78	A	C5-C6-N1	8.13	121.77	117.70
21	AA	1229	A	N1-C6-N6	-8.13	113.72	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	943	A	N1-C6-N6	-8.13	113.72	118.60
22	A1	9	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	282	A	C5-C6-N1	8.12	121.76	117.70
21	AA	1375	A	N1-C6-N6	-8.12	113.72	118.60
21	AA	1533	C	N3-C2-O2	-8.12	116.21	121.90
22	A1	75	C	N3-C2-O2	-8.13	116.21	121.90
24	A3	45	A	N1-C6-N6	-8.12	113.72	118.60
21	AA	373	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	502	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	1519	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1264	A	C5-C6-N1	8.12	121.76	117.70
55	BB	39	A	C5-C6-N1	8.12	121.76	117.70
21	AA	648	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1700	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	8	A	C5-C6-N1	8.12	121.76	117.70
54	BA	861	A	C4-C5-C6	-8.11	112.94	117.00
54	BA	981	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2740	A	C1'-O4'-C4'	-8.11	103.41	109.90
25	BC	181	ARG	NE-CZ-NH1	8.11	124.35	120.30
54	BA	1597	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2564	A	C5-C6-N1	8.11	121.75	117.70
54	BA	1050	A	N1-C6-N6	-8.11	113.74	118.60
55	BB	15	A	C5-C6-N1	8.10	121.75	117.70
21	AA	432	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	282	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1175	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	2439	A	C5-C6-N1	8.10	121.75	117.70
21	AA	120	A	N1-C6-N6	-8.09	113.74	118.60
21	AA	1180	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	947	A	N1-C6-N6	-8.09	113.74	118.60
23	A2	82	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2589	A	C4-C5-C6	-8.09	112.95	117.00
21	AA	1239	A	N1-C6-N6	-8.09	113.75	118.60
22	A1	38	A	C5-C6-N1	8.09	121.74	117.70
54	BA	21	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	1848	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	1821	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	330	A	O4'-C1'-N9	8.08	114.66	108.20
54	BA	995	C	N3-C2-O2	-8.08	116.24	121.90
54	BA	2275	C	N3-C2-O2	-8.08	116.24	121.90
54	BA	1632	A	C5-C6-N1	8.08	121.74	117.70
54	BA	1786	A	C5-C6-N1	8.08	121.74	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1405	U	O4'-C1'-N1	8.07	114.66	108.20
21	AA	432	A	C5-C6-N1	8.07	121.73	117.70
54	BA	199	A	C5-C6-N1	8.07	121.73	117.70
54	BA	2453	A	C5-C6-N1	8.07	121.73	117.70
6	AG	95	ARG	NE-CZ-NH1	8.06	124.33	120.30
21	AA	1285	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	262	A	N1-C6-N6	-8.06	113.77	118.60
21	AA	899	C	O4'-C1'-N1	8.06	114.64	108.20
27	BE	117	ARG	NE-CZ-NH1	8.06	124.33	120.30
54	BA	980	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	2013	A	N1-C6-N6	-8.05	113.77	118.60
14	AO	76	ARG	NE-CZ-NH1	8.05	124.33	120.30
21	AA	547	A	C5-C6-N1	8.05	121.73	117.70
21	AA	1534	A	C5-C6-N1	8.05	121.73	117.70
54	BA	63	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	74	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	1020	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	933	A	C5-C6-N1	8.04	121.72	117.70
54	BA	878	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	1815	A	C5-C6-N1	8.04	121.72	117.70
21	AA	366	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	768	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	1451	U	O4'-C1'-N1	8.04	114.63	108.20
21	AA	728	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1705	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	2322	A	N1-C6-N6	-8.04	113.78	118.60
46	BX	36	ARG	NE-CZ-NH1	8.03	124.32	120.30
22	A1	16	C	N3-C2-O2	-8.03	116.28	121.90
54	BA	2879	A	C5-C6-N1	8.03	121.71	117.70
55	BB	39	A	C4-C5-C6	-8.03	112.99	117.00
54	BA	1583	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2713	U	O4'-C1'-N1	8.03	114.62	108.20
54	BA	2765	A	C5-C6-N1	8.03	121.71	117.70
54	BA	181	A	N1-C6-N6	-8.02	113.78	118.60
54	BA	2211	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	1239	A	C5-C6-N1	8.01	121.71	117.70
54	BA	1027	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	2311	A	C5-C6-N1	8.01	121.71	117.70
11	AL	13	ARG	NE-CZ-NH1	8.01	124.31	120.30
21	AA	1257	A	C5-C6-N1	8.01	121.70	117.70
21	AA	95	C	N3-C2-O2	-8.01	116.30	121.90
54	BA	422	A	N1-C6-N6	-8.01	113.80	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	73	A	C5-C6-N1	8.01	121.70	117.70
45	BW	40	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	825	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1419	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1808	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2317	A	N1-C6-N6	-8.00	113.80	118.60
8	AI	129	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	915	C	N3-C2-O2	-8.00	116.30	121.90
51	B2	3	ARG	NE-CZ-NH2	8.00	124.30	120.30
54	BA	2267	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2600	A	C5-C6-N1	8.00	121.70	117.70
54	BA	866	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2212	A	N1-C6-N6	-8.00	113.80	118.60
55	BB	57	A	C5-C6-N1	8.00	121.70	117.70
54	BA	149	A	C4-C5-C6	-7.99	113.00	117.00
54	BA	2598	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	1130	A	C5-C6-N1	7.99	121.69	117.70
56	B5	71	ARG	NE-CZ-NH1	7.99	124.30	120.30
21	AA	1501	C	N3-C2-O2	-7.99	116.31	121.90
21	AA	1067	A	C5-C6-N1	7.99	121.69	117.70
54	BA	265	A	C5-C6-N1	7.99	121.69	117.70
54	BA	1189	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	2531	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	71	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	1253	A	C5-C6-N1	7.98	121.69	117.70
8	AI	44	ARG	NE-CZ-NH1	7.98	124.29	120.30
21	AA	794	A	C5-C6-N1	7.98	121.69	117.70
21	AA	1363	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	99	U	N3-C2-O2	-7.97	116.62	122.20
54	BA	2566	A	C5-C6-N1	7.97	121.69	117.70
54	BA	223	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	279	A	C5-C6-N1	7.97	121.68	117.70
21	AA	665	A	C5-C6-N1	7.97	121.68	117.70
21	AA	1362	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	946	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	2281	A	C5-C6-N1	7.96	121.68	117.70
54	BA	2639	A	C5-C6-N1	7.96	121.68	117.70
21	AA	60	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	1453	A	C5-C6-N1	7.96	121.68	117.70
54	BA	2837	A	C5-C6-N1	7.96	121.68	117.70
21	AA	1492	A	C5-C6-N1	7.96	121.68	117.70
21	AA	1163	A	C5-C6-N1	7.96	121.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1281	C	N3-C2-O2	-7.96	116.33	121.90
54	BA	896	A	C5-C6-N1	7.96	121.68	117.70
21	AA	1431	A	C5-C6-N1	7.96	121.68	117.70
54	BA	105	C	N3-C2-O2	-7.96	116.33	121.90
54	BA	227	A	C5-C6-N1	7.96	121.68	117.70
28	BF	124	ARG	NE-CZ-NH1	7.95	124.28	120.30
54	BA	2835	A	C5-C6-N1	7.95	121.68	117.70
21	AA	1289	A	C5-C6-N1	7.95	121.68	117.70
21	AA	262	A	C5-C6-N1	7.95	121.68	117.70
21	AA	518	C	N3-C2-O2	-7.95	116.33	121.90
21	AA	74	A	C5-C6-N1	7.95	121.67	117.70
54	BA	63	A	C5-C6-N1	7.94	121.67	117.70
21	AA	608	A	N1-C6-N6	-7.94	113.83	118.60
48	BZ	29	ARG	NE-CZ-NH1	7.94	124.27	120.30
21	AA	1049	U	C1'-O4'-C4'	-7.94	103.55	109.90
54	BA	1679	A	C5-C6-N1	7.94	121.67	117.70
54	BA	2094	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	2478	A	C5-C6-N1	7.94	121.67	117.70
21	AA	749	A	N1-C6-N6	-7.94	113.84	118.60
21	AA	1433	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	256	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	2406	A	C5-C6-N1	7.94	121.67	117.70
54	BA	190	A	N1-C6-N6	-7.94	113.84	118.60
21	AA	635	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	195	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	466	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	2051	A	C5-C6-N1	7.93	121.67	117.70
21	AA	373	A	C5-C6-N1	7.93	121.67	117.70
54	BA	472	A	C5-C6-N1	7.93	121.66	117.70
54	BA	1952	A	C5-C6-N1	7.93	121.66	117.70
21	AA	630	A	C5-C6-N1	7.93	121.66	117.70
21	AA	694	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1522	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1596	A	C4-C5-C6	-7.92	113.04	117.00
2	AC	126	ARG	NE-CZ-NH1	7.92	124.26	120.30
54	BA	1048	A	C5-C6-N1	7.92	121.66	117.70
21	AA	649	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1503	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1428	C	N3-C2-O2	-7.92	116.36	121.90
54	BA	2530	A	C5-C6-N1	7.92	121.66	117.70
54	BA	2278	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	2378	A	N1-C6-N6	-7.92	113.85	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	2	ARG	NE-CZ-NH1	7.92	124.26	120.30
54	BA	1535	A	C5-C6-N1	7.92	121.66	117.70
21	AA	1092	A	N1-C6-N6	-7.91	113.85	118.60
21	AA	1158	C	N3-C2-O2	-7.91	116.36	121.90
54	BA	791	C	N3-C2-O2	-7.91	116.36	121.90
54	BA	233	A	C5-C6-N1	7.91	121.66	117.70
12	AM	56	ARG	NE-CZ-NH1	7.91	124.25	120.30
21	AA	572	A	C5-C6-N1	7.91	121.65	117.70
21	AA	958	A	C5-C6-N1	7.91	121.65	117.70
21	AA	1476	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	945	A	N1-C6-N6	-7.91	113.86	118.60
21	AA	1196	A	C5-C6-N1	7.91	121.65	117.70
54	BA	627	A	C5-C6-N1	7.91	121.65	117.70
54	BA	352	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	607	A	C5-C6-N1	7.90	121.65	117.70
54	BA	1359	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	816	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1256	A	C5-C6-N1	7.89	121.65	117.70
38	BP	61	ARG	NE-CZ-NH1	7.89	124.25	120.30
54	BA	142	A	N1-C6-N6	-7.89	113.86	118.60
25	BC	155	ARG	NE-CZ-NH1	7.89	124.25	120.30
54	BA	221	A	C5-C6-N1	7.89	121.65	117.70
54	BA	1525	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	2013	A	C5-C6-N1	7.89	121.65	117.70
54	BA	936	A	C5-C6-N1	7.89	121.64	117.70
54	BA	226	A	C5-C6-N1	7.89	121.64	117.70
22	A1	74	C	N1-C2-O2	7.89	123.63	118.90
54	BA	1010	A	C5-C6-N1	7.89	121.64	117.70
19	AT	59	ARG	NE-CZ-NH1	7.89	124.24	120.30
21	AA	143	A	C5-C6-N1	7.88	121.64	117.70
21	AA	353	A	C5-C6-N1	7.88	121.64	117.70
21	AA	1269	A	C5-C6-N1	7.88	121.64	117.70
54	BA	103	A	C5-C6-N1	7.88	121.64	117.70
54	BA	2019	A	N1-C6-N6	-7.88	113.87	118.60
21	AA	66	A	N1-C6-N6	-7.88	113.87	118.60
21	AA	149	A	N1-C6-N6	-7.88	113.87	118.60
21	AA	328	C	N3-C2-O2	-7.88	116.39	121.90
54	BA	1572	A	C5-C6-N1	7.88	121.64	117.70
33	BK	70	ARG	NE-CZ-NH1	7.88	124.24	120.30
54	BA	861	A	C5-C6-N1	7.87	121.64	117.70
54	BA	984	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1144	A	C5-C6-N1	7.87	121.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	250	A	C5-C6-N1	7.87	121.63	117.70
21	AA	1170	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	330	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	563	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2170	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	1928	A	N1-C6-N6	-7.86	113.88	118.60
23	A2	79	A	C5-C6-N1	7.86	121.63	117.70
13	AN	90	ARG	NE-CZ-NH1	7.86	124.23	120.30
54	BA	1597	A	C5-C6-N1	7.86	121.63	117.70
21	AA	1054	C	N1-C2-O2	7.85	123.61	118.90
21	AA	1465	A	N1-C6-N6	-7.85	113.89	118.60
21	AA	356	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2826	A	N1-C6-N6	-7.85	113.89	118.60
21	AA	1225	A	C5-C6-N1	7.85	121.62	117.70
54	BA	602	A	C5-C6-N1	7.85	121.62	117.70
54	BA	750	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	706	A	C5-C6-N1	7.85	121.62	117.70
19	AT	28	ARG	NE-CZ-NH1	7.84	124.22	120.30
54	BA	204	A	C4-C5-C6	-7.84	113.08	117.00
54	BA	1088	A	O4'-C1'-N9	7.84	114.48	108.20
54	BA	2328	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2335	A	N1-C6-N6	-7.84	113.89	118.60
21	AA	1201	A	C5-C6-N1	7.84	121.62	117.70
54	BA	928	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	1586	A	C5-C6-N1	7.84	121.62	117.70
26	BD	33	ARG	NE-CZ-NH1	7.84	124.22	120.30
41	BS	18	ARG	NE-CZ-NH1	7.84	124.22	120.30
54	BA	1213	A	C5-C6-N1	7.84	121.62	117.70
22	A1	56	C	N3-C2-O2	-7.84	116.42	121.90
21	AA	994	A	C5-C6-N1	7.83	121.62	117.70
54	BA	1384	A	C5-C6-N1	7.83	121.62	117.70
54	BA	1616	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1952	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	371	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1096	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1320	C	N1-C2-O2	7.83	123.60	118.90
53	B4	36	ARG	NE-CZ-NH1	7.83	124.21	120.30
54	BA	1504	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1009	A	C5-C6-N1	7.82	121.61	117.70
37	BO	111	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	507	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1607	C	N3-C2-O2	-7.82	116.43	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1870	C	N1-C2-O2	7.82	123.59	118.90
54	BA	2101	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	2274	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	119	A	C5-C6-N1	7.82	121.61	117.70
21	AA	190	A	C5-C6-N1	7.82	121.61	117.70
54	BA	574	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	592	A	N1-C6-N6	-7.82	113.91	118.60
21	AA	345	C	N3-C2-O2	-7.81	116.43	121.90
54	BA	456	C	O4'-C1'-N1	7.81	114.45	108.20
54	BA	2740	A	C5'-C4'-O4'	7.81	118.48	109.10
21	AA	452	A	N1-C6-N6	-7.81	113.91	118.60
21	AA	1441	A	N1-C6-N6	-7.81	113.91	118.60
24	A3	11	A	C5-C6-N1	7.81	121.61	117.70
21	AA	1394	A	C5-C6-N1	7.81	121.60	117.70
21	AA	110	C	N3-C2-O2	-7.81	116.44	121.90
21	AA	970	C	N3-C2-O2	-7.81	116.44	121.90
54	BA	19	A	C5-C6-N1	7.81	121.60	117.70
54	BA	1932	A	C5-C6-N1	7.81	121.60	117.70
54	BA	2712	C	N3-C2-O2	-7.81	116.44	121.90
54	BA	2809	A	C5-C6-N1	7.81	121.60	117.70
21	AA	766	A	C5-C6-N1	7.80	121.60	117.70
54	BA	1969	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	1082	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	1377	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	2858	C	N3-C2-O2	-7.80	116.44	121.90
54	BA	1672	A	C5-C6-N1	7.80	121.60	117.70
21	AA	197	A	C5-C6-N1	7.79	121.60	117.70
21	AA	1036	A	N1-C6-N6	-7.79	113.92	118.60
54	BA	125	A	N1-C6-N6	-7.79	113.92	118.60
21	AA	523	A	N1-C6-N6	-7.79	113.92	118.60
38	BP	38	ARG	NE-CZ-NH1	7.79	124.19	120.30
54	BA	1571	A	N1-C6-N6	-7.79	113.93	118.60
46	BX	10	ARG	NE-CZ-NH1	7.79	124.19	120.30
54	BA	299	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	1169	A	C5-C6-N1	7.79	121.59	117.70
21	AA	704	A	C5-C6-N1	7.78	121.59	117.70
21	AA	900	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2173	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	443	A	C5-C6-N1	7.78	121.59	117.70
54	BA	1580	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	2340	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	878	A	N1-C6-N6	-7.78	113.93	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	983	A	C5-C6-N1	7.78	121.59	117.70
54	BA	1287	A	C5-C6-N1	7.78	121.59	117.70
21	AA	907	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	1456	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	146	A	C5-C6-N1	7.78	121.59	117.70
54	BA	563	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2095	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	228	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	2284	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	1155	A	C4-C5-C6	-7.78	113.11	117.00
21	AA	152	A	C5-C6-N1	7.77	121.59	117.70
54	BA	996	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	562	U	O4'-C1'-N1	7.77	114.42	108.20
21	AA	938	A	N1-C6-N6	-7.77	113.94	118.60
24	A3	60	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2376	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2327	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2212	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2247	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1451	C	N3-C2-O2	-7.76	116.47	121.90
21	AA	77	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	756	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1580	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1847	A	C5-C6-N1	7.76	121.58	117.70
54	BA	783	A	C5-C6-N1	7.76	121.58	117.70
22	A1	58	A	C5-C6-N1	7.76	121.58	117.70
24	A3	70	C	N3-C2-O2	-7.76	116.47	121.90
54	BA	101	A	C5-C6-N1	7.75	121.58	117.70
54	BA	1960	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	1429	A	C5-C6-N1	7.75	121.58	117.70
38	BP	87	ARG	NE-CZ-NH1	7.75	124.18	120.30
54	BA	749	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1098	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	768	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2042	A	C5-C6-N1	7.75	121.58	117.70
54	BA	217	A	C5-C6-N1	7.75	121.58	117.70
29	BG	54	ARG	NE-CZ-NH1	7.75	124.17	120.30
54	BA	1342	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1634	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	2170	A	C5-C6-N1	7.75	121.58	117.70
21	AA	1046	A	C5-C6-N1	7.75	121.57	117.70
38	BP	20	ARG	NE-CZ-NH1	7.75	124.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	BY	23	ARG	NE-CZ-NH1	7.75	124.17	120.30
21	AA	564	C	N3-C2-O2	-7.75	116.48	121.90
54	BA	1373	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	161	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	727	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1163	A	N1-C6-N6	-7.74	113.95	118.60
25	BC	166	ARG	NE-CZ-NH1	7.74	124.17	120.30
54	BA	1008	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1084	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1195	C	N3-C2-O2	-7.74	116.48	121.90
54	BA	19	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	710	U	O4'-C1'-N1	7.74	114.39	108.20
54	BA	1987	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	2191	A	C5-C6-N1	7.74	121.57	117.70
54	BA	311	A	C5-C6-N1	7.74	121.57	117.70
24	A3	22	A	C5-C6-N1	7.73	121.57	117.70
54	BA	490	C	N3-C2-O2	-7.73	116.49	121.90
54	BA	1274	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	1366	A	C5-C6-N1	7.73	121.57	117.70
21	AA	790	A	C5-C6-N1	7.73	121.56	117.70
21	AA	1248	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	195	A	C5-C6-N1	7.73	121.56	117.70
54	BA	479	A	C5-C6-N1	7.73	121.56	117.70
54	BA	1943	U	N3-C2-O2	-7.73	116.79	122.20
21	AA	621	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	1029	A	C5-C6-N1	7.73	121.56	117.70
54	BA	1069	A	C5-C6-N1	7.73	121.56	117.70
54	BA	2727	A	C5-C6-N1	7.73	121.56	117.70
2	AC	163	ARG	NE-CZ-NH1	7.73	124.16	120.30
21	AA	1246	A	C5-C6-N1	7.72	121.56	117.70
54	BA	233	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	833	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	167	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	1468	A	C5-C6-N1	7.72	121.56	117.70
21	AA	251	G	O4'-C1'-N9	7.72	114.38	108.20
54	BA	1618	A	O4'-C1'-N9	7.72	114.38	108.20
54	BA	1403	A	C5-C6-N1	7.72	121.56	117.70
21	AA	583	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	1236	A	C5-C6-N1	7.71	121.56	117.70
54	BA	608	A	C5-C6-N1	7.71	121.56	117.70
54	BA	838	C	N3-C2-O2	-7.71	116.50	121.90
54	BA	1054	A	C5-C6-N1	7.71	121.56	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1363	A	C5-C6-N1	7.71	121.56	117.70
54	BA	177	G	O4'-C1'-N9	7.71	114.37	108.20
54	BA	2163	A	C5-C6-N1	7.71	121.56	117.70
54	BA	2088	A	N1-C6-N6	-7.71	113.97	118.60
5	AF	91	ARG	NE-CZ-NH1	7.71	124.15	120.30
21	AA	288	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	972	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	1040	A	N1-C6-N6	-7.71	113.98	118.60
21	AA	819	A	C5-C6-N1	7.71	121.55	117.70
54	BA	735	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	1970	A	C5-C6-N1	7.71	121.55	117.70
54	BA	2270	A	N1-C6-N6	-7.71	113.98	118.60
21	AA	1434	A	N1-C6-N6	-7.70	113.98	118.60
22	A1	73	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1144	A	N1-C6-N6	-7.70	113.98	118.60
55	BB	36	C	N3-C2-O2	-7.70	116.51	121.90
54	BA	1032	A	C5-C6-N1	7.70	121.55	117.70
21	AA	120	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1640	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2333	A	C5-C6-N1	7.70	121.55	117.70
11	AL	85	ARG	NE-CZ-NH1	7.70	124.15	120.30
21	AA	1428	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1393	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2147	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	2516	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	195	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1480	C	O4'-C1'-N1	7.70	114.36	108.20
21	AA	1158	C	N1-C2-O2	7.69	123.52	118.90
55	BB	45	A	N1-C6-N6	-7.69	113.98	118.60
2	AC	155	ARG	NE-CZ-NH1	7.69	124.15	120.30
21	AA	250	A	O4'-C1'-N9	7.69	114.35	108.20
21	AA	729	A	C5-C6-N1	7.69	121.55	117.70
21	AA	977	A	N1-C6-N6	-7.69	113.98	118.60
54	BA	213	A	C5-C6-N1	7.69	121.55	117.70
54	BA	2114	A	C5-C6-N1	7.69	121.55	117.70
36	BN	45	ARG	NE-CZ-NH1	7.69	124.15	120.30
54	BA	2448	A	N1-C6-N6	-7.69	113.99	118.60
21	AA	451	A	C5-C6-N1	7.69	121.54	117.70
21	AA	478	A	C5-C6-N1	7.69	121.54	117.70
33	BK	105	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	863	A	C5-C6-N1	7.68	121.54	117.70
54	BA	2518	A	N1-C6-N6	-7.68	113.99	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	573	A	C5-C6-N1	7.68	121.54	117.70
21	AA	622	A	C5-C6-N1	7.68	121.54	117.70
54	BA	279	A	C5-C6-N1	7.68	121.54	117.70
54	BA	925	A	C5-C6-N1	7.68	121.54	117.70
54	BA	2342	C	N3-C2-O2	-7.68	116.53	121.90
21	AA	182	A	C5-C6-N1	7.68	121.54	117.70
54	BA	218	A	N1-C6-N6	-7.68	114.00	118.60
54	BA	278	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1632	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2764	A	C5-C6-N1	7.68	121.54	117.70
54	BA	480	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2886	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	71	A	C5-C6-N1	7.67	121.54	117.70
54	BA	76	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	1057	A	C5-C6-N1	7.67	121.54	117.70
54	BA	1470	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	1598	A	C5-C6-N1	7.67	121.54	117.70
54	BA	1854	A	C5-C6-N1	7.67	121.54	117.70
54	BA	761	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1566	A	C5-C6-N1	7.67	121.53	117.70
54	BA	2564	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2635	A	C4-C5-C6	-7.67	113.17	117.00
54	BA	2422	C	N1-C2-O2	7.67	123.50	118.90
54	BA	2587	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1392	A	C5-C6-N1	7.67	121.53	117.70
21	AA	1082	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2748	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2771	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	362	A	N1-C6-N6	-7.66	114.00	118.60
54	BA	1079	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	2108	A	N1-C6-N6	-7.66	114.00	118.60
55	BB	94	A	C5-C6-N1	7.66	121.53	117.70
20	AU	46	ARG	NE-CZ-NH2	7.66	124.13	120.30
54	BA	982	C	N1-C2-O2	7.66	123.50	118.90
54	BA	1321	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2613	U	O4'-C1'-N1	7.66	114.33	108.20
8	AI	122	ARG	NE-CZ-NH1	7.66	124.13	120.30
16	AQ	5	ARG	NE-CZ-NH1	7.66	124.13	120.30
54	BA	1637	A	N1-C6-N6	-7.66	114.01	118.60
21	AA	780	A	C5-C6-N1	7.65	121.53	117.70
54	BA	1757	A	C5-C6-N1	7.65	121.53	117.70
54	BA	1815	A	N1-C6-N6	-7.65	114.01	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	510	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	699	A	C5-C6-N1	7.65	121.53	117.70
54	BA	1609	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	538	A	N1-C6-N6	-7.65	114.01	118.60
21	AA	560	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	1126	A	C4-C5-C6	-7.65	113.18	117.00
54	BA	1274	A	C5-C6-N1	7.65	121.52	117.70
54	BA	1308	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	1509	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	2860	A	C5-C6-N1	7.65	121.52	117.70
21	AA	1180	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2750	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2886	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2736	A	N1-C6-N6	-7.64	114.02	118.60
16	AQ	64	ARG	NE-CZ-NH1	7.64	124.12	120.30
54	BA	670	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	2407	A	C5-C6-N1	7.64	121.52	117.70
54	BA	920	A	C5-C6-N1	7.64	121.52	117.70
54	BA	1322	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2727	A	C4-C5-C6	-7.63	113.18	117.00
54	BA	255	A	C5-C6-N1	7.63	121.52	117.70
54	BA	794	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	923	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	1503	A	C5-C6-N1	7.63	121.51	117.70
54	BA	225	C	O4'-C1'-N1	7.63	114.30	108.20
54	BA	443	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	1574	C	N3-C2-O2	-7.63	116.56	121.90
54	BA	1829	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	2886	A	O4'-C1'-N9	7.63	114.30	108.20
21	AA	130	A	C4-C5-C6	-7.63	113.19	117.00
21	AA	487	A	C5-C6-N1	7.63	121.51	117.70
54	BA	368	A	C5-C6-N1	7.63	121.51	117.70
21	AA	493	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2738	A	C5-C6-N1	7.62	121.51	117.70
21	AA	1183	U	C1'-O4'-C4'	-7.62	103.80	109.90
54	BA	2749	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	103	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	637	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	1307	A	N1-C6-N6	-7.62	114.03	118.60
8	AI	11	ARG	NE-CZ-NH1	7.62	124.11	120.30
54	BA	348	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	759	A	N1-C6-N6	-7.62	114.03	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2288	A	C5-C6-N1	7.62	121.51	117.70
21	AA	81	A	C5-C6-N1	7.62	121.51	117.70
21	AA	496	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	1735	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	267	C	O4'-C1'-N1	7.61	114.29	108.20
54	BA	1981	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	1101	A	C5-C6-N1	7.61	121.50	117.70
21	AA	60	A	C5-C6-N1	7.61	121.50	117.70
21	AA	1267	C	N3-C2-O2	-7.61	116.58	121.90
39	BQ	91	ARG	NE-CZ-NH1	7.61	124.10	120.30
54	BA	877	A	C5-C6-N1	7.61	121.50	117.70
17	AR	42	ARG	NE-CZ-NH1	7.60	124.10	120.30
54	BA	131	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	98	A	C5-C6-N1	7.60	121.50	117.70
54	BA	2850	A	C5-C6-N1	7.60	121.50	117.70
46	BX	56	ARG	NE-CZ-NH1	7.60	124.10	120.30
54	BA	1626	A	C5-C6-N1	7.60	121.50	117.70
54	BA	2781	A	C5-C6-N1	7.60	121.50	117.70
21	AA	793	U	C1'-O4'-C4'	-7.60	103.82	109.90
54	BA	947	A	C5-C6-N1	7.60	121.50	117.70
54	BA	982	C	N3-C2-O2	-7.60	116.58	121.90
21	AA	44	A	N1-C6-N6	-7.59	114.04	118.60
21	AA	546	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1077	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	1307	A	C5-C6-N1	7.59	121.50	117.70
54	BA	2020	A	N1-C6-N6	-7.59	114.04	118.60
21	AA	81	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	910	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1314	C	N3-C2-O2	-7.59	116.59	121.90
55	BB	66	A	C5-C6-N1	7.59	121.50	117.70
21	AA	495	A	N1-C6-N6	-7.59	114.05	118.60
21	AA	892	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1040	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1490	A	O4'-C1'-N9	7.59	114.27	108.20
2	AC	53	ARG	NE-CZ-NH1	7.59	124.09	120.30
21	AA	1238	A	C5-C6-N1	7.59	121.49	117.70
54	BA	1493	C	N3-C2-O2	-7.59	116.59	121.90
54	BA	2270	A	C5-C6-N1	7.59	121.49	117.70
54	BA	1618	A	C5-C6-N1	7.58	121.49	117.70
54	BA	346	A	C5-C6-N1	7.58	121.49	117.70
21	AA	448	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2589	A	C5-C6-N1	7.58	121.49	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	784	A	N1-C6-N6	-7.58	114.05	118.60
21	AA	1311	A	C4-C5-C6	-7.58	113.21	117.00
54	BA	13	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1117	A	N1-C6-N6	-7.58	114.05	118.60
24	A3	75	C	N3-C2-O2	-7.58	116.60	121.90
54	BA	1434	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2468	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2170	A	C4-C5-C6	-7.57	113.21	117.00
55	BB	108	A	C5-C6-N1	7.57	121.49	117.70
21	AA	315	A	C5-C6-N1	7.57	121.49	117.70
54	BA	643	A	C5-C6-N1	7.57	121.49	117.70
54	BA	1900	A	C5-C6-N1	7.57	121.49	117.70
21	AA	221	C	N3-C2-O2	-7.57	116.60	121.90
21	AA	1357	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1552	A	C5-C6-N1	7.57	121.48	117.70
56	B5	162	ARG	NE-CZ-NH1	7.57	124.08	120.30
54	BA	83	A	C5-C6-N1	7.57	121.48	117.70
54	BA	781	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1382	G	O4'-C1'-N9	7.57	114.25	108.20
21	AA	553	A	C4-C5-C6	-7.56	113.22	117.00
21	AA	1500	A	C4-C5-C6	-7.56	113.22	117.00
54	BA	2225	A	C5-C6-N1	7.56	121.48	117.70
21	AA	274	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1427	A	C4-C5-C6	-7.56	113.22	117.00
54	BA	2021	C	N3-C2-O2	-7.56	116.61	121.90
21	AA	583	A	C5-C6-N1	7.56	121.48	117.70
54	BA	960	A	C5-C6-N1	7.56	121.48	117.70
54	BA	693	A	N1-C6-N6	-7.56	114.07	118.60
54	BA	439	A	N1-C6-N6	-7.56	114.07	118.60
54	BA	793	A	N1-C6-N6	-7.55	114.07	118.60
4	AE	28	ARG	NE-CZ-NH1	7.55	124.08	120.30
26	BD	46	ARG	NE-CZ-NH1	7.55	124.08	120.30
54	BA	1508	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1689	A	C5-C6-N1	7.55	121.47	117.70
54	BA	706	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1755	A	C5-C6-N1	7.55	121.47	117.70
21	AA	336	A	C5-C6-N1	7.55	121.47	117.70
54	BA	203	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	575	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1606	C	N3-C2-O2	-7.55	116.62	121.90
54	BA	1664	A	C5-C6-N1	7.54	121.47	117.70
54	BA	323	C	N3-C2-O2	-7.54	116.62	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	804	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	1789	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	1829	A	C5-C6-N1	7.54	121.47	117.70
54	BA	513	A	C5-C6-N1	7.54	121.47	117.70
54	BA	2565	A	C5-C6-N1	7.54	121.47	117.70
21	AA	889	A	C5-C6-N1	7.54	121.47	117.70
21	AA	1227	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	298	A	C4-C5-C6	-7.54	113.23	117.00
37	BO	7	ARG	NE-CZ-NH1	7.54	124.07	120.30
21	AA	10	A	C5-C6-N1	7.54	121.47	117.70
21	AA	1303	C	N3-C2-O2	-7.54	116.63	121.90
54	BA	204	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	1454	C	N1-C2-O2	7.54	123.42	118.90
21	AA	1274	A	C5-C6-N1	7.53	121.47	117.70
54	BA	574	A	C5-C6-N1	7.53	121.47	117.70
21	AA	1005	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	819	A	N1-C6-N6	-7.53	114.08	118.60
21	AA	765	G	O4'-C1'-N9	7.52	114.22	108.20
54	BA	2005	A	C5-C6-N1	7.52	121.46	117.70
54	BA	2134	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	1668	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	573	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	787	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	263	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	1217	C	O4'-C1'-N1	7.52	114.21	108.20
54	BA	2434	A	C5-C6-N1	7.52	121.46	117.70
11	AL	82	ARG	NE-CZ-NH1	7.51	124.06	120.30
21	AA	1251	A	C5-C6-N1	7.51	121.46	117.70
54	BA	1328	A	C4-C5-C6	-7.51	113.25	117.00
54	BA	2009	A	C4-C5-C6	-7.51	113.25	117.00
2	AC	125	ARG	NE-CZ-NH1	7.51	124.05	120.30
21	AA	363	A	C5-C6-N1	7.51	121.45	117.70
40	BR	90	ARG	NE-CZ-NH1	7.51	124.05	120.30
44	BV	21	ARG	NE-CZ-NH1	-7.51	116.55	120.30
21	AA	308	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	743	A	N1-C6-N6	-7.51	114.10	118.60
54	BA	1030	C	N3-C2-O2	-7.50	116.65	121.90
21	AA	901	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2733	A	N1-C6-N6	-7.50	114.10	118.60
24	A3	1	C	N3-C2-O2	-7.50	116.65	121.90
54	BA	218	A	C5-C6-N1	7.50	121.45	117.70
54	BA	632	A	N1-C6-N6	-7.50	114.10	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	655	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1000	A	C5-C6-N1	7.50	121.45	117.70
54	BA	513	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	886	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1434	A	O4'-C1'-N9	7.50	114.20	108.20
54	BA	2113	U	O4'-C1'-N1	7.50	114.20	108.20
54	BA	2837	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	637	A	C5-C6-N1	7.50	121.45	117.70
54	BA	909	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	1686	C	N3-C2-O2	-7.50	116.65	121.90
21	AA	1201	A	P-O3'-C3'	7.50	128.69	119.70
21	AA	845	A	C5-C6-N1	7.49	121.45	117.70
22	A1	23	A	C5-C6-N1	7.49	121.45	117.70
54	BA	244	A	N1-C6-N6	-7.49	114.10	118.60
54	BA	374	A	N1-C6-N6	-7.49	114.10	118.60
54	BA	2250	G	O4'-C1'-N9	7.49	114.19	108.20
54	BA	2820	A	N1-C6-N6	-7.49	114.10	118.60
54	BA	889	C	N3-C2-O2	-7.49	116.66	121.90
54	BA	716	A	C5-C6-N1	7.49	121.44	117.70
54	BA	975	A	C5-C6-N1	7.49	121.44	117.70
54	BA	1046	A	C5-C6-N1	7.49	121.44	117.70
54	BA	1420	A	C5-C6-N1	7.49	121.44	117.70
21	AA	695	A	C5-C6-N1	7.49	121.44	117.70
21	AA	1395	C	N3-C2-O2	-7.49	116.66	121.90
21	AA	600	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	1254	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	2547	A	N1-C6-N6	-7.49	114.11	118.60
21	AA	784	A	C5-C6-N1	7.48	121.44	117.70
10	AK	12	ARG	NE-CZ-NH1	7.48	124.04	120.30
21	AA	131	A	C4-C5-C6	-7.48	113.26	117.00
21	AA	167	A	C5-C6-N1	7.48	121.44	117.70
54	BA	1810	A	C5-C6-N1	7.48	121.44	117.70
7	AH	79	ARG	NE-CZ-NH1	7.48	124.04	120.30
21	AA	968	A	C5-C6-N1	7.48	121.44	117.70
54	BA	689	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	888	C	N3-C2-O2	-7.48	116.67	121.90
54	BA	2336	A	C5-C6-N1	7.48	121.44	117.70
54	BA	345	A	C5-C6-N1	7.48	121.44	117.70
54	BA	324	A	N1-C6-N6	-7.47	114.11	118.60
54	BA	1067	A	N1-C6-N6	-7.47	114.11	118.60
54	BA	1821	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2327	A	N1-C6-N6	-7.47	114.11	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2394	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	2781	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	2281	A	N1-C6-N6	-7.47	114.12	118.60
21	AA	1180	A	C4-C5-C6	-7.47	113.27	117.00
21	AA	1214	C	N1-C2-O2	7.47	123.38	118.90
54	BA	644	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2158	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	342	A	N1-C6-N6	-7.47	114.12	118.60
21	AA	1255	G	N3-C2-N2	-7.47	114.67	119.90
54	BA	2058	A	C5-C6-N1	7.47	121.43	117.70
54	BA	156	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	125	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1551	A	N1-C6-N6	-7.46	114.12	118.60
21	AA	1152	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1433	A	C5-C6-N1	7.46	121.43	117.70
54	BA	10	A	N1-C6-N6	-7.46	114.12	118.60
21	AA	109	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1246	A	C4-C5-C6	-7.46	113.27	117.00
21	AA	1500	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1610	A	N1-C6-N6	-7.46	114.13	118.60
54	BA	1858	A	N1-C6-N6	-7.46	114.13	118.60
54	BA	2459	A	N1-C6-N6	-7.46	114.13	118.60
54	BA	1260	A	C4-C5-C6	-7.46	113.27	117.00
54	BA	1272	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1590	A	C4-C5-C6	-7.46	113.27	117.00
21	AA	51	A	C4-C5-C6	-7.45	113.27	117.00
21	AA	794	A	C4-C5-C6	-7.45	113.27	117.00
21	AA	1110	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	183	C	O4'-C1'-N1	7.45	114.16	108.20
21	AA	675	A	P-O3'-C3'	7.45	128.64	119.70
21	AA	119	A	C5-C6-N1	7.45	121.42	117.70
21	AA	513	C	N3-C2-O2	-7.45	116.69	121.90
28	BF	109	ARG	NE-CZ-NH1	7.45	124.02	120.30
54	BA	1070	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1073	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2469	A	N1-C6-N6	-7.45	114.13	118.60
8	AI	123	ARG	NE-CZ-NH1	7.45	124.02	120.30
21	AA	642	A	C5-C6-N1	7.45	121.42	117.70
44	BV	93	ARG	NE-CZ-NH1	7.45	124.02	120.30
54	BA	1755	A	C4-C5-C6	-7.45	113.28	117.00
54	BA	2433	A	C5-C6-N1	7.45	121.42	117.70
21	AA	643	C	N3-C2-O2	-7.44	116.69	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	74	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2215	C	O4'-C1'-N1	7.44	114.15	108.20
21	AA	1476	A	C5-C6-N1	7.44	121.42	117.70
23	A2	91	A	C5-C6-N1	7.44	121.42	117.70
54	BA	269	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	1067	A	C5-C6-N1	7.44	121.42	117.70
21	AA	408	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	309	A	C5-C6-N1	7.44	121.42	117.70
54	BA	943	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	356	A	C5-C6-N1	7.44	121.42	117.70
54	BA	118	A	C5-C6-N1	7.44	121.42	117.70
54	BA	176	A	C5-C6-N1	7.44	121.42	117.70
2	AC	10	ARG	NE-CZ-NH1	7.43	124.02	120.30
21	AA	665	A	C4-C5-C6	-7.43	113.28	117.00
21	AA	1252	A	C5-C6-N1	7.43	121.42	117.70
21	AA	1418	A	N1-C6-N6	-7.43	114.14	118.60
9	AJ	68	ARG	NE-CZ-NH1	7.43	124.02	120.30
21	AA	1519	A	C5-C6-N1	7.43	121.42	117.70
54	BA	532	A	C5-C6-N1	7.43	121.42	117.70
21	AA	1324	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	1168	U	O4'-C1'-N1	7.43	114.14	108.20
22	A1	76	A	C5-C6-N1	7.43	121.41	117.70
54	BA	2298	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	2378	A	C5-C6-N1	7.43	121.41	117.70
21	AA	236	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	1080	A	C4-C5-C6	-7.42	113.29	117.00
34	BL	21	ARG	NE-CZ-NH1	7.42	124.01	120.30
54	BA	540	C	N3-C2-O2	-7.42	116.70	121.90
54	BA	1367	A	C5-C6-N1	7.42	121.41	117.70
54	BA	2386	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	8	A	C4-C5-C6	-7.42	113.29	117.00
54	BA	2368	C	N3-C2-O2	-7.42	116.71	121.90
21	AA	1518	A	N1-C6-N6	-7.42	114.15	118.60
49	B0	12	ARG	NE-CZ-NH1	7.42	124.01	120.30
24	A3	36	A	C5-C6-N1	7.42	121.41	117.70
54	BA	310	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	272	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1322	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	320	A	C5-C6-N1	7.41	121.41	117.70
54	BA	2154	A	N1-C6-N6	-7.41	114.15	118.60
21	AA	66	A	C5-C6-N1	7.41	121.41	117.70
54	BA	2711	A	C5-C6-N1	7.41	121.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	927	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	1143	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	1103	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	1175	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2205	A	C5-C6-N1	7.41	121.40	117.70
54	BA	1705	A	C5-C6-N1	7.40	121.40	117.70
21	AA	160	A	C5-C6-N1	7.40	121.40	117.70
21	AA	371	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	749	A	C5-C6-N1	7.40	121.40	117.70
49	B0	9	ARG	NE-CZ-NH1	7.40	124.00	120.30
54	BA	740	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	503	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	322	A	C5-C6-N1	7.39	121.40	117.70
54	BA	1328	A	C5-C6-N1	7.39	121.40	117.70
54	BA	1966	A	C5-C6-N1	7.39	121.40	117.70
34	BL	69	ARG	NE-CZ-NH1	7.39	124.00	120.30
54	BA	866	A	C5-C6-N1	7.39	121.40	117.70
54	BA	1532	A	C5-C6-N1	7.39	121.40	117.70
54	BA	1591	A	C5-C6-N1	7.39	121.40	117.70
54	BA	104	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	1801	A	C5-C6-N1	7.39	121.39	117.70
21	AA	51	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1284	A	C5-C6-N1	7.39	121.39	117.70
21	AA	1446	A	C5-C6-N1	7.39	121.39	117.70
24	A3	77	A	C5-C6-N1	7.39	121.39	117.70
54	BA	863	A	N1-C6-N6	-7.39	114.17	118.60
22	A1	14	A	C5-C6-N1	7.38	121.39	117.70
54	BA	979	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2266	A	C4-C5-C6	-7.38	113.31	117.00
55	BB	90	C	O4'-C1'-N1	7.38	114.11	108.20
21	AA	1396	A	C5-C6-N1	7.38	121.39	117.70
29	BG	2	ARG	NE-CZ-NH1	7.38	123.99	120.30
54	BA	825	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2534	A	C5-C6-N1	7.38	121.39	117.70
16	AQ	39	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	393	A	N1-C6-N6	-7.38	114.17	118.60
21	AA	502	A	C5-C6-N1	7.38	121.39	117.70
54	BA	514	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2600	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	590	A	O4'-C1'-N9	7.38	114.10	108.20
54	BA	1504	A	C4-C5-C6	-7.38	113.31	117.00
21	AA	1130	A	C4-C5-C6	-7.38	113.31	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1431	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	900	A	N1-C6-N6	-7.38	114.17	118.60
21	AA	1188	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2426	A	C4-C5-C6	-7.37	113.31	117.00
54	BA	2614	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1048	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	1143	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1606	C	N1-C2-O2	7.37	123.32	118.90
51	B2	19	ARG	NE-CZ-NH1	7.37	123.98	120.30
54	BA	1021	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2882	A	C5-C6-N1	7.37	121.38	117.70
21	AA	919	A	C4-C5-C6	-7.37	113.32	117.00
21	AA	1219	A	C5-C6-N1	7.37	121.38	117.70
54	BA	693	A	C5-C6-N1	7.37	121.38	117.70
21	AA	777	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	1308	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1596	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2198	A	N1-C6-N6	-7.36	114.18	118.60
43	BU	5	ARG	NE-CZ-NH1	7.36	123.98	120.30
21	AA	171	A	C5-C6-N1	7.36	121.38	117.70
54	BA	508	A	C5-C6-N1	7.36	121.38	117.70
54	BA	614	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	1427	A	C5-C6-N1	7.36	121.38	117.70
21	AA	532	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1329	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2077	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	2184	A	N1-C6-N6	-7.36	114.19	118.60
21	AA	1287	A	C5-C6-N1	7.36	121.38	117.70
54	BA	374	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2778	A	C5-C6-N1	7.36	121.38	117.70
21	AA	936	C	N3-C2-O2	-7.35	116.75	121.90
6	AG	9	ARG	NE-CZ-NH1	7.35	123.98	120.30
21	AA	1484	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	415	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2283	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	238	A	N1-C6-N6	-7.35	114.19	118.60
24	A3	17	C	N3-C2-O2	-7.35	116.75	121.90
25	BC	12	ARG	NE-CZ-NH1	7.35	123.97	120.30
54	BA	2328	A	C4-C5-C6	-7.35	113.33	117.00
21	AA	1342	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	1269	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1301	A	C5-C6-N1	7.34	121.37	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	560	A	C5-C6-N1	7.34	121.37	117.70
54	BA	751	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1928	A	C5-C6-N1	7.34	121.37	117.70
21	AA	716	A	C4-C5-C6	-7.34	113.33	117.00
21	AA	767	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1321	A	N1-C6-N6	-7.34	114.19	118.60
54	BA	2142	A	N1-C6-N6	-7.34	114.19	118.60
54	BA	2333	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	1169	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2452	C	N3-C2-O2	-7.34	116.76	121.90
16	AQ	61	ARG	NE-CZ-NH1	7.33	123.97	120.30
3	AD	80	ARG	NE-CZ-NH1	7.33	123.97	120.30
21	AA	509	A	C5-C6-N1	7.33	121.37	117.70
24	A3	73	A	C5-C6-N1	7.33	121.37	117.70
14	AO	63	ARG	NE-CZ-NH1	7.33	123.97	120.30
21	AA	63	C	N3-C2-O2	-7.33	116.77	121.90
21	AA	977	A	C5-C6-N1	7.33	121.36	117.70
54	BA	626	A	C5-C6-N1	7.33	121.37	117.70
54	BA	1241	A	C5-C6-N1	7.33	121.36	117.70
54	BA	1889	A	C4-C5-C6	-7.33	113.33	117.00
54	BA	2851	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2726	A	O4'-C1'-N9	7.33	114.06	108.20
14	AO	62	ARG	NE-CZ-NH1	7.33	123.96	120.30
21	AA	1285	A	C5-C6-N1	7.32	121.36	117.70
54	BA	146	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	222	A	C5-C6-N1	7.32	121.36	117.70
21	AA	320	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	1311	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1783	A	C4-C5-C6	-7.32	113.34	117.00
21	AA	1317	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	2515	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	2660	A	C5-C6-N1	7.32	121.36	117.70
54	BA	742	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2350	C	O4'-C1'-N1	7.32	114.06	108.20
21	AA	315	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	906	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	1353	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1549	A	C5-C6-N1	7.32	121.36	117.70
21	AA	132	C	N3-C2-O2	-7.32	116.78	121.90
21	AA	949	A	C4-C5-C6	-7.31	113.34	117.00
54	BA	614	A	C5-C6-N1	7.31	121.36	117.70
54	BA	1230	A	N1-C6-N6	-7.31	114.21	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1226	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2062	A	C5-C6-N1	7.31	121.36	117.70
14	AO	57	ARG	NE-CZ-NH1	7.31	123.96	120.30
24	A3	73	A	O4'-C1'-N9	7.31	114.05	108.20
21	AA	797	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	471	A	C5-C6-N1	7.31	121.36	117.70
54	BA	1134	A	N1-C6-N6	-7.31	114.21	118.60
54	BA	2432	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2614	A	N1-C6-N6	-7.31	114.22	118.60
21	AA	964	A	C5-C6-N1	7.31	121.35	117.70
21	AA	1271	A	C5-C6-N1	7.31	121.35	117.70
19	AT	24	ARG	NE-CZ-NH1	7.31	123.95	120.30
21	AA	872	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	1827	U	O4'-C1'-N1	7.30	114.04	108.20
54	BA	2711	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	460	A	N1-C6-N6	-7.30	114.22	118.60
21	AA	795	C	N1-C2-O2	7.30	123.28	118.90
24	A3	74	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2381	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	2628	C	N1-C2-O2	7.30	123.28	118.90
54	BA	2666	C	O4'-C1'-N1	7.30	114.04	108.20
21	AA	53	A	C5-C6-N1	7.30	121.35	117.70
21	AA	792	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1447	A	C5-C6-N1	7.30	121.35	117.70
54	BA	53	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1548	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	1668	A	C5-C6-N1	7.30	121.35	117.70
54	BA	10	A	C5-C6-N1	7.29	121.35	117.70
54	BA	613	A	C5-C6-N1	7.29	121.35	117.70
54	BA	2059	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	579	A	C5-C6-N1	7.29	121.35	117.70
54	BA	632	A	C5-C6-N1	7.29	121.35	117.70
21	AA	196	A	C4-C5-C6	-7.29	113.35	117.00
21	AA	938	A	C5-C6-N1	7.29	121.35	117.70
21	AA	962	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	1403	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	2632	A	C4-C5-C6	-7.29	113.35	117.00
12	AM	108	ARG	NE-CZ-NH1	7.29	123.94	120.30
54	BA	1507	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	1439	A	C5-C6-N1	7.29	121.34	117.70
54	BA	60	G	N3-C2-N2	-7.29	114.80	119.90
21	AA	1378	C	N3-C2-O2	-7.28	116.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1938	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	468	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1616	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2145	C	N3-C2-O2	-7.28	116.80	121.90
21	AA	1456	A	C5-C6-N1	7.28	121.34	117.70
32	BJ	120	ARG	NE-CZ-NH1	7.28	123.94	120.30
21	AA	116	A	C5-C6-N1	7.28	121.34	117.70
21	AA	595	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	264	C	N3-C2-O2	-7.28	116.80	121.90
54	BA	526	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	1204	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	943	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1194	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	1480	C	N3-C2-O2	-7.28	116.81	121.90
54	BA	1551	A	C5-C6-N1	7.28	121.34	117.70
55	BB	50	A	C5-C6-N1	7.28	121.34	117.70
3	AD	187	ARG	NE-CZ-NH1	7.27	123.94	120.30
54	BA	1385	A	C5-C6-N1	7.27	121.34	117.70
21	AA	1362	A	C5-C6-N1	7.27	121.34	117.70
54	BA	2154	A	C5-C6-N1	7.27	121.34	117.70
54	BA	2273	A	C5-C6-N1	7.27	121.34	117.70
21	AA	59	A	C5-C6-N1	7.27	121.33	117.70
22	A1	26	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1739	A	C5-C6-N1	7.27	121.33	117.70
54	BA	522	A	C5-C6-N1	7.27	121.33	117.70
55	BB	71	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	217	A	C4-C5-C6	-7.27	113.37	117.00
54	BA	718	A	O4'-C1'-N9	7.27	114.01	108.20
18	AS	54	ARG	NE-CZ-NH1	7.26	123.93	120.30
24	A3	40	C	N3-C2-O2	-7.26	116.81	121.90
21	AA	1081	A	N1-C6-N6	-7.26	114.24	118.60
54	BA	1890	A	C5-C6-N1	7.26	121.33	117.70
21	AA	899	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	2497	A	C5-C6-N1	7.26	121.33	117.70
21	AA	80	A	C5-C6-N1	7.26	121.33	117.70
21	AA	130	A	C5-C6-N1	7.26	121.33	117.70
21	AA	228	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1509	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1433	A	C5-C6-N1	7.26	121.33	117.70
38	BP	102	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	1609	A	C5-C6-N1	7.26	121.33	117.70
21	AA	431	A	C5-C6-N1	7.25	121.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1605	C	N3-C2-O2	-7.25	116.82	121.90
54	BA	2503	A	C5-C6-N1	7.25	121.33	117.70
21	AA	574	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	1165	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	1899	A	N1-C6-N6	-7.25	114.25	118.60
12	AM	91	ARG	NE-CZ-NH1	7.25	123.92	120.30
21	AA	108	G	O4'-C1'-N9	7.25	114.00	108.20
21	AA	466	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1502	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	2055	C	N3-C2-O2	-7.25	116.83	121.90
54	BA	621	A	C5-C6-N1	7.25	121.32	117.70
54	BA	668	A	N1-C6-N6	-7.25	114.25	118.60
21	AA	796	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	1324	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1679	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	2461	A	C5-C6-N1	7.25	121.32	117.70
54	BA	730	A	N1-C6-N6	-7.24	114.25	118.60
21	AA	151	A	C5-C6-N1	7.24	121.32	117.70
21	AA	840	C	N3-C2-O2	-7.24	116.83	121.90
37	BO	94	ARG	NE-CZ-NH1	7.24	123.92	120.30
21	AA	959	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	821	A	C5-C6-N1	7.24	121.32	117.70
8	AI	98	ARG	NE-CZ-NH1	7.24	123.92	120.30
21	AA	1430	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1142	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	1978	A	C5-C6-N1	7.23	121.32	117.70
54	BA	2810	A	C5-C6-N1	7.23	121.32	117.70
21	AA	364	A	C5-C6-N1	7.23	121.32	117.70
21	AA	366	A	C5-C6-N1	7.23	121.32	117.70
21	AA	1167	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	420	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	752	A	C5-C6-N1	7.23	121.32	117.70
54	BA	1591	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	2590	A	C5-C6-N1	7.23	121.32	117.70
54	BA	1095	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1650	A	C4-C5-C6	-7.23	113.39	117.00
54	BA	1937	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2741	A	C5-C6-N1	7.23	121.32	117.70
21	AA	205	A	C5-C6-N1	7.23	121.31	117.70
54	BA	560	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	1059	C	N3-C2-O2	-7.23	116.84	121.90
22	A1	56	C	N1-C2-O2	7.23	123.24	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	6	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	675	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1977	A	C5-C6-N1	7.23	121.31	117.70
21	AA	576	C	N3-C2-O2	-7.22	116.84	121.90
21	AA	1110	A	C5-C6-N1	7.22	121.31	117.70
24	A3	11	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	229	C	N3-C2-O2	-7.22	116.84	121.90
21	AA	71	A	C5-C6-N1	7.22	121.31	117.70
21	AA	329	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	2090	A	C5-C6-N1	7.22	121.31	117.70
2	AC	142	ARG	NE-CZ-NH1	7.22	123.91	120.30
21	AA	196	A	C5-C6-N1	7.22	121.31	117.70
21	AA	872	A	C5-C6-N1	7.22	121.31	117.70
21	AA	1280	A	C5-C6-N1	7.22	121.31	117.70
21	AA	1437	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	2483	C	N3-C2-O2	-7.22	116.85	121.90
55	BB	108	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	767	U	O4'-C1'-N1	7.22	113.97	108.20
54	BA	1803	A	C5-C6-N1	7.22	121.31	117.70
21	AA	640	A	C5-C6-N1	7.22	121.31	117.70
21	AA	1469	C	N3-C2-O2	-7.22	116.85	121.90
42	BT	12	ARG	NE-CZ-NH1	7.22	123.91	120.30
54	BA	183	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	847	U	N3-C2-O2	-7.22	117.15	122.20
54	BA	1365	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2542	A	C5-C6-N1	7.22	121.31	117.70
21	AA	316	C	N3-C2-O2	-7.21	116.85	121.90
36	BN	12	ARG	NE-CZ-NH1	7.21	123.91	120.30
54	BA	2285	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	2392	A	C5-C6-N1	7.21	121.31	117.70
54	BA	482	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	1603	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	2868	A	C5-C6-N1	7.21	121.31	117.70
21	AA	414	A	C5-C6-N1	7.21	121.30	117.70
54	BA	216	A	N1-C6-N6	-7.21	114.28	118.60
54	BA	510	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	2199	A	C5-C6-N1	7.21	121.30	117.70
21	AA	1480	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	1134	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1441	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1304	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1470	A	C5-C6-N1	7.20	121.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	129	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1227	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1275	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1508	A	C5-C6-N1	7.20	121.30	117.70
51	B2	41	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	2767	C	O4'-C1'-N1	7.20	113.96	108.20
21	AA	374	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	990	A	C5-C6-N1	7.20	121.30	117.70
21	AA	381	C	N3-C2-O2	-7.19	116.86	121.90
54	BA	2037	A	N1-C6-N6	-7.19	114.28	118.60
21	AA	1499	A	C5-C6-N1	7.19	121.30	117.70
54	BA	654	A	C5-C6-N1	7.19	121.30	117.70
21	AA	716	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2634	A	C5-C6-N1	7.19	121.30	117.70
21	AA	476	U	O4'-C1'-N1	7.19	113.95	108.20
54	BA	2705	A	C5-C6-N1	7.19	121.29	117.70
6	AG	142	ARG	NE-CZ-NH1	7.18	123.89	120.30
21	AA	461	A	C5-C6-N1	7.18	121.29	117.70
39	BQ	69	ARG	NE-CZ-NH1	7.18	123.89	120.30
54	BA	1805	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2654	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2734	A	C5-C6-N1	7.18	121.29	117.70
21	AA	696	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	94	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1392	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1583	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1726	C	O4'-C1'-N1	7.18	113.94	108.20
21	AA	629	A	C5-C6-N1	7.18	121.29	117.70
21	AA	754	C	N3-C2-O2	-7.18	116.88	121.90
21	AA	969	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1413	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	1499	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	1590	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2699	C	N3-C2-O2	-7.18	116.88	121.90
21	AA	80	A	N1-C6-N6	-7.17	114.30	118.60
21	AA	1274	A	N1-C6-N6	-7.17	114.30	118.60
21	AA	1418	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1877	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2721	A	C5-C6-N1	7.17	121.29	117.70
21	AA	327	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1117	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1518	A	C5-C6-N1	7.17	121.29	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1005	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1787	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	2284	A	C5-C6-N1	7.17	121.29	117.70
54	BA	282	A	C5-C6-N1	7.17	121.28	117.70
54	BA	572	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1289	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	1383	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1544	A	C5-C6-N1	7.17	121.28	117.70
26	BD	179	ARG	NE-CZ-NH1	7.17	123.89	120.30
54	BA	401	A	N1-C6-N6	-7.17	114.30	118.60
13	AN	69	ARG	NE-CZ-NH1	7.17	123.88	120.30
54	BA	436	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	1889	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1086	A	C5-C6-N1	7.16	121.28	117.70
22	A1	21	A	C4-C5-C6	-7.16	113.42	117.00
54	BA	899	A	C5-C6-N1	7.16	121.28	117.70
21	AA	210	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	152	A	C5-C6-N1	7.16	121.28	117.70
54	BA	236	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	1579	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2023	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	142	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2733	A	C5-C6-N1	7.16	121.28	117.70
54	BA	753	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2082	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	472	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	896	A	O4'-C1'-N9	7.16	113.92	108.20
54	BA	2366	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	332	A	C4-C5-C6	-7.15	113.42	117.00
21	AA	892	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	219	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1987	A	C5-C6-N1	7.15	121.28	117.70
21	AA	1014	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1211	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	2135	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	2757	A	C5-C6-N1	7.15	121.27	117.70
21	AA	327	A	N1-C6-N6	-7.14	114.31	118.60
21	AA	465	A	O4'-C1'-N9	7.14	113.92	108.20
54	BA	2347	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	2558	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	427	U	O4'-C1'-N1	7.14	113.91	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	89	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	2019	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2173	A	C5-C6-N1	7.14	121.27	117.70
24	A3	59	A	C5-C6-N1	7.14	121.27	117.70
54	BA	422	A	C5-C6-N1	7.14	121.27	117.70
54	BA	633	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	456	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	84	A	C5-C6-N1	7.14	121.27	117.70
21	AA	523	A	C4-C5-C6	-7.13	113.43	117.00
43	BU	6	ARG	NE-CZ-NH1	7.13	123.87	120.30
54	BA	2381	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2814	A	C5-C6-N1	7.13	121.27	117.70
54	BA	265	A	C4-C5-C6	-7.13	113.43	117.00
54	BA	2164	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	2717	C	N3-C2-O2	-7.13	116.91	121.90
10	AK	105	ARG	NE-CZ-NH1	7.13	123.86	120.30
21	AA	673	A	C5-C6-N1	7.13	121.26	117.70
54	BA	846	U	O4'-C1'-N1	7.13	113.90	108.20
54	BA	1912	A	C5-C6-N1	7.13	121.26	117.70
21	AA	546	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	1113	C	N3-C2-O2	-7.12	116.91	121.90
21	AA	1480	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1439	A	O4'-C1'-N9	7.12	113.90	108.20
54	BA	1654	A	C5-C6-N1	7.12	121.26	117.70
21	AA	53	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	298	A	C5-C6-N1	7.12	121.26	117.70
26	BD	128	ARG	NE-CZ-NH1	7.12	123.86	120.30
54	BA	2706	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	525	U	O4'-C1'-N1	7.12	113.89	108.20
54	BA	38	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1194	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1569	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2147	A	C5-C6-N1	7.11	121.26	117.70
21	AA	602	A	C5-C6-N1	7.11	121.25	117.70
21	AA	994	A	N1-C6-N6	-7.11	114.33	118.60
54	BA	631	A	C5-C6-N1	7.11	121.26	117.70
54	BA	634	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	645	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	1635	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2566	A	N1-C6-N6	-7.11	114.33	118.60
54	BA	2665	A	C5-C6-N1	7.11	121.25	117.70
21	AA	873	A	N1-C6-N6	-7.11	114.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1102	A	C5-C6-N1	7.11	121.25	117.70
21	AA	1167	A	C5-C6-N1	7.11	121.25	117.70
21	AA	1399	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	1505	A	C5-C6-N1	7.11	121.25	117.70
21	AA	547	A	C4-C5-C6	-7.11	113.45	117.00
21	AA	1216	A	N1-C6-N6	-7.11	114.34	118.60
54	BA	516	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	1932	A	C4-C5-C6	-7.11	113.45	117.00
21	AA	344	A	C5-C6-N1	7.11	121.25	117.70
54	BA	428	A	N1-C6-N6	-7.11	114.34	118.60
54	BA	1027	A	C5-C6-N1	7.11	121.25	117.70
54	BA	157	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	864	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	616	A	C5-C6-N1	7.10	121.25	117.70
54	BA	951	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	1373	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1670	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	1790	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	495	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2434	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	2682	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2687	U	O4'-C1'-N1	7.10	113.88	108.20
39	BQ	32	ARG	NE-CZ-NH1	7.10	123.85	120.30
54	BA	844	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	854	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	972	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2020	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2501	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	1306	A	C4-C5-C6	-7.10	113.45	117.00
24	A3	45	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1477	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2459	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1700	A	C5-C6-N1	7.09	121.25	117.70
22	A1	6	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2300	C	O4'-C1'-N1	7.09	113.87	108.20
21	AA	482	A	C5-C6-N1	7.09	121.25	117.70
21	AA	753	A	C5-C6-N1	7.09	121.24	117.70
21	AA	881	G	O4'-C1'-N9	7.09	113.87	108.20
21	AA	1196	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	1603	A	C5-C6-N1	7.09	121.24	117.70
54	BA	2411	A	C5-C6-N1	7.09	121.24	117.70
28	BF	70	ARG	NE-CZ-NH2	-7.09	116.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	340	A	C5-C6-N1	7.09	121.24	117.70
54	BA	920	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	2366	A	C5-C6-N1	7.09	121.24	117.70
21	AA	349	A	C4-C5-C6	-7.09	113.46	117.00
21	AA	383	A	C5-C6-N1	7.09	121.24	117.70
22	A1	66	A	C5-C6-N1	7.09	121.24	117.70
54	BA	255	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	412	A	C4-C5-C6	-7.09	113.46	117.00
54	BA	1020	A	C5-C6-N1	7.09	121.24	117.70
21	AA	32	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2278	A	C5-C6-N1	7.08	121.24	117.70
54	BA	95	A	C5-C6-N1	7.08	121.24	117.70
54	BA	165	A	C5-C6-N1	7.08	121.24	117.70
54	BA	730	A	C5-C6-N1	7.08	121.24	117.70
54	BA	794	A	C5-C6-N1	7.08	121.24	117.70
54	BA	984	A	O4'-C1'-N9	7.08	113.87	108.20
54	BA	2579	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	382	A	C5-C6-N1	7.08	121.24	117.70
21	AA	718	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1247	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	279	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	2005	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	2425	A	C5-C6-N1	7.08	121.24	117.70
21	AA	1000	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	262	A	C5-C6-N1	7.08	121.24	117.70
21	AA	595	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1965	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	2610	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	131	A	C5-C6-N1	7.08	121.24	117.70
54	BA	207	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	227	A	N1-C6-N6	-7.08	114.36	118.60
54	BA	2587	A	C4-C5-C6	-7.08	113.46	117.00
55	BB	109	A	C5-C6-N1	7.08	121.24	117.70
6	AG	101	ARG	NE-CZ-NH1	7.07	123.84	120.30
21	AA	10	A	C4-C5-C6	-7.07	113.46	117.00
21	AA	831	A	C4-C5-C6	-7.07	113.46	117.00
54	BA	165	A	C4-C5-C6	-7.07	113.46	117.00
54	BA	721	A	C4-C5-C6	-7.07	113.46	117.00
54	BA	845	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	2856	A	C5-C6-N1	7.07	121.24	117.70
54	BA	959	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	1262	A	C5-C6-N1	7.07	121.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2761	A	C5-C6-N1	7.07	121.24	117.70
54	BA	515	A	C5-C6-N1	7.07	121.24	117.70
54	BA	945	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	1398	C	N3-C2-O2	-7.07	116.95	121.90
49	B0	15	ARG	NE-CZ-NH1	7.07	123.83	120.30
54	BA	197	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1608	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	370	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	609	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1285	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1961	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	1219	A	C4-C5-C6	-7.07	113.47	117.00
21	AA	1238	A	C4-C5-C6	-7.07	113.47	117.00
21	AA	732	C	N3-C2-O2	-7.06	116.95	121.90
21	AA	460	A	C5-C6-N1	7.06	121.23	117.70
21	AA	878	A	C5-C6-N1	7.06	121.23	117.70
21	AA	1287	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	430	A	C5-C6-N1	7.06	121.23	117.70
55	BB	58	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	1085	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1953	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	1635	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2572	A	C5-C6-N1	7.06	121.23	117.70
55	BB	58	A	C5-C6-N1	7.06	121.23	117.70
21	AA	162	A	C5-C6-N1	7.05	121.23	117.70
54	BA	324	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1270	C	N3-C2-O2	-7.05	116.96	121.90
54	BA	1336	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1533	C	N3-C2-O2	-7.05	116.96	121.90
21	AA	860	A	C5-C6-N1	7.05	121.23	117.70
54	BA	2888	C	N3-C2-O2	-7.05	116.96	121.90
22	A1	38	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	2079	U	O4'-C1'-N1	7.05	113.84	108.20
55	BB	94	A	C4-C5-C6	-7.05	113.47	117.00
13	AN	13	ARG	NE-CZ-NH1	7.05	123.83	120.30
21	AA	181	A	C5-C6-N1	7.05	121.22	117.70
21	AA	355	C	N3-C2-O2	-7.05	116.97	121.90
55	BB	89	U	N3-C2-O2	-7.05	117.27	122.20
54	BA	849	A	C5-C6-N1	7.05	121.22	117.70
54	BA	980	A	C5-C6-N1	7.05	121.22	117.70
21	AA	26	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1328	C	N3-C2-O2	-7.05	116.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	603	A	C4-C5-C6	-7.05	113.48	117.00
54	BA	2227	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1866	A	C4-C5-C6	-7.04	113.48	117.00
55	BB	27	C	N3-C2-O2	-7.04	116.97	121.90
12	AM	86	ARG	NE-CZ-NH1	7.04	123.82	120.30
21	AA	412	A	C5-C6-N1	7.04	121.22	117.70
54	BA	239	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	750	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2214	C	N3-C2-O2	-7.04	116.97	121.90
55	BB	99	A	C5-C6-N1	7.04	121.22	117.70
21	AA	183	C	N1-C2-O2	7.04	123.12	118.90
21	AA	596	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1360	A	C5-C6-N1	7.04	121.22	117.70
54	BA	802	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1611	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	2313	C	O4'-C1'-N1	7.04	113.83	108.20
21	AA	101	A	C5-C6-N1	7.04	121.22	117.70
24	A3	39	A	C5-C6-N1	7.04	121.22	117.70
54	BA	19	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	2635	A	C5-C6-N1	7.04	121.22	117.70
21	AA	430	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	1350	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1819	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2823	A	N1-C6-N6	-7.03	114.38	118.60
55	BB	30	C	N3-C2-O2	-7.03	116.98	121.90
19	AT	9	ARG	NE-CZ-NH1	7.03	123.82	120.30
21	AA	65	A	C5-C6-N1	7.03	121.22	117.70
21	AA	815	A	C5-C6-N1	7.03	121.22	117.70
21	AA	1197	A	C5-C6-N1	7.03	121.22	117.70
54	BA	453	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1427	A	P-O3'-C3'	7.03	128.14	119.70
54	BA	947	A	C4-C5-C6	-7.03	113.48	117.00
21	AA	696	A	C5-C6-N1	7.03	121.21	117.70
21	AA	1014	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	792	A	C5-C6-N1	7.03	121.21	117.70
54	BA	937	C	N3-C2-O2	-7.03	116.98	121.90
21	AA	1191	A	C5-C6-N1	7.03	121.21	117.70
22	A1	41	A	C5-C6-N1	7.03	121.21	117.70
21	AA	401	C	N3-C2-O2	-7.02	116.98	121.90
34	BL	47	ARG	NE-CZ-NH1	7.02	123.81	120.30
36	BN	30	ARG	NE-CZ-NH1	7.02	123.81	120.30
21	AA	73	C	N3-C2-O2	-7.02	116.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1513	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	423	A	C5-C6-N1	7.02	121.21	117.70
54	BA	439	A	C5-C6-N1	7.02	121.21	117.70
54	BA	761	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	1089	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	1260	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1610	A	C1'-O4'-C4'	-7.02	104.28	109.90
55	BB	29	A	C4-C5-C6	-7.02	113.49	117.00
55	BB	45	A	C5-C6-N1	7.02	121.21	117.70
21	AA	178	C	N3-C2-O2	-7.02	116.99	121.90
21	AA	918	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	2377	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	981	A	C5-C6-N1	7.02	121.21	117.70
21	AA	87	C	N3-C2-O2	-7.02	116.99	121.90
21	AA	1093	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2213	U	N3-C2-O2	-7.01	117.29	122.20
54	BA	2340	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1654	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	2006	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	631	C	N1-C2-O2	7.01	123.11	118.90
54	BA	2419	U	O4'-C1'-N1	7.01	113.81	108.20
54	BA	1276	A	C4-C5-C6	-7.01	113.50	117.00
54	BA	2654	A	C4-C5-C6	-7.01	113.50	117.00
22	A1	70	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	191	A	C5-C6-N1	7.01	121.20	117.70
54	BA	1942	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	1513	A	C5-C6-N1	7.01	121.20	117.70
54	BA	670	A	C5-C6-N1	7.01	121.20	117.70
54	BA	1399	C	N3-C2-O2	-7.01	117.00	121.90
13	AN	59	ARG	NE-CZ-NH1	7.00	123.80	120.30
21	AA	262	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	42	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	1339	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	1493	A	C5-C6-N1	7.00	121.20	117.70
54	BA	352	A	C5-C6-N1	7.00	121.20	117.70
54	BA	432	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1854	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	238	A	C5-C6-N1	7.00	121.20	117.70
47	BY	29	ARG	NE-CZ-NH1	7.00	123.80	120.30
54	BA	1287	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1043	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	1411	C	N3-C2-O2	-7.00	117.00	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1830	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	915	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1089	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1378	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1689	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	28	A	C4-C5-C6	-7.00	113.50	117.00
30	BH	68	ARG	NE-CZ-NH1	7.00	123.80	120.30
54	BA	330	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1103	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1515	A	C5-C6-N1	6.99	121.20	117.70
21	AA	139	A	C4-C5-C6	-6.99	113.50	117.00
21	AA	578	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	466	A	C5-C6-N1	6.99	121.20	117.70
54	BA	817	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	28	A	C5-C6-N1	6.99	121.19	117.70
21	AA	1269	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	1794	A	C5-C6-N1	6.99	121.20	117.70
54	BA	2062	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	2736	A	C5-C6-N1	6.99	121.19	117.70
21	AA	217	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	1057	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	1384	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	1156	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2542	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	479	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	554	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	1064	G	P-O3'-C3'	6.98	128.08	119.70
31	BI	64	ARG	NE-CZ-NH1	6.98	123.79	120.30
54	BA	1385	A	N1-C6-N6	-6.98	114.41	118.60
21	AA	611	C	N3-C2-O2	-6.98	117.01	121.90
21	AA	946	A	C5-C6-N1	6.98	121.19	117.70
21	AA	1000	A	C5-C6-N1	6.98	121.19	117.70
21	AA	1293	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	1152	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	2847	U	O4'-C1'-N1	6.98	113.78	108.20
22	A1	36	C	N3-C2-O2	-6.98	117.02	121.90
21	AA	779	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	49	A	C5-C6-N1	6.98	121.19	117.70
54	BA	144	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1890	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	143	A	N1-C6-N6	-6.98	114.41	118.60
21	AA	411	A	C5-C6-N1	6.97	121.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BK	30	ARG	NE-CZ-NH1	6.97	123.79	120.30
54	BA	300	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2799	A	C5-C6-N1	6.97	121.19	117.70
54	BA	160	A	C5-C6-N1	6.97	121.19	117.70
54	BA	804	A	C5-C6-N1	6.97	121.19	117.70
21	AA	817	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	1093	A	C5-C6-N1	6.97	121.19	117.70
54	BA	241	A	C5-C6-N1	6.97	121.19	117.70
21	AA	7	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1634	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2657	A	C5-C6-N1	6.97	121.19	117.70
21	AA	712	A	C5-C6-N1	6.97	121.18	117.70
54	BA	61	C	N3-C2-O2	-6.97	117.02	121.90
22	A1	6	A	C5-C6-N1	6.97	121.18	117.70
22	A1	73	A	C1'-O4'-C4'	-6.97	104.33	109.90
54	BA	1670	C	O4'-C1'-N1	6.97	113.77	108.20
54	BA	2806	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2620	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	485	C	O4'-C1'-N1	6.96	113.77	108.20
54	BA	2094	A	C5-C6-N1	6.96	121.18	117.70
3	AD	61	ARG	NE-CZ-NH1	6.96	123.78	120.30
54	BA	71	A	O4'-C1'-N9	6.96	113.77	108.20
54	BA	789	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2880	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	1286	A	C5-C6-N1	6.96	121.18	117.70
21	AA	937	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	412	A	C5-C6-N1	6.96	121.18	117.70
54	BA	523	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	274	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1323	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	1730	C	N1-C2-O2	6.96	123.07	118.90
54	BA	1858	A	C5-C6-N1	6.96	121.18	117.70
55	BB	59	A	C5-C6-N1	6.96	121.18	117.70
21	AA	436	C	N3-C2-O2	-6.95	117.03	121.90
21	AA	660	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	877	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	1788	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	1916	A	C5-C6-N1	6.95	121.18	117.70
54	BA	2346	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	2395	C	N3-C2-O2	-6.95	117.03	121.90
21	AA	172	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	11	C	N1-C2-O2	6.95	123.07	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2573	C	N1-C2-O2	6.95	123.07	118.90
21	AA	476	U	P-O3'-C3'	6.95	128.04	119.70
21	AA	694	A	C5-C6-N1	6.95	121.17	117.70
54	BA	787	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	1541	C	N3-C2-O2	-6.95	117.04	121.90
51	B2	28	ARG	NE-CZ-NH1	6.95	123.77	120.30
54	BA	941	A	C5-C6-N1	6.95	121.17	117.70
21	AA	389	A	C5-C6-N1	6.95	121.17	117.70
21	AA	456	A	C5-C6-N1	6.95	121.17	117.70
42	BT	73	ARG	NE-CZ-NH1	6.95	123.77	120.30
54	BA	190	A	C5-C6-N1	6.95	121.17	117.70
54	BA	627	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	1772	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	2072	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	2850	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	460	A	C5-C6-N1	6.94	121.17	117.70
21	AA	747	A	C5-C6-N1	6.94	121.17	117.70
1	AB	224	ARG	NE-CZ-NH1	6.94	123.77	120.30
21	AA	199	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1133	A	C5-C6-N1	6.94	121.17	117.70
54	BA	2119	A	N1-C6-N6	-6.94	114.44	118.60
54	BA	2517	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	523	A	C5-C6-N1	6.94	121.17	117.70
21	AA	1035	A	C5-C6-N1	6.94	121.17	117.70
54	BA	480	A	C5-C6-N1	6.94	121.17	117.70
6	AG	3	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	1244	A	C5-C6-N1	6.93	121.17	117.70
54	BA	2873	A	C5-C6-N1	6.93	121.17	117.70
54	BA	819	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1084	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	2077	A	C5-C6-N1	6.93	121.17	117.70
21	AA	67	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	648	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1155	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1250	A	C5-C6-N1	6.93	121.17	117.70
28	BF	177	ARG	NE-CZ-NH1	6.93	123.76	120.30
54	BA	1247	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1780	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	397	A	C5-C6-N1	6.93	121.16	117.70
54	BA	1181	U	O4'-C1'-N1	6.93	113.74	108.20
54	BA	1819	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	2741	A	C4-C5-C6	-6.93	113.54	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2758	A	C5-C6-N1	6.93	121.16	117.70
21	AA	98	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1044	C	N3-C2-O2	-6.92	117.05	121.90
52	B3	7	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	2155	U	O4'-C1'-N1	6.92	113.74	108.20
22	A1	31	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	38	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	820	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1512	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	1028	A	N1-C6-N6	-6.92	114.45	118.60
55	BB	29	A	C5-C6-N1	6.92	121.16	117.70
54	BA	164	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	764	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	2761	A	N1-C6-N6	-6.92	114.45	118.60
40	BR	21	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	2033	A	C5-C6-N1	6.91	121.16	117.70
54	BA	192	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	294	A	C5-C6-N1	6.91	121.16	117.70
54	BA	676	A	C5-C6-N1	6.91	121.16	117.70
54	BA	792	A	N1-C6-N6	-6.91	114.45	118.60
21	AA	896	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	1257	A	C4-C5-C6	-6.91	113.55	117.00
21	AA	1531	A	C5-C6-N1	6.91	121.16	117.70
54	BA	76	C	N1-C2-O2	6.91	123.05	118.90
54	BA	965	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	1999	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	2050	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	782	A	C5-C6-N1	6.91	121.15	117.70
21	AA	1188	A	N1-C6-N6	-6.91	114.46	118.60
54	BA	1749	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2126	A	C5-C6-N1	6.91	121.15	117.70
54	BA	2313	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	1097	C	N3-C2-O2	-6.91	117.07	121.90
21	AA	1430	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	1269	A	N1-C6-N6	-6.91	114.46	118.60
21	AA	50	A	C5-C6-N1	6.90	121.15	117.70
21	AA	309	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2450	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	99	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	313	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1357	A	N1-C6-N6	-6.90	114.46	118.60
24	A3	58	A	C5-C6-N1	6.90	121.15	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	504	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1705	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	2003	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2297	A	C5-C6-N1	6.90	121.15	117.70
15	AP	56	ARG	NE-CZ-NH1	6.90	123.75	120.30
54	BA	211	C	O4'-C1'-N1	6.90	113.72	108.20
54	BA	311	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	344	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2326	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	441	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1413	A	C5-C6-N1	6.90	121.15	117.70
21	AA	197	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	1142	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2635	A	O4'-C1'-N9	6.90	113.72	108.20
15	AP	14	ARG	NE-CZ-NH1	6.89	123.75	120.30
21	AA	937	A	C5-C6-N1	6.89	121.15	117.70
21	AA	1192	C	N3-C2-O2	-6.89	117.07	121.90
21	AA	1254	A	C5-C6-N1	6.89	121.15	117.70
54	BA	592	A	C5-C6-N1	6.89	121.15	117.70
54	BA	734	A	C5-C6-N1	6.89	121.15	117.70
54	BA	973	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1626	A	N1-C6-N6	-6.89	114.46	118.60
54	BA	1918	A	C5-C6-N1	6.89	121.15	117.70
54	BA	2045	C	N3-C2-O2	-6.89	117.07	121.90
47	BY	7	ARG	NE-CZ-NH1	6.89	123.75	120.30
54	BA	1169	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	1748	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	2468	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	1305	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1553	A	C5-C6-N1	6.89	121.14	117.70
21	AA	306	A	C5-C6-N1	6.89	121.14	117.70
21	AA	746	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1377	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1502	A	C5-C6-N1	6.89	121.14	117.70
54	BA	483	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	2893	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1302	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1618	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	1936	A	C5-C6-N1	6.89	121.14	117.70
54	BA	2475	C	N3-C2-O2	-6.89	117.08	121.90
18	AS	36	ARG	NE-CZ-NH1	6.89	123.74	120.30
21	AA	825	A	C4-C5-C6	-6.89	113.56	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	270	A	C5-C6-N1	6.89	121.14	117.70
54	BA	1969	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1080	A	C5-C6-N1	6.88	121.14	117.70
21	AA	1429	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	541	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1021	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2265	U	O4'-C1'-N1	6.88	113.71	108.20
21	AA	167	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	411	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	865	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1375	A	C5-C6-N1	6.88	121.14	117.70
54	BA	821	A	C4-C5-C6	-6.88	113.56	117.00
55	BB	114	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	743	A	C5-C6-N1	6.88	121.14	117.70
24	A3	16	C	N3-C2-O2	-6.88	117.09	121.90
54	BA	1809	A	C5-C6-N1	6.88	121.14	117.70
21	AA	389	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2336	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2551	C	N3-C2-O2	-6.88	117.09	121.90
54	BA	2070	A	C5-C6-N1	6.88	121.14	117.70
21	AA	1042	A	C5-C6-N1	6.87	121.14	117.70
21	AA	1252	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	1368	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	1396	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	623	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	73	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	354	A	C5-C6-N1	6.87	121.14	117.70
54	BA	2726	A	C5-C6-N1	6.87	121.14	117.70
54	BA	2823	A	C5-C6-N1	6.87	121.14	117.70
54	BA	2841	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	800	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	223	A	C5-C6-N1	6.87	121.14	117.70
54	BA	603	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1565	C	N3-C2-O2	-6.87	117.09	121.90
35	BM	81	ARG	NE-CZ-NH1	6.87	123.73	120.30
21	AA	608	A	C5-C6-N1	6.87	121.13	117.70
54	BA	756	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	1204	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1717	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	2424	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	2494	G	N1-C6-O6	-6.87	115.78	119.90
21	AA	655	A	N1-C6-N6	-6.86	114.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1044	A	C5-C6-N1	6.86	121.13	117.70
40	BR	78	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	371	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	1284	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	2792	A	C5-C6-N1	6.86	121.13	117.70
21	AA	430	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1815	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	2893	A	N1-C6-N6	-6.86	114.48	118.60
21	AA	1151	A	C5-C6-N1	6.86	121.13	117.70
54	BA	181	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2273	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	323	C	C1'-O4'-C4'	-6.86	104.41	109.90
54	BA	1650	A	C5-C6-N1	6.86	121.13	117.70
22	A1	60	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2126	A	N1-C6-N6	-6.86	114.49	118.60
54	BA	791	C	O4'-C1'-N1	6.85	113.68	108.20
54	BA	2350	C	N3-C2-O2	-6.85	117.10	121.90
6	AG	69	ARG	NE-CZ-NH1	6.85	123.73	120.30
7	AH	14	ARG	NE-CZ-NH1	6.85	123.73	120.30
21	AA	663	A	C5-C6-N1	6.85	121.13	117.70
21	AA	790	A	N1-C6-N6	-6.85	114.49	118.60
24	A3	72	C	N3-C2-O2	-6.85	117.10	121.90
54	BA	1853	A	C5-C6-N1	6.85	121.13	117.70
21	AA	1035	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	1483	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	2287	A	C5-C6-N1	6.85	121.12	117.70
21	AA	307	C	N3-C2-O2	-6.85	117.11	121.90
54	BA	398	C	N3-C2-O2	-6.85	117.11	121.90
54	BA	2037	A	C5-C6-N1	6.85	121.12	117.70
54	BA	677	A	C5-C6-N1	6.85	121.12	117.70
54	BA	722	A	C5-C6-N1	6.85	121.12	117.70
21	AA	1510	C	N3-C2-O2	-6.85	117.11	121.90
54	BA	1571	A	C5-C6-N1	6.85	121.12	117.70
54	BA	505	A	N1-C6-N6	-6.84	114.49	118.60
54	BA	633	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2073	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	2175	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	2241	A	C5-C6-N1	6.84	121.12	117.70
21	AA	199	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	382	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	2708	G	O4'-C1'-N9	6.84	113.67	108.20
19	AT	23	ARG	NE-CZ-NH1	6.84	123.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	777	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1063	C	N3-C2-O2	-6.84	117.11	121.90
29	BG	93	TYR	CB-CG-CD2	-6.84	116.90	121.00
36	BN	69	ARG	NE-CZ-NH1	6.84	123.72	120.30
54	BA	384	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1005	C	N3-C2-O2	-6.84	117.11	121.90
12	AM	2	ARG	NE-CZ-NH2	6.84	123.72	120.30
21	AA	825	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1129	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2448	A	C5-C6-N1	6.84	121.12	117.70
21	AA	151	A	C4-C5-C6	-6.84	113.58	117.00
21	AA	759	A	C5-C6-N1	6.84	121.12	117.70
37	BO	33	ARG	NE-CZ-NH1	6.84	123.72	120.30
54	BA	1214	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1469	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1728	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1871	A	C5-C6-N1	6.84	121.12	117.70
21	AA	909	A	C4-C5-C6	-6.83	113.58	117.00
21	AA	1201	A	O4'-C1'-N9	6.83	113.67	108.20
50	B1	43	ARG	NE-CZ-NH1	6.83	123.72	120.30
54	BA	979	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	1414	C	N3-C2-O2	-6.83	117.11	121.90
21	AA	1398	A	C5-C6-N1	6.83	121.12	117.70
24	A3	62	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	705	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2632	A	C5-C6-N1	6.83	121.12	117.70
21	AA	349	A	C5-C6-N1	6.83	121.12	117.70
21	AA	975	A	C5-C6-N1	6.83	121.12	117.70
21	AA	1261	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1338	G	N1-C6-O6	-6.83	115.80	119.90
21	AA	1408	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	127	A	C5-C6-N1	6.83	121.12	117.70
54	BA	620	G	O4'-C1'-N9	6.83	113.67	108.20
21	AA	1145	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	91	A	C5-C6-N1	6.83	121.11	117.70
21	AA	787	A	C5-C6-N1	6.83	121.11	117.70
54	BA	1453	A	C4-C5-C6	-6.83	113.59	117.00
55	BB	104	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	1998	A	C5-C6-N1	6.83	121.11	117.70
21	AA	510	A	C5-C6-N1	6.83	121.11	117.70
21	AA	642	A	C4-C5-C6	-6.83	113.59	117.00
21	AA	1446	A	O4'-C1'-N9	6.83	113.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1803	A	C4-C5-C6	-6.83	113.59	117.00
21	AA	747	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1359	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	109	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	1352	U	N3-C2-O2	-6.82	117.42	122.20
21	AA	1534	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	692	C	N3-C2-O2	-6.82	117.12	121.90
21	AA	1157	A	C4-C5-C6	-6.82	113.59	117.00
33	BK	108	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	1701	A	C5-C6-N1	6.82	121.11	117.70
19	AT	73	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	961	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	1346	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2065	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	2416	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	459	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	849	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	1741	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	2700	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2752	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	1483	A	C5-C6-N1	6.81	121.11	117.70
54	BA	1075	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	364	A	N1-C6-N6	-6.81	114.51	118.60
21	AA	533	A	N1-C6-N6	-6.81	114.51	118.60
22	A1	69	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	2723	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	1214	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	1646	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	2795	C	N3-C2-O2	-6.81	117.13	121.90
55	BB	34	A	C5-C6-N1	6.81	121.11	117.70
21	AA	1169	A	C4-C5-C6	-6.81	113.60	117.00
54	BA	342	A	C5-C6-N1	6.81	121.10	117.70
54	BA	527	C	N1-C2-O2	6.81	122.98	118.90
55	BB	12	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	299	A	C5-C6-N1	6.81	121.10	117.70
21	AA	315	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	702	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1110	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	1746	A	N1-C6-N6	-6.80	114.52	118.60
54	BA	1919	A	C5-C6-N1	6.80	121.10	117.70
21	AA	959	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1209	C	N3-C2-O2	-6.80	117.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1400	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	1028	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1608	A	C5-C6-N1	6.80	121.10	117.70
21	AA	161	A	C5-C6-N1	6.80	121.10	117.70
21	AA	325	A	C5-C6-N1	6.80	121.10	117.70
21	AA	735	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	1132	C	N3-C2-O2	-6.80	117.14	121.90
22	A1	35	A	C5-C6-N1	6.80	121.10	117.70
22	A1	66	A	C4-C5-C6	-6.80	113.60	117.00
26	BD	148	GLN	C-N-CA	6.80	138.70	121.70
54	BA	844	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2014	A	C5-C6-N1	6.80	121.10	117.70
54	BA	440	C	O4'-C1'-N1	6.80	113.64	108.20
54	BA	2639	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	408	A	C5-C6-N1	6.80	121.10	117.70
54	BA	231	A	C5-C6-N1	6.80	121.10	117.70
54	BA	449	A	C5-C6-N1	6.80	121.10	117.70
54	BA	482	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1731	G	O4'-C1'-N9	6.80	113.64	108.20
55	BB	99	A	N1-C6-N6	-6.80	114.52	118.60
21	AA	459	A	C5-C6-N1	6.79	121.10	117.70
54	BA	300	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	309	A	C4-C5-C6	-6.79	113.60	117.00
24	A3	38	A	C5-C6-N1	6.79	121.10	117.70
21	AA	889	A	C4-C5-C6	-6.79	113.60	117.00
21	AA	1163	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	1413	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	2755	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	2766	A	C5-C6-N1	6.79	121.09	117.70
54	BA	173	A	N1-C6-N6	-6.79	114.53	118.60
54	BA	1894	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	18	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	124	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	912	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	974	A	C4-C5-C6	-6.79	113.61	117.00
53	B4	24	ARG	NE-CZ-NH1	6.79	123.69	120.30
54	BA	2225	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	2749	A	C5-C6-N1	6.79	121.09	117.70
25	BC	101	ARG	NE-CZ-NH1	6.79	123.69	120.30
54	BA	878	A	C5-C6-N1	6.79	121.09	117.70
21	AA	575	G	P-O3'-C3'	6.79	127.84	119.70
54	BA	21	A	C5-C6-N1	6.79	121.09	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2600	A	O4'-C1'-N9	6.79	113.63	108.20
21	AA	913	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	140	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	240	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	1368	A	C5-C6-N1	6.78	121.09	117.70
54	BA	689	A	C4-C5-C6	-6.78	113.61	117.00
11	AL	30	ARG	NE-CZ-NH2	-6.78	116.91	120.30
21	AA	152	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	1237	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1462	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	2590	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1055	A	C5-C6-N1	6.78	121.09	117.70
21	AA	1408	A	C5-C6-N1	6.78	121.09	117.70
39	BQ	49	ARG	NE-CZ-NH1	6.78	123.69	120.30
21	AA	189	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	624	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	790	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	735	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1387	A	C5-C6-N1	6.78	121.09	117.70
21	AA	1155	A	C4-C5-C6	-6.78	113.61	117.00
55	BB	53	A	C5-C6-N1	6.78	121.09	117.70
54	BA	556	A	C5-C6-N1	6.77	121.09	117.70
54	BA	501	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2471	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	155	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	215	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	386	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	535	A	C5-C6-N1	6.77	121.08	117.70
21	AA	1339	A	C5-C6-N1	6.77	121.08	117.70
21	AA	1403	C	N3-C2-O2	-6.77	117.16	121.90
45	BW	76	ARG	NE-CZ-NH1	6.77	123.69	120.30
54	BA	2342	C	N1-C2-O2	6.77	122.96	118.90
54	BA	2785	C	N3-C2-O2	-6.77	117.16	121.90
23	A2	82	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1077	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2009	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2346	A	C5-C6-N1	6.77	121.08	117.70
54	BA	478	A	C5-C6-N1	6.77	121.08	117.70
54	BA	547	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1488	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	908	A	C5-C6-N1	6.76	121.08	117.70
24	A3	14	A	N1-C6-N6	-6.76	114.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	69	C	N3-C2-O2	-6.76	117.16	121.90
54	BA	161	A	C5-C6-N1	6.76	121.08	117.70
29	BG	169	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	586	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1342	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1746	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1374	A	C5-C6-N1	6.76	121.08	117.70
54	BA	795	C	N3-C2-O2	-6.76	117.17	121.90
16	AQ	76	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	1248	A	C5-C6-N1	6.76	121.08	117.70
54	BA	415	A	C5-C6-N1	6.76	121.08	117.70
54	BA	586	A	N1-C6-N6	-6.76	114.55	118.60
54	BA	1597	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1810	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	2774	C	N3-C2-O2	-6.76	117.17	121.90
10	AK	55	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	630	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	1136	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1092	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1536	C	N1-C2-O2	6.76	122.95	118.90
21	AA	313	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	1354	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1561	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	2753	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	666	A	C5-C6-N1	6.75	121.08	117.70
54	BA	719	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	1029	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	1545	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1575	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	2025	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	2670	A	C5-C6-N1	6.75	121.08	117.70
21	AA	728	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	1261	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	1909	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	1916	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	2274	A	C5-C6-N1	6.75	121.08	117.70
4	AE	111	ARG	NE-CZ-NH1	6.75	123.67	120.30
54	BA	348	A	C5-C6-N1	6.75	121.07	117.70
54	BA	685	A	C5-C6-N1	6.75	121.07	117.70
54	BA	1545	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	2880	C	O4'-C1'-N1	6.75	113.60	108.20
54	BA	483	A	C5-C6-N1	6.75	121.07	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2376	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	2636	C	C5'-C4'-C3'	-6.75	105.21	116.00
21	AA	19	A	C5-C6-N1	6.75	121.07	117.70
22	A1	38	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	649	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1809	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1885	A	C5-C6-N1	6.74	121.07	117.70
54	BA	197	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1296	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	611	C	O4'-C1'-N1	6.74	113.59	108.20
21	AA	373	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1874	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	2071	A	C5-C6-N1	6.74	121.07	117.70
21	AA	288	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1690	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2776	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1665	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2530	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2725	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2726	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1021	A	C4-C5-C6	-6.73	113.63	117.00
54	BA	685	A	C4-C5-C6	-6.73	113.63	117.00
21	AA	186	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	1452	C	P-O3'-C3'	6.73	127.78	119.70
54	BA	557	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1801	A	C4-C5-C6	-6.73	113.63	117.00
54	BA	2101	A	C5-C6-N1	6.73	121.07	117.70
21	AA	831	A	C5-C6-N1	6.73	121.06	117.70
54	BA	960	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	1639	C	O4'-C1'-N1	6.73	113.58	108.20
54	BA	2036	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1265	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	2169	A	C5-C6-N1	6.73	121.06	117.70
21	AA	883	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	969	A	C4-C5-C6	-6.73	113.64	117.00
21	AA	155	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	739	A	N1-C6-N6	-6.73	114.56	118.60
21	AA	559	A	C5-C6-N1	6.72	121.06	117.70
21	AA	1521	C	N3-C2-O2	-6.72	117.19	121.90
22	A1	21	A	C5-C6-N1	6.72	121.06	117.70
54	BA	1669	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2711	A	C4-C5-C6	-6.72	113.64	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	311	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	640	A	N1-C6-N6	-6.72	114.57	118.60
21	AA	914	A	C5-C6-N1	6.72	121.06	117.70
21	AA	1146	A	C5-C6-N1	6.72	121.06	117.70
54	BA	723	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	1080	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	1332	A	C4-C5-C6	-6.72	113.64	117.00
24	A3	44	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2766	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	935	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1549	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1691	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	2035	G	O4'-C1'-N9	6.72	113.58	108.20
54	BA	2856	A	C4-C5-C6	-6.72	113.64	117.00
37	BO	25	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	893	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	988	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2114	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	923	A	C5-C6-N1	6.72	121.06	117.70
54	BA	368	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	527	C	P-O3'-C3'	6.72	127.76	119.70
54	BA	542	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	2176	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	668	A	C5-C6-N1	6.71	121.06	117.70
54	BA	6	A	C5-C6-N1	6.71	121.06	117.70
54	BA	611	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	996	A	C5-C6-N1	6.71	121.06	117.70
54	BA	37	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	2135	A	C5-C6-N1	6.71	121.06	117.70
54	BA	2142	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1072	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	233	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	505	A	C5-C6-N1	6.71	121.05	117.70
54	BA	541	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1327	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1592	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1749	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1806	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	913	A	P-O3'-C3'	6.71	127.75	119.70
21	AA	1518	A	C4-C5-C6	-6.71	113.65	117.00
24	A3	14	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1285	A	C4-C5-C6	-6.71	113.65	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1335	C	O4'-C1'-N1	6.71	113.57	108.20
54	BA	1525	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1698	A	C5-C6-N1	6.71	121.05	117.70
21	AA	586	C	N3-C2-O2	-6.71	117.21	121.90
21	AA	1218	C	N3-C2-O2	-6.71	117.21	121.90
54	BA	1304	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	884	U	O4'-C1'-N1	6.70	113.56	108.20
54	BA	1518	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2432	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2868	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	716	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	913	A	C5-C6-N1	6.70	121.05	117.70
30	BH	27	ARG	NE-CZ-NH1	6.70	123.65	120.30
54	BA	64	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	151	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	207	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1585	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2314	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2418	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1617	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2030	A	C5-C6-N1	6.70	121.05	117.70
21	AA	1105	A	C5-C6-N1	6.70	121.05	117.70
54	BA	126	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1794	A	N1-C6-N6	-6.70	114.58	118.60
21	AA	65	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	622	A	C4-C5-C6	-6.70	113.65	117.00
22	A1	9	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1086	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1787	A	C5-C6-N1	6.70	121.05	117.70
21	AA	802	A	C5-C6-N1	6.69	121.05	117.70
21	AA	1507	A	C5-C6-N1	6.69	121.05	117.70
54	BA	2333	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	2617	U	O4'-C1'-N1	6.69	113.56	108.20
56	B5	7	ARG	NE-CZ-NH1	6.69	123.65	120.30
21	AA	918	A	C5-C6-N1	6.69	121.05	117.70
21	AA	1011	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	1037	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	1479	C	N3-C2-O2	-6.69	117.22	121.90
50	B1	27	ARG	NE-CZ-NH1	6.69	123.64	120.30
54	BA	2358	A	C5-C6-N1	6.69	121.05	117.70
21	AA	982	U	P-O3'-C3'	6.69	127.73	119.70
21	AA	1111	A	C5-C6-N1	6.69	121.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1349	A	C5-C6-N1	6.69	121.04	117.70
54	BA	1698	A	N1-C6-N6	-6.69	114.59	118.60
21	AA	1230	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2612	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2866	U	O4'-C1'-N1	6.69	113.55	108.20
54	BA	1054	A	C4-C5-C6	-6.69	113.66	117.00
18	AS	35	ARG	NE-CZ-NH1	6.68	123.64	120.30
21	AA	172	A	C4-C5-C6	-6.68	113.66	117.00
22	A1	14	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	89	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	226	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	227	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	270	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	2652	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	533	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1448	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1701	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	2078	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	2427	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	722	A	C4-C5-C6	-6.68	113.66	117.00
21	AA	77	A	C5-C6-N1	6.68	121.04	117.70
21	AA	320	A	C5-C6-N1	6.68	121.04	117.70
21	AA	974	A	C5-C6-N1	6.68	121.04	117.70
22	A1	73	A	C5'-C4'-C3'	-6.68	105.31	116.00
35	BM	59	ARG	NE-CZ-NH1	6.68	123.64	120.30
54	BA	2134	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2309	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2560	A	C5-C6-N1	6.68	121.04	117.70
21	AA	363	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	890	C	N3-C2-O2	-6.68	117.23	121.90
21	AA	673	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	2227	A	C4-C5-C6	-6.68	113.66	117.00
25	BC	62	ARG	NE-CZ-NH1	6.67	123.64	120.30
54	BA	440	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	321	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	1288	A	C5-C6-N1	6.67	121.04	117.70
22	A1	48	C	N1-C2-O2	6.67	122.90	118.90
54	BA	182	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2329	U	O4'-C1'-N1	6.67	113.54	108.20
21	AA	781	A	N1-C6-N6	-6.67	114.60	118.60
28	BF	91	ARG	NE-CZ-NH1	6.67	123.64	120.30
54	BA	1494	A	C5-C6-N1	6.67	121.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1398	A	C4-C5-C6	-6.67	113.67	117.00
35	BM	50	ARG	NE-CZ-NH1	6.67	123.63	120.30
54	BA	119	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	609	A	C5-C6-N1	6.67	121.03	117.70
54	BA	643	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	1357	C	O4'-C1'-N1	6.67	113.53	108.20
21	AA	655	A	C5-C6-N1	6.67	121.03	117.70
54	BA	1451	C	P-O3'-C3'	6.67	127.70	119.70
55	BB	26	C	N3-C2-O2	-6.67	117.23	121.90
56	B5	53	ARG	NE-CZ-NH1	6.67	123.63	120.30
54	BA	104	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2860	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	1096	C	N3-C2-O2	-6.66	117.23	121.90
54	BA	5	A	C5-C6-N1	6.66	121.03	117.70
54	BA	128	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1805	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2547	A	C5-C6-N1	6.66	121.03	117.70
21	AA	767	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	1251	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	1318	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1049	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1554	U	N3-C2-O2	-6.66	117.54	122.20
54	BA	1600	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	2089	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	536	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	812	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1008	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1127	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2014	A	N1-C6-N6	-6.66	114.61	118.60
54	BA	2872	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1135	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	2090	A	N1-C6-N6	-6.66	114.61	118.60
54	BA	2704	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	33	A	C5-C6-N1	6.66	121.03	117.70
21	AA	452	A	C5-C6-N1	6.66	121.03	117.70
54	BA	788	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1630	A	C5-C6-N1	6.66	121.03	117.70
54	BA	910	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	1039	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1096	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1275	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	1359	A	C5-C6-N1	6.65	121.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2028	U	O4'-C1'-N1	6.65	113.52	108.20
54	BA	2902	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	382	A	C5-C6-N1	6.65	121.03	117.70
54	BA	502	A	C5-C6-N1	6.65	121.03	117.70
54	BA	781	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	1278	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	2560	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	1228	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1295	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1378	A	O4'-C1'-N9	6.65	113.52	108.20
54	BA	1526	C	O4'-C1'-N1	6.65	113.52	108.20
21	AA	1213	A	C5-C6-N1	6.65	121.02	117.70
27	BE	21	ARG	NE-CZ-NH1	6.65	123.62	120.30
54	BA	471	A	N1-C6-N6	-6.65	114.61	118.60
54	BA	1301	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	52	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	1319	A	C5-C6-N1	6.64	121.02	117.70
21	AA	1394	A	N1-C6-N6	-6.64	114.61	118.60
23	A2	79	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1395	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2320	U	O4'-C1'-N1	6.64	113.52	108.20
55	BB	91	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	243	A	C5-C6-N1	6.64	121.02	117.70
21	AA	1197	A	N1-C6-N6	-6.64	114.61	118.60
54	BA	1347	A	C5-C6-N1	6.64	121.02	117.70
54	BA	155	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1548	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2374	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2388	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2119	A	C5-C6-N1	6.64	121.02	117.70
21	AA	16	A	C5-C6-N1	6.64	121.02	117.70
21	AA	23	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1332	G	C3'-C2'-C1'	6.64	106.81	101.50
54	BA	2171	A	O4'-C1'-N9	6.64	113.51	108.20
55	BB	52	A	C5-C6-N1	6.64	121.02	117.70
21	AA	177	G	N3-C4-C5	-6.63	125.28	128.60
29	BG	162	ARG	NE-CZ-NH1	6.63	123.62	120.30
46	BX	73	ARG	NE-CZ-NH1	6.63	123.62	120.30
54	BA	980	A	C4-C5-C6	-6.63	113.68	117.00
1	AB	221	ARG	NE-CZ-NH1	6.63	123.62	120.30
21	AA	325	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	290	C	N3-C2-O2	-6.63	117.26	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1210	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	130	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	774	G	O4'-C1'-N9	6.63	113.50	108.20
54	BA	829	A	C5-C6-N1	6.63	121.02	117.70
54	BA	1069	A	O4'-C1'-N9	6.63	113.51	108.20
54	BA	1759	A	C5-C6-N1	6.63	121.02	117.70
54	BA	1789	A	C5-C6-N1	6.63	121.02	117.70
54	BA	2070	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	1049	U	C5'-C4'-C3'	-6.63	105.39	116.00
54	BA	249	C	O4'-C1'-N1	6.63	113.50	108.20
54	BA	650	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1664	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	2030	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	1069	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	1467	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	2809	A	N1-C6-N6	-6.63	114.62	118.60
3	AD	110	ARG	NE-CZ-NH1	6.63	123.61	120.30
54	BA	251	A	C5-C6-N1	6.63	121.01	117.70
54	BA	776	G	N1-C6-O6	-6.63	115.92	119.90
54	BA	945	A	C5-C6-N1	6.63	121.01	117.70
54	BA	2327	A	C4-C5-C6	-6.63	113.69	117.00
24	A3	32	G	N1-C6-O6	-6.62	115.92	119.90
54	BA	582	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	1383	C	N3-C2-O2	-6.62	117.26	121.90
22	A1	16	C	N1-C2-O2	6.62	122.87	118.90
54	BA	286	U	O4'-C1'-N1	6.62	113.50	108.20
21	AA	72	A	N1-C6-N6	-6.62	114.63	118.60
21	AA	432	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	851	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1005	C	O4'-C1'-N1	6.62	113.50	108.20
55	BB	8	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	666	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	2343	U	O4'-C1'-N1	6.62	113.50	108.20
21	AA	280	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	978	A	C5-C6-N1	6.62	121.01	117.70
54	BA	802	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1711	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	2161	C	N3-C2-O2	-6.62	117.27	121.90
12	AM	89	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	856	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1685	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1960	A	C5-C6-N1	6.62	121.01	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2386	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2767	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	1101	A	N1-C6-N6	-6.61	114.63	118.60
21	AA	1531	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	477	A	C5-C6-N1	6.61	121.01	117.70
54	BA	1610	A	C5-C6-N1	6.61	121.00	117.70
54	BA	2191	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	2887	A	C5-C6-N1	6.61	121.00	117.70
21	AA	996	A	C5-C6-N1	6.61	121.00	117.70
21	AA	1524	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	457	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	655	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	1151	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1816	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	1853	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	1081	A	C5-C6-N1	6.61	121.00	117.70
21	AA	1389	C	N3-C2-O2	-6.61	117.28	121.90
21	AA	1410	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	911	A	C5-C6-N1	6.61	121.00	117.70
54	BA	2700	A	C4-C5-C6	-6.61	113.70	117.00
24	A3	22	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	987	C	O4'-C1'-N1	6.60	113.48	108.20
54	BA	1326	U	O4'-C1'-N1	6.60	113.48	108.20
21	AA	1352	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	293	U	O4'-C1'-N1	6.60	113.48	108.20
3	AD	103	ARG	NE-CZ-NH1	6.60	123.60	120.30
21	AA	807	A	C5-C6-N1	6.60	121.00	117.70
54	BA	310	A	C5-C6-N1	6.60	121.00	117.70
54	BA	2601	C	N3-C2-O2	-6.60	117.28	121.90
20	AU	34	ARG	NE-CZ-NH1	6.60	123.60	120.30
21	AA	512	U	O4'-C1'-N1	6.60	113.48	108.20
21	AA	1004	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	507	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	1039	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	1515	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	2088	A	C5-C6-N1	6.60	121.00	117.70
54	BA	21	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	205	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	104	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1262	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1872	A	N1-C6-N6	-6.59	114.64	118.60
11	AL	109	ARG	NE-CZ-NH1	6.59	123.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	781	A	C5-C6-N1	6.59	121.00	117.70
54	BA	478	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1431	A	C5-C6-N1	6.59	121.00	117.70
54	BA	2471	A	C5-C6-N1	6.59	121.00	117.70
54	BA	353	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	699	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	825	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1032	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1147	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	2000	C	N3-C2-O2	-6.59	117.29	121.90
27	BE	114	ARG	NE-CZ-NH1	6.59	123.59	120.30
40	BR	79	ARG	NE-CZ-NH1	6.59	123.59	120.30
54	BA	1395	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1499	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	2176	A	C5-C6-N1	6.59	121.00	117.70
54	BA	2183	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	1044	A	C4-C5-C6	-6.59	113.71	117.00
21	AA	1151	A	C4-C5-C6	-6.59	113.71	117.00
21	AA	106	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	501	C	N3-C2-O2	-6.59	117.29	121.90
24	A3	41	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	272	A	N1-C6-N6	-6.59	114.65	118.60
54	BA	354	A	N1-C6-N6	-6.59	114.65	118.60
54	BA	606	U	O4'-C1'-N1	6.59	113.47	108.20
54	BA	739	A	C5-C6-N1	6.59	120.99	117.70
54	BA	2206	C	O4'-C1'-N1	6.59	113.47	108.20
21	AA	77	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	497	A	C5-C6-N1	6.58	120.99	117.70
21	AA	873	A	C5-C6-N1	6.58	120.99	117.70
32	BJ	69	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	1403	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1652	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1744	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2171	A	C5-C6-N1	6.58	120.99	117.70
56	B5	162	ARG	NE-CZ-NH2	-6.58	117.01	120.30
54	BA	86	G	C1'-O4'-C4'	-6.58	104.64	109.90
54	BA	176	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2678	C	O4'-C1'-N1	6.58	113.46	108.20
21	AA	338	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1978	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	393	A	C5-C6-N1	6.58	120.99	117.70
21	AA	466	A	C4-C5-C6	-6.58	113.71	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1507	A	N1-C6-N6	-6.58	114.66	118.60
54	BA	173	A	C5-C6-N1	6.58	120.99	117.70
54	BA	758	C	O4'-C1'-N1	6.58	113.46	108.20
54	BA	1098	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2117	A	C5-C6-N1	6.58	120.99	117.70
55	BB	59	A	N1-C6-N6	-6.58	114.66	118.60
21	AA	680	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	1157	A	C5-C6-N1	6.57	120.99	117.70
21	AA	1216	A	C5-C6-N1	6.57	120.99	117.70
54	BA	262	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	1172	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2821	A	N1-C6-N6	-6.57	114.66	118.60
55	BB	70	C	N3-C2-O2	-6.57	117.30	121.90
56	B5	74	ARG	NE-CZ-NH1	6.57	123.59	120.30
21	AA	1128	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	751	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	1237	A	O4'-C1'-N9	6.57	113.46	108.20
54	BA	2469	A	C5-C6-N1	6.57	120.99	117.70
54	BA	2821	A	C5-C6-N1	6.57	120.98	117.70
21	AA	522	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	574	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	2385	C	O4'-C1'-N1	6.57	113.45	108.20
54	BA	2513	A	C5-C6-N1	6.57	120.98	117.70
21	AA	816	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2672	U	O4'-C1'-N1	6.57	113.45	108.20
54	BA	2705	A	C4-C5-C6	-6.57	113.72	117.00
21	AA	374	A	C5-C6-N1	6.57	120.98	117.70
21	AA	511	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	1374	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	44	A	C5-C6-N1	6.57	120.98	117.70
54	BA	1039	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	1335	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1678	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	1970	A	C4-C5-C6	-6.57	113.72	117.00
37	BO	30	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	1795	C	O4'-C1'-N1	6.56	113.45	108.20
21	AA	1350	A	N1-C6-N6	-6.56	114.66	118.60
54	BA	984	A	N1-C6-N6	-6.56	114.66	118.60
54	BA	1147	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2150	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	370	C	N1-C2-O2	6.56	122.84	118.90
54	BA	2037	A	C4-C5-C6	-6.56	113.72	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2321	U	O4'-C1'-N1	6.56	113.45	108.20
55	BB	104	A	C5-C6-N1	6.56	120.98	117.70
54	BA	394	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1261	C	O4'-C1'-N1	6.56	113.44	108.20
54	BA	2851	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	271	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	574	A	C5-C6-N1	6.55	120.98	117.70
21	AA	1217	C	P-O3'-C3'	6.55	127.56	119.70
54	BA	72	U	O4'-C1'-N1	6.55	113.44	108.20
54	BA	1757	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1877	A	C5-C6-N1	6.55	120.98	117.70
54	BA	2738	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	1050	A	C5-C6-N1	6.55	120.98	117.70
54	BA	2818	U	O4'-C1'-N1	6.55	113.44	108.20
55	BB	97	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1028	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	935	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2566	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1876	A	C5-C6-N1	6.55	120.97	117.70
54	BA	2215	C	N3-C2-O2	-6.55	117.32	121.90
21	AA	1239	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	1111	A	C5-C6-N1	6.55	120.97	117.70
54	BA	2420	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	985	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1128	G	C1'-O4'-C4'	-6.54	104.66	109.90
54	BA	1417	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1745	A	C5-C6-N1	6.54	120.97	117.70
25	BC	79	ARG	NE-CZ-NH1	6.54	123.57	120.30
29	BG	68	ARG	NE-CZ-NH1	6.54	123.57	120.30
21	AA	1437	A	C5-C6-N1	6.54	120.97	117.70
54	BA	925	A	N1-C6-N6	-6.54	114.68	118.60
54	BA	1354	A	N1-C6-N6	-6.54	114.68	118.60
54	BA	2107	G	N3-C2-N2	-6.54	115.32	119.90
21	AA	649	A	C5-C6-N1	6.54	120.97	117.70
54	BA	404	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1934	C	O4'-C1'-N1	6.54	113.43	108.20
54	BA	2060	A	C5-C6-N1	6.54	120.97	117.70
21	AA	58	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	244	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1226	A	N1-C6-N6	-6.54	114.68	118.60
54	BA	1580	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2710	C	N3-C2-O2	-6.54	117.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	139	A	C5-C6-N1	6.54	120.97	117.70
21	AA	1105	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1353	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1437	C	O4'-C1'-N1	6.54	113.43	108.20
22	A1	51	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	693	A	C4-C5-C6	-6.53	113.73	117.00
6	AG	77	ARG	NE-CZ-NH1	6.53	123.56	120.30
21	AA	519	C	N3-C2-O2	-6.53	117.33	121.90
33	BK	78	ARG	NE-CZ-NH1	6.53	123.56	120.30
54	BA	482	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	2883	A	C5-C6-N1	6.53	120.97	117.70
21	AA	602	A	C4-C5-C6	-6.53	113.74	117.00
22	A1	72	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1221	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1637	A	C5-C6-N1	6.53	120.96	117.70
54	BA	2497	A	C4-C5-C6	-6.53	113.74	117.00
2	AC	168	ARG	NE-CZ-NH1	6.53	123.56	120.30
21	AA	539	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	599	A	C5-C6-N1	6.53	120.96	117.70
54	BA	989	G	N1-C6-O6	-6.53	115.98	119.90
54	BA	1226	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1237	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1761	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	2332	C	O4'-C1'-N1	6.53	113.42	108.20
55	BB	34	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	351	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	1443	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	933	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	379	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	900	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1535	A	N1-C6-N6	-6.52	114.69	118.60
21	AA	270	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	1112	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	626	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	958	U	O4'-C1'-N1	6.52	113.41	108.20
21	AA	1360	A	N1-C6-N6	-6.52	114.69	118.60
54	BA	2764	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	681	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	152	A	N1-C6-N6	-6.51	114.69	118.60
54	BA	748	G	N1-C6-O6	-6.51	115.99	119.90
54	BA	1566	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	1570	A	C5-C6-N1	6.51	120.96	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1711	A	C5-C6-N1	6.51	120.96	117.70
54	BA	2461	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	1250	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	309	A	C4-C5-C6	-6.51	113.75	117.00
21	AA	658	C	N3-C2-O2	-6.51	117.34	121.90
25	BC	132	ARG	NE-CZ-NH1	6.51	123.56	120.30
54	BA	282	A	C4-C5-C6	-6.51	113.75	117.00
55	BB	66	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1990	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	312	C	N3-C2-O2	-6.51	117.35	121.90
21	AA	1140	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	2080	A	C5-C6-N1	6.51	120.95	117.70
54	BA	2813	A	C5-C6-N1	6.51	120.95	117.70
21	AA	720	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	759	A	C4-C5-C6	-6.50	113.75	117.00
41	BS	11	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	566	U	O4'-C1'-N1	6.50	113.40	108.20
54	BA	602	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	899	C	N1-C2-O2	6.50	122.80	118.90
54	BA	1156	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2826	A	C5-C6-N1	6.50	120.95	117.70
21	AA	338	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1224	U	O4'-C1'-N1	6.50	113.40	108.20
36	BN	17	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	364	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	734	A	C4-C5-C6	-6.50	113.75	117.00
6	AG	118	ARG	NE-CZ-NH1	6.50	123.55	120.30
21	AA	1191	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1243	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	742	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	991	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1258	U	O4'-C1'-N1	6.50	113.40	108.20
55	BB	78	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	182	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	392	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	1019	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1419	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1593	A	C4-C5-C6	-6.50	113.75	117.00
55	BB	62	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	231	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	517	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	715	A	C5-C6-N1	6.50	120.95	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	743	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	1275	A	C5-C6-N1	6.49	120.95	117.70
54	BA	2715	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	48	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	172	A	C5-C6-N1	6.49	120.95	117.70
21	AA	1375	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	635	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2211	A	C5-C6-N1	6.49	120.95	117.70
54	BA	14	A	C5-C6-N1	6.49	120.94	117.70
21	AA	435	A	C4-C5-C6	-6.49	113.75	117.00
46	BX	26	ARG	NE-CZ-NH1	6.49	123.55	120.30
54	BA	531	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	908	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	201	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	864	A	C5-C6-N1	6.49	120.94	117.70
21	AA	1465	A	C4-C5-C6	-6.49	113.76	117.00
34	BL	48	ARG	NE-CZ-NH1	6.49	123.54	120.30
54	BA	256	A	C5-C6-N1	6.49	120.94	117.70
54	BA	470	A	C5-C6-N1	6.49	120.94	117.70
54	BA	2872	A	N1-C6-N6	-6.48	114.71	118.60
21	AA	43	C	N3-C2-O2	-6.48	117.36	121.90
38	BP	88	ARG	NE-CZ-NH2	-6.48	117.06	120.30
54	BA	1706	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1722	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1735	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1900	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	1109	C	N3-C2-O2	-6.48	117.36	121.90
25	BC	51	ARG	NE-CZ-NH1	6.48	123.54	120.30
54	BA	1257	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1607	C	N1-C2-O2	6.48	122.79	118.90
54	BA	1764	C	O4'-C1'-N1	6.48	113.38	108.20
54	BA	2205	A	O4'-C1'-N9	6.48	113.38	108.20
21	AA	914	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	64	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1665	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1101	A	P-O3'-C3'	6.48	127.47	119.70
21	AA	1103	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	1364	U	N3-C2-O2	-6.48	117.67	122.20
54	BA	1713	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2178	C	N3-C2-O2	-6.48	117.37	121.90
4	AE	44	ARG	NE-CZ-NH1	6.48	123.54	120.30
54	BA	239	C	O4'-C1'-N1	6.48	113.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1952	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2808	G	N1-C6-O6	-6.48	116.02	119.90
21	AA	403	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1319	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2254	C	N3-C2-O2	-6.47	117.37	121.90
22	A1	27	C	N3-C2-O2	-6.47	117.37	121.90
24	A3	35	C	N1-C2-O2	6.47	122.78	118.90
54	BA	1027	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1167	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	676	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	1276	A	C5-C6-N1	6.47	120.94	117.70
54	BA	2791	G	O4'-C1'-N9	6.47	113.38	108.20
21	AA	1035	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	1045	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	487	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	1055	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1014	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1677	A	C5-C6-N1	6.47	120.93	117.70
54	BA	2503	A	O4'-C1'-N9	6.47	113.37	108.20
21	AA	1170	A	C5-C6-N1	6.47	120.93	117.70
54	BA	2084	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	263	A	C5-C6-N1	6.46	120.93	117.70
21	AA	282	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	582	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2095	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2725	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1254	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1261	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	33	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	281	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2251	G	N3-C2-N2	-6.46	115.38	119.90
54	BA	2707	U	O4'-C1'-N1	6.46	113.37	108.20
21	AA	393	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1267	C	N1-C2-O2	6.46	122.78	118.90
54	BA	1472	C	N3-C2-O2	-6.46	117.38	121.90
13	AN	81	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	54	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	419	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	503	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1090	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	2541	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1764	C	N3-C2-O2	-6.46	117.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1913	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1141	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	815	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	1252	G	N3-C2-N2	-6.45	115.38	119.90
54	BA	1625	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	1785	A	C5-C6-N1	6.45	120.93	117.70
54	BA	2486	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	1998	A	C4-C5-C6	-6.45	113.77	117.00
21	AA	977	A	O4'-C1'-N9	6.45	113.36	108.20
21	AA	1217	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1508	A	C5-C6-N1	6.45	120.92	117.70
54	BA	8	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	661	A	C5-C6-N1	6.45	120.93	117.70
54	BA	909	A	C5-C6-N1	6.45	120.92	117.70
54	BA	2058	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	2800	A	C5-C6-N1	6.45	120.93	117.70
54	BA	2829	A	C5-C6-N1	6.45	120.92	117.70
22	A1	11	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1783	A	C5-C6-N1	6.45	120.92	117.70
54	BA	1908	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	2171	A	N1-C6-N6	-6.45	114.73	118.60
54	BA	2387	U	N3-C2-O2	-6.45	117.69	122.20
54	BA	2824	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1322	C	N1-C2-O2	6.45	122.77	118.90
21	AA	1434	A	C5-C6-N1	6.45	120.92	117.70
54	BA	1146	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1570	A	C4-C5-C6	-6.45	113.78	117.00
1	AB	94	ARG	NE-CZ-NH1	6.45	123.52	120.30
16	AQ	10	ARG	NE-CZ-NH1	6.45	123.52	120.30
21	AA	248	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1327	C	N3-C2-O2	-6.45	117.39	121.90
39	BQ	44	TYR	CB-CG-CD2	-6.45	117.13	121.00
54	BA	156	A	C5-C6-N1	6.45	120.92	117.70
54	BA	920	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1586	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	2789	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	952	U	O4'-C1'-N1	6.44	113.36	108.20
54	BA	1001	A	C5-C6-N1	6.44	120.92	117.70
21	AA	737	C	N3-C2-O2	-6.44	117.39	121.90
22	A1	35	A	N1-C6-N6	-6.44	114.73	118.60
54	BA	242	G	O4'-C1'-N9	6.44	113.35	108.20
54	BA	2636	C	N3-C2-O2	-6.44	117.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	88	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	229	C	O4'-C1'-N1	6.44	113.35	108.20
54	BA	331	C	N1-C2-O2	6.44	122.76	118.90
54	BA	814	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	927	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1244	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1799	G	O4'-C1'-N9	6.44	113.35	108.20
54	BA	1936	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2646	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	169	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	1152	A	C4-C5-C6	-6.44	113.78	117.00
22	A1	69	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1772	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1892	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	196	A	C5-C6-N1	6.44	120.92	117.70
21	AA	496	A	C1'-O4'-C4'	-6.43	104.75	109.90
21	AA	1509	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	343	C	N3-C2-O2	-6.43	117.39	121.90
54	BA	529	A	C5-C6-N1	6.43	120.92	117.70
54	BA	599	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1493	C	N1-C2-O2	6.43	122.76	118.90
21	AA	174	A	C5-C6-N1	6.43	120.92	117.70
21	AA	285	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	1162	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	986	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2117	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	347	A	C5-C6-N1	6.43	120.92	117.70
54	BA	2090	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	2655	G	O4'-C1'-N9	6.43	113.34	108.20
54	BA	203	A	C5-C6-N1	6.43	120.92	117.70
54	BA	2805	C	O4'-C1'-N1	6.43	113.34	108.20
55	BB	73	A	C5-C6-N1	6.43	120.92	117.70
21	AA	7	A	N1-C6-N6	-6.43	114.74	118.60
21	AA	415	A	N1-C6-N6	-6.43	114.74	118.60
45	BW	24	ARG	NE-CZ-NH1	6.43	123.51	120.30
54	BA	1048	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	1178	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1366	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	1960	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	171	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2153	C	N3-C2-O2	-6.42	117.40	121.90
54	BA	2369	A	C4-C5-C6	-6.42	113.79	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2314	A	C5-C6-N1	6.42	120.91	117.70
21	AA	50	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	311	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1000	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1040	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1558	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	2559	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	2649	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	687	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2417	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1533	C	N1-C2-O2	6.42	122.75	118.90
54	BA	1773	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1920	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	2108	A	C5-C6-N1	6.42	120.91	117.70
21	AA	251	G	P-O3'-C3'	6.42	127.40	119.70
54	BA	101	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1213	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	181	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1647	U	O4'-C1'-N1	6.42	113.33	108.20
54	BA	2667	C	N1-C2-O2	6.42	122.75	118.90
21	AA	984	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	1046	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	1738	G	O4'-C1'-N9	6.41	113.33	108.20
54	BA	2377	A	C5-C6-N1	6.41	120.91	117.70
54	BA	2427	C	O4'-C1'-N1	6.41	113.33	108.20
54	BA	2589	A	C6-C5-N7	6.41	136.79	132.30
8	AI	84	ARG	NE-CZ-NH1	6.41	123.50	120.30
54	BA	718	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	994	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1595	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	959	A	C5-C6-N1	6.41	120.90	117.70
54	BA	1272	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1669	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2901	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	144	A	N1-C6-N6	-6.41	114.76	118.60
54	BA	654	A	N1-C6-N6	-6.41	114.76	118.60
54	BA	1117	C	O4'-C1'-N1	6.41	113.32	108.20
54	BA	1997	C	N3-C2-O2	-6.41	117.42	121.90
21	AA	339	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1064	C	O4'-C1'-N1	6.40	113.32	108.20
38	BP	108	ARG	NE-CZ-NH2	6.40	123.50	120.30
54	BA	89	A	C5-C6-N1	6.40	120.90	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	470	A	N1-C6-N6	-6.40	114.76	118.60
54	BA	5	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	184	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	323	C	N1-C2-O2	6.40	122.74	118.90
21	AA	526	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	535	A	N1-C6-N6	-6.40	114.76	118.60
21	AA	681	A	C5-C6-N1	6.40	120.90	117.70
21	AA	758	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	455	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	975	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1529	G	O4'-C1'-N9	6.40	113.32	108.20
54	BA	1938	A	C5-C6-N1	6.40	120.90	117.70
55	BB	46	A	C5-C6-N1	6.40	120.90	117.70
21	AA	1382	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	111	A	C5-C6-N1	6.39	120.90	117.70
54	BA	1638	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	1962	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	715	A	C5-C6-N1	6.39	120.90	117.70
21	AA	909	A	C5-C6-N1	6.39	120.90	117.70
21	AA	1319	A	C4-C5-C6	-6.39	113.80	117.00
34	BL	2	ARG	NE-CZ-NH2	6.39	123.50	120.30
54	BA	918	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	1614	A	C5-C6-N1	6.39	120.90	117.70
21	AA	1520	C	N3-C2-O2	-6.39	117.43	121.90
41	BS	11	ARG	NE-CZ-NH2	-6.39	117.10	120.30
54	BA	57	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2899	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	1022	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	2332	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2815	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	162	A	N1-C6-N6	-6.39	114.77	118.60
21	AA	750	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	754	C	N1-C2-O2	6.39	122.73	118.90
21	AA	1350	A	C5-C6-N1	6.39	120.89	117.70
21	AA	1462	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1528	A	C5-C6-N1	6.39	120.89	117.70
21	AA	609	A	C4-C5-C6	-6.38	113.81	117.00
24	A3	74	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	990	A	O4'-C1'-N9	6.38	113.31	108.20
54	BA	1264	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1370	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	1675	C	N3-C2-O2	-6.38	117.43	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2753	A	C5-C6-N1	6.38	120.89	117.70
21	AA	161	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	179	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	865	A	C5-C6-N1	6.38	120.89	117.70
21	AA	1092	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1615	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	924	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	637	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	1100	C	O4'-C1'-N1	6.38	113.30	108.20
21	AA	1150	A	C5-C6-N1	6.38	120.89	117.70
21	AA	1346	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1351	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	190	A	C4-C5-C6	-6.38	113.81	117.00
24	A3	24	C	N3-C2-O2	-6.38	117.44	121.90
24	A3	68	C	N3-C2-O2	-6.38	117.44	121.90
27	BE	49	ARG	NE-CZ-NH2	-6.38	117.11	120.30
54	BA	590	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1899	A	C5-C6-N1	6.38	120.89	117.70
21	AA	460	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	679	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	243	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	328	C	N1-C2-O2	6.37	122.72	118.90
21	AA	1200	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1369	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	16	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	485	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1289	C	C3'-C2'-C1'	6.37	106.60	101.50
21	AA	188	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	302	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1654	A	O4'-C1'-N9	6.37	113.30	108.20
54	BA	2080	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2183	A	C5-C6-N1	6.37	120.89	117.70
54	BA	2284	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2305	U	O4'-C1'-N1	6.37	113.30	108.20
54	BA	2788	C	N3-C2-O2	-6.37	117.44	121.90
12	AM	97	ARG	NE-CZ-NH2	-6.37	117.11	120.30
21	AA	490	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	433	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	905	A	C5-C6-N1	6.37	120.89	117.70
54	BA	2258	C	N3-C2-O2	-6.37	117.44	121.90
55	BB	53	A	N1-C6-N6	-6.37	114.78	118.60
21	AA	807	A	C4-C5-C6	-6.37	113.82	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	932	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1005	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	429	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	717	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2757	A	N1-C6-N6	-6.37	114.78	118.60
54	BA	919	U	O4'-C1'-N1	6.37	113.29	108.20
21	AA	1245	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	575	A	C5-C6-N1	6.37	120.88	117.70
54	BA	1170	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2281	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2813	A	C4-C5-C6	-6.36	113.82	117.00
15	AP	35	ARG	NE-CZ-NH1	6.36	123.48	120.30
54	BA	1102	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	73	A	N1-C6-N6	-6.36	114.78	118.60
54	BA	1451	C	N1-C2-O2	6.36	122.72	118.90
54	BA	1522	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1848	A	C5-C6-N1	6.36	120.88	117.70
54	BA	2247	A	C5-C6-N1	6.36	120.88	117.70
54	BA	2480	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2616	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	1501	C	N1-C2-O2	6.36	122.72	118.90
54	BA	1100	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2794	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	63	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1013	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2453	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	808	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	819	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	1111	A	C4-C5-C6	-6.36	113.82	117.00
51	B2	14	ARG	NE-CZ-NH1	6.36	123.48	120.30
54	BA	1977	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2147	A	O4'-C1'-N9	6.36	113.28	108.20
54	BA	2800	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	415	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	2810	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	195	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	556	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	1407	C	N3-C2-O2	-6.35	117.45	121.90
22	A1	58	A	N1-C6-N6	-6.35	114.79	118.60
54	BA	1768	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	129	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	256	U	O4'-C1'-N1	6.35	113.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	461	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	677	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	702	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	1329	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	853	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	900	A	C5-C6-N1	6.35	120.88	117.70
54	BA	2008	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	2207	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	689	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	826	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	1161	C	N3-C2-O2	-6.35	117.46	121.90
24	A3	13	C	N3-C2-O2	-6.35	117.46	121.90
25	BC	42	ARG	NE-CZ-NH1	6.35	123.47	120.30
54	BA	2048	G	N1-C6-O6	-6.35	116.09	119.90
54	BA	2147	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	749	A	C5-C6-N1	6.34	120.87	117.70
54	BA	357	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	472	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1799	G	P-O3'-C3'	6.34	127.31	119.70
54	BA	1967	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2059	A	C5-C6-N1	6.34	120.87	117.70
21	AA	539	A	C5-C6-N1	6.34	120.87	117.70
21	AA	908	A	N1-C6-N6	-6.34	114.79	118.60
21	AA	300	A	C5-C6-N1	6.34	120.87	117.70
21	AA	848	C	N3-C2-O2	-6.34	117.46	121.90
37	BO	7	ARG	NE-CZ-NH2	-6.34	117.13	120.30
39	BQ	29	ARG	NE-CZ-NH1	6.34	123.47	120.30
54	BA	191	A	N1-C6-N6	-6.34	114.80	118.60
54	BA	280	U	N3-C2-O2	-6.34	117.76	122.20
54	BA	2356	U	O4'-C1'-N1	6.34	113.27	108.20
54	BA	2518	A	C4-C5-C6	-6.34	113.83	117.00
55	BB	19	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2364	C	O4'-C1'-N1	6.34	113.27	108.20
54	BA	2720	U	O4'-C1'-N1	6.34	113.27	108.20
24	A3	76	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	53	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	640	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	19	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	228	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	743	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1065	U	O4'-C1'-N1	6.34	113.27	108.20
54	BA	2799	A	O4'-C1'-N9	6.34	113.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	179	A	C5-C6-N1	6.33	120.87	117.70
4	AE	53	ARG	NE-CZ-NH1	6.33	123.47	120.30
21	AA	1172	C	N3-C2-O2	-6.33	117.47	121.90
37	BO	9	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	218	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	753	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	987	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1762	A	C5-C6-N1	6.33	120.87	117.70
54	BA	2248	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2362	C	N3-C2-O2	-6.33	117.47	121.90
15	AP	70	ARG	NE-CZ-NH1	6.33	123.47	120.30
21	AA	321	A	C5-C6-N1	6.33	120.87	117.70
54	BA	403	U	O4'-C1'-N1	6.33	113.27	108.20
54	BA	2322	A	C5-C6-N1	6.33	120.87	117.70
21	AA	498	A	C5-C6-N1	6.33	120.86	117.70
35	BM	10	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	345	A	N1-C6-N6	-6.33	114.80	118.60
54	BA	503	A	C5-C6-N1	6.33	120.86	117.70
54	BA	816	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1644	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2001	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2773	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2863	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1271	A	C4-C5-C6	-6.33	113.84	117.00
39	BQ	57	ARG	NE-CZ-NH1	6.33	123.46	120.30
54	BA	615	U	O4'-C1'-N1	6.33	113.26	108.20
54	BA	2541	A	C4-C5-C6	-6.33	113.83	117.00
21	AA	499	A	C1'-O4'-C4'	-6.33	104.84	109.90
21	AA	1508	A	C4-C5-C6	-6.33	113.84	117.00
49	B0	39	ARG	NE-CZ-NH1	6.33	123.46	120.30
54	BA	595	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	675	A	C5-C6-N1	6.33	120.86	117.70
24	A3	63	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1014	A	C5-C6-N1	6.33	120.86	117.70
54	BA	1158	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2239	G	N3-C2-N2	-6.33	115.47	119.90
54	BA	2510	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	746	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	806	C	N3-C2-O2	-6.32	117.47	121.90
21	AA	1325	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	453	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	837	C	N3-C2-O2	-6.32	117.47	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2072	C	C4'-C3'-C2'	-6.32	96.28	102.60
54	BA	2452	C	O4'-C1'-N1	6.32	113.26	108.20
54	BA	2598	A	C5-C6-N1	6.32	120.86	117.70
26	BD	141	ARG	NE-CZ-NH1	6.32	123.46	120.30
54	BA	1302	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1708	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2510	C	O4'-C1'-N1	6.32	113.26	108.20
54	BA	163	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	501	A	N1-C6-N6	-6.32	114.81	118.60
55	BB	49	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	246	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	360	U	O4'-C1'-N1	6.32	113.25	108.20
54	BA	2658	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2666	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	853	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	1465	A	C5-C6-N1	6.32	120.86	117.70
54	BA	449	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1879	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2385	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	949	A	C5-C6-N1	6.31	120.86	117.70
21	AA	1502	A	O4'-C1'-N9	6.31	113.25	108.20
21	AA	634	C	N3-C2-O2	-6.31	117.48	121.90
22	A1	68	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	617	G	O4'-C1'-N9	6.31	113.25	108.20
54	BA	917	A	N1-C6-N6	-6.31	114.81	118.60
21	AA	269	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	563	A	N1-C6-N6	-6.31	114.82	118.60
54	BA	2159	G	N1-C6-O6	-6.31	116.12	119.90
54	BA	2691	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	1413	A	C5-C6-N1	6.31	120.85	117.70
54	BA	251	A	N1-C6-N6	-6.31	114.82	118.60
54	BA	1183	U	O4'-C1'-N1	6.31	113.24	108.20
54	BA	1502	A	C5-C6-N1	6.31	120.85	117.70
21	AA	163	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1176	A	C5-C6-N1	6.30	120.85	117.70
21	AA	1333	A	C5-C6-N1	6.30	120.85	117.70
21	AA	1366	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1412	C	N3-C2-O2	-6.30	117.49	121.90
28	BF	114	ARG	NE-CZ-NH1	6.30	123.45	120.30
54	BA	52	A	C5-C6-N1	6.30	120.85	117.70
54	BA	447	A	C5-C6-N1	6.30	120.85	117.70
17	AR	56	ARG	NE-CZ-NH1	6.30	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	254	G	N1-C6-O6	-6.30	116.12	119.90
24	A3	39	A	C4-C5-C6	-6.30	113.85	117.00
27	BE	79	ARG	NE-CZ-NH1	6.30	123.45	120.30
54	BA	762	U	P-O3'-C3'	6.30	127.26	119.70
21	AA	545	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	126	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	556	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1298	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1460	U	O4'-C1'-N1	6.30	113.24	108.20
54	BA	1924	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2482	A	C5-C6-N1	6.30	120.85	117.70
54	BA	2539	C	N3-C2-O2	-6.30	117.49	121.90
55	BB	115	A	N1-C6-N6	-6.30	114.82	118.60
21	AA	706	A	C5-C6-N1	6.30	120.85	117.70
49	B0	51	ARG	NE-CZ-NH1	6.30	123.45	120.30
54	BA	125	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	133	U	O4'-C1'-N1	6.30	113.24	108.20
54	BA	213	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1795	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2268	A	C5-C6-N1	6.30	120.85	117.70
55	BB	69	G	O4'-C1'-N9	6.30	113.24	108.20
54	BA	793	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	1397	C	N1-C2-O2	6.29	122.68	118.90
54	BA	1144	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	1268	A	C5-C6-N1	6.29	120.85	117.70
21	AA	452	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	878	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	1496	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1612	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2600	A	C1'-O4'-C4'	-6.29	104.87	109.90
54	BA	1582	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2298	A	C5-C6-N1	6.29	120.84	117.70
54	BA	743	A	C5-C6-N1	6.29	120.84	117.70
21	AA	78	A	C5-C6-N1	6.29	120.84	117.70
21	AA	400	C	O4'-C1'-N1	6.29	113.23	108.20
54	BA	2060	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	174	A	N1-C6-N6	-6.29	114.83	118.60
21	AA	923	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	1019	A	C5-C6-N1	6.29	120.84	117.70
54	BA	84	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	1872	A	C5-C6-N1	6.29	120.84	117.70
54	BA	807	U	O4'-C1'-N1	6.28	113.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	931	U	N3-C2-O2	-6.28	117.80	122.20
54	BA	1230	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1404	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2403	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2456	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2665	A	O4'-C1'-N9	6.28	113.23	108.20
8	AI	32	ARG	NE-CZ-NH1	6.28	123.44	120.30
21	AA	559	A	N1-C6-N6	-6.28	114.83	118.60
54	BA	1564	C	N3-C2-O2	-6.28	117.50	121.90
8	AI	10	ARG	NE-CZ-NH1	6.28	123.44	120.30
21	AA	1150	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	679	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	800	A	C5-C6-N1	6.28	120.84	117.70
21	AA	74	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	422	C	N3-C2-O2	-6.28	117.51	121.90
21	AA	528	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	66	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	1469	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2311	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2738	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	490	C	O4'-C1'-N1	6.27	113.22	108.20
54	BA	2015	A	C5-C6-N1	6.27	120.84	117.70
21	AA	175	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	554	A	C5-C6-N1	6.27	120.84	117.70
54	BA	492	A	C5-C6-N1	6.27	120.84	117.70
54	BA	671	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1291	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1357	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1759	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	1384	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	372	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1084	G	N1-C6-O6	-6.27	116.14	119.90
54	BA	840	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1021	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	2765	A	N1-C6-N6	-6.27	114.84	118.60
21	AA	978	A	N1-C6-N6	-6.27	114.84	118.60
21	AA	1117	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	1468	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	20	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	609	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	917	A	C5-C6-N1	6.27	120.83	117.70
54	BA	990	A	N1-C6-N6	-6.27	114.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1672	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	910	C	N3-C2-O2	-6.26	117.52	121.90
23	A2	91	A	C4-C5-C6	-6.26	113.87	117.00
35	BM	6	ARG	NE-CZ-NH1	6.26	123.43	120.30
35	BM	51	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	56	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1247	A	O4'-C1'-N9	6.26	113.21	108.20
54	BA	1498	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2026	U	O4'-C1'-N1	6.26	113.21	108.20
24	A3	44	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	676	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	1394	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	988	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2440	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	903	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2270	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	84	U	N3-C2-O2	-6.26	117.82	122.20
21	AA	553	A	C5-C6-N1	6.26	120.83	117.70
54	BA	118	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2771	C	N1-C2-O2	6.26	122.66	118.90
54	BA	1052	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	222	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	1229	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	1246	A	C5-C6-N1	6.25	120.83	117.70
54	BA	1927	A	C5-C6-N1	6.25	120.83	117.70
54	BA	2260	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	2781	A	C4-C5-C6	-6.25	113.87	117.00
30	BH	50	ARG	NE-CZ-NH1	6.25	123.42	120.30
54	BA	703	U	O4'-C1'-N1	6.25	113.20	108.20
21	AA	1476	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2476	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2814	A	C4-C5-C6	-6.25	113.88	117.00
13	AN	24	ARG	NE-CZ-NH1	6.25	123.42	120.30
21	AA	155	A	C5-C6-N1	6.24	120.82	117.70
21	AA	833	G	N1-C6-O6	-6.24	116.15	119.90
21	AA	930	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	1364	U	C3'-C2'-C1'	6.24	106.50	101.50
54	BA	79	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1532	A	C4-C5-C6	-6.24	113.88	117.00
41	BS	95	ARG	NE-CZ-NH1	6.24	123.42	120.30
54	BA	1912	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2675	A	C5-C6-N1	6.24	120.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1456	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	180	G	C1'-O4'-C4'	-6.24	104.91	109.90
54	BA	1481	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	1495	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2154	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2478	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	704	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	983	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1046	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1383	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1525	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1800	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1868	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	618	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2699	C	O4'-C1'-N1	6.24	113.19	108.20
21	AA	964	A	C4-C5-C6	-6.24	113.88	117.00
24	A3	42	C	N3-C2-O2	-6.24	117.53	121.90
40	BR	13	ARG	NE-CZ-NH1	6.24	123.42	120.30
54	BA	508	A	N1-C6-N6	-6.24	114.86	118.60
54	BA	1791	A	N1-C6-N6	-6.24	114.86	118.60
54	BA	1914	C	O4'-C1'-N1	6.24	113.19	108.20
54	BA	2463	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	216	A	C5-C6-N1	6.23	120.82	117.70
21	AA	100	G	N1-C6-O6	-6.23	116.16	119.90
21	AA	739	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	872	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	979	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	430	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	686	U	O4'-C1'-N1	6.23	113.19	108.20
54	BA	2392	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	1519	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	320	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	601	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1270	C	N3-C4-C5	6.23	124.39	121.90
54	BA	2879	A	O4'-C1'-N9	6.23	113.19	108.20
55	BB	63	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	614	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	695	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	1340	A	C4-C5-C6	-6.23	113.89	117.00
24	A3	58	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	208	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2823	A	C4-C5-C6	-6.23	113.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2205	A	N1-C6-N6	-6.23	114.86	118.60
21	AA	329	A	C5-C6-N1	6.22	120.81	117.70
21	AA	573	A	C3'-C2'-C1'	6.22	106.48	101.50
54	BA	221	A	N1-C6-N6	-6.22	114.86	118.60
54	BA	1070	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1453	A	O4'-C1'-N9	6.22	113.18	108.20
54	BA	97	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1035	U	O4'-C1'-N1	6.22	113.18	108.20
54	BA	820	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	1557	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	1487	G	N3-C2-N2	-6.22	115.55	119.90
54	BA	210	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	384	A	C4-C5-C6	-6.22	113.89	117.00
55	BB	57	A	N1-C6-N6	-6.22	114.87	118.60
21	AA	270	A	C5-C6-N1	6.22	120.81	117.70
54	BA	238	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1760	C	N3-C2-O2	-6.22	117.55	121.90
11	AL	13	ARG	NE-CZ-NH2	-6.22	117.19	120.30
54	BA	42	A	C5-C6-N1	6.22	120.81	117.70
54	BA	417	C	O4'-C1'-N1	6.22	113.17	108.20
54	BA	1528	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	1632	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	475	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1223	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1073	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1348	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1495	A	C5-C6-N1	6.21	120.81	117.70
54	BA	2626	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1036	A	C5-C6-N1	6.21	120.81	117.70
54	BA	129	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2358	A	C4-C5-C6	-6.21	113.89	117.00
27	BE	40	ARG	NE-CZ-NH1	6.21	123.41	120.30
54	BA	1081	U	O4'-C1'-N1	6.21	113.17	108.20
12	AM	112	ARG	NE-CZ-NH1	6.21	123.40	120.30
54	BA	56	A	C5-C6-N1	6.21	120.80	117.70
54	BA	941	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1833	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2891	U	O4'-C1'-N1	6.21	113.17	108.20
21	AA	687	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	2231	U	O4'-C1'-N1	6.21	113.17	108.20
21	AA	101	A	N1-C6-N6	-6.21	114.88	118.60
23	A2	79	A	O4'-C1'-N9	6.21	113.16	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1732	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	277	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	509	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1012	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2042	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	655	A	C4-C5-C6	-6.20	113.90	117.00
25	BC	174	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	AA	192	A	C5-C6-N1	6.20	120.80	117.70
21	AA	1314	C	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1189	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2174	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2393	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	2418	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2482	A	N1-C6-N6	-6.20	114.88	118.60
21	AA	1055	A	O4'-C1'-N9	6.20	113.16	108.20
54	BA	31	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	366	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	806	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1611	C	N1-C2-O2	6.20	122.62	118.90
54	BA	1739	A	N1-C6-N6	-6.20	114.88	118.60
21	AA	968	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1248	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1881	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	712	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	880	C	N3-C2-O2	-6.20	117.56	121.90
22	A1	75	C	N1-C2-O2	6.20	122.62	118.90
54	BA	613	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1322	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1658	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1832	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2721	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2837	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	621	A	C5-C6-N1	6.19	120.80	117.70
54	BA	1233	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1771	C	N3-C2-O2	-6.19	117.56	121.90
21	AA	90	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	990	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1336	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1446	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	279	A	N1-C6-N6	-6.19	114.89	118.60
54	BA	1246	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	1704	C	N3-C2-O2	-6.19	117.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2527	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	306	A	C4-C5-C6	-6.19	113.91	117.00
28	BF	109	ARG	NE-CZ-NH2	-6.19	117.21	120.30
21	AA	985	C	N3-C2-O2	-6.19	117.57	121.90
24	A3	52	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	272	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	592	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	2634	A	C6-C5-N7	6.19	136.63	132.30
55	BB	109	A	N1-C6-N6	-6.19	114.89	118.60
21	AA	83	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	907	A	C5-C6-N1	6.19	120.79	117.70
25	BC	188	ARG	NE-CZ-NH1	6.19	123.39	120.30
54	BA	833	A	C5-C6-N1	6.19	120.79	117.70
54	BA	1205	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	572	A	N1-C6-N6	-6.18	114.89	118.60
54	BA	828	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	2236	U	O4'-C1'-N1	6.18	113.15	108.20
21	AA	582	C	N1-C2-O2	6.18	122.61	118.90
36	BN	96	ARG	NE-CZ-NH1	6.18	123.39	120.30
42	BT	6	ARG	NE-CZ-NH2	-6.18	117.21	120.30
54	BA	558	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	838	C	N1-C2-O2	6.18	122.61	118.90
54	BA	928	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	721	A	C5-C6-N1	6.18	120.79	117.70
21	AA	729	A	C4-C5-C6	-6.18	113.91	117.00
24	A3	11	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	709	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	1675	C	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2494	G	O4'-C1'-N9	6.18	113.14	108.20
21	AA	646	G	N1-C6-O6	-6.18	116.19	119.90
21	AA	882	C	N3-C2-O2	-6.18	117.58	121.90
24	A3	49	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	1285	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	973	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1145	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1652	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2268	A	N1-C6-N6	-6.18	114.89	118.60
21	AA	468	A	O4'-C1'-N9	6.17	113.14	108.20
21	AA	607	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	980	C	N3-C2-O2	-6.17	117.58	121.90
22	A1	71	C	N3-C2-O2	-6.17	117.58	121.90
24	A3	36	A	C4-C5-C6	-6.17	113.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	352	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	490	C	N1-C2-O2	6.17	122.61	118.90
54	BA	1793	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2177	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2291	U	O4'-C1'-N1	6.17	113.14	108.20
54	BA	2335	A	C5-C6-N1	6.17	120.79	117.70
55	BB	50	A	C4-C5-C6	-6.17	113.91	117.00
36	BN	8	ARG	NE-CZ-NH1	6.17	123.39	120.30
54	BA	1624	U	O4'-C1'-N1	6.17	113.14	108.20
21	AA	149	A	C5-C6-N1	6.17	120.79	117.70
54	BA	336	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1069	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	2378	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	590	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	303	A	C5-C6-N1	6.17	120.78	117.70
21	AA	815	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	337	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1090	A	C5-C6-N1	6.17	120.78	117.70
54	BA	2439	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	935	A	C5-C6-N1	6.17	120.78	117.70
21	AA	1314	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1821	A	C4-C5-C6	-6.17	113.92	117.00
55	BB	3	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	976	G	N3-C2-N2	-6.17	115.58	119.90
54	BA	1253	A	C1'-O4'-C4'	-6.17	104.97	109.90
54	BA	2531	A	C5-C6-N1	6.17	120.78	117.70
21	AA	1082	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	1203	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	922	C	N3-C2-O2	-6.16	117.58	121.90
54	BA	998	C	N3-C2-O2	-6.16	117.58	121.90
54	BA	1461	C	N3-C2-O2	-6.16	117.59	121.90
55	BB	63	C	O4'-C1'-N1	6.16	113.13	108.20
14	AO	53	ARG	NE-CZ-NH1	6.16	123.38	120.30
21	AA	230	G	N3-C2-N2	-6.16	115.59	119.90
21	AA	938	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	2054	A	C5-C6-N1	6.16	120.78	117.70
54	BA	2321	U	N3-C2-O2	-6.16	117.89	122.20
21	AA	1259	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	115	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	353	A	O4'-C1'-N9	6.16	113.13	108.20
54	BA	992	C	N3-C2-O2	-6.16	117.59	121.90
26	BD	77	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	318	C	O4'-C1'-N1	6.16	113.12	108.20
54	BA	1386	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	431	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1676	A	C5-C6-N1	6.15	120.78	117.70
54	BA	2208	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	635	A	C5-C6-N1	6.15	120.78	117.70
54	BA	362	A	C5-C6-N1	6.15	120.78	117.70
54	BA	1463	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2792	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	2264	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	246	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	925	A	C4-C5-C6	-6.15	113.92	117.00
21	AA	71	A	C4-C5-C6	-6.15	113.93	117.00
21	AA	520	A	C5-C6-N1	6.15	120.77	117.70
54	BA	678	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	1958	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	2364	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	2467	C	N3-C2-O2	-6.15	117.60	121.90
21	AA	653	U	N3-C2-O2	-6.15	117.90	122.20
21	AA	1114	C	N3-C2-O2	-6.15	117.60	121.90
35	BM	38	ARG	NE-CZ-NH1	6.15	123.37	120.30
54	BA	2406	A	N1-C6-N6	-6.15	114.91	118.60
21	AA	66	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	901	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	936	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1006	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1499	C	O4'-C1'-N1	6.14	113.12	108.20
54	BA	2157	G	O4'-C1'-N9	6.14	113.12	108.20
54	BA	2594	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2657	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	322	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	999	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	335	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	783	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1339	G	O4'-C1'-N9	6.14	113.11	108.20
28	BF	166	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	2082	A	C5-C6-N1	6.14	120.77	117.70
5	AF	45	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	660	C	N3-C2-O2	-6.14	117.60	121.90
8	AI	105	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	28	A	N1-C6-N6	-6.14	114.92	118.60
54	BA	456	C	N1-C2-O2	6.14	122.58	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1327	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2199	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2352	A	N1-C6-N6	-6.14	114.92	118.60
21	AA	768	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	538	A	C5-C6-N1	6.13	120.77	117.70
54	BA	2442	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2896	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	960	U	N3-C2-O2	-6.13	117.91	122.20
21	AA	1234	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	22	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	580	C	N3-C2-O2	-6.13	117.61	121.90
35	BM	114	ARG	NE-CZ-NH1	6.13	123.36	120.30
54	BA	2198	A	C5-C6-N1	6.13	120.77	117.70
54	BA	2564	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	2748	A	N1-C6-N6	-6.13	114.92	118.60
55	BB	80	U	O4'-C1'-N1	6.13	113.11	108.20
15	AP	51	ARG	NE-CZ-NH1	6.13	123.36	120.30
39	BQ	2	ARG	NE-CZ-NH1	6.13	123.36	120.30
54	BA	347	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2130	U	O4'-C1'-N1	6.13	113.10	108.20
54	BA	2241	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	802	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	1503	A	C4-C5-C6	-6.13	113.94	117.00
53	B4	12	ARG	NE-CZ-NH1	6.13	123.36	120.30
43	BU	93	ARG	NE-CZ-NH1	6.13	123.36	120.30
54	BA	443	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	504	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	1330	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	507	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1001	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	435	A	C5-C6-N1	6.12	120.76	117.70
21	AA	995	C	N3-C2-O2	-6.12	117.61	121.90
24	A3	14	A	C4-C5-C6	-6.12	113.94	117.00
46	BX	71	ARG	NE-CZ-NH1	6.12	123.36	120.30
54	BA	672	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	2451	A	C5-C6-N1	6.12	120.76	117.70
8	AI	108	ARG	NE-CZ-NH1	6.12	123.36	120.30
21	AA	47	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	322	A	O4'-C1'-N9	6.12	113.10	108.20
54	BA	737	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	756	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	382	A	C4-C5-C6	-6.12	113.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	708	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	564	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	738	G	N1-C6-O6	-6.12	116.23	119.90
54	BA	2459	A	C4-C5-C6	-6.12	113.94	117.00
25	BC	213	ARG	NE-CZ-NH1	6.12	123.36	120.30
24	A3	45	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	225	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1020	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2825	G	N3-C4-C5	-6.12	125.54	128.60
54	BA	1848	A	C4-C5-C6	-6.11	113.94	117.00
21	AA	744	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	487	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2288	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	2184	A	C5-C6-N1	6.11	120.76	117.70
54	BA	794	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	845	A	C5-C6-N1	6.11	120.75	117.70
12	AM	70	ARG	NE-CZ-NH1	6.11	123.35	120.30
21	AA	448	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	2762	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	1176	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	1230	A	C5-C6-N1	6.11	120.75	117.70
21	AA	266	G	O4'-C1'-N9	6.10	113.08	108.20
21	AA	608	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	936	A	O4'-C1'-N9	6.10	113.08	108.20
54	BA	1690	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2829	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	675	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	1332	A	C5-C6-N1	6.10	120.75	117.70
28	BF	94	ARG	NE-CZ-NH1	6.10	123.35	120.30
54	BA	1437	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	560	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	1016	A	C5-C6-N1	6.10	120.75	117.70
54	BA	294	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1143	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1596	A	C6-C5-N7	6.10	136.57	132.30
21	AA	1492	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	759	G	N3-C4-C5	-6.10	125.55	128.60
54	BA	948	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1937	A	O4'-C1'-N9	6.10	113.08	108.20
54	BA	2900	A	C5-C6-N1	6.10	120.75	117.70
54	BA	1385	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	2835	A	C4-C5-C6	-6.09	113.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AP	5	ARG	NE-CZ-NH1	6.09	123.35	120.30
32	BJ	96	ARG	NE-CZ-NH1	6.09	123.35	120.30
54	BA	513	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	192	A	C4-C5-C6	-6.09	113.95	117.00
32	BJ	99	ARG	NE-CZ-NH1	6.09	123.34	120.30
54	BA	2575	C	N3-C2-O2	-6.09	117.64	121.90
34	BL	126	ARG	NE-CZ-NH1	6.09	123.34	120.30
54	BA	544	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	10	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	334	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	804	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	2793	C	N3-C2-O2	-6.09	117.64	121.90
3	AD	72	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	2103	C	N3-C2-O2	-6.08	117.64	121.90
55	BB	6	G	O4'-C1'-N9	6.08	113.07	108.20
21	AA	288	A	C4-C5-C6	-6.08	113.96	117.00
22	A1	20	G	O4'-C1'-N9	6.08	113.07	108.20
54	BA	344	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	908	C	O4'-C1'-N1	6.08	113.07	108.20
54	BA	1775	U	O4'-C1'-N1	6.08	113.07	108.20
54	BA	2200	C	O4'-C1'-N1	6.08	113.07	108.20
21	AA	1226	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	1274	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1196	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	840	C	N1-C2-O2	6.08	122.55	118.90
21	AA	876	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2499	C	O4'-C1'-N1	6.08	113.06	108.20
54	BA	2734	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	96	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	95	C	N1-C2-O2	6.08	122.55	118.90
21	AA	136	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	1049	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	1966	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2682	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	118	A	C5'-C4'-O4'	6.07	116.39	109.10
54	BA	1088	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	2776	A	N1-C6-N6	-6.07	114.96	118.60
21	AA	498	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	393	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	782	A	C5-C6-N1	6.07	120.74	117.70
54	BA	968	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1754	A	C5-C6-N1	6.07	120.74	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BC	47	ARG	NE-CZ-NH1	6.07	123.34	120.30
54	BA	83	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	111	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	1941	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2085	U	O4'-C1'-N1	6.07	113.06	108.20
38	BP	50	ARG	NE-CZ-NH1	6.07	123.33	120.30
54	BA	47	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	95	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	2222	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2870	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	1092	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	1277	C	N3-C2-O2	-6.07	117.66	121.90
54	BA	1200	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2192	U	O4'-C1'-N1	6.07	113.05	108.20
21	AA	832	G	N1-C6-O6	-6.06	116.26	119.90
21	AA	676	A	C5-C6-N1	6.06	120.73	117.70
21	AA	1362	A	C4-C5-C6	-6.06	113.97	117.00
39	BQ	47	ARG	NE-CZ-NH1	6.06	123.33	120.30
54	BA	2507	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2678	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	496	A	C5-C6-N1	6.06	120.73	117.70
54	BA	244	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1785	A	C4-C5-C6	-6.06	113.97	117.00
32	BJ	27	ARG	NE-CZ-NH1	6.06	123.33	120.30
51	B2	33	ARG	NE-CZ-NH1	6.06	123.33	120.30
54	BA	764	A	C5-C6-N1	6.06	120.73	117.70
54	BA	2520	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2882	A	C4-C5-C6	-6.06	113.97	117.00
55	BB	14	U	N3-C2-O2	-6.06	117.96	122.20
14	AO	71	ARG	NE-CZ-NH1	6.06	123.33	120.30
54	BA	1079	C	N1-C2-O2	6.06	122.53	118.90
54	BA	1583	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2565	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	225	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	575	A	C4-C5-C6	-6.06	113.97	117.00
15	AP	28	ARG	NE-CZ-NH1	6.05	123.33	120.30
21	AA	451	A	P-O3'-C3'	6.05	126.97	119.70
21	AA	489	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	222	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	528	A	C5-C6-N1	6.05	120.73	117.70
54	BA	1117	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	1513	U	O4'-C1'-N1	6.05	113.04	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2352	A	C5-C6-N1	6.05	120.73	117.70
54	BA	274	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	423	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	497	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	1204	A	C5-C6-N1	6.05	120.72	117.70
54	BA	750	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	2858	C	N1-C2-O2	6.05	122.53	118.90
21	AA	502	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1547	C	N3-C2-O2	-6.05	117.67	121.90
55	BB	60	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	653	U	O4'-C1'-N1	6.05	113.04	108.20
21	AA	897	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	1377	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	385	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1314	C	N1-C2-O2	6.05	122.53	118.90
54	BA	2412	A	C5-C6-N1	6.05	120.72	117.70
55	BB	55	U	O4'-C1'-N1	6.05	113.04	108.20
55	BB	71	C	O4'-C1'-N1	6.05	113.04	108.20
54	BA	1095	A	N1-C6-N6	-6.04	114.97	118.60
54	BA	2369	A	C5-C6-N1	6.04	120.72	117.70
4	AE	44	ARG	NE-CZ-NH2	-6.04	117.28	120.30
21	AA	441	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	658	U	O4'-C1'-N1	6.04	113.03	108.20
22	A1	23	A	C4-C5-C6	-6.04	113.98	117.00
25	BC	202	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	731	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	1480	A	C4-C5-C6	-6.04	113.98	117.00
22	A1	25	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1189	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1243	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1569	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1773	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2045	C	O4'-C1'-N1	6.04	113.03	108.20
54	BA	616	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1433	A	N1-C6-N6	-6.04	114.98	118.60
54	BA	1734	G	O4'-C1'-N9	6.04	113.03	108.20
54	BA	2200	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	385	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	1213	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	47	C	O4'-C1'-N1	6.03	113.03	108.20
54	BA	2095	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2397	G	N3-C2-N2	-6.03	115.68	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1503	A	C5-C6-N1	6.03	120.72	117.70
54	BA	2101	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2586	U	O4'-C1'-N1	6.03	113.03	108.20
21	AA	1410	A	C5-C6-N1	6.03	120.72	117.70
22	A1	41	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	202	U	O4'-C1'-N1	6.03	113.02	108.20
54	BA	268	C	N3-C2-O2	-6.03	117.68	121.90
11	AL	85	ARG	NE-CZ-NH2	-6.03	117.29	120.30
21	AA	272	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	689	C	O4'-C1'-N1	6.03	113.02	108.20
21	AA	699	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	147	C	O4'-C1'-N1	6.03	113.02	108.20
54	BA	509	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1313	U	N3-C2-O2	-6.03	117.98	122.20
54	BA	2097	A	C5-C6-N1	6.03	120.71	117.70
54	BA	2143	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	264	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	334	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	1022	A	C5-C6-N1	6.03	120.71	117.70
39	BQ	12	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	172	A	C5-C6-N1	6.03	120.71	117.70
54	BA	426	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	601	C	O4'-C1'-N1	6.03	113.02	108.20
54	BA	1104	C	N3-C2-O2	-6.03	117.68	121.90
55	BB	42	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	701	U	P-O3'-C3'	6.02	126.93	119.70
21	AA	1273	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	1296	C	N1-C2-O2	6.02	122.51	118.90
54	BA	981	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	559	A	C1'-O4'-C4'	-6.02	105.08	109.90
54	BA	378	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1363	C	N3-C2-O2	-6.02	117.69	121.90
55	BB	115	A	C5-C6-N1	6.02	120.71	117.70
21	AA	119	A	C4-C5-C6	-6.02	113.99	117.00
23	A2	92	U	O4'-C1'-N1	6.02	113.02	108.20
54	BA	1293	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1754	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	1131	G	N3-C2-N2	-6.02	115.69	119.90
54	BA	1130	U	O4'-C1'-N1	6.02	113.01	108.20
54	BA	1294	U	O4'-C1'-N1	6.02	113.01	108.20
54	BA	2142	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	946	A	C4-C5-C6	-6.01	113.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	143	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	179	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	435	C	N1-C2-O2	6.01	122.51	118.90
54	BA	2596	U	O4'-C1'-N1	6.01	113.01	108.20
22	A1	36	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	401	A	C5-C6-N1	6.01	120.70	117.70
54	BA	1165	A	C5-C6-N1	6.01	120.71	117.70
54	BA	1306	C	N3-C2-O2	-6.01	117.69	121.90
55	BB	113	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	814	A	C5-C6-N1	6.01	120.70	117.70
54	BA	1829	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	719	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	211	C	N3-C2-O2	-6.01	117.70	121.90
54	BA	257	C	N3-C2-O2	-6.01	117.70	121.90
54	BA	1417	C	O4'-C1'-N1	6.01	113.00	108.20
21	AA	1237	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2232	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2274	A	C4-C5-C6	-6.00	114.00	117.00
11	AL	120	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	680	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1118	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2745	C	N3-C2-O2	-6.00	117.70	121.90
55	BB	68	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	214	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	469	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1328	C	N3-C4-C5	6.00	124.30	121.90
25	BC	257	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	1004	U	O4'-C1'-N1	6.00	113.00	108.20
54	BA	1009	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1253	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1902	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2706	A	C5-C6-N1	6.00	120.70	117.70
21	AA	263	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	414	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	583	A	C4-C5-C6	-6.00	114.00	117.00
47	BY	52	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	1447	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1509	A	O4'-C1'-N9	6.00	113.00	108.20
54	BA	1836	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	766	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1541	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	2099	U	O4'-C1'-N1	6.00	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2435	A	C5-C6-N1	6.00	120.70	117.70
21	AA	1201	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	1262	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1510	G	O4'-C1'-N9	6.00	113.00	108.20
21	AA	1016	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	661	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	2158	A	C4-C5-C6	-5.99	114.00	117.00
9	AJ	16	ARG	NE-CZ-NH1	5.99	123.30	120.30
54	BA	1947	C	N3-C2-O2	-5.99	117.70	121.90
21	AA	412	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	514	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	959	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1503	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	1168	U	N3-C2-O2	-5.99	118.01	122.20
21	AA	1482	G	N1-C6-O6	-5.99	116.31	119.90
54	BA	491	G	O4'-C1'-N9	5.99	112.99	108.20
54	BA	2626	C	O4'-C1'-N1	5.99	112.99	108.20
54	BA	2424	C	N1-C2-O2	5.99	122.49	118.90
21	AA	40	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	1404	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	466	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1523	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	2577	A	N1-C6-N6	-5.99	115.01	118.60
54	BA	2650	U	O4'-C1'-N1	5.98	112.99	108.20
21	AA	1184	G	C3'-C2'-C1'	5.98	106.29	101.50
21	AA	1256	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1402	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	372	G	O4'-C1'-N9	5.98	112.99	108.20
54	BA	529	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1376	C	N3-C2-O2	-5.98	117.71	121.90
55	BB	46	A	C4-C5-C6	-5.98	114.01	117.00
4	AE	156	ARG	NE-CZ-NH2	5.98	123.29	120.30
21	AA	563	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1170	A	C4-C5-C6	-5.98	114.01	117.00
48	BZ	30	ARG	NE-CZ-NH2	5.98	123.29	120.30
54	BA	55	G	N1-C6-O6	-5.98	116.31	119.90
54	BA	1150	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	1123	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	2032	G	O4'-C1'-N9	5.98	112.98	108.20
54	BA	2295	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	972	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	1433	A	C4-C5-C6	-5.98	114.01	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1802	A	C5-C6-N1	5.98	120.69	117.70
54	BA	2263	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	2317	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1274	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1804	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	36	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2465	C	O4'-C1'-N1	5.97	112.98	108.20
21	AA	1149	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1917	U	O4'-C1'-N1	5.97	112.98	108.20
54	BA	2615	U	N3-C2-O2	-5.97	118.02	122.20
21	AA	664	G	N3-C2-N2	-5.97	115.72	119.90
54	BA	844	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	946	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	657	U	O4'-C1'-N1	5.97	112.98	108.20
54	BA	744	U	O4'-C1'-N1	5.97	112.97	108.20
54	BA	2359	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	267	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2428	G	P-O3'-C3'	5.97	126.86	119.70
21	AA	34	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	1129	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1365	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	477	C	N3-C2-O2	-5.96	117.72	121.90
21	AA	1038	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	1449	C	N3-C2-O2	-5.96	117.72	121.90
45	BW	10	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	361	G	O4'-C1'-N9	5.96	112.97	108.20
27	BE	67	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	195	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	888	C	N1-C2-O2	5.96	122.48	118.90
54	BA	2449	U	O4'-C1'-N1	5.96	112.97	108.20
21	AA	286	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	445	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1553	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2096	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	374	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	138	U	O4'-C1'-N1	5.96	112.97	108.20
54	BA	1315	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2498	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	184	C	O4'-C1'-N1	5.96	112.97	108.20
54	BA	451	U	C1'-O4'-C4'	-5.96	105.14	109.90
54	BA	1954	G	O4'-C4'-C3'	5.96	110.86	106.10
54	BA	2767	C	N1-C2-O2	5.96	122.47	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1179	A	C5-C6-N1	5.95	120.68	117.70
22	A1	29	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	1142	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	1967	C	O4'-C1'-N1	5.95	112.96	108.20
54	BA	2602	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	2740	A	O4'-C4'-C3'	-5.95	98.05	104.00
54	BA	2840	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	892	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	1038	G	C5'-C4'-C3'	-5.95	106.48	116.00
54	BA	2830	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	199	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	345	C	N1-C2-O2	5.95	122.47	118.90
21	AA	1428	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	754	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	928	A	C5-C6-N1	5.95	120.67	117.70
54	BA	1236	G	N3-C2-N2	-5.95	115.74	119.90
54	BA	2883	A	C4-C5-C6	-5.95	114.03	117.00
27	BE	88	ARG	NE-CZ-NH1	5.95	123.27	120.30
54	BA	1151	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	356	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	1328	C	N1-C2-O2	5.95	122.47	118.90
54	BA	1297	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1344	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	2206	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	2381	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1655	A	N1-C6-N6	-5.94	115.03	118.60
54	BA	2540	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	1014	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	584	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	905	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2091	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2512	C	O4'-C1'-N1	5.94	112.95	108.20
54	BA	2799	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2874	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	510	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	1380	U	C1'-O4'-C4'	-5.94	105.15	109.90
54	BA	528	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1584	U	N3-C2-O2	-5.94	118.04	122.20
54	BA	2889	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	1265	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1064	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2651	C	N3-C2-O2	-5.94	117.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	994	A	C4-C5-C6	-5.93	114.03	117.00
23	A2	80	C	N3-C4-C5	5.93	124.27	121.90
24	A3	57	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	644	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1289	C	N1-C2-O2	5.93	122.46	118.90
54	BA	2148	G	O4'-C1'-N9	5.93	112.95	108.20
32	BJ	116	ARG	NE-CZ-NH1	5.93	123.27	120.30
54	BA	1986	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	2250	G	N1-C6-O6	-5.93	116.34	119.90
21	AA	839	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	422	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1489	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	2514	U	O4'-C1'-N1	5.93	112.94	108.20
21	AA	868	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1484	C	N1-C2-O2	5.93	122.46	118.90
21	AA	44	A	C5-C6-N1	5.93	120.66	117.70
21	AA	174	A	C4-C5-C6	-5.93	114.04	117.00
21	AA	1452	C	N3-C2-O2	-5.93	117.75	121.90
55	BB	118	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	1762	A	C4-C5-C6	-5.93	114.04	117.00
54	BA	2317	A	C5-C6-N1	5.93	120.66	117.70
21	AA	1460	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	845	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	957	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1350	C	O4'-C1'-N1	5.92	112.94	108.20
54	BA	1477	A	N1-C6-N6	-5.92	115.05	118.60
54	BA	1843	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	2196	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	2338	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	2824	C	O4'-C1'-N1	5.92	112.94	108.20
21	AA	246	A	C5-C6-N1	5.92	120.66	117.70
54	BA	706	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1028	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1431	A	C4-C5-C6	-5.92	114.04	117.00
55	BB	45	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	470	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	172	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	971	G	C4'-C3'-C2'	-5.92	96.68	102.60
54	BA	2662	A	C5-C6-N1	5.92	120.66	117.70
54	BA	2817	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	421	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	2238	G	N3-C4-C5	-5.92	125.64	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	101	A	C5-C6-N1	5.92	120.66	117.70
21	AA	787	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	885	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	1654	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2739	U	N3-C2-O2	-5.92	118.06	122.20
21	AA	236	A	C5-C6-N1	5.92	120.66	117.70
54	BA	752	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	269	C	O4'-C1'-N1	5.92	112.93	108.20
54	BA	348	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1314	C	N3-C4-C5	5.92	124.27	121.90
54	BA	1812	U	O4'-C1'-N1	5.92	112.93	108.20
54	BA	2160	C	O4'-C1'-N1	5.92	112.93	108.20
54	BA	2655	G	N1-C6-O6	-5.92	116.35	119.90
9	AJ	7	ARG	NE-CZ-NH1	5.91	123.26	120.30
21	AA	813	U	O4'-C1'-N1	5.91	112.93	108.20
21	AA	879	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1061	U	O4'-C1'-N1	5.91	112.93	108.20
54	BA	1599	U	C1'-O4'-C4'	-5.91	105.17	109.90
54	BA	2574	G	N1-C6-O6	-5.91	116.35	119.90
54	BA	2703	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2749	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	1128	G	N1-C6-O6	-5.91	116.35	119.90
54	BA	1837	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	610	C	O4'-C1'-N1	5.91	112.93	108.20
54	BA	702	U	O4'-C1'-N1	5.91	112.93	108.20
21	AA	418	C	N3-C2-O2	-5.91	117.77	121.90
21	AA	883	C	N1-C2-O2	5.91	122.44	118.90
21	AA	1340	A	C5-C6-N1	5.91	120.65	117.70
54	BA	314	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	414	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	691	C	O4'-C1'-N1	5.91	112.93	108.20
54	BA	1954	G	C3'-C2'-C1'	5.91	106.23	101.50
21	AA	1320	C	N3-C2-O2	-5.91	117.77	121.90
21	AA	1388	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	1272	A	O4'-C1'-N9	5.91	112.93	108.20
12	AM	69	ARG	NE-CZ-NH1	5.91	123.25	120.30
22	A1	18	G	O4'-C1'-N9	5.91	112.92	108.20
22	A1	70	C	N1-C2-O2	5.91	122.44	118.90
54	BA	2422	C	O4'-C1'-N1	5.90	112.92	108.20
21	AA	253	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	396	C	N3-C2-O2	-5.90	117.77	121.90
38	BP	71	ARG	NE-CZ-NH1	5.90	123.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	403	C	O4'-C1'-N1	5.90	112.92	108.20
21	AA	782	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1053	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	2426	A	P-O3'-C3'	5.90	126.78	119.70
54	BA	587	C	N1-C2-O2	5.90	122.44	118.90
54	BA	2071	A	C4-C5-C6	-5.90	114.05	117.00
7	AH	76	ARG	NE-CZ-NH1	5.90	123.25	120.30
24	A3	66	C	N3-C2-O2	-5.90	117.77	121.90
2	AC	163	ARG	NE-CZ-NH2	-5.89	117.35	120.30
54	BA	418	C	N3-C2-O2	-5.89	117.77	121.90
54	BA	550	C	N3-C2-O2	-5.89	117.77	121.90
54	BA	1085	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	2044	C	N3-C2-O2	-5.89	117.77	121.90
54	BA	2760	C	N3-C2-O2	-5.89	117.77	121.90
55	BB	21	G	N1-C6-O6	-5.89	116.36	119.90
21	AA	1281	C	N1-C2-O2	5.89	122.44	118.90
54	BA	1286	A	N1-C6-N6	-5.89	115.06	118.60
54	BA	2380	C	N3-C2-O2	-5.89	117.78	121.90
24	A3	60	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	736	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	1204	A	C6-C5-N7	5.89	136.42	132.30
40	BR	80	ARG	NE-CZ-NH2	-5.89	117.36	120.30
54	BA	610	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	909	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	1656	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2471	A	O4'-C1'-N9	5.89	112.91	108.20
54	BA	2681	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2698	U	O4'-C1'-N1	5.89	112.91	108.20
21	AA	1094	G	O4'-C1'-N9	5.89	112.91	108.20
54	BA	964	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1395	A	O4'-C1'-N9	5.89	112.91	108.20
54	BA	247	G	N1-C6-O6	-5.89	116.37	119.90
54	BA	386	G	O4'-C1'-N9	5.89	112.91	108.20
54	BA	846	U	C1'-O4'-C4'	-5.89	105.19	109.90
54	BA	1765	U	O4'-C1'-N1	5.89	112.91	108.20
54	BA	1969	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	116	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1786	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	147	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	732	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	963	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	1052	C	N1-C2-O2	5.88	122.43	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	341	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1447	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	1280	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	876	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	2553	G	O4'-C1'-N9	5.88	112.90	108.20
21	AA	493	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	635	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	919	A	O4'-C1'-N9	5.88	112.90	108.20
25	BC	269	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	91	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	549	G	O4'-C1'-N9	5.88	112.90	108.20
54	BA	867	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	1005	C	C3'-C2'-C1'	5.88	106.20	101.50
21	AA	156	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	2750	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	819	A	C1'-O4'-C4'	-5.87	105.20	109.90
21	AA	1027	C	N3-C2-O2	-5.87	117.79	121.90
24	A3	7	G	O4'-C1'-N9	5.87	112.90	108.20
54	BA	691	C	N3-C2-O2	-5.87	117.79	121.90
4	AE	149	PRO	C-N-CA	5.87	136.38	121.70
21	AA	25	C	N3-C2-O2	-5.87	117.79	121.90
29	BG	162	ARG	NE-CZ-NH2	-5.87	117.36	120.30
54	BA	1846	G	C3'-C2'-C1'	5.87	106.20	101.50
55	BB	88	C	N1-C2-O2	5.87	122.42	118.90
54	BA	318	C	N3-C2-O2	-5.87	117.79	121.90
9	AJ	37	ARG	NE-CZ-NH1	5.87	123.23	120.30
54	BA	2052	A	C4-C5-C6	-5.87	114.07	117.00
20	AU	16	ARG	NE-CZ-NH1	5.86	123.23	120.30
21	AA	966	G	C5-C6-N1	5.86	114.43	111.50
21	AA	1161	C	C1'-O4'-C4'	-5.86	105.21	109.90
21	AA	1367	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	32	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	829	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1241	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	430	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1537	G	C1'-O4'-C4'	-5.86	105.21	109.90
54	BA	1940	U	O4'-C1'-N1	5.86	112.89	108.20
21	AA	193	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1432	G	N1-C6-O6	-5.86	116.39	119.90
54	BA	1644	C	O4'-C1'-N1	5.86	112.89	108.20
21	AA	1177	G	N3-C2-N2	-5.86	115.80	119.90
54	BA	532	A	C4-C5-C6	-5.86	114.07	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2758	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1067	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1171	A	C5-C6-N1	5.86	120.63	117.70
55	BB	52	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1298	U	O4'-C1'-N1	5.85	112.88	108.20
21	AA	59	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	284	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	736	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	788	A	N1-C6-N6	-5.85	115.09	118.60
54	BA	1164	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	1446	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	105	C	N1-C2-O2	5.85	122.41	118.90
54	BA	264	C	N1-C2-O2	5.85	122.41	118.90
55	BB	48	U	O4'-C1'-N1	5.85	112.88	108.20
21	AA	600	A	C5-C6-N1	5.85	120.62	117.70
39	BQ	50	ARG	NE-CZ-NH1	5.85	123.22	120.30
54	BA	161	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1994	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	2434	A	C6-C5-N7	5.85	136.40	132.30
21	AA	483	C	N3-C2-O2	-5.85	117.81	121.90
22	A1	76	A	O4'-C1'-N9	5.85	112.88	108.20
54	BA	486	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	1755	A	C6-C5-N7	5.85	136.39	132.30
21	AA	948	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	503	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1150	C	O4'-C1'-N1	5.84	112.88	108.20
28	BF	79	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	AA	810	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	1161	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	2845	U	O4'-C1'-N1	5.84	112.87	108.20
22	A1	23	A	N1-C6-N6	-5.84	115.10	118.60
54	BA	413	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1240	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	1505	A	C4-C5-C6	-5.84	114.08	117.00
8	AI	17	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	AA	143	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1643	G	O4'-C1'-N9	5.84	112.87	108.20
21	AA	486	U	O4'-C1'-N1	5.83	112.87	108.20
36	BN	4	ARG	NE-CZ-NH1	5.83	123.22	120.30
54	BA	1579	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	1612	C	O4'-C1'-N1	5.83	112.87	108.20
22	A1	74	C	O4'-C1'-N1	5.83	112.87	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	241	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	772	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	912	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1111	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	1939	U	O4'-C1'-N1	5.83	112.87	108.20
54	BA	2443	C	N3-C2-O2	-5.83	117.82	121.90
55	BB	37	C	N3-C2-O2	-5.83	117.82	121.90
10	AK	68	ARG	NE-CZ-NH1	5.83	123.22	120.30
21	AA	251	G	N3-C4-C5	-5.83	125.68	128.60
54	BA	316	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	748	G	C1'-O4'-C4'	-5.83	105.23	109.90
21	AA	504	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1180	U	O4'-C1'-N1	5.83	112.86	108.20
21	AA	233	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2827	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	252	G	N1-C6-O6	-5.83	116.40	119.90
54	BA	2431	U	N3-C2-O2	-5.83	118.12	122.20
24	A3	70	C	N1-C2-O2	5.83	122.39	118.90
54	BA	93	G	N1-C6-O6	-5.83	116.41	119.90
54	BA	2094	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	2709	G	O4'-C1'-N9	5.83	112.86	108.20
54	BA	2887	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	2146	C	N3-C2-O2	-5.82	117.82	121.90
54	BA	1591	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	499	A	C6-C5-N7	5.82	136.38	132.30
54	BA	1691	C	N1-C2-O2	5.82	122.39	118.90
54	BA	2716	C	N3-C2-O2	-5.82	117.83	121.90
55	BB	4	C	N3-C2-O2	-5.82	117.83	121.90
44	BV	79	ARG	NE-CZ-NH1	5.82	123.21	120.30
54	BA	2145	C	N1-C2-O2	5.82	122.39	118.90
49	B0	16	ARG	NE-CZ-NH1	5.82	123.21	120.30
54	BA	897	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1312	U	P-O3'-C3'	5.82	126.68	119.70
54	BA	2888	C	O4'-C1'-N1	5.82	112.86	108.20
21	AA	72	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	267	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	295	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	249	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	698	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	898	C	N3-C2-O2	-5.82	117.83	121.90
27	BE	44	ARG	NE-CZ-NH1	5.81	123.21	120.30
54	BA	1796	U	N3-C2-O2	-5.81	118.13	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	57	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	345	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2287	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	765	G	N3-C4-C5	-5.81	125.69	128.60
21	AA	859	G	N1-C6-O6	-5.81	116.41	119.90
21	AA	940	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	1036	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2354	C	N3-C2-O2	-5.81	117.83	121.90
42	BT	69	ARG	NE-CZ-NH1	5.81	123.20	120.30
54	BA	775	G	O4'-C1'-N9	5.81	112.85	108.20
54	BA	1630	A	C6-C5-N7	5.81	136.37	132.30
55	BB	38	C	N3-C2-O2	-5.81	117.83	121.90
10	AK	97	ARG	NE-CZ-NH1	5.81	123.20	120.30
21	AA	55	A	C5-C6-N1	5.81	120.60	117.70
25	BC	261	ARG	NE-CZ-NH1	5.81	123.20	120.30
43	BU	21	ARG	NE-CZ-NH1	5.81	123.20	120.30
54	BA	633	A	O4'-C1'-N9	5.81	112.85	108.20
54	BA	692	C	N1-C2-O2	5.81	122.39	118.90
54	BA	1077	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	2875	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	730	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	866	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	206	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	939	G	O4'-C1'-N9	5.80	112.84	108.20
54	BA	1308	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	823	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	892	A	C5-C6-N1	5.80	120.60	117.70
54	BA	1617	C	N1-C2-O2	5.80	122.38	118.90
54	BA	1641	A	C5-C6-N1	5.80	120.60	117.70
54	BA	2278	A	C4-C5-C6	-5.80	114.10	117.00
8	AI	112	ARG	NE-CZ-NH1	5.80	123.20	120.30
21	AA	1119	C	N3-C2-O2	-5.80	117.84	121.90
22	A1	20	G	N3-C2-N2	-5.80	115.84	119.90
54	BA	477	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	876	C	O4'-C1'-N1	5.80	112.84	108.20
54	BA	984	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2066	C	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2073	C	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2313	C	N1-C2-O2	5.80	122.38	118.90
21	AA	217	C	N1-C2-O2	5.80	122.38	118.90
21	AA	488	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	1126	U	C3'-C2'-C1'	5.80	106.14	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	366	C	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2033	A	N1-C6-N6	-5.80	115.12	118.60
21	AA	1437	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	1745	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	2870	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	321	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1075	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2238	G	O4'-C1'-N9	5.79	112.83	108.20
54	BA	441	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	416	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1121	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1307	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2670	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	81	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2439	A	O4'-C1'-N9	5.79	112.83	108.20
54	BA	2503	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2704	C	O4'-C1'-N1	5.79	112.83	108.20
21	AA	234	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	968	A	O4'-C1'-N9	5.78	112.83	108.20
54	BA	1923	U	O4'-C1'-N1	5.78	112.83	108.20
21	AA	303	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1300	G	P-O3'-C3'	5.78	126.64	119.70
54	BA	1349	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2064	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2462	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2043	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	932	U	N3-C2-O2	-5.78	118.16	122.20
54	BA	2466	C	N3-C2-O2	-5.78	117.86	121.90
4	AE	19	ARG	NE-CZ-NH1	5.78	123.19	120.30
21	AA	135	C	N3-C2-O2	-5.78	117.86	121.90
21	AA	210	C	O4'-C4'-C3'	5.78	110.72	106.10
21	AA	223	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1411	C	N1-C2-O2	5.78	122.37	118.90
54	BA	820	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2425	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2732	G	N3-C4-C5	-5.78	125.71	128.60
54	BA	1668	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2512	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	2755	C	O4'-C1'-N1	5.78	112.82	108.20
54	BA	2765	A	O4'-C1'-N9	5.78	112.82	108.20
24	A3	35	C	N3-C4-N4	-5.77	113.96	118.00
54	BA	2347	C	N1-C2-O2	5.77	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AC	87	ARG	NE-CZ-NH1	5.77	123.18	120.30
21	AA	398	U	O4'-C1'-N1	5.77	112.82	108.20
21	AA	1409	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	2226	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	2282	G	N1-C6-O6	-5.77	116.44	119.90
54	BA	1076	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	2088	A	C4-C5-C6	-5.77	114.12	117.00
55	BB	59	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	1229	A	C5-C6-N1	5.76	120.58	117.70
44	BV	18	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	44	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1140	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	1340	U	N3-C2-O2	-5.76	118.16	122.20
54	BA	2339	C	O4'-C1'-N1	5.76	112.81	108.20
21	AA	520	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	624	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2538	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	32	A	N1-C6-N6	-5.76	115.14	118.60
21	AA	1422	G	O4'-C1'-N9	5.76	112.81	108.20
54	BA	2611	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	454	A	C5-C6-N1	5.76	120.58	117.70
54	BA	2319	G	O4'-C1'-N9	5.76	112.81	108.20
54	BA	765	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	1800	C	N1-C2-O2	5.76	122.36	118.90
54	BA	2534	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	758	C	N1-C2-O2	5.76	122.35	118.90
54	BA	1135	C	N1-C2-O2	5.76	122.35	118.90
54	BA	2739	U	O4'-C1'-N1	5.76	112.81	108.20
54	BA	28	A	C5-C6-N1	5.75	120.58	117.70
21	AA	715	A	C4-C5-C6	-5.75	114.12	117.00
36	BN	46	ARG	NE-CZ-NH1	5.75	123.18	120.30
54	BA	514	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	1686	C	N1-C2-O2	5.75	122.35	118.90
54	BA	1822	C	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2063	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	2205	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	687	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	1248	G	C3'-C2'-C1'	5.75	106.10	101.50
54	BA	1640	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2117	A	O4'-C1'-N9	5.75	112.80	108.20
21	AA	78	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	1951	U	O4'-C1'-N1	5.75	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2163	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2536	G	N1-C6-O6	-5.75	116.45	119.90
54	BA	1808	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	1919	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	2441	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2496	C	N3-C2-O2	-5.75	117.88	121.90
55	BB	93	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	1393	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	2696	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	1115	G	N3-C2-N2	-5.74	115.88	119.90
54	BA	2675	A	N1-C6-N6	-5.74	115.15	118.60
54	BA	959	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	726	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	845	A	C4-C5-C6	-5.74	114.13	117.00
27	BE	102	ARG	NE-CZ-NH1	5.74	123.17	120.30
54	BA	237	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	462	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	690	G	N1-C6-O6	-5.74	116.45	119.90
54	BA	2526	G	N1-C6-O6	-5.74	116.46	119.90
54	BA	2736	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	816	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	502	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	921	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1254	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	784	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2577	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	279	A	P-O3'-C3'	5.73	126.58	119.70
21	AA	1288	A	C4-C5-C6	-5.73	114.13	117.00
21	AA	86	G	O4'-C1'-N9	5.73	112.78	108.20
21	AA	366	A	C4-C5-C6	-5.73	114.13	117.00
22	A1	65	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2013	A	C4-C5-C6	-5.73	114.13	117.00
55	BB	12	C	N1-C2-O2	5.73	122.34	118.90
21	AA	16	A	C4-C5-C6	-5.73	114.13	117.00
21	AA	1278	G	N1-C6-O6	-5.73	116.46	119.90
54	BA	34	U	O4'-C1'-N1	5.73	112.78	108.20
54	BA	398	C	O4'-C1'-N1	5.73	112.78	108.20
54	BA	2591	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	335	C	N3-C2-O2	-5.73	117.89	121.90
22	A1	49	G	N1-C6-O6	-5.73	116.46	119.90
24	A3	3	C	N1-C2-O2	5.73	122.34	118.90
54	BA	475	C	O4'-C1'-N1	5.73	112.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1893	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	1145	A	C4-C5-C6	-5.73	114.14	117.00
21	AA	1507	A	C4-C5-C6	-5.73	114.14	117.00
43	BU	81	ARG	NE-CZ-NH2	-5.73	117.44	120.30
21	AA	1263	C	N3-C2-O2	-5.72	117.89	121.90
22	A1	26	A	C4-C5-C6	-5.72	114.14	117.00
23	A2	82	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2166	U	O4'-C1'-N1	5.72	112.78	108.20
54	BA	2433	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2647	U	O4'-C1'-N1	5.72	112.78	108.20
54	BA	2861	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	578	C	N1-C2-O2	5.72	122.33	118.90
54	BA	268	C	O4'-C1'-N1	5.72	112.78	108.20
54	BA	342	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	893	C	O4'-C1'-N1	5.72	112.78	108.20
54	BA	1161	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	817	C	N1-C2-O2	5.72	122.33	118.90
54	BA	203	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	758	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	796	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	1550	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	2315	G	O4'-C1'-N9	5.72	112.78	108.20
54	BA	428	A	C5-C6-N1	5.72	120.56	117.70
54	BA	103	A	C6-C5-N7	5.72	136.30	132.30
54	BA	545	U	O4'-C1'-N1	5.72	112.77	108.20
54	BA	752	A	O4'-C1'-N9	5.72	112.77	108.20
54	BA	872	U	O4'-C1'-N1	5.72	112.77	108.20
54	BA	1974	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	492	C	N3-C2-O2	-5.71	117.90	121.90
22	A1	16	C	O4'-C1'-N1	5.71	112.77	108.20
54	BA	835	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	1496	A	C5-C6-N1	5.71	120.56	117.70
54	BA	2054	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2197	U	O4'-C1'-N1	5.71	112.77	108.20
36	BN	90	ARG	NE-CZ-NH1	5.71	123.16	120.30
54	BA	130	C	N3-C4-N4	-5.71	114.00	118.00
54	BA	1397	U	O4'-C1'-N1	5.71	112.77	108.20
54	BA	1096	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1676	A	C4-C5-C6	-5.71	114.14	117.00
1	AB	112	ARG	NE-CZ-NH1	5.71	123.15	120.30
21	AA	402	G	O4'-C1'-N9	5.71	112.77	108.20
54	BA	1626	A	C4-C5-C6	-5.71	114.15	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1636	U	O4'-C1'-N1	5.71	112.77	108.20
54	BA	2152	G	O4'-C1'-N9	5.71	112.77	108.20
54	BA	2715	C	O4'-C1'-N1	5.71	112.77	108.20
54	BA	2899	A	C5-C6-N1	5.71	120.55	117.70
21	AA	478	A	N1-C6-N6	-5.71	115.18	118.60
21	AA	1259	C	N1-C2-O2	5.71	122.32	118.90
22	A1	28	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	507	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	2653	U	O4'-C1'-N1	5.71	112.77	108.20
21	AA	1042	A	C4-C5-C6	-5.70	114.15	117.00
45	BW	13	ARG	NE-CZ-NH1	5.70	123.15	120.30
54	BA	1254	A	C5-C6-N1	5.70	120.55	117.70
54	BA	2019	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	454	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1727	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	549	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	564	C	N1-C2-O2	5.70	122.32	118.90
21	AA	596	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2816	G	N1-C6-O6	-5.70	116.48	119.90
21	AA	1402	C	O4'-C1'-N1	5.70	112.76	108.20
21	AA	1466	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	2572	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2778	A	N1-C6-N6	-5.70	115.18	118.60
21	AA	1181	G	O4'-C1'-N9	5.70	112.76	108.20
54	BA	911	A	C4-C5-C6	-5.70	114.15	117.00
5	AF	44	ARG	NE-CZ-NH1	5.70	123.15	120.30
21	AA	116	A	N1-C6-N6	-5.70	115.18	118.60
21	AA	933	G	N1-C6-O6	-5.70	116.48	119.90
21	AA	1101	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	166	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1205	A	O4'-C1'-N9	5.70	112.76	108.20
21	AA	794	A	C6-C5-N7	5.69	136.29	132.30
54	BA	2300	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	35	G	N1-C6-O6	-5.69	116.48	119.90
21	AA	292	G	N1-C6-O6	-5.69	116.48	119.90
21	AA	1427	C	N3-C2-O2	-5.69	117.92	121.90
24	A3	67	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	49	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2606	C	N3-C4-C5	5.69	124.18	121.90
21	AA	321	A	C6-C5-N7	5.69	136.28	132.30
54	BA	429	A	C5-C6-N1	5.69	120.55	117.70
54	BA	581	C	N3-C2-O2	-5.69	117.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	873	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	2614	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2763	G	N3-C2-N2	-5.69	115.92	119.90
3	AD	183	ARG	NE-CZ-NH1	5.69	123.14	120.30
21	AA	153	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	1098	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1347	A	C4-C5-C6	-5.69	114.16	117.00
21	AA	1147	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	673	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	223	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	787	C	N3-C4-C5	5.69	124.17	121.90
54	BA	2368	C	N1-C2-O2	5.69	122.31	118.90
21	AA	329	A	C4-C5-C6	-5.68	114.16	117.00
46	BX	2	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	219	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1387	A	O4'-C1'-N9	5.68	112.75	108.20
54	BA	1387	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	2858	C	C3'-C2'-C1'	5.68	106.05	101.50
24	A3	1	C	N1-C2-O2	5.68	122.31	118.90
21	AA	314	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	1178	C	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1722	A	N1-C6-N6	-5.68	115.19	118.60
54	BA	2855	C	N3-C2-O2	-5.68	117.92	121.90
21	AA	770	C	N3-C2-O2	-5.68	117.92	121.90
21	AA	886	G	N3-C2-N2	-5.68	115.92	119.90
21	AA	1395	C	N1-C2-O2	5.68	122.31	118.90
54	BA	139	U	N3-C2-O2	-5.68	118.22	122.20
54	BA	305	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	612	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	1822	C	N3-C2-O2	-5.68	117.92	121.90
55	BB	39	A	C6-C5-N7	5.68	136.28	132.30
5	AF	86	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	226	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	482	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	440	C	C5'-C4'-O4'	5.68	115.91	109.10
21	AA	951	G	N3-C4-C5	-5.67	125.76	128.60
54	BA	1913	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1593	A	C5-C6-N1	5.67	120.54	117.70
21	AA	1225	A	C2-N3-C4	5.67	113.44	110.60
25	BC	181	ARG	NE-CZ-NH2	-5.67	117.47	120.30
38	BP	52	ARG	NE-CZ-NH1	5.67	123.14	120.30
54	BA	1427	A	C6-C5-N7	5.67	136.27	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	69	C	N3-C2-O2	-5.67	117.93	121.90
12	AM	106	ARG	NE-CZ-NH1	5.67	123.14	120.30
21	AA	109	A	P-O3'-C3'	5.67	126.50	119.70
24	A3	26	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	340	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	996	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	2772	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	12	U	O4'-C1'-N1	5.67	112.73	108.20
21	AA	694	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	783	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1357	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	650	C	N3-C4-N4	-5.66	114.03	118.00
54	BA	668	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	787	C	N1-C2-O2	5.66	122.30	118.90
21	AA	236	A	C4-C5-C6	-5.66	114.17	117.00
49	B0	51	ARG	NE-CZ-NH2	-5.66	117.47	120.30
21	AA	403	C	C1'-O4'-C4'	-5.66	105.37	109.90
21	AA	638	U	O4'-C1'-N1	5.66	112.73	108.20
21	AA	647	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1179	A	C4-C5-C6	-5.66	114.17	117.00
35	BM	18	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	819	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1328	A	C6-C5-N7	5.66	136.26	132.30
54	BA	1726	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	2610	C	N1-C2-O2	5.66	122.30	118.90
21	AA	880	C	O4'-C1'-N1	5.66	112.73	108.20
21	AA	1107	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1135	U	O4'-C1'-N1	5.66	112.73	108.20
25	BC	176	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	2826	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	1397	C	N3-C4-N4	-5.66	114.04	118.00
21	AA	1229	A	C4-C5-C6	-5.66	114.17	117.00
26	BD	184	ARG	NE-CZ-NH1	5.66	123.13	120.30
55	BB	43	C	N3-C2-O2	-5.66	117.94	121.90
22	A1	59	U	N3-C2-O2	-5.65	118.24	122.20
54	BA	2606	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	648	A	C4-C5-C6	-5.65	114.17	117.00
25	BC	100	ARG	NE-CZ-NH1	5.65	123.13	120.30
33	BK	17	ARG	NE-CZ-NH1	5.65	123.13	120.30
54	BA	688	U	O4'-C1'-N1	5.65	112.72	108.20
2	AC	71	ARG	NE-CZ-NH1	5.65	123.12	120.30
7	AH	12	ARG	NE-CZ-NH1	5.65	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2009	A	C6-C5-N7	5.65	136.26	132.30
54	BA	540	C	N1-C2-O2	5.65	122.29	118.90
54	BA	1175	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	1137	C	N3-C2-O2	-5.65	117.95	121.90
21	AA	1275	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	683	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	2662	A	N1-C6-N6	-5.65	115.21	118.60
55	BB	110	C	N3-C2-O2	-5.65	117.95	121.90
21	AA	862	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	48	G	N1-C6-O6	-5.64	116.51	119.90
54	BA	663	G	C5-C6-N1	5.64	114.32	111.50
54	BA	2212	A	O4'-C1'-N9	5.64	112.72	108.20
21	AA	303	A	N1-C6-N6	-5.64	115.22	118.60
21	AA	451	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	1141	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	2097	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2132	U	N3-C2-O2	-5.64	118.25	122.20
54	BA	2310	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2521	C	N3-C2-O2	-5.64	117.95	121.90
55	BB	15	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	1225	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	896	C	N1-C2-O2	5.64	122.28	118.90
54	BA	432	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	1081	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	71	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2727	A	C6-C5-N7	5.64	136.25	132.30
21	AA	1020	G	N1-C6-O6	-5.64	116.52	119.90
24	A3	16	C	N1-C2-O2	5.64	122.28	118.90
54	BA	142	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1510	G	N1-C6-O6	-5.64	116.52	119.90
54	BA	2619	C	N3-C2-O2	-5.64	117.95	121.90
8	AI	121	ARG	NE-CZ-NH1	5.63	123.12	120.30
54	BA	785	G	N3-C2-N2	-5.63	115.95	119.90
54	BA	1981	A	C5-C6-N1	5.63	120.52	117.70
54	BA	2143	C	O4'-C1'-N1	5.63	112.71	108.20
21	AA	860	A	C4-C5-C6	-5.63	114.18	117.00
3	AD	69	ARG	NE-CZ-NH1	5.63	123.11	120.30
54	BA	1102	C	O4'-C1'-N1	5.63	112.71	108.20
54	BA	1129	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	2646	C	O4'-C1'-N1	5.63	112.70	108.20
21	AA	753	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1171	A	C4-C5-C6	-5.63	114.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	154	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	1382	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	1895	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	2247	A	O4'-C1'-N9	5.63	112.70	108.20
21	AA	320	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	397	A	C4-C5-C6	-5.63	114.19	117.00
52	B3	12	ARG	NE-CZ-NH1	5.63	123.11	120.30
21	AA	120	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	796	C	N1-C2-O2	5.62	122.28	118.90
54	BA	41	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	1121	C	O4'-C1'-N1	5.62	112.70	108.20
21	AA	495	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	522	C	O4'-C1'-N1	5.62	112.70	108.20
21	AA	623	C	N3-C2-O2	-5.62	117.96	121.90
21	AA	735	C	N1-C2-O2	5.62	122.27	118.90
54	BA	2451	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2834	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	478	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1451	U	N3-C2-O2	-5.62	118.27	122.20
54	BA	1126	A	P-O3'-C3'	5.62	126.44	119.70
41	BS	110	ARG	NE-CZ-NH2	5.62	123.11	120.30
21	AA	573	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1086	U	N3-C2-O2	-5.62	118.27	122.20
54	BA	1784	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1457	G	O4'-C1'-N9	5.62	112.69	108.20
34	BL	33	ARG	NE-CZ-NH1	5.62	123.11	120.30
54	BA	727	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	789	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1752	C	O4'-C1'-N1	5.62	112.69	108.20
21	AA	355	C	N1-C2-O2	5.61	122.27	118.90
21	AA	1317	C	N1-C2-O2	5.61	122.27	118.90
54	BA	515	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	1127	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	1194	A	O4'-C1'-N9	5.61	112.69	108.20
54	BA	1577	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1905	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	2562	U	O4'-C1'-N1	5.61	112.69	108.20
21	AA	773	G	O4'-C1'-N9	5.61	112.69	108.20
21	AA	610	U	N3-C2-O2	-5.61	118.27	122.20
21	AA	793	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2679	A	C5-C6-N1	5.61	120.50	117.70
21	AA	1279	G	N3-C4-C5	-5.61	125.80	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	93	G	O4'-C1'-N9	5.61	112.69	108.20
21	AA	1018	G	C1'-O4'-C4'	-5.61	105.42	109.90
48	BZ	44	ARG	NE-CZ-NH1	5.61	123.10	120.30
54	BA	162	U	N3-C2-O2	-5.61	118.28	122.20
54	BA	2119	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	532	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	805	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	2386	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	776	G	N3-C2-N2	-5.60	115.98	119.90
54	BA	2184	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	958	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1270	C	N1-C2-O2	5.60	122.26	118.90
54	BA	1332	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	1902	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2063	C	O4'-C1'-N1	5.60	112.68	108.20
21	AA	1284	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	190	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	436	C	N1-C2-O2	5.60	122.26	118.90
21	AA	471	U	O4'-C1'-N1	5.59	112.67	108.20
21	AA	857	C	N3-C2-O2	-5.59	117.98	121.90
45	BW	38	ARG	NE-CZ-NH2	-5.59	117.50	120.30
54	BA	1382	G	N3-C4-C5	-5.59	125.80	128.60
54	BA	1571	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	2051	A	C4-C5-C6	-5.59	114.20	117.00
55	BB	92	C	N3-C2-O2	-5.59	117.98	121.90
27	BE	49	ARG	NE-CZ-NH1	5.59	123.10	120.30
54	BA	324	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	386	G	P-O3'-C3'	5.59	126.41	119.70
54	BA	1901	A	C5-C6-N1	5.59	120.50	117.70
21	AA	920	U	N3-C2-O2	-5.59	118.28	122.20
21	AA	1018	G	O4'-C1'-N9	5.59	112.67	108.20
54	BA	461	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	1813	G	O4'-C1'-N9	5.59	112.67	108.20
54	BA	2129	C	N3-C2-O2	-5.59	117.98	121.90
21	AA	612	C	N3-C2-O2	-5.59	117.99	121.90
29	BG	34	ARG	NE-CZ-NH1	5.59	123.09	120.30
54	BA	205	G	N3-C4-C5	-5.59	125.81	128.60
54	BA	484	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2621	G	O4'-C1'-N9	5.59	112.67	108.20
54	BA	308	G	C3'-C2'-C1'	5.59	105.97	101.50
54	BA	1101	U	O4'-C1'-N1	5.59	112.67	108.20
21	AA	207	C	N3-C2-O2	-5.58	117.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	572	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2806	C	N1-C2-O2	5.58	122.25	118.90
54	BA	180	G	N1-C6-O6	-5.58	116.55	119.90
54	BA	310	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	522	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1207	C	O4'-C1'-N1	5.58	112.67	108.20
54	BA	2411	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2425	A	P-O3'-C3'	5.58	126.40	119.70
54	BA	2717	C	N1-C2-O2	5.58	122.25	118.90
54	BA	1529	G	N3-C2-N2	-5.58	115.99	119.90
54	BA	1548	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1896	G	N1-C6-O6	-5.58	116.55	119.90
54	BA	2419	U	C1'-O4'-C4'	-5.58	105.44	109.90
54	BA	2723	C	N1-C2-O2	5.58	122.25	118.90
21	AA	1434	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	523	C	N1-C2-O2	5.58	122.25	118.90
6	AG	52	ARG	NE-CZ-NH2	-5.58	117.51	120.30
21	AA	400	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	402	A	N1-C6-N6	-5.57	115.26	118.60
54	BA	554	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	2556	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	2809	A	C4-C5-C6	-5.57	114.21	117.00
2	AC	178	ARG	NE-CZ-NH1	5.57	123.09	120.30
24	A3	38	A	C4-C5-C6	-5.57	114.21	117.00
22	A1	67	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	257	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	1045	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	1051	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1825	U	O4'-C1'-N1	5.57	112.66	108.20
55	BB	51	G	C3'-C2'-C1'	5.57	105.95	101.50
21	AA	70	U	N3-C2-O2	-5.57	118.30	122.20
21	AA	724	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	680	C	C5'-C4'-O4'	5.57	115.78	109.10
54	BA	851	C	N1-C2-O2	5.57	122.24	118.90
54	BA	1832	C	O4'-C1'-N1	5.57	112.65	108.20
54	BA	2469	A	C4-C5-C6	-5.57	114.22	117.00
55	BB	36	C	N1-C2-O2	5.57	122.24	118.90
51	B2	34	ARG	NE-CZ-NH2	-5.57	117.52	120.30
54	BA	69	C	O4'-C1'-N1	5.57	112.65	108.20
54	BA	1538	G	O4'-C1'-N9	5.57	112.65	108.20
54	BA	2003	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	706	A	C4-C5-C6	-5.56	114.22	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1018	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	1067	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1792	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	2077	A	C4-C5-C6	-5.56	114.22	117.00
55	BB	17	C	N3-C2-O2	-5.56	118.01	121.90
21	AA	1344	C	N3-C2-O2	-5.56	118.01	121.90
24	A3	30	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	480	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	873	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1114	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1789	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	223	A	C5-C6-N1	5.56	120.48	117.70
54	BA	1267	U	O4'-C1'-N1	5.56	112.65	108.20
54	BA	1921	G	N1-C6-O6	-5.56	116.56	119.90
21	AA	641	U	N3-C2-O2	-5.56	118.31	122.20
54	BA	1080	A	C5-C6-N1	5.56	120.48	117.70
54	BA	2052	A	N1-C6-N6	-5.56	115.27	118.60
54	BA	546	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	557	C	N1-C2-O2	5.55	122.23	118.90
54	BA	871	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1590	A	C6-C5-N7	5.55	136.19	132.30
54	BA	2624	G	N3-C2-N2	-5.55	116.01	119.90
21	AA	1363	A	C4-C5-C6	-5.55	114.22	117.00
31	BI	102	ARG	NE-CZ-NH1	5.55	123.08	120.30
54	BA	192	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1010	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1066	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1367	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1419	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1667	G	N1-C6-O6	-5.55	116.57	119.90
55	BB	37	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	439	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1604	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	2313	C	N3-C4-N4	-5.55	114.11	118.00
54	BA	2606	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1551	A	C4-C5-C6	-5.55	114.23	117.00
55	BB	73	A	C4-C5-C6	-5.55	114.23	117.00
21	AA	31	G	O4'-C1'-N9	5.55	112.64	108.20
21	AA	342	C	N3-C2-O2	-5.55	118.02	121.90
21	AA	518	C	N1-C2-O2	5.55	122.23	118.90
21	AA	576	C	N1-C2-O2	5.55	122.23	118.90
21	AA	651	C	N3-C2-O2	-5.55	118.02	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1936	A	P-O3'-C3'	5.55	126.36	119.70
54	BA	417	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	1987	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	756	C	N1-C2-O2	5.54	122.23	118.90
54	BA	31	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1615	C	O4'-C1'-N1	5.54	112.64	108.20
54	BA	2135	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2346	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	724	U	C1'-O4'-C4'	-5.54	105.47	109.90
54	BA	1408	G	C5-C6-N1	5.54	114.27	111.50
54	BA	13	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2740	A	C5-C6-N1	5.54	120.47	117.70
21	AA	253	A	C5-C6-N1	5.54	120.47	117.70
54	BA	106	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	407	G	N1-C6-O6	-5.54	116.58	119.90
54	BA	1316	U	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1893	C	N1-C2-O2	5.54	122.22	118.90
22	A1	61	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	47	C	N1-C2-O2	5.54	122.22	118.90
55	BB	77	U	O4'-C1'-N1	5.54	112.63	108.20
11	AL	35	ARG	NH1-CZ-NH2	-5.53	113.31	119.40
21	AA	456	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	669	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	1477	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1609	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1702	G	O4'-C1'-N9	5.53	112.63	108.20
54	BA	1934	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2483	C	N1-C2-O2	5.53	122.22	118.90
54	BA	776	G	N3-C4-C5	-5.53	125.83	128.60
54	BA	1742	U	O4'-C1'-N1	5.53	112.62	108.20
21	AA	490	C	N1-C2-O2	5.53	122.22	118.90
21	AA	1408	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	1486	G	N3-C2-N2	-5.53	116.03	119.90
43	BU	21	ARG	NE-CZ-NH2	-5.53	117.53	120.30
54	BA	372	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	786	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	1082	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	749	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	547	A	C1'-O4'-C4'	-5.53	105.48	109.90
54	BA	2072	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	2468	A	O4'-C1'-N9	5.53	112.62	108.20
21	AA	1289	A	C4-C5-C6	-5.53	114.24	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	253	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	435	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	886	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	1331	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	1378	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	1942	C	N1-C2-O2	5.52	122.21	118.90
54	BA	2601	C	N1-C2-O2	5.52	122.22	118.90
21	AA	108	G	N3-C4-C5	-5.52	125.84	128.60
21	AA	1241	G	C5-C6-N1	5.52	114.26	111.50
54	BA	20	C	N1-C2-O2	5.52	122.21	118.90
54	BA	1095	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2303	G	N1-C6-O6	-5.52	116.59	119.90
54	BA	2374	C	N1-C2-O2	5.52	122.21	118.90
21	AA	546	A	C1'-O4'-C4'	-5.52	105.48	109.90
54	BA	395	U	O4'-C1'-N1	5.52	112.62	108.20
54	BA	2072	C	N1-C2-O2	5.52	122.21	118.90
54	BA	2496	C	N3-C4-C5	5.52	124.11	121.90
20	AU	44	ARG	NE-CZ-NH2	5.52	123.06	120.30
21	AA	579	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	629	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	792	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	1385	G	N1-C6-O6	-5.52	116.59	119.90
54	BA	251	A	C4'-C3'-C2'	-5.52	97.08	102.60
54	BA	402	A	C5-C6-N1	5.52	120.46	117.70
54	BA	2047	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	2280	G	N1-C6-O6	-5.52	116.59	119.90
21	AA	406	G	N1-C6-O6	-5.52	116.59	119.90
21	AA	1283	U	C5-C6-N1	-5.52	119.94	122.70
54	BA	505	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1406	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	1715	G	O4'-C1'-N9	5.52	112.61	108.20
54	BA	1720	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	2730	C	O4'-C1'-N1	5.52	112.61	108.20
21	AA	1342	C	N3-C4-N4	-5.52	114.14	118.00
42	BT	3	ARG	NE-CZ-NH1	5.52	123.06	120.30
54	BA	990	A	C4-C5-C6	-5.52	114.24	117.00
55	BB	58	A	C4-C5-C6	-5.52	114.24	117.00
55	BB	114	C	N1-C2-O2	5.52	122.21	118.90
2	AC	106	ARG	NE-CZ-NH1	5.51	123.06	120.30
21	AA	823	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	299	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	2339	C	N3-C2-O2	-5.51	118.04	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	8	C	N1-C2-O2	5.51	122.21	118.90
54	BA	127	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	901	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	1362	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	1337	G	C5'-C4'-C3'	-5.51	107.18	116.00
54	BA	1434	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	1641	A	C4-C5-C6	-5.51	114.24	117.00
21	AA	502	A	O4'-C1'-N9	5.51	112.61	108.20
21	AA	1167	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	234	U	N1-C2-N3	5.51	118.21	114.90
21	AA	16	A	C3'-C2'-C1'	5.51	105.91	101.50
21	AA	780	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	167	A	C5-C6-N1	5.51	120.45	117.70
21	AA	235	C	N3-C2-O2	-5.51	118.05	121.90
21	AA	341	C	N3-C2-O2	-5.51	118.05	121.90
21	AA	643	C	N1-C2-O2	5.51	122.20	118.90
21	AA	843	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	1728	C	O4'-C1'-N1	5.51	112.61	108.20
54	BA	447	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	60	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1890	A	C6-C5-N7	5.50	136.15	132.30
54	BA	1957	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	1063	C	N1-C2-O2	5.50	122.20	118.90
54	BA	587	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1112	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	2596	U	N3-C2-O2	-5.50	118.35	122.20
54	BA	2793	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1928	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	931	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	634	C	N1-C2-O2	5.50	122.20	118.90
54	BA	1605	C	N1-C2-O2	5.50	122.20	118.90
54	BA	2666	C	C5'-C4'-O4'	5.50	115.70	109.10
54	BA	2669	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	884	U	N3-C2-O2	-5.50	118.35	122.20
21	AA	1128	C	N1-C2-O2	5.50	122.20	118.90
54	BA	122	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	791	C	N3-C4-N4	-5.50	114.15	118.00
54	BA	899	A	C4-C5-C6	-5.50	114.25	117.00
24	A3	24	C	N1-C2-O2	5.50	122.20	118.90
54	BA	1741	C	N1-C2-O2	5.50	122.20	118.90
21	AA	80	A	C4-C5-C6	-5.49	114.25	117.00
21	AA	1433	A	C4-C5-C6	-5.49	114.25	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1706	C	N1-C2-O2	5.49	122.20	118.90
21	AA	1093	A	C1'-O4'-C4'	-5.49	105.51	109.90
54	BA	181	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	2695	U	O4'-C1'-N1	5.49	112.59	108.20
21	AA	949	A	C6-C5-N7	5.49	136.14	132.30
54	BA	1735	A	C4-C5-C6	-5.49	114.25	117.00
20	AU	17	ARG	NE-CZ-NH1	5.49	123.04	120.30
21	AA	574	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	243	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	1866	A	O4'-C1'-N9	5.49	112.59	108.20
54	BA	2108	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	1268	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	1494	A	C4-C5-C6	-5.49	114.26	117.00
21	AA	98	A	C6-C5-N7	5.49	136.14	132.30
21	AA	162	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	284	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	209	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	2412	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	569	C	N3-C2-O2	-5.48	118.06	121.90
32	BJ	13	ARG	NE-CZ-NH1	5.48	123.04	120.30
54	BA	383	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	1502	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2787	C	N3-C2-O2	-5.48	118.06	121.90
55	BB	71	C	C5'-C4'-O4'	5.48	115.68	109.10
21	AA	336	A	C6-C5-N7	5.48	136.14	132.30
21	AA	814	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	1349	A	N1-C6-N6	-5.48	115.31	118.60
54	BA	354	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2805	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	1474	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2465	C	N3-C2-O2	-5.48	118.06	121.90
8	AI	118	ARG	NE-CZ-NH1	5.48	123.04	120.30
33	BK	18	ARG	NE-CZ-NH1	5.48	123.04	120.30
54	BA	834	G	O4'-C1'-N9	5.48	112.58	108.20
54	BA	1442	U	O4'-C1'-N1	5.48	112.58	108.20
21	AA	44	A	C4-C5-C6	-5.48	114.26	117.00
22	A1	30	C	N3-C2-O2	-5.48	118.07	121.90
54	BA	960	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2283	C	N1-C2-O2	5.48	122.19	118.90
13	AN	63	ARG	NE-CZ-NH1	5.47	123.04	120.30
21	AA	238	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	1224	U	N3-C2-O2	-5.47	118.37	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BN	2	ARG	NE-CZ-NH1	5.47	123.04	120.30
54	BA	723	C	N1-C2-O2	5.47	122.19	118.90
54	BA	817	C	N1-C2-O2	5.47	122.19	118.90
54	BA	1428	C	N3-C4-C5	5.47	124.09	121.90
21	AA	465	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	1102	A	N1-C6-N6	-5.47	115.32	118.60
54	BA	128	C	N1-C2-O2	5.47	122.18	118.90
54	BA	555	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	715	A	C4-C5-C6	-5.47	114.26	117.00
54	BA	1295	C	C4'-C3'-C2'	-5.47	97.13	102.60
54	BA	1576	U	O4'-C1'-N1	5.47	112.58	108.20
9	AJ	31	ARG	NE-CZ-NH1	5.47	123.04	120.30
21	AA	229	U	N3-C2-O2	-5.47	118.37	122.20
54	BA	119	A	O4'-C1'-N9	5.47	112.58	108.20
55	BB	17	C	O4'-C1'-N1	5.47	112.58	108.20
21	AA	353	A	C4-C5-C6	-5.47	114.27	117.00
21	AA	841	C	C1'-O4'-C4'	-5.47	105.52	109.90
21	AA	1071	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	1438	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	565	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	705	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	2665	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	1476	U	C1'-O4'-C4'	-5.47	105.53	109.90
54	BA	639	U	O4'-C1'-N1	5.47	112.57	108.20
14	AO	52	ARG	NE-CZ-NH1	5.46	123.03	120.30
21	AA	1032	G	O4'-C1'-N9	5.46	112.57	108.20
21	AA	1441	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	278	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	866	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1874	C	N1-C2-O2	5.46	122.18	118.90
54	BA	2516	A	C6-C5-N7	5.46	136.13	132.30
54	BA	149	A	C6-C5-N7	5.46	136.12	132.30
54	BA	1172	C	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1392	A	C6-C5-N7	5.46	136.12	132.30
21	AA	131	A	C1'-O4'-C4'	-5.46	105.53	109.90
22	A1	31	C	N1-C2-O2	5.46	122.17	118.90
54	BA	1700	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2267	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	663	A	N1-C6-N6	-5.46	115.33	118.60
40	BR	84	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	983	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1100	C	O4'-C1'-N1	5.46	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1863	G	N1-C6-O6	-5.46	116.63	119.90
54	BA	1838	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	2760	C	O4'-C1'-N1	5.46	112.56	108.20
54	BA	2430	A	C6-N1-C2	-5.45	115.33	118.60
21	AA	998	C	N1-C2-O2	5.45	122.17	118.90
21	AA	1356	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	85	G	O4'-C1'-N9	5.45	112.56	108.20
54	BA	1877	A	C4-C5-C6	-5.45	114.28	117.00
3	AD	43	ARG	NE-CZ-NH1	5.45	123.02	120.30
21	AA	525	C	N3-C2-O2	-5.45	118.09	121.90
48	BZ	15	ARG	NE-CZ-NH2	-5.45	117.58	120.30
54	BA	149	A	C5'-C4'-O4'	5.45	115.64	109.10
54	BA	889	C	N1-C2-O2	5.45	122.17	118.90
54	BA	1526	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	1695	G	N3-C4-C5	-5.45	125.88	128.60
54	BA	2198	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2896	C	O4'-C1'-N1	5.45	112.56	108.20
55	BB	54	G	O4'-C1'-N9	5.45	112.56	108.20
54	BA	145	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	182	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	346	G	N3-C4-C5	-5.45	125.88	128.60
54	BA	1476	U	N3-C2-O2	-5.45	118.39	122.20
54	BA	1990	C	N1-C2-O2	5.44	122.17	118.90
54	BA	2165	C	N3-C2-O2	-5.44	118.09	121.90
21	AA	1059	C	N1-C2-O2	5.44	122.17	118.90
46	BX	56	ARG	NE-CZ-NH2	-5.44	117.58	120.30
54	BA	896	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1288	G	O4'-C1'-N9	5.44	112.55	108.20
54	BA	1894	C	N1-C2-O2	5.44	122.17	118.90
21	AA	1066	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	2767	C	N3-C4-C5	5.44	124.08	121.90
54	BA	1290	C	N3-C2-O2	-5.44	118.09	121.90
55	BB	101	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	94	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1167	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	1761	C	N1-C2-O2	5.44	122.16	118.90
54	BA	2160	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	259	G	O4'-C1'-N9	5.43	112.55	108.20
54	BA	1286	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	1731	G	N3-C4-C5	-5.43	125.88	128.60
9	AJ	45	ARG	NE-CZ-NH1	5.43	123.02	120.30
21	AA	1303	C	N1-C2-O2	5.43	122.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	60	G	O4'-C1'-N9	5.43	112.55	108.20
54	BA	1933	G	N3-C4-C5	-5.43	125.89	128.60
21	AA	653	U	C3'-C2'-C1'	5.43	105.84	101.50
21	AA	749	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	106	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	1050	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	1311	A	C6-C5-N7	5.43	136.10	132.30
54	BA	371	A	O4'-C1'-N9	5.43	112.54	108.20
55	BB	111	U	P-O3'-C3'	5.43	126.21	119.70
10	AK	52	ARG	NE-CZ-NH1	5.43	123.01	120.30
21	AA	173	U	N3-C2-O2	-5.43	118.40	122.20
54	BA	458	G	C5-C6-N1	5.43	114.21	111.50
54	BA	590	A	C1'-O4'-C4'	-5.43	105.56	109.90
21	AA	777	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1188	A	O4'-C1'-N9	5.42	112.54	108.20
54	BA	97	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	2062	A	O4'-C1'-N9	5.42	112.54	108.20
54	BA	2499	C	C5'-C4'-O4'	5.42	115.61	109.10
45	BW	24	ARG	NE-CZ-NH2	-5.42	117.59	120.30
54	BA	269	C	N1-C2-O2	5.42	122.15	118.90
54	BA	496	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	927	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	6	G	N3-C4-C5	-5.42	125.89	128.60
21	AA	116	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	625	U	N3-C2-O2	-5.42	118.41	122.20
21	AA	1299	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	37	C	N1-C2-O2	5.42	122.15	118.90
54	BA	331	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	745	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	1746	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2261	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	2708	G	N1-C6-O6	-5.42	116.65	119.90
55	BB	3	C	N1-C2-O2	5.42	122.15	118.90
21	AA	517	G	O4'-C1'-N9	5.42	112.54	108.20
21	AA	973	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	650	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	1918	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2023	C	N1-C2-O2	5.42	122.15	118.90
21	AA	26	A	C4-C5-C6	-5.42	114.29	117.00
36	BN	64	ARG	NE-CZ-NH1	5.42	123.01	120.30
54	BA	138	U	N1-C2-N3	5.42	118.15	114.90
54	BA	216	A	C4-C5-C6	-5.42	114.29	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1253	A	C5'-C4'-O4'	5.42	115.60	109.10
3	AD	55	ARG	NE-CZ-NH1	5.42	123.01	120.30
22	A1	76	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	198	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	460	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1057	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1302	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1681	G	O4'-C1'-N9	5.42	112.53	108.20
54	BA	1937	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2322	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1637	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	2559	C	O4'-C1'-N1	5.41	112.53	108.20
21	AA	160	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	560	C	N1-C2-O2	5.41	122.15	118.90
54	BA	979	A	C6-C5-N7	5.41	136.09	132.30
54	BA	1207	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	1359	A	C4-C5-C6	-5.41	114.29	117.00
21	AA	221	C	N1-C2-O2	5.41	122.15	118.90
21	AA	660	C	N1-C2-O2	5.41	122.15	118.90
21	AA	1096	C	N1-C2-O2	5.41	122.15	118.90
54	BA	337	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	465	G	N1-C6-O6	-5.41	116.65	119.90
54	BA	1252	G	N1-C6-O6	-5.41	116.65	119.90
54	BA	1414	C	N1-C2-O2	5.41	122.15	118.90
55	BB	81	G	N1-C6-O6	-5.41	116.65	119.90
21	AA	1282	C	N1-C2-O2	5.41	122.14	118.90
22	A1	26	A	N1-C6-N6	-5.41	115.35	118.60
54	BA	2900	A	C4-C5-C6	-5.41	114.30	117.00
4	AE	137	ARG	NE-CZ-NH1	5.41	123.00	120.30
54	BA	127	A	O4'-C4'-C3'	5.41	110.43	106.10
13	AN	53	ARG	NE-CZ-NH1	5.41	123.00	120.30
54	BA	968	C	N1-C2-O2	5.41	122.14	118.90
54	BA	2050	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	632	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1558	C	N1-C2-O2	5.40	122.14	118.90
54	BA	2777	G	N3-C4-C5	-5.40	125.90	128.60
21	AA	24	U	O4'-C1'-N1	5.40	112.52	108.20
21	AA	454	G	N7-C8-N9	5.40	115.80	113.10
21	AA	1417	G	C5-C6-N1	5.40	114.20	111.50
54	BA	6	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	214	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	1163	G	N1-C6-O6	-5.40	116.66	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1739	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1985	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2633	G	O4'-C1'-N9	5.40	112.52	108.20
21	AA	1065	U	N3-C2-O2	-5.40	118.42	122.20
21	AA	1473	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	269	C	C5'-C4'-O4'	5.40	115.58	109.10
54	BA	391	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1134	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	784	G	N3-C4-C5	-5.40	125.90	128.60
54	BA	2888	C	N3-C4-C5	5.40	124.06	121.90
21	AA	55	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	1487	G	O4'-C1'-N9	5.40	112.52	108.20
54	BA	944	C	C5'-C4'-O4'	5.40	115.58	109.10
54	BA	1285	A	C6-C5-N7	5.40	136.08	132.30
54	BA	1439	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2024	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	2513	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	199	A	C6-C5-N7	5.40	136.08	132.30
54	BA	229	C	N1-C2-O2	5.40	122.14	118.90
54	BA	1791	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2833	U	N3-C2-O2	-5.40	118.42	122.20
21	AA	501	C	N1-C2-O2	5.39	122.14	118.90
21	AA	1010	U	O4'-C1'-N1	5.39	112.52	108.20
21	AA	1196	A	C1'-O4'-C4'	-5.39	105.58	109.90
54	BA	1496	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	2087	G	N1-C6-O6	-5.39	116.66	119.90
55	BB	65	U	O4'-C1'-N1	5.39	112.52	108.20
22	A1	73	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	721	A	C6-C5-N7	5.39	136.07	132.30
54	BA	2018	G	O4'-C1'-N9	5.39	112.51	108.20
54	BA	2375	G	O4'-C1'-N9	5.39	112.52	108.20
22	A1	13	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	2746	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	84	A	O4'-C1'-N9	5.39	112.51	108.20
54	BA	152	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	2066	C	N3-C2-O2	-5.39	118.13	121.90
21	AA	344	A	C4-C5-C6	-5.39	114.31	117.00
21	AA	665	A	C6-C5-N7	5.39	136.07	132.30
55	BB	22	U	O4'-C1'-N1	5.39	112.51	108.20
21	AA	395	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	107	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	1446	C	O4'-C1'-N1	5.39	112.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1794	A	C4-C5-C6	-5.39	114.31	117.00
21	AA	513	C	N1-C2-O2	5.38	122.13	118.90
21	AA	722	G	N1-C6-O6	-5.38	116.67	119.90
46	BX	17	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BA	2407	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	640	A	C4-C5-C6	-5.38	114.31	117.00
16	AQ	26	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BA	1498	C	N1-C2-O2	5.38	122.13	118.90
54	BA	1616	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1676	A	N1-C6-N6	-5.38	115.37	118.60
54	BA	2470	G	N3-C2-N2	-5.38	116.13	119.90
21	AA	196	A	C6-C5-N7	5.38	136.07	132.30
24	A3	9	G	C3'-C2'-C1'	5.38	105.80	101.50
54	BA	2354	C	O4'-C1'-N1	5.38	112.50	108.20
13	AN	81	ARG	NE-CZ-NH2	-5.38	117.61	120.30
21	AA	935	A	C6-C5-N7	5.38	136.06	132.30
21	AA	1324	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	1352	C	N1-C2-O2	5.38	122.13	118.90
54	BA	2539	C	O4'-C1'-N1	5.38	112.50	108.20
55	BB	97	C	O4'-C1'-N1	5.38	112.50	108.20
21	AA	1067	A	N1-C6-N6	-5.38	115.38	118.60
54	BA	621	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	954	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1013	C	O4'-C1'-N1	5.38	112.50	108.20
54	BA	2586	U	N3-C2-O2	-5.38	118.44	122.20
45	BW	38	ARG	NE-CZ-NH1	5.37	122.99	120.30
54	BA	2755	C	N1-C2-O2	5.37	122.12	118.90
54	BA	1709	U	O4'-C1'-N1	5.37	112.50	108.20
54	BA	2515	C	O4'-C1'-N1	5.37	112.50	108.20
21	AA	1290	G	N7-C8-N9	5.37	115.78	113.10
21	AA	1500	A	C6-C5-N7	5.37	136.06	132.30
54	BA	150	U	O4'-C1'-N1	5.37	112.49	108.20
22	A1	8	U	N3-C2-O2	-5.37	118.44	122.20
54	BA	1929	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	945	G	C5-C6-N1	5.37	114.18	111.50
24	A3	29	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	341	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	1211	C	N1-C2-O2	5.37	122.12	118.90
54	BA	1507	C	N1-C2-O2	5.37	122.12	118.90
54	BA	144	A	O4'-C1'-N9	5.36	112.49	108.20
54	BA	677	A	O4'-C1'-N9	5.36	112.49	108.20
54	BA	997	G	O4'-C1'-N9	5.36	112.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1719	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	2618	G	C5'-C4'-O4'	5.36	115.53	109.10
21	AA	443	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	1331	G	N1-C6-O6	-5.36	116.68	119.90
54	BA	240	C	N1-C2-O2	5.36	122.12	118.90
54	BA	972	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1565	C	O4'-C1'-N1	5.36	112.49	108.20
21	AA	1160	G	N3-C2-N2	-5.36	116.15	119.90
25	BC	216	ARG	NH1-CZ-NH2	-5.36	113.51	119.40
54	BA	2733	A	C4-C5-C6	-5.36	114.32	117.00
47	BY	47	ARG	NE-CZ-NH1	5.36	122.98	120.30
54	BA	383	C	O4'-C1'-N1	5.36	112.48	108.20
54	BA	958	U	C1'-O4'-C4'	-5.36	105.61	109.90
54	BA	1909	C	N1-C2-O2	5.36	122.11	118.90
54	BA	2109	U	O4'-C1'-N1	5.36	112.48	108.20
54	BA	2504	U	C3'-C2'-C1'	5.36	105.78	101.50
21	AA	1053	G	N1-C6-O6	-5.35	116.69	119.90
21	AA	234	C	O4'-C1'-N1	5.35	112.48	108.20
21	AA	620	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	451	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	608	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	1373	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	517	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	669	G	C3'-C2'-C1'	5.35	105.78	101.50
54	BA	2283	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2761	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	101	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	70	G	N7-C8-N9	5.35	115.78	113.10
54	BA	1940	U	N3-C2-O2	-5.35	118.45	122.20
21	AA	457	G	N1-C6-O6	-5.35	116.69	119.90
21	AA	589	U	O4'-C1'-N1	5.35	112.48	108.20
21	AA	939	G	C1'-O4'-C4'	-5.35	105.62	109.90
21	AA	1120	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	1993	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2654	A	O4'-C1'-N9	5.35	112.48	108.20
21	AA	954	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	854	C	N1-C2-O2	5.34	122.11	118.90
54	BA	1881	C	N1-C2-O2	5.34	122.11	118.90
54	BA	2340	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2489	U	N3-C2-O2	-5.34	118.46	122.20
54	BA	234	U	N3-C2-O2	-5.34	118.46	122.20
54	BA	907	G	N1-C6-O6	-5.34	116.69	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	315	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	2547	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	635	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1152	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1730	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1752	C	N3-C2-O2	-5.34	118.16	121.90
55	BB	71	C	N1-C2-O2	5.34	122.10	118.90
54	BA	405	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1173	U	O4'-C1'-N1	5.33	112.47	108.20
55	BB	47	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	483	A	C6-C5-N7	5.33	136.03	132.30
54	BA	528	A	O4'-C1'-N9	5.33	112.47	108.20
54	BA	1072	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	2458	G	N3-C4-C5	-5.33	125.93	128.60
54	BA	2519	U	O4'-C1'-N1	5.33	112.47	108.20
54	BA	2853	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	1127	G	C5-C6-N1	5.33	114.17	111.50
54	BA	1043	C	N1-C2-O2	5.33	122.10	118.90
54	BA	1367	A	O4'-C1'-N9	5.33	112.47	108.20
54	BA	2033	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	2463	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	337	C	C4'-C3'-C2'	-5.33	97.27	102.60
54	BA	818	G	P-O3'-C3'	5.33	126.10	119.70
54	BA	2421	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	1363	A	O4'-C1'-N9	5.33	112.46	108.20
22	A1	9	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	508	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	613	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	614	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	1850	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	2395	C	C4'-C3'-C2'	-5.33	97.27	102.60
55	BB	28	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	300	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	697	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	2133	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	717	U	O4'-C1'-N1	5.32	112.46	108.20
54	BA	922	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	952	G	N1-C6-O6	-5.32	116.70	119.90
54	BA	1565	C	N1-C2-O2	5.32	122.09	118.90
54	BA	2443	C	O4'-C1'-N1	5.32	112.46	108.20
55	BB	104	A	C4-C5-C6	-5.32	114.34	117.00
55	BB	111	U	O4'-C1'-N1	5.32	112.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	169	C	C1'-O4'-C4'	-5.32	105.64	109.90
21	AA	403	C	N1-C2-O2	5.32	122.09	118.90
21	AA	856	C	N1-C2-O2	5.32	122.09	118.90
54	BA	404	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	2073	C	N1-C2-O2	5.32	122.09	118.90
54	BA	2222	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	2542	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	2195	U	O4'-C1'-N1	5.32	112.45	108.20
8	AI	84	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
54	BA	479	A	C6-C5-N7	5.32	136.02	132.30
54	BA	643	A	C1'-O4'-C4'	-5.32	105.65	109.90
54	BA	99	U	N1-C2-O2	5.32	126.52	122.80
54	BA	274	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1703	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	2336	A	C6-C5-N7	5.32	136.02	132.30
21	AA	202	G	N1-C6-O6	-5.31	116.71	119.90
21	AA	358	U	O4'-C1'-N1	5.31	112.45	108.20
21	AA	830	G	N1-C6-O6	-5.31	116.71	119.90
21	AA	1244	G	C8-N9-C4	-5.31	104.27	106.40
44	BV	21	ARG	CD-NE-CZ	5.31	131.04	123.60
54	BA	985	C	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1239	G	O4'-C1'-N9	5.31	112.45	108.20
54	BA	1854	A	C6-C5-N7	5.31	136.02	132.30
54	BA	1887	C	N3-C2-O2	-5.31	118.18	121.90
36	BN	103	ARG	NE-CZ-NH1	5.31	122.95	120.30
55	BB	97	C	N1-C2-O2	5.31	122.08	118.90
21	AA	20	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1070	A	O4'-C1'-N9	5.31	112.45	108.20
54	BA	2558	C	N1-C2-O2	5.31	122.08	118.90
21	AA	1128	C	O4'-C1'-N1	5.31	112.44	108.20
21	AA	291	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	535	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	861	A	C6-C5-N7	5.30	136.01	132.30
54	BA	1138	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	1317	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	1633	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	1679	A	C6-C5-N7	5.30	136.01	132.30
54	BA	2113	U	C1'-O4'-C4'	-5.30	105.66	109.90
54	BA	2580	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	2628	C	C3'-C2'-C1'	5.30	105.74	101.50
54	BA	2689	U	N3-C2-O2	-5.30	118.49	122.20
55	BB	99	A	C4-C5-C6	-5.30	114.35	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	264	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	493	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	454	G	C5-C6-N1	5.30	114.15	111.50
21	AA	840	C	C3'-C2'-C1'	5.30	105.74	101.50
54	BA	584	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1972	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	2751	G	N3-C4-C5	-5.30	125.95	128.60
21	AA	561	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	841	C	N3-C2-O2	-5.30	118.19	121.90
21	AA	865	A	C6-C5-N7	5.30	136.01	132.30
54	BA	1688	U	N1-C2-N3	5.30	118.08	114.90
54	BA	2561	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	592	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	1803	A	C6-C5-N7	5.30	136.01	132.30
21	AA	67	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1376	C	O4'-C1'-N1	5.30	112.44	108.20
21	AA	85	U	C1'-O4'-C4'	-5.29	105.66	109.90
21	AA	194	C	C2-N1-C1'	5.29	124.62	118.80
21	AA	1347	G	N3-C2-N2	-5.29	116.19	119.90
10	AK	126	ARG	CD-NE-CZ	5.29	131.01	123.60
54	BA	78	U	O4'-C1'-N1	5.29	112.44	108.20
21	AA	557	G	N1-C6-O6	-5.29	116.72	119.90
25	BC	268	ARG	NE-CZ-NH1	5.29	122.95	120.30
54	BA	739	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	791	C	N1-C2-O2	5.29	122.08	118.90
54	BA	1918	A	C3'-C2'-C1'	5.29	105.73	101.50
54	BA	2673	G	N3-C2-N2	-5.29	116.20	119.90
56	B5	12	ARG	NE-CZ-NH1	5.29	122.95	120.30
12	AM	92	ARG	NE-CZ-NH1	5.29	122.94	120.30
21	AA	876	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	33	C	N3-C2-O2	-5.29	118.20	121.90
54	BA	434	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	527	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	580	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1224	U	C5-C6-N1	-5.29	120.06	122.70
54	BA	1563	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1574	C	N1-C2-O2	5.29	122.07	118.90
8	AI	84	ARG	NE-CZ-NH2	5.29	122.94	120.30
54	BA	520	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	1607	C	N3-C4-N4	-5.29	114.30	118.00
21	AA	1484	C	O4'-C1'-N1	5.29	112.43	108.20
34	BL	78	ARG	NE-CZ-NH1	5.29	122.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1729	U	N3-C2-O2	-5.29	118.50	122.20
54	BA	2752	C	O4'-C1'-N1	5.29	112.43	108.20
21	AA	893	C	N3-C2-O2	-5.28	118.20	121.90
54	BA	38	A	C6-C5-N7	5.28	136.00	132.30
54	BA	1320	C	O4'-C1'-N1	5.28	112.43	108.20
54	BA	1847	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	2450	A	C6-C5-N7	5.28	136.00	132.30
22	A1	47	U	C1'-O4'-C4'	-5.28	105.67	109.90
54	BA	1598	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	2104	C	N3-C2-O2	-5.28	118.20	121.90
54	BA	2769	U	O4'-C1'-N1	5.28	112.42	108.20
55	BB	24	G	C5-C6-N1	5.28	114.14	111.50
21	AA	177	G	O4'-C1'-N9	5.28	112.42	108.20
21	AA	1443	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	806	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	1536	C	O4'-C1'-N1	5.28	112.42	108.20
21	AA	155	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	20	C	C1'-O4'-C4'	-5.28	105.68	109.90
21	AA	1216	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	2171	A	P-O3'-C3'	5.28	126.03	119.70
54	BA	2297	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	2499	C	C1'-O4'-C4'	-5.28	105.68	109.90
54	BA	2564	A	O4'-C1'-N9	5.28	112.42	108.20
21	AA	605	U	O4'-C1'-N1	5.27	112.42	108.20
22	A1	72	C	N1-C2-O2	5.27	122.06	118.90
54	BA	943	A	C6-C5-N7	5.27	135.99	132.30
54	BA	2323	G	C8-N9-C4	-5.27	104.29	106.40
54	BA	349	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	742	A	O4'-C1'-N9	5.27	112.42	108.20
54	BA	1512	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2258	C	N1-C2-O2	5.27	122.06	118.90
21	AA	176	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	545	C	N1-C2-O2	5.27	122.06	118.90
54	BA	2021	C	N1-C2-O2	5.27	122.06	118.90
54	BA	2697	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	2872	A	C4-C5-C6	-5.27	114.37	117.00
56	B5	53	ARG	NE-CZ-NH2	-5.27	117.67	120.30
21	AA	132	C	N1-C2-O2	5.27	122.06	118.90
21	AA	1162	C	N1-C2-O2	5.27	122.06	118.90
54	BA	1208	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	1864	U	O4'-C1'-N1	5.27	112.41	108.20
55	BB	109	A	C4-C5-C6	-5.27	114.37	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1218	C	O4'-C1'-N1	5.27	112.41	108.20
21	AA	454	G	N3-C2-N2	-5.26	116.22	119.90
21	AA	727	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	1164	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	1959	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	547	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1153	C	N3-C2-O2	-5.26	118.22	121.90
54	BA	1219	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	332	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	559	A	O4'-C1'-N9	5.26	112.41	108.20
21	AA	1078	U	C5-C6-N1	-5.26	120.07	122.70
54	BA	607	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	994	C	N1-C2-O2	5.26	122.06	118.90
54	BA	2168	G	C5-C6-N1	5.26	114.13	111.50
54	BA	2350	C	C4'-C3'-C2'	-5.26	97.34	102.60
21	AA	38	G	N9-C1'-C2'	-5.26	106.21	112.00
54	BA	1260	A	C6-C5-N7	5.26	135.98	132.30
54	BA	1885	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1203	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	277	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	2492	U	N3-C2-O2	-5.26	118.52	122.20
21	AA	327	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1120	C	O4'-C1'-N1	5.26	112.41	108.20
21	AA	1180	A	C6-C5-N7	5.26	135.98	132.30
54	BA	212	G	N1-C6-O6	-5.26	116.75	119.90
54	BA	361	G	N1-C6-O6	-5.26	116.75	119.90
54	BA	560	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	1981	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2006	C	N1-C2-O2	5.26	122.05	118.90
54	BA	2031	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	848	C	N3-C2-O2	-5.25	118.22	121.90
54	BA	2019	A	C3'-C2'-C1'	5.25	105.70	101.50
21	AA	110	C	N1-C2-O2	5.25	122.05	118.90
54	BA	538	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	865	C	N3-C2-O2	-5.25	118.22	121.90
54	BA	2326	C	N1-C2-O2	5.25	122.05	118.90
21	AA	197	A	C6-C5-N7	5.25	135.98	132.30
21	AA	1236	A	C4-C5-C6	-5.25	114.37	117.00
21	AA	1241	G	N3-C4-C5	-5.25	125.97	128.60
21	AA	1510	C	N1-C2-O2	5.25	122.05	118.90
54	BA	39	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	232	G	N1-C6-O6	-5.25	116.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	995	C	N1-C2-O2	5.25	122.05	118.90
54	BA	1177	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	1515	A	C6-C5-N7	5.25	135.97	132.30
54	BA	1874	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2164	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2177	C	N1-C2-O2	5.25	122.05	118.90
54	BA	8	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	436	C	C5'-C4'-O4'	5.25	115.40	109.10
54	BA	1204	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	1247	A	C6-C5-N7	5.25	135.97	132.30
54	BA	2211	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	2893	A	C4-C5-C6	-5.25	114.38	117.00
55	BB	26	C	N1-C2-O2	5.25	122.05	118.90
21	AA	1146	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	1185	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	1062	G	N3-C4-C5	-5.25	125.98	128.60
21	AA	149	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	969	A	C6-C5-N7	5.24	135.97	132.30
54	BA	219	A	C5'-C4'-O4'	5.24	115.39	109.10
54	BA	1303	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	2740	A	N1-C6-N6	-5.24	115.45	118.60
54	BA	2850	A	C6-C5-N7	5.24	135.97	132.30
54	BA	1474	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2301	C	N3-C2-O2	-5.24	118.23	121.90
21	AA	411	A	C6-C5-N7	5.24	135.97	132.30
21	AA	1191	A	C6-C5-N7	5.24	135.97	132.30
33	BK	98	ARG	NE-CZ-NH2	-5.24	117.68	120.30
54	BA	1561	C	N1-C2-O2	5.24	122.04	118.90
54	BA	1816	C	N1-C2-O2	5.24	122.04	118.90
54	BA	1036	G	C5'-C4'-O4'	5.24	115.39	109.10
54	BA	1332	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	1713	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	2502	G	O4'-C1'-N9	5.24	112.39	108.20
21	AA	974	A	C6-C5-N7	5.24	135.97	132.30
54	BA	2395	C	N1-C2-O2	5.24	122.04	118.90
21	AA	1029	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	165	A	C6-C5-N7	5.24	135.97	132.30
54	BA	1999	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2025	C	N1-C2-O2	5.24	122.04	118.90
54	BA	2491	U	O4'-C1'-N1	5.24	112.39	108.20
18	AS	80	ARG	NE-CZ-NH1	5.23	122.92	120.30
21	AA	625	U	O4'-C1'-N1	5.23	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	444	C	O4'-C1'-N1	5.23	112.39	108.20
54	BA	1401	G	O4'-C1'-N9	5.23	112.39	108.20
54	BA	1689	A	C4-C5-C6	-5.23	114.38	117.00
21	AA	911	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	740	C	O4'-C1'-N1	5.23	112.39	108.20
54	BA	1744	A	C4-C5-C6	-5.23	114.38	117.00
54	BA	1955	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2404	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2551	C	N1-C2-O2	5.23	122.04	118.90
21	AA	13	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	194	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	2059	A	C4-C5-C6	-5.23	114.39	117.00
21	AA	912	C	N1-C2-O2	5.23	122.04	118.90
21	AA	1055	A	C6-C5-N7	5.23	135.96	132.30
54	BA	1809	A	C6-C5-N7	5.23	135.96	132.30
54	BA	2676	C	N3-C2-O2	-5.23	118.24	121.90
21	AA	316	C	N1-C2-O2	5.23	122.03	118.90
21	AA	73	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2153	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2556	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	764	C	N3-C2-O2	-5.22	118.24	121.90
54	BA	25	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	1255	U	N3-C2-O2	-5.22	118.54	122.20
21	AA	994	A	O4'-C1'-N9	5.22	112.38	108.20
54	BA	177	G	N3-C4-C5	-5.22	125.99	128.60
21	AA	25	C	N1-C2-O2	5.22	122.03	118.90
21	AA	219	U	O4'-C1'-N1	5.22	112.38	108.20
21	AA	634	C	N1-C2-O2	5.22	122.03	118.90
21	AA	716	A	C6-C5-N7	5.22	135.95	132.30
54	BA	288	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	1723	G	N3-C2-N2	-5.22	116.25	119.90
54	BA	1822	C	C4'-C3'-C2'	-5.22	97.38	102.60
54	BA	2730	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	2852	G	C5-C6-N1	5.22	114.11	111.50
21	AA	275	G	C5-C6-N1	5.22	114.11	111.50
35	BM	44	ARG	NE-CZ-NH1	5.22	122.91	120.30
54	BA	1060	U	N3-C2-O2	-5.22	118.55	122.20
54	BA	1806	C	N1-C2-O2	5.22	122.03	118.90
21	AA	67	C	C1'-O4'-C4'	-5.22	105.73	109.90
21	AA	394	G	C5-C6-N1	5.22	114.11	111.50
21	AA	554	A	C6-C5-N7	5.22	135.95	132.30
54	BA	1508	A	C4-C5-C6	-5.22	114.39	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1802	A	N1-C6-N6	-5.22	115.47	118.60
54	BA	1901	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	2897	U	O4'-C1'-N1	5.22	112.37	108.20
54	BA	1999	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2558	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2638	G	N3-C4-C5	-5.21	125.99	128.60
22	A1	35	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	1556	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	1879	C	O4'-C1'-N1	5.21	112.37	108.20
21	AA	881	G	N1-C6-O6	-5.21	116.77	119.90
21	AA	1502	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	589	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	2201	G	C5'-C4'-O4'	5.21	115.35	109.10
21	AA	1049	U	N3-C2-O2	-5.21	118.55	122.20
24	A3	9	G	N3-C4-C5	-5.21	126.00	128.60
21	AA	211	G	N3-C4-C5	-5.21	126.00	128.60
21	AA	1080	A	C6-C5-N7	5.21	135.95	132.30
22	A1	47	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	289	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	459	U	O4'-C1'-N1	5.21	112.37	108.20
21	AA	308	C	N1-C2-O2	5.21	122.02	118.90
21	AA	751	U	O4'-C1'-N1	5.21	112.36	108.20
21	AA	1208	C	N3-C2-O2	-5.21	118.26	121.90
21	AA	1469	C	N3-C4-N4	-5.21	114.36	118.00
54	BA	156	A	C4-C5-C6	-5.21	114.40	117.00
54	BA	1614	A	C4-C5-C6	-5.21	114.40	117.00
55	BB	95	U	O4'-C1'-N1	5.21	112.36	108.20
21	AA	18	C	N1-C2-O2	5.21	122.02	118.90
54	BA	263	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	878	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	1402	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2888	C	N1-C2-O2	5.20	122.02	118.90
55	BB	60	C	O4'-C1'-N1	5.20	112.36	108.20
13	AN	61	ARG	NE-CZ-NH1	5.20	122.90	120.30
21	AA	570	G	N3-C2-N2	-5.20	116.26	119.90
54	BA	2879	A	C4-C5-C6	-5.20	114.40	117.00
21	AA	480	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	473	G	O4'-C1'-N9	5.20	112.36	108.20
54	BA	906	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1288	G	N3-C4-C5	-5.20	126.00	128.60
54	BA	2464	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	2487	G	N1-C6-O6	-5.20	116.78	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2573	C	C1'-O4'-C4'	-5.20	105.74	109.90
54	BA	792	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	877	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1399	C	N1-C2-O2	5.20	122.02	118.90
54	BA	1462	C	N1-C2-O2	5.20	122.02	118.90
54	BA	1684	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	2600	A	C6-C5-N7	5.20	135.94	132.30
54	BA	2751	G	N3-C2-N2	-5.20	116.26	119.90
55	BB	19	C	N1-C2-O2	5.20	122.02	118.90
23	A2	90	U	C5'-C4'-C3'	-5.20	107.69	116.00
54	BA	300	A	C6-C5-N7	5.20	135.94	132.30
54	BA	367	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	673	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1139	G	C5-C6-N1	5.20	114.10	111.50
54	BA	2427	C	N1-C2-O2	5.20	122.02	118.90
19	AT	17	ARG	NE-CZ-NH1	5.19	122.90	120.30
21	AA	1243	C	N1-C2-O2	5.19	122.02	118.90
21	AA	1358	U	C5-C6-N1	-5.19	120.10	122.70
21	AA	1501	C	N3-C4-C5	5.19	123.98	121.90
54	BA	812	C	N1-C2-O2	5.19	122.02	118.90
54	BA	2107	G	N9-C4-C5	5.19	107.48	105.40
20	AU	35	GLU	C-N-CA	5.19	134.68	121.70
54	BA	245	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	1298	C	N1-C2-O2	5.19	122.01	118.90
54	BA	2768	U	O4'-C1'-N1	5.19	112.35	108.20
21	AA	185	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	471	A	C4-C5-C6	-5.19	114.41	117.00
5	AF	2	ARG	NE-CZ-NH1	5.19	122.89	120.30
21	AA	313	A	C6-C5-N7	5.19	135.93	132.30
21	AA	379	C	N1-C2-O2	5.19	122.01	118.90
21	AA	621	A	C4-C5-C6	-5.19	114.41	117.00
21	AA	926	G	N1-C6-O6	-5.19	116.79	119.90
21	AA	977	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	346	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	489	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	1222	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	2435	A	C4-C5-C6	-5.19	114.41	117.00
21	AA	330	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	2092	U	N3-C2-O2	-5.19	118.57	122.20
21	AA	620	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	832	U	O4'-C1'-N1	5.18	112.35	108.20
54	BA	2463	C	N1-C2-O2	5.18	122.01	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2712	C	N1-C2-O2	5.18	122.01	118.90
55	BB	10	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	415	A	O4'-C1'-N9	5.18	112.34	108.20
21	AA	808	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1132	C	N1-C2-O2	5.18	122.01	118.90
22	A1	76	A	C8-N9-C4	-5.18	103.73	105.80
54	BA	986	C	N1-C2-O2	5.18	122.01	118.90
54	BA	1687	G	N7-C8-N9	5.18	115.69	113.10
54	BA	2457	U	N3-C2-O2	-5.18	118.58	122.20
54	BA	2765	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	302	G	N3-C2-N2	-5.18	116.28	119.90
21	AA	806	C	N1-C2-O2	5.18	122.01	118.90
54	BA	1428	C	N1-C2-O2	5.18	122.01	118.90
54	BA	2516	A	O4'-C1'-N9	5.18	112.34	108.20
21	AA	421	U	O4'-C1'-N1	5.17	112.34	108.20
21	AA	1032	G	N3-C4-C5	-5.17	126.01	128.60
21	AA	1371	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1192	G	O4'-C1'-N9	5.17	112.34	108.20
55	BB	25	U	O4'-C1'-N1	5.17	112.34	108.20
21	AA	779	C	N1-C2-O2	5.17	122.00	118.90
21	AA	1011	C	N1-C2-O2	5.17	122.00	118.90
54	BA	250	G	O4'-C1'-N9	5.17	112.34	108.20
55	BB	56	G	N3-C4-C5	-5.17	126.01	128.60
21	AA	1105	A	C6-C5-N7	5.17	135.92	132.30
21	AA	1317	C	O4'-C1'-N1	5.17	112.34	108.20
24	A3	48	U	C1'-O4'-C4'	-5.17	105.76	109.90
54	BA	217	A	C6-C5-N7	5.17	135.92	132.30
54	BA	430	A	C6-C5-N7	5.17	135.92	132.30
54	BA	2563	U	C5'-C4'-O4'	5.17	115.31	109.10
21	AA	139	A	C6-C5-N7	5.17	135.92	132.30
21	AA	426	U	O4'-C1'-N1	5.17	112.33	108.20
21	AA	726	C	N1-C2-O2	5.17	122.00	118.90
21	AA	1093	A	C6-C5-N7	5.17	135.92	132.30
30	BH	51	ARG	NE-CZ-NH1	5.17	122.88	120.30
54	BA	1518	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1892	C	O4'-C1'-N1	5.17	112.33	108.20
24	A3	59	A	C4-C5-C6	-5.17	114.42	117.00
54	BA	158	U	O4'-C1'-N1	5.17	112.33	108.20
54	BA	1869	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	2289	G	N3-C2-N2	-5.17	116.28	119.90
21	AA	1227	A	C4-C5-C6	-5.17	114.42	117.00
54	BA	1299	G	N7-C8-N9	5.17	115.68	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	22	G	N3-C4-C5	-5.16	126.02	128.60
21	AA	831	A	C6-C5-N7	5.16	135.91	132.30
54	BA	206	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1259	G	N7-C8-N9	5.16	115.68	113.10
54	BA	1558	C	N3-C4-C5	5.16	123.97	121.90
54	BA	1599	U	C5-C6-N1	-5.16	120.12	122.70
54	BA	1985	C	N3-C2-O2	-5.16	118.28	121.90
54	BA	2014	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	412	A	C6-C5-N7	5.16	135.91	132.30
54	BA	2342	C	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	2656	U	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1389	C	N1-C2-O2	5.16	122.00	118.90
54	BA	859	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	1592	C	N1-C2-O2	5.16	122.00	118.90
54	BA	1830	C	C6-N1-C2	-5.16	118.23	120.30
54	BA	1872	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1925	C	N3-C2-O2	-5.16	118.29	121.90
54	BA	2139	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	2325	G	N3-C4-C5	-5.16	126.02	128.60
54	BA	2666	C	C1'-O4'-C4'	-5.16	105.77	109.90
21	AA	679	C	N1-C2-O2	5.16	122.00	118.90
21	AA	718	A	N1-C6-N6	-5.16	115.50	118.60
21	AA	945	G	N3-C4-C5	-5.16	126.02	128.60
25	BC	62	ARG	NE-CZ-NH2	-5.16	117.72	120.30
54	BA	564	C	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1097	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1233	C	N1-C2-O2	5.16	121.99	118.90
54	BA	1639	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	255	G	N1-C6-O6	-5.16	116.81	119.90
21	AA	1143	G	N1-C6-O6	-5.16	116.81	119.90
21	AA	1413	A	C6-C5-N7	5.16	135.91	132.30
54	BA	492	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1736	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1792	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	1986	C	C5'-C4'-O4'	5.16	115.29	109.10
54	BA	1509	A	C4-C5-C6	-5.15	114.42	117.00
55	BB	11	C	N3-C2-O2	-5.15	118.29	121.90
21	AA	553	A	C6-C5-N7	5.15	135.91	132.30
54	BA	1802	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	2645	G	N3-C2-N2	-5.15	116.29	119.90
54	BA	2782	G	N1-C6-O6	-5.15	116.81	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	81	G	N3-C2-N2	-5.15	116.29	119.90
54	BA	1841	U	O4'-C1'-N1	5.15	112.32	108.20
21	AA	600	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	710	G	N1-C6-O6	-5.15	116.81	119.90
4	AE	68	ARG	NE-CZ-NH1	5.15	122.87	120.30
21	AA	732	C	N1-C2-O2	5.15	121.99	118.90
21	AA	1278	G	O4'-C1'-N9	5.15	112.32	108.20
54	BA	119	A	C6-C5-N7	5.15	135.90	132.30
54	BA	229	C	N3-C4-C5	5.15	123.96	121.90
54	BA	637	A	C6-C5-N7	5.15	135.90	132.30
54	BA	757	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1146	C	N1-C2-O2	5.15	121.99	118.90
54	BA	2309	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	404	G	C5-C6-N1	5.15	114.07	111.50
21	AA	935	A	C5-C6-N6	5.15	127.82	123.70
21	AA	1315	U	N3-C2-O2	-5.15	118.60	122.20
21	AA	113	G	N1-C6-O6	-5.14	116.81	119.90
21	AA	908	A	C4-C5-C6	-5.14	114.43	117.00
24	A3	49	C	C5'-C4'-C3'	-5.14	107.77	116.00
41	BS	84	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	1420	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2635	A	C6-C5-N7	5.14	135.90	132.30
6	AG	91	ARG	NE-CZ-NH1	5.14	122.87	120.30
21	AA	383	A	C4-C5-C6	-5.14	114.43	117.00
21	AA	540	G	N3-C2-N2	-5.14	116.30	119.90
21	AA	738	C	N3-C2-O2	-5.14	118.30	121.90
21	AA	907	A	C4-C5-C6	-5.14	114.43	117.00
21	AA	1244	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	61	C	N1-C2-O2	5.14	121.98	118.90
54	BA	567	U	N1-C1'-C2'	-5.14	106.34	112.00
54	BA	654	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	737	C	C4'-C3'-C2'	-5.14	97.46	102.60
54	BA	2636	C	N1-C2-O2	5.14	121.99	118.90
54	BA	944	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	1470	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2377	A	C4-C5-C6	-5.14	114.43	117.00
21	AA	352	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	519	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	945	A	C3'-C2'-C1'	-5.14	97.39	101.50
54	BA	2134	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	737	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2387	U	N1-C2-N3	5.14	117.98	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2828	G	C5'-C4'-O4'	5.14	115.27	109.10
21	AA	67	C	N1-C2-O2	5.14	121.98	118.90
21	AA	311	C	N1-C2-O2	5.14	121.98	118.90
54	BA	1956	U	N3-C2-O2	-5.14	118.61	122.20
21	AA	1000	A	C6-C5-N7	5.13	135.90	132.30
54	BA	1753	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	20	U	N1-C2-N3	5.13	117.98	114.90
21	AA	391	G	C8-N9-C4	-5.13	104.35	106.40
21	AA	757	U	O4'-C1'-N1	5.13	112.31	108.20
28	BF	124	ARG	NH1-CZ-NH2	-5.13	113.76	119.40
54	BA	174	U	O4'-C1'-N1	5.13	112.31	108.20
54	BA	458	G	O4'-C1'-N9	5.13	112.30	108.20
54	BA	2880	C	N1-C2-O2	5.13	121.98	118.90
21	AA	1242	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	1339	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	1162	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	90	C	N1-C2-O2	5.13	121.98	118.90
21	AA	284	C	O4'-C1'-N1	5.13	112.30	108.20
21	AA	868	C	N1-C2-O2	5.13	121.98	118.90
54	BA	444	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	791	C	C1'-O4'-C4'	-5.13	105.80	109.90
54	BA	1291	C	C5'-C4'-O4'	5.13	115.25	109.10
54	BA	1748	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2426	A	C6-C5-N7	5.13	135.89	132.30
55	BB	32	U	O4'-C1'-N1	5.13	112.30	108.20
21	AA	43	C	N1-C2-O2	5.13	121.97	118.90
21	AA	64	G	C3'-C2'-C1'	5.13	105.60	101.50
21	AA	274	A	O4'-C1'-N9	5.13	112.30	108.20
21	AA	423	G	N3-C4-C5	-5.13	126.04	128.60
21	AA	599	C	N3-C2-O2	-5.13	118.31	121.90
50	B1	5	ARG	NE-CZ-NH1	5.13	122.86	120.30
54	BA	193	U	O4'-C1'-N1	5.13	112.30	108.20
54	BA	1068	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1334	G	N3-C2-N2	-5.13	116.31	119.90
54	BA	1545	A	C6-C5-N7	5.13	135.89	132.30
54	BA	1708	C	O4'-C1'-N1	5.13	112.30	108.20
54	BA	2247	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	302	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	3	U	C4'-C3'-C2'	-5.12	97.47	102.60
54	BA	635	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1170	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1319	C	N1-C2-O2	5.12	121.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2885	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	112	G	C5-C6-N1	5.12	114.06	111.50
21	AA	824	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	96	C	N1-C2-O2	5.12	121.97	118.90
54	BA	795	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1763	G	O4'-C1'-N9	5.12	112.30	108.20
21	AA	562	U	C1'-O4'-C4'	-5.12	105.80	109.90
21	AA	1188	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1269	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2840	C	O4'-C1'-N1	5.12	112.30	108.20
21	AA	864	A	C6-C5-N7	5.12	135.88	132.30
54	BA	2286	G	C3'-C2'-C1'	5.12	105.60	101.50
54	BA	2452	C	C1'-O4'-C4'	-5.12	105.80	109.90
21	AA	1423	G	O4'-C1'-N9	5.12	112.29	108.20
53	B4	4	ARG	NE-CZ-NH1	5.12	122.86	120.30
54	BA	327	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1292	G	C5'-C4'-O4'	5.12	115.24	109.10
54	BA	1562	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1608	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2073	C	N3-C4-N4	-5.12	114.42	118.00
54	BA	2161	C	C1'-O4'-C4'	-5.12	105.81	109.90
54	BA	2164	C	N1-C2-O2	5.12	121.97	118.90
54	BA	2348	U	O4'-C1'-N1	5.12	112.30	108.20
55	BB	64	G	N1-C6-O6	-5.12	116.83	119.90
24	A3	77	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2065	C	N3-C4-C5	5.12	123.95	121.90
54	BA	2233	U	O4'-C1'-N1	5.12	112.29	108.20
11	AL	55	ARG	NE-CZ-NH1	5.12	122.86	120.30
21	AA	595	A	C4-C5-C6	-5.12	114.44	117.00
55	BB	68	C	O4'-C1'-N1	5.12	112.29	108.20
21	AA	198	G	N3-C2-N2	-5.11	116.32	119.90
24	A3	23	G	N3-C2-N2	-5.11	116.32	119.90
54	BA	1410	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	2055	C	N1-C2-O2	5.11	121.97	118.90
54	BA	2813	A	O4'-C1'-N9	5.11	112.29	108.20
54	BA	1615	C	N3-C4-C5	5.11	123.94	121.90
41	BS	92	ARG	NE-CZ-NH1	5.11	122.85	120.30
54	BA	1471	G	N1-C6-O6	-5.11	116.83	119.90
6	AG	2	ARG	NE-CZ-NH2	5.11	122.85	120.30
21	AA	22	G	C5-C6-N1	5.11	114.05	111.50
54	BA	956	G	N1-C6-O6	-5.11	116.84	119.90
54	BA	1384	A	C6-C5-N7	5.11	135.87	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2542	A	O4'-C1'-N9	5.11	112.28	108.20
21	AA	298	A	C6-C5-N7	5.10	135.87	132.30
21	AA	737	C	O4'-C1'-N1	5.10	112.28	108.20
22	A1	50	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	1354	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2010	G	N3-C4-C5	-5.10	126.05	128.60
55	BB	31	C	N3-C2-O2	-5.10	118.33	121.90
21	AA	481	G	C1'-O4'-C4'	-5.10	105.82	109.90
54	BA	390	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	615	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	2622	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1431	A	C6-C5-N7	5.10	135.87	132.30
22	A1	76	A	C2-N3-C4	5.10	113.15	110.60
54	BA	1792	G	C5-C6-N1	5.10	114.05	111.50
54	BA	2307	G	N3-C4-C5	-5.10	126.05	128.60
54	BA	2385	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1504	G	N1-C6-O6	-5.10	116.84	119.90
22	A1	45	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	214	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	253	C	N3-C2-O2	-5.10	118.33	121.90
54	BA	379	G	C5-C6-N1	5.10	114.05	111.50
54	BA	2468	A	C6-C5-N7	5.10	135.87	132.30
54	BA	568	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	130	A	C6-C5-N7	5.09	135.87	132.30
21	AA	216	U	O4'-C1'-N1	5.09	112.28	108.20
21	AA	775	G	N3-C2-N2	-5.09	116.33	119.90
54	BA	1544	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	1836	C	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1968	G	O4'-C1'-N9	5.09	112.28	108.20
54	BA	2598	A	C4-C5-C6	-5.09	114.45	117.00
21	AA	420	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	1059	G	O4'-C1'-N9	5.09	112.27	108.20
54	BA	1141	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	2050	C	N1-C2-O2	5.09	121.96	118.90
54	BA	2706	A	C4-C5-C6	-5.09	114.45	117.00
21	AA	672	U	C5-C6-N1	-5.09	120.16	122.70
21	AA	1195	C	N1-C2-O2	5.09	121.95	118.90
21	AA	1332	A	C6-C5-N7	5.09	135.86	132.30
54	BA	1223	G	N1-C6-O6	-5.09	116.85	119.90
54	BA	1871	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	1889	A	C6-C5-N7	5.09	135.86	132.30
54	BA	2437	G	N1-C6-O6	-5.09	116.85	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1387	G	N3-C2-N2	-5.09	116.34	119.90
54	BA	1234	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	1345	C	N3-C2-O2	-5.09	118.34	121.90
54	BA	2005	A	C6-C5-N7	5.09	135.86	132.30
21	AA	75	G	N1-C6-O6	-5.09	116.85	119.90
21	AA	942	G	N1-C6-O6	-5.09	116.85	119.90
54	BA	256	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	550	C	N1-C2-O2	5.09	121.95	118.90
54	BA	728	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	628	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1030	C	N1-C2-O2	5.08	121.95	118.90
54	BA	1114	C	N1-C2-O2	5.08	121.95	118.90
19	AT	73	ARG	NE-CZ-NH2	-5.08	117.76	120.30
21	AA	186	C	N1-C2-O2	5.08	121.95	118.90
21	AA	740	U	O4'-C1'-N1	5.08	112.27	108.20
21	AA	1450	U	N3-C2-O2	-5.08	118.64	122.20
21	AA	1496	C	N1-C2-O2	5.08	121.95	118.90
54	BA	1000	A	C5'-C4'-O4'	5.08	115.20	109.10
54	BA	1381	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1918	A	O4'-C4'-C3'	5.08	110.17	106.10
54	BA	2825	G	C8-N9-C4	-5.08	104.37	106.40
55	BB	54	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2401	U	O4'-C1'-N1	5.08	112.27	108.20
21	AA	483	C	C3'-C2'-C1'	5.08	105.56	101.50
54	BA	74	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	888	C	N3-C4-C5	5.08	123.93	121.90
54	BA	903	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1075	C	N3-C4-N4	-5.08	114.44	118.00
18	AS	77	ARG	NE-CZ-NH2	5.08	122.84	120.30
21	AA	658	C	N1-C2-O2	5.08	121.95	118.90
21	AA	970	C	N1-C2-O2	5.08	121.95	118.90
22	A1	36	C	N1-C2-O2	5.08	121.95	118.90
54	BA	694	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	1533	C	N1-C2-O2	5.08	121.95	118.90
54	BA	1905	C	C5'-C4'-O4'	5.08	115.19	109.10
21	AA	256	U	C5-C6-N1	-5.08	120.16	122.70
54	BA	1186	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1472	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2692	G	C5-C6-N1	5.08	114.04	111.50
21	AA	549	C	O4'-C1'-N1	5.08	112.26	108.20
21	AA	858	G	N3-C2-N2	-5.08	116.35	119.90
21	AA	1350	A	C4-C5-C6	-5.08	114.46	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	295	G	C5'-C4'-O4'	5.08	115.19	109.10
54	BA	741	U	C4-C5-C6	5.08	122.75	119.70
54	BA	1194	A	C6-C5-N7	5.08	135.85	132.30
54	BA	2767	C	C3'-C2'-C1'	5.08	105.56	101.50
21	AA	816	A	C5'-C4'-C3'	-5.07	107.88	116.00
21	AA	1302	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1289	C	O4'-C1'-N1	5.07	112.26	108.20
54	BA	1983	G	N3-C2-N2	-5.07	116.35	119.90
54	BA	2045	C	N1-C2-O2	5.07	121.94	118.90
54	BA	2078	C	N1-C2-O2	5.07	121.94	118.90
54	BA	2557	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2867	G	N3-C2-N2	-5.07	116.35	119.90
54	BA	1165	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	1488	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1271	G	C5'-C4'-O4'	5.07	115.19	109.10
21	AA	1140	C	C5'-C4'-O4'	5.07	115.18	109.10
21	AA	1398	A	C6-C5-N7	5.07	135.85	132.30
54	BA	531	C	N1-C2-O2	5.07	121.94	118.90
54	BA	533	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	1784	A	N1-C6-N6	-5.07	115.56	118.60
21	AA	1161	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1464	G	C8-N9-C4	-5.07	104.37	106.40
54	BA	1497	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	2475	C	N1-C2-O2	5.07	121.94	118.90
55	BB	113	C	O4'-C1'-N1	5.07	112.25	108.20
21	AA	956	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	129	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	375	G	N3-C4-C5	-5.07	126.07	128.60
54	BA	451	U	C5'-C4'-O4'	5.07	115.18	109.10
54	BA	485	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1323	C	N1-C2-O2	5.07	121.94	118.90
55	BB	72	G	C3'-C2'-C1'	5.07	105.55	101.50
54	BA	330	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	1508	A	C1'-O4'-C4'	-5.06	105.85	109.90
54	BA	2652	C	N1-C2-O2	5.06	121.94	118.90
21	AA	408	A	C6-C5-N7	5.06	135.84	132.30
21	AA	972	C	C1'-O4'-C4'	-5.06	105.85	109.90
26	BD	33	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
54	BA	55	G	C4'-C3'-C2'	-5.06	97.54	102.60
54	BA	334	C	N1-C2-O2	5.06	121.94	118.90
54	BA	2347	C	N3-C4-C5	5.06	123.92	121.90
21	AA	542	G	N1-C6-O6	-5.06	116.86	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1068	G	C5'-C4'-O4'	5.06	115.17	109.10
54	BA	322	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	1593	A	C6-C5-N7	5.06	135.84	132.30
54	BA	2048	G	C5-C6-N1	5.06	114.03	111.50
54	BA	2324	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2599	G	N1-C6-O6	-5.06	116.86	119.90
55	BB	51	G	N1-C6-O6	-5.06	116.86	119.90
21	AA	115	G	C5-C6-N1	5.06	114.03	111.50
21	AA	792	A	C1'-O4'-C4'	-5.06	105.85	109.90
21	AA	909	A	C6-C5-N7	5.06	135.84	132.30
24	A3	64	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	411	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	2618	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	2632	A	C6-C5-N7	5.06	135.84	132.30
54	BA	2888	C	C5'-C4'-O4'	5.06	115.17	109.10
21	AA	422	C	O4'-C1'-N1	5.06	112.25	108.20
21	AA	1064	G	N3-C2-N2	-5.06	116.36	119.90
40	BR	80	ARG	NE-CZ-NH1	5.06	122.83	120.30
54	BA	164	C	N1-C2-O2	5.06	121.94	118.90
54	BA	1083	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	698	C	N1-C2-O2	5.06	121.93	118.90
54	BA	1188	U	O4'-C1'-N1	5.06	112.24	108.20
21	AA	556	C	N1-C2-O2	5.05	121.93	118.90
21	AA	978	A	C4-C5-C6	-5.05	114.47	117.00
21	AA	1469	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	837	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1126	A	C6-C5-N7	5.05	135.84	132.30
54	BA	2406	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	2902	C	N1-C2-O2	5.05	121.93	118.90
54	BA	37	C	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	1772	A	C6-C5-N7	5.05	135.84	132.30
54	BA	1855	U	O4'-C1'-N1	5.05	112.24	108.20
21	AA	526	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1385	G	C5-C6-N1	5.05	114.03	111.50
54	BA	114	U	N3-C2-O2	-5.05	118.66	122.20
54	BA	210	C	N1-C2-O2	5.05	121.93	118.90
54	BA	917	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	1301	A	O4'-C1'-N9	5.05	112.24	108.20
54	BA	1305	C	N3-C4-C5	5.05	123.92	121.90
55	BB	95	U	N3-C2-O2	-5.05	118.66	122.20
21	AA	792	A	O4'-C1'-N9	5.05	112.24	108.20
21	AA	889	A	C1'-O4'-C4'	-5.05	105.86	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	290	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	833	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	1288	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1475	G	N3-C4-C5	-5.05	126.08	128.60
21	AA	962	C	O4'-C1'-N1	5.05	112.24	108.20
21	AA	967	C	N3-C2-O2	-5.05	118.37	121.90
24	A3	20	G	N1-C6-O6	-5.05	116.87	119.90
26	BD	83	ARG	NE-CZ-NH2	-5.05	117.78	120.30
54	BA	1052	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	1248	G	N3-C4-C5	-5.05	126.08	128.60
54	BA	1899	A	C4-C5-C6	-5.05	114.48	117.00
21	AA	1249	C	N3-C2-O2	-5.04	118.37	121.90
24	A3	69	C	N1-C2-O2	5.04	121.93	118.90
21	AA	134	G	N1-C6-O6	-5.04	116.87	119.90
21	AA	975	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	197	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1655	A	C5-C6-N1	5.04	120.22	117.70
54	BA	1952	A	C3'-C2'-C1'	5.04	105.53	101.50
21	AA	1217	C	N1-C2-O2	5.04	121.92	118.90
21	AA	1423	G	C5-C6-N1	5.04	114.02	111.50
54	BA	759	G	C8-N9-C4	-5.04	104.38	106.40
54	BA	1266	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2084	C	N3-C4-C5	5.04	123.92	121.90
3	AD	62	ARG	NE-CZ-NH1	5.04	122.82	120.30
21	AA	36	C	N1-C2-O2	5.04	121.92	118.90
54	BA	1044	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	1638	C	N1-C2-O2	5.04	121.92	118.90
54	BA	2027	G	N7-C8-N9	5.04	115.62	113.10
54	BA	132	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	542	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	1025	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	1564	C	N1-C2-O2	5.04	121.92	118.90
21	AA	154	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	401	C	N1-C2-O2	5.04	121.92	118.90
21	AA	1001	C	N3-C2-O2	-5.04	118.38	121.90
21	AA	1287	A	C6-C5-N7	5.04	135.82	132.30
49	B0	49	ARG	NE-CZ-NH1	5.04	122.82	120.30
52	B3	39	ARG	NE-CZ-NH1	5.04	122.82	120.30
54	BA	140	C	N1-C2-O2	5.04	121.92	118.90
54	BA	1196	C	N1-C2-O2	5.04	121.92	118.90
54	BA	1537	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	1858	A	C4-C5-C6	-5.04	114.48	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1982	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	2620	C	N1-C2-O2	5.04	121.92	118.90
54	BA	2831	G	N1-C6-O6	-5.04	116.88	119.90
55	BB	90	C	N3-C2-O2	-5.04	118.38	121.90
21	AA	465	A	C1'-O4'-C4'	-5.03	105.87	109.90
21	AA	1123	U	N3-C2-O2	-5.03	118.68	122.20
24	A3	49	C	O4'-C1'-N1	5.03	112.23	108.20
54	BA	1030	C	O4'-C1'-N1	5.03	112.23	108.20
54	BA	1671	U	O4'-C1'-N1	5.03	112.23	108.20
54	BA	2251	G	O4'-C1'-N9	5.03	112.23	108.20
54	BA	2266	A	C6-C5-N7	5.03	135.82	132.30
24	A3	73	A	C5'-C4'-C3'	-5.03	107.95	116.00
54	BA	363	G	N3-C4-C5	-5.03	126.08	128.60
54	BA	680	C	N1-C2-O2	5.03	121.92	118.90
54	BA	1094	U	C5'-C4'-O4'	5.03	115.14	109.10
54	BA	2155	U	C1'-O4'-C4'	-5.03	105.87	109.90
21	AA	471	U	C5-C6-N1	-5.03	120.19	122.70
21	AA	1153	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	1522	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	177	G	N3-C2-N2	-5.03	116.38	119.90
54	BA	304	U	O4'-C1'-N1	5.03	112.22	108.20
2	AC	39	ARG	NE-CZ-NH1	5.03	122.81	120.30
21	AA	383	A	O4'-C1'-N9	5.03	112.22	108.20
21	AA	934	C	N3-C2-O2	-5.03	118.38	121.90
54	BA	1837	C	O4'-C1'-N1	5.03	112.22	108.20
21	AA	99	C	N1-C2-O2	5.03	121.92	118.90
21	AA	184	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	571	U	C5-C6-N1	-5.03	120.19	122.70
21	AA	819	A	O4'-C1'-N9	5.03	112.22	108.20
21	AA	1012	A	C4-C5-C6	-5.03	114.49	117.00
21	AA	1114	C	N1-C2-O2	5.03	121.92	118.90
21	AA	1238	A	C6-C5-N7	5.03	135.82	132.30
21	AA	1318	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	578	G	C5-C6-N1	5.03	114.01	111.50
54	BA	947	A	C4'-C3'-C2'	-5.03	97.57	102.60
54	BA	2858	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	2873	A	C4-C5-C6	-5.03	114.49	117.00
21	AA	293	G	N3-C2-N2	-5.03	116.38	119.90
21	AA	601	G	N1-C6-O6	-5.03	116.89	119.90
54	BA	146	A	C6-C5-N7	5.03	135.82	132.30
54	BA	634	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	664	G	O4'-C1'-N9	5.03	112.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1092	C	N1-C2-O2	5.03	121.92	118.90
54	BA	1703	G	C5'-C4'-O4'	5.03	115.13	109.10
54	BA	1929	G	O4'-C1'-N9	5.03	112.22	108.20
54	BA	2416	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2433	A	P-O3'-C3'	5.03	125.73	119.70
54	BA	2621	G	N1-C6-O6	-5.03	116.89	119.90
54	BA	2753	A	C6-C5-N7	5.03	135.82	132.30
55	BB	5	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	353	C	N1-C2-O2	5.02	121.92	118.90
54	BA	1301	A	O4'-C1'-C2'	-5.02	100.78	105.80
54	BA	1512	C	C5'-C4'-O4'	5.02	115.13	109.10
54	BA	2417	C	N1-C2-O2	5.02	121.91	118.90
54	BA	631	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	1305	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2173	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	2528	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	1475	G	N1-C6-O6	-5.02	116.89	119.90
22	A1	62	C	N3-C2-O2	-5.02	118.39	121.90
54	BA	316	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1282	U	N3-C2-O2	-5.02	118.69	122.20
21	AA	40	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	740	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1186	G	O4'-C1'-N9	5.02	112.21	108.20
54	BA	2448	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	2510	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2570	G	C5-C6-N1	5.02	114.01	111.50
21	AA	274	A	C6-C5-N7	5.02	135.81	132.30
21	AA	339	C	N1-C2-O2	5.02	121.91	118.90
21	AA	381	C	N1-C2-O2	5.02	121.91	118.90
55	BB	110	C	O4'-C1'-N1	5.02	112.21	108.20
21	AA	364	A	C4-C5-C6	-5.01	114.49	117.00
21	AA	1176	A	C6-C5-N7	5.01	135.81	132.30
54	BA	48	G	C5'-C4'-O4'	5.01	115.12	109.10
54	BA	1724	G	C5-C6-N1	5.01	114.01	111.50
54	BA	2035	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	2515	C	C4'-C3'-C2'	-5.01	97.58	102.60
54	BA	2613	U	C5-C6-N1	-5.01	120.19	122.70
56	B5	134	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	440	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1248	G	C8-N9-C4	-5.01	104.39	106.40
54	BA	2012	G	N3-C4-C5	-5.01	126.09	128.60
54	BA	748	G	O4'-C1'-N9	5.01	112.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1818	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	1964	G	N3-C4-C5	-5.01	126.09	128.60
55	BB	35	C	C5'-C4'-O4'	5.01	115.11	109.10
23	A2	90	U	N3-C2-O2	-5.01	118.69	122.20
24	A3	16	C	N3-C4-C5	5.01	123.90	121.90
54	BA	2499	C	N3-C2-O2	-5.01	118.39	121.90
21	AA	1130	A	C6-C5-N7	5.01	135.81	132.30
54	BA	974	G	N3-C4-C5	-5.01	126.10	128.60
54	BA	1459	G	N3-C2-N2	-5.01	116.39	119.90
54	BA	2431	U	N1-C2-N3	5.01	117.91	114.90
54	BA	578	G	N1-C6-O6	-5.01	116.90	119.90
54	BA	623	C	N1-C2-O2	5.01	121.90	118.90
54	BA	871	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	2350	C	N3-C4-N4	-5.01	114.50	118.00
54	BA	1293	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	436	C	N1-C2-O2	5.00	121.90	118.90
21	AA	674	G	C8-N9-C4	-5.00	104.40	106.40
54	BA	583	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	862	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	1880	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	2555	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	2676	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	800	G	N3-C4-C5	-5.00	126.10	128.60
21	AA	1417	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	2113	U	C5-C6-N1	-5.00	120.20	122.70

There are no chirality outliers.

All (1084) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	12	U	Sidechain
22	A1	20	G	Sidechain
22	A1	27	C	Sidechain
22	A1	32	C	Sidechain
22	A1	42	G	Sidechain
22	A1	43	G	Sidechain
22	A1	44	G	Sidechain
22	A1	45	G	Sidechain
22	A1	47	U	Sidechain
22	A1	50	G	Sidechain
22	A1	53	G	Sidechain
22	A1	65	C	Sidechain

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Mol	Chain	Res	Type	Group
22	A1	73	A	Sidechain
22	A1	76	A	Sidechain
23	A2	79	A	Sidechain
23	A2	80	C	Sidechain
23	A2	84	G	Sidechain
23	A2	90	U	Sidechain
23	A2	92	U	Sidechain
24	A3	16	C	Sidechain
24	A3	23	G	Sidechain
24	A3	24	C	Sidechain
24	A3	39	A	Sidechain
24	A3	4	G	Sidechain
24	A3	44	A	Sidechain
24	A3	46	G	Sidechain
24	A3	54	G	Sidechain
24	A3	60	A	Sidechain
24	A3	61	U	Sidechain
24	A3	64	G	Sidechain
24	A3	65	G	Sidechain
24	A3	66	C	Sidechain
24	A3	7	G	Sidechain
24	A3	74	A	Sidechain
24	A3	76	C	Sidechain
21	AA	1001	C	Sidechain
21	AA	1005	A	Sidechain
21	AA	1013	G	Sidechain
21	AA	1014	A	Sidechain
21	AA	1024	G	Sidechain
21	AA	1025	U	Sidechain
21	AA	1040	U	Sidechain
21	AA	1049	U	Sidechain
21	AA	1051	C	Sidechain
21	AA	1052	U	Sidechain
21	AA	1053	G	Sidechain
21	AA	1054	C	Sidechain
21	AA	1055	A	Sidechain
21	AA	1062	U	Sidechain
21	AA	1064	G	Sidechain
21	AA	1072	G	Sidechain
21	AA	1073	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	1079	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	108	G	Sidechain
21	AA	1081	A	Sidechain
21	AA	1085	U	Sidechain
21	AA	1086	U	Sidechain
21	AA	1087	G	Sidechain
21	AA	1093	A	Sidechain
21	AA	1095	U	Sidechain
21	AA	1098	C	Sidechain
21	AA	1107	C	Sidechain
21	AA	1108	G	Sidechain
21	AA	1118	U	Sidechain
21	AA	1120	C	Sidechain
21	AA	1121	U	Sidechain
21	AA	1124	G	Sidechain
21	AA	1126	U	Sidechain
21	AA	1128	C	Sidechain
21	AA	1131	G	Sidechain
21	AA	1139	G	Sidechain
21	AA	115	G	Sidechain
21	AA	1155	A	Sidechain
21	AA	1156	G	Sidechain
21	AA	1158	C	Sidechain
21	AA	1159	U	Sidechain
21	AA	1166	G	Sidechain
21	AA	1174	G	Sidechain
21	AA	1178	G	Sidechain
21	AA	1183	U	Sidechain
21	AA	1185	G	Sidechain
21	AA	1187	G	Sidechain
21	AA	1190	G	Sidechain
21	AA	1192	C	Sidechain
21	AA	1195	C	Sidechain
21	AA	1203	C	Sidechain
21	AA	1206	G	Sidechain
21	AA	1207	G	Sidechain
21	AA	121	U	Sidechain
21	AA	1211	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1222	G	Sidechain
21	AA	1225	A	Sidechain
21	AA	1226	C	Sidechain
21	AA	1228	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1231	G	Sidechain
21	AA	1236	A	Sidechain
21	AA	124	C	Sidechain
21	AA	1244	G	Sidechain
21	AA	1246	A	Sidechain
21	AA	1250	A	Sidechain
21	AA	1259	C	Sidechain
21	AA	1264	U	Sidechain
21	AA	1266	G	Sidechain
21	AA	1269	A	Sidechain
21	AA	1278	G	Sidechain
21	AA	1282	C	Sidechain
21	AA	1283	U	Sidechain
21	AA	1287	A	Sidechain
21	AA	129	A	Sidechain
21	AA	1300	G	Sidechain
21	AA	1303	C	Sidechain
21	AA	1304	G	Sidechain
21	AA	1306	A	Sidechain
21	AA	1311	A	Sidechain
21	AA	1316	G	Sidechain
21	AA	1319	A	Sidechain
21	AA	1329	A	Sidechain
21	AA	1332	A	Sidechain
21	AA	1342	C	Sidechain
21	AA	1345	U	Sidechain
21	AA	1351	U	Sidechain
21	AA	1358	U	Sidechain
21	AA	1359	C	Sidechain
21	AA	1361	G	Sidechain
21	AA	1362	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	1368	A	Sidechain
21	AA	1373	G	Sidechain
21	AA	1377	A	Sidechain
21	AA	1380	U	Sidechain
21	AA	1384	C	Sidechain
21	AA	1386	G	Sidechain
21	AA	1390	U	Sidechain
21	AA	1391	U	Sidechain
21	AA	14	U	Sidechain
21	AA	1411	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1419	G	Sidechain
21	AA	1422	G	Sidechain
21	AA	1427	C	Sidechain
21	AA	143	A	Sidechain
21	AA	144	G	Sidechain
21	AA	1446	A	Sidechain
21	AA	145	G	Sidechain
21	AA	1451	U	Sidechain
21	AA	1467	C	Sidechain
21	AA	1473	G	Sidechain
21	AA	1486	G	Sidechain
21	AA	1487	G	Sidechain
21	AA	1491	G	Sidechain
21	AA	1495	U	Sidechain
21	AA	1502	A	Sidechain
21	AA	1506	U	Sidechain
21	AA	1510	C	Sidechain
21	AA	1513	A	Sidechain
21	AA	1517	G	Sidechain
21	AA	1519	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1525	G	Sidechain
21	AA	1528	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1530	G	Sidechain
21	AA	1532	U	Sidechain
21	AA	158	G	Sidechain
21	AA	159	G	Sidechain
21	AA	163	C	Sidechain
21	AA	164	G	Sidechain
21	AA	167	A	Sidechain
21	AA	173	U	Sidechain
21	AA	179	A	Sidechain
21	AA	181	A	Sidechain
21	AA	183	C	Sidechain
21	AA	187	G	Sidechain
21	AA	188	C	Sidechain
21	AA	193	C	Sidechain
21	AA	196	A	Sidechain
21	AA	197	A	Sidechain
21	AA	209	U	Sidechain
21	AA	217	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	219	U	Sidechain
21	AA	227	G	Sidechain
21	AA	230	G	Sidechain
21	AA	236	A	Sidechain
21	AA	239	U	Sidechain
21	AA	241	G	Sidechain
21	AA	243	A	Sidechain
21	AA	251	G	Sidechain
21	AA	263	A	Sidechain
21	AA	264	C	Sidechain
21	AA	266	G	Sidechain
21	AA	273	U	Sidechain
21	AA	278	G	Sidechain
21	AA	293	G	Sidechain
21	AA	296	U	Sidechain
21	AA	297	G	Sidechain
21	AA	301	G	Sidechain
21	AA	310	G	Sidechain
21	AA	315	A	Sidechain
21	AA	324	G	Sidechain
21	AA	333	U	Sidechain
21	AA	337	G	Sidechain
21	AA	34	C	Sidechain
21	AA	341	C	Sidechain
21	AA	352	C	Sidechain
21	AA	353	A	Sidechain
21	AA	354	G	Sidechain
21	AA	355	C	Sidechain
21	AA	362	G	Sidechain
21	AA	367	U	Sidechain
21	AA	370	C	Sidechain
21	AA	372	C	Sidechain
21	AA	374	A	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	382	A	Sidechain
21	AA	391	G	Sidechain
21	AA	394	G	Sidechain
21	AA	395	C	Sidechain
21	AA	401	C	Sidechain
21	AA	402	G	Sidechain
21	AA	403	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	404	G	Sidechain
21	AA	407	U	Sidechain
21	AA	41	G	Sidechain
21	AA	414	A	Sidechain
21	AA	415	A	Sidechain
21	AA	416	G	Sidechain
21	AA	429	U	Sidechain
21	AA	430	A	Sidechain
21	AA	431	A	Sidechain
21	AA	433	G	Sidechain
21	AA	438	U	Sidechain
21	AA	440	C	Sidechain
21	AA	441	A	Sidechain
21	AA	442	G	Sidechain
21	AA	445	G	Sidechain
21	AA	449	G	Sidechain
21	AA	450	G	Sidechain
21	AA	466	A	Sidechain
21	AA	467	U	Sidechain
21	AA	470	C	Sidechain
21	AA	474	G	Sidechain
21	AA	479	U	Sidechain
21	AA	481	G	Sidechain
21	AA	484	G	Sidechain
21	AA	487	A	Sidechain
21	AA	492	C	Sidechain
21	AA	494	G	Sidechain
21	AA	497	G	Sidechain
21	AA	499	A	Sidechain
21	AA	502	A	Sidechain
21	AA	51	A	Sidechain
21	AA	512	U	Sidechain
21	AA	513	C	Sidechain
21	AA	515	G	Sidechain
21	AA	516	U	Sidechain
21	AA	517	G	Sidechain
21	AA	523	A	Sidechain
21	AA	524	G	Sidechain
21	AA	529	G	Sidechain
21	AA	533	A	Sidechain
21	AA	537	G	Sidechain
21	AA	541	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	547	A	Sidechain
21	AA	553	A	Sidechain
21	AA	557	G	Sidechain
21	AA	558	G	Sidechain
21	AA	563	A	Sidechain
21	AA	566	G	Sidechain
21	AA	568	G	Sidechain
21	AA	58	C	Sidechain
21	AA	582	C	Sidechain
21	AA	584	G	Sidechain
21	AA	592	G	Sidechain
21	AA	593	U	Sidechain
21	AA	594	U	Sidechain
21	AA	595	A	Sidechain
21	AA	6	G	Sidechain
21	AA	611	C	Sidechain
21	AA	612	C	Sidechain
21	AA	622	A	Sidechain
21	AA	623	C	Sidechain
21	AA	625	U	Sidechain
21	AA	626	G	Sidechain
21	AA	632	U	Sidechain
21	AA	633	G	Sidechain
21	AA	640	A	Sidechain
21	AA	643	C	Sidechain
21	AA	65	A	Sidechain
21	AA	650	G	Sidechain
21	AA	653	U	Sidechain
21	AA	654	G	Sidechain
21	AA	656	G	Sidechain
21	AA	66	A	Sidechain
21	AA	660	C	Sidechain
21	AA	661	G	Sidechain
21	AA	662	U	Sidechain
21	AA	664	G	Sidechain
21	AA	665	A	Sidechain
21	AA	67	C	Sidechain
21	AA	69	G	Sidechain
21	AA	695	A	Sidechain
21	AA	697	U	Sidechain
21	AA	701	U	Sidechain
21	AA	709	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	71	A	Sidechain
21	AA	717	U	Sidechain
21	AA	724	G	Sidechain
21	AA	727	G	Sidechain
21	AA	738	C	Sidechain
21	AA	740	U	Sidechain
21	AA	742	G	Sidechain
21	AA	745	G	Sidechain
21	AA	748	G	Sidechain
21	AA	751	U	Sidechain
21	AA	753	A	Sidechain
21	AA	754	C	Sidechain
21	AA	758	C	Sidechain
21	AA	766	A	Sidechain
21	AA	768	A	Sidechain
21	AA	773	G	Sidechain
21	AA	778	G	Sidechain
21	AA	785	G	Sidechain
21	AA	796	C	Sidechain
21	AA	800	G	Sidechain
21	AA	801	U	Sidechain
21	AA	804	U	Sidechain
21	AA	805	C	Sidechain
21	AA	813	U	Sidechain
21	AA	820	U	Sidechain
21	AA	830	G	Sidechain
21	AA	838	G	Sidechain
21	AA	844	G	Sidechain
21	AA	845	A	Sidechain
21	AA	852	G	Sidechain
21	AA	858	G	Sidechain
21	AA	859	G	Sidechain
21	AA	86	G	Sidechain
21	AA	863	U	Sidechain
21	AA	864	A	Sidechain
21	AA	869	G	Sidechain
21	AA	873	A	Sidechain
21	AA	874	G	Sidechain
21	AA	877	G	Sidechain
21	AA	879	C	Sidechain
21	AA	883	C	Sidechain
21	AA	885	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	886	G	Sidechain
21	AA	89	U	Sidechain
21	AA	891	U	Sidechain
21	AA	898	G	Sidechain
21	AA	90	C	Sidechain
21	AA	901	A	Sidechain
21	AA	902	G	Sidechain
21	AA	906	A	Sidechain
21	AA	907	A	Sidechain
21	AA	909	A	Sidechain
21	AA	91	U	Sidechain
21	AA	916	U	Sidechain
21	AA	919	A	Sidechain
21	AA	925	G	Sidechain
21	AA	926	G	Sidechain
21	AA	927	G	Sidechain
21	AA	932	C	Sidechain
21	AA	933	G	Sidechain
21	AA	938	A	Sidechain
21	AA	940	C	Sidechain
21	AA	941	G	Sidechain
21	AA	942	G	Sidechain
21	AA	946	A	Sidechain
21	AA	952	U	Sidechain
21	AA	954	G	Sidechain
21	AA	957	U	Sidechain
21	AA	967	C	Sidechain
21	AA	97	G	Sidechain
21	AA	972	C	Sidechain
21	AA	973	G	Sidechain
21	AA	976	G	Sidechain
21	AA	977	A	Sidechain
21	AA	98	A	Sidechain
21	AA	983	A	Sidechain
21	AA	987	G	Sidechain
21	AA	991	U	Sidechain
21	AA	994	A	Sidechain
3	AD	3	TYR	Sidechain
3	AD	36	ALA	Peptide
4	AE	148	SER	Peptide
54	BA	1	G	Sidechain
54	BA	1002	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1006	C	Sidechain
54	BA	1008	A	Sidechain
54	BA	101	A	Sidechain
54	BA	1014	A	Sidechain
54	BA	1015	U	Sidechain
54	BA	1016	G	Sidechain
54	BA	1017	G	Sidechain
54	BA	1018	U	Sidechain
54	BA	1019	U	Sidechain
54	BA	1020	A	Sidechain
54	BA	1028	A	Sidechain
54	BA	1030	C	Sidechain
54	BA	1033	U	Sidechain
54	BA	1039	A	Sidechain
54	BA	1044	C	Sidechain
54	BA	1045	C	Sidechain
54	BA	1050	A	Sidechain
54	BA	1051	G	Sidechain
54	BA	1056	G	Sidechain
54	BA	1059	G	Sidechain
54	BA	1069	A	Sidechain
54	BA	1070	A	Sidechain
54	BA	1072	C	Sidechain
54	BA	1077	A	Sidechain
54	BA	1079	C	Sidechain
54	BA	1081	U	Sidechain
54	BA	1089	A	Sidechain
54	BA	109	C	Sidechain
54	BA	1099	G	Sidechain
54	BA	11	C	Sidechain
54	BA	1100	C	Sidechain
54	BA	1107	G	Sidechain
54	BA	1115	G	Sidechain
54	BA	1119	U	Sidechain
54	BA	1125	G	Sidechain
54	BA	1126	A	Sidechain
54	BA	114	U	Sidechain
54	BA	1142	A	Sidechain
54	BA	1144	A	Sidechain
54	BA	1158	C	Sidechain
54	BA	1162	G	Sidechain
54	BA	1167	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1171	G	Sidechain
54	BA	1175	A	Sidechain
54	BA	1184	U	Sidechain
54	BA	1186	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1202	G	Sidechain
54	BA	1210	G	Sidechain
54	BA	1215	G	Sidechain
54	BA	1223	G	Sidechain
54	BA	1224	U	Sidechain
54	BA	1227	G	Sidechain
54	BA	1229	C	Sidechain
54	BA	1234	U	Sidechain
54	BA	1236	G	Sidechain
54	BA	1239	G	Sidechain
54	BA	1251	C	Sidechain
54	BA	1261	C	Sidechain
54	BA	1263	U	Sidechain
54	BA	1265	A	Sidechain
54	BA	1269	A	Sidechain
54	BA	1270	C	Sidechain
54	BA	1273	U	Sidechain
54	BA	1274	A	Sidechain
54	BA	1277	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	129	C	Sidechain
54	BA	1291	C	Sidechain
54	BA	1306	C	Sidechain
54	BA	1315	C	Sidechain
54	BA	1319	C	Sidechain
54	BA	1320	C	Sidechain
54	BA	1325	U	Sidechain
54	BA	1326	U	Sidechain
54	BA	1327	A	Sidechain
54	BA	1331	G	Sidechain
54	BA	1332	G	Sidechain
54	BA	1333	G	Sidechain
54	BA	1334	G	Sidechain
54	BA	134	G	Sidechain
54	BA	1343	G	Sidechain
54	BA	1344	U	Sidechain
54	BA	1355	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1364	G	Sidechain
54	BA	1368	G	Sidechain
54	BA	1370	C	Sidechain
54	BA	1376	C	Sidechain
54	BA	1387	A	Sidechain
54	BA	1390	U	Sidechain
54	BA	1391	U	Sidechain
54	BA	1392	A	Sidechain
54	BA	1398	C	Sidechain
54	BA	1399	C	Sidechain
54	BA	14	A	Sidechain
54	BA	141	G	Sidechain
54	BA	1410	G	Sidechain
54	BA	1419	A	Sidechain
54	BA	142	A	Sidechain
54	BA	1423	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1426	G	Sidechain
54	BA	1427	A	Sidechain
54	BA	1428	C	Sidechain
54	BA	143	C	Sidechain
54	BA	1436	G	Sidechain
54	BA	1438	U	Sidechain
54	BA	1440	U	Sidechain
54	BA	1444	G	Sidechain
54	BA	1448	G	Sidechain
54	BA	1457	U	Sidechain
54	BA	146	A	Sidechain
54	BA	1464	G	Sidechain
54	BA	1465	G	Sidechain
54	BA	1474	U	Sidechain
54	BA	1475	G	Sidechain
54	BA	1478	G	Sidechain
54	BA	1483	G	Sidechain
54	BA	1492	G	Sidechain
54	BA	1493	C	Sidechain
54	BA	1495	A	Sidechain
54	BA	15	G	Sidechain
54	BA	150	U	Sidechain
54	BA	1509	A	Sidechain
54	BA	1515	A	Sidechain
54	BA	1517	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	153	U	Sidechain
54	BA	1530	G	Sidechain
54	BA	1531	C	Sidechain
54	BA	1534	U	Sidechain
54	BA	1540	G	Sidechain
54	BA	1544	A	Sidechain
54	BA	1546	G	Sidechain
54	BA	1548	A	Sidechain
54	BA	1552	A	Sidechain
54	BA	1554	U	Sidechain
54	BA	1555	G	Sidechain
54	BA	1559	U	Sidechain
54	BA	1561	C	Sidechain
54	BA	1565	C	Sidechain
54	BA	1567	G	Sidechain
54	BA	1569	A	Sidechain
54	BA	1573	G	Sidechain
54	BA	1581	G	Sidechain
54	BA	1584	U	Sidechain
54	BA	1585	C	Sidechain
54	BA	1592	C	Sidechain
54	BA	1598	A	Sidechain
54	BA	1602	U	Sidechain
54	BA	1612	C	Sidechain
54	BA	1613	G	Sidechain
54	BA	1617	C	Sidechain
54	BA	1628	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1642	G	Sidechain
54	BA	1646	C	Sidechain
54	BA	1652	A	Sidechain
54	BA	1653	G	Sidechain
54	BA	1656	C	Sidechain
54	BA	1664	A	Sidechain
54	BA	1667	G	Sidechain
54	BA	168	G	Sidechain
54	BA	1680	U	Sidechain
54	BA	1681	G	Sidechain
54	BA	1684	G	Sidechain
54	BA	169	G	Sidechain
54	BA	1692	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1696	G	Sidechain
54	BA	1699	G	Sidechain
54	BA	1705	A	Sidechain
54	BA	1706	C	Sidechain
54	BA	1707	G	Sidechain
54	BA	1709	U	Sidechain
54	BA	171	U	Sidechain
54	BA	1711	A	Sidechain
54	BA	1714	U	Sidechain
54	BA	1716	U	Sidechain
54	BA	1723	G	Sidechain
54	BA	1725	U	Sidechain
54	BA	1729	U	Sidechain
54	BA	173	A	Sidechain
54	BA	1737	G	Sidechain
54	BA	1738	G	Sidechain
54	BA	1743	G	Sidechain
54	BA	1744	A	Sidechain
54	BA	1747	U	Sidechain
54	BA	1753	G	Sidechain
54	BA	1759	A	Sidechain
54	BA	177	G	Sidechain
54	BA	1772	A	Sidechain
54	BA	1774	C	Sidechain
54	BA	1778	U	Sidechain
54	BA	1779	U	Sidechain
54	BA	1789	A	Sidechain
54	BA	179	C	Sidechain
54	BA	1792	G	Sidechain
54	BA	1797	G	Sidechain
54	BA	1798	U	Sidechain
54	BA	180	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1803	A	Sidechain
54	BA	1804	C	Sidechain
54	BA	1808	A	Sidechain
54	BA	1821	A	Sidechain
54	BA	1823	G	Sidechain
54	BA	1837	C	Sidechain
54	BA	1838	C	Sidechain
54	BA	1840	G	Sidechain
54	BA	1845	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1852	U	Sidechain
54	BA	1854	A	Sidechain
54	BA	1859	U	Sidechain
54	BA	1865	U	Sidechain
54	BA	1869	G	Sidechain
54	BA	187	G	Sidechain
54	BA	1884	G	Sidechain
54	BA	1887	C	Sidechain
54	BA	1890	A	Sidechain
54	BA	1891	G	Sidechain
54	BA	1892	C	Sidechain
54	BA	1893	C	Sidechain
54	BA	1896	G	Sidechain
54	BA	1897	G	Sidechain
54	BA	1903	G	Sidechain
54	BA	1908	C	Sidechain
54	BA	1912	A	Sidechain
54	BA	1913	A	Sidechain
54	BA	1915	U	Sidechain
54	BA	1918	A	Sidechain
54	BA	1919	A	Sidechain
54	BA	1927	A	Sidechain
54	BA	193	U	Sidechain
54	BA	1935	G	Sidechain
54	BA	1938	A	Sidechain
54	BA	194	G	Sidechain
54	BA	1941	C	Sidechain
54	BA	1942	C	Sidechain
54	BA	1945	G	Sidechain
54	BA	1946	U	Sidechain
54	BA	1948	G	Sidechain
54	BA	1952	A	Sidechain
54	BA	1955	U	Sidechain
54	BA	196	A	Sidechain
54	BA	1964	G	Sidechain
54	BA	1967	C	Sidechain
54	BA	1968	G	Sidechain
54	BA	1971	U	Sidechain
54	BA	1975	G	Sidechain
54	BA	1976	U	Sidechain
54	BA	1978	A	Sidechain
54	BA	1993	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1995	U	Sidechain
54	BA	1997	C	Sidechain
54	BA	1998	A	Sidechain
54	BA	200	U	Sidechain
54	BA	2005	A	Sidechain
54	BA	2006	C	Sidechain
54	BA	2007	U	Sidechain
54	BA	2010	G	Sidechain
54	BA	2012	G	Sidechain
54	BA	2016	U	Sidechain
54	BA	2022	U	Sidechain
54	BA	2024	G	Sidechain
54	BA	2029	G	Sidechain
54	BA	2034	U	Sidechain
54	BA	2037	A	Sidechain
54	BA	204	A	Sidechain
54	BA	2044	C	Sidechain
54	BA	2047	C	Sidechain
54	BA	2049	G	Sidechain
54	BA	205	G	Sidechain
54	BA	2050	C	Sidechain
54	BA	2052	A	Sidechain
54	BA	2054	A	Sidechain
54	BA	2056	G	Sidechain
54	BA	206	U	Sidechain
54	BA	2063	C	Sidechain
54	BA	2065	C	Sidechain
54	BA	2068	U	Sidechain
54	BA	207	A	Sidechain
54	BA	2071	A	Sidechain
54	BA	2074	U	Sidechain
54	BA	2076	U	Sidechain
54	BA	2078	C	Sidechain
54	BA	2080	A	Sidechain
54	BA	2086	U	Sidechain
54	BA	2093	G	Sidechain
54	BA	2095	A	Sidechain
54	BA	2103	C	Sidechain
54	BA	2113	U	Sidechain
54	BA	2116	G	Sidechain
54	BA	2123	G	Sidechain
54	BA	2132	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2134	A	Sidechain
54	BA	2147	A	Sidechain
54	BA	215	G	Sidechain
54	BA	2152	G	Sidechain
54	BA	2157	G	Sidechain
54	BA	2158	A	Sidechain
54	BA	2160	C	Sidechain
54	BA	2161	C	Sidechain
54	BA	2163	A	Sidechain
54	BA	2165	C	Sidechain
54	BA	2166	U	Sidechain
54	BA	2168	G	Sidechain
54	BA	218	A	Sidechain
54	BA	2181	U	Sidechain
54	BA	2186	G	Sidechain
54	BA	2193	G	Sidechain
54	BA	2196	C	Sidechain
54	BA	2203	U	Sidechain
54	BA	2205	A	Sidechain
54	BA	2207	C	Sidechain
54	BA	221	A	Sidechain
54	BA	2210	U	Sidechain
54	BA	2212	A	Sidechain
54	BA	2215	C	Sidechain
54	BA	2224	G	Sidechain
54	BA	2226	C	Sidechain
54	BA	2228	G	Sidechain
54	BA	2230	G	Sidechain
54	BA	2236	U	Sidechain
54	BA	2242	G	Sidechain
54	BA	2249	U	Sidechain
54	BA	2250	G	Sidechain
54	BA	2252	G	Sidechain
54	BA	2257	U	Sidechain
54	BA	2260	C	Sidechain
54	BA	2262	U	Sidechain
54	BA	2264	C	Sidechain
54	BA	227	A	Sidechain
54	BA	2271	G	Sidechain
54	BA	2282	G	Sidechain
54	BA	2286	G	Sidechain
54	BA	2293	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2297	A	Sidechain
54	BA	2299	U	Sidechain
54	BA	2304	G	Sidechain
54	BA	2306	C	Sidechain
54	BA	2309	A	Sidechain
54	BA	2310	C	Sidechain
54	BA	232	G	Sidechain
54	BA	2321	U	Sidechain
54	BA	2323	G	Sidechain
54	BA	2324	U	Sidechain
54	BA	2325	G	Sidechain
54	BA	2327	A	Sidechain
54	BA	2328	A	Sidechain
54	BA	2336	A	Sidechain
54	BA	235	U	Sidechain
54	BA	2352	A	Sidechain
54	BA	2358	A	Sidechain
54	BA	236	C	Sidechain
54	BA	2375	G	Sidechain
54	BA	2376	A	Sidechain
54	BA	238	C	Sidechain
54	BA	2384	U	Sidechain
54	BA	2387	U	Sidechain
54	BA	2391	G	Sidechain
54	BA	2397	G	Sidechain
54	BA	2398	U	Sidechain
54	BA	240	C	Sidechain
54	BA	2415	G	Sidechain
54	BA	2418	A	Sidechain
54	BA	2421	G	Sidechain
54	BA	2422	C	Sidechain
54	BA	2431	U	Sidechain
54	BA	2432	A	Sidechain
54	BA	2437	G	Sidechain
54	BA	244	A	Sidechain
54	BA	2440	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2445	G	Sidechain
54	BA	2446	G	Sidechain
54	BA	2449	U	Sidechain
54	BA	2453	A	Sidechain
54	BA	2455	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2458	G	Sidechain
54	BA	2461	A	Sidechain
54	BA	2462	C	Sidechain
54	BA	2468	A	Sidechain
54	BA	2469	A	Sidechain
54	BA	247	G	Sidechain
54	BA	2474	U	Sidechain
54	BA	2475	C	Sidechain
54	BA	2476	A	Sidechain
54	BA	2486	C	Sidechain
54	BA	2487	G	Sidechain
54	BA	2488	G	Sidechain
54	BA	2499	C	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2502	G	Sidechain
54	BA	2506	U	Sidechain
54	BA	2507	C	Sidechain
54	BA	2509	G	Sidechain
54	BA	251	A	Sidechain
54	BA	2513	A	Sidechain
54	BA	2516	A	Sidechain
54	BA	2524	G	Sidechain
54	BA	2529	G	Sidechain
54	BA	2530	A	Sidechain
54	BA	2541	A	Sidechain
54	BA	2550	G	Sidechain
54	BA	2552	U	Sidechain
54	BA	2557	G	Sidechain
54	BA	2560	A	Sidechain
54	BA	2562	U	Sidechain
54	BA	2572	A	Sidechain
54	BA	2574	G	Sidechain
54	BA	2575	C	Sidechain
54	BA	2579	C	Sidechain
54	BA	2580	U	Sidechain
54	BA	2587	A	Sidechain
54	BA	2588	G	Sidechain
54	BA	2597	G	Sidechain
54	BA	2602	A	Sidechain
54	BA	2608	G	Sidechain
54	BA	2609	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2618	G	Sidechain
54	BA	2627	G	Sidechain
54	BA	2628	C	Sidechain
54	BA	2630	G	Sidechain
54	BA	2631	G	Sidechain
54	BA	2637	U	Sidechain
54	BA	2639	A	Sidechain
54	BA	2640	G	Sidechain
54	BA	2643	G	Sidechain
54	BA	2647	U	Sidechain
54	BA	2648	G	Sidechain
54	BA	2650	U	Sidechain
54	BA	2654	A	Sidechain
54	BA	2659	G	Sidechain
54	BA	2660	A	Sidechain
54	BA	2661	G	Sidechain
54	BA	2664	G	Sidechain
54	BA	267	C	Sidechain
54	BA	2678	C	Sidechain
54	BA	2682	A	Sidechain
54	BA	2683	C	Sidechain
54	BA	2686	G	Sidechain
54	BA	2695	U	Sidechain
54	BA	2700	A	Sidechain
54	BA	2711	A	Sidechain
54	BA	2713	U	Sidechain
54	BA	2720	U	Sidechain
54	BA	2723	C	Sidechain
54	BA	273	G	Sidechain
54	BA	274	C	Sidechain
54	BA	2753	A	Sidechain
54	BA	2756	U	Sidechain
54	BA	2759	G	Sidechain
54	BA	2760	C	Sidechain
54	BA	2762	C	Sidechain
54	BA	2763	G	Sidechain
54	BA	2765	A	Sidechain
54	BA	277	G	Sidechain
54	BA	2771	C	Sidechain
54	BA	2777	G	Sidechain
54	BA	278	A	Sidechain
54	BA	2780	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2783	U	Sidechain
54	BA	2788	C	Sidechain
54	BA	2797	U	Sidechain
54	BA	2798	U	Sidechain
54	BA	2799	A	Sidechain
54	BA	2806	C	Sidechain
54	BA	2816	G	Sidechain
54	BA	282	A	Sidechain
54	BA	2829	A	Sidechain
54	BA	2832	U	Sidechain
54	BA	2836	U	Sidechain
54	BA	2840	C	Sidechain
54	BA	2844	G	Sidechain
54	BA	2854	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2862	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	287	G	Sidechain
54	BA	2872	A	Sidechain
54	BA	2874	C	Sidechain
54	BA	2883	A	Sidechain
54	BA	2885	G	Sidechain
54	BA	2893	A	Sidechain
54	BA	2899	A	Sidechain
54	BA	29	U	Sidechain
54	BA	2900	A	Sidechain
54	BA	291	G	Sidechain
54	BA	293	U	Sidechain
54	BA	30	G	Sidechain
54	BA	304	U	Sidechain
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	310	A	Sidechain
54	BA	313	G	Sidechain
54	BA	314	C	Sidechain
54	BA	316	C	Sidechain
54	BA	319	G	Sidechain
54	BA	327	G	Sidechain
54	BA	328	U	Sidechain
54	BA	344	A	Sidechain
54	BA	352	A	Sidechain
54	BA	354	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	360	U	Sidechain
54	BA	361	G	Sidechain
54	BA	364	C	Sidechain
54	BA	365	U	Sidechain
54	BA	370	G	Sidechain
54	BA	374	A	Sidechain
54	BA	385	C	Sidechain
54	BA	389	G	Sidechain
54	BA	392	U	Sidechain
54	BA	395	U	Sidechain
54	BA	417	C	Sidechain
54	BA	418	C	Sidechain
54	BA	426	C	Sidechain
54	BA	429	A	Sidechain
54	BA	43	G	Sidechain
54	BA	44	A	Sidechain
54	BA	441	U	Sidechain
54	BA	443	A	Sidechain
54	BA	449	A	Sidechain
54	BA	452	G	Sidechain
54	BA	462	C	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	475	C	Sidechain
54	BA	477	A	Sidechain
54	BA	479	A	Sidechain
54	BA	48	G	Sidechain
54	BA	487	C	Sidechain
54	BA	488	G	Sidechain
54	BA	49	A	Sidechain
54	BA	494	G	Sidechain
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain
54	BA	502	A	Sidechain
54	BA	506	G	Sidechain
54	BA	511	U	Sidechain
54	BA	519	U	Sidechain
54	BA	521	U	Sidechain
54	BA	524	G	Sidechain
54	BA	526	A	Sidechain
54	BA	529	A	Sidechain
54	BA	532	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	54	G	Sidechain
54	BA	542	C	Sidechain
54	BA	556	A	Sidechain
54	BA	561	G	Sidechain
54	BA	563	A	Sidechain
54	BA	565	C	Sidechain
54	BA	567	U	Sidechain
54	BA	568	U	Sidechain
54	BA	571	U	Sidechain
54	BA	572	A	Sidechain
54	BA	575	A	Sidechain
54	BA	577	G	Sidechain
54	BA	579	G	Sidechain
54	BA	580	U	Sidechain
54	BA	581	C	Sidechain
54	BA	585	G	Sidechain
54	BA	586	A	Sidechain
54	BA	597	G	Sidechain
54	BA	600	G	Sidechain
54	BA	608	A	Sidechain
54	BA	617	G	Sidechain
54	BA	628	G	Sidechain
54	BA	629	G	Sidechain
54	BA	63	A	Sidechain
54	BA	630	G	Sidechain
54	BA	631	A	Sidechain
54	BA	633	A	Sidechain
54	BA	64	A	Sidechain
54	BA	640	C	Sidechain
54	BA	641	U	Sidechain
54	BA	646	U	Sidechain
54	BA	647	G	Sidechain
54	BA	653	U	Sidechain
54	BA	659	G	Sidechain
54	BA	671	C	Sidechain
54	BA	672	C	Sidechain
54	BA	675	A	Sidechain
54	BA	680	C	Sidechain
54	BA	688	U	Sidechain
54	BA	689	A	Sidechain
54	BA	70	G	Sidechain
54	BA	706	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	718	A	Sidechain
54	BA	723	C	Sidechain
54	BA	724	U	Sidechain
54	BA	726	G	Sidechain
54	BA	729	G	Sidechain
54	BA	732	C	Sidechain
54	BA	733	G	Sidechain
54	BA	738	G	Sidechain
54	BA	74	A	Sidechain
54	BA	748	G	Sidechain
54	BA	755	U	Sidechain
54	BA	759	G	Sidechain
54	BA	765	C	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain
54	BA	776	G	Sidechain
54	BA	780	G	Sidechain
54	BA	784	G	Sidechain
54	BA	789	A	Sidechain
54	BA	800	A	Sidechain
54	BA	804	A	Sidechain
54	BA	809	G	Sidechain
54	BA	810	U	Sidechain
54	BA	813	U	Sidechain
54	BA	818	G	Sidechain
54	BA	822	G	Sidechain
54	BA	828	U	Sidechain
54	BA	833	A	Sidechain
54	BA	837	C	Sidechain
54	BA	841	G	Sidechain
54	BA	845	A	Sidechain
54	BA	846	U	Sidechain
54	BA	847	U	Sidechain
54	BA	848	C	Sidechain
54	BA	85	G	Sidechain
54	BA	854	C	Sidechain
54	BA	858	G	Sidechain
54	BA	862	G	Sidechain
54	BA	866	A	Sidechain
54	BA	869	G	Sidechain
54	BA	870	U	Sidechain
54	BA	883	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	884	U	Sidechain
54	BA	89	A	Sidechain
54	BA	890	C	Sidechain
54	BA	894	U	Sidechain
54	BA	9	G	Sidechain
54	BA	901	C	Sidechain
54	BA	904	G	Sidechain
54	BA	912	C	Sidechain
54	BA	918	A	Sidechain
54	BA	922	C	Sidechain
54	BA	923	G	Sidechain
54	BA	932	U	Sidechain
54	BA	935	C	Sidechain
54	BA	94	A	Sidechain
54	BA	942	G	Sidechain
54	BA	944	C	Sidechain
54	BA	945	A	Sidechain
54	BA	954	G	Sidechain
54	BA	959	A	Sidechain
54	BA	96	C	Sidechain
54	BA	964	C	Sidechain
54	BA	967	U	Sidechain
54	BA	969	G	Sidechain
54	BA	973	A	Sidechain
54	BA	974	G	Sidechain
54	BA	982	C	Sidechain
54	BA	988	A	Sidechain
54	BA	989	G	Sidechain
54	BA	99	U	Sidechain
54	BA	993	G	Sidechain
54	BA	999	U	Sidechain
55	BB	10	G	Sidechain
55	BB	108	A	Sidechain
55	BB	109	A	Sidechain
55	BB	111	U	Sidechain
55	BB	112	G	Sidechain
55	BB	18	G	Sidechain
55	BB	23	G	Sidechain
55	BB	24	G	Sidechain
55	BB	27	C	Sidechain
55	BB	3	C	Sidechain
55	BB	30	C	Sidechain

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Mol	Chain	Res	Type	Group
55	BB	31	C	Sidechain
55	BB	32	U	Sidechain
55	BB	40	U	Sidechain
55	BB	41	G	Sidechain
55	BB	42	C	Sidechain
55	BB	43	C	Sidechain
55	BB	48	U	Sidechain
55	BB	49	C	Sidechain
55	BB	57	A	Sidechain
55	BB	58	A	Sidechain
55	BB	6	G	Sidechain
55	BB	60	C	Sidechain
55	BB	66	A	Sidechain
55	BB	75	G	Sidechain
55	BB	84	G	Sidechain
55	BB	88	C	Sidechain
55	BB	92	C	Sidechain
55	BB	93	C	Sidechain
55	BB	94	A	Sidechain
55	BB	99	A	Sidechain
25	BC	42	ARG	Sidechain
38	BP	113	LEU	Mainchain

5.2 Too-close contacts ⓘ

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	1	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16522	4	0
22	A1	1627	0	832	1	0
23	A2	309	0	156	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	1	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	1	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	BA	62317	0	31339	3	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99657	11	0

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

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.76	0.51
21:AA:730:G:C5	21:AA:731:G:H1'	2.48	0.48
6:AG:148:LYS:HE3	10:AK:60:PHE:CZ	2.48	0.47
26:BD:125:TRP:CE3	26:BD:160:LYS:HE3	2.48	0.47
29:BG:1:SER:HA	54:BA:2749:A:OP1	2.18	0.43
54:BA:1760:C:H5''	54:BA:1761:C:C5	2.55	0.42
21:AA:22:G:H4'	21:AA:885:G:C8	2.55	0.42
21:AA:1063:C:H2'	21:AA:1064:G:C8	2.55	0.42
14:AO:50:HIS:CD2	21:AA:666:G:H21	2.38	0.41
22:A1:54:5MU:H73	22:A1:55:PSU:O2	2.20	0.41
54:BA:616:A:HO2'	54:BA:617:G:H8	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AB	218/220 (99%)	202 (93%)	15 (7%)	1 (0%)	34 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	205/208 (99%)	190 (93%)	12 (6%)	3 (2%)	13	57
3	AD	203/206 (98%)	189 (93%)	10 (5%)	4 (2%)	9	51
4	AE	150/152 (99%)	135 (90%)	11 (7%)	4 (3%)	6	45
5	AF	99/101 (98%)	90 (91%)	4 (4%)	5 (5%)	2	30
6	AG	150/152 (99%)	130 (87%)	18 (12%)	2 (1%)	15	60
7	AH	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	24	69
8	AI	126/128 (98%)	114 (90%)	11 (9%)	1 (1%)	24	69
9	AJ	98/100 (98%)	92 (94%)	3 (3%)	3 (3%)	5	42
10	AK	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	21	67
11	AL	121/124 (98%)	108 (89%)	11 (9%)	2 (2%)	11	55
12	AM	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	11	53
13	AN	98/101 (97%)	90 (92%)	6 (6%)	2 (2%)	9	51
14	AO	86/89 (97%)	76 (88%)	7 (8%)	3 (4%)	4	39
15	AP	79/81 (98%)	65 (82%)	11 (14%)	3 (4%)	4	37
16	AQ	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	7	46
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	11	53
18	AS	79/81 (98%)	73 (92%)	5 (6%)	1 (1%)	15	60
19	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	AU	51/53 (96%)	36 (71%)	12 (24%)	3 (6%)	2	27
25	BC	270/273 (99%)	241 (89%)	22 (8%)	7 (3%)	7	45
26	BD	207/209 (99%)	172 (83%)	20 (10%)	15 (7%)	1	22
27	BE	199/201 (99%)	179 (90%)	17 (8%)	3 (2%)	13	57
28	BF	176/179 (98%)	142 (81%)	25 (14%)	9 (5%)	2	30
29	BG	174/177 (98%)	156 (90%)	15 (9%)	3 (2%)	11	55
30	BH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	5	40
31	BI	139/142 (98%)	128 (92%)	9 (6%)	2 (1%)	14	58
32	BJ	140/142 (99%)	128 (91%)	10 (7%)	2 (1%)	14	58
33	BK	121/123 (98%)	102 (84%)	15 (12%)	4 (3%)	5	40
34	BL	141/144 (98%)	111 (79%)	19 (14%)	11 (8%)	1	20
35	BM	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	8	49
36	BN	119/121 (98%)	108 (91%)	9 (8%)	2 (2%)	11	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BO	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
38	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	6	45
39	BQ	115/118 (98%)	103 (90%)	9 (8%)	3 (3%)	7	45
40	BR	101/103 (98%)	92 (91%)	7 (7%)	2 (2%)	9	51
41	BS	108/110 (98%)	95 (88%)	13 (12%)	0	100	100
42	BT	92/94 (98%)	77 (84%)	12 (13%)	3 (3%)	5	40
43	BU	101/104 (97%)	83 (82%)	12 (12%)	6 (6%)	2	27
44	BV	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	17	63
45	BW	78/80 (98%)	64 (82%)	10 (13%)	4 (5%)	2	30
46	BX	75/79 (95%)	66 (88%)	8 (11%)	1 (1%)	15	60
47	BY	61/63 (97%)	54 (88%)	6 (10%)	1 (2%)	12	56
48	BZ	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	2	29
49	B0	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
50	B1	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1	19
51	B2	44/46 (96%)	38 (86%)	5 (11%)	1 (2%)	8	48
52	B3	62/65 (95%)	55 (89%)	7 (11%)	0	100	100
53	B4	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	2	28
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	34	77
All	All	5876/6008 (98%)	5234 (89%)	497 (8%)	145 (2%)	11	46

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	AH	105	THR
9	AJ	74	VAL
12	AM	65	GLU
14	AO	45	HIS
16	AQ	39	ARG
25	BC	191	LEU
26	BD	51	THR
33	BK	103	VAL
34	BL	21	ARG
34	BL	101	ILE
35	BM	135	VAL
38	BP	63	ILE
43	BU	43	LYS

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Mol	Chain	Res	Type
43	BU	70	ALA
44	BV	14	LYS
48	BZ	31	ILE
50	B1	36	LYS
2	AC	171	ARG
2	AC	195	ILE
4	AE	105	ILE
5	AF	63	ASN
5	AF	90	MET
8	AI	57	VAL
9	AJ	57	VAL
9	AJ	75	ASP
12	AM	42	VAL
13	AN	63	ARG
15	AP	11	ALA
25	BC	161	VAL
26	BD	80	TRP
26	BD	203	VAL
28	BF	133	GLU
28	BF	176	PHE
29	BG	9	VAL
29	BG	151	ARG
31	BI	12	VAL
32	BJ	81	ILE
38	BP	2	ASN
38	BP	26	GLU
39	BQ	90	ASP
42	BT	11	LEU
43	BU	12	VAL
43	BU	85	ARG
43	BU	102	ILE
46	BX	34	SER
53	B4	16	ILE
3	AD	29	THR
5	AF	36	ILE
5	AF	39	LEU
6	AG	2	ARG
10	AK	49	SER
11	AL	33	CYS
14	AO	43	ALA
15	AP	17	TYR
17	AR	69	TYR

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Mol	Chain	Res	Type
20	AU	34	ARG
20	AU	35	GLU
26	BD	7	LYS
26	BD	49	GLN
26	BD	82	PHE
26	BD	149	ASN
28	BF	87	LYS
28	BF	136	ILE
29	BG	16	VAL
30	BH	104	THR
33	BK	2	ILE
34	BL	29	LYS
36	BN	3	HIS
39	BQ	5	ARG
39	BQ	91	ARG
40	BR	9	GLY
40	BR	53	PHE
42	BT	63	VAL
42	BT	88	LYS
43	BU	59	GLU
45	BW	53	GLY
47	BY	9	LYS
56	B5	91	GLY
3	AD	204	SER
4	AE	43	GLY
4	AE	106	ALA
20	AU	4	LYS
25	BC	153	LEU
26	BD	34	VAL
26	BD	144	GLY
26	BD	201	LEU
27	BE	147	LEU
30	BH	10	ALA
30	BH	39	ALA
33	BK	32	TYR
34	BL	30	THR
34	BL	68	SER
35	BM	2	LEU
35	BM	21	ALA
36	BN	104	ALA
45	BW	23	LYS
45	BW	38	ARG

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Mol	Chain	Res	Type
48	BZ	9	THR
48	BZ	30	ARG
50	B1	6	GLU
51	B2	44	VAL
1	AB	129	THR
2	AC	14	VAL
3	AD	203	TYR
5	AF	6	ILE
11	AL	78	VAL
13	AN	38	ASP
15	AP	40	ASN
18	AS	79	TYR
25	BC	144	GLU
26	BD	43	ASP
26	BD	119	ALA
27	BE	165	HIS
28	BF	155	ILE
30	BH	88	GLY
30	BH	121	VAL
32	BJ	72	LYS
33	BK	25	LEU
34	BL	36	LYS
34	BL	66	PHE
53	B4	2	LYS
4	AE	54	GLU
6	AG	74	VAL
14	AO	18	ALA
25	BC	185	ALA
26	BD	37	VAL
26	BD	138	LEU
27	BE	160	ALA
34	BL	12	SER
34	BL	55	MET
45	BW	16	GLU
50	B1	45	HIS
50	B1	50	GLU
3	AD	41	GLY
25	BC	123	ILE
26	BD	5	VAL
31	BI	18	ASN
34	BL	130	GLY
16	AQ	82	VAL

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Mol	Chain	Res	Type
28	BF	12	VAL
28	BF	88	VAL
25	BC	253	GLY
28	BF	103	ILE
34	BL	65	GLY
28	BF	175	PRO

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%)	180 (100%)	0	100	100
2	AC	170/171 (99%)	170 (100%)	0	100	100
3	AD	172/173 (99%)	172 (100%)	0	100	100
4	AE	113/113 (100%)	112 (99%)	1 (1%)	84	93
5	AF	87/87 (100%)	85 (98%)	2 (2%)	58	83
6	AG	123/123 (100%)	121 (98%)	2 (2%)	70	88
7	AH	104/105 (99%)	103 (99%)	1 (1%)	82	92
8	AI	105/105 (100%)	104 (99%)	1 (1%)	82	92
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	101 (98%)	2 (2%)	65	86
12	AM	91/92 (99%)	90 (99%)	1 (1%)	80	91
13	AN	83/84 (99%)	78 (94%)	5 (6%)	24	60
14	AO	76/77 (99%)	76 (100%)	0	100	100
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	52	79
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	70 (100%)	0	100	100
19	AT	65/65 (100%)	64 (98%)	1 (2%)	72	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AU	44/44 (100%)	42 (96%)	2 (4%)	34	69
25	BC	216/217 (100%)	214 (99%)	2 (1%)	84	93
26	BD	164/164 (100%)	162 (99%)	2 (1%)	78	90
27	BE	165/165 (100%)	156 (94%)	9 (6%)	27	63
28	BF	149/150 (99%)	146 (98%)	3 (2%)	63	85
29	BG	137/138 (99%)	135 (98%)	2 (2%)	72	88
30	BH	114/114 (100%)	112 (98%)	2 (2%)	66	87
31	BI	109/110 (99%)	107 (98%)	2 (2%)	66	87
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	68	87
33	BK	103/103 (100%)	102 (99%)	1 (1%)	82	92
34	BL	102/103 (99%)	100 (98%)	2 (2%)	63	85
35	BM	109/109 (100%)	106 (97%)	3 (3%)	51	78
36	BN	100/100 (100%)	98 (98%)	2 (2%)	63	85
37	BO	86/87 (99%)	85 (99%)	1 (1%)	78	90
38	BP	99/100 (99%)	98 (99%)	1 (1%)	82	92
39	BQ	89/90 (99%)	89 (100%)	0	100	100
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	92 (99%)	1 (1%)	80	91
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	57	82
44	BV	78/78 (100%)	76 (97%)	2 (3%)	54	80
45	BW	59/59 (100%)	57 (97%)	2 (3%)	44	75
46	BX	67/68 (98%)	64 (96%)	3 (4%)	34	69
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	47 (98%)	1 (2%)	61	84
49	B0	47/48 (98%)	46 (98%)	1 (2%)	61	84
50	B1	45/45 (100%)	44 (98%)	1 (2%)	60	83
51	B2	38/38 (100%)	37 (97%)	1 (3%)	54	80
52	B3	51/52 (98%)	50 (98%)	1 (2%)	63	85
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	170 (98%)	3 (2%)	68	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4842/4870 (99%)	4769 (98%)	73 (2%)	74 88

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AE	47	PHE
5	AF	52	ASN
5	AF	68	GLN
6	AG	65	LEU
6	AG	102	TRP
7	AH	66	GLN
8	AI	56	MET
11	AL	94	TYR
11	AL	113	ARG
12	AM	96	VAL
13	AN	3	LYS
13	AN	38	ASP
13	AN	42	TRP
13	AN	62	ASN
13	AN	101	TRP
16	AQ	20	ILE
16	AQ	64	ARG
19	AT	25	SER
20	AU	6	ARG
20	AU	13	VAL
25	BC	57	HIS
25	BC	188	ARG
26	BD	91	THR
26	BD	154	LYS
27	BE	7	ASP
27	BE	33	VAL
27	BE	47	LYS
27	BE	53	THR
27	BE	99	LYS
27	BE	105	LEU
27	BE	147	LEU
27	BE	163	ASN
27	BE	187	VAL
28	BF	12	VAL
28	BF	80	GLN
28	BF	151	LEU
29	BG	37	ASN

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Mol	Chain	Res	Type
29	BG	103	ASN
30	BH	44	ILE
30	BH	135	HIS
31	BI	67	THR
31	BI	89	SER
32	BJ	43	GLU
32	BJ	47	HIS
33	BK	32	TYR
34	BL	79	LEU
34	BL	104	GLN
35	BM	96	ILE
35	BM	97	GLN
35	BM	126	ILE
36	BN	1	MET
36	BN	18	GLN
37	BO	38	GLN
38	BP	50	ARG
40	BR	27	ILE
41	BS	33	LEU
43	BU	44	HIS
43	BU	61	GLU
44	BV	44	HIS
44	BV	51	GLN
45	BW	23	LYS
45	BW	35	ILE
46	BX	26	ARG
46	BX	31	ASN
46	BX	65	THR
48	BZ	33	HIS
49	B0	45	ASP
50	B1	39	ASP
51	B2	43	THR
52	B3	33	THR
56	B5	18	THR
56	B5	40	GLU
56	B5	165	ASN

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

Mol	Chain	Res	Type
10	AK	23	HIS
34	BL	35	HIS

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Mol	Chain	Res	Type
44	BV	88	HIS
49	B0	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	251 (16%)	84 (5%)
22	A1	73/76 (96%)	10 (13%)	4 (5%)
23	A2	14/15 (93%)	8 (57%)	2 (14%)
24	A3	76/77 (98%)	13 (17%)	2 (2%)
54	BA	2902/2903 (99%)	462 (15%)	119 (4%)
55	BB	117/118 (99%)	18 (15%)	6 (5%)
All	All	4712/4722 (99%)	762 (16%)	217 (4%)

All (762) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	16	A
21	AA	17	U
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	50	A
21	AA	51	A
21	AA	52	C
21	AA	66	A
21	AA	67	C
21	AA	83	C
21	AA	84	U
21	AA	85	U
21	AA	86	G
21	AA	87	C
21	AA	109	A
21	AA	110	C
21	AA	120	A
21	AA	122	G

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Mol	Chain	Res	Type
21	AA	163	C
21	AA	182	A
21	AA	183	C
21	AA	184	G
21	AA	191	G
21	AA	194	C
21	AA	195	A
21	AA	198	G
21	AA	211	G
21	AA	212	G
21	AA	237	G
21	AA	240	G
21	AA	245	U
21	AA	247	G
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	267	C
21	AA	280	C
21	AA	289	G
21	AA	306	A
21	AA	329	A
21	AA	330	C
21	AA	332	G
21	AA	346	G
21	AA	347	G
21	AA	351	G
21	AA	352	C
21	AA	354	G
21	AA	357	G
21	AA	358	U
21	AA	361	G
21	AA	366	A
21	AA	367	U
21	AA	368	U
21	AA	372	C
21	AA	373	A
21	AA	381	C
21	AA	392	C
21	AA	397	A
21	AA	398	U
21	AA	411	A

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Mol	Chain	Res	Type
21	AA	412	A
21	AA	414	A
21	AA	415	A
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	446	G
21	AA	452	A
21	AA	455	G
21	AA	456	A
21	AA	461	A
21	AA	462	G
21	AA	463	U
21	AA	464	U
21	AA	467	U
21	AA	468	A
21	AA	476	U
21	AA	477	C
21	AA	481	G
21	AA	482	A
21	AA	484	G
21	AA	497	G
21	AA	500	G
21	AA	510	A
21	AA	511	C
21	AA	512	U
21	AA	514	C
21	AA	527	G
21	AA	532	A
21	AA	547	A
21	AA	559	A
21	AA	564	C
21	AA	565	U
21	AA	567	G
21	AA	572	A
21	AA	573	A
21	AA	576	C
21	AA	611	C
21	AA	612	C
21	AA	632	U
21	AA	665	A
21	AA	675	A

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Mol	Chain	Res	Type
21	AA	676	A
21	AA	700	G
21	AA	701	U
21	AA	702	A
21	AA	703	G
21	AA	704	A
21	AA	705	G
21	AA	718	A
21	AA	719	C
21	AA	721	G
21	AA	722	G
21	AA	723	U
21	AA	724	G
21	AA	755	G
21	AA	767	A
21	AA	777	A
21	AA	794	A
21	AA	812	G
21	AA	817	C
21	AA	819	A
21	AA	821	G
21	AA	828	U
21	AA	840	C
21	AA	841	C
21	AA	845	A
21	AA	846	G
21	AA	869	G
21	AA	872	A
21	AA	873	A
21	AA	876	C
21	AA	899	C
21	AA	902	G
21	AA	914	A
21	AA	920	U
21	AA	926	G
21	AA	927	G
21	AA	934	C
21	AA	935	A
21	AA	936	C
21	AA	939	G
21	AA	945	G
21	AA	958	A

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Mol	Chain	Res	Type
21	AA	959	A
21	AA	960	U
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	972	C
21	AA	977	A
21	AA	978	A
21	AA	979	C
21	AA	981	U
21	AA	983	A
21	AA	984	C
21	AA	993	G
21	AA	995	C
21	AA	1004	A
21	AA	1026	G
21	AA	1030	U
21	AA	1031	C
21	AA	1045	C
21	AA	1046	A
21	AA	1049	U
21	AA	1050	G
21	AA	1056	U
21	AA	1064	G
21	AA	1065	U
21	AA	1068	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1130	A
21	AA	1137	C
21	AA	1139	G
21	AA	1140	C
21	AA	1146	A
21	AA	1147	C
21	AA	1152	A
21	AA	1167	A
21	AA	1183	U
21	AA	1185	G
21	AA	1189	U
21	AA	1191	A
21	AA	1194	U

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Mol	Chain	Res	Type
21	AA	1195	C
21	AA	1196	A
21	AA	1201	A
21	AA	1202	U
21	AA	1218	C
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1229	A
21	AA	1233	G
21	AA	1238	A
21	AA	1240	U
21	AA	1241	G
21	AA	1251	A
21	AA	1256	A
21	AA	1257	A
21	AA	1278	G
21	AA	1279	G
21	AA	1282	C
21	AA	1285	A
21	AA	1286	U
21	AA	1298	U
21	AA	1300	G
21	AA	1301	U
21	AA	1303	C
21	AA	1305	G
21	AA	1337	G
21	AA	1338	G
21	AA	1346	A
21	AA	1362	A
21	AA	1363	A
21	AA	1379	G
21	AA	1380	U
21	AA	1381	U
21	AA	1382	C
21	AA	1394	A
21	AA	1397	C
21	AA	1398	A
21	AA	1399	C
21	AA	1400	C
21	AA	1401	G
21	AA	1419	G

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Mol	Chain	Res	Type
21	AA	1432	G
21	AA	1446	A
21	AA	1447	A
21	AA	1448	C
21	AA	1452	C
21	AA	1453	G
21	AA	1491	G
21	AA	1493	A
21	AA	1494	G
21	AA	1503	A
21	AA	1505	G
21	AA	1506	U
21	AA	1511	G
21	AA	1517	G
21	AA	1529	G
21	AA	1530	G
21	AA	1534	A
22	A1	10	G
22	A1	16	C
22	A1	18	G
22	A1	20	G
22	A1	47	U
22	A1	48	C
22	A1	59	U
22	A1	73	A
22	A1	74	C
22	A1	76	A
23	A2	80	C
23	A2	81	U
23	A2	82	A
23	A2	83	U
23	A2	84	G
23	A2	85	G
23	A2	88	U
23	A2	92	U
24	A3	5	G
24	A3	9	G
24	A3	10	G
24	A3	17	C
24	A3	19	G
24	A3	21	H2U
24	A3	22	A

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Mol	Chain	Res	Type
24	A3	32	G
24	A3	33	OMC
24	A3	49	C
24	A3	62	C
24	A3	71	G
24	A3	72	C
54	BA	9	G
54	BA	13	A
54	BA	15	G
54	BA	20	C
54	BA	34	U
54	BA	39	G
54	BA	71	A
54	BA	72	U
54	BA	74	A
54	BA	75	G
54	BA	85	G
54	BA	86	G
54	BA	88	G
54	BA	98	G
54	BA	100	U
54	BA	101	A
54	BA	102	U
54	BA	103	A
54	BA	112	U
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	127	A
54	BA	128	C
54	BA	139	U
54	BA	140	C
54	BA	141	G
54	BA	143	C
54	BA	149	A
54	BA	163	C
54	BA	180	G
54	BA	181	A
54	BA	196	A
54	BA	204	A
54	BA	205	G

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Mol	Chain	Res	Type
54	BA	216	A
54	BA	222	A
54	BA	228	C
54	BA	248	G
54	BA	249	C
54	BA	255	A
54	BA	256	A
54	BA	265	A
54	BA	266	G
54	BA	272	A
54	BA	278	A
54	BA	294	A
54	BA	299	A
54	BA	302	C
54	BA	316	C
54	BA	327	G
54	BA	330	A
54	BA	346	A
54	BA	370	G
54	BA	386	G
54	BA	387	U
54	BA	388	G
54	BA	389	G
54	BA	390	U
54	BA	404	A
54	BA	405	U
54	BA	411	G
54	BA	428	A
54	BA	451	U
54	BA	455	C
54	BA	457	A
54	BA	475	C
54	BA	482	A
54	BA	504	A
54	BA	505	A
54	BA	506	G
54	BA	508	A
54	BA	526	A
54	BA	528	A
54	BA	529	A
54	BA	530	G
54	BA	531	C

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Mol	Chain	Res	Type
54	BA	532	A
54	BA	533	G
54	BA	546	U
54	BA	549	G
54	BA	562	U
54	BA	563	A
54	BA	573	U
54	BA	574	A
54	BA	575	A
54	BA	588	U
54	BA	590	A
54	BA	603	A
54	BA	607	U
54	BA	613	A
54	BA	615	U
54	BA	616	A
54	BA	617	G
54	BA	627	A
54	BA	631	A
54	BA	632	A
54	BA	637	A
54	BA	643	A
54	BA	644	A
54	BA	653	U
54	BA	654	A
54	BA	655	A
54	BA	672	C
54	BA	686	U
54	BA	719	C
54	BA	724	U
54	BA	726	G
54	BA	730	A
54	BA	736	C
54	BA	743	A
54	BA	747	U
54	BA	762	U
54	BA	763	G
54	BA	764	A
54	BA	765	C
54	BA	775	G
54	BA	776	G
54	BA	782	A

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Mol	Chain	Res	Type
54	BA	784	G
54	BA	793	A
54	BA	800	A
54	BA	805	G
54	BA	812	C
54	BA	814	C
54	BA	819	A
54	BA	827	U
54	BA	846	U
54	BA	847	U
54	BA	852	U
54	BA	858	G
54	BA	859	G
54	BA	866	A
54	BA	867	C
54	BA	889	C
54	BA	890	C
54	BA	896	A
54	BA	897	C
54	BA	914	G
54	BA	915	C
54	BA	932	U
54	BA	934	U
54	BA	935	C
54	BA	945	A
54	BA	958	U
54	BA	961	C
54	BA	962	G
54	BA	973	A
54	BA	974	G
54	BA	980	A
54	BA	981	A
54	BA	983	A
54	BA	985	C
54	BA	994	C
54	BA	996	A
54	BA	1005	C
54	BA	1011	G
54	BA	1022	G
54	BA	1024	G
54	BA	1025	G
54	BA	1026	G

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Mol	Chain	Res	Type
54	BA	1033	U
54	BA	1046	A
54	BA	1047	G
54	BA	1060	U
54	BA	1067	A
54	BA	1069	A
54	BA	1070	A
54	BA	1072	C
54	BA	1073	A
54	BA	1078	U
54	BA	1088	A
54	BA	1089	A
54	BA	1094	U
54	BA	1112	G
54	BA	1127	A
54	BA	1129	A
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1142	A
54	BA	1143	A
54	BA	1175	A
54	BA	1204	A
54	BA	1205	A
54	BA	1206	G
54	BA	1211	C
54	BA	1241	A
54	BA	1242	U
54	BA	1254	A
54	BA	1256	G
54	BA	1266	G
54	BA	1272	A
54	BA	1273	U
54	BA	1274	A
54	BA	1276	A
54	BA	1289	C
54	BA	1290	C
54	BA	1300	G
54	BA	1301	A
54	BA	1306	C
54	BA	1313	U
54	BA	1317	G

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Mol	Chain	Res	Type
54	BA	1320	C
54	BA	1321	A
54	BA	1325	U
54	BA	1332	G
54	BA	1340	U
54	BA	1341	G
54	BA	1345	C
54	BA	1365	A
54	BA	1378	A
54	BA	1379	U
54	BA	1383	A
54	BA	1384	A
54	BA	1388	G
54	BA	1399	C
54	BA	1416	G
54	BA	1420	A
54	BA	1421	G
54	BA	1427	A
54	BA	1428	C
54	BA	1435	G
54	BA	1452	G
54	BA	1453	A
54	BA	1454	C
54	BA	1459	G
54	BA	1475	G
54	BA	1482	G
54	BA	1493	C
54	BA	1497	U
54	BA	1508	A
54	BA	1511	G
54	BA	1515	A
54	BA	1523	U
54	BA	1538	G
54	BA	1539	U
54	BA	1560	G
54	BA	1565	C
54	BA	1568	G
54	BA	1570	A
54	BA	1578	U
54	BA	1584	U
54	BA	1599	U
54	BA	1608	A

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Mol	Chain	Res	Type
54	BA	1610	A
54	BA	1611	C
54	BA	1617	C
54	BA	1618	A
54	BA	1628	G
54	BA	1629	U
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1654	A
54	BA	1668	A
54	BA	1669	A
54	BA	1670	C
54	BA	1674	G
54	BA	1711	A
54	BA	1715	G
54	BA	1730	C
54	BA	1731	G
54	BA	1732	C
54	BA	1733	G
54	BA	1734	G
54	BA	1758	U
54	BA	1760	C
54	BA	1761	C
54	BA	1764	C
54	BA	1773	A
54	BA	1776	G
54	BA	1780	A
54	BA	1781	U
54	BA	1782	U
54	BA	1784	A
54	BA	1800	C
54	BA	1802	A
54	BA	1803	A
54	BA	1808	A
54	BA	1816	C
54	BA	1848	A
54	BA	1870	C
54	BA	1871	A
54	BA	1872	A
54	BA	1877	A
54	BA	1888	G

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Mol	Chain	Res	Type
54	BA	1906	G
54	BA	1913	A
54	BA	1914	C
54	BA	1929	G
54	BA	1930	G
54	BA	1931	U
54	BA	1937	A
54	BA	1940	U
54	BA	1943	U
54	BA	1945	G
54	BA	1953	A
54	BA	1955	U
54	BA	1963	U
54	BA	1971	U
54	BA	1972	G
54	BA	1993	U
54	BA	1997	C
54	BA	2022	U
54	BA	2023	C
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2043	C
54	BA	2055	C
54	BA	2059	A
54	BA	2060	A
54	BA	2061	G
54	BA	2062	A
54	BA	2063	C
54	BA	2068	U
54	BA	2069	G
54	BA	2072	C
54	BA	2092	U
54	BA	2113	U
54	BA	2114	A
54	BA	2126	A
54	BA	2132	U
54	BA	2133	G
54	BA	2135	A
54	BA	2155	U
54	BA	2157	G
54	BA	2159	G

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Mol	Chain	Res	Type
54	BA	2160	C
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2181	U
54	BA	2199	A
54	BA	2203	U
54	BA	2204	G
54	BA	2206	C
54	BA	2211	A
54	BA	2214	C
54	BA	2238	G
54	BA	2245	U
54	BA	2262	U
54	BA	2266	A
54	BA	2267	A
54	BA	2269	G
54	BA	2275	C
54	BA	2283	C
54	BA	2288	A
54	BA	2289	G
54	BA	2305	U
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2310	C
54	BA	2311	A
54	BA	2312	U
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2322	A
54	BA	2325	G
54	BA	2326	C
54	BA	2333	A
54	BA	2335	A
54	BA	2339	C
54	BA	2345	G
54	BA	2346	A
54	BA	2347	C
54	BA	2353	G
54	BA	2383	G

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Mol	Chain	Res	Type
54	BA	2385	C
54	BA	2387	U
54	BA	2388	A
54	BA	2403	C
54	BA	2406	A
54	BA	2419	U
54	BA	2425	A
54	BA	2426	A
54	BA	2427	C
54	BA	2428	G
54	BA	2429	G
54	BA	2430	A
54	BA	2431	U
54	BA	2434	A
54	BA	2435	A
54	BA	2441	U
54	BA	2444	G
54	BA	2448	A
54	BA	2449	U
54	BA	2469	A
54	BA	2470	G
54	BA	2476	A
54	BA	2491	U
54	BA	2492	U
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2505	G
54	BA	2518	A
54	BA	2529	G
54	BA	2531	A
54	BA	2532	G
54	BA	2540	C
54	BA	2547	A
54	BA	2554	U
54	BA	2555	U
54	BA	2564	A
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2572	A
54	BA	2573	C

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Mol	Chain	Res	Type
54	BA	2574	G
54	BA	2578	G
54	BA	2581	G
54	BA	2584	U
54	BA	2587	A
54	BA	2596	U
54	BA	2599	G
54	BA	2600	A
54	BA	2613	U
54	BA	2614	A
54	BA	2615	U
54	BA	2629	U
54	BA	2645	G
54	BA	2646	C
54	BA	2655	G
54	BA	2660	A
54	BA	2674	G
54	BA	2684	U
54	BA	2689	U
54	BA	2690	U
54	BA	2709	G
54	BA	2714	G
54	BA	2726	A
54	BA	2732	G
54	BA	2733	A
54	BA	2740	A
54	BA	2744	G
54	BA	2765	A
54	BA	2766	A
54	BA	2778	A
54	BA	2779	U
54	BA	2791	G
54	BA	2797	U
54	BA	2808	G
54	BA	2820	A
54	BA	2821	A
54	BA	2823	A
54	BA	2830	C
54	BA	2850	A
54	BA	2858	C
54	BA	2859	G
54	BA	2868	A

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Mol	Chain	Res	Type
54	BA	2879	A
54	BA	2880	C
54	BA	2881	U
54	BA	2886	A
54	BA	2894	G
54	BA	2895	G
55	BB	3	C
55	BB	5	U
55	BB	13	G
55	BB	14	U
55	BB	15	A
55	BB	16	G
55	BB	25	U
55	BB	35	C
55	BB	42	C
55	BB	44	G
55	BB	66	A
55	BB	73	A
55	BB	88	C
55	BB	89	U
55	BB	90	C
55	BB	108	A
55	BB	109	A
55	BB	112	G

All (217) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	13	U
21	AA	16	A
21	AA	50	A
21	AA	51	A
21	AA	59	A
21	AA	64	G
21	AA	66	A
21	AA	84	U
21	AA	109	A
21	AA	181	A
21	AA	251	G
21	AA	266	G
21	AA	279	A

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Mol	Chain	Res	Type
21	AA	346	G
21	AA	351	G
21	AA	357	G
21	AA	372	C
21	AA	412	A
21	AA	451	A
21	AA	455	G
21	AA	461	A
21	AA	465	A
21	AA	467	U
21	AA	476	U
21	AA	481	G
21	AA	483	C
21	AA	499	A
21	AA	500	G
21	AA	510	A
21	AA	559	A
21	AA	573	A
21	AA	575	G
21	AA	607	A
21	AA	611	C
21	AA	630	A
21	AA	675	A
21	AA	701	U
21	AA	703	G
21	AA	704	A
21	AA	718	A
21	AA	721	G
21	AA	753	A
21	AA	755	G
21	AA	758	C
21	AA	804	U
21	AA	819	A
21	AA	840	C
21	AA	844	G
21	AA	872	A
21	AA	913	A
21	AA	938	A
21	AA	958	A
21	AA	959	A
21	AA	980	C
21	AA	982	U

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Mol	Chain	Res	Type
21	AA	983	A
21	AA	1049	U
21	AA	1053	G
21	AA	1064	G
21	AA	1101	A
21	AA	1117	A
21	AA	1146	A
21	AA	1166	G
21	AA	1171	A
21	AA	1184	G
21	AA	1190	G
21	AA	1194	U
21	AA	1195	C
21	AA	1201	A
21	AA	1217	C
21	AA	1225	A
21	AA	1233	G
21	AA	1298	U
21	AA	1337	G
21	AA	1380	U
21	AA	1397	C
21	AA	1399	C
21	AA	1446	A
21	AA	1447	A
21	AA	1452	C
21	AA	1476	A
21	AA	1493	A
21	AA	1529	G
22	A1	10	G
22	A1	18	G
22	A1	47	U
22	A1	75	C
23	A2	80	C
23	A2	84	G
24	A3	21	H2U
24	A3	71	G
54	BA	14	A
54	BA	34	U
54	BA	48	G
54	BA	71	A
54	BA	102	U
54	BA	118	A

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Mol	Chain	Res	Type
54	BA	119	A
54	BA	125	A
54	BA	127	A
54	BA	180	G
54	BA	196	A
54	BA	199	A
54	BA	255	A
54	BA	278	A
54	BA	323	C
54	BA	386	G
54	BA	387	U
54	BA	388	G
54	BA	503	A
54	BA	505	A
54	BA	527	C
54	BA	547	A
54	BA	573	U
54	BA	615	U
54	BA	631	A
54	BA	643	A
54	BA	748	G
54	BA	762	U
54	BA	764	A
54	BA	818	G
54	BA	827	U
54	BA	846	U
54	BA	896	A
54	BA	934	U
54	BA	958	U
54	BA	1005	C
54	BA	1033	U
54	BA	1088	A
54	BA	1126	A
54	BA	1128	G
54	BA	1141	U
54	BA	1142	A
54	BA	1204	A
54	BA	1205	A
54	BA	1210	G
54	BA	1273	U
54	BA	1289	C
54	BA	1300	G

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Mol	Chain	Res	Type
54	BA	1301	A
54	BA	1312	U
54	BA	1320	C
54	BA	1383	A
54	BA	1385	A
54	BA	1420	A
54	BA	1427	A
54	BA	1451	C
54	BA	1453	A
54	BA	1490	A
54	BA	1512	C
54	BA	1537	G
54	BA	1560	G
54	BA	1607	C
54	BA	1610	A
54	BA	1617	C
54	BA	1628	G
54	BA	1647	U
54	BA	1668	A
54	BA	1730	C
54	BA	1732	C
54	BA	1760	C
54	BA	1780	A
54	BA	1799	G
54	BA	1802	A
54	BA	1847	A
54	BA	1871	A
54	BA	1930	G
54	BA	1936	A
54	BA	1939	U
54	BA	1952	A
54	BA	1955	U
54	BA	1981	A
54	BA	2034	U
54	BA	2060	A
54	BA	2062	A
54	BA	2071	A
54	BA	2113	U
54	BA	2132	U
54	BA	2133	G
54	BA	2145	C
54	BA	2171	A

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Mol	Chain	Res	Type
54	BA	2172	U
54	BA	2180	U
54	BA	2286	G
54	BA	2288	A
54	BA	2321	U
54	BA	2325	G
54	BA	2345	G
54	BA	2402	U
54	BA	2418	A
54	BA	2425	A
54	BA	2427	C
54	BA	2428	G
54	BA	2429	G
54	BA	2433	A
54	BA	2503	A
54	BA	2531	A
54	BA	2564	A
54	BA	2571	U
54	BA	2573	C
54	BA	2575	C
54	BA	2596	U
54	BA	2712	C
54	BA	2732	G
54	BA	2740	A
54	BA	2778	A
54	BA	2790	U
54	BA	2829	A
54	BA	2832	U
54	BA	2858	C
55	BB	2	G
55	BB	4	C
55	BB	14	U
55	BB	15	A
55	BB	57	A
55	BB	111	U

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CM0	A1	34	22,23	15,26,27	1.82	3 (20%)	18,37,40	3.15	2 (11%)
22	6MZ	A1	37	22	17,25,26	0.96	0	15,36,39	1.49	2 (13%)
22	7MG	A1	46	22	20,26,27	2.23	4 (20%)	23,39,42	2.10	2 (8%)
22	5MU	A1	54	22	13,22,23	1.20	2 (15%)	16,32,35	4.70	2 (12%)
22	PSU	A1	55	22	15,21,22	1.08	1 (6%)	16,30,33	3.28	4 (25%)
22	4SU	A1	7	22	12,21,22	1.01	0	15,30,33	2.13	1 (6%)
24	H2U	A3	21	24	17,21,22	1.35	2 (11%)	23,30,33	1.49	4 (17%)
24	OMC	A3	33	24	15,22,23	1.04	0	20,31,34	0.76	0
24	5MU	A3	55	24	13,22,23	0.94	1 (7%)	16,32,35	4.74	2 (12%)
24	PSU	A3	56	24	15,21,22	1.11	1 (6%)	16,30,33	3.51	5 (31%)
24	4SU	A3	8	24	12,21,22	1.21	2 (16%)	15,30,33	2.12	1 (6%)

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

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.32	1.33	1.45
22	A1	34	CM0	O5-C5	-5.63	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	21	H2U	C4-N3	-3.33	1.32	1.37
24	A3	21	H2U	C2-N3	-3.15	1.32	1.38
22	A1	46	7MG	C8-N7	-2.86	1.30	1.43
22	A1	54	5MU	O4'-C1'	2.02	1.44	1.41
22	A1	46	7MG	C4-N3	2.15	1.37	1.34
24	A3	56	PSU	C4-N3	2.16	1.36	1.33
24	A3	8	4SU	C6-N1	2.22	1.38	1.35
22	A1	55	PSU	C4-N3	2.36	1.37	1.33
24	A3	8	4SU	O4'-C1'	2.37	1.44	1.41
24	A3	55	5MU	C4-N3	2.52	1.37	1.33
22	A1	34	CM0	C4-N3	2.53	1.37	1.33
22	A1	34	CM0	C4-C5	2.61	1.47	1.40
22	A1	46	7MG	C6-N1	2.71	1.37	1.33
22	A1	54	5MU	C4-N3	2.72	1.37	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	55	5MU	C5-C4-N3	-13.25	114.23	125.35
22	A1	54	5MU	C5-C4-N3	-12.76	114.64	125.35
22	A1	7	4SU	C5-C4-N3	-7.53	115.58	123.56
24	A3	8	4SU	C5-C4-N3	-7.36	115.75	123.56
22	A1	46	7MG	C5-C6-N1	-6.79	113.28	123.39
24	A3	56	PSU	C5-C6-N1	-3.22	119.89	124.38
24	A3	56	PSU	C5-C1'-C2'	-2.96	110.42	115.44
24	A3	56	PSU	C4'-O4'-C1'	-2.87	106.59	109.54
22	A1	37	6MZ	C1'-N9-C4	-2.74	123.75	126.81
22	A1	55	PSU	C5-C6-N1	-2.68	120.64	124.38
22	A1	55	PSU	C5-C1'-C2'	-2.29	111.54	115.44
24	A3	21	H2U	O4'-C4'-C3'	2.27	109.77	105.16
24	A3	21	H2U	C5-C6-N1	2.69	113.71	110.76
24	A3	21	H2U	C5-C4-N3	2.83	119.61	116.62
22	A1	55	PSU	O4'-C1'-C2'	3.02	107.95	104.69
24	A3	21	H2U	N3-C2-N1	3.38	119.77	116.64
22	A1	34	CM0	C7-O5-C5	3.50	124.26	117.83
22	A1	37	6MZ	C2-N1-C6	3.77	119.18	116.47
24	A3	56	PSU	O4'-C1'-C2'	3.93	108.94	104.69
22	A1	46	7MG	C6-N1-C2	6.78	123.83	115.88
22	A1	55	PSU	C4-N3-C2	11.86	125.06	115.16
22	A1	34	CM0	C4-N3-C2	12.20	125.34	115.16
24	A3	56	PSU	C4-N3-C2	12.24	125.37	115.16
24	A3	55	5MU	C4-N3-C2	13.18	126.16	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C4-N3-C2	13.28	126.24	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A1	54	5MU	1	0
22	A1	55	PSU	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	VAL	A1	101	58,22	5,6,7	0.61	0	5,7,9	1.78	1 (20%)
58	FME	BA	3001	57	8,9,10	0.72	0	5,9,11	1.57	2 (40%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
58	BA	3001	FME	O-C-CA	-2.67	118.39	125.69
58	BA	3001	FME	O1-CN-N	-2.17	121.47	124.80
57	A1	101	VAL	C-CA-N	3.57	117.84	109.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.