



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:03 PM BST

PDB ID : 4V76
EMDB ID: : EMD-1722
Title : E. coli 70S-fMetVal-tRNAVal-tRNA^fMet complex in intermediate post-translocation state (post2a)
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on : 2013-10-14
Resolution : 17.00 Å (reported)
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

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

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

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

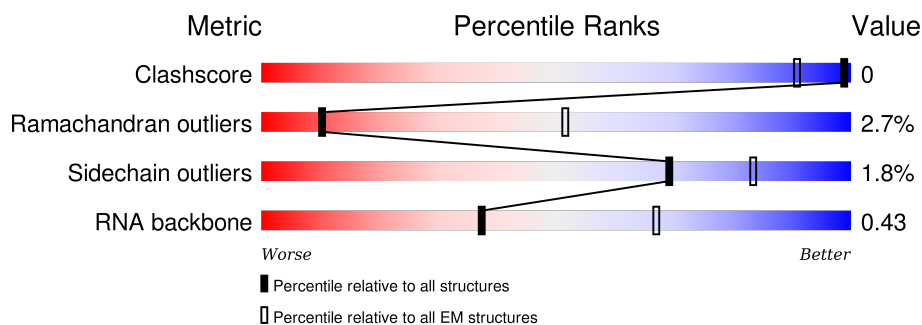
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 Å.

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














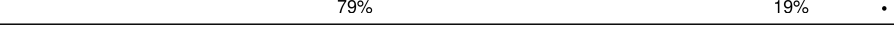
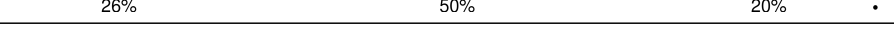


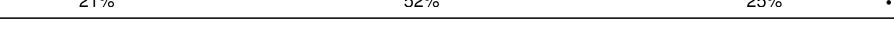



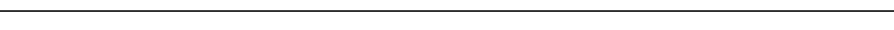

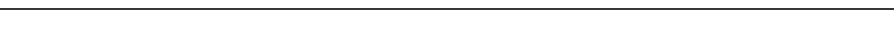
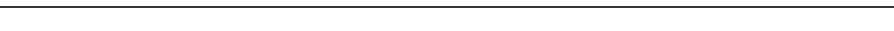


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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	91% 9%
2	AC	208	90% 9%
3	AD	206	89% 10% .
4	AE	152	91% 9%
5	AF	101	87% 13%
6	AG	152	86% 14% .
7	AH	130	91% 8% .
8	AI	128	90% 9% .













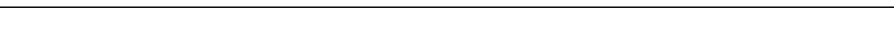



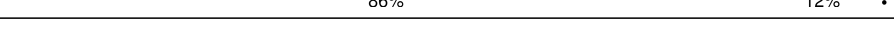




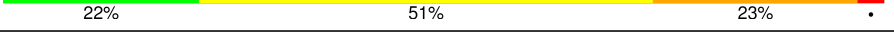
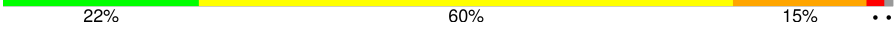
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Mol	Chain	Length	Quality of chain
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	A3	77	
25	BC	273	
26	BD	209	
27	BE	201	
28	BF	179	
29	BG	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	 86% 13% .
35	BM	136	 90% 10%
36	BN	121	 85% 15%
37	BO	117	 88% 11% .
38	BP	115	 85% 12% ..
39	BQ	118	 84% 14% ..
40	BR	103	 93% 7%
41	BS	110	 91% 9%
42	BT	94	 89% 11%
43	BU	104	 85% 13% ..
44	BV	94	 94% 6%
45	BW	80	 79% 18% .
46	BX	79	 84% 13% ..
47	BY	63	 89% 11%
48	BZ	59	 88% 8% ..
49	B0	57	 86% 12% .
50	B1	52	 92% 6% .
51	B2	46	 76% 22% .
52	B3	65	 80% 18% .
53	B4	38	 84% 16%
54	BA	2903	 22% 51% 23% .
55	BB	118	 22% 60% 15% ..
56	B5	234	 88% 7% 5%

2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

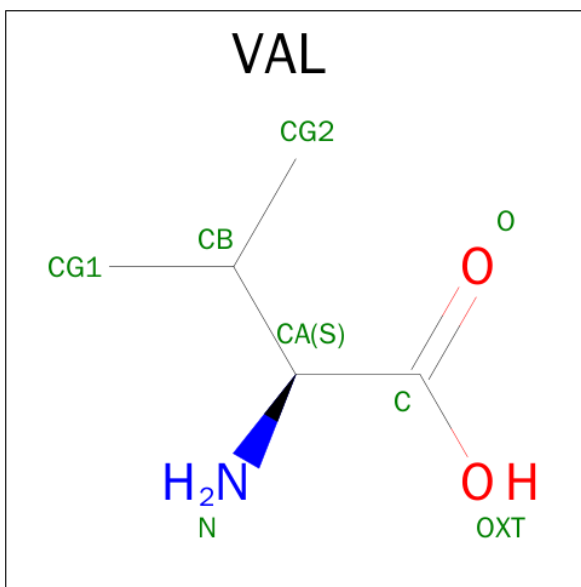
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

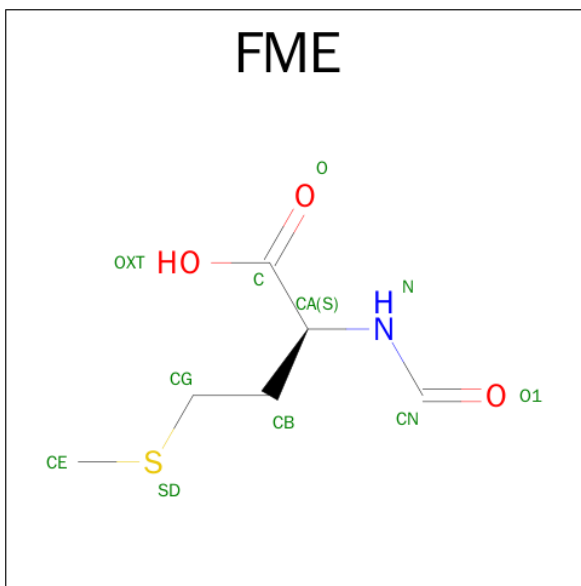
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



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

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).

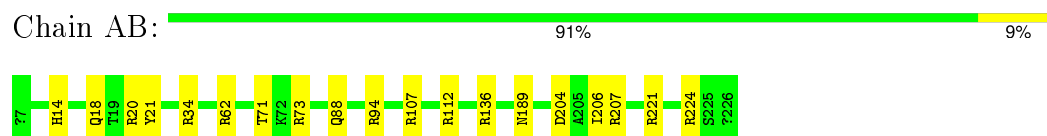


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

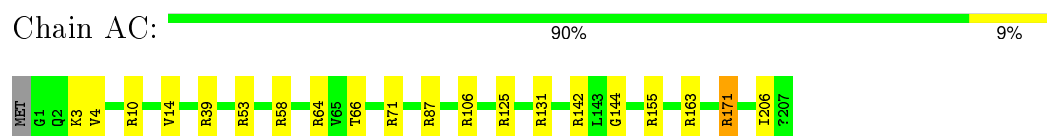
3 Residue-property plots [i](#)

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

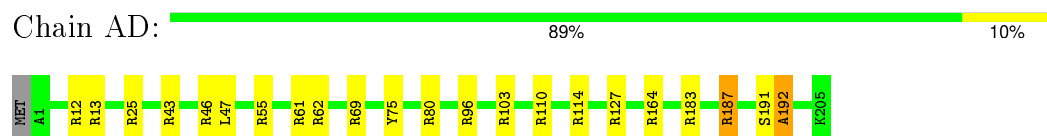
- Molecule 1: 30S ribosomal protein S2



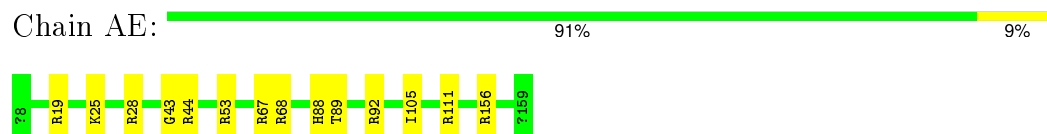
- Molecule 2: 30S ribosomal protein S3



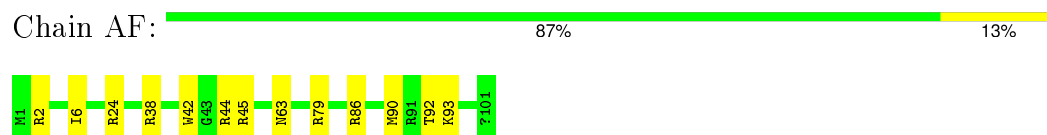
- Molecule 3: 30S ribosomal protein S4



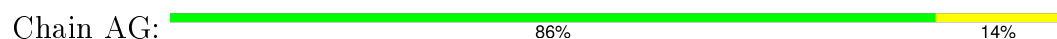
- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S7





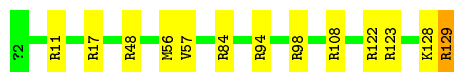
- Molecule 7: 30S ribosomal protein S8

Chain AH: 91% 8%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 90% 9%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 85% 13%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 89% 9%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 81% 16%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 82% 17%

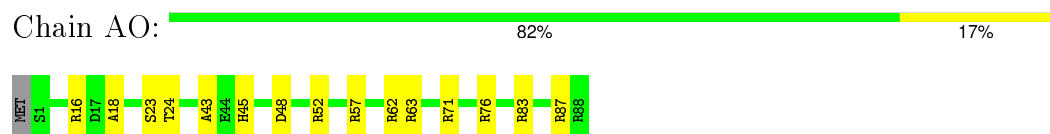


- Molecule 13: 30S ribosomal protein S14

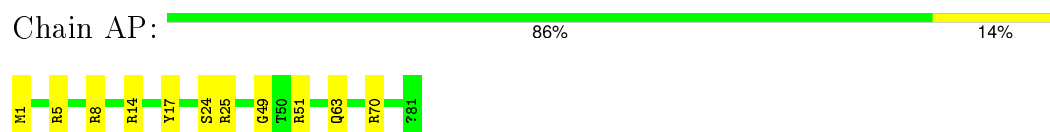
Chain AN: 82% 17%



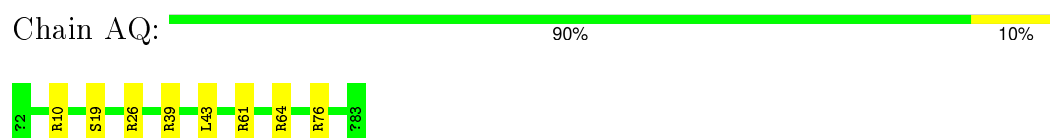
- Molecule 14: 30S ribosomal protein S15



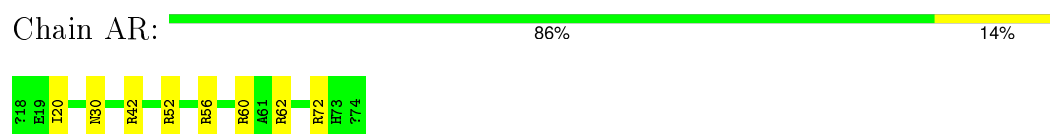
- Molecule 15: 30S ribosomal protein S16



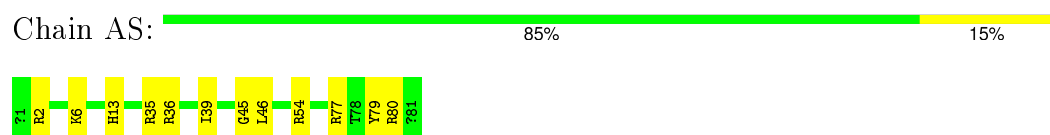
- Molecule 16: 30S ribosomal protein S17



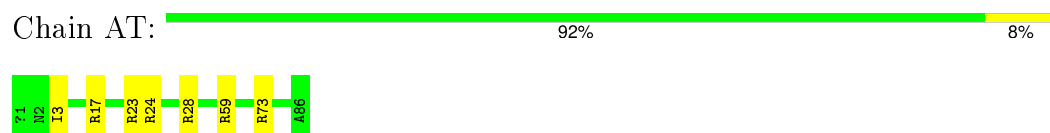
- Molecule 17: 30S ribosomal protein S18



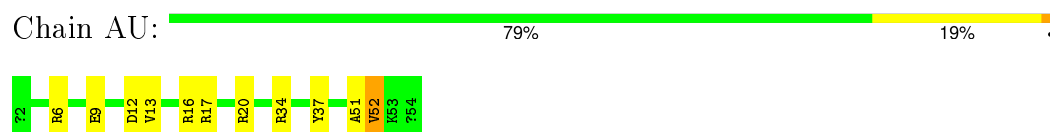
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



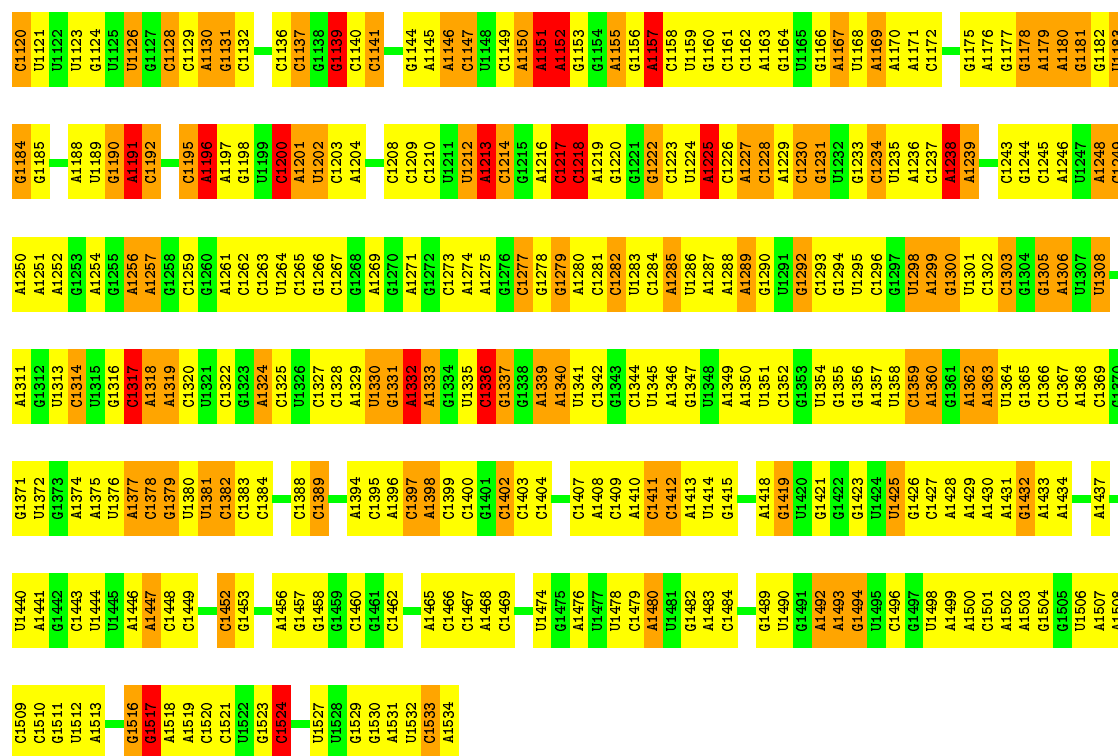
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA



C1051	C1052	C1053	C1054	C1055	C1056	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	A1080	A1081	A1082	A1083	A1092	A1093	A1094	A1095	A1096	A1097	C1098	C1099	C1100	A1101	A1102	C1103	C1104	A1105	C1106	C1107	C1108	C1109	A1110	A1111	C1112	C1113	C1114	C1115	A1116	A1117	A1118	C1119											
C985	C986	U989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	A1000	C1001	C1002	C1003	A1004	A1005	U1010	C1011	C1012	A1013	A1014	C1015	A1016	C1017	C1018	C1019	A1020	A1021	A1022	U1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	A1035	C1036	C1037	C1038	G1041	A1042	C1043	C1044	C1045	A1046	C1047	C1048	U1049	C1050										
C857	C858	C859	A860	C861	C862	C863	A864	A865	C866	C867	C868	C869	U870	U871	C872	A873	C874	C875	C876	C877	A878	C879	C880	C881	C882	C883	U884	C885	C886	C887	C888	A889	C890	A891	A892	C893	C894	C895	C896	C897	C898	C899	A900	A901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	A913	A914	A915	U916								
G917	A918	A919	U920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	G944	C945	A946	C947	C948	C949	G954	U957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984								
C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	
C786	A787	U788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855
C857	C858	C859	A860	C861	C862	C863	A864	A865	C866	C867	C868	C869	U870	U871	C872	A873	C874	C875	C876	C877	A878	C879	C880	C881	C882	C883	U884	C885	C886	C887	C888	A889	C890	A891	A892	C893	C894	C895	C896	C897	C898	C899	A900	A901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	A913	A914	A915	U916								
G917	A918	A919	U920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	G944	C945	A946	C947	C948	C949	G954	U957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984								
C1051	C1052	C1053	C1054	C1055	C1056	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	A1080	A1081	A1082	A1083	A1092	A1093	A1094	A1095	A1096	A1097	C1098	C1099	C1100	A1101	A1102	C1103	C1104	A1105	C1106	C1107	C1108	C1109	A1110	A1111	C1112	C1113	C1114	C1115	A1116	A1117	A1118	C1119											
C985	C986	U989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	A1000	C1001	C1002	C1003	A1004	A1005	U1010	C1011	C1012	A1013	A1014	C1015	A1016	C1017	C1018	C1019	A1020	A1021	A1022	U1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	A1035	C1036	C1037	C1038	G1041	A1042	C1043	C1044	C1045	A1046	C1047	C1048	U1049	C1050										
C857	C858	C859	A860	C861	C862	C863	A864	A865	C866	C867	C868	C869	U870	U871	C872	A873	C874	C875	C876	C877	A878	C879	C880	C881	C882	C883	U884	C885	C886	C887	C888	A889	C890	A891	A892	C893	C894	C895	C896	C897	C898	C899	A900	A901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	A913	A914	A915	U916								
G917	A918	A919	U920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	G944	C945	A946	C947	C948	C949	G954	U957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984								



• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 32% 51% 13%



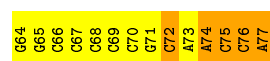
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

Chain A2: 13% 47% 27% 13%



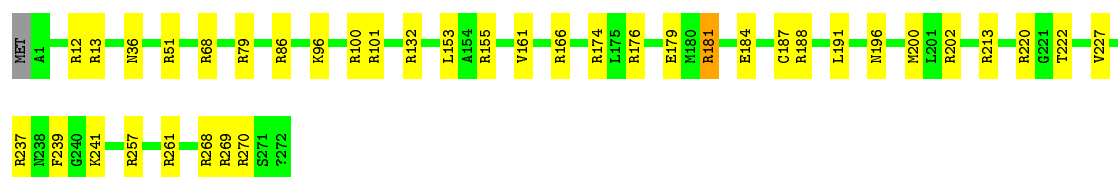
• Molecule 24: tRNA-fMet

Chain A3: 21% 52% 25%



• Molecule 25: 50S ribosomal protein L2

Chain BC: 86% 14%



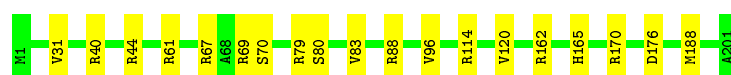
- Molecule 26: 50S ribosomal protein L3

Chain BD: 91% 8%



- Molecule 27: 50S ribosomal protein L4

Chain BE: 91% 9%



- Molecule 28: 50S ribosomal protein L5

Chain BF: 89% 9% ..



- Molecule 29: 50S ribosomal protein L6

Chain BG: 93% 6% ..



- Molecule 30: 50S ribosomal protein L9

Chain BH: 94% 6%



- Molecule 31: 50S ribosomal protein L11

Chain BI: 95% ..



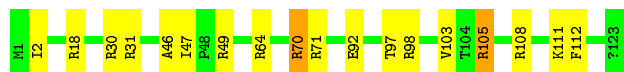
- Molecule 32: 50S ribosomal protein L13

Chain BJ: 90% 9% .



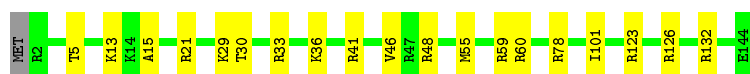
- Molecule 33: 50S ribosomal protein L14

Chain BK: 85% 13%



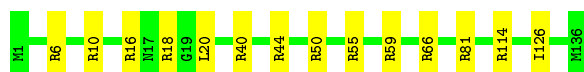
- Molecule 34: 50S ribosomal protein L15

Chain BL: 86% 13%



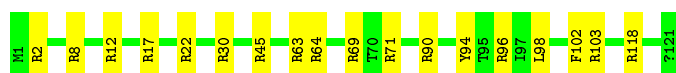
- Molecule 35: 50S ribosomal protein L16

Chain BM: 90% 10%



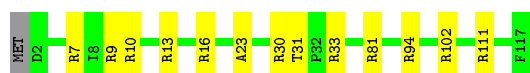
- Molecule 36: 50S ribosomal protein L17

Chain BN: 85% 15%



- Molecule 37: 50S ribosomal protein L18

Chain BO: 88% 11%



- Molecule 38: 50S ribosomal protein L19

Chain BP: 85% 12%

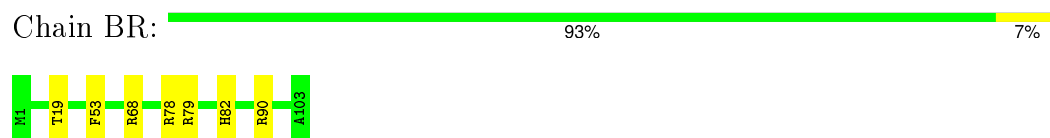


- Molecule 39: 50S ribosomal protein L20

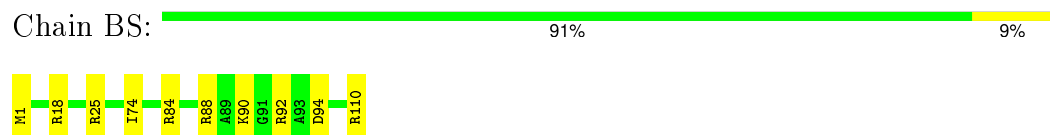
Chain BQ: 84% 14%



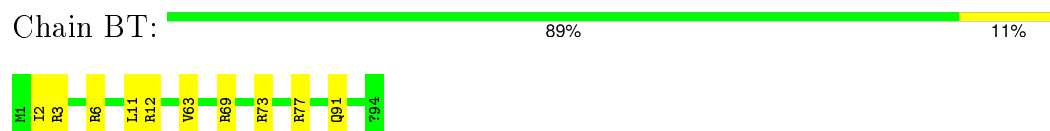
- Molecule 40: 50S ribosomal protein L21



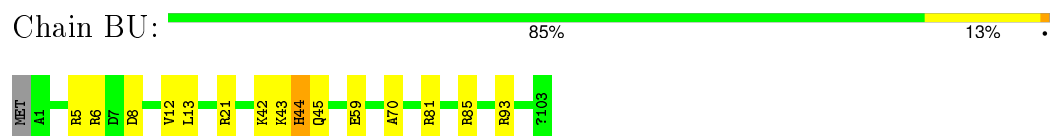
- Molecule 41: 50S ribosomal protein L22



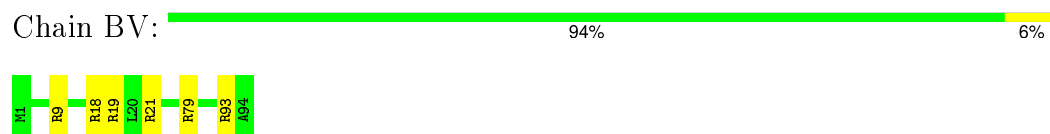
- Molecule 42: 50S ribosomal protein L23



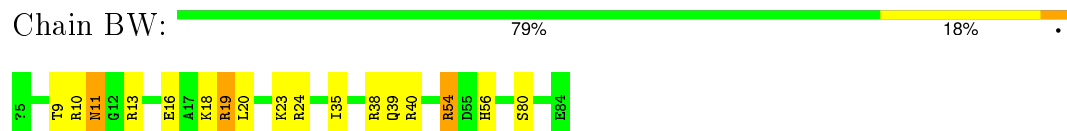
- Molecule 43: 50S ribosomal protein L24



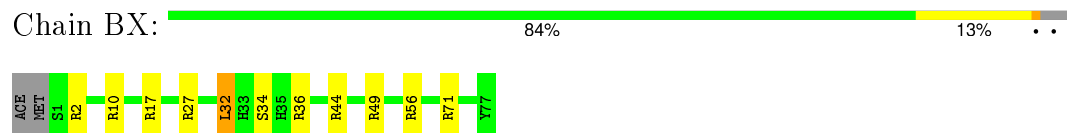
- Molecule 44: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L28




- Molecule 47: 50S ribosomal protein L29

Chain BY:  89% 11%




- Molecule 48: 50S ribosomal protein L30

Chain BZ:  88% 8% ..



- Molecule 49: 50S ribosomal protein L32

Chain B0:  86% 12% .




- Molecule 50: 50S ribosomal protein L33

Chain B1:  92% 6% .




- Molecule 51: 50S ribosomal protein L34

Chain B2:  76% 22% .




- Molecule 52: 50S ribosomal protein L35

Chain B3:  80% 18% .



- Molecule 53: 50S ribosomal protein L36

Chain B4:  84% 16%

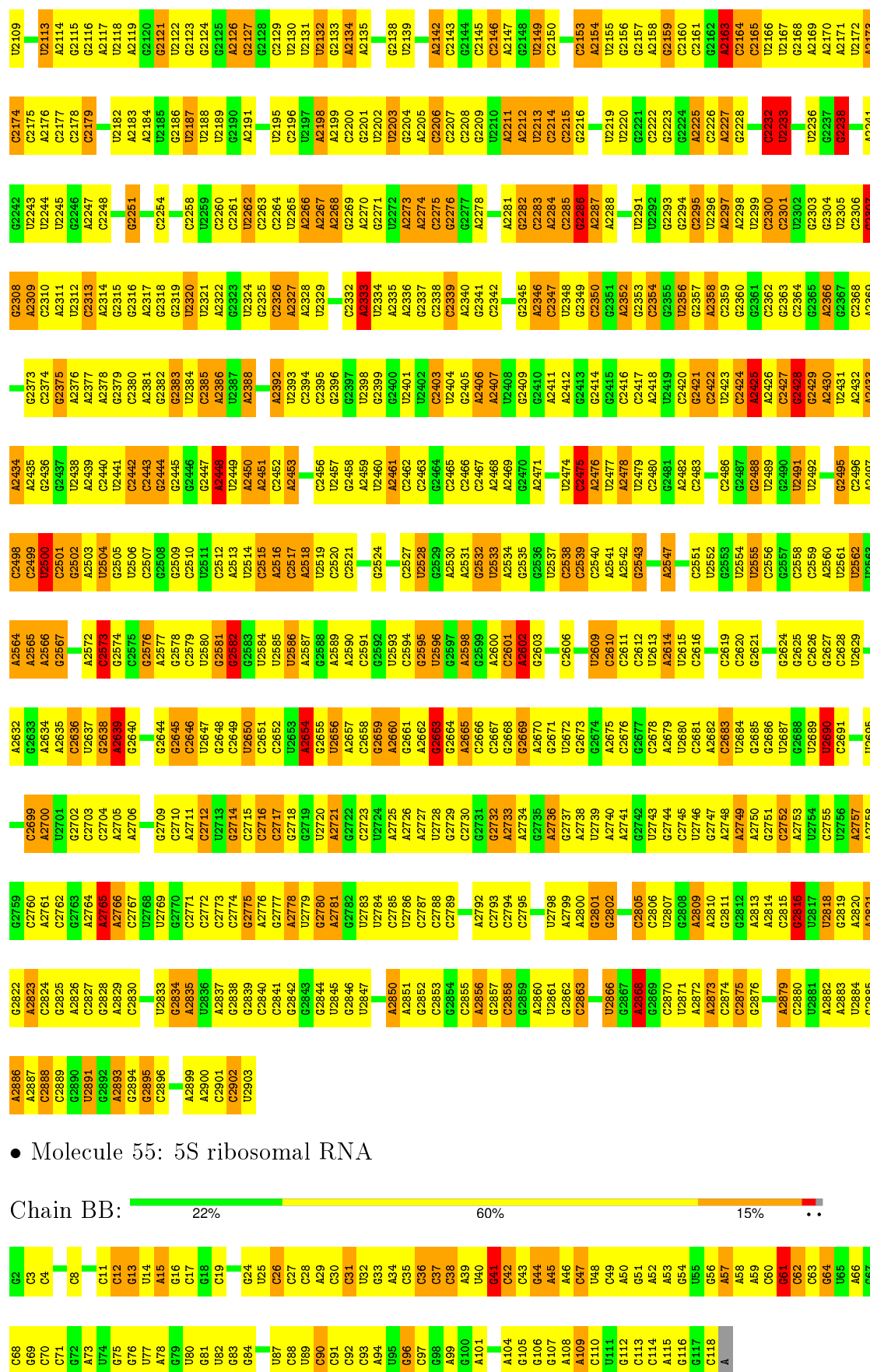


- Molecule 54: 23S ribosomal RNA

Chain BA:  22% 51% 23% .

A1028	C964	C902	U839	C772	U710	C640	G577	U448	G317	G250	G189	A126	U62	G1
A1029	C965	C903	C840	U773	G711	U641	G578	A449	C318	A251	A190	A127	A63	G2
G1030	G904	G905	G841	G774	G714	A642	G579	U450	G319	G252	A191	C128	A64	U3
A1031	G969	A905	A844	G775	A715	A643	U580	U451	A320	C253	A192	C129	U65	U4
A1032	U970	C908	A845	A781	A716	A644	C581	A452	U321	G254	U193	C130	C66	A5
G1033	G971	A909	U846	A782	A717	C645	A582	A453	A322	A255	G194	A131	U67	A6
G1034	G972	A910	U847	A783	G717	U646	G583	A454	C323	A256	A195	G132	G68	G7
U1035	A973	A911	C848	G784	A718	G647	C584	C455	A324	C257	A196	U133	G69	G8
G1038	G974	U912	U849	G785	C719	C650	G585	C456	G327	G260	C198	G134	G70	G9
A1039	A975	U913	A850	C786	A720	U653	A586	A457	U328	G261	A199	U138	A71	C11
A1040	G976	C915	C851	C787	A722	U654	C587	U459	G329	A262	U200	U139	U72	C12
C1043	A979	G916	U852	A788	C723	U655	A590	A460	A330	G263	C201	A140	A73	U12
C1044	A980	A917	C853	A789	U724	A855	U591	C461	C331	C264	U202	G141	A74	U13
C1045	A981	A918	G854	U790	G726	G856	A592	C462	A332	A265	A203	A142	G75	A14
A1046	A982	A919	C855	C791	A727	U658	C595	U463	G333	G266	A204	A143	C76	C16
C1047	A983	U919	C856	A792	A728	C659	U596	U464	C334	C267	G205	A144	U78	G17
A1048	A984	A920	C857	A793	G728	C660	G597	A466	C335	C268	U206	A145	C79	U18
C1049	A985	C921	G858	A794	G729	A661	U598	A467	C336	C269	A207	A146	U82	A19
U1050	C986	G922	G859	C795	A730	G662	U599	C468	C337	A270	C208	C147	A83	C20
G1051	C987	G923	U860	C796	C732	A663	G600	A469	G338	G271	C209	U148	A84	C22
C1052	A988	A925	G862	G733	G733	A666	C601	A470	U339	A272	C210	U150	G85	G23
C1053	G989	G926	A863	G801	A734	U667	A603	A471	C341	C274	C211	C151	G86	G24
A1054	A990	A927	C864	A802	A735	A668	A603	A472	A342	C275	A213	A152	U89	U25
G1055	C991	A928	C865	U803	C736	G669	A603	A473	C343	U276	U153	U153	A89	G26
U1056	C992	U929	A866	A804	C737	A670	U606	C476	A344	G277	A216	U154	U90	G27
A1057	C993	G930	C867	G805	G738	C671	U607	A477	A345	A278	A217	U155	A91	A28
U1060	C994	U931	C868	C906	A739	C672	A608	A478	A346	A279	A218	U156	U92	U29
G1061	C995	U932	U871	U807	C740	C673	A609	A479	A347	U280	A219	C157	G93	G30
G1062	A996	A933	G872	U741	U741	G674	C610	A480	A348	C281	G220	U158	A94	C31
G1063	C997	U934	C873	A742	A742	A675	C611	A481	U349	A282	A221	G159	A95	C32
U1064	C998	C935	C874	U743	U743	A676	U612	A482	G350	G283	A222	U160	C96	C33
G1065	U999	A936	C875	G744	G744	A677	A613	A483	C351	U284	U223	U161	C97	U34
U1066	A1001	G938	C876	U745	U745	C678	A614	A484	A352	U284	U224	U162	G98	
A1067	G1004	G938	C877	U746	U746	C679	U615	C485	C353	U290	C225	C163	U99	C37
G1068	C1005	A941	C878	U747	U747	C680	A616	A486	A354	G291	A226	C164	U100	A38
A1069	C1006	G942	C879	G748	G748	A685	U617	C487	C357	U292	A227	A165	A101	G39
A1070	C1007	A943	G880	A749	A749	U686	U618	U488	U357	U293	C228	U166	U102	U40
G1071	U1008	G944	C881	A750	A750	U686	U619	A489	U358	A294	C229	A167	A103	C41
C1072	A1008	A945	C882	A751	A751	A689	G620	C490	G361	U296	A231	G168	A104	A42
A1073	A1009	C946	C883	A752	A752	A689	A621	C491	A362	U297	G232	U170	C105	G43
G1074	U1010	A947	C884	A753	U753	G690	G622	A492	A363	G297	G233	U171	C106	A44
C1075	G1011	C948	C885	U754	U754	C691	C623	A493	G363	G298	A234	A172	G107	G45
U1076	U1012	U949	A886	U755	U755	C692	C624	A494	C364	A299	U235	A173	G108	G46
C1077	C1013	G950	U887	G756	G756	A693	G625	A495	U365	A300	C236	U174	G110	G48
U1078	A1014	C951	C888	G757	G757	G696	A626	A496	G366	G301	C237	G175	G111	C48
C1079	U1015	G952	C889	U758	U758	G697	A627	A497	G367	C302	C238	A176	A111	
A1080	U1016	G953	C890	G759	G759	G698	G628	A498	A368	G305	C239	G177	U50	G51
U1081	U1017	C954	C891	U760	U760	A699	G629	G500	U369	C306	C240	G178	C115	G52
U1082	U1018	U955	A892	A761	A761	A699	G630	A501	G370	U307	A241	G179	G117	A53
U1083	A1020	G956	C893	U762	U762	U702	A632	A502	A371	G308	G242	G180	A118	G54
A1084	A1021	C957	C894	G763	G763	U703	A633	A503	G372	A309	U243	G181	A119	G55
A1085	U1022	U958	C895	A764	A764	G704	C634	A504	U373	A310	G244	A182	U120	A56
A1086	G1023	G959	C896	G765	G765	A705	C635	A505	A374	A311	G245	C183	G121	C57
G1087	U1024	A960	C897	U766	U766	A706	G636	A506	G375	G376	C246	C184	G122	G58
A1088	G1025	C961	C898	U767	U767	G707	A637	A507	C377	C314	G247	G187	G123	G59
A1089	G1026	G962	C899	G770	G770	U708	G638	A508	C378	G315	G248	G187	G124	G60
A1090	A1027	U963	C901	G771	G771	U709	U639	C510	G379	C316	C249	G188	A125	G61


C2045	G1980	A1789	C1728	A1665	U1602	G1540	G1478	C1417	G1346	A1285	C1221	G1154	G1091
G2046	A1981	C1790	U1729	G1666	A1603	C1541	G1479	C1418	A1347	A1286	C1221	A1154	C1092
C2047	U1982	A1791	G1730	G1667	C1604	C1542	U1480	A1419	C1348	A1287	U1224	A1155	G1093
G2048	U1855	G1792	G1731	A1668	C1605	G1543	U1481	A1420	C1349	G1288	G1225	G1157	U1094
G2049	G1857	C1793	C1732	A1669	C1606	A1544	G1482	G1421	C1350	C1289	G1226	A1096	A1095
C2050	A1858	A1794	G1733	C1670	G1607	A1545	G1483	G1422	C1351	C1290	G1227	U1158	A1096
A2051	U1859	C1795	G1734	A1671	A1608	G1546	U1484	G1423	C1352	G1291	G1228	G1160	U1097
A2052	U1926	A1796	U1735	A1672	A1609	C1547	U1485	G1424	A1353	G1292	C1229	C1161	A1098
G2053	A1927	U1797	U1736	G1673	A1610	A1548	U1486	G1425	A1354	G1293	C1230	G1162	G1099
C2054	U1929	G1798	G1737	A1674	C1611	A1549	U1487	G1426	G1355	U1294	U1231	G1163	C1100
A2055	G1930	G1799	G1738	C1675	C1612	C1550	U1488	A1427	G1356	C1295	G1232	G1164	U1101
A2056	U1931	C1800	A1739	A1676	G1613	A1551	G1489	G1428	G1357	G1296	C1233	A1165	C1102
A2057	A1932	A1801	G1740	A1677	A1614	A1552	A1490	G1429	G1358	C1297	U1234	G1166	A1103
A2058	U1933	A1802	C1741	A1678	C1615	A1553	G1491	G1430	A1359	C1298	G1235	C1167	C1104
A2059	U1934	C1803	U1742	A1679	A1616	U1554	G1492	A1431	C1362	G1299	G1236	G1168	U1105
A2060	U1935	A1804	G1743	U1680	C1617	C1555	G1493	G1432	G1300	G1300	A1237	A1169	G1106
A2061	G1936	A1805	A1744	G1681	A1618	C1556	A1494	A1433	A1363	A1301	G1238	C1170	G1107
A2062	A1937	A1806	A1745	G1682	G1619	C1557	A1495	A1434	G1364	A1302	G1239	C1171	U1108
C2063	C1938	G1807	A1746	U1683	G1620	C1558	A1496	G1435	A1365	G1303	U1240	C1172	U1109
C2064	U1939	A1808	U1747	G1684	U1624	U1559	U1497	G1436	A1366	A1304	U1241	G1110	G1110
C2065	U1940	A1809	C1748	C1685	C1625	U1562	C1498	G1437	A1367	C1305	U1242	A1175	A1111
C2066	C1941	A1810	A1749	C1686	A1626	U1562	C1499	U1438	G1368	A1307	A1244	U1176	G1112
C2067	G2004	G1811	U1750	C1687	U1626	U1562	C1499	A1439	G1369	A1307	A1244	G1177	U1113
C2068	U1943	A1812	G1752	A1689	U1629	C1563	A1502	U1441	G1370	A1308	A1246	G1178	C1114
C2069	A1944	G1813	G1753	A1690	A1630	C1564	A1503	U1442	U1372	G1311	A1247	U1180	G1116
A2071	G1945	U1814	A1754	C1691	A1630	C1565	A1504	U1443	A1373	U1312	G1248	G1185	C1117
C2072	U1946	A1815	G1755	U1687	G1631	A1566	A1505	U1444	G1374	U1313	U1249	G1186	G1118
C2073	C1947	U1816	G1756	G1695	A1632	G1567	U1506	G1444	U1375	C1314	G1250	G1187	C1121
U2074	G1948	G1817	A1757	G1696	G1633	G1568	C1507	G1445	C1376	C1315	C1251	U1188	C1122
U2075	G1949	A1818	U1758	A1697	A1634	A1569	A1508	G1446	G1377	U1316	G1252	U1189	C1123
U2076	U1950	A1819	A1759	U1698	G1635	A1570	A1509	C1447	A1378	G1317	A1253	A1189	C1124
A2077	U1951	U1820	C1760	A1698	U1636	A1571	G1510	G1448	A1379	U1318	A1254	G1190	G1125
C2078	A1952	A1821	C1761	G1699	A1637	A1572	C1512	C1451	A1383	C1320	U1255	G1191	G1126
U2079	U1953	G1822	A1762	A1700	C1638	C1574	G1513	A1452	A1384	A1321	G1256	G1192	A1126
A2080	G1954	G1823	G1763	A1701	A1640	C1575	A1453	A1453	A1385	A1322	C1257	G1193	A1127
A2081	U1955	U1824	C1764	G1702	A1641	U1576	G1514	C1454	A1386	A1328	U1258	A1194	G1128
A2082	C1892	G1825	U1765	G1703	G1642	C1577	G1515	G1455	C1386	C1323	G1259	G1195	A1129
G2083	C1893	U1827	G1766	C1704	G1642	C1577	G1516	G1456	A1387	G1324	A1260	G1196	U1130
C2084	C1894	G1828	G1767	A1705	G1643	U1578	G1517	U1457	U1391	U1326	C1261	U1199	G1131
U2085	C1895	A1829	C1768	C1706	C1644	A1579	G1518	U1458	A1392	A1327	A1262	U1199	U1132
U2086	A1899	G1830	U1769	G1707	G1645	C1580	U1520	U1459	A1393	A1328	U1263	C1200	A1133
G2087	A1900	C1831	G1770	G1708	C1646	G1581	G1521	U1460	A1393	A1328	A1264	C1200	A1134
C2088	A1901	C1832	C1771	U1709	U1647	C1582	A1522	C1461	U1394	U1329	A1265	U1201	A1135
C2089	C1902	C1833	A1772	G1710	U1648	A1583	U1523	C1461	A1395	C1330	G1266	A1204	G1136
A2090	U1964	A1773	A1773	U1711	G1649	U1584	G1524	C1462	A1395	G1330	G1266	A1205	G1137
C2091	C1965	C1836	C1774	U1712	A1650	C1585	A1525	C1463	U1396	U1267	A1267	G1206	U1140
U2092	A1966	C1837	U1775	A1713	G1651	A1586	C1526	C1464	U1397	A1268	A1268	G1207	U1141
C2093	C1967	G1838	G1776	U1714	A1652	A1586	G1527	G1465	C1398	G1333	A1269	C1207	A1142
A2094	A1968	G1839	U1777	G1715	G1653	A1590	A1528	U1466	C1399	G1334	G1270	G1208	U1143
A2095	C1909	U1841	U1778	U1716	A1654	A1591	G1529	U1467	U1402	G1335	G1271	U1209	A1143
C2096	G1910	G1842	U1779	G1717	C1655	C1592	G1530	U1468	U1403	A1336	A1272	G1210	A1144
A2097	U1911	C1843	U1780	G1718	A1656	A1593	C1531	A1469	A1403	U1273	A1272	C1211	A1145
G2100	A1912	C1844	U1781	G1719	U1657	U1594	A1532	A1470	U1404	G1338	A1274	G1212	C1146
A2101	G1972	G1845	U1782	C1658	C1658	C1595	C1533	G1471	U1405	G1339	A1275	A1213	A1147
G2102	C1974	A1783	A1783	G1659	G1659	A1596	U1534	C1472	U1406	U1340	A1276	G1214	A1147
A2103	G1975	G1846	A1784	A1597	G1660	A1597	U1535	G1473	U1406	G1341	G1277	G1215	U1150
C2104	U1976	A1847	A1785	G1724	G1661	A1598	C1536	U1474	A1413	A1342	C1278	G1216	A1151
A2108	A1977	U1848	A1786	U1725	U1662	U1599	G1537	U1475	U1414	G1343	U1283	G1217	A1152
	C2042	A1978	A1787	G1726	G1663	U1600	G1538	U1476	U1415	U1344	G1283	G1218	C1153
	C2044	U1979	C1727	A1664	A1664	G1601	U1539	A1477	G1416	C1345	A1284		



- Molecule 55: 5S ribosomal RNA

Chain BB:

● Molecule 56: 50S ribosomal protein L1

Chain B5:  88% 7% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	5656	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	161000	Depositor
Image detector	4k CCD camera (TVIPS)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	AB	0.69	0/1736	1.04	13/2340 (0.6%)
10	AK	0.73	0/894	1.19	10/1207 (0.8%)
11	AL	0.74	0/969	1.23	16/1300 (1.2%)
12	AM	0.74	0/884	1.35	18/1181 (1.5%)
13	AN	0.77	0/817	1.35	14/1088 (1.3%)
14	AO	0.70	0/722	1.26	10/964 (1.0%)
15	AP	0.75	0/648	1.16	7/870 (0.8%)
16	AQ	0.69	0/658	1.15	6/883 (0.7%)
17	AR	0.78	0/463	1.19	6/623 (1.0%)
18	AS	0.74	0/653	1.23	6/879 (0.7%)
19	AT	0.68	0/672	1.06	6/890 (0.7%)
2	AC	0.71	0/1651	1.12	15/2225 (0.7%)
20	AU	0.83	0/431	1.55	6/572 (1.0%)
21	AA	1.57	0/36759	2.22	1953/57346 (3.4%)
22	A1	1.59	0/1668	2.19	92/2595 (3.5%)
23	A2	1.54	0/343	2.27	23/531 (4.3%)
24	A3	1.58	1/1722 (0.1%)	2.19	93/2685 (3.5%)
25	BC	0.72	0/2121	1.26	26/2852 (0.9%)
26	BD	0.66	0/1586	1.19	13/2134 (0.6%)
27	BE	0.66	0/1571	1.13	10/2113 (0.5%)
28	BF	0.73	0/1444	1.17	10/1937 (0.5%)
29	BG	0.68	0/1343	1.18	11/1816 (0.6%)
3	AD	0.75	0/1665	1.23	21/2227 (0.9%)
30	BH	0.64	0/1122	1.12	5/1515 (0.3%)
31	BI	0.63	0/1046	1.07	4/1410 (0.3%)
32	BJ	0.70	0/1152	1.17	10/1551 (0.6%)
33	BK	0.69	0/947	1.22	10/1268 (0.8%)
34	BL	0.74	0/1054	1.31	10/1403 (0.7%)
35	BM	0.74	0/1093	1.23	12/1460 (0.8%)
36	BN	0.75	0/973	1.41	17/1301 (1.3%)
37	BO	0.71	0/902	1.24	11/1209 (0.9%)
38	BP	0.72	0/929	1.32	15/1242 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.77	0/960	1.34	18/1278 (1.4%)
4	AE	0.68	0/1119	1.06	8/1506 (0.5%)
40	BR	0.68	0/829	1.10	4/1107 (0.4%)
41	BS	0.64	0/864	1.15	6/1156 (0.5%)
42	BT	0.64	0/744	1.22	7/994 (0.7%)
43	BU	0.68	0/787	1.16	6/1051 (0.6%)
44	BV	0.68	0/766	1.19	8/1025 (0.8%)
45	BW	0.75	0/604	1.28	6/799 (0.8%)
46	BX	0.74	0/635	1.38	9/848 (1.1%)
47	BY	0.66	0/510	1.16	5/677 (0.7%)
48	BZ	0.69	0/453	1.24	3/605 (0.5%)
49	B0	0.73	0/450	1.24	5/599 (0.8%)
5	AF	0.71	0/835	1.13	8/1128 (0.7%)
50	B1	0.69	0/417	1.04	2/556 (0.4%)
51	B2	0.81	0/380	1.47	11/498 (2.2%)
52	B3	0.72	0/513	1.20	6/676 (0.9%)
53	B4	0.67	0/303	1.22	4/397 (1.0%)
54	BA	1.44	16/69796 (0.0%)	2.22	4183/108888 (3.8%)
55	BB	1.46	0/2800	2.16	142/4367 (3.3%)
56	B5	0.63	0/1673	1.11	10/2255 (0.4%)
6	AG	0.73	0/1188	1.19	15/1593 (0.9%)
7	AH	0.69	0/989	1.09	10/1326 (0.8%)
8	AI	0.78	0/1035	1.20	10/1377 (0.7%)
9	AJ	0.72	0/797	1.23	13/1079 (1.2%)
All	All	1.31	17/160085 (0.0%)	2.00	6978/239402 (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
11	AL	0	1
18	AS	0	1
21	AA	0	346
22	A1	0	12
23	A2	0	4
24	A3	0	13
3	AD	0	2
38	BP	0	1
4	AE	0	1
50	B1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	BA	0	647
55	BB	0	19
56	B5	0	1
8	AI	0	1
9	AJ	0	1
All	All	0	1051

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1784	A	N3-C4	5.88	1.38	1.34
54	BA	2405	G	C2-N2	-5.24	1.29	1.34
54	BA	901	C	C4-N4	-5.22	1.29	1.33
54	BA	192	C	C4-N4	-5.21	1.29	1.33
54	BA	2332	C	C4-N4	-5.19	1.29	1.33
54	BA	2676	C	C4-N4	-5.15	1.29	1.33
54	BA	435	C	C4-N4	-5.11	1.29	1.33
54	BA	1617	C	C4-N4	-5.10	1.29	1.33
54	BA	2902	C	C4-N4	-5.10	1.29	1.33
54	BA	1788	C	C4-N4	-5.08	1.29	1.33
54	BA	2232	C	C4-N4	-5.08	1.29	1.33
54	BA	2045	C	C4-N4	-5.06	1.29	1.33
54	BA	1631	G	C2-N2	-5.05	1.29	1.34
24	A3	4	G	C2-N2	-5.03	1.29	1.34
54	BA	229	C	C4-N4	-5.03	1.29	1.33
54	BA	2855	C	C4-N4	-5.03	1.29	1.33
54	BA	1558	C	C4-N4	-5.01	1.29	1.33

All (6978) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2063	C	N3-C2-O2	-17.09	109.94	121.90
54	BA	614	A	O4'-C1'-N9	14.96	120.17	108.20
22	A1	73	A	N1-C6-N6	-14.17	110.10	118.60
54	BA	548	G	O4'-C1'-N9	12.93	118.55	108.20
54	BA	2114	A	N1-C6-N6	-12.72	110.97	118.60
54	BA	218	A	N1-C6-N6	-12.35	111.19	118.60
55	BB	34	A	N1-C6-N6	-12.28	111.23	118.60
21	AA	1225	A	N1-C6-N6	-12.21	111.27	118.60
21	AA	131	A	N1-C6-N6	-12.21	111.28	118.60
54	BA	2317	A	N1-C6-N6	-12.20	111.28	118.60
26	BD	124	ARG	NE-CZ-NH1	12.14	126.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	313	A	N1-C6-N6	-12.10	111.34	118.60
21	AA	913	A	N1-C6-N6	-11.96	111.43	118.60
21	AA	825	A	N1-C6-N6	-11.87	111.48	118.60
54	BA	984	A	N1-C6-N6	-11.87	111.48	118.60
54	BA	743	A	N1-C6-N6	-11.75	111.55	118.60
54	BA	1009	A	N1-C6-N6	-11.71	111.58	118.60
21	AA	1350	A	N1-C6-N6	-11.59	111.65	118.60
54	BA	280	U	O4'-C1'-N1	11.56	117.45	108.20
21	AA	1105	A	N1-C6-N6	-11.55	111.67	118.60
54	BA	490	C	O4'-C1'-N1	11.46	117.37	108.20
30	BH	51	ARG	NE-CZ-NH1	11.43	126.02	120.30
54	BA	1427	A	N1-C6-N6	-11.40	111.76	118.60
54	BA	2063	C	N1-C2-O2	11.38	125.73	118.90
21	AA	563	A	N1-C6-N6	-11.38	111.77	118.60
21	AA	130	A	N1-C6-N6	-11.38	111.78	118.60
54	BA	2320	U	O4'-C1'-N1	11.36	117.29	108.20
54	BA	1241	A	N1-C6-N6	-11.35	111.79	118.60
54	BA	783	A	N1-C6-N6	-11.34	111.80	118.60
21	AA	532	A	N1-C6-N6	-11.33	111.80	118.60
54	BA	896	A	N1-C6-N6	-11.32	111.81	118.60
54	BA	1505	A	N1-C6-N6	-11.32	111.81	118.60
54	BA	196	A	O4'-C1'-N9	11.31	117.25	108.20
54	BA	481	G	O4'-C1'-N9	11.29	117.23	108.20
54	BA	2358	A	N1-C6-N6	-11.28	111.83	118.60
54	BA	2288	A	N1-C6-N6	-11.27	111.84	118.60
54	BA	973	A	N1-C6-N6	-11.22	111.87	118.60
21	AA	171	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	872	A	C1'-O4'-C4'	-11.18	100.96	109.90
54	BA	432	A	N1-C6-N6	-11.15	111.91	118.60
21	AA	1311	A	N1-C6-N6	-11.13	111.92	118.60
21	AA	704	A	N1-C6-N6	-11.13	111.92	118.60
21	AA	766	A	N1-C6-N6	-11.12	111.93	118.60
9	AJ	62	ARG	NE-CZ-NH1	11.04	125.82	120.30
54	BA	1755	A	N1-C6-N6	-11.03	111.98	118.60
54	BA	1046	A	N1-C6-N6	-11.03	111.98	118.60
55	BB	94	A	N1-C6-N6	-11.01	112.00	118.60
54	BA	53	A	N1-C6-N6	-11.00	112.00	118.60
54	BA	2679	A	N1-C6-N6	-11.00	112.00	118.60
21	AA	994	A	N1-C6-N6	-10.96	112.02	118.60
54	BA	1086	A	N1-C6-N6	-10.96	112.02	118.60
54	BA	2267	A	N1-C6-N6	-10.95	112.03	118.60
21	AA	546	A	N1-C6-N6	-10.93	112.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1490	A	O4'-C1'-N9	10.91	116.93	108.20
54	BA	2758	A	N1-C6-N6	-10.89	112.06	118.60
21	AA	50	A	N1-C6-N6	-10.88	112.08	118.60
21	AA	1357	A	N1-C6-N6	-10.87	112.08	118.60
21	AA	520	A	N1-C6-N6	-10.86	112.08	118.60
21	AA	493	A	N1-C6-N6	-10.84	112.10	118.60
54	BA	613	A	N1-C6-N6	-10.83	112.10	118.60
21	AA	918	A	N1-C6-N6	-10.81	112.11	118.60
21	AA	1287	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	792	A	N1-C6-N6	-10.79	112.12	118.60
21	AA	547	A	N1-C6-N6	-10.79	112.13	118.60
55	BB	45	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	1932	A	N1-C6-N6	-10.77	112.14	118.60
21	AA	101	A	N1-C6-N6	-10.75	112.15	118.60
54	BA	1664	A	N1-C6-N6	-10.74	112.15	118.60
54	BA	1175	A	N1-C6-N6	-10.73	112.16	118.60
54	BA	262	A	N1-C6-N6	-10.72	112.17	118.60
21	AA	499	A	N1-C6-N6	-10.70	112.18	118.60
21	AA	1434	A	N1-C6-N6	-10.69	112.18	118.60
21	AA	889	A	N1-C6-N6	-10.69	112.19	118.60
54	BA	2657	A	N1-C6-N6	-10.68	112.19	118.60
54	BA	905	A	N1-C6-N6	-10.68	112.19	118.60
21	AA	579	A	N1-C6-N6	-10.67	112.20	118.60
54	BA	71	A	N1-C6-N6	-10.67	112.20	118.60
54	BA	1014	A	N1-C6-N6	-10.66	112.20	118.60
54	BA	323	C	O4'-C1'-N1	10.65	116.72	108.20
54	BA	2564	A	N1-C6-N6	-10.65	112.21	118.60
33	BK	64	ARG	NE-CZ-NH1	10.65	125.62	120.30
54	BA	2766	A	N1-C6-N6	-10.64	112.21	118.60
21	AA	1368	A	N1-C6-N6	-10.63	112.22	118.60
54	BA	323	C	N3-C2-O2	-10.62	114.46	121.90
54	BA	975	A	N1-C6-N6	-10.62	112.23	118.60
54	BA	1759	A	N1-C6-N6	-10.62	112.23	118.60
54	BA	2800	A	N1-C6-N6	-10.62	112.23	118.60
54	BA	2169	A	O4'-C1'-N9	10.61	116.69	108.20
21	AA	320	A	N1-C6-N6	-10.59	112.25	118.60
54	BA	1713	A	N1-C6-N6	-10.57	112.26	118.60
21	AA	919	A	N1-C6-N6	-10.56	112.27	118.60
54	BA	1156	A	N1-C6-N6	-10.55	112.27	118.60
54	BA	1853	A	N1-C6-N6	-10.55	112.27	118.60
54	BA	751	A	N1-C6-N6	-10.53	112.28	118.60
54	BA	2733	A	N1-C6-N6	-10.51	112.29	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2734	A	N1-C6-N6	-10.51	112.30	118.60
21	AA	935	A	N1-C6-N6	-10.50	112.30	118.60
21	AA	609	A	N1-C6-N6	-10.49	112.31	118.60
54	BA	945	A	N1-C6-N6	-10.49	112.31	118.60
54	BA	1801	A	N1-C6-N6	-10.49	112.31	118.60
54	BA	404	A	N1-C6-N6	-10.48	112.31	118.60
38	BP	100	ARG	NE-CZ-NH1	10.47	125.53	120.30
54	BA	1607	C	O4'-C1'-N1	10.46	116.57	108.20
34	BL	21	ARG	NE-CZ-NH1	10.45	125.53	120.30
54	BA	1385	A	N1-C6-N6	-10.45	112.33	118.60
54	BA	2030	A	N1-C6-N6	-10.44	112.34	118.60
21	AA	1340	A	N1-C6-N6	-10.42	112.35	118.60
21	AA	1288	A	N1-C6-N6	-10.39	112.37	118.60
54	BA	265	A	O4'-C1'-N9	10.38	116.51	108.20
54	BA	5	A	N1-C6-N6	-10.38	112.38	118.60
54	BA	2726	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	2482	A	N1-C6-N6	-10.36	112.38	118.60
54	BA	528	A	N1-C6-N6	-10.36	112.39	118.60
54	BA	699	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	2003	A	N1-C6-N6	-10.34	112.40	118.60
21	AA	1204	A	N1-C6-N6	-10.33	112.40	118.60
54	BA	959	A	N1-C6-N6	-10.32	112.41	118.60
39	BQ	29	ARG	NE-CZ-NH1	10.32	125.46	120.30
54	BA	2170	A	N1-C6-N6	-10.32	112.41	118.60
54	BA	2327	A	N1-C6-N6	-10.31	112.41	118.60
21	AA	466	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	1938	A	N1-C6-N6	-10.29	112.43	118.60
21	AA	914	A	N1-C6-N6	-10.25	112.45	118.60
56	B5	134	ARG	NE-CZ-NH1	10.25	125.42	120.30
54	BA	1877	A	N1-C6-N6	-10.22	112.47	118.60
54	BA	2059	A	N1-C6-N6	-10.21	112.47	118.60
54	BA	1265	A	N1-C6-N6	-10.21	112.48	118.60
54	BA	633	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	1274	A	N1-C6-N6	-10.20	112.48	118.60
21	AA	461	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	1630	A	N1-C6-N6	-10.20	112.48	118.60
21	AA	635	A	N1-C6-N6	-10.19	112.49	118.60
54	BA	2213	U	O4'-C1'-N1	10.17	116.34	108.20
54	BA	1073	A	O4'-C1'-N9	10.17	116.34	108.20
54	BA	2134	A	N1-C6-N6	-10.17	112.50	118.60
54	BA	2126	A	O4'-C1'-N9	10.16	116.33	108.20
54	BA	2753	A	N1-C6-N6	-10.16	112.50	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	861	A	N1-C6-N6	-10.16	112.50	118.60
21	AA	74	A	N1-C6-N6	-10.16	112.51	118.60
21	AA	1502	A	N1-C6-N6	-10.14	112.51	118.60
21	AA	1418	A	N1-C6-N6	-10.14	112.51	118.60
21	AA	1398	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	2092	U	O4'-C1'-N1	10.14	116.31	108.20
54	BA	1420	A	N1-C6-N6	-10.13	112.52	118.60
21	AA	1275	A	N1-C6-N6	-10.12	112.53	118.60
54	BA	2145	C	N3-C2-O2	-10.12	114.81	121.90
54	BA	299	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	1603	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	515	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	2547	A	N1-C6-N6	-10.11	112.54	118.60
21	AA	665	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	1253	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	1022	A	N1-C6-N6	-10.09	112.54	118.60
54	BA	1308	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	1632	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	925	A	N1-C6-N6	-10.08	112.55	118.60
45	BW	38	ARG	NE-CZ-NH1	10.07	125.33	120.30
54	BA	1054	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	2270	A	N1-C6-N6	-10.06	112.56	118.60
20	AU	20	ARG	NE-CZ-NH1	10.06	125.33	120.30
54	BA	788	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	538	A	N1-C6-N6	-10.06	112.57	118.60
54	BA	1549	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	451	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	1606	C	O4'-C1'-N1	10.05	116.24	108.20
3	AD	114	ARG	NE-CZ-NH1	10.05	125.32	120.30
21	AA	1396	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	1570	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	784	G	O4'-C1'-N9	10.04	116.23	108.20
54	BA	1711	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	1970	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	340	A	N1-C6-N6	-10.03	112.58	118.60
21	AA	408	A	N1-C6-N6	-10.02	112.59	118.60
54	BA	2108	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	478	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	860	A	N1-C6-N6	-10.01	112.59	118.60
21	AA	1014	A	N1-C6-N6	-10.01	112.59	118.60
21	AA	729	A	N1-C6-N6	-10.01	112.60	118.60
54	BA	322	A	N1-C6-N6	-10.00	112.60	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1127	A	N1-C6-N6	-10.00	112.60	118.60
36	BN	118	ARG	NE-CZ-NH1	10.00	125.30	120.30
21	AA	1447	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	1057	A	N1-C6-N6	-9.99	112.60	118.60
54	BA	1021	A	N1-C6-N6	-9.99	112.61	118.60
19	AT	28	ARG	NE-CZ-NH1	9.98	125.29	120.30
21	AA	718	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	2425	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	1810	A	N1-C6-N6	-9.98	112.61	118.60
23	A2	91	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	1678	A	N1-C6-N6	-9.97	112.62	118.60
21	AA	983	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	2706	A	N1-C6-N6	-9.97	112.62	118.60
21	AA	781	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	309	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	422	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	1360	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	1876	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	2031	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	152	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	825	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	84	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	1248	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	780	A	N1-C6-N6	-9.91	112.65	118.60
21	AA	197	A	N1-C6-N6	-9.91	112.65	118.60
21	AA	622	A	N1-C6-N6	-9.91	112.66	118.60
54	BA	706	A	N1-C6-N6	-9.91	112.65	118.60
54	BA	103	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	716	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	1167	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	2513	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	969	A	N1-C6-N6	-9.89	112.66	118.60
21	AA	968	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	1607	C	N3-C2-O2	-9.88	114.98	121.90
54	BA	1566	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	735	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	1552	A	N1-C6-N6	-9.88	112.67	118.60
21	AA	502	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	532	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	342	A	N1-C6-N6	-9.86	112.68	118.60
21	AA	468	A	N1-C6-N6	-9.86	112.69	118.60
54	BA	1522	A	N1-C6-N6	-9.86	112.69	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	807	A	N1-C6-N6	-9.85	112.69	118.60
51	B2	34	ARG	NE-CZ-NH1	9.85	125.22	120.30
54	BA	2376	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	2589	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	401	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	990	A	N1-C6-N6	-9.83	112.70	118.60
21	AA	1067	A	N1-C6-N6	-9.82	112.70	118.60
54	BA	730	A	N1-C6-N6	-9.82	112.71	118.60
54	BA	1327	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	1384	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	727	A	N1-C6-N6	-9.80	112.72	118.60
21	AA	759	A	N1-C6-N6	-9.79	112.73	118.60
21	AA	363	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	412	A	N1-C6-N6	-9.78	112.73	118.60
12	AM	106	ARG	NE-CZ-NH1	9.77	125.19	120.30
54	BA	119	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	1251	A	N1-C6-N6	-9.76	112.75	118.60
40	BR	78	ARG	NE-CZ-NH1	9.76	125.18	120.30
21	AA	397	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	1937	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	503	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	928	A	N1-C6-N6	-9.75	112.75	118.60
21	AA	192	A	N1-C6-N6	-9.74	112.76	118.60
21	AA	1179	A	N1-C6-N6	-9.74	112.76	118.60
21	AA	815	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	877	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	21	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1607	C	N1-C2-O2	9.72	124.73	118.90
54	BA	677	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	878	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	2064	C	N3-C2-O2	-9.72	115.10	121.90
54	BA	1336	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1731	G	O4'-C1'-N9	9.70	115.96	108.20
54	BA	936	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	687	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	2247	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	300	A	N1-C6-N6	-9.68	112.80	118.60
21	AA	162	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	1626	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	2748	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	1606	C	N3-C2-O2	-9.67	115.13	121.90
21	AA	938	A	N1-C6-N6	-9.66	112.80	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	988	A	N1-C6-N6	-9.66	112.80	118.60
54	BA	1088	A	N1-C6-N6	-9.66	112.80	118.60
54	BA	42	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	1960	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	2198	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	2858	C	O4'-C1'-N1	9.66	115.93	108.20
26	BD	83	ARG	NE-CZ-NH1	9.65	125.13	120.30
21	AA	1318	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	821	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	139	A	N1-C6-N6	-9.64	112.81	118.60
21	AA	1431	A	N1-C6-N6	-9.64	112.81	118.60
23	A2	82	A	N1-C6-N6	-9.64	112.81	118.60
54	BA	278	A	N1-C6-N6	-9.64	112.82	118.60
16	AQ	10	ARG	NE-CZ-NH1	9.64	125.12	120.30
54	BA	2205	A	N1-C6-N6	-9.64	112.82	118.60
21	AA	1256	A	N1-C6-N6	-9.63	112.82	118.60
22	A1	26	A	N1-C6-N6	-9.63	112.82	118.60
21	AA	977	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	833	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1301	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2665	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	348	A	N1-C6-N6	-9.61	112.84	118.60
54	BA	1126	A	N1-C6-N6	-9.61	112.84	118.60
54	BA	2227	A	N1-C6-N6	-9.60	112.84	118.60
3	AD	12	ARG	NE-CZ-NH1	9.59	125.10	120.30
54	BA	1854	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	752	A	N1-C6-N6	-9.59	112.85	118.60
38	BP	87	ARG	NE-CZ-NH1	9.57	125.08	120.30
54	BA	430	A	N1-C6-N6	-9.57	112.86	118.60
21	AA	1145	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	749	A	N1-C6-N6	-9.56	112.87	118.60
54	BA	1454	C	N3-C2-O2	-9.56	115.21	121.90
21	AA	389	A	N1-C6-N6	-9.55	112.87	118.60
42	BT	12	ARG	NE-CZ-NH1	9.54	125.07	120.30
21	AA	55	A	N1-C6-N6	-9.54	112.87	118.60
21	AA	1171	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	1366	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	2308	G	O4'-C1'-N9	9.54	115.83	108.20
54	BA	2176	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	1329	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	1227	A	N1-C6-N6	-9.53	112.89	118.60
54	BA	2810	A	N1-C6-N6	-9.53	112.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	29	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	1055	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	323	C	N1-C2-O2	9.52	124.61	118.90
54	BA	2654	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	94	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	602	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	753	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2602	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	2572	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	845	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	2019	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	2378	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	300	A	N1-C6-N6	-9.50	112.90	118.60
21	AA	872	A	O4'-C1'-N9	9.49	115.79	108.20
21	AA	629	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	866	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	696	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	1492	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	886	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	2634	A	N1-C6-N6	-9.47	112.92	118.60
22	A1	59	U	O4'-C1'-N1	9.46	115.77	108.20
21	AA	607	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	1789	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	2418	A	N1-C6-N6	-9.46	112.92	118.60
21	AA	702	A	N1-C6-N6	-9.46	112.92	118.60
55	BB	15	A	N1-C6-N6	-9.46	112.92	118.60
21	AA	1035	A	N1-C6-N6	-9.46	112.93	118.60
36	BN	63	ARG	NE-CZ-NH1	9.46	125.03	120.30
21	AA	782	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	509	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1523	U	O4'-C1'-N1	9.45	115.76	108.20
21	AA	1534	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	1069	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	1469	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	2900	A	N1-C6-N6	-9.44	112.94	118.60
9	AJ	31	ARG	NE-CZ-NH1	9.44	125.02	120.30
54	BA	478	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	346	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	1080	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	83	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	2476	A	N1-C6-N6	-9.43	112.94	118.60
24	A3	73	A	N1-C6-N6	-9.43	112.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	71	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	91	A	O4'-C1'-N9	9.41	115.73	108.20
21	AA	194	C	N3-C2-O2	-9.40	115.32	121.90
21	AA	1197	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	1480	A	N1-C6-N6	-9.40	112.96	118.60
24	A3	77	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	728	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	2042	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	2879	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	1319	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	614	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	149	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	19	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	2450	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	1110	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	1821	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	2284	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	447	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	983	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	750	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	1493	C	O4'-C1'-N1	9.37	115.70	108.20
54	BA	2761	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1395	A	N1-C6-N6	-9.37	112.98	118.60
56	B5	9	ARG	NE-CZ-NH1	9.37	124.98	120.30
54	BA	2117	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	2211	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	1569	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	2451	A	N1-C6-N6	-9.35	112.99	118.60
21	AA	539	A	N1-C6-N6	-9.34	112.99	118.60
21	AA	600	A	N1-C6-N6	-9.34	113.00	118.60
22	A1	21	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	2266	A	N1-C6-N6	-9.33	113.00	118.60
3	AD	55	ARG	NE-CZ-NH1	9.32	124.96	120.30
21	AA	908	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	1238	A	N1-C6-N6	-9.32	113.01	118.60
25	BC	220	ARG	NE-CZ-NH1	9.32	124.96	120.30
54	BA	2097	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	1616	A	N1-C6-N6	-9.31	113.01	118.60
27	BE	88	ARG	NE-CZ-NH1	9.31	124.95	120.30
16	AQ	39	ARG	NE-CZ-NH1	9.31	124.95	120.30
21	AA	174	A	N1-C6-N6	-9.31	113.02	118.60
54	BA	330	A	N1-C6-N6	-9.30	113.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2799	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	320	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	2600	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	119	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	222	A	N1-C6-N6	-9.29	113.03	118.60
18	AS	77	ARG	NE-CZ-NH2	9.29	124.94	120.30
54	BA	849	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	1548	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2886	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	2407	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	1496	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	1815	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	1634	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	1500	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1591	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	1092	A	N1-C6-N6	-9.26	113.04	118.60
28	BF	147	ARG	NE-CZ-NH1	9.26	124.93	120.30
54	BA	443	A	N1-C6-N6	-9.26	113.04	118.60
54	BA	160	A	N1-C6-N6	-9.26	113.05	118.60
54	BA	599	A	N1-C6-N6	-9.26	113.05	118.60
21	AA	602	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	10	A	N1-C6-N6	-9.24	113.05	118.60
21	AA	1152	A	N1-C6-N6	-9.24	113.05	118.60
21	AA	1219	A	N1-C6-N6	-9.24	113.05	118.60
21	AA	784	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	1885	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	432	A	N1-C6-N6	-9.23	113.06	118.60
25	BC	269	ARG	NE-CZ-NH1	9.23	124.92	120.30
54	BA	203	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	181	A	N1-C6-N6	-9.23	113.06	118.60
54	BA	721	A	N1-C6-N6	-9.23	113.06	118.60
6	AG	118	ARG	NE-CZ-NH1	9.22	124.91	120.30
54	BA	2516	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1654	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1347	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1927	A	N1-C6-N6	-9.22	113.07	118.60
21	AA	1513	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	632	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	2736	A	N1-C6-N6	-9.21	113.08	118.60
54	BA	2565	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	415	A	N1-C6-N6	-9.20	113.08	118.60
42	BT	69	ARG	NE-CZ-NH1	9.20	124.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2882	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	2850	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	1609	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	931	U	O4'-C1'-N1	9.19	115.55	108.20
21	AA	306	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	627	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	2274	A	N1-C6-N6	-9.18	113.09	118.60
20	AU	6	ARG	NE-CZ-NH1	9.18	124.89	120.30
24	A3	45	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1085	A	N1-C6-N6	-9.17	113.10	118.60
34	BL	48	ARG	NE-CZ-NH1	9.17	124.89	120.30
44	BV	21	ARG	NE-CZ-NH2	9.17	124.88	120.30
3	AD	61	ARG	NE-CZ-NH1	9.16	124.88	120.30
54	BA	64	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	1413	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	2813	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	325	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	1103	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	146	A	N1-C6-N6	-9.14	113.11	118.60
54	BA	590	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	626	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	1637	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	431	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	583	A	N1-C6-N6	-9.11	113.13	118.60
21	AA	1016	A	N1-C6-N6	-9.11	113.13	118.60
30	BH	97	ARG	NE-CZ-NH1	9.11	124.86	120.30
54	BA	1029	A	N1-C6-N6	-9.11	113.13	118.60
21	AA	182	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	2764	A	N1-C6-N6	-9.11	113.14	118.60
21	AA	1363	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	1508	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2184	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	1289	A	N1-C6-N6	-9.10	113.14	118.60
3	AD	183	ARG	NE-CZ-NH1	9.09	124.85	120.30
54	BA	608	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	2090	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	382	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	2412	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	911	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	1981	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	60	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	78	A	N1-C6-N6	-9.07	113.16	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1142	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	81	A	N1-C6-N6	-9.07	113.16	118.60
37	BO	13	ARG	NE-CZ-NH1	9.06	124.83	120.30
54	BA	1269	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	238	A	N1-C6-N6	-9.06	113.17	118.60
21	AA	1216	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	1434	A	N1-C6-N6	-9.06	113.17	118.60
21	AA	366	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1067	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	2322	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	439	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1701	A	N1-C6-N6	-9.05	113.17	118.60
27	BE	67	ARG	NE-CZ-NH1	9.05	124.82	120.30
12	AM	86	ARG	NE-CZ-NH1	9.04	124.82	120.30
21	AA	1188	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2158	A	N1-C6-N6	-9.04	113.18	118.60
38	BP	38	ARG	NE-CZ-NH1	9.03	124.82	120.30
54	BA	1528	A	N1-C6-N6	-9.03	113.18	118.60
55	BB	50	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	197	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	1998	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2628	C	N3-C2-O2	-9.02	115.58	121.90
54	BA	2721	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	559	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	479	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	1008	A	N1-C6-N6	-9.01	113.19	118.60
21	AA	298	A	C5-C6-N1	9.01	122.20	117.70
21	AA	915	A	C5-C6-N1	9.00	122.20	117.70
54	BA	2273	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	1019	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1808	A	C5-C6-N1	9.00	122.20	117.70
21	AA	33	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	722	A	N1-C6-N6	-8.99	113.20	118.60
54	BA	1717	A	N1-C6-N6	-8.99	113.20	118.60
21	AA	329	A	C5-C6-N1	8.99	122.20	117.70
21	AA	246	A	N1-C6-N6	-8.99	113.21	118.60
44	BV	79	ARG	NE-CZ-NH1	8.99	124.80	120.30
21	AA	364	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	586	A	N1-C6-N6	-8.99	113.21	118.60
12	AM	91	ARG	NE-CZ-NH1	8.98	124.79	120.30
54	BA	2009	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2541	A	N1-C6-N6	-8.98	113.21	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2542	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	223	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	1205	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	1858	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2468	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	345	C	N3-C2-O2	-8.97	115.62	121.90
54	BA	1566	A	C5-C6-N1	8.97	122.19	117.70
54	BA	1668	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	8	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1641	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1729	U	O4'-C1'-N1	8.97	115.38	108.20
54	BA	1809	A	N1-C6-N6	-8.97	113.22	118.60
24	A3	39	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1096	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1525	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	1324	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1928	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	715	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	160	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	553	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	804	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1785	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	393	A	N1-C6-N6	-8.96	113.23	118.60
54	BA	1848	A	N1-C6-N6	-8.95	113.23	118.60
46	BX	2	ARG	NE-CZ-NH1	8.94	124.77	120.30
54	BA	563	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	452	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	1021	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	1144	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	915	A	N1-C6-N6	-8.93	113.25	118.60
54	BA	889	C	N3-C2-O2	-8.93	115.65	121.90
54	BA	2145	C	N1-C2-O2	8.92	124.25	118.90
54	BA	781	A	N1-C6-N6	-8.92	113.25	118.60
14	AO	76	ARG	NE-CZ-NH1	8.92	124.76	120.30
21	AA	901	A	N1-C6-N6	-8.92	113.25	118.60
21	AA	1080	A	N1-C6-N6	-8.92	113.25	118.60
21	AA	1362	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	2366	A	N1-C6-N6	-8.92	113.25	118.60
21	AA	1000	A	N1-C6-N6	-8.91	113.25	118.60
21	AA	1196	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	63	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1387	A	N1-C6-N6	-8.90	113.26	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1791	A	N1-C6-N6	-8.89	113.26	118.60
21	AA	1213	A	N1-C6-N6	-8.89	113.26	118.60
54	BA	1387	A	O4'-C1'-N9	8.89	115.31	108.20
54	BA	1786	A	N1-C6-N6	-8.89	113.26	118.60
54	BA	1454	C	N1-C2-O2	8.89	124.23	118.90
54	BA	1583	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	263	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	1109	C	N3-C2-O2	-8.89	115.68	121.90
54	BA	2369	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	909	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	1433	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	668	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	2062	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	974	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	7	A	N1-C6-N6	-8.88	113.28	118.60
21	AA	98	A	N1-C6-N6	-8.88	113.28	118.60
54	BA	513	A	N1-C6-N6	-8.88	113.28	118.60
39	BQ	49	ARG	NE-CZ-NH1	8.87	124.73	120.30
54	BA	1077	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	1650	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	777	A	N1-C6-N6	-8.86	113.28	118.60
20	AU	16	ARG	NE-CZ-NH1	8.86	124.73	120.30
54	BA	2860	A	N1-C6-N6	-8.86	113.29	118.60
54	BA	716	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	1246	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	465	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	1084	A	C5-C6-N1	8.85	122.12	117.70
21	AA	665	A	C5-C6-N1	8.84	122.12	117.70
54	BA	1916	A	N1-C6-N6	-8.84	113.30	118.60
21	AA	411	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	449	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	483	A	N1-C6-N6	-8.84	113.30	118.60
21	AA	1519	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	644	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	497	A	N1-C6-N6	-8.83	113.30	118.60
21	AA	1157	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	219	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	72	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	1900	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	383	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	960	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	1031	C	N3-C2-O2	-8.81	115.73	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	947	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1912	A	N1-C6-N6	-8.81	113.32	118.60
21	AA	460	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	1515	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	2227	A	C5-C6-N1	8.80	122.10	117.70
54	BA	718	A	O4'-C1'-N9	8.80	115.24	108.20
54	BA	1307	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	767	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	465	A	C1'-O4'-C4'	-8.79	102.87	109.90
54	BA	182	A	N1-C6-N6	-8.79	113.33	118.60
22	A1	74	C	N3-C2-O2	-8.79	115.75	121.90
54	BA	204	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	1167	A	C5-C6-N1	8.77	122.09	117.70
54	BA	2381	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2088	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	1333	A	N1-C6-N6	-8.77	113.34	118.60
34	BL	59	ARG	NE-CZ-NH1	8.76	124.68	120.30
54	BA	2163	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	243	A	N1-C6-N6	-8.76	113.35	118.60
54	BA	764	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	2154	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	2883	A	C5-C6-N1	8.74	122.07	117.70
54	BA	1151	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	2020	A	N1-C6-N6	-8.74	113.36	118.60
44	BV	19	ARG	NE-CZ-NH1	8.74	124.67	120.30
21	AA	790	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1614	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1241	A	C5-C6-N1	8.73	122.07	117.70
54	BA	2883	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	2278	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	780	A	C5-C6-N1	8.73	122.06	117.70
21	AA	1434	A	C5-C6-N1	8.73	122.06	117.70
54	BA	1176	U	O4'-C1'-N1	8.73	115.18	108.20
54	BA	1314	C	N3-C2-O2	-8.73	115.79	121.90
54	BA	1032	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	1252	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	802	A	N1-C6-N6	-8.72	113.37	118.60
16	AQ	26	ARG	NE-CZ-NH1	8.72	124.66	120.30
24	A3	44	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	2666	C	N3-C2-O2	-8.71	115.80	121.90
54	BA	639	U	O4'-C1'-N1	8.71	115.17	108.20
54	BA	933	A	N1-C6-N6	-8.71	113.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2778	A	N1-C6-N6	-8.71	113.37	118.60
39	BQ	5	ARG	NE-CZ-NH1	8.71	124.65	120.30
54	BA	1048	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	2071	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	666	A	N1-C6-N6	-8.70	113.38	118.60
48	BZ	15	ARG	NE-CZ-NH1	8.70	124.65	120.30
54	BA	1805	A	N1-C6-N6	-8.70	113.38	118.60
21	AA	975	A	C5-C6-N1	8.69	122.05	117.70
54	BA	1365	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	1204	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	1287	A	N1-C6-N6	-8.69	113.39	118.60
46	BX	17	ARG	NE-CZ-NH1	8.69	124.64	120.30
54	BA	347	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1260	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	80	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	172	A	N1-C6-N6	-8.68	113.39	118.60
55	BB	73	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1730	C	N3-C2-O2	-8.68	115.83	121.90
3	AD	164	ARG	NE-CZ-NH1	8.67	124.64	120.30
54	BA	466	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	65	A	C5-C6-N1	8.67	122.03	117.70
54	BA	643	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	1117	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	2070	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	1272	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	541	A	N1-C6-N6	-8.66	113.41	118.60
54	BA	368	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	120	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	1276	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	176	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	2809	A	N1-C6-N6	-8.64	113.41	118.60
21	AA	19	A	N1-C6-N6	-8.64	113.41	118.60
21	AA	279	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	676	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	560	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1439	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1955	U	O4'-C1'-N1	8.64	115.11	108.20
54	BA	2675	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	927	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	2711	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	2013	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	1772	A	N1-C6-N6	-8.63	113.42	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2060	A	C5-C6-N1	8.63	122.01	117.70
54	BA	2170	A	C5-C6-N1	8.63	122.02	117.70
54	BA	2776	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	152	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	183	C	N3-C2-O2	-8.62	115.87	121.90
21	AA	1346	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	231	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	1700	A	N1-C6-N6	-8.62	113.43	118.60
39	BQ	63	ARG	NE-CZ-NH1	8.61	124.61	120.30
21	AA	958	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	173	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	2435	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	1913	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	2241	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	789	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	1244	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	2573	C	N3-C2-O2	-8.60	115.88	121.90
21	AA	608	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	649	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1669	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	1101	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	1084	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	739	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	637	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	415	A	N1-C6-N6	-8.58	113.45	118.60
55	BB	15	A	C5-C6-N1	8.57	121.99	117.70
21	AA	1196	A	C5-C6-N1	8.57	121.99	117.70
54	BA	1247	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2173	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2899	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	250	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	829	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	673	A	N1-C6-N6	-8.56	113.47	118.60
54	BA	1537	G	O4'-C1'-N9	8.56	115.05	108.20
54	BA	2471	A	N1-C6-N6	-8.56	113.47	118.60
54	BA	1610	A	O4'-C1'-N9	8.55	115.04	108.20
54	BA	2497	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	51	A	N1-C6-N6	-8.55	113.47	118.60
22	A1	66	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2033	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2377	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	802	A	N1-C6-N6	-8.54	113.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2860	A	C5-C6-N1	8.54	121.97	117.70
21	AA	274	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	550	C	N3-C2-O2	-8.54	115.92	121.90
54	BA	1194	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	171	A	C5-C6-N1	8.53	121.97	117.70
33	BK	18	ARG	NE-CZ-NH1	8.53	124.57	120.30
54	BA	546	U	O4'-C1'-N1	8.53	115.03	108.20
54	BA	2080	A	N1-C6-N6	-8.53	113.48	118.60
46	BX	56	ARG	NE-CZ-NH1	8.52	124.56	120.30
21	AA	964	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	1098	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	10	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	1981	A	C5-C6-N1	8.52	121.96	117.70
21	AA	321	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	2054	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	533	A	C5-C6-N1	8.51	121.95	117.70
36	BN	22	ARG	NE-CZ-NH1	8.51	124.55	120.30
54	BA	1652	A	N1-C6-N6	-8.51	113.50	118.60
5	AF	38	ARG	NE-CZ-NH1	8.50	124.55	120.30
21	AA	1456	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1265	A	C5-C6-N1	8.50	121.95	117.70
21	AA	706	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	197	A	C5-C6-N1	8.50	121.95	117.70
54	BA	1359	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	878	A	N1-C6-N6	-8.49	113.51	118.60
34	BL	60	ARG	NE-CZ-NH1	8.49	124.54	120.30
21	AA	1158	C	N3-C2-O2	-8.48	115.96	121.90
54	BA	1021	A	C5-C6-N1	8.48	121.94	117.70
54	BA	2461	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1590	A	N1-C6-N6	-8.48	113.52	118.60
54	BA	2198	A	O4'-C1'-N9	8.47	114.98	108.20
54	BA	1143	A	N1-C6-N6	-8.47	113.52	118.60
21	AA	1311	A	C4-C5-C6	-8.47	112.77	117.00
21	AA	327	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1000	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	704	A	C5-C6-N1	8.46	121.93	117.70
21	AA	747	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	346	A	C5-C6-N1	8.46	121.93	117.70
54	BA	2809	A	C5-C6-N1	8.46	121.93	117.70
54	BA	2810	A	C5-C6-N1	8.46	121.93	117.70
54	BA	2062	A	C5-C6-N1	8.45	121.92	117.70
21	AA	872	A	N1-C6-N6	-8.45	113.53	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1507	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	336	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	227	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	1451	C	O4'-C1'-N1	8.45	114.96	108.20
21	AA	189	A	C5-C6-N1	8.45	121.92	117.70
54	BA	1089	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	642	A	N1-C6-N6	-8.44	113.53	118.60
55	BB	39	A	N1-C6-N6	-8.44	113.53	118.60
1	AB	73	ARG	NE-CZ-NH1	8.44	124.52	120.30
21	AA	1042	A	N1-C6-N6	-8.44	113.53	118.60
21	AA	814	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	299	A	C5-C6-N1	8.44	121.92	117.70
21	AA	190	A	N1-C6-N6	-8.43	113.54	118.60
25	BC	155	ARG	NE-CZ-NH2	-8.43	116.09	120.30
14	AO	63	ARG	NE-CZ-NH1	8.42	124.51	120.30
54	BA	654	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	165	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	847	U	O4'-C1'-N1	8.42	114.94	108.20
54	BA	2478	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	1133	A	C5-C6-N1	8.42	121.91	117.70
54	BA	1373	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	749	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	1169	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	1978	A	N1-C6-N6	-8.41	113.55	118.60
55	BB	115	A	N1-C6-N6	-8.41	113.56	118.60
3	AD	127	ARG	NE-CZ-NH1	8.41	124.50	120.30
21	AA	1493	A	N1-C6-N6	-8.41	113.56	118.60
25	BC	213	ARG	NE-CZ-NH1	8.41	124.50	120.30
21	AA	371	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2287	A	N1-C6-N6	-8.40	113.56	118.60
2	AC	87	ARG	NE-CZ-NH1	8.40	124.50	120.30
22	A1	16	C	N3-C2-O2	-8.40	116.02	121.90
24	A3	22	A	C5-C6-N1	8.40	121.90	117.70
21	AA	328	C	N3-C2-O2	-8.40	116.02	121.90
21	AA	199	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2433	A	N1-C6-N6	-8.40	113.56	118.60
55	BB	99	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	978	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	1672	A	N1-C6-N6	-8.39	113.56	118.60
13	AN	75	ARG	NE-CZ-NH1	8.39	124.50	120.30
54	BA	233	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2825	G	O4'-C1'-N9	8.39	114.91	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1191	A	N1-C6-N6	-8.39	113.57	118.60
24	A3	76	C	C1'-O4'-C4'	-8.39	103.19	109.90
22	A1	41	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	155	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	1285	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	1304	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	2346	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	1340	U	O4'-C1'-N1	8.38	114.90	108.20
51	B2	35	ARG	NE-CZ-NH1	8.38	124.49	120.30
52	B3	7	ARG	NE-CZ-NH1	8.38	124.49	120.30
55	BB	66	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	490	C	N3-C2-O2	-8.37	116.04	121.90
21	AA	563	A	C4-C5-C6	-8.37	112.81	117.00
21	AA	596	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	2856	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1780	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1952	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	1082	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	911	A	C5-C6-N1	8.37	121.88	117.70
54	BA	1431	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1847	A	O4'-C1'-N9	8.37	114.89	108.20
21	AA	1430	A	N1-C6-N6	-8.36	113.58	118.60
29	BG	68	ARG	NE-CZ-NH1	8.36	124.48	120.30
54	BA	672	C	O4'-C1'-N1	8.36	114.89	108.20
54	BA	1774	C	N3-C2-O2	-8.36	116.05	121.90
21	AA	493	A	C5-C6-N1	8.36	121.88	117.70
24	A3	74	A	N1-C6-N6	-8.36	113.59	118.60
54	BA	2700	A	N1-C6-N6	-8.36	113.59	118.60
54	BA	2851	A	C5-C6-N1	8.36	121.88	117.70
22	A1	14	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	415	A	C5-C6-N1	8.35	121.88	117.70
21	AA	864	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	621	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	681	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	792	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	1679	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	2459	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	277	G	O4'-C1'-N9	8.34	114.87	108.20
54	BA	1226	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	941	A	N1-C6-N6	-8.34	113.60	118.60
21	AA	461	A	C5-C6-N1	8.33	121.87	117.70
54	BA	2534	A	N1-C6-N6	-8.33	113.60	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2670	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	1382	C	N3-C2-O2	-8.33	116.07	121.90
54	BA	794	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	2058	A	N1-C6-N6	-8.33	113.60	118.60
55	BB	101	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	2422	C	N3-C2-O2	-8.33	116.07	121.90
21	AA	44	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	476	U	P-O3'-C3'	8.32	129.69	119.70
54	BA	1353	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	2727	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	2426	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	892	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	126	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	1408	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	1090	A	C5-C6-N1	8.31	121.86	117.70
54	BA	1829	A	N1-C6-N6	-8.31	113.61	118.60
26	BD	83	ARG	NE-CZ-NH2	-8.31	116.14	120.30
14	AO	52	ARG	NE-CZ-NH1	8.31	124.45	120.30
21	AA	1274	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	996	A	N1-C6-N6	-8.31	113.62	118.60
24	A3	16	C	N3-C2-O2	-8.30	116.09	121.90
54	BA	2632	A	N1-C6-N6	-8.30	113.62	118.60
24	A3	59	A	C5-C6-N1	8.30	121.85	117.70
54	BA	2434	A	N1-C6-N6	-8.30	113.62	118.60
22	A1	23	A	N1-C6-N6	-8.30	113.62	118.60
1	AB	224	ARG	NE-CZ-NH1	8.29	124.45	120.30
21	AA	459	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	1470	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	161	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	216	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	384	A	C5-C6-N1	8.29	121.85	117.70
21	AA	622	A	C5-C6-N1	8.29	121.84	117.70
21	AA	946	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1090	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1253	A	C5-C6-N1	8.29	121.84	117.70
21	AA	356	A	N1-C6-N6	-8.28	113.63	118.60
45	BW	19	ARG	NE-CZ-NH1	8.28	124.44	120.30
54	BA	44	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	2430	A	C5-C6-N1	8.28	121.84	117.70
54	BA	2328	A	N1-C6-N6	-8.28	113.63	118.60
21	AA	1349	A	N1-C6-N6	-8.28	113.64	118.60
54	BA	1544	A	N1-C6-N6	-8.27	113.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1914	C	N3-C2-O2	-8.27	116.11	121.90
21	AA	1299	A	C5-C6-N1	8.27	121.83	117.70
54	BA	2738	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	504	A	N1-C6-N6	-8.26	113.64	118.60
55	BB	109	A	N1-C6-N6	-8.26	113.64	118.60
21	AA	648	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	10	A	C5-C6-N1	8.26	121.83	117.70
54	BA	670	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	1746	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	1773	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2669	G	O4'-C1'-N9	8.25	114.80	108.20
54	BA	2598	A	N1-C6-N6	-8.25	113.65	118.60
21	AA	50	A	C5-C6-N1	8.24	121.82	117.70
21	AA	329	A	N1-C6-N6	-8.24	113.65	118.60
21	AA	353	A	N1-C6-N6	-8.24	113.65	118.60
10	AK	55	ARG	NE-CZ-NH1	8.24	124.42	120.30
21	AA	1308	U	N3-C2-O2	-8.24	116.43	122.20
54	BA	453	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	2199	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	344	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	712	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	53	A	C4-C5-C6	-8.24	112.88	117.00
56	B5	122	ARG	NE-CZ-NH1	8.24	124.42	120.30
21	AA	900	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	74	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	1362	A	C5-C6-N1	8.23	121.82	117.70
54	BA	621	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	1095	A	N1-C6-N6	-8.23	113.66	118.60
22	A1	38	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	793	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	362	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	371	A	C5-C6-N1	8.22	121.81	117.70
54	BA	2439	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	298	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	819	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	1519	A	C5-C6-N1	8.22	121.81	117.70
26	BD	169	ARG	NE-CZ-NH1	8.22	124.41	120.30
54	BA	1070	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	522	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1451	C	N3-C2-O2	-8.22	116.15	121.90
54	BA	1780	A	C5-C6-N1	8.21	121.81	117.70
54	BA	2169	A	N1-C6-N6	-8.21	113.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	111	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	613	A	C5-C6-N1	8.21	121.81	117.70
21	AA	572	A	C5-C6-N1	8.21	121.80	117.70
21	AA	729	A	C5-C6-N1	8.21	121.80	117.70
54	BA	294	A	C5-C6-N1	8.21	121.80	117.70
54	BA	1580	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	1819	A	C5-C6-N1	8.21	121.81	117.70
54	BA	2750	A	C5-C6-N1	8.21	121.80	117.70
24	A3	35	C	N3-C2-O2	-8.20	116.16	121.90
37	BO	10	ARG	NE-CZ-NH2	-8.21	116.20	120.30
54	BA	2666	C	N1-C2-O2	8.20	123.82	118.90
21	AA	608	A	C5-C6-N1	8.20	121.80	117.70
54	BA	1204	A	O4'-C1'-N9	8.20	114.76	108.20
54	BA	251	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	73	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	1117	A	C5-C6-N1	8.20	121.80	117.70
54	BA	718	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1551	A	N1-C6-N6	-8.19	113.68	118.60
21	AA	554	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	899	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	1320	C	N3-C2-O2	-8.19	116.17	121.90
54	BA	742	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	766	A	C5-C6-N1	8.18	121.79	117.70
23	A2	79	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1494	A	C5-C6-N1	8.18	121.79	117.70
21	AA	1429	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	716	A	C5-C6-N1	8.18	121.79	117.70
21	AA	746	A	N1-C6-N6	-8.18	113.69	118.60
2	AC	64	ARG	NE-CZ-NH1	8.18	124.39	120.30
54	BA	458	G	O4'-C1'-N9	8.18	114.74	108.20
21	AA	923	A	N1-C6-N6	-8.17	113.70	118.60
21	AA	1285	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	1722	A	N1-C6-N6	-8.17	113.70	118.60
26	BD	13	ARG	NE-CZ-NH1	8.17	124.39	120.30
7	AH	116	ARG	NE-CZ-NH1	8.17	124.39	120.30
21	AA	1377	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2868	A	N1-C6-N6	-8.17	113.70	118.60
21	AA	546	A	C5-C6-N1	8.17	121.78	117.70
54	BA	1593	A	N1-C6-N6	-8.17	113.70	118.60
10	AK	121	ARG	NE-CZ-NH1	8.16	124.38	120.30
21	AA	179	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1584	U	O4'-C1'-N1	8.16	114.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	547	A	C5-C6-N1	8.16	121.78	117.70
21	AA	313	A	C4-C5-C6	-8.15	112.92	117.00
54	BA	167	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	2311	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	205	G	O4'-C1'-N9	8.15	114.72	108.20
21	AA	16	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	529	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1128	G	O4'-C1'-N9	8.15	114.72	108.20
54	BA	2064	C	N1-C2-O2	8.15	123.79	118.90
54	BA	460	A	C5-C6-N1	8.14	121.77	117.70
21	AA	495	A	N1-C6-N6	-8.14	113.71	118.60
54	BA	1392	A	C5-C6-N1	8.14	121.77	117.70
54	BA	2639	A	N1-C6-N6	-8.14	113.71	118.60
21	AA	753	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	49	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	482	A	N1-C6-N6	-8.14	113.72	118.60
21	AA	344	A	O4'-C1'-N9	8.14	114.71	108.20
21	AA	872	A	C5-C6-N1	8.14	121.77	117.70
54	BA	1010	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	1606	C	N1-C2-O2	8.14	123.78	118.90
54	BA	1532	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	499	A	C5-C6-N1	8.13	121.77	117.70
21	AA	532	A	C5-C6-N1	8.13	121.77	117.70
54	BA	508	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1494	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1936	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	1383	C	N3-C2-O2	-8.13	116.21	121.90
54	BA	2358	A	C5-C6-N1	8.13	121.77	117.70
54	BA	1284	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	384	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1213	A	N1-C6-N6	-8.12	113.72	118.60
54	BA	1810	A	C5-C6-N1	8.13	121.76	117.70
54	BA	1237	A	N1-C6-N6	-8.12	113.72	118.60
54	BA	1490	A	C5-C6-N1	8.12	121.76	117.70
54	BA	1598	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	819	A	C5-C6-N1	8.12	121.76	117.70
54	BA	56	A	C5-C6-N1	8.12	121.76	117.70
54	BA	1938	A	C5-C6-N1	8.12	121.76	117.70
54	BA	2781	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	1441	A	C5-C6-N1	8.12	121.76	117.70
54	BA	1088	A	C5-C6-N1	8.12	121.76	117.70
24	A3	38	A	N1-C6-N6	-8.12	113.73	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BC	51	ARG	NE-CZ-NH1	8.12	124.36	120.30
21	AA	155	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	144	A	N1-C6-N6	-8.11	113.73	118.60
6	AG	101	ARG	NE-CZ-NH1	8.11	124.36	120.30
17	AR	52	ARG	NE-CZ-NH1	8.11	124.36	120.30
21	AA	1100	C	N3-C2-O2	-8.11	116.22	121.90
29	BG	162	ARG	NE-CZ-NH1	8.11	124.35	120.30
54	BA	342	A	C4-C5-C6	-8.11	112.95	117.00
54	BA	1155	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	1502	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	2191	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	2792	A	N1-C6-N6	-8.11	113.74	118.60
21	AA	1111	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1509	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1580	A	C5-C6-N1	8.10	121.75	117.70
54	BA	2051	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	352	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1535	A	O4'-C1'-N9	8.10	114.68	108.20
54	BA	1900	A	C5-C6-N1	8.10	121.75	117.70
54	BA	53	A	C5-C6-N1	8.10	121.75	117.70
54	BA	2547	A	O4'-C1'-N9	8.10	114.68	108.20
3	AD	110	ARG	NE-CZ-NH1	8.09	124.35	120.30
14	AO	87	ARG	NE-CZ-NH1	8.09	124.35	120.30
54	BA	1027	A	N1-C6-N6	-8.09	113.74	118.60
2	AC	131	ARG	NE-CZ-NH1	8.09	124.34	120.30
54	BA	13	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2031	A	C5-C6-N1	8.09	121.74	117.70
54	BA	2748	A	C5-C6-N1	8.09	121.74	117.70
54	BA	244	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	1500	A	C5-C6-N1	8.08	121.74	117.70
54	BA	257	C	N3-C2-O2	-8.08	116.24	121.90
54	BA	2835	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	552	U	O4'-C1'-N1	8.08	114.66	108.20
54	BA	2392	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	1049	U	P-O3'-C3'	8.07	129.39	119.70
46	BX	49	ARG	NE-CZ-NH1	8.07	124.34	120.30
54	BA	2682	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2176	A	C5-C6-N1	8.07	121.74	117.70
21	AA	152	A	C5-C6-N1	8.07	121.73	117.70
29	BG	93	TYR	CB-CG-CD2	-8.07	116.16	121.00
54	BA	575	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2573	C	O4'-C1'-N1	8.07	114.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AN	53	ARG	NE-CZ-NH1	8.07	124.33	120.30
54	BA	1030	C	N3-C2-O2	-8.07	116.25	121.90
54	BA	1248	G	O4'-C1'-N9	8.06	114.65	108.20
54	BA	2826	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	190	A	C5-C6-N1	8.06	121.73	117.70
21	AA	1274	A	C5-C6-N1	8.06	121.73	117.70
35	BM	114	ARG	NE-CZ-NH1	8.06	124.33	120.30
21	AA	728	A	C5-C6-N1	8.06	121.73	117.70
54	BA	1244	A	C5-C6-N1	8.06	121.73	117.70
54	BA	1387	A	C5-C6-N1	8.05	121.73	117.70
54	BA	2665	A	C5-C6-N1	8.05	121.73	117.70
26	BD	46	ARG	NE-CZ-NH1	8.05	124.33	120.30
21	AA	151	A	N1-C6-N6	-8.04	113.77	118.60
21	AA	907	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1406	U	O4'-C1'-N1	8.04	114.63	108.20
54	BA	1730	C	N1-C2-O2	8.04	123.72	118.90
54	BA	2675	A	C5-C6-N1	8.04	121.72	117.70
54	BA	620	G	O4'-C1'-N9	8.04	114.63	108.20
54	BA	1254	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	913	A	C4-C5-C6	-8.03	112.98	117.00
54	BA	91	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	655	A	C5-C6-N1	8.03	121.72	117.70
54	BA	2268	A	N1-C6-N6	-8.03	113.78	118.60
9	AJ	16	ARG	NE-CZ-NH1	8.03	124.31	120.30
22	A1	58	A	C5-C6-N1	8.03	121.72	117.70
54	BA	125	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	792	A	C5-C6-N1	8.03	121.71	117.70
54	BA	2094	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	794	A	C5-C6-N1	8.03	121.71	117.70
54	BA	1635	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2530	A	C5-C6-N1	8.03	121.71	117.70
54	BA	2712	C	N3-C2-O2	-8.03	116.28	121.90
54	BA	2835	A	C5-C6-N1	8.02	121.71	117.70
21	AA	1256	A	C5-C6-N1	8.02	121.71	117.70
21	AA	182	A	C5-C6-N1	8.02	121.71	117.70
21	AA	559	A	C5-C6-N1	8.02	121.71	117.70
21	AA	1269	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	2850	A	C5-C6-N1	8.02	121.71	117.70
54	BA	423	A	N1-C6-N6	-8.01	113.79	118.60
21	AA	243	A	C5-C6-N1	8.01	121.71	117.70
54	BA	910	A	C5-C6-N1	8.01	121.71	117.70
54	BA	2158	A	C5-C6-N1	8.01	121.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2766	A	C5-C6-N1	8.01	121.71	117.70
21	AA	65	A	N1-C6-N6	-8.01	113.80	118.60
21	AA	356	A	C5-C6-N1	8.01	121.70	117.70
21	AA	665	A	C4-C5-C6	-8.01	113.00	117.00
54	BA	1378	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	2453	A	C5-C6-N1	8.01	121.70	117.70
46	BX	71	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	1960	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2448	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	968	A	C5-C6-N1	8.00	121.70	117.70
54	BA	1439	A	O4'-C1'-N9	8.00	114.60	108.20
54	BA	2450	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2211	A	O4'-C1'-N9	8.00	114.60	108.20
21	AA	1150	A	N1-C6-N6	-8.00	113.80	118.60
36	BN	12	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	1808	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	1227	A	C5-C6-N1	7.99	121.70	117.70
54	BA	1503	A	N1-C6-N6	-7.99	113.80	118.60
54	BA	1046	A	C5-C6-N1	7.99	121.70	117.70
21	AA	282	A	N1-C6-N6	-7.99	113.81	118.60
25	BC	270	ARG	NE-CZ-NH1	7.99	124.30	120.30
21	AA	1214	C	N3-C2-O2	-7.99	116.31	121.90
54	BA	2518	A	C5-C6-N1	7.99	121.69	117.70
35	BM	81	ARG	NE-CZ-NH1	7.99	124.29	120.30
21	AA	1137	C	N3-C2-O2	-7.99	116.31	121.90
54	BA	980	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	1044	A	N1-C6-N6	-7.98	113.81	118.60
31	BI	64	ARG	NE-CZ-NH1	7.98	124.29	120.30
54	BA	1919	A	N1-C6-N6	-7.98	113.81	118.60
41	BS	84	ARG	NE-CZ-NH1	7.98	124.29	120.30
21	AA	143	A	C5-C6-N1	7.98	121.69	117.70
54	BA	947	A	C5-C6-N1	7.98	121.69	117.70
21	AA	1238	A	C5-C6-N1	7.97	121.69	117.70
21	AA	1163	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	2411	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	676	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	315	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	845	A	C5-C6-N1	7.97	121.68	117.70
54	BA	1050	A	C5-C6-N1	7.97	121.68	117.70
54	BA	2888	C	N3-C2-O2	-7.97	116.32	121.90
52	B3	41	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	889	C	N1-C2-O2	7.96	123.68	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	454	A	N1-C6-N6	-7.96	113.82	118.60
5	AF	44	ARG	NE-CZ-NH1	7.96	124.28	120.30
51	B2	33	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	2453	A	C4-C5-C6	-7.96	113.02	117.00
54	BA	920	A	N1-C6-N6	-7.96	113.83	118.60
54	BA	1049	C	N3-C2-O2	-7.96	116.33	121.90
54	BA	1301	A	C5-C6-N1	7.96	121.68	117.70
54	BA	2129	C	N3-C2-O2	-7.96	116.33	121.90
14	AO	71	ARG	NE-CZ-NH1	7.96	124.28	120.30
21	AA	970	C	N3-C2-O2	-7.96	116.33	121.90
54	BA	634	C	N3-C2-O2	-7.95	116.33	121.90
54	BA	734	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	498	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	223	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1205	A	C5-C6-N1	7.95	121.68	117.70
54	BA	1477	A	N1-C6-N6	-7.95	113.83	118.60
17	AR	42	ARG	NE-CZ-NH1	7.95	124.27	120.30
54	BA	371	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1175	A	C5-C6-N1	7.95	121.67	117.70
21	AA	794	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	8	A	C5-C6-N1	7.94	121.67	117.70
54	BA	354	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	2778	A	C5-C6-N1	7.94	121.67	117.70
54	BA	457	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	1342	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	2590	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	1165	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	1953	A	C5-C6-N1	7.93	121.67	117.70
54	BA	1966	A	C5-C6-N1	7.93	121.67	117.70
54	BA	2799	A	C5-C6-N1	7.93	121.67	117.70
21	AA	937	A	C5-C6-N1	7.93	121.67	117.70
54	BA	2851	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	324	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	1531	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	262	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	189	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	2037	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	2317	A	C5-C6-N1	7.92	121.66	117.70
54	BA	428	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1504	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	1225	A	C5-C6-N1	7.91	121.66	117.70
54	BA	1665	A	N1-C6-N6	-7.91	113.85	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AC	71	ARG	NE-CZ-NH1	7.91	124.25	120.30
21	AA	1229	A	N1-C6-N6	-7.91	113.85	118.60
25	BC	257	ARG	NE-CZ-NH1	7.91	124.26	120.30
54	BA	2212	A	N1-C6-N6	-7.91	113.85	118.60
4	AE	28	ARG	NE-CZ-NH1	7.91	124.25	120.30
21	AA	448	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	1698	A	C5-C6-N1	7.91	121.65	117.70
54	BA	2829	A	N1-C6-N6	-7.91	113.85	118.60
21	AA	66	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	675	A	C5-C6-N1	7.90	121.65	117.70
54	BA	845	A	N1-C6-N6	-7.90	113.86	118.60
22	A1	73	A	C5-C6-N1	7.90	121.65	117.70
54	BA	937	C	N3-C2-O2	-7.90	116.37	121.90
54	BA	73	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2660	A	C5-C6-N1	7.90	121.65	117.70
21	AA	510	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	1784	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2837	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	2749	A	N1-C6-N6	-7.89	113.86	118.60
30	BH	50	ARG	NE-CZ-NH1	7.89	124.25	120.30
21	AA	338	A	C4-C5-C6	-7.89	113.06	117.00
22	A1	69	A	N1-C6-N6	-7.89	113.87	118.60
54	BA	270	A	C5-C6-N1	7.89	121.64	117.70
54	BA	1508	A	N1-C6-N6	-7.89	113.87	118.60
54	BA	199	A	N1-C6-N6	-7.89	113.87	118.60
54	BA	1086	A	C5-C6-N1	7.89	121.64	117.70
54	BA	91	A	C5-C6-N1	7.89	121.64	117.70
54	BA	330	A	O4'-C1'-N9	7.89	114.51	108.20
54	BA	1672	A	C5-C6-N1	7.88	121.64	117.70
54	BA	925	A	C4-C5-C6	-7.88	113.06	117.00
54	BA	1634	A	C5-C6-N1	7.88	121.64	117.70
21	AA	1418	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1213	A	C5-C6-N1	7.88	121.64	117.70
23	A2	91	A	C5-C6-N1	7.88	121.64	117.70
21	AA	937	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	1678	A	C5-C6-N1	7.87	121.64	117.70
54	BA	2386	A	N1-C6-N6	-7.87	113.88	118.60
24	A3	11	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	38	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	2163	A	C5-C6-N1	7.87	121.64	117.70
54	BA	572	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	2135	A	N1-C6-N6	-7.87	113.88	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	B3	12	ARG	NE-CZ-NH1	7.86	124.23	120.30
54	BA	705	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	742	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1745	A	N1-C6-N6	-7.86	113.88	118.60
22	A1	38	A	C5-C6-N1	7.86	121.63	117.70
55	BB	59	A	N1-C6-N6	-7.86	113.88	118.60
21	AA	338	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	505	A	N1-C6-N6	-7.86	113.89	118.60
55	BB	45	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1147	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	2503	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2666	C	O4'-C1'-N1	7.86	114.48	108.20
21	AA	1254	A	N1-C6-N6	-7.85	113.89	118.60
21	AA	353	A	C5-C6-N1	7.85	121.63	117.70
21	AA	1519	A	C4-C5-C6	-7.85	113.07	117.00
54	BA	756	A	C5-C6-N1	7.85	121.62	117.70
12	AM	106	ARG	CD-NE-CZ	7.85	134.59	123.60
54	BA	1189	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2565	A	C5-C6-N1	7.85	121.62	117.70
14	AO	83	ARG	NE-CZ-NH1	7.84	124.22	120.30
21	AA	84	U	O4'-C1'-N1	7.84	114.47	108.20
54	BA	101	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	1127	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2451	A	C5-C6-N1	7.84	121.62	117.70
21	AA	1014	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2311	A	C5-C6-N1	7.84	121.62	117.70
21	AA	1239	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	1677	A	N1-C6-N6	-7.84	113.90	118.60
21	AA	563	A	C5-C6-N1	7.84	121.62	117.70
21	AA	366	A	C5-C6-N1	7.84	121.62	117.70
21	AA	1534	A	C5-C6-N1	7.84	121.62	117.70
32	BJ	37	ARG	NE-CZ-NH1	7.83	124.22	120.30
21	AA	1168	U	N3-C2-O2	-7.83	116.72	122.20
21	AA	171	A	C4-C5-C6	-7.83	113.08	117.00
54	BA	1646	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	1749	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	2503	A	N1-C6-N6	-7.83	113.90	118.60
6	AG	110	ARG	NE-CZ-NH1	7.83	124.21	120.30
54	BA	1598	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1610	A	C5-C6-N1	7.83	121.61	117.70
55	BB	104	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	2587	A	N1-C6-N6	-7.83	113.90	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	412	A	N1-C6-N6	-7.83	113.91	118.60
21	AA	1357	A	C4-C5-C6	-7.83	113.09	117.00
54	BA	354	A	C5-C6-N1	7.83	121.61	117.70
21	AA	374	A	C5-C6-N1	7.82	121.61	117.70
36	BN	45	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	56	A	N1-C6-N6	-7.82	113.91	118.60
15	AP	51	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	527	C	N3-C2-O2	-7.82	116.43	121.90
54	BA	2430	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	1679	A	C5-C6-N1	7.82	121.61	117.70
54	BA	2381	A	C5-C6-N1	7.82	121.61	117.70
54	BA	710	U	O4'-C1'-N1	7.81	114.45	108.20
54	BA	1085	A	C5-C6-N1	7.81	121.61	117.70
54	BA	218	A	C5-C6-N1	7.81	121.61	117.70
21	AA	411	A	C5-C6-N1	7.81	121.60	117.70
21	AA	906	A	C5-C6-N1	7.81	121.60	117.70
56	B5	164	ARG	NE-CZ-NH1	7.81	124.20	120.30
11	AL	82	ARG	NE-CZ-NH1	7.81	124.20	120.30
24	A3	75	C	N3-C2-O2	-7.80	116.44	121.90
54	BA	877	A	C5-C6-N1	7.80	121.60	117.70
54	BA	1783	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	1597	A	C5-C6-N1	7.80	121.60	117.70
54	BA	63	A	C5-C6-N1	7.80	121.60	117.70
54	BA	477	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	608	A	C5-C6-N1	7.80	121.60	117.70
54	BA	2741	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	1168	U	O4'-C1'-N1	7.80	114.44	108.20
54	BA	2184	A	C5-C6-N1	7.80	121.60	117.70
54	BA	127	A	N1-C6-N6	-7.79	113.92	118.60
21	AA	496	A	O4'-C1'-N9	7.79	114.44	108.20
21	AA	611	C	N3-C2-O2	-7.79	116.44	121.90
21	AA	1246	A	C5-C6-N1	7.79	121.60	117.70
22	A1	21	A	C4-C5-C6	-7.79	113.10	117.00
21	AA	228	A	N1-C6-N6	-7.79	113.92	118.60
54	BA	1027	A	C5-C6-N1	7.79	121.60	117.70
22	A1	26	A	C5-C6-N1	7.79	121.59	117.70
54	BA	2019	A	C5-C6-N1	7.79	121.59	117.70
54	BA	627	A	C5-C6-N1	7.78	121.59	117.70
21	AA	974	A	C5-C6-N1	7.78	121.59	117.70
21	AA	975	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	1413	A	C5-C6-N1	7.78	121.59	117.70
54	BA	160	A	C5-C6-N1	7.78	121.59	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1664	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1340	A	C4-C5-C6	-7.78	113.11	117.00
54	BA	149	A	C5-C6-N1	7.78	121.59	117.70
54	BA	1069	A	C5-C6-N1	7.78	121.59	117.70
54	BA	282	A	C5-C6-N1	7.77	121.59	117.70
54	BA	344	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	1031	C	N1-C2-O2	7.77	123.56	118.90
21	AA	1036	A	C5-C6-N1	7.77	121.59	117.70
21	AA	1329	A	C5-C6-N1	7.77	121.58	117.70
54	BA	718	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1508	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1638	C	N3-C2-O2	-7.77	116.46	121.90
21	AA	1093	A	N1-C6-N6	-7.77	113.94	118.60
22	A1	35	A	N1-C6-N6	-7.76	113.94	118.60
36	BN	96	ARG	NE-CZ-NH1	7.76	124.18	120.30
54	BA	99	U	O4'-C1'-N1	7.76	114.41	108.20
54	BA	943	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	2750	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1928	A	C5-C6-N1	7.76	121.58	117.70
21	AA	109	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	482	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2434	A	C5-C6-N1	7.76	121.58	117.70
21	AA	151	A	C4-C5-C6	-7.75	113.12	117.00
1	AB	207	ARG	NE-CZ-NH1	7.75	124.18	120.30
21	AA	195	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	155	A	C4-C5-C6	-7.75	113.12	117.00
54	BA	2676	C	N3-C2-O2	-7.75	116.47	121.90
54	BA	155	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2587	A	C5-C6-N1	7.75	121.58	117.70
54	BA	981	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	45	G	O4'-C1'-N9	7.75	114.40	108.20
54	BA	603	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1089	A	C5-C6-N1	7.75	121.57	117.70
54	BA	196	A	C5-C6-N1	7.75	121.57	117.70
54	BA	892	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	435	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	61	C	N3-C2-O2	-7.75	116.48	121.90
54	BA	1545	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	1014	A	C4-C5-C6	-7.74	113.13	117.00
24	A3	36	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	526	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	2327	A	C4-C5-C6	-7.74	113.13	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2670	A	C5-C6-N1	7.74	121.57	117.70
4	AE	111	ARG	NE-CZ-NH1	7.74	124.17	120.30
54	BA	6	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	1549	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1923	U	O4'-C1'-N1	7.74	114.39	108.20
54	BA	2587	A	C4-C5-C6	-7.74	113.13	117.00
54	BA	2886	A	C5-C6-N1	7.74	121.57	117.70
21	AA	498	A	C5-C6-N1	7.74	121.57	117.70
21	AA	607	A	C5-C6-N1	7.74	121.57	117.70
24	A3	58	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	181	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	502	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	2030	A	C5-C6-N1	7.74	121.57	117.70
21	AA	958	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1229	A	C5-C6-N1	7.74	121.57	117.70
54	BA	973	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2425	A	C5-C6-N1	7.74	121.57	117.70
54	BA	569	U	O4'-C1'-N1	7.73	114.39	108.20
54	BA	984	A	C5-C6-N1	7.73	121.57	117.70
54	BA	2655	G	O4'-C1'-N9	7.73	114.39	108.20
21	AA	906	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	104	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	1803	A	N1-C6-N6	-7.73	113.96	118.60
55	BB	108	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	655	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	344	A	C5-C6-N1	7.73	121.56	117.70
54	BA	161	A	C5-C6-N1	7.73	121.56	117.70
54	BA	979	A	C5-C6-N1	7.73	121.56	117.70
54	BA	1143	A	C5-C6-N1	7.73	121.56	117.70
21	AA	1476	A	N1-C6-N6	-7.73	113.97	118.60
37	BO	10	ARG	NE-CZ-NH1	7.73	124.16	120.30
21	AA	1158	C	N1-C2-O2	7.72	123.53	118.90
21	AA	1429	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1169	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2887	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1579	A	C5-C6-N1	7.72	121.56	117.70
21	AA	72	A	C5-C6-N1	7.72	121.56	117.70
21	AA	1374	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	1508	A	C5-C6-N1	7.72	121.56	117.70
54	BA	719	C	N3-C2-O2	-7.72	116.50	121.90
54	BA	1758	U	O4'-C1'-N1	7.72	114.37	108.20
54	BA	2342	C	N3-C2-O2	-7.71	116.50	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1505	A	C5-C6-N1	7.71	121.56	117.70
6	AG	94	ARG	NE-CZ-NH1	7.71	124.16	120.30
54	BA	1773	A	C5-C6-N1	7.71	121.56	117.70
54	BA	2082	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	969	A	C5-C6-N1	7.71	121.56	117.70
54	BA	510	C	N3-C2-O2	-7.71	116.50	121.90
54	BA	1535	A	N1-C6-N6	-7.71	113.97	118.60
56	B5	12	ARG	NE-CZ-NH1	7.71	124.16	120.30
54	BA	508	A	C5-C6-N1	7.71	121.55	117.70
54	BA	514	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	1596	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	2021	C	N3-C2-O2	-7.71	116.51	121.90
54	BA	2378	A	C4-C5-C6	-7.71	113.15	117.00
13	AN	85	ARG	NE-CZ-NH1	7.70	124.15	120.30
21	AA	65	A	C4-C5-C6	-7.70	113.15	117.00
54	BA	1427	A	C5-C6-N1	7.70	121.55	117.70
55	BB	35	C	N3-C2-O2	-7.70	116.51	121.90
21	AA	919	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2521	C	O4'-C1'-N1	7.70	114.36	108.20
21	AA	507	C	N3-C2-O2	-7.70	116.51	121.90
21	AA	977	A	C5-C6-N1	7.70	121.55	117.70
54	BA	241	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	743	A	C4-C5-C6	-7.70	113.15	117.00
54	BA	2660	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	644	A	C5-C6-N1	7.69	121.55	117.70
43	BU	85	ARG	NE-CZ-NH1	7.69	124.15	120.30
21	AA	535	A	N1-C6-N6	-7.69	113.98	118.60
21	AA	572	A	N1-C6-N6	-7.69	113.99	118.60
21	AA	1250	A	N1-C6-N6	-7.69	113.98	118.60
54	BA	643	A	C5-C6-N1	7.69	121.55	117.70
54	BA	1713	A	C4-C5-C6	-7.69	113.16	117.00
55	BB	53	A	C5-C6-N1	7.69	121.55	117.70
54	BA	582	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	961	C	N3-C2-O2	-7.69	116.52	121.90
54	BA	1123	C	O4'-C1'-N1	7.69	114.35	108.20
54	BA	1889	A	C5-C6-N1	7.69	121.54	117.70
56	B5	7	ARG	NE-CZ-NH1	7.69	124.14	120.30
21	AA	28	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	1054	A	C4-C5-C6	-7.69	113.16	117.00
21	AA	250	A	O4'-C1'-N9	7.68	114.35	108.20
21	AA	262	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1427	A	C4-C5-C6	-7.68	113.16	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	529	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1819	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2333	A	C5-C6-N1	7.68	121.54	117.70
54	BA	2381	A	C4-C5-C6	-7.68	113.16	117.00
54	BA	204	A	C5-C6-N1	7.68	121.54	117.70
54	BA	761	A	C5-C6-N1	7.68	121.54	117.70
21	AA	130	A	C5-C6-N1	7.68	121.54	117.70
54	BA	592	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2113	U	O4'-C1'-N1	7.68	114.34	108.20
54	BA	2225	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2757	A	N1-C6-N6	-7.68	113.99	118.60
10	AK	36	ARG	NE-CZ-NH1	7.68	124.14	120.30
21	AA	288	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	456	A	N1-C6-N6	-7.68	113.99	118.60
22	A1	38	A	C4-C5-C6	-7.68	113.16	117.00
54	BA	2266	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1525	A	C4-C5-C6	-7.67	113.16	117.00
28	BF	91	ARG	NE-CZ-NH1	7.67	124.14	120.30
54	BA	1266	G	O4'-C1'-N9	7.67	114.34	108.20
54	BA	2358	A	C4-C5-C6	-7.67	113.17	117.00
21	AA	631	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	2160	C	N3-C2-O2	-7.67	116.53	121.90
55	BB	46	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1132	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	1009	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1353	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1783	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1937	A	C5-C6-N1	7.66	121.53	117.70
22	A1	16	C	N1-C2-O2	7.66	123.50	118.90
2	AC	53	ARG	NE-CZ-NH1	7.66	124.13	120.30
21	AA	160	A	C5-C6-N1	7.66	121.53	117.70
54	BA	71	A	C5-C6-N1	7.66	121.53	117.70
54	BA	470	A	N1-C6-N6	-7.66	114.00	118.60
54	BA	2711	A	C5-C6-N1	7.66	121.53	117.70
21	AA	768	A	C5-C6-N1	7.66	121.53	117.70
54	BA	345	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	2094	A	C5-C6-N1	7.66	121.53	117.70
21	AA	1257	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	1204	A	C5-C6-N1	7.65	121.53	117.70
54	BA	1395	A	C5-C6-N1	7.65	121.53	117.70
54	BA	1427	A	P-O3'-C3'	7.65	128.88	119.70
54	BA	2376	A	C5-C6-N1	7.65	121.53	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1067	A	C5-C6-N1	7.65	121.52	117.70
29	BG	2	ARG	NE-CZ-NH1	7.65	124.12	120.30
33	BK	98	ARG	NE-CZ-NH1	7.65	124.12	120.30
54	BA	866	A	C5-C6-N1	7.65	121.52	117.70
21	AA	1004	A	N1-C6-N6	-7.64	114.01	118.60
22	A1	76	A	N1-C6-N6	-7.64	114.01	118.60
54	BA	1451	C	N1-C2-O2	7.64	123.49	118.90
54	BA	2628	C	O4'-C1'-N1	7.64	114.31	108.20
21	AA	825	A	C5-C6-N1	7.64	121.52	117.70
21	AA	59	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	480	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	2171	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2198	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2117	A	C5-C6-N1	7.64	121.52	117.70
21	AA	383	A	C5-C6-N1	7.63	121.52	117.70
49	B0	16	ARG	NE-CZ-NH1	7.63	124.12	120.30
21	AA	274	A	C5-C6-N1	7.63	121.52	117.70
36	BN	30	ARG	NE-CZ-NH1	7.63	124.12	120.30
54	BA	2142	A	C5-C6-N1	7.63	121.52	117.70
21	AA	373	A	C5-C6-N1	7.63	121.51	117.70
54	BA	1458	U	C1'-O4'-C4'	-7.63	103.80	109.90
54	BA	2281	A	C5-C6-N1	7.63	121.51	117.70
54	BA	2328	A	C5-C6-N1	7.63	121.52	117.70
54	BA	2346	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2792	A	C5-C6-N1	7.62	121.51	117.70
56	B5	74	ARG	NE-CZ-NH1	7.62	124.11	120.30
35	BM	59	ARG	NE-CZ-NH1	7.62	124.11	120.30
54	BA	1901	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	1035	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1640	A	C5-C6-N1	7.62	121.51	117.70
21	AA	1467	C	N3-C2-O2	-7.62	116.57	121.90
54	BA	2333	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1144	A	C5-C6-N1	7.62	121.51	117.70
23	A2	79	A	C5-C6-N1	7.62	121.51	117.70
54	BA	310	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1730	C	O4'-C1'-N1	7.62	114.29	108.20
55	BB	57	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	423	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2851	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	547	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	1761	C	N3-C2-O2	-7.61	116.57	121.90
21	AA	816	A	N1-C6-N6	-7.61	114.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	228	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	2740	A	C5-C6-N1	7.61	121.50	117.70
21	AA	923	A	C5-C6-N1	7.61	121.50	117.70
54	BA	362	A	C5-C6-N1	7.61	121.50	117.70
55	BB	57	A	C5-C6-N1	7.61	121.50	117.70
54	BA	221	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	1969	A	C5-C6-N1	7.60	121.50	117.70
21	AA	780	A	C4-C5-C6	-7.60	113.20	117.00
54	BA	453	A	C5-C6-N1	7.60	121.50	117.70
54	BA	959	A	C5-C6-N1	7.60	121.50	117.70
54	BA	2542	A	C5-C6-N1	7.60	121.50	117.70
39	BQ	47	ARG	NE-CZ-NH1	7.60	124.10	120.30
54	BA	221	A	C5-C6-N1	7.60	121.50	117.70
54	BA	1832	C	N3-C2-O2	-7.60	116.58	121.90
21	AA	250	A	C5-C6-N1	7.59	121.50	117.70
39	BQ	2	ARG	NE-CZ-NH1	7.59	124.10	120.30
54	BA	457	A	C5-C6-N1	7.59	121.50	117.70
54	BA	863	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	1552	A	C5-C6-N1	7.59	121.50	117.70
54	BA	2432	A	C5-C6-N1	7.59	121.50	117.70
21	AA	1145	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1354	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	2439	A	C5-C6-N1	7.59	121.50	117.70
21	AA	595	A	N1-C6-N6	-7.59	114.05	118.60
21	AA	466	A	C5-C6-N1	7.59	121.49	117.70
21	AA	307	C	N3-C2-O2	-7.59	116.59	121.90
21	AA	1252	A	C5-C6-N1	7.58	121.49	117.70
54	BA	980	A	C5-C6-N1	7.58	121.49	117.70
21	AA	795	C	N3-C2-O2	-7.58	116.59	121.90
54	BA	284	U	O4'-C1'-N1	7.58	114.27	108.20
21	AA	253	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	332	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	877	A	C4-C5-C6	-7.58	113.21	117.00
54	BA	2882	A	C5-C6-N1	7.58	121.49	117.70
21	AA	935	A	C5-C6-N1	7.58	121.49	117.70
21	AA	907	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	262	A	C5-C6-N1	7.57	121.49	117.70
54	BA	507	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	974	G	N3-C2-N2	-7.57	114.60	119.90
21	AA	994	A	C5-C6-N1	7.57	121.49	117.70
11	AL	8	ARG	NE-CZ-NH1	7.57	124.08	120.30
21	AA	1398	A	C5-C6-N1	7.57	121.48	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2700	A	C5-C6-N1	7.57	121.48	117.70
22	A1	6	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	309	A	C5-C6-N1	7.57	121.48	117.70
21	AA	1080	A	C5-C6-N1	7.57	121.48	117.70
24	A3	40	C	N3-C2-O2	-7.57	116.60	121.90
54	BA	1111	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	1912	A	C5-C6-N1	7.57	121.48	117.70
21	AA	1397	C	N3-C2-O2	-7.57	116.60	121.90
54	BA	2422	C	N1-C2-O2	7.57	123.44	118.90
54	BA	661	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	717	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	960	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1787	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2821	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2858	C	N3-C2-O2	-7.56	116.61	121.90
21	AA	143	A	N1-C6-N6	-7.56	114.07	118.60
21	AA	1446	A	C5-C6-N1	7.56	121.48	117.70
54	BA	821	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1786	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1787	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	2590	A	C5-C6-N1	7.55	121.48	117.70
21	AA	1394	A	N1-C6-N6	-7.55	114.07	118.60
8	AI	48	ARG	NE-CZ-NH1	7.55	124.07	120.30
21	AA	889	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1350	A	C4-C5-C6	-7.55	113.23	117.00
21	AA	1396	A	C5-C6-N1	7.55	121.47	117.70
21	AA	663	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1110	A	C4-C5-C6	-7.55	113.23	117.00
54	BA	1226	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2309	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	2734	A	C5-C6-N1	7.55	121.47	117.70
54	BA	909	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1287	A	C5-C6-N1	7.54	121.47	117.70
21	AA	167	A	N1-C6-N6	-7.54	114.07	118.60
54	BA	330	A	C5-C6-N1	7.54	121.47	117.70
54	BA	775	G	O4'-C1'-N9	7.54	114.23	108.20
54	BA	1802	A	N1-C6-N6	-7.54	114.07	118.60
54	BA	2614	A	C5-C6-N1	7.54	121.47	117.70
21	AA	1287	A	C5-C6-N1	7.54	121.47	117.70
54	BA	2288	A	C5-C6-N1	7.54	121.47	117.70
54	BA	311	A	N1-C6-N6	-7.54	114.08	118.60
48	BZ	29	ARG	NE-CZ-NH1	7.54	124.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	119	A	C5-C6-N1	7.54	121.47	117.70
22	A1	56	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	2518	A	N1-C6-N6	-7.53	114.08	118.60
21	AA	718	A	C5-C6-N1	7.53	121.47	117.70
54	BA	2765	A	C5-C6-N1	7.53	121.47	117.70
54	BA	2003	A	C4-C5-C6	-7.53	113.24	117.00
54	BA	278	A	C5-C6-N1	7.53	121.46	117.70
54	BA	1871	A	O4'-C1'-N9	7.52	114.22	108.20
54	BA	197	A	C5-C6-N1	7.52	121.46	117.70
21	AA	983	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1518	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	761	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	1383	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2614	A	N1-C6-N6	-7.52	114.09	118.60
11	AL	85	ARG	NE-CZ-NH1	7.52	124.06	120.30
21	AA	167	A	C5-C6-N1	7.52	121.46	117.70
8	AI	108	ARG	NE-CZ-NH1	7.52	124.06	120.30
21	AA	414	A	C5-C6-N1	7.52	121.46	117.70
24	A3	59	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2159	G	O4'-C1'-N9	7.51	114.21	108.20
54	BA	2837	A	C5-C6-N1	7.51	121.46	117.70
21	AA	1375	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	290	U	O4'-C1'-N1	7.51	114.21	108.20
54	BA	670	A	C5-C6-N1	7.51	121.46	117.70
54	BA	1029	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2872	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	1515	A	C5-C6-N1	7.51	121.45	117.70
54	BA	1133	A	N1-C6-N6	-7.51	114.10	118.60
54	BA	1854	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2820	A	N1-C6-N6	-7.51	114.10	118.60
21	AA	345	C	N1-C2-O2	7.50	123.40	118.90
29	BG	54	ARG	NE-CZ-NH1	7.50	124.05	120.30
32	BJ	96	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	484	C	N3-C2-O2	-7.50	116.65	121.90
21	AA	1081	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1054	A	C5-C6-N1	7.50	121.45	117.70
21	AA	487	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	622	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	1525	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1545	A	C5-C6-N1	7.50	121.45	117.70
21	AA	149	A	C5-C6-N1	7.50	121.45	117.70
21	AA	808	C	N3-C2-O2	-7.50	116.65	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	706	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1757	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	2336	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	2749	A	C5-C6-N1	7.50	121.45	117.70
21	AA	655	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	1431	A	C5-C6-N1	7.50	121.45	117.70
54	BA	226	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	1101	A	P-O3'-C3'	7.49	128.69	119.70
21	AA	1311	A	C5-C6-N1	7.49	121.45	117.70
54	BA	146	A	C5-C6-N1	7.49	121.45	117.70
54	BA	1384	A	C5-C6-N1	7.49	121.45	117.70
54	BA	2711	A	C4-C5-C6	-7.49	113.25	117.00
21	AA	1151	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	678	C	N3-C2-O2	-7.49	116.66	121.90
54	BA	1987	A	C5-C6-N1	7.49	121.44	117.70
21	AA	1465	A	N1-C6-N6	-7.49	114.11	118.60
21	AA	131	A	C5-C6-N1	7.49	121.44	117.70
21	AA	715	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	2281	A	N1-C6-N6	-7.49	114.11	118.60
21	AA	1285	A	C5-C6-N1	7.48	121.44	117.70
54	BA	11	C	N3-C2-O2	-7.48	116.66	121.90
54	BA	1118	C	N3-C2-O2	-7.48	116.66	121.90
54	BA	1608	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2706	A	C4-C5-C6	-7.48	113.26	117.00
21	AA	174	A	C5-C6-N1	7.48	121.44	117.70
21	AA	1300	G	O4'-C1'-N9	7.48	114.19	108.20
38	BP	112	ARG	NE-CZ-NH1	7.48	124.04	120.30
54	BA	111	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2052	A	N1-C6-N6	-7.48	114.11	118.60
21	AA	1001	C	N3-C2-O2	-7.48	116.67	121.90
54	BA	1914	C	N1-C2-O2	7.48	123.39	118.90
54	BA	439	A	C5-C6-N1	7.48	121.44	117.70
54	BA	1791	A	C5-C6-N1	7.48	121.44	117.70
21	AA	767	A	C5-C6-N1	7.47	121.44	117.70
54	BA	501	A	N1-C6-N6	-7.47	114.11	118.60
54	BA	833	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1962	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	1938	A	C1'-O4'-C4'	-7.47	103.92	109.90
54	BA	2211	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2377	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1383	A	C5-C6-N1	7.47	121.44	117.70
54	BA	730	A	C5-C6-N1	7.47	121.44	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	747	A	C5-C6-N1	7.47	121.43	117.70
54	BA	95	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	1754	A	N1-C6-N6	-7.47	114.12	118.60
21	AA	1428	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	644	A	C4-C5-C6	-7.46	113.27	117.00
54	BA	2411	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2628	C	N1-C2-O2	7.46	123.38	118.90
54	BA	1134	A	C5-C6-N1	7.46	121.43	117.70
21	AA	129	A	N1-C6-N6	-7.46	114.12	118.60
37	BO	16	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	1040	A	N1-C6-N6	-7.46	114.12	118.60
21	AA	308	C	N3-C2-O2	-7.46	116.68	121.90
21	AA	634	C	N3-C2-O2	-7.46	116.68	121.90
21	AA	1170	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2340	A	N1-C6-N6	-7.46	114.13	118.60
21	AA	432	A	C5-C6-N1	7.46	121.43	117.70
21	AA	370	C	N3-C2-O2	-7.45	116.68	121.90
21	AA	1502	A	C5-C6-N1	7.45	121.43	117.70
54	BA	504	A	C5-C6-N1	7.45	121.43	117.70
54	BA	2530	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	393	A	C4-C5-C6	-7.45	113.27	117.00
21	AA	1197	A	C5-C6-N1	7.45	121.43	117.70
54	BA	1453	A	C5-C6-N1	7.45	121.43	117.70
21	AA	478	A	C5-C6-N1	7.45	121.42	117.70
54	BA	460	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	1098	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1414	C	N3-C2-O2	-7.45	116.69	121.90
54	BA	2433	A	C5-C6-N1	7.45	121.42	117.70
21	AA	371	A	C5-C6-N1	7.45	121.42	117.70
25	BC	79	ARG	NE-CZ-NH1	7.45	124.02	120.30
54	BA	1970	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2705	A	C5-C6-N1	7.45	121.42	117.70
21	AA	172	A	N1-C6-N6	-7.44	114.14	118.60
21	AA	1179	A	C5-C6-N1	7.44	121.42	117.70
21	AA	873	A	N1-C6-N6	-7.44	114.14	118.60
21	AA	1374	A	C5-C6-N1	7.44	121.42	117.70
54	BA	782	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	1847	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1858	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2354	C	O4'-C1'-N1	7.44	114.15	108.20
54	BA	2566	A	C5-C6-N1	7.44	121.42	117.70
21	AA	642	A	C5-C6-N1	7.43	121.42	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	829	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2459	A	C5-C6-N1	7.43	121.42	117.70
21	AA	251	G	O4'-C1'-N9	7.43	114.15	108.20
21	AA	487	A	C5-C6-N1	7.43	121.42	117.70
21	AA	873	A	C5-C6-N1	7.43	121.42	117.70
21	AA	1447	A	C5-C6-N1	7.43	121.42	117.70
54	BA	1918	A	C5-C6-N1	7.43	121.42	117.70
54	BA	195	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	1341	G	O4'-C1'-N9	7.43	114.14	108.20
21	AA	629	A	C5-C6-N1	7.43	121.42	117.70
54	BA	52	A	C5-C6-N1	7.43	121.42	117.70
54	BA	1853	A	C4-C5-C6	-7.43	113.29	117.00
54	BA	2090	A	C4-C5-C6	-7.43	113.29	117.00
54	BA	2516	A	C5-C6-N1	7.43	121.41	117.70
21	AA	395	C	N3-C2-O2	-7.42	116.70	121.90
21	AA	964	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1308	U	O4'-C1'-N1	7.42	114.14	108.20
54	BA	1887	C	N3-C2-O2	-7.42	116.71	121.90
21	AA	949	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1395	C	N3-C2-O2	-7.42	116.71	121.90
54	BA	925	A	C5-C6-N1	7.42	121.41	117.70
54	BA	661	A	C5-C6-N1	7.42	121.41	117.70
54	BA	2388	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	415	A	O4'-C1'-N9	7.41	114.13	108.20
54	BA	2369	A	C4-C5-C6	-7.41	113.29	117.00
54	BA	2900	A	C5-C6-N1	7.41	121.41	117.70
54	BA	631	A	C5-C6-N1	7.41	121.40	117.70
54	BA	668	A	C5-C6-N1	7.41	121.40	117.70
55	BB	101	A	C5-C6-N1	7.41	121.40	117.70
21	AA	129	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2386	A	C4-C5-C6	-7.41	113.30	117.00
54	BA	2761	A	C5-C6-N1	7.41	121.40	117.70
21	AA	1195	C	N3-C2-O2	-7.41	116.72	121.90
54	BA	743	A	C5-C6-N1	7.41	121.40	117.70
54	BA	1084	A	C4-C5-C6	-7.41	113.30	117.00
54	BA	118	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1386	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	2119	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	412	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1501	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	1410	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1762	A	C5-C6-N1	7.40	121.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2691	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	116	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1392	A	C4-C5-C6	-7.40	113.30	117.00
21	AA	71	A	C5-C6-N1	7.40	121.40	117.70
21	AA	161	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	959	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	1340	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2121	G	N3-C2-N2	-7.40	114.72	119.90
54	BA	528	A	C5-C6-N1	7.39	121.40	117.70
54	BA	1076	C	O4'-C1'-N1	7.39	114.11	108.20
21	AA	967	C	N3-C2-O2	-7.39	116.72	121.90
35	BM	10	ARG	NE-CZ-NH1	7.39	124.00	120.30
36	BN	69	ARG	NE-CZ-NH1	7.39	124.00	120.30
54	BA	2014	A	N1-C6-N6	-7.39	114.16	118.60
54	BA	2327	A	C5-C6-N1	7.39	121.40	117.70
21	AA	139	A	C4-C5-C6	-7.39	113.31	117.00
21	AA	743	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	941	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1636	U	O4'-C1'-N1	7.39	114.11	108.20
21	AA	10	A	C5-C6-N1	7.39	121.39	117.70
54	BA	905	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1544	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1057	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1866	A	C5-C6-N1	7.39	121.39	117.70
21	AA	1492	A	C5-C6-N1	7.38	121.39	117.70
54	BA	616	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	2284	A	C5-C6-N1	7.38	121.39	117.70
21	AA	640	A	N1-C6-N6	-7.38	114.17	118.60
21	AA	825	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	2332	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	311	A	C5-C6-N1	7.38	121.39	117.70
21	AA	495	A	C5-C6-N1	7.38	121.39	117.70
25	BC	86	ARG	NE-CZ-NH1	7.38	123.99	120.30
22	A1	9	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	1307	A	C5-C6-N1	7.38	121.39	117.70
21	AA	1110	A	C5-C6-N1	7.37	121.39	117.70
24	A3	36	A	C5-C6-N1	7.37	121.39	117.70
54	BA	888	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	896	A	C5-C6-N1	7.37	121.39	117.70
42	BT	3	ARG	NE-CZ-NH1	7.37	123.98	120.30
54	BA	158	U	O4'-C1'-N1	7.37	114.10	108.20
54	BA	1039	A	C5-C6-N1	7.37	121.39	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1919	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2335	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1308	A	C5-C6-N1	7.37	121.39	117.70
7	AH	113	ARG	NE-CZ-NH1	7.37	123.98	120.30
21	AA	431	A	C5-C6-N1	7.37	121.38	117.70
21	AA	621	A	C5-C6-N1	7.37	121.38	117.70
54	BA	2534	A	C5-C6-N1	7.37	121.38	117.70
21	AA	151	A	C5-C6-N1	7.37	121.38	117.70
54	BA	919	U	O4'-C1'-N1	7.37	114.09	108.20
4	AE	19	ARG	NE-CZ-NH1	7.36	123.98	120.30
21	AA	908	A	C4-C5-C6	-7.36	113.32	117.00
54	BA	1020	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1977	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	2014	A	C5-C6-N1	7.36	121.38	117.70
55	BB	73	A	C5-C6-N1	7.36	121.38	117.70
54	BA	466	A	C5-C6-N1	7.36	121.38	117.70
54	BA	982	C	N3-C2-O2	-7.36	116.75	121.90
21	AA	1533	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	1551	A	C5-C6-N1	7.36	121.38	117.70
24	A3	3	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	118	A	C5-C6-N1	7.36	121.38	117.70
54	BA	947	A	C4-C5-C6	-7.35	113.32	117.00
54	BA	1230	A	C5-C6-N1	7.35	121.38	117.70
3	AD	13	ARG	NE-CZ-NH1	7.35	123.98	120.30
21	AA	1201	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	1413	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	2222	C	N3-C2-O2	-7.35	116.75	121.90
16	AQ	76	ARG	NE-CZ-NH1	7.35	123.97	120.30
21	AA	1204	A	C4-C5-C6	-7.35	113.33	117.00
54	BA	909	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	2482	A	C5-C6-N1	7.35	121.37	117.70
54	BA	2682	A	C5-C6-N1	7.35	121.37	117.70
54	BA	621	A	C5-C6-N1	7.35	121.37	117.70
54	BA	1689	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1700	A	C5-C6-N1	7.35	121.37	117.70
54	BA	1801	A	C4-C5-C6	-7.35	113.33	117.00
21	AA	1180	A	N1-C6-N6	-7.34	114.19	118.60
54	BA	52	A	N1-C6-N6	-7.34	114.19	118.60
54	BA	219	A	C5-C6-N1	7.34	121.37	117.70
54	BA	164	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	980	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	1586	A	N1-C6-N6	-7.34	114.19	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AN	63	ARG	NE-CZ-NH1	7.34	123.97	120.30
21	AA	766	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	528	A	C4-C5-C6	-7.34	113.33	117.00
21	AA	51	A	C5-C6-N1	7.34	121.37	117.70
43	BU	6	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	28	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	633	A	C5-C6-N1	7.34	121.37	117.70
45	BW	24	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	794	A	C5-C6-N1	7.34	121.37	117.70
21	AA	1105	A	C5-C6-N1	7.34	121.37	117.70
54	BA	142	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	144	A	C5-C6-N1	7.34	121.37	117.70
54	BA	226	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1932	A	C5-C6-N1	7.34	121.37	117.70
54	BA	412	A	C5-C6-N1	7.33	121.37	117.70
21	AA	270	A	N1-C6-N6	-7.33	114.20	118.60
18	AS	80	ARG	NE-CZ-NH1	7.33	123.97	120.30
54	BA	173	A	C5-C6-N1	7.33	121.37	117.70
54	BA	693	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	849	A	C5-C6-N1	7.33	121.37	117.70
21	AA	1280	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	2051	A	C5-C6-N1	7.33	121.36	117.70
54	BA	988	A	C5-C6-N1	7.33	121.36	117.70
54	BA	1123	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	2274	A	C5-C6-N1	7.33	121.36	117.70
43	BU	21	ARG	NE-CZ-NH1	7.32	123.96	120.30
54	BA	2873	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	109	A	C5-C6-N1	7.32	121.36	117.70
21	AA	915	A	C4-C5-C6	-7.32	113.34	117.00
21	AA	78	A	C5-C6-N1	7.32	121.36	117.70
21	AA	712	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1596	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2727	A	C5-C6-N1	7.32	121.36	117.70
21	AA	364	A	C5-C6-N1	7.32	121.36	117.70
21	AA	787	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	1434	A	C5-C6-N1	7.32	121.36	117.70
54	BA	456	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	1372	U	O4'-C1'-N1	7.31	114.05	108.20
21	AA	782	A	C5-C6-N1	7.31	121.36	117.70
54	BA	196	A	N1-C6-N6	-7.31	114.21	118.60
54	BA	586	A	C5-C6-N1	7.31	121.36	117.70
54	BA	1815	A	C4-C5-C6	-7.31	113.34	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AI	84	ARG	NE-CZ-NH1	7.31	123.95	120.30
21	AA	509	A	C5-C6-N1	7.31	121.35	117.70
21	AA	1082	A	C4-C5-C6	-7.31	113.35	117.00
21	AA	1479	C	N3-C2-O2	-7.31	116.79	121.90
19	AT	24	ARG	NE-CZ-NH1	7.30	123.95	120.30
21	AA	389	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1437	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	614	A	C5-C6-N1	7.30	121.35	117.70
54	BA	654	A	C5-C6-N1	7.30	121.35	117.70
54	BA	715	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1135	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	1403	A	C5-C6-N1	7.30	121.35	117.70
21	AA	325	A	C5-C6-N1	7.30	121.35	117.70
36	BN	2	ARG	NE-CZ-NH1	7.30	123.95	120.30
21	AA	313	A	C5-C6-N1	7.30	121.35	117.70
21	AA	702	A	C5-C6-N1	7.30	121.35	117.70
25	BC	155	ARG	NE-CZ-NH1	7.29	123.95	120.30
54	BA	2899	A	C5-C6-N1	7.29	121.35	117.70
21	AA	315	A	C5-C6-N1	7.29	121.35	117.70
54	BA	101	A	C5-C6-N1	7.29	121.35	117.70
54	BA	863	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1505	A	C4-C5-C6	-7.29	113.35	117.00
54	BA	2879	A	C5-C6-N1	7.29	121.35	117.70
25	BC	220	ARG	NE-CZ-NH2	-7.29	116.65	120.30
28	BF	109	ARG	NE-CZ-NH1	7.29	123.95	120.30
54	BA	1698	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	2432	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	1042	A	C5-C6-N1	7.29	121.34	117.70
54	BA	353	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	2883	A	C4-C5-C6	-7.29	113.36	117.00
13	AN	13	ARG	NE-CZ-NH1	7.29	123.94	120.30
21	AA	959	A	C5-C6-N1	7.29	121.34	117.70
54	BA	983	A	C5-C6-N1	7.29	121.34	117.70
54	BA	10	A	C4-C5-C6	-7.29	113.36	117.00
54	BA	101	A	O4'-C1'-N9	7.29	114.03	108.20
54	BA	229	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	1879	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	368	A	C5-C6-N1	7.28	121.34	117.70
21	AA	675	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	899	A	C5-C6-N1	7.28	121.34	117.70
54	BA	943	A	C5-C6-N1	7.28	121.34	117.70
21	AA	578	C	N3-C2-O2	-7.28	116.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	781	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1262	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	241	A	C5-C6-N1	7.28	121.34	117.70
54	BA	556	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	1899	A	C5-C6-N1	7.28	121.34	117.70
21	AA	630	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	977	A	O4'-C1'-N9	7.28	114.02	108.20
21	AA	1441	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	749	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1128	G	C1'-O4'-C4'	-7.28	104.08	109.90
54	BA	1616	A	C5-C6-N1	7.28	121.34	117.70
54	BA	972	A	C5-C6-N1	7.28	121.34	117.70
21	AA	743	A	C5-C6-N1	7.27	121.34	117.70
21	AA	1204	A	C5-C6-N1	7.27	121.34	117.70
21	AA	1319	A	C5-C6-N1	7.27	121.34	117.70
21	AA	1350	A	C5-C6-N1	7.27	121.34	117.70
21	AA	342	C	N3-C2-O2	-7.27	116.81	121.90
21	AA	860	A	C5-C6-N1	7.27	121.33	117.70
22	A1	66	A	C5-C6-N1	7.27	121.33	117.70
54	BA	756	A	N1-C6-N6	-7.27	114.24	118.60
54	BA	1936	A	C5-C6-N1	7.27	121.33	117.70
54	BA	2227	A	C4-C5-C6	-7.27	113.36	117.00
30	BH	123	ARG	NE-CZ-NH1	7.27	123.93	120.30
54	BA	222	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1508	A	O4'-C1'-N9	7.27	114.01	108.20
54	BA	2513	A	C5-C6-N1	7.27	121.33	117.70
54	BA	2795	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	2847	U	O4'-C1'-N1	7.27	114.01	108.20
54	BA	447	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1745	A	C4-C5-C6	-7.27	113.37	117.00
54	BA	1745	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1274	A	C5-C6-N1	7.26	121.33	117.70
21	AA	1289	A	C5-C6-N1	7.26	121.33	117.70
11	AL	113	ARG	NE-CZ-NH1	7.26	123.93	120.30
21	AA	694	A	N1-C6-N6	-7.26	114.24	118.60
21	AA	1368	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	1461	C	N3-C2-O2	-7.26	116.82	121.90
21	AA	572	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	217	A	N1-C6-N6	-7.26	114.25	118.60
54	BA	1996	C	N3-C2-O2	-7.26	116.82	121.90
21	AA	919	A	C4-C5-C6	-7.25	113.37	117.00
21	AA	889	A	C4-C5-C6	-7.25	113.37	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	727	A	C5-C6-N1	7.25	121.33	117.70
54	BA	788	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1918	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	2766	A	C4-C5-C6	-7.25	113.37	117.00
21	AA	1000	A	C4-C5-C6	-7.25	113.38	117.00
22	A1	17	U	O4'-C1'-N1	7.25	114.00	108.20
54	BA	2170	A	C4-C5-C6	-7.25	113.37	117.00
55	BB	50	A	C5-C6-N1	7.25	121.33	117.70
2	AC	58	ARG	NE-CZ-NH1	7.25	123.92	120.30
54	BA	2050	C	N3-C2-O2	-7.25	116.83	121.90
54	BA	2278	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	2418	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	2003	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1553	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	1953	A	N1-C6-N6	-7.25	114.25	118.60
55	BB	94	A	C4-C5-C6	-7.25	113.38	117.00
21	AA	179	A	C5-C6-N1	7.24	121.32	117.70
21	AA	767	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	2270	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1264	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1586	A	C5-C6-N1	7.24	121.32	117.70
21	AA	60	A	C5-C6-N1	7.24	121.32	117.70
21	AA	579	A	C5-C6-N1	7.24	121.32	117.70
54	BA	94	A	C5-C6-N1	7.24	121.32	117.70
54	BA	918	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	2829	A	C5-C6-N1	7.24	121.32	117.70
21	AA	946	A	C5-C6-N1	7.24	121.32	117.70
54	BA	791	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	1320	C	O4'-C1'-N1	7.24	113.99	108.20
54	BA	1871	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2856	A	C5-C6-N1	7.24	121.32	117.70
21	AA	1130	A	C5-C6-N1	7.23	121.32	117.70
21	AA	77	A	N1-C6-N6	-7.23	114.26	118.60
21	AA	797	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	975	A	C4-C5-C6	-7.23	113.38	117.00
54	BA	2154	A	C5-C6-N1	7.23	121.32	117.70
10	AK	12	ARG	NE-CZ-NH1	7.23	123.92	120.30
21	AA	321	A	C5-C6-N1	7.23	121.31	117.70
21	AA	349	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	391	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1713	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2421	G	O4'-C1'-N9	7.23	113.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2776	A	C5-C6-N1	7.23	121.31	117.70
21	AA	309	A	N1-C6-N6	-7.23	114.26	118.60
21	AA	924	C	N3-C2-O2	-7.22	116.84	121.90
54	BA	480	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2063	C	C2-N3-C4	-7.22	116.29	119.90
54	BA	2395	C	N3-C2-O2	-7.22	116.84	121.90
54	BA	1352	U	O4'-C1'-N1	7.22	113.98	108.20
54	BA	2527	C	N3-C2-O2	-7.22	116.84	121.90
21	AA	759	A	C5-C6-N1	7.22	121.31	117.70
21	AA	938	A	C5-C6-N1	7.22	121.31	117.70
54	BA	306	U	O4'-C1'-N1	7.22	113.98	108.20
54	BA	676	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1340	U	N3-C2-O2	-7.22	117.15	122.20
21	AA	1049	U	N3-C2-O2	-7.22	117.15	122.20
54	BA	609	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	783	A	C5-C6-N1	7.22	121.31	117.70
21	AA	1179	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	374	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1668	A	C5-C6-N1	7.22	121.31	117.70
21	AA	188	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	815	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1366	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	806	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	1275	A	N1-C6-N6	-7.21	114.27	118.60
21	AA	386	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	826	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	472	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1325	U	O4'-C1'-N1	7.21	113.97	108.20
54	BA	2814	A	C5-C6-N1	7.21	121.31	117.70
21	AA	396	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	279	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1480	A	C4-C5-C6	-7.21	113.39	117.00
21	AA	1483	A	N1-C6-N6	-7.21	114.27	118.60
24	A3	45	A	C5-C6-N1	7.21	121.30	117.70
54	BA	1603	A	C4-C5-C6	-7.21	113.39	117.00
7	AH	14	ARG	NE-CZ-NH1	7.21	123.90	120.30
21	AA	306	A	C5-C6-N1	7.21	121.30	117.70
22	A1	9	A	C5-C6-N1	7.21	121.30	117.70
54	BA	751	A	C4-C5-C6	-7.21	113.40	117.00
54	BA	1417	C	N3-C2-O2	-7.21	116.86	121.90
21	AA	80	A	C5-C6-N1	7.21	121.30	117.70
21	AA	595	A	C5-C6-N1	7.21	121.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A2	82	A	C5-C6-N1	7.21	121.30	117.70
2	AC	155	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	1571	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	195	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1032	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1156	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2497	A	C5-C6-N1	7.20	121.30	117.70
55	BB	109	A	C5-C6-N1	7.20	121.30	117.70
21	AA	913	A	C5-C6-N1	7.20	121.30	117.70
44	BV	93	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	740	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	981	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2009	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2126	A	C5-C6-N1	7.20	121.30	117.70
55	BB	45	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	1711	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1239	A	C5-C6-N1	7.20	121.30	117.70
54	BA	177	G	O4'-C1'-N9	7.20	113.96	108.20
54	BA	1008	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1493	C	N3-C2-O2	-7.20	116.86	121.90
32	BJ	27	ARG	NE-CZ-NH1	7.19	123.90	120.30
21	AA	560	A	C5-C6-N1	7.19	121.30	117.70
21	AA	1248	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2823	A	N1-C6-N6	-7.19	114.28	118.60
54	BA	2077	A	C5-C6-N1	7.19	121.30	117.70
21	AA	528	C	N3-C2-O2	-7.19	116.87	121.90
54	BA	2810	A	C4-C5-C6	-7.19	113.41	117.00
21	AA	1146	A	N1-C6-N6	-7.19	114.29	118.60
24	A3	74	A	C5-C6-N1	7.19	121.29	117.70
21	AA	718	A	C4-C5-C6	-7.19	113.41	117.00
54	BA	104	A	C5-C6-N1	7.19	121.29	117.70
54	BA	256	A	C5-C6-N1	7.19	121.29	117.70
21	AA	59	A	C5-C6-N1	7.18	121.29	117.70
21	AA	602	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	979	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	2169	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2298	A	N1-C6-N6	-7.18	114.29	118.60
21	AA	26	A	N1-C6-N6	-7.18	114.29	118.60
21	AA	136	C	N3-C2-O2	-7.18	116.87	121.90
21	AA	371	A	C4-C5-C6	-7.18	113.41	117.00
47	BY	23	ARG	NE-CZ-NH1	7.18	123.89	120.30
54	BA	1998	A	C5-C6-N1	7.18	121.29	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1468	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	1063	G	O4'-C1'-N9	7.18	113.94	108.20
54	BA	1580	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	2386	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1339	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	477	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1000	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1571	A	C5-C6-N1	7.18	121.29	117.70
21	AA	908	A	C5-C6-N1	7.18	121.29	117.70
42	BT	6	ARG	NE-CZ-NH2	7.18	123.89	120.30
54	BA	1265	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	196	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	972	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	1760	C	N3-C2-O2	-7.18	116.88	121.90
54	BA	2043	C	N3-C2-O2	-7.18	116.88	121.90
54	BA	2275	C	N3-C2-O2	-7.18	116.88	121.90
21	AA	7	A	C5-C6-N1	7.17	121.29	117.70
1	AB	112	ARG	NE-CZ-NH1	7.17	123.89	120.30
13	AN	24	ARG	NE-CZ-NH1	7.17	123.89	120.30
21	AA	81	A	C5-C6-N1	7.17	121.29	117.70
21	AA	681	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1103	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	74	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1246	A	N1-C6-N6	-7.17	114.30	118.60
21	AA	756	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	526	A	C5-C6-N1	7.17	121.28	117.70
54	BA	156	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2173	A	C5-C6-N1	7.16	121.28	117.70
21	AA	124	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	272	A	N1-C6-N6	-7.16	114.30	118.60
54	BA	364	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	2352	A	N1-C6-N6	-7.16	114.30	118.60
21	AA	972	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	1499	A	C5-C6-N1	7.16	121.28	117.70
43	BU	81	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	1927	A	C5-C6-N1	7.16	121.28	117.70
21	AA	320	A	C4-C5-C6	-7.16	113.42	117.00
54	BA	814	C	O4'-C1'-N1	7.16	113.93	108.20
54	BA	1987	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	2080	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2273	A	C5-C6-N1	7.16	121.28	117.70
54	BA	1813	G	O4'-C1'-N9	7.16	113.93	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1847	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	348	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2784	U	O4'-C1'-N1	7.16	113.92	108.20
21	AA	279	A	C5-C6-N1	7.15	121.28	117.70
24	A3	58	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1319	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	1366	A	C5-C6-N1	7.15	121.28	117.70
22	A1	76	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1433	A	C5-C6-N1	7.15	121.27	117.70
54	BA	2114	A	C5-C6-N1	7.15	121.27	117.70
21	AA	1157	A	C4-C5-C6	-7.15	113.43	117.00
54	BA	265	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	1711	A	C4-C5-C6	-7.15	113.43	117.00
54	BA	2478	A	C5-C6-N1	7.15	121.27	117.70
54	BA	603	A	C5-C6-N1	7.14	121.27	117.70
21	AA	363	A	C5-C6-N1	7.14	121.27	117.70
54	BA	560	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	825	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2516	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	253	A	C5-C6-N1	7.14	121.27	117.70
21	AA	996	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1430	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	2359	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	263	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1518	A	C5-C6-N1	7.14	121.27	117.70
54	BA	163	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	374	A	N1-C6-N6	-7.14	114.32	118.60
54	BA	945	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1354	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2176	A	C4-C5-C6	-7.14	113.43	117.00
55	BB	29	A	C5-C6-N1	7.14	121.27	117.70
1	AB	20	ARG	NE-CZ-NH1	7.13	123.87	120.30
24	A3	14	A	C5-C6-N1	7.13	121.27	117.70
21	AA	1178	G	N1-C6-O6	-7.13	115.62	119.90
21	AA	1377	A	C5-C6-N1	7.13	121.27	117.70
54	BA	84	A	C5-C6-N1	7.13	121.27	117.70
56	B5	71	ARG	NE-CZ-NH1	7.13	123.87	120.30
54	BA	540	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	1717	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1914	C	O4'-C1'-N1	7.13	113.90	108.20
54	BA	917	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	702	A	C4-C5-C6	-7.12	113.44	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1314	C	N1-C2-O2	7.12	123.17	118.90
21	AA	53	A	N1-C6-N6	-7.12	114.33	118.60
21	AA	1201	A	P-O3'-C3'	7.12	128.25	119.70
21	AA	1250	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1373	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1503	A	C5-C6-N1	7.12	121.26	117.70
7	AH	127	TYR	CB-CG-CD2	-7.12	116.73	121.00
54	BA	294	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	455	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	1640	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2560	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2577	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1853	A	C5-C6-N1	7.12	121.26	117.70
21	AA	329	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	1705	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2055	C	N3-C2-O2	-7.12	116.92	121.90
9	AJ	9	ARG	NE-CZ-NH1	7.12	123.86	120.30
21	AA	1410	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1169	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1531	A	C5-C6-N1	7.12	121.26	117.70
22	A1	23	A	C5-C6-N1	7.12	121.26	117.70
38	BP	61	ARG	NE-CZ-NH1	7.12	123.86	120.30
54	BA	2531	A	N1-C6-N6	-7.12	114.33	118.60
10	AK	126	ARG	NE-CZ-NH1	7.11	123.86	120.30
54	BA	563	A	C5-C6-N1	7.11	121.26	117.70
54	BA	1289	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	1378	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	821	A	C4-C5-C6	-7.11	113.44	117.00
54	BA	2451	A	C4-C5-C6	-7.11	113.44	117.00
3	AD	62	ARG	NE-CZ-NH1	7.11	123.86	120.30
21	AA	781	A	C5-C6-N1	7.11	121.25	117.70
54	BA	223	A	C5-C6-N1	7.11	121.25	117.70
54	BA	1603	A	C5-C6-N1	7.11	121.25	117.70
21	AA	1016	A	C5-C6-N1	7.11	121.25	117.70
54	BA	347	A	C5-C6-N1	7.11	121.25	117.70
54	BA	1947	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	865	A	N1-C6-N6	-7.10	114.34	118.60
29	BG	151	ARG	NE-CZ-NH1	7.10	123.85	120.30
51	B2	12	ARG	NE-CZ-NH1	7.10	123.85	120.30
54	BA	412	A	C4-C5-C6	-7.10	113.45	117.00
21	AA	397	A	C5-C6-N1	7.10	121.25	117.70
21	AA	98	A	C4-C5-C6	-7.10	113.45	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1004	A	C5-C6-N1	7.10	121.25	117.70
54	BA	218	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	685	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	878	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1308	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	1509	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2104	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	42	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	554	U	O4'-C1'-N1	7.10	113.88	108.20
54	BA	2254	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	74	A	C4-C5-C6	-7.09	113.45	117.00
21	AA	1155	A	C5-C6-N1	7.09	121.25	117.70
39	BQ	27	ARG	NE-CZ-NH1	7.09	123.85	120.30
54	BA	217	A	C5-C6-N1	7.09	121.25	117.70
54	BA	354	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2614	A	C4-C5-C6	-7.09	113.45	117.00
21	AA	754	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	16	C	O4'-C1'-N1	7.09	113.87	108.20
54	BA	276	U	O4'-C1'-N1	7.09	113.87	108.20
21	AA	422	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	510	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1889	A	N1-C6-N6	-7.09	114.34	118.60
21	AA	101	A	C5-C6-N1	7.09	121.25	117.70
21	AA	649	A	C5-C6-N1	7.09	121.25	117.70
21	AA	1214	C	N1-C2-O2	7.09	123.15	118.90
54	BA	279	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	497	A	C5-C6-N1	7.09	121.24	117.70
54	BA	750	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1095	A	C5-C6-N1	7.09	121.24	117.70
54	BA	1366	A	C4-C5-C6	-7.09	113.46	117.00
21	AA	715	A	C5-C6-N1	7.09	121.24	117.70
21	AA	1046	A	C5-C6-N1	7.09	121.24	117.70
22	A1	61	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	1077	A	C5-C6-N1	7.09	121.24	117.70
54	BA	1328	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	1350	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	1394	A	C5-C6-N1	7.08	121.24	117.70
55	BB	99	A	C5-C6-N1	7.08	121.24	117.70
21	AA	768	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	1147	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2427	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	363	A	C4-C5-C6	-7.08	113.46	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1082	A	C5-C6-N1	7.08	121.24	117.70
21	AA	1296	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	1408	A	C5-C6-N1	7.08	121.24	117.70
54	BA	849	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	990	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2377	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	635	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	640	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	1272	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1522	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2541	A	C5-C6-N1	7.08	121.24	117.70
24	A3	44	A	C5-C6-N1	7.08	121.24	117.70
54	BA	483	A	C5-C6-N1	7.08	121.24	117.70
54	BA	449	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1020	A	N1-C6-N6	-7.08	114.36	118.60
21	AA	841	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	1188	A	C5-C6-N1	7.07	121.24	117.70
54	BA	564	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1286	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	2856	A	C4-C5-C6	-7.07	113.46	117.00
21	AA	502	A	C4-C5-C6	-7.07	113.46	117.00
54	BA	1876	A	C5-C6-N1	7.07	121.24	117.70
18	AS	36	ARG	NE-CZ-NH2	7.07	123.83	120.30
21	AA	392	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1012	U	O4'-C1'-N1	7.07	113.86	108.20
54	BA	1126	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1991	U	O4'-C1'-N1	7.07	113.86	108.20
54	BA	2771	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	1318	A	C5-C6-N1	7.07	121.23	117.70
12	AM	2	ARG	NE-CZ-NH2	7.07	123.83	120.30
21	AA	1269	A	C5-C6-N1	7.07	121.23	117.70
47	BY	47	ARG	NE-CZ-NH1	7.07	123.83	120.30
54	BA	1021	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	2020	A	C4-C5-C6	-7.07	113.47	117.00
21	AA	1357	A	C5-C6-N1	7.06	121.23	117.70
24	A3	60	A	C5-C6-N1	7.06	121.23	117.70
21	AA	901	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1676	A	C5-C6-N1	7.06	121.23	117.70
21	AA	16	A	C5-C6-N1	7.06	121.23	117.70
21	AA	328	C	N1-C2-O2	7.06	123.14	118.90
54	BA	2084	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	436	C	N3-C2-O2	-7.06	116.96	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1744	A	N1-C6-N6	-7.06	114.37	118.60
54	BA	1789	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2412	A	C5-C6-N1	7.06	121.23	117.70
21	AA	382	A	C5-C6-N1	7.05	121.23	117.70
21	AA	408	A	C5-C6-N1	7.05	121.23	117.70
21	AA	938	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	721	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1630	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	2406	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	2700	A	C4-C5-C6	-7.05	113.47	117.00
55	BB	47	C	O4'-C1'-N1	7.05	113.84	108.20
21	AA	236	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	844	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	2147	A	N1-C6-N6	-7.05	114.37	118.60
21	AA	1226	C	N3-C2-O2	-7.05	116.96	121.90
54	BA	1585	C	N3-C2-O2	-7.05	116.96	121.90
21	AA	238	A	C5-C6-N1	7.05	121.22	117.70
21	AA	546	A	C4-C5-C6	-7.05	113.48	117.00
54	BA	984	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	1230	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	2435	A	C5-C6-N1	7.05	121.22	117.70
21	AA	223	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1288	A	C5-C6-N1	7.05	121.22	117.70
25	BC	132	ARG	NE-CZ-NH1	7.05	123.82	120.30
54	BA	1572	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2307	G	O4'-C1'-N9	7.05	113.84	108.20
21	AA	1425	U	O4'-C1'-N1	7.04	113.84	108.20
54	BA	1618	A	N1-C6-N6	-7.04	114.37	118.60
8	AI	17	ARG	NE-CZ-NH1	7.04	123.82	120.30
21	AA	523	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1073	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1085	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	32	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	1129	C	N3-C2-O2	-7.04	116.97	121.90
22	A1	26	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	492	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	802	A	C5-C6-N1	7.04	121.22	117.70
54	BA	912	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	1916	A	C5-C6-N1	7.04	121.22	117.70
54	BA	606	U	O4'-C1'-N1	7.04	113.83	108.20
54	BA	1815	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2483	C	N3-C2-O2	-7.04	116.97	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AN	41	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	1189	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1200	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	1285	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2392	A	C5-C6-N1	7.04	121.22	117.70
21	AA	482	A	C5-C6-N1	7.04	121.22	117.70
21	AA	648	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1866	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	2247	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	1456	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1142	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	1632	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2094	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	1494	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	2147	A	C5-C6-N1	7.03	121.22	117.70
2	AC	39	ARG	NE-CZ-NH1	7.03	123.82	120.30
21	AA	1021	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1611	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1626	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1828	G	N1-C6-O6	-7.03	115.68	119.90
54	BA	2725	A	C5-C6-N1	7.03	121.22	117.70
55	BB	52	A	C5-C6-N1	7.03	121.22	117.70
55	BB	58	A	N1-C6-N6	-7.03	114.38	118.60
21	AA	1044	A	C5-C6-N1	7.03	121.22	117.70
54	BA	13	A	C5-C6-N1	7.03	121.21	117.70
54	BA	2870	C	N3-C2-O2	-7.03	116.98	121.90
21	AA	1093	A	C5-C6-N1	7.03	121.21	117.70
48	BZ	37	ARG	NE-CZ-NH1	7.03	123.81	120.30
54	BA	56	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	468	G	O4'-C1'-N9	7.03	113.82	108.20
54	BA	2433	A	C4-C5-C6	-7.03	113.49	117.00
21	AA	914	A	C5-C6-N1	7.03	121.21	117.70
54	BA	282	A	N1-C6-N6	-7.03	114.39	118.60
11	AL	49	ARG	NE-CZ-NH1	7.02	123.81	120.30
54	BA	2753	A	C5-C6-N1	7.02	121.21	117.70
55	BB	58	A	C5-C6-N1	7.02	121.21	117.70
21	AA	99	C	N3-C2-O2	-7.02	116.98	121.90
21	AA	374	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	2073	C	N3-C2-O2	-7.02	116.98	121.90
21	AA	1346	A	C5-C6-N1	7.02	121.21	117.70
54	BA	748	G	O4'-C1'-N9	7.02	113.81	108.20
54	BA	1654	A	C5-C6-N1	7.02	121.21	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2097	A	C5-C6-N1	7.02	121.21	117.70
54	BA	2225	A	C5-C6-N1	7.02	121.21	117.70
21	AA	999	C	N3-C2-O2	-7.02	116.99	121.90
54	BA	131	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	1610	A	N1-C6-N6	-7.02	114.39	118.60
21	AA	640	A	C5-C6-N1	7.02	121.21	117.70
21	AA	381	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	706	A	C5-C6-N1	7.01	121.21	117.70
54	BA	64	A	C5-C6-N1	7.01	121.21	117.70
54	BA	83	A	C5-C6-N1	7.01	121.21	117.70
54	BA	819	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1938	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2726	A	C5-C6-N1	7.01	121.21	117.70
21	AA	860	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	522	A	C5-C6-N1	7.01	121.21	117.70
21	AA	1283	U	O4'-C1'-N1	7.01	113.81	108.20
21	AA	1428	A	C5-C6-N1	7.01	121.21	117.70
35	BM	66	ARG	NE-CZ-NH1	7.01	123.81	120.30
54	BA	240	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	601	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	236	A	N1-C6-N6	-7.01	114.39	118.60
21	AA	1105	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	1176	A	N1-C6-N6	-7.01	114.39	118.60
21	AA	1261	A	C5-C6-N1	7.01	121.20	117.70
24	A3	73	A	C5-C6-N1	7.01	121.20	117.70
54	BA	89	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	219	A	C4-C5-C6	-7.01	113.50	117.00
54	BA	1420	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2806	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	496	A	N1-C6-N6	-7.01	114.39	118.60
55	BB	90	C	O4'-C1'-N1	7.01	113.81	108.20
21	AA	574	A	N1-C6-N6	-7.01	114.40	118.60
21	AA	1005	A	N1-C6-N6	-7.01	114.40	118.60
21	AA	408	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1735	A	C5-C6-N1	7.00	121.20	117.70
21	AA	1219	A	C5-C6-N1	7.00	121.20	117.70
22	A1	14	A	C5-C6-N1	7.00	121.20	117.70
36	BN	71	ARG	NE-CZ-NH1	7.00	123.80	120.30
54	BA	611	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2020	A	C5-C6-N1	7.00	121.20	117.70
21	AA	1493	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1741	C	N3-C2-O2	-7.00	117.00	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2889	C	N3-C2-O2	-7.00	117.00	121.90
56	B5	162	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	AC	163	ARG	NE-CZ-NH1	7.00	123.80	120.30
21	AA	54	C	C1'-O4'-C4'	-7.00	104.30	109.90
21	AA	805	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	1196	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	1237	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	747	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	448	A	C5-C6-N1	7.00	121.20	117.70
21	AA	1425	U	P-O3'-C3'	7.00	128.09	119.70
54	BA	1833	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2005	A	C5-C6-N1	7.00	121.20	117.70
21	AA	303	A	C4-C5-C6	-6.99	113.50	117.00
22	A1	74	C	N1-C2-O2	6.99	123.10	118.90
54	BA	422	A	C5-C6-N1	6.99	121.20	117.70
54	BA	1749	A	C5-C6-N1	6.99	121.20	117.70
21	AA	478	A	C4-C5-C6	-6.99	113.50	117.00
21	AA	1012	A	C5-C6-N1	6.99	121.19	117.70
5	AF	86	ARG	NE-CZ-NH1	6.99	123.79	120.30
21	AA	1496	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	149	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	936	A	C5-C6-N1	6.99	121.19	117.70
54	BA	996	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2287	A	C5-C6-N1	6.99	121.19	117.70
21	AA	309	A	C5-C6-N1	6.99	121.19	117.70
54	BA	190	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1076	C	C1'-O4'-C4'	-6.99	104.31	109.90
54	BA	2723	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	1170	A	N1-C6-N6	-6.99	114.41	118.60
21	AA	1468	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1794	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	2350	C	N3-C2-O2	-6.99	117.01	121.90
28	BF	79	ARG	NE-CZ-NH1	6.98	123.79	120.30
21	AA	655	A	C5-C6-N1	6.98	121.19	117.70
54	BA	677	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	722	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	2335	A	N1-C6-N6	-6.98	114.41	118.60
55	BB	97	C	N3-C2-O2	-6.98	117.01	121.90
21	AA	1228	C	C1'-O4'-C4'	-6.98	104.31	109.90
21	AA	583	A	C5-C6-N1	6.98	121.19	117.70
21	AA	1016	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	1163	A	C5-C6-N1	6.98	121.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	227	A	C5-C6-N1	6.98	121.19	117.70
54	BA	430	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1393	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	2352	A	C5-C6-N1	6.98	121.19	117.70
21	AA	432	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	1229	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	2683	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	2882	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	228	A	C5-C6-N1	6.98	121.19	117.70
21	AA	1101	A	C5-C6-N1	6.97	121.19	117.70
21	AA	1306	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	1610	A	C1'-O4'-C4'	-6.97	104.32	109.90
54	BA	1937	A	O4'-C1'-N9	6.97	113.78	108.20
54	BA	1952	A	C5-C6-N1	6.97	121.19	117.70
54	BA	401	A	C5-C6-N1	6.97	121.19	117.70
21	AA	1248	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	1439	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1342	A	C5-C6-N1	6.97	121.18	117.70
54	BA	2283	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	120	A	C5-C6-N1	6.96	121.18	117.70
21	AA	327	A	C5-C6-N1	6.96	121.18	117.70
21	AA	430	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1446	A	N1-C6-N6	-6.96	114.42	118.60
54	BA	1669	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1779	U	O4'-C1'-N1	6.96	113.77	108.20
54	BA	2440	C	N3-C2-O2	-6.96	117.02	121.90
55	BB	11	C	N3-C2-O2	-6.96	117.03	121.90
55	BB	110	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	531	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	181	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	513	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	513	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1960	A	C4-C5-C6	-6.96	113.52	117.00
11	AL	93	ARG	NE-CZ-NH1	6.96	123.78	120.30
22	A1	21	A	C5-C6-N1	6.96	121.18	117.70
54	BA	435	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	1504	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	777	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1236	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1324	A	C5-C6-N1	6.96	121.18	117.70
54	BA	14	A	C5-C6-N1	6.96	121.18	117.70
54	BA	31	C	N3-C2-O2	-6.96	117.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	104	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1805	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1809	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2019	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	2309	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2406	A	C5-C6-N1	6.96	121.18	117.70
54	BA	960	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1535	A	C5-C6-N1	6.96	121.18	117.70
3	AD	46	ARG	NE-CZ-NH1	6.95	123.78	120.30
6	AG	4	ARG	NE-CZ-NH1	6.95	123.78	120.30
21	AA	73	C	N3-C2-O2	-6.95	117.03	121.90
21	AA	313	A	C6-C5-N7	6.95	137.17	132.30
54	BA	574	A	N1-C6-N6	-6.95	114.43	118.60
21	AA	303	A	C5-C6-N1	6.95	121.18	117.70
54	BA	479	A	C5-C6-N1	6.95	121.18	117.70
54	BA	1848	A	C5-C6-N1	6.95	121.18	117.70
21	AA	610	U	O4'-C1'-N1	6.95	113.76	108.20
21	AA	1413	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	1570	A	C5-C6-N1	6.95	121.17	117.70
21	AA	983	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	1048	A	C5-C6-N1	6.95	121.17	117.70
54	BA	670	A	O4'-C1'-N9	-6.95	102.64	108.20
21	AA	320	A	C5-C6-N1	6.95	121.17	117.70
21	AA	83	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	1579	A	N1-C6-N6	-6.94	114.43	118.60
21	AA	1225	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	1827	U	O4'-C1'-N1	6.94	113.75	108.20
21	AA	1271	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1014	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	1155	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1662	U	O4'-C1'-N1	6.94	113.75	108.20
54	BA	1759	A	C5-C6-N1	6.94	121.17	117.70
54	BA	2813	A	C5-C6-N1	6.94	121.17	117.70
55	BB	50	A	C4-C5-C6	-6.94	113.53	117.00
38	BP	20	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	820	A	N1-C6-N6	-6.94	114.44	118.60
54	BA	2612	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	1509	C	N3-C2-O2	-6.94	117.04	121.90
24	A3	69	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	582	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1142	A	C5-C6-N1	6.94	121.17	117.70
54	BA	2733	A	C5-C6-N1	6.94	121.17	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	113	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	608	A	C4-C5-C6	-6.94	113.53	117.00
21	AA	600	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1155	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	685	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1126	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	1532	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1597	A	O4'-C1'-N9	6.93	113.75	108.20
54	BA	1829	A	C5-C6-N1	6.93	121.17	117.70
54	BA	79	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	590	A	C5-C6-N1	6.93	121.17	117.70
54	BA	2066	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	790	A	C5-C6-N1	6.93	121.17	117.70
54	BA	721	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	2458	G	O4'-C1'-N9	6.93	113.74	108.20
54	BA	2501	C	N3-C2-O2	-6.93	117.05	121.90
55	BB	66	A	C5-C6-N1	6.93	121.17	117.70
22	A1	73	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	1490	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	865	A	C5-C6-N1	6.93	121.16	117.70
54	BA	272	A	C5-C6-N1	6.93	121.16	117.70
54	BA	614	A	C1'-O4'-C4'	-6.93	104.36	109.90
54	BA	1495	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	787	A	C5-C6-N1	6.92	121.16	117.70
54	BA	64	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	788	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	994	C	N3-C2-O2	-6.92	117.05	121.90
21	AA	300	A	C5-C6-N1	6.92	121.16	117.70
21	AA	729	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	599	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	2212	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2818	U	O4'-C1'-N1	6.92	113.74	108.20
21	AA	1363	A	C5-C6-N1	6.92	121.16	117.70
54	BA	959	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	866	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	1360	A	C5-C6-N1	6.92	121.16	117.70
54	BA	239	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	1247	A	O4'-C1'-N9	6.92	113.73	108.20
54	BA	2634	A	C5-C6-N1	6.92	121.16	117.70
21	AA	36	C	N3-C2-O2	-6.92	117.06	121.90
24	A3	38	A	C5-C6-N1	6.92	121.16	117.70
21	AA	716	A	C4-C5-C6	-6.92	113.54	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	19	A	C4-C5-C6	-6.92	113.54	117.00
8	AI	122	ARG	NE-CZ-NH1	6.91	123.76	120.30
21	AA	270	A	C5-C6-N1	6.91	121.16	117.70
21	AA	132	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	478	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1040	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1247	A	C5-C6-N1	6.91	121.16	117.70
54	BA	2902	C	N3-C2-O2	-6.91	117.06	121.90
2	AC	106	ARG	NE-CZ-NH1	6.91	123.76	120.30
21	AA	152	A	C4-C5-C6	-6.91	113.55	117.00
21	AA	549	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	1384	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2297	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	2369	A	C5-C6-N1	6.91	121.16	117.70
21	AA	161	A	C5-C6-N1	6.91	121.15	117.70
54	BA	689	A	N1-C6-N6	-6.91	114.46	118.60
21	AA	430	A	N1-C6-N6	-6.91	114.46	118.60
54	BA	125	A	C5-C6-N1	6.91	121.15	117.70
54	BA	602	A	C5-C6-N1	6.91	121.15	117.70
54	BA	1419	A	C5-C6-N1	6.91	121.15	117.70
54	BA	2468	A	C5-C6-N1	6.91	121.15	117.70
28	BF	124	ARG	NE-CZ-NH1	6.90	123.75	120.30
43	BU	93	ARG	NE-CZ-NH1	6.90	123.75	120.30
54	BA	973	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	1549	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	205	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1150	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1267	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	1367	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	1067	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	1049	U	O4'-C1'-N1	6.90	113.72	108.20
54	BA	21	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	1029	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	1654	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	2184	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	2841	C	N3-C2-O2	-6.90	117.07	121.90
12	AM	97	ARG	NE-CZ-NH1	6.90	123.75	120.30
54	BA	1378	A	C5-C6-N1	6.90	121.15	117.70
18	AS	2	ARG	NE-CZ-NH1	6.90	123.75	120.30
21	AA	749	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1428	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	1900	A	C4-C5-C6	-6.90	113.55	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2205	A	C4-C5-C6	-6.89	113.55	117.00
55	BB	52	A	N1-C6-N6	-6.89	114.46	118.60
21	AA	312	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	1466	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1014	A	C5-C6-N1	6.89	121.15	117.70
21	AA	612	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	490	C	N1-C2-O2	6.89	123.03	118.90
54	BA	1802	A	C5-C6-N1	6.89	121.14	117.70
54	BA	2317	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	2745	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	435	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1333	A	C5-C6-N1	6.89	121.14	117.70
54	BA	699	A	C5-C6-N1	6.89	121.14	117.70
54	BA	1044	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	2760	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	101	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	92	U	O4'-C1'-N1	6.89	113.71	108.20
21	AA	26	A	C5-C6-N1	6.88	121.14	117.70
21	AA	78	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	403	U	O4'-C1'-N1	6.88	113.71	108.20
54	BA	1701	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2407	A	C5-C6-N1	6.88	121.14	117.70
21	AA	214	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	1055	A	C5-C6-N1	6.88	121.14	117.70
54	BA	176	A	C5-C6-N1	6.88	121.14	117.70
54	BA	633	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2226	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	802	A	C5-C6-N1	6.88	121.14	117.70
54	BA	84	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	728	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1433	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	19	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1073	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	13	U	C1'-O4'-C4'	-6.87	104.40	109.90
21	AA	637	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1748	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	2815	C	N3-C2-O2	-6.87	117.09	121.90
6	AG	142	ARG	NE-CZ-NH1	6.87	123.74	120.30
21	AA	629	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	1067	A	C5-C6-N1	6.87	121.14	117.70
25	BC	181	ARG	NE-CZ-NH1	6.87	123.73	120.30
54	BA	532	A	C5-C6-N1	6.87	121.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	927	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1609	A	C5-C6-N1	6.87	121.14	117.70
54	BA	2326	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	332	A	C5-C6-N1	6.87	121.14	117.70
54	BA	825	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	632	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1722	A	C5-C6-N1	6.87	121.13	117.70
21	AA	1092	A	C5-C6-N1	6.87	121.13	117.70
21	AA	1430	A	C5-C6-N1	6.87	121.13	117.70
21	AA	1434	A	C4-C5-C6	-6.87	113.57	117.00
23	A2	93	U	C1'-O4'-C4'	-6.87	104.41	109.90
54	BA	1069	A	C4-C5-C6	-6.87	113.57	117.00
7	AH	12	ARG	NE-CZ-NH1	6.86	123.73	120.30
21	AA	1257	A	C5-C6-N1	6.86	121.13	117.70
21	AA	1280	A	C5-C6-N1	6.86	121.13	117.70
21	AA	1317	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2336	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2134	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	876	C	P-O3'-C3'	6.86	127.93	119.70
54	BA	1403	A	N1-C6-N6	-6.86	114.49	118.60
54	BA	1507	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2023	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2855	C	N3-C2-O2	-6.86	117.10	121.90
55	BB	34	A	C4-C5-C6	-6.86	113.57	117.00
7	AH	83	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	265	A	C5-C6-N1	6.86	121.13	117.70
54	BA	507	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1284	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2594	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	1974	C	N3-C2-O2	-6.85	117.10	121.90
54	BA	233	A	C5-C6-N1	6.85	121.13	117.70
54	BA	2760	C	O4'-C1'-N1	6.85	113.68	108.20
54	BA	2872	A	C5-C6-N1	6.85	121.13	117.70
21	AA	95	C	N3-C2-O2	-6.85	117.10	121.90
54	BA	735	A	C5-C6-N1	6.85	121.12	117.70
55	BB	58	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	1419	A	N1-C6-N6	-6.85	114.49	118.60
54	BA	1890	A	N1-C6-N6	-6.85	114.49	118.60
54	BA	1953	A	C4-C5-C6	-6.85	113.58	117.00
12	AM	56	ARG	NE-CZ-NH1	6.85	123.72	120.30
36	BN	8	ARG	NE-CZ-NH1	6.85	123.72	120.30
54	BA	330	A	C4-C5-C6	-6.85	113.58	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1140	C	N3-C2-O2	-6.85	117.11	121.90
54	BA	1237	A	C5-C6-N1	6.85	121.12	117.70
6	AG	78	ARG	NE-CZ-NH1	6.84	123.72	120.30
25	BC	166	ARG	NE-CZ-NH1	6.84	123.72	120.30
54	BA	1129	A	N1-C6-N6	-6.84	114.49	118.60
21	AA	251	G	P-O3'-C3'	6.84	127.91	119.70
21	AA	1483	A	C5-C6-N1	6.84	121.12	117.70
54	BA	722	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2434	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	2517	C	N3-C2-O2	-6.84	117.11	121.90
13	AN	59	ARG	NE-CZ-NH1	6.84	123.72	120.30
19	AT	73	ARG	NE-CZ-NH1	6.84	123.72	120.30
21	AA	596	A	C5-C6-N1	6.84	121.12	117.70
54	BA	103	A	C5-C6-N1	6.84	121.12	117.70
54	BA	471	A	C5-C6-N1	6.84	121.12	117.70
54	BA	310	A	C5-C6-N1	6.84	121.12	117.70
21	AA	857	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	1320	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	264	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	882	C	N3-C2-O2	-6.83	117.11	121.90
21	AA	1167	A	C4-C5-C6	-6.83	113.58	117.00
21	AA	1230	C	N3-C2-O2	-6.83	117.12	121.90
24	A3	39	A	C5-C6-N1	6.83	121.12	117.70
33	BK	108	ARG	NE-CZ-NH1	6.83	123.72	120.30
54	BA	1652	A	C5-C6-N1	6.83	121.12	117.70
21	AA	750	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1503	A	C5-C6-N1	6.83	121.11	117.70
54	BA	131	A	C5-C6-N1	6.83	121.11	117.70
54	BA	1365	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2314	A	N1-C6-N6	-6.83	114.50	118.60
55	BB	26	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	893	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	73	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	2340	A	C5-C6-N1	6.83	121.11	117.70
21	AA	873	A	C4-C5-C6	-6.83	113.59	117.00
21	AA	930	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1246	A	C4-C5-C6	-6.83	113.58	117.00
22	A1	74	C	O4'-C1'-N1	6.83	113.66	108.20
46	BX	10	ARG	NE-CZ-NH1	6.83	123.71	120.30
54	BA	1081	U	O4'-C1'-N1	6.83	113.66	108.20
21	AA	1201	A	O4'-C1'-N9	6.83	113.66	108.20
54	BA	1772	A	C4-C5-C6	-6.83	113.59	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2374	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	470	C	N3-C2-O2	-6.82	117.12	121.90
21	AA	1283	U	N3-C2-O2	-6.82	117.42	122.20
21	AA	1412	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	142	A	O4'-C1'-N9	6.82	113.66	108.20
54	BA	1278	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	2238	G	N1-C6-O6	-6.82	115.81	119.90
21	AA	189	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1462	C	N3-C2-O2	-6.82	117.12	121.90
24	A3	77	A	C5-C6-N1	6.82	121.11	117.70
54	BA	671	C	N3-C2-O2	-6.82	117.12	121.90
21	AA	719	C	N3-C2-O2	-6.82	117.13	121.90
51	B2	28	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	817	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	928	A	C5-C6-N1	6.82	121.11	117.70
21	AA	177	G	N3-C4-C5	-6.82	125.19	128.60
21	AA	969	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1117	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	318	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	1269	A	C4-C5-C6	-6.82	113.59	117.00
37	BO	102	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	309	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	1793	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	374	A	N1-C6-N6	-6.81	114.51	118.60
49	B0	39	ARG	NE-CZ-NH1	6.81	123.71	120.30
54	BA	1270	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	451	A	C5-C6-N1	6.81	121.11	117.70
21	AA	694	A	C5-C6-N1	6.81	121.11	117.70
21	AA	1469	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	1363	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	142	A	C5-C6-N1	6.81	121.11	117.70
54	BA	2090	A	C5-C6-N1	6.81	121.10	117.70
54	BA	2706	A	C5-C6-N1	6.81	121.11	117.70
54	BA	2868	A	C5-C6-N1	6.81	121.11	117.70
21	AA	978	A	C5-C6-N1	6.81	121.10	117.70
54	BA	1591	A	C4-C5-C6	-6.81	113.60	117.00
54	BA	497	A	C4-C5-C6	-6.81	113.60	117.00
54	BA	2095	A	N1-C6-N6	-6.81	114.52	118.60
54	BA	975	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2267	A	C5-C6-N1	6.80	121.10	117.70
21	AA	194	C	N1-C2-O2	6.80	122.98	118.90
21	AA	1036	A	N1-C6-N6	-6.80	114.52	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	77	A	O4'-C1'-N9	6.80	113.64	108.20
21	AA	172	A	C5-C6-N1	6.80	121.10	117.70
21	AA	315	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	203	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1088	A	O4'-C1'-N9	6.80	113.64	108.20
21	AA	303	A	N1-C6-N6	-6.80	114.52	118.60
21	AA	502	A	C5-C6-N1	6.80	121.10	117.70
54	BA	817	C	O4'-C1'-N1	6.80	113.64	108.20
54	BA	918	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1772	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2887	A	N1-C6-N6	-6.80	114.52	118.60
55	BB	39	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1092	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	352	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	511	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	1493	A	O4'-C1'-N9	6.80	113.64	108.20
54	BA	2757	A	C5-C6-N1	6.80	121.10	117.70
55	BB	34	A	C5-C6-N1	6.79	121.10	117.70
21	AA	311	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	590	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	2054	A	C5-C6-N1	6.79	121.10	117.70
21	AA	620	C	N3-C2-O2	-6.79	117.14	121.90
21	AA	741	G	N3-C2-N2	-6.79	115.15	119.90
21	AA	1287	A	C4-C5-C6	-6.79	113.61	117.00
24	A3	62	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	886	A	C5-C6-N1	6.79	121.09	117.70
54	BA	1413	A	C5-C6-N1	6.79	121.10	117.70
54	BA	2037	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	54	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	288	A	C5-C6-N1	6.79	121.09	117.70
21	AA	1427	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	514	A	C5-C6-N1	6.79	121.09	117.70
54	BA	1293	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	1346	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	275	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	572	A	C5-C6-N1	6.79	121.09	117.70
54	BA	2734	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	1329	A	C4-C5-C6	-6.79	113.61	117.00
22	A1	23	A	C4-C5-C6	-6.79	113.61	117.00
22	A1	41	A	C5-C6-N1	6.79	121.09	117.70
54	BA	556	A	C5-C6-N1	6.79	121.09	117.70
54	BA	742	A	C4-C5-C6	-6.79	113.61	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2556	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	389	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	764	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	1508	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2738	A	C5-C6-N1	6.78	121.09	117.70
21	AA	32	A	C5-C6-N1	6.78	121.09	117.70
54	BA	74	A	O4'-C1'-N9	6.78	113.62	108.20
54	BA	1913	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2513	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	792	A	C5-C6-N1	6.78	121.09	117.70
21	AA	923	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1280	A	C1'-O4'-C4'	-6.78	104.47	109.90
54	BA	1039	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1169	A	C5-C6-N1	6.78	121.09	117.70
54	BA	689	A	C5-C6-N1	6.78	121.09	117.70
29	BG	148	ARG	NE-CZ-NH1	6.78	123.69	120.30
21	AA	949	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	457	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	1446	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	1578	U	O4'-C1'-N1	6.78	113.62	108.20
54	BA	94	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	391	A	N1-C6-N6	-6.77	114.54	118.60
54	BA	1096	A	C5-C6-N1	6.77	121.09	117.70
21	AA	414	A	N1-C6-N6	-6.77	114.54	118.60
21	AA	535	A	C5-C6-N1	6.77	121.09	117.70
21	AA	946	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	501	A	C5-C6-N1	6.77	121.09	117.70
10	AK	127	ARG	NE-CZ-NH1	6.77	123.69	120.30
11	AL	98	ARG	NE-CZ-NH1	6.77	123.69	120.30
54	BA	151	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	574	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1678	A	C4-C5-C6	-6.77	113.62	117.00
54	BA	1639	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1001	A	C5-C6-N1	6.76	121.08	117.70
54	BA	2013	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	2461	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1059	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	175	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	553	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	630	A	C5-C6-N1	6.76	121.08	117.70
54	BA	342	A	C5-C6-N1	6.76	121.08	117.70
54	BA	844	A	C5-C6-N1	6.76	121.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1039	A	N1-C6-N6	-6.76	114.55	118.60
54	BA	2418	A	C5-C6-N1	6.76	121.08	117.70
54	BA	402	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1320	C	N1-C2-O2	6.76	122.95	118.90
54	BA	69	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	550	C	N1-C2-O2	6.76	122.95	118.90
54	BA	1932	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	2539	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	979	A	N1-C6-N6	-6.75	114.55	118.60
54	BA	1322	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1347	A	C5-C6-N1	6.75	121.08	117.70
54	BA	156	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	2088	A	O4'-C1'-N9	6.75	113.60	108.20
21	AA	1136	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	1256	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	5	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	1498	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	1590	A	C5-C6-N1	6.75	121.08	117.70
21	AA	28	A	C5-C6-N1	6.75	121.08	117.70
54	BA	28	A	C5-C6-N1	6.75	121.08	117.70
54	BA	251	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	441	A	C5-C6-N1	6.75	121.07	117.70
21	AA	676	A	C5-C6-N1	6.75	121.07	117.70
54	BA	2378	A	C5-C6-N1	6.75	121.07	117.70
43	BU	5	ARG	NE-CZ-NH1	6.75	123.67	120.30
54	BA	1650	A	C5-C6-N1	6.75	121.07	117.70
21	AA	181	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1503	A	N1-C6-N6	-6.74	114.56	118.60
54	BA	1028	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1804	C	N3-C2-O2	-6.74	117.18	121.90
51	B2	34	ARG	NE-CZ-NH2	-6.74	116.93	120.30
54	BA	982	C	O4'-C1'-N1	6.74	113.59	108.20
54	BA	1241	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2506	U	O4'-C1'-N1	6.74	113.59	108.20
54	BA	1614	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1111	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1322	C	N3-C2-O2	-6.74	117.19	121.90
54	BA	676	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2033	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2704	C	N3-C2-O2	-6.74	117.19	121.90
21	AA	1411	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1321	A	N1-C6-N6	-6.73	114.56	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2313	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2382	G	O4'-C1'-N9	6.73	113.59	108.20
21	AA	298	A	C4-C5-C6	-6.73	113.63	117.00
21	AA	518	C	N3-C2-O2	-6.73	117.19	121.90
31	BI	133	ARG	NE-CZ-NH1	6.73	123.67	120.30
54	BA	2326	C	N1-C2-O2	6.73	122.94	118.90
21	AA	1152	A	C5-C6-N1	6.73	121.06	117.70
21	AA	1197	A	C4-C5-C6	-6.73	113.64	117.00
21	AA	1251	A	C5-C6-N1	6.73	121.07	117.70
54	BA	322	A	C5-C6-N1	6.73	121.06	117.70
54	BA	251	A	C5-C6-N1	6.73	121.06	117.70
55	BB	60	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	1012	A	N1-C6-N6	-6.73	114.56	118.60
21	AA	1306	A	C5-C6-N1	6.73	121.06	117.70
54	BA	42	A	C5-C6-N1	6.73	121.06	117.70
54	BA	300	A	C5-C6-N1	6.73	121.06	117.70
54	BA	1376	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	330	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	2205	A	C5-C6-N1	6.72	121.06	117.70
54	BA	675	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	1786	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1912	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2268	A	C5-C6-N1	6.72	121.06	117.70
21	AA	675	A	C5-C6-N1	6.72	121.06	117.70
54	BA	592	A	C5-C6-N1	6.72	121.06	117.70
13	AN	9	ARG	NE-CZ-NH1	6.72	123.66	120.30
24	A3	44	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1816	C	N3-C2-O2	-6.72	117.20	121.90
14	AO	16	ARG	NE-CZ-NH2	-6.72	116.94	120.30
21	AA	687	A	C5-C6-N1	6.72	121.06	117.70
54	BA	229	C	O4'-C1'-N1	6.72	113.57	108.20
54	BA	415	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1321	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1757	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1677	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1894	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	2248	C	N3-C2-O2	-6.71	117.20	121.90
1	AB	94	ARG	NE-CZ-NH1	6.71	123.66	120.30
54	BA	1591	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1637	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1801	A	C5-C6-N1	6.71	121.06	117.70
21	AA	614	C	N3-C2-O2	-6.71	117.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	816	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1819	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2426	A	C5-C6-N1	6.71	121.05	117.70
21	AA	246	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	533	A	N1-C6-N6	-6.71	114.58	118.60
22	A1	71	C	N3-C2-O2	-6.71	117.21	121.90
41	BS	92	ARG	NE-CZ-NH1	6.71	123.65	120.30
54	BA	730	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	1550	C	N3-C2-O2	-6.71	117.21	121.90
54	BA	2705	A	N1-C6-N6	-6.71	114.58	118.60
54	BA	161	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	1575	C	N3-C2-O2	-6.71	117.21	121.90
21	AA	1402	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1691	C	N3-C2-O2	-6.70	117.21	121.90
35	BM	114	ARG	NE-CZ-NH2	-6.70	116.95	120.30
21	AA	267	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	471	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	515	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2060	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2565	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1359	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1838	C	O4'-C1'-N1	6.70	113.56	108.20
54	BA	2042	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1414	C	O4'-C1'-N1	6.70	113.56	108.20
21	AA	264	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	1299	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	199	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	244	A	C5-C6-N1	6.70	121.05	117.70
54	BA	944	C	O4'-C1'-N1	6.70	113.56	108.20
54	BA	1214	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	1590	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1597	A	C4-C5-C6	-6.70	113.65	117.00
28	BF	149	ARG	NE-CZ-NH1	6.69	123.65	120.30
54	BA	1385	A	C5-C6-N1	6.69	121.05	117.70
54	BA	2153	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2717	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	98	A	C5-C6-N1	6.69	121.05	117.70
21	AA	784	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1502	A	C5-C6-N1	6.69	121.05	117.70
21	AA	779	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	213	A	C5-C6-N1	6.69	121.04	117.70
54	BA	1477	A	C5-C6-N1	6.69	121.05	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	602	A	C5-C6-N1	6.69	121.04	117.70
54	BA	432	A	C5-C6-N1	6.69	121.04	117.70
54	BA	1685	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2600	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	782	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	807	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	2463	C	N3-C2-O2	-6.69	117.22	121.90
55	BB	90	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	1739	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1920	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	613	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	2858	C	N1-C2-O2	6.68	122.91	118.90
21	AA	704	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1551	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	2824	C	O4'-C1'-N1	6.68	113.54	108.20
8	AI	94	ARG	NE-CZ-NH1	6.67	123.64	120.30
54	BA	761	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	1625	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1686	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2632	A	C5-C6-N1	6.67	121.04	117.70
21	AA	282	A	C5-C6-N1	6.67	121.04	117.70
21	AA	753	A	P-O3'-C3'	6.67	127.71	119.70
38	BP	88	ARG	NE-CZ-NH1	6.67	123.64	120.30
54	BA	876	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2042	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	1130	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	900	A	C5-C6-N1	6.67	121.04	117.70
54	BA	181	A	C5-C6-N1	6.67	121.03	117.70
6	AG	3	ARG	NE-CZ-NH1	6.67	123.64	120.30
21	AA	199	A	C5-C6-N1	6.67	121.03	117.70
54	BA	631	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	804	A	C5-C6-N1	6.67	121.03	117.70
54	BA	1194	A	C5-C6-N1	6.67	121.03	117.70
21	AA	74	A	C5-C6-N1	6.67	121.03	117.70
21	AA	1400	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1504	A	C5-C6-N1	6.67	121.03	117.70
54	BA	936	A	C1'-O4'-C4'	-6.67	104.57	109.90
54	BA	2008	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2058	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2183	A	C5-C6-N1	6.67	121.03	117.70
21	AA	1396	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1260	A	C5-C6-N1	6.66	121.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	335	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	655	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1393	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1584	U	N3-C2-O2	-6.66	117.54	122.20
15	AP	70	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	1534	A	C1'-O4'-C4'	-6.66	104.57	109.90
54	BA	517	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1565	C	O4'-C1'-N1	6.66	113.53	108.20
21	AA	968	A	O4'-C1'-N9	6.66	113.53	108.20
54	BA	2071	A	C5-C6-N1	6.66	121.03	117.70
55	BB	36	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1152	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2264	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1336	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	2761	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	2540	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	215	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	1201	A	C5-C6-N1	6.65	121.03	117.70
21	AA	440	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	1288	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	466	A	O4'-C1'-N9	6.65	113.52	108.20
21	AA	58	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	1022	A	C5-C6-N1	6.64	121.02	117.70
35	BM	16	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	443	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1348	C	O4'-C1'-N1	6.64	113.51	108.20
54	BA	1734	G	O4'-C1'-N9	6.64	113.51	108.20
54	BA	2114	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	848	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1312	U	P-O3'-C3'	6.64	127.67	119.70
21	AA	34	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	1000	A	C5-C6-N1	6.64	121.02	117.70
21	AA	1130	A	N1-C6-N6	-6.64	114.62	118.60
54	BA	734	A	C5-C6-N1	6.64	121.02	117.70
21	AA	80	A	C4-C5-C6	-6.63	113.68	117.00
22	A1	60	C	N3-C2-O2	-6.63	117.25	121.90
54	BA	1732	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	2821	A	N1-C6-N6	-6.63	114.62	118.60
55	BB	8	C	N3-C2-O2	-6.63	117.25	121.90
21	AA	482	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	2404	U	O4'-C1'-N1	6.63	113.51	108.20
21	AA	53	A	C5-C6-N1	6.63	121.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	403	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	468	A	C5-C6-N1	6.63	121.02	117.70
21	AA	744	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	1513	A	C5-C6-N1	6.63	121.02	117.70
54	BA	352	A	C5-C6-N1	6.63	121.02	117.70
54	BA	2119	A	C5-C6-N1	6.63	121.02	117.70
54	BA	2265	U	O4'-C1'-N1	6.63	113.50	108.20
21	AA	1339	A	C5-C6-N1	6.63	121.02	117.70
9	AJ	45	ARG	NE-CZ-NH1	6.63	123.61	120.30
54	BA	727	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	1762	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	2476	A	C5-C6-N1	6.63	121.01	117.70
21	AA	280	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	2432	A	C1'-O4'-C4'	-6.63	104.60	109.90
6	AG	69	ARG	NE-CZ-NH1	6.62	123.61	120.30
54	BA	2101	A	C5-C6-N1	6.62	121.01	117.70
21	AA	816	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2134	A	C5-C6-N1	6.62	121.01	117.70
55	BB	115	A	C5-C6-N1	6.62	121.01	117.70
8	AI	98	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	547	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	1520	C	N3-C2-O2	-6.62	117.27	121.90
47	BY	52	ARG	NE-CZ-NH1	6.62	123.61	120.30
55	BB	3	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	833	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1431	A	C5-C6-N1	6.62	121.01	117.70
54	BA	637	A	C5-C6-N1	6.62	121.01	117.70
54	BA	861	A	C5-C6-N1	6.62	121.01	117.70
54	BA	998	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	299	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	1597	A	N1-C6-N6	-6.61	114.63	118.60
54	BA	1630	A	C5-C6-N1	6.61	121.01	117.70
21	AA	1285	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	936	A	O4'-C1'-N9	6.61	113.49	108.20
54	BA	2045	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1079	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	2453	A	N1-C6-N6	-6.61	114.63	118.60
54	BA	1090	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	752	A	C5-C6-N1	6.61	121.00	117.70
55	BB	94	A	C5-C6-N1	6.61	121.00	117.70
54	BA	765	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	1304	A	C4-C5-C6	-6.61	113.70	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2139	U	O4'-C1'-N1	6.61	113.48	108.20
54	BA	2270	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	918	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	439	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1877	A	C5-C6-N1	6.60	121.00	117.70
1	AB	107	ARG	NE-CZ-NH1	6.60	123.60	120.30
54	BA	820	A	C5-C6-N1	6.60	121.00	117.70
54	BA	2054	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	2778	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	2829	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	231	U	O4'-C1'-N1	6.60	113.48	108.20
55	BB	78	A	N1-C6-N6	-6.60	114.64	118.60
21	AA	19	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	459	A	C5-C6-N1	6.60	121.00	117.70
21	AA	642	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	1271	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	320	A	C5-C6-N1	6.60	121.00	117.70
54	BA	693	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1387	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1978	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	119	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	920	A	C5-C6-N1	6.60	121.00	117.70
54	BA	2420	C	N3-C2-O2	-6.60	117.28	121.90
41	BS	18	ARG	NE-CZ-NH1	6.60	123.60	120.30
21	AA	274	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	1492	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	2620	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	1194	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	401	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	419	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	345	A	C5-C6-N1	6.59	121.00	117.70
54	BA	905	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	505	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	917	A	C5-C6-N1	6.59	121.00	117.70
54	BA	1260	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1595	C	N3-C2-O2	-6.59	117.29	121.90
27	BE	44	ARG	NE-CZ-NH1	6.59	123.59	120.30
37	BO	94	ARG	NE-CZ-NH1	6.59	123.59	120.30
21	AA	456	A	C5-C6-N1	6.59	120.99	117.70
26	BD	124	ARG	CD-NE-CZ	6.59	132.82	123.60
41	BS	25	ARG	NE-CZ-NH1	6.59	123.59	120.30
54	BA	1306	C	N3-C2-O2	-6.59	117.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AH	76	ARG	NE-CZ-NH1	6.58	123.59	120.30
35	BM	55	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	538	A	C5-C6-N1	6.58	120.99	117.70
54	BA	751	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1453	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	1480	C	N3-C2-O2	-6.58	117.29	121.90
55	BB	108	A	C5-C6-N1	6.58	120.99	117.70
21	AA	143	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1423	G	N1-C6-O6	-6.58	115.95	119.90
54	BA	1302	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1704	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	651	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1990	C	N3-C2-O2	-6.58	117.30	121.90
24	A3	66	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	2765	A	N1-C6-N6	-6.58	114.65	118.60
21	AA	673	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	676	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1070	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2679	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	452	A	C5-C6-N1	6.57	120.99	117.70
21	AA	1223	C	N3-C2-O2	-6.57	117.30	121.90
24	A3	26	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	16	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	660	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	800	A	C5-C6-N1	6.57	120.99	117.70
54	BA	1789	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	2062	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	2727	A	C4-C5-C6	-6.57	113.71	117.00
10	AK	92	ARG	NE-CZ-NH1	6.57	123.59	120.30
21	AA	460	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	1063	G	C1'-O4'-C4'	-6.57	104.64	109.90
54	BA	1634	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	2342	C	N1-C2-O2	6.57	122.84	118.90
54	BA	2471	A	C5-C6-N1	6.57	120.99	117.70
21	AA	1375	A	C5-C6-N1	6.57	120.98	117.70
54	BA	1785	A	C5-C6-N1	6.57	120.98	117.70
21	AA	1359	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	1480	A	C5-C6-N1	6.57	120.98	117.70
54	BA	750	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	2247	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2284	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	401	A	C4-C5-C6	-6.56	113.72	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	192	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2161	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2514	U	O4'-C1'-N1	6.56	113.45	108.20
19	AT	23	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	1615	C	N3-C2-O2	-6.56	117.31	121.90
10	AK	97	ARG	NE-CZ-NH1	6.56	123.58	120.30
21	AA	40	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	461	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	753	A	C5-C6-N1	6.56	120.98	117.70
54	BA	129	C	O4'-C1'-N1	6.56	113.45	108.20
54	BA	575	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1103	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1196	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2150	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2564	A	C5-C6-N1	6.56	120.98	117.70
21	AA	817	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	919	A	O4'-C1'-N9	6.56	113.45	108.20
29	BG	93	TYR	CB-CG-CD1	6.56	124.94	121.00
54	BA	795	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1213	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	1635	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2676	C	N1-C2-O2	6.56	122.83	118.90
54	BA	128	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	503	A	C4-C5-C6	-6.55	113.72	117.00
26	BD	128	ARG	NE-CZ-NH1	6.55	123.58	120.30
54	BA	1385	A	O4'-C1'-N9	6.55	113.44	108.20
21	AA	160	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1080	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1522	A	O4'-C1'-N9	6.55	113.44	108.20
54	BA	1676	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1893	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	2421	G	N3-C2-N2	-6.55	115.31	119.90
54	BA	2753	A	C4-C5-C6	-6.55	113.72	117.00
1	AB	136	ARG	NE-CZ-NH1	6.55	123.58	120.30
54	BA	1472	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	2261	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	48	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	1392	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	2158	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	781	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	1145	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	1830	C	N3-C2-O2	-6.55	117.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1169	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	116	A	N1-C6-N6	-6.54	114.67	118.60
21	AA	807	A	C5-C6-N1	6.54	120.97	117.70
54	BA	493	G	O4'-C1'-N9	6.54	113.44	108.20
54	BA	654	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	174	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	624	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	2080	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2380	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	2579	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1938	A	O4'-C1'-N9	6.54	113.43	108.20
21	AA	1245	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1322	A	N1-C6-N6	-6.54	114.68	118.60
54	BA	1961	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	2159	G	N1-C6-O6	-6.54	115.98	119.90
54	BA	2888	C	N1-C2-O2	6.54	122.82	118.90
54	BA	1512	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1569	A	C5-C6-N1	6.54	120.97	117.70
21	AA	536	C	N3-C2-O2	-6.54	117.33	121.90
21	AA	1109	C	N1-C2-O2	6.54	122.82	118.90
22	A1	36	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	603	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2286	G	N3-C2-N2	-6.54	115.33	119.90
2	AC	10	ARG	NE-CZ-NH1	6.53	123.57	120.30
21	AA	696	A	C5-C6-N1	6.53	120.97	117.70
21	AA	768	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	2577	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	2660	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	1872	A	C5-C6-N1	6.53	120.97	117.70
54	BA	2241	A	C5-C6-N1	6.53	120.97	117.70
54	BA	2717	C	O4'-C1'-N1	6.53	113.42	108.20
21	AA	749	A	C4-C5-C6	-6.53	113.73	117.00
21	AA	1216	A	C4-C5-C6	-6.53	113.73	117.00
29	BG	152	ARG	NE-CZ-NH1	6.53	123.57	120.30
39	BQ	12	ARG	NE-CZ-NH1	6.53	123.56	120.30
39	BQ	32	ARG	NE-CZ-NH1	6.53	123.57	120.30
54	BA	14	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	191	A	C5-C6-N1	6.53	120.97	117.70
54	BA	281	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	282	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	1151	A	C5-C6-N1	6.53	120.97	117.70
54	BA	2005	A	C4-C5-C6	-6.53	113.73	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2602	A	C5-C6-N1	6.53	120.97	117.70
21	AA	309	A	C4-C5-C6	-6.53	113.74	117.00
22	A1	16	C	O4'-C1'-N1	6.53	113.42	108.20
54	BA	269	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	248	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	787	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1803	A	C5-C6-N1	6.53	120.96	117.70
54	BA	1999	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	2013	A	C5-C6-N1	6.53	120.96	117.70
24	A3	68	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	344	A	C5-C6-N1	6.53	120.96	117.70
54	BA	677	A	C5-C6-N1	6.53	120.96	117.70
54	BA	716	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1011	G	O4'-C1'-N9	6.53	113.42	108.20
54	BA	1264	A	N1-C6-N6	-6.53	114.69	118.60
54	BA	1963	U	O4'-C1'-N1	6.53	113.42	108.20
54	BA	2781	A	C5-C6-N1	6.53	120.96	117.70
21	AA	262	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	334	C	N3-C2-O2	-6.52	117.33	121.90
24	A3	11	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1254	A	C5-C6-N1	6.52	120.96	117.70
54	BA	2089	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	573	A	C5-C6-N1	6.52	120.96	117.70
22	A1	62	C	N3-C2-O2	-6.52	117.33	121.90
22	A1	65	C	N3-C2-O2	-6.52	117.33	121.90
33	BK	105	ARG	NE-CZ-NH1	6.52	123.56	120.30
54	BA	320	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	575	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	737	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	2469	A	N1-C6-N6	-6.52	114.69	118.60
54	BA	2781	A	C4-C5-C6	-6.52	113.74	117.00
55	BB	109	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1370	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	498	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	631	C	N1-C2-O2	6.52	122.81	118.90
21	AA	1399	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	2174	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	1210	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	256	A	N1-C6-N6	-6.52	114.69	118.60
54	BA	2199	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	1332	A	C5-C6-N1	6.51	120.96	117.70
21	AA	1209	C	N3-C2-O2	-6.51	117.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1349	C	O4'-C1'-N1	6.51	113.41	108.20
54	BA	2009	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	867	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1573	G	O4'-C1'-N9	6.51	113.41	108.20
54	BA	2758	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	1051	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	44	A	C5-C6-N1	6.51	120.95	117.70
54	BA	294	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1246	A	C5-C6-N1	6.51	120.95	117.70
54	BA	1650	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	378	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1744	A	C5-C6-N1	6.51	120.95	117.70
21	AA	501	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	982	C	N1-C2-O2	6.51	122.80	118.90
54	BA	1788	C	N3-C2-O2	-6.51	117.35	121.90
54	BA	1848	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	2654	A	C5-C6-N1	6.51	120.95	117.70
54	BA	1053	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2006	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2037	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2101	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	861	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1583	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2675	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2820	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	839	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	962	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	602	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1570	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2088	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2515	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	8	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	161	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1369	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	626	A	C5-C6-N1	6.50	120.95	117.70
54	BA	673	C	O4'-C1'-N1	6.50	113.40	108.20
21	AA	1262	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1129	A	C5-C6-N1	6.50	120.95	117.70
21	AA	1282	C	N3-C2-O2	-6.50	117.35	121.90
39	BQ	2	ARG	NE-CZ-NH2	-6.50	117.05	120.30
54	BA	911	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1114	C	N3-C2-O2	-6.49	117.35	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1302	C	N3-C2-O2	-6.49	117.35	121.90
54	BA	1268	A	N1-C6-N6	-6.49	114.70	118.60
54	BA	1874	C	N3-C2-O2	-6.49	117.35	121.90
54	BA	2213	U	C1'-O4'-C4'	-6.49	104.70	109.90
54	BA	2606	C	N3-C2-O2	-6.49	117.35	121.90
21	AA	110	C	N3-C2-O2	-6.49	117.36	121.90
38	BP	87	ARG	NE-CZ-NH2	-6.49	117.05	120.30
54	BA	6	A	C5-C6-N1	6.49	120.95	117.70
54	BA	41	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1722	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1771	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	135	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	173	U	N3-C2-O2	-6.49	117.66	122.20
21	AA	958	A	C4-C5-C6	-6.49	113.76	117.00
21	AA	1344	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	165	A	C5-C6-N1	6.49	120.94	117.70
54	BA	1307	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	1876	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	2171	A	N1-C6-N6	-6.49	114.71	118.60
21	AA	600	A	C4-C5-C6	-6.49	113.76	117.00
42	BT	73	ARG	NE-CZ-NH1	6.49	123.54	120.30
47	BY	29	ARG	NE-CZ-NH1	6.49	123.54	120.30
54	BA	438	G	N1-C6-O6	-6.49	116.01	119.90
21	AA	1518	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	140	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2785	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	995	C	N3-C2-O2	-6.48	117.36	121.90
29	BG	34	ARG	NE-CZ-NH1	6.48	123.54	120.30
21	AA	155	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1368	A	C5-C6-N1	6.48	120.94	117.70
54	BA	165	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	262	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	627	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1143	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2611	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1453	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	752	G	O4'-C1'-N9	6.48	113.38	108.20
53	B4	24	ARG	NE-CZ-NH1	6.48	123.54	120.30
54	BA	2456	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	1046	A	N1-C6-N6	-6.48	114.71	118.60
21	AA	1306	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	145	C	N3-C2-O2	-6.48	117.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1871	A	N1-C6-N6	-6.48	114.72	118.60
54	BA	1899	A	N1-C6-N6	-6.48	114.71	118.60
54	BA	2654	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	67	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1325	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	147	C	O4'-C1'-N1	6.47	113.38	108.20
54	BA	337	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	789	A	C5-C6-N1	6.47	120.94	117.70
54	BA	1367	A	C5-C6-N1	6.47	120.94	117.70
54	BA	2461	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	2746	U	O4'-C1'-N1	6.47	113.38	108.20
54	BA	2901	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	880	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1157	A	C5-C6-N1	6.47	120.94	117.70
54	BA	111	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	176	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	910	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1303	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1045	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	720	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1314	C	N3-C2-O2	-6.47	117.37	121.90
24	A3	1	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1885	A	C5-C6-N1	6.47	120.94	117.70
54	BA	2547	A	C5-C6-N1	6.47	120.94	117.70
21	AA	130	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	668	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	163	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	340	A	C5-C6-N1	6.47	120.93	117.70
54	BA	502	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	732	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2196	C	O4'-C1'-N1	6.47	113.37	108.20
54	BA	2559	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	475	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1774	C	N1-C2-O2	6.46	122.78	118.90
54	BA	2480	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2880	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	933	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	2164	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2115	G	O4'-C1'-N9	6.46	113.37	108.20
54	BA	2314	A	C5-C6-N1	6.46	120.93	117.70
11	AL	35	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	1433	A	C5-C6-N1	6.46	120.93	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1554	U	N3-C2-O2	-6.46	117.68	122.20
54	BA	1986	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2813	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	854	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2199	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2366	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	2699	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2814	A	N1-C6-N6	-6.46	114.72	118.60
4	AE	67	ARG	NE-CZ-NH1	6.46	123.53	120.30
18	AS	35	ARG	NE-CZ-NH1	6.46	123.53	120.30
20	AU	17	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	618	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	831	A	C5-C6-N1	6.46	120.93	117.70
54	BA	302	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1616	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1958	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2126	A	N1-C6-N6	-6.46	114.73	118.60
54	BA	2744	G	O4'-C1'-N9	6.46	113.36	108.20
55	BB	66	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	508	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	19	A	C5-C6-N1	6.45	120.93	117.70
21	AA	1054	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	1069	C	N3-C2-O2	-6.45	117.38	121.90
40	BR	68	ARG	NE-CZ-NH1	6.45	123.53	120.30
54	BA	587	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	1783	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	2560	A	N1-C6-N6	-6.45	114.73	118.60
21	AA	1328	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	1534	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1881	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	2558	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	204	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	921	C	N3-C2-O2	-6.45	117.39	121.90
55	BB	31	C	N3-C2-O2	-6.45	117.39	121.90
46	BX	44	ARG	NE-CZ-NH1	6.45	123.52	120.30
21	AA	223	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	1380	U	O4'-C1'-N1	6.45	113.36	108.20
54	BA	1111	A	C5-C6-N1	6.45	120.92	117.70
54	BA	1328	A	C5-C6-N1	6.45	120.92	117.70
55	BB	39	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	196	A	C5-C6-N1	6.44	120.92	117.70
21	AA	335	C	N3-C2-O2	-6.44	117.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	460	A	C5-C6-N1	6.44	120.92	117.70
21	AA	726	C	N3-C2-O2	-6.44	117.39	121.90
36	BN	17	ARG	NE-CZ-NH1	6.44	123.52	120.30
54	BA	509	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	452	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	648	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	201	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	169	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2530	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	1081	A	C4-C5-C6	-6.43	113.78	117.00
44	BV	21	ARG	NE-CZ-NH1	-6.43	117.08	120.30
54	BA	1305	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2335	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	97	C	O4'-C1'-N1	6.43	113.35	108.20
54	BA	2845	U	O4'-C1'-N1	6.43	113.34	108.20
21	AA	222	C	N3-C2-O2	-6.43	117.40	121.90
22	A1	48	C	N3-C2-O2	-6.43	117.40	121.90
36	BN	90	ARG	NE-CZ-NH1	6.43	123.51	120.30
54	BA	1349	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2748	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	10	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	900	A	C5-C6-N1	6.43	120.91	117.70
24	A3	73	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	1679	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	1746	A	C5-C6-N1	6.43	120.91	117.70
54	BA	2278	A	C5-C6-N1	6.43	120.91	117.70
21	AA	1404	C	N3-C2-O2	-6.42	117.40	121.90
22	A1	59	U	N3-C2-O2	-6.42	117.70	122.20
54	BA	176	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1676	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	1905	C	N3-C2-O2	-6.42	117.40	121.90
54	BA	1298	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	878	A	C5-C6-N1	6.42	120.91	117.70
42	BT	6	ARG	NE-CZ-NH1	-6.42	117.09	120.30
54	BA	470	A	C5-C6-N1	6.42	120.91	117.70
54	BA	792	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	47	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1890	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2072	C	O4'-C1'-N1	6.42	113.34	108.20
21	AA	1208	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	382	A	C5-C6-N1	6.42	120.91	117.70
54	BA	523	C	N3-C2-O2	-6.42	117.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	52	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	621	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1081	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	790	U	N3-C2-O2	-6.42	117.71	122.20
54	BA	909	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1178	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1251	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	2800	A	C5-C6-N1	6.42	120.91	117.70
21	AA	487	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	522	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1477	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	395	U	O4'-C1'-N1	6.41	113.33	108.20
54	BA	414	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	108	G	O4'-C1'-N9	6.41	113.33	108.20
21	AA	372	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1046	A	O4'-C1'-N9	6.41	113.33	108.20
54	BA	1618	A	C5-C6-N1	6.41	120.91	117.70
54	BA	2322	A	C4-C5-C6	-6.41	113.79	117.00
21	AA	1249	C	N3-C2-O2	-6.41	117.41	121.90
55	BB	37	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	234	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	708	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	1349	A	C5-C6-N1	6.41	120.91	117.70
54	BA	310	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	739	A	C5-C6-N1	6.41	120.90	117.70
54	BA	945	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2328	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	205	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	545	C	N3-C2-O2	-6.41	117.42	121.90
31	BI	126	ARG	NE-CZ-NH1	6.41	123.50	120.30
4	AE	92	ARG	NE-CZ-NH1	6.41	123.50	120.30
21	AA	162	A	C5-C6-N1	6.41	120.90	117.70
21	AA	186	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	866	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2366	A	C5-C6-N1	6.41	120.90	117.70
54	BA	2538	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	2758	A	C5-C6-N1	6.41	120.90	117.70
21	AA	1046	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1226	A	C4-C5-C6	-6.40	113.80	117.00
14	AO	57	ARG	NE-CZ-NH1	6.40	123.50	120.30
21	AA	1037	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	1141	C	N3-C2-O2	-6.40	117.42	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1246	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1564	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	316	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1548	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2317	A	O4'-C1'-N9	6.40	113.32	108.20
21	AA	1423	G	O4'-C1'-N9	6.40	113.32	108.20
40	BR	90	ARG	NE-CZ-NH1	6.40	123.50	120.30
54	BA	2681	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	1384	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1032	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	86	G	O4'-C1'-N9	6.39	113.31	108.20
54	BA	429	A	C5-C6-N1	6.39	120.90	117.70
54	BA	623	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	1780	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	2030	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	2191	A	C5-C6-N1	6.39	120.90	117.70
54	BA	2755	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	81	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	695	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	1429	A	C4-C5-C6	-6.39	113.80	117.00
34	BL	33	ARG	NE-CZ-NH1	6.39	123.50	120.30
54	BA	2725	A	N1-C6-N6	-6.39	114.76	118.60
22	A1	27	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	274	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	831	A	N1-C6-N6	-6.39	114.77	118.60
21	AA	1510	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1794	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2636	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	634	C	N1-C2-O2	6.39	122.73	118.90
54	BA	1357	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1528	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2662	A	N1-C6-N6	-6.39	114.77	118.60
21	AA	325	A	C4-C5-C6	-6.39	113.81	117.00
21	AA	1421	G	N1-C6-O6	-6.39	116.07	119.90
54	BA	896	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1086	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1420	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	503	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1221	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2448	A	C5-C6-N1	6.38	120.89	117.70
14	AO	62	ARG	NE-CZ-NH2	6.38	123.49	120.30
12	AM	69	ARG	NE-CZ-NH1	6.38	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	191	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	505	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1177	G	O4'-C1'-N9	6.38	113.31	108.20
21	AA	918	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2886	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	716	A	C5-C6-N1	6.38	120.89	117.70
21	AA	1120	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	582	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	607	U	O4'-C1'-N1	6.38	113.30	108.20
54	BA	631	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	957	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	1165	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2320	U	N3-C2-O2	-6.38	117.73	122.20
21	AA	490	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	1363	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	908	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	2175	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	2805	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	696	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	126	A	C5-C6-N1	6.37	120.89	117.70
54	BA	1304	A	C5-C6-N1	6.37	120.89	117.70
54	BA	2001	C	O4'-C1'-N1	6.37	113.30	108.20
21	AA	55	A	C5-C6-N1	6.37	120.89	117.70
21	AA	131	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	368	U	C1'-O4'-C4'	-6.37	104.80	109.90
21	AA	1155	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	1318	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	1352	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	666	A	C5-C6-N1	6.37	120.89	117.70
54	BA	922	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2200	C	O4'-C1'-N1	6.37	113.30	108.20
21	AA	1162	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1219	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2469	A	C5-C6-N1	6.37	120.88	117.70
54	BA	522	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	2589	A	C5-C6-N1	6.37	120.88	117.70
54	BA	2799	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	1795	C	O4'-C1'-N1	6.37	113.29	108.20
54	BA	1928	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	2528	U	O4'-C1'-N1	6.37	113.29	108.20
54	BA	2873	A	C5-C6-N1	6.37	120.88	117.70
12	AM	92	ARG	NE-CZ-NH1	6.36	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	393	C	N3-C2-O2	-6.36	117.44	121.90
21	AA	580	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	1036	A	C4-C5-C6	-6.36	113.82	117.00
24	A3	9	G	O4'-C1'-N9	6.36	113.29	108.20
54	BA	300	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	1278	G	O4'-C1'-N9	6.36	113.29	108.20
21	AA	1448	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1117	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1963	U	N3-C2-O2	-6.36	117.75	122.20
54	BA	2561	U	O4'-C1'-N1	6.36	113.29	108.20
21	AA	271	C	N3-C2-O2	-6.36	117.45	121.90
22	A1	41	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	443	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	609	A	C5-C6-N1	6.36	120.88	117.70
21	AA	1113	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2734	A	O4'-C1'-N9	6.36	113.28	108.20
54	BA	2063	C	N1-C2-N3	6.35	123.65	119.20
54	BA	2288	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	2403	C	O4'-C1'-N1	6.35	113.28	108.20
54	BA	420	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	637	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	1165	A	C5-C6-N1	6.35	120.88	117.70
54	BA	2208	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	1043	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	2716	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	1035	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	242	G	O4'-C1'-N9	6.35	113.28	108.20
54	BA	2840	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	715	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	1080	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	97	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	1046	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	2016	U	O4'-C1'-N1	6.35	113.28	108.20
6	AG	91	ARG	NE-CZ-NH1	6.34	123.47	120.30
21	AA	139	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1805	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	2507	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2752	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	532	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	270	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	357	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	404	A	C5-C6-N1	6.34	120.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	691	C	O4'-C1'-N1	6.34	113.27	108.20
54	BA	1070	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	2646	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	732	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1313	U	N3-C2-O2	-6.34	117.76	122.20
21	AA	1005	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1104	C	N3-C2-O2	-6.34	117.47	121.90
54	BA	2667	C	N3-C2-O2	-6.34	117.47	121.90
54	BA	2733	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1937	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	2291	U	O4'-C1'-N1	6.33	113.27	108.20
54	BA	2566	A	N1-C6-N6	-6.33	114.80	118.60
54	BA	2591	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	671	G	N3-C2-N2	-6.33	115.47	119.90
54	BA	608	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	1335	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1499	A	N1-C6-N6	-6.33	114.80	118.60
54	BA	1005	C	C3'-C2'-C1'	6.33	106.56	101.50
21	AA	689	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1484	C	N3-C2-O2	-6.33	117.47	121.90
22	A1	30	C	N3-C2-O2	-6.33	117.47	121.90
27	BE	114	ARG	NE-CZ-NH1	6.33	123.46	120.30
54	BA	1799	G	P-O3'-C3'	6.33	127.29	119.70
54	BA	2634	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	1020	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	1870	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2258	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2809	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	50	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	539	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	1038	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	486	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	702	U	O4'-C1'-N1	6.33	113.26	108.20
54	BA	767	U	O4'-C1'-N1	6.33	113.26	108.20
54	BA	1088	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	878	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	192	C	N3-C2-O2	-6.32	117.47	121.90
21	AA	217	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	1257	C	N3-C2-O2	-6.32	117.47	121.90
3	AD	69	ARG	NE-CZ-NH1	6.32	123.46	120.30
54	BA	661	A	C4-C5-C6	-6.32	113.84	117.00
55	BB	19	C	N3-C2-O2	-6.32	117.48	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	119	A	C5-C6-N1	6.32	120.86	117.70
21	AA	815	A	C4-C5-C6	-6.32	113.84	117.00
24	A3	29	C	N3-C2-O2	-6.32	117.48	121.90
24	A3	63	C	N3-C2-O2	-6.32	117.48	121.90
50	B1	27	ARG	NE-CZ-NH1	6.32	123.46	120.30
54	BA	207	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2767	C	N3-C2-O2	-6.32	117.48	121.90
9	AJ	72	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	864	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	1275	A	C5-C6-N1	6.32	120.86	117.70
54	BA	127	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1705	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1964	G	N3-C4-C5	-6.32	125.44	128.60
54	BA	2088	A	C5-C6-N1	6.32	120.86	117.70
21	AA	1100	C	N1-C2-O2	6.31	122.69	118.90
54	BA	1175	A	C4-C5-C6	-6.31	113.84	117.00
11	AL	53	ARG	NE-CZ-NH1	6.31	123.46	120.30
15	AP	25	ARG	NE-CZ-NH2	-6.31	117.14	120.30
21	AA	892	A	C5-C6-N1	6.31	120.86	117.70
21	AA	971	G	C1'-O4'-C4'	-6.31	104.85	109.90
21	AA	1236	A	N1-C6-N6	-6.31	114.81	118.60
54	BA	1102	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1147	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1515	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	2774	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	912	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1009	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	2893	A	C5-C6-N1	6.31	120.86	117.70
21	AA	1028	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	183	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	673	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1689	A	C5-C6-N1	6.31	120.85	117.70
54	BA	2059	A	C4-C5-C6	-6.31	113.85	117.00
21	AA	1407	C	N3-C2-O2	-6.31	117.49	121.90
55	BB	115	A	C4-C5-C6	-6.31	113.85	117.00
21	AA	712	A	C4-C5-C6	-6.30	113.85	117.00
22	A1	28	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	37	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	324	A	C5-C6-N1	6.30	120.85	117.70
54	BA	698	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1275	A	C5-C6-N1	6.30	120.85	117.70
21	AA	120	A	C4-C5-C6	-6.30	113.85	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	556	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	193	C	N3-C2-O2	-6.30	117.49	121.90
27	BE	162	ARG	NE-CZ-NH1	6.30	123.45	120.30
54	BA	1057	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2362	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	331	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	987	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2639	A	C5-C6-N1	6.30	120.85	117.70
21	AA	172	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	1191	A	C5-C6-N1	6.30	120.85	117.70
52	B3	29	ARG	NE-CZ-NH2	6.30	123.45	120.30
54	BA	890	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2430	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2635	A	C5-C6-N1	6.30	120.85	117.70
54	BA	118	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	1179	A	C3'-C2'-C1'	6.29	106.53	101.50
21	AA	1180	A	C5-C6-N1	6.29	120.85	117.70
54	BA	2015	A	C5-C6-N1	6.29	120.85	117.70
54	BA	2521	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	736	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	764	A	C5-C6-N1	6.29	120.85	117.70
54	BA	902	C	O4'-C1'-N1	6.29	113.23	108.20
54	BA	63	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	268	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	162	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	233	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	208	C	O4'-C1'-N1	6.29	113.23	108.20
54	BA	1788	C	N1-C2-O2	6.29	122.67	118.90
21	AA	411	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	695	A	N1-C6-N6	-6.29	114.83	118.60
21	AA	876	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	1071	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	478	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	758	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1502	A	C4-C5-C6	-6.29	113.86	117.00
55	BB	29	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	1362	A	C4-C5-C6	-6.28	113.86	117.00
22	A1	69	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2332	C	O4'-C1'-N1	6.28	113.23	108.20
55	BB	27	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1045	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1098	C	N3-C2-O2	-6.28	117.50	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	216	A	C5-C6-N1	6.28	120.84	117.70
54	BA	2762	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	994	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	1011	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	22	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	586	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1469	A	C5-C6-N1	6.28	120.84	117.70
21	AA	23	C	N3-C2-O2	-6.28	117.51	121.90
25	BC	101	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	1269	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1533	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	1755	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2820	A	C5-C6-N1	6.28	120.84	117.70
21	AA	1327	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	477	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	884	U	O4'-C1'-N1	6.28	113.22	108.20
21	AA	640	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	1431	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	2497	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	1153	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1474	U	O4'-C1'-N1	6.27	113.22	108.20
54	BA	27	G	O4'-C1'-N9	6.27	113.22	108.20
54	BA	632	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	2616	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	398	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1275	A	O4'-C1'-N9	6.27	113.22	108.20
54	BA	2476	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	575	G	P-O3'-C3'	6.27	127.22	119.70
21	AA	1044	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	1311	A	C6-C5-N7	6.27	136.69	132.30
21	AA	1398	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	231	A	C5-C6-N1	6.27	120.83	117.70
54	BA	1632	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	573	A	N1-C6-N6	-6.27	114.84	118.60
21	AA	899	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	725	G	N1-C6-O6	-6.26	116.14	119.90
54	BA	867	C	O4'-C1'-N1	6.26	113.21	108.20
56	B5	60	ARG	NE-CZ-NH1	6.26	123.43	120.30
21	AA	738	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	1418	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1694	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1916	A	C4-C5-C6	-6.26	113.87	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	673	A	C5-C6-N1	6.26	120.83	117.70
21	AA	680	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	726	G	O4'-C1'-N9	6.26	113.21	108.20
54	BA	992	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1496	A	C5-C6-N1	6.26	120.83	117.70
54	BA	1626	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1672	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2142	A	N1-C6-N6	-6.26	114.84	118.60
54	BA	2183	A	N1-C6-N6	-6.26	114.84	118.60
54	BA	2503	A	O4'-C1'-N9	6.26	113.21	108.20
54	BA	1274	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	177	G	O4'-C1'-N9	6.26	113.20	108.20
21	AA	356	A	C4-C5-C6	-6.26	113.87	117.00
39	BQ	44	TYR	CB-CG-CD2	-6.26	117.25	121.00
54	BA	1437	C	O4'-C1'-N1	6.26	113.20	108.20
54	BA	2902	C	N1-C2-O2	6.26	122.65	118.90
21	AA	853	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	611	C	N1-C2-O2	6.25	122.65	118.90
21	AA	932	C	P-O3'-C3'	6.25	127.20	119.70
21	AA	1265	C	N3-C2-O2	-6.25	117.52	121.90
23	A2	80	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	991	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	1171	A	C4-C5-C6	-6.25	113.87	117.00
34	BL	41	ARG	NE-CZ-NH1	6.25	123.43	120.30
54	BA	423	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	2658	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	246	A	C5-C6-N1	6.25	120.83	117.70
23	A2	90	U	C1'-O4'-C4'	-6.25	104.90	109.90
54	BA	705	A	C5-C6-N1	6.25	120.83	117.70
54	BA	2078	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	87	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	355	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	794	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1644	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	2439	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	155	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	197	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1214	A	C5-C6-N1	6.25	120.82	117.70
55	BB	38	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	511	C	O4'-C1'-N1	6.24	113.19	108.20
21	AA	349	A	C5-C6-N1	6.24	120.82	117.70
54	BA	60	G	N3-C2-N2	-6.24	115.53	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AM	106	ARG	C-N-CA	6.24	137.30	121.70
21	AA	1324	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	941	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1553	A	C5-C6-N1	6.24	120.82	117.70
55	BB	88	C	N3-C2-O2	-6.24	117.53	121.90
9	AJ	89	ARG	NE-CZ-NH1	6.24	123.42	120.30
54	BA	109	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1152	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	586	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	695	A	C5-C6-N1	6.24	120.82	117.70
54	BA	787	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	523	A	N1-C6-N6	-6.24	114.86	118.60
54	BA	599	A	C5-C6-N1	6.24	120.82	117.70
54	BA	944	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	978	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	666	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2823	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2863	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	327	A	P-O3'-C3'	6.23	127.18	119.70
21	AA	1019	A	C5-C6-N1	6.23	120.82	117.70
54	BA	318	C	O4'-C1'-N1	6.23	113.19	108.20
54	BA	449	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	149	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	932	C	N3-C2-O2	-6.23	117.54	121.90
55	BB	46	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	613	C	N3-C2-O2	-6.23	117.54	121.90
55	BB	46	A	C5-C6-N1	6.23	120.81	117.70
21	AA	228	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	946	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2468	A	C4-C5-C6	-6.23	113.89	117.00
13	AN	90	ARG	NE-CZ-NH1	6.23	123.41	120.30
21	AA	574	A	C5-C6-N1	6.23	120.81	117.70
54	BA	1462	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1101	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	964	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	199	A	C5-C6-N1	6.22	120.81	117.70
54	BA	433	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	748	G	N1-C6-O6	-6.22	116.17	119.90
54	BA	1075	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1151	A	C4-C5-C6	-6.22	113.89	117.00
55	BB	26	C	N1-C2-O2	6.22	122.63	118.90
54	BA	1013	C	N3-C2-O2	-6.22	117.55	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	753	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1244	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	195	A	C5-C6-N1	6.22	120.81	117.70
54	BA	706	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1221	C	O4'-C1'-N1	6.22	113.17	108.20
21	AA	341	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	116	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	231	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1665	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2632	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1554	U	O4'-C1'-N1	6.21	113.17	108.20
54	BA	2712	C	N1-C2-O2	6.21	122.63	118.90
21	AA	1146	A	C5-C6-N1	6.21	120.81	117.70
22	A1	6	A	C5-C6-N1	6.21	120.81	117.70
54	BA	1028	A	N1-C6-N6	-6.21	114.87	118.60
54	BA	1755	A	C5-C6-N1	6.21	120.81	117.70
54	BA	2626	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	229	C	N1-C2-O2	6.21	122.63	118.90
54	BA	2823	A	C5-C6-N1	6.21	120.81	117.70
54	BA	2826	A	C5-C6-N1	6.21	120.81	117.70
54	BA	1880	U	O4'-C1'-N1	6.21	113.17	108.20
54	BA	2830	C	N3-C2-O2	-6.21	117.55	121.90
3	AD	43	ARG	NE-CZ-NH1	6.21	123.40	120.30
21	AA	59	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	393	A	C5-C6-N1	6.21	120.80	117.70
21	AA	1277	C	N3-C2-O2	-6.21	117.56	121.90
35	BM	18	ARG	NE-CZ-NH1	6.21	123.40	120.30
46	BX	36	ARG	NE-CZ-NH1	6.21	123.40	120.30
54	BA	527	C	N1-C2-O2	6.21	122.62	118.90
54	BA	592	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	994	C	N1-C2-O2	6.21	122.62	118.90
21	AA	435	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1902	C	N3-C2-O2	-6.20	117.56	121.90
16	AQ	64	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	AA	238	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	643	A	O4'-C1'-N9	6.20	113.16	108.20
54	BA	1230	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1286	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2721	A	C5-C6-N1	6.20	120.80	117.70
54	BA	227	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	793	A	C5-C6-N1	6.20	120.80	117.70
54	BA	1574	C	N3-C2-O2	-6.20	117.56	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1690	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2443	C	N3-C2-O2	-6.20	117.56	121.90
12	AM	108	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	BA	1571	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2005	A	N1-C6-N6	-6.20	114.88	118.60
54	BA	1233	C	N3-C2-O2	-6.19	117.56	121.90
10	AK	52	ARG	NE-CZ-NH1	6.19	123.40	120.30
54	BA	1134	A	N1-C6-N6	-6.19	114.89	118.60
54	BA	1258	U	O4'-C1'-N1	6.19	113.15	108.20
54	BA	1735	A	N1-C6-N6	-6.19	114.89	118.60
21	AA	794	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	948	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1238	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	1965	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	2232	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	2298	A	C5-C6-N1	6.19	120.80	117.70
54	BA	1998	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	483	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1128	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1495	A	C5-C6-N1	6.19	120.79	117.70
54	BA	2103	C	N3-C2-O2	-6.19	117.57	121.90
55	BB	28	C	N3-C2-O2	-6.19	117.57	121.90
55	BB	30	C	O4'-C1'-N1	6.19	113.15	108.20
21	AA	182	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	814	A	C5-C6-N1	6.18	120.79	117.70
21	AA	1507	A	C5-C6-N1	6.18	120.79	117.70
54	BA	2728	U	O4'-C1'-N1	6.18	113.15	108.20
21	AA	33	A	C5-C6-N1	6.18	120.79	117.70
21	AA	33	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	935	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	2896	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	579	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	311	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	341	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1941	C	N3-C2-O2	-6.18	117.57	121.90
25	BC	12	ARG	NE-CZ-NH1	6.18	123.39	120.30
54	BA	173	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	184	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	753	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1013	C	O4'-C1'-N1	6.18	113.14	108.20
54	BA	1752	C	N3-C2-O2	-6.18	117.58	121.90
3	AD	61	ARG	NE-CZ-NH2	-6.18	117.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2266	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2368	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	190	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	353	A	O4'-C1'-N9	6.18	113.14	108.20
21	AA	373	A	N1-C6-N6	-6.18	114.89	118.60
21	AA	1336	C	N3-C2-O2	-6.18	117.58	121.90
24	A3	52	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	454	A	C5-C6-N1	6.18	120.79	117.70
54	BA	845	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2182	U	O4'-C1'-N1	6.18	113.14	108.20
21	AA	777	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	1170	A	C4-C5-C6	-6.17	113.91	117.00
23	A2	90	U	C5'-C4'-O4'	6.17	116.51	109.10
54	BA	487	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	699	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	1261	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1417	C	O4'-C1'-N1	6.17	113.14	108.20
54	BA	1536	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2119	A	O4'-C1'-N9	6.17	113.14	108.20
54	BA	2036	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2780	G	O4'-C1'-N9	6.17	113.14	108.20
21	AA	909	A	C5-C6-N1	6.17	120.79	117.70
22	A1	75	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	38	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	106	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	995	C	O4'-C1'-N1	6.17	113.14	108.20
54	BA	1548	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	2649	C	N3-C2-O2	-6.17	117.58	121.90
22	A1	69	A	C5-C6-N1	6.17	120.78	117.70
54	BA	1243	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1866	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	694	A	C4-C5-C6	-6.17	113.92	117.00
24	A3	60	A	N1-C6-N6	-6.17	114.90	118.60
54	BA	430	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	515	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	1010	A	C5-C6-N1	6.17	120.78	117.70
54	BA	1822	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2059	A	O4'-C1'-N9	6.17	113.14	108.20
54	BA	2163	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	2598	A	C5-C6-N1	6.17	120.78	117.70
21	AA	66	A	C5-C6-N1	6.17	120.78	117.70
21	AA	1022	A	C4-C5-C6	-6.17	113.92	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A2	91	A	C3'-C2'-C1'	6.17	106.43	101.50
54	BA	129	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1146	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	57	G	N1-C6-O6	-6.17	116.20	119.90
54	BA	624	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1594	U	O4'-C1'-N1	6.17	113.13	108.20
54	BA	1705	A	C4-C5-C6	-6.17	113.92	117.00
36	BN	64	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	541	A	C5-C6-N1	6.16	120.78	117.70
54	BA	1311	G	N1-C6-O6	-6.16	116.20	119.90
54	BA	2108	A	C5-C6-N1	6.16	120.78	117.70
54	BA	846	U	O4'-C1'-N1	6.16	113.13	108.20
54	BA	1586	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	533	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	941	G	N3-C2-N2	-6.16	115.59	119.90
54	BA	415	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1048	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1399	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	339	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	792	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	1112	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	82	U	O4'-C1'-N1	6.16	113.13	108.20
54	BA	147	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1064	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2406	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	1517	G	N3-C2-N2	-6.16	115.59	119.90
25	BC	100	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	479	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1327	A	C5-C6-N1	6.15	120.78	117.70
21	AA	663	A	N1-C6-N6	-6.15	114.91	118.60
47	BY	7	ARG	NE-CZ-NH1	6.15	123.38	120.30
54	BA	985	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2828	G	N7-C8-N9	6.15	116.18	113.10
55	BB	42	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	305	G	C5'-C4'-C3'	-6.15	106.16	116.00
52	B3	44	ARG	NE-CZ-NH1	6.15	123.38	120.30
54	BA	2195	U	O4'-C1'-N1	6.15	113.12	108.20
55	BB	41	G	O4'-C1'-N9	6.15	113.12	108.20
21	AA	338	A	C5-C6-N1	6.15	120.78	117.70
22	A1	13	C	N3-C2-O2	-6.15	117.60	121.90
21	AA	1097	C	N3-C2-O2	-6.15	117.60	121.90
21	AA	1176	A	C5-C6-N1	6.15	120.77	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	547	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	2424	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	800	A	N1-C6-N6	-6.15	114.91	118.60
21	AA	1042	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	807	U	O4'-C1'-N1	6.14	113.11	108.20
54	BA	1291	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1955	U	C1'-O4'-C4'	-6.14	104.98	109.90
54	BA	1974	C	N1-C2-O2	6.14	122.59	118.90
21	AA	253	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	336	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1512	C	O4'-C1'-N1	6.14	113.11	108.20
54	BA	2619	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	1330	U	O4'-C1'-N1	6.14	113.11	108.20
21	AA	1331	G	O4'-C1'-N9	6.14	113.11	108.20
54	BA	464	U	O4'-C1'-N1	6.14	113.11	108.20
54	BA	1614	A	C4-C5-C6	-6.14	113.93	117.00
6	AG	9	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	49	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1858	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1408	A	C4-C5-C6	-6.13	113.93	117.00
55	BB	40	U	O4'-C1'-N1	6.13	113.11	108.20
54	BA	143	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	964	C	N3-C2-O2	-6.13	117.61	121.90
15	AP	25	ARG	NE-CZ-NH1	6.13	123.37	120.30
21	AA	1012	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	1052	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1552	A	O4'-C1'-N9	6.13	113.11	108.20
21	AA	1261	A	N1-C6-N6	-6.13	114.92	118.60
38	BP	50	ARG	NE-CZ-NH1	6.13	123.36	120.30
54	BA	128	C	O4'-C1'-N1	6.13	113.10	108.20
54	BA	696	G	N1-C6-O6	-6.13	116.22	119.90
54	BA	1072	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1158	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1518	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	514	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	222	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	845	A	C5-C6-N1	6.13	120.77	117.70
54	BA	1434	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	399	U	O4'-C1'-N1	6.13	113.10	108.20
54	BA	898	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1795	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2177	C	N3-C2-O2	-6.13	117.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	173	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	209	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	2827	C	N3-C2-O2	-6.12	117.61	121.90
22	A1	58	A	N1-C6-N6	-6.12	114.92	118.60
54	BA	672	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1172	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1236	G	O4'-C1'-N9	6.12	113.10	108.20
21	AA	1217	C	P-O3'-C3'	6.12	127.05	119.70
54	BA	626	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1121	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1289	C	C3'-C2'-C1'	6.12	106.40	101.50
54	BA	1290	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1605	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1909	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	897	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	1217	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	1452	C	N3-C2-O2	-6.12	117.62	121.90
22	A1	51	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2651	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	974	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	394	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1979	U	O4'-C1'-N1	6.12	113.09	108.20
54	BA	2860	A	O4'-C1'-N9	6.12	113.09	108.20
55	BB	114	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	90	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	106	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	344	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	723	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1843	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2726	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	225	C	O4'-C1'-N1	6.11	113.09	108.20
54	BA	1207	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	897	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2837	A	C4-C5-C6	-6.11	113.94	117.00
21	AA	879	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	844	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	2741	A	C5-C6-N1	6.11	120.75	117.70
15	AP	5	ARG	NE-CZ-NH1	6.11	123.35	120.30
21	AA	28	A	C4-C5-C6	-6.11	113.95	117.00
21	AA	1492	A	C3'-C2'-C1'	6.11	106.39	101.50
54	BA	382	A	N1-C6-N6	-6.11	114.94	118.60
54	BA	1952	A	O4'-C1'-N9	6.11	113.09	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	883	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	5	A	C5-C6-N1	6.11	120.75	117.70
54	BA	76	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	457	A	O4'-C1'-N9	6.11	113.08	108.20
54	BA	910	A	N1-C6-N6	-6.11	114.94	118.60
54	BA	972	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	2385	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	96	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	246	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1600	C	N3-C2-O2	-6.10	117.63	121.90
8	AI	11	ARG	NE-CZ-NH1	6.10	123.35	120.30
54	BA	933	A	C5-C6-N1	6.10	120.75	117.70
55	BB	113	C	N1-C2-O2	6.10	122.56	118.90
21	AA	1107	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	156	A	C5-C6-N1	6.10	120.75	117.70
54	BA	544	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	1691	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	1727	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	2750	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	806	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	2025	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	2407	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2482	A	C4-C5-C6	-6.10	113.95	117.00
55	BB	59	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	1213	A	C5-C6-N1	6.10	120.75	117.70
54	BA	1670	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1810	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	211	C	N3-C2-O2	-6.09	117.63	121.90
54	BA	352	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	485	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2824	C	N3-C2-O2	-6.09	117.64	121.90
22	A1	35	A	C5-C6-N1	6.09	120.75	117.70
54	BA	2564	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	353	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	502	A	C5-C6-N1	6.09	120.74	117.70
54	BA	1617	C	N3-C4-C5	6.09	124.33	121.90
54	BA	38	A	C5-C6-N1	6.09	120.74	117.70
54	BA	371	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	692	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	793	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	1161	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2657	A	C5-C6-N1	6.09	120.74	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2741	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	272	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	1779	U	C1'-O4'-C4'	-6.08	105.03	109.90
53	B4	19	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	1547	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2214	C	N3-C2-O2	-6.08	117.64	121.90
55	BB	104	A	C5-C6-N1	6.08	120.74	117.70
21	AA	466	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	523	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	560	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	190	A	N1-C6-N6	-6.08	114.95	118.60
54	BA	1027	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1566	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2108	A	C4-C5-C6	-6.08	113.96	117.00
5	AF	24	ARG	NE-CZ-NH1	6.08	123.34	120.30
21	AA	859	G	N1-C6-O6	-6.08	116.25	119.90
21	AA	1274	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1952	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	322	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	931	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	292	U	O4'-C1'-N1	6.07	113.06	108.20
54	BA	689	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	734	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	2602	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	1785	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	2182	U	C1'-O4'-C4'	-6.07	105.04	109.90
21	AA	1257	A	C4-C5-C6	-6.07	113.97	117.00
39	BQ	10	ARG	NE-CZ-NH1	6.07	123.33	120.30
54	BA	181	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	609	A	C5-C6-N1	6.07	120.73	117.70
54	BA	1957	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1995	U	O4'-C1'-N1	6.07	113.05	108.20
55	BB	61	G	N3-C4-C5	-6.07	125.57	128.60
21	AA	243	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	412	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	906	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	1149	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	1200	C	N3-C2-O2	-6.07	117.66	121.90
39	BQ	57	ARG	NE-CZ-NH1	6.07	123.33	120.30
54	BA	348	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	544	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1717	A	C4-C5-C6	-6.07	113.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2135	A	C4-C5-C6	-6.07	113.97	117.00
25	BC	202	ARG	NE-CZ-NH1	6.06	123.33	120.30
21	AA	1377	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	225	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	334	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1215	G	N3-C2-N2	-6.06	115.66	119.90
54	BA	1264	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1288	G	N3-C2-N2	-6.06	115.66	119.90
21	AA	236	A	C5-C6-N1	6.06	120.73	117.70
21	AA	758	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	1267	C	N1-C2-O2	6.06	122.54	118.90
21	AA	1409	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2425	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2572	A	C5-C6-N1	6.06	120.73	117.70
54	BA	707	G	C5-C6-N1	6.06	114.53	111.50
54	BA	1728	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1746	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1812	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	1391	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	1561	C	N3-C2-O2	-6.06	117.66	121.90
55	BB	30	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	949	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	1531	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1253	A	O4'-C1'-N9	6.05	113.04	108.20
54	BA	2000	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	2364	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	1977	A	C5-C6-N1	6.05	120.73	117.70
54	BA	1997	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	2044	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	2332	C	N1-C2-O2	6.05	122.53	118.90
54	BA	2730	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	937	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	920	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1597	A	C3'-C2'-C1'	6.05	106.34	101.50
21	AA	77	A	C5-C6-N1	6.05	120.72	117.70
54	BA	848	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1040	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	2764	A	C5-C6-N1	6.05	120.72	117.70
54	BA	1668	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1446	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	819	A	N1-C6-N6	-6.04	114.97	118.60
54	BA	2135	A	C5-C6-N1	6.04	120.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1500	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	996	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2033	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	948	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2509	G	O4'-C1'-N9	6.04	113.03	108.20
54	BA	743	A	C6-C5-N7	6.04	136.53	132.30
54	BA	1077	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	958	A	C3'-C2'-C1'	6.04	106.33	101.50
21	AA	535	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1443	C	N3-C2-O2	-6.04	117.68	121.90
54	BA	1675	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2347	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	445	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	958	U	O4'-C1'-N1	6.03	113.03	108.20
54	BA	1495	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	1701	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2059	A	C5-C6-N1	6.03	120.72	117.70
38	BP	108	ARG	NE-CZ-NH2	-6.03	117.28	120.30
54	BA	279	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	172	A	C5-C6-N1	6.03	120.72	117.70
54	BA	557	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1080	A	C5-C6-N1	6.03	120.72	117.70
54	BA	2108	A	O4'-C1'-N9	6.03	113.02	108.20
54	BA	2661	G	O4'-C1'-N9	6.03	113.02	108.20
21	AA	496	A	C5-C6-N1	6.03	120.72	117.70
54	BA	635	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	914	G	O4'-C1'-N9	6.03	113.02	108.20
54	BA	2085	U	O4'-C1'-N1	6.03	113.02	108.20
21	AA	1096	C	N3-C2-O2	-6.03	117.68	121.90
22	A1	14	A	C4-C5-C6	-6.03	113.99	117.00
22	A1	16	C	N3-C4-C5	6.03	124.31	121.90
54	BA	1166	G	N3-C2-N2	-6.03	115.68	119.90
54	BA	1905	C	O4'-C1'-N1	6.03	113.02	108.20
54	BA	2589	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	1259	C	N3-C2-O2	-6.03	117.68	121.90
23	A2	82	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	965	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1141	U	O4'-C4'-C3'	6.03	110.92	106.10
54	BA	1934	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2014	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	2349	G	O4'-C1'-N9	6.03	113.02	108.20
21	AA	71	A	C4-C5-C6	-6.02	113.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	770	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	441	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	572	A	O4'-C1'-N9	6.02	113.02	108.20
24	A3	70	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	693	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1892	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	327	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	547	A	C5-C6-N1	6.02	120.71	117.70
21	AA	1019	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1733	G	P-O3'-C3'	6.02	126.92	119.70
55	BB	70	C	O4'-C1'-N1	6.02	113.02	108.20
21	AA	336	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2244	U	O4'-C1'-N1	6.02	113.01	108.20
54	BA	2887	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	440	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	436	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	510	A	C4-C5-C6	-6.01	113.99	117.00
24	A3	16	C	N1-C2-O2	6.01	122.51	118.90
54	BA	28	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	1541	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1925	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2662	A	C5-C6-N1	6.01	120.71	117.70
21	AA	373	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	1213	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	1276	A	C5-C6-N1	6.01	120.71	117.70
54	BA	1909	C	O4'-C1'-N1	6.01	113.01	108.20
21	AA	210	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	660	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1379	U	O4'-C1'-N1	6.01	113.01	108.20
54	BA	1877	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2673	G	N3-C2-N2	-6.01	115.69	119.90
21	AA	1389	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	782	A	C5-C6-N1	6.01	120.70	117.70
21	AA	192	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	157	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	238	C	N3-C2-O2	-6.01	117.70	121.90
54	BA	1005	C	N3-C2-O2	-6.01	117.70	121.90
54	BA	1250	G	O4'-C1'-N9	6.01	113.01	108.20
54	BA	2066	C	O4'-C1'-N1	6.01	113.00	108.20
21	AA	1243	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2745	C	O4'-C1'-N1	6.00	113.00	108.20
21	AA	421	U	O4'-C1'-N1	6.00	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	796	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	95	A	C5-C6-N1	6.00	120.70	117.70
54	BA	315	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	1364	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	2873	A	O4'-C1'-N9	6.00	113.00	108.20
54	BA	529	A	C4-C5-C6	-6.00	114.00	117.00
55	BB	4	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1250	A	C4-C5-C6	-6.00	114.00	117.00
22	A1	25	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1402	U	O4'-C1'-N1	6.00	113.00	108.20
54	BA	2635	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2789	C	N3-C2-O2	-6.00	117.70	121.90
5	AF	79	ARG	NE-CZ-NH1	6.00	123.30	120.30
9	AJ	48	ARG	NE-CZ-NH1	6.00	123.30	120.30
15	AP	8	ARG	NE-CZ-NH1	6.00	123.30	120.30
21	AA	72	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	943	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1447	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2471	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2220	U	O4'-C1'-N1	6.00	113.00	108.20
21	AA	290	C	N3-C2-O2	-6.00	117.70	121.90
22	A1	31	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2442	C	N3-C2-O2	-6.00	117.70	121.90
24	A3	7	G	N1-C6-O6	-5.99	116.30	119.90
54	BA	814	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	2165	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	2600	A	C5-C6-N1	5.99	120.70	117.70
55	BB	17	C	N3-C2-O2	-5.99	117.70	121.90
55	BB	60	C	O4'-C1'-N1	5.99	113.00	108.20
21	AA	84	U	N3-C2-O2	-5.99	118.01	122.20
54	BA	504	A	C4-C5-C6	-5.99	114.00	117.00
11	AL	55	ARG	NE-CZ-NH1	5.99	123.30	120.30
54	BA	951	C	N3-C2-O2	-5.99	117.71	121.90
55	BB	15	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	305	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1049	C	N1-C2-O2	5.99	122.49	118.90
54	BA	1229	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2143	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2531	A	C5-C6-N1	5.99	120.69	117.70
54	BA	2665	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	2855	C	N1-C2-O2	5.99	122.49	118.90
12	AM	78	ARG	NE-CZ-NH1	5.99	123.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	493	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	979	C	N1-C2-O2	5.99	122.49	118.90
21	AA	1067	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	2339	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	746	A	C5-C6-N1	5.99	120.69	117.70
21	AA	1281	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	483	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1098	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1757	A	O4'-C1'-N9	5.99	112.99	108.20
54	BA	2072	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2359	C	O4'-C1'-N1	5.99	112.99	108.20
54	BA	2794	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	456	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	959	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1228	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	841	G	C5'-C4'-O4'	5.98	116.28	109.10
55	BB	78	A	C5-C6-N1	5.98	120.69	117.70
21	AA	44	A	C5-C6-N1	5.98	120.69	117.70
21	AA	1216	A	C5-C6-N1	5.98	120.69	117.70
21	AA	1453	G	O4'-C1'-N9	5.98	112.98	108.20
28	BF	101	ARG	NE-CZ-NH1	5.98	123.29	120.30
54	BA	61	C	N1-C2-O2	5.98	122.49	118.90
54	BA	2322	A	C5-C6-N1	5.98	120.69	117.70
54	BA	172	A	O4'-C1'-N9	5.98	112.98	108.20
54	BA	2635	A	N1-C6-N6	-5.98	115.01	118.60
21	AA	314	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	720	U	O4'-C1'-N1	5.98	112.98	108.20
21	AA	984	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	828	U	N3-C2-O2	-5.98	118.02	122.20
51	B2	19	ARG	NE-CZ-NH1	5.97	123.29	120.30
54	BA	887	U	O4'-C1'-N1	5.97	112.98	108.20
54	BA	142	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	265	A	C1'-O4'-C4'	-5.97	105.12	109.90
54	BA	936	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	539	A	C5-C6-N1	5.97	120.69	117.70
54	BA	573	U	N3-C2-O2	-5.97	118.02	122.20
54	BA	2703	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	576	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	555	G	N1-C6-O6	-5.97	116.32	119.90
54	BA	614	A	C5'-C4'-O4'	5.97	116.26	109.10
54	BA	1469	A	C4-C5-C6	-5.97	114.02	117.00
55	BB	118	C	N3-C2-O2	-5.97	117.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1066	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	2376	A	C4-C5-C6	-5.96	114.02	117.00
55	BB	63	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	434	U	O4'-C1'-N1	5.96	112.97	108.20
54	BA	783	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1339	G	N3-C2-N2	-5.96	115.73	119.90
21	AA	526	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	270	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	454	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	786	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1509	A	C4-C5-C6	-5.96	114.02	117.00
27	BE	88	ARG	NE-CZ-NH2	-5.96	117.32	120.30
33	BK	30	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	1353	A	C5'-C4'-O4'	5.96	116.25	109.10
54	BA	1806	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	167	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	1263	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1007	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1262	A	C5-C6-N1	5.96	120.68	117.70
54	BA	2307	G	N3-C2-N2	-5.96	115.73	119.90
54	BA	2590	A	C4-C5-C6	-5.96	114.02	117.00
32	BJ	95	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	1808	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	1468	A	C4-C5-C6	-5.95	114.02	117.00
42	BT	77	ARG	NE-CZ-NH1	5.95	123.28	120.30
54	BA	1348	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	1618	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	2215	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	286	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	935	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	507	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	2082	A	C5-C6-N1	5.95	120.67	117.70
54	BA	2306	C	N3-C2-O2	-5.95	117.74	121.90
21	AA	630	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	595	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1655	A	C5-C6-N1	5.95	120.67	117.70
54	BA	428	A	C5-C6-N1	5.95	120.67	117.70
21	AA	331	G	C3'-C2'-C1'	5.94	106.25	101.50
54	BA	340	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	1169	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	1203	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	426	C	N3-C2-O2	-5.94	117.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1947	C	N1-C2-O2	5.94	122.46	118.90
54	BA	2179	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2340	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2401	U	O4'-C1'-N1	5.94	112.95	108.20
54	BA	2462	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2788	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2860	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	465	A	C5-C6-N1	5.94	120.67	117.70
54	BA	255	A	N1-C6-N6	-5.94	115.04	118.60
54	BA	384	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1470	A	C5-C6-N1	5.94	120.67	117.70
54	BA	1604	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2764	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	837	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1577	C	N3-C2-O2	-5.94	117.75	121.90
21	AA	1252	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	1296	C	N1-C2-O2	5.93	122.46	118.90
54	BA	182	A	C5-C6-N1	5.93	120.67	117.70
54	BA	1393	A	C4'-C3'-C2'	-5.93	96.67	102.60
54	BA	2749	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2893	A	C4-C5-C6	-5.93	114.03	117.00
24	A3	39	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1844	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	2492	U	O4'-C1'-N1	5.93	112.94	108.20
21	AA	1275	A	C4-C5-C6	-5.93	114.03	117.00
33	BK	71	ARG	NE-CZ-NH1	5.93	123.27	120.30
54	BA	679	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	892	A	C5-C6-N1	5.93	120.67	117.70
54	BA	1189	A	C4'-C3'-C2'	-5.93	96.67	102.60
54	BA	1715	G	O4'-C1'-N9	5.93	112.94	108.20
54	BA	2122	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	2207	C	N3-C2-O2	-5.93	117.75	121.90
37	BO	7	ARG	NE-CZ-NH1	5.93	123.26	120.30
54	BA	1888	G	N3-C4-C5	-5.93	125.64	128.60
21	AA	1293	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	150	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	482	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1155	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1283	G	N1-C6-O6	-5.92	116.34	119.90
54	BA	1592	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1651	G	N1-C6-O6	-5.92	116.35	119.90
54	BA	1777	U	O4'-C1'-N1	5.92	112.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2051	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1496	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	645	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	1395	A	C4-C5-C6	-5.92	114.04	117.00
9	AJ	48	ARG	NE-CZ-NH2	-5.92	117.34	120.30
54	BA	20	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	952	G	N1-C6-O6	-5.92	116.35	119.90
54	BA	1665	A	C5-C6-N1	5.92	120.66	117.70
55	BB	97	C	N1-C2-O2	5.92	122.45	118.90
54	BA	1828	G	C5-C6-N1	5.92	114.46	111.50
3	AD	25	ARG	NE-CZ-NH1	5.91	123.26	120.30
21	AA	124	C	N1-C2-O2	5.91	122.45	118.90
54	BA	2785	C	O4'-C1'-N1	5.91	112.93	108.20
13	AN	65	ARG	NE-CZ-NH1	5.91	123.26	120.30
54	BA	1484	U	O4'-C1'-N1	5.91	112.93	108.20
17	AR	56	ARG	NE-CZ-NH1	5.91	123.25	120.30
21	AA	284	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	790	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	2814	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	1140	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	115	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	582	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	1433	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1943	U	N3-C2-O2	-5.91	118.06	122.20
54	BA	1987	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	399	G	C1'-O4'-C4'	-5.91	105.18	109.90
23	A2	92	U	N3-C2-O2	-5.91	118.07	122.20
40	BR	79	ARG	NE-CZ-NH1	5.91	123.25	120.30
54	BA	1289	C	N1-C2-O2	5.91	122.44	118.90
54	BA	2518	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	610	U	C1'-O4'-C4'	-5.90	105.18	109.90
21	AA	663	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	679	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1231	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	1456	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	131	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	460	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1208	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1690	A	N1-C6-N6	-5.90	115.06	118.60
54	BA	2117	A	O4'-C1'-N9	5.90	112.92	108.20
54	BA	362	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	910	A	C4-C5-C6	-5.90	114.05	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1167	C	N3-C2-O2	-5.90	117.77	121.90
11	AL	30	ARG	NE-CZ-NH1	5.90	123.25	120.30
21	AA	397	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	1147	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1269	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	509	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	466	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1327	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	55	A	C4-C5-C6	-5.89	114.05	117.00
21	AA	279	A	C4-C5-C6	-5.89	114.05	117.00
21	AA	913	A	P-O3'-C3'	5.89	126.77	119.70
54	BA	755	U	O4'-C1'-N1	5.89	112.92	108.20
54	BA	2423	U	O4'-C1'-N1	5.89	112.92	108.20
54	BA	2853	C	N3-C2-O2	-5.89	117.77	121.90
21	AA	857	C	N1-C2-O2	5.89	122.44	118.90
54	BA	492	A	C5-C6-N1	5.89	120.65	117.70
54	BA	2202	U	O4'-C1'-N1	5.89	112.91	108.20
54	BA	1977	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	2498	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	225	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	840	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1656	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1981	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	1100	C	O4'-C1'-N1	5.89	112.91	108.20
54	BA	2682	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	295	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	650	G	N1-C6-O6	-5.89	116.37	119.90
54	BA	2584	U	O4'-C1'-N1	5.89	112.91	108.20
54	BA	2871	U	O4'-C1'-N1	5.89	112.91	108.20
21	AA	108	G	N3-C4-C5	-5.88	125.66	128.60
54	BA	133	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	2241	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	1504	G	N1-C6-O6	-5.88	116.37	119.90
54	BA	823	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	930	C	O4'-C1'-N1	5.88	112.91	108.20
54	BA	981	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2309	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	783	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	650	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1582	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	236	A	O4'-C1'-N9	5.88	112.90	108.20
21	AA	376	G	N1-C6-O6	-5.88	116.37	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1151	A	C5-C6-N1	5.88	120.64	117.70
21	AA	1465	A	C5-C6-N1	5.88	120.64	117.70
54	BA	968	C	O4'-C1'-N1	5.88	112.90	108.20
54	BA	1489	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1652	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	381	C	N1-C2-O2	5.88	122.43	118.90
54	BA	1821	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	51	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1404	C	N3-C2-O2	-5.88	117.79	121.90
21	AA	810	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1218	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1794	A	C4-C5-C6	-5.87	114.06	117.00
5	AF	2	ARG	NE-CZ-NH1	5.87	123.23	120.30
21	AA	583	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	1188	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	461	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	739	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	964	C	O4'-C1'-N1	5.87	112.90	108.20
54	BA	1800	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2262	U	O4'-C1'-N1	5.87	112.90	108.20
21	AA	316	C	N3-C2-O2	-5.87	117.79	121.90
32	BJ	116	ARG	NE-CZ-NH1	5.87	123.23	120.30
45	BW	40	ARG	NE-CZ-NH1	5.87	123.23	120.30
54	BA	228	C	N1-C2-O2	5.87	122.42	118.90
54	BA	680	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2669	G	C1'-O4'-C4'	-5.87	105.20	109.90
54	BA	2850	A	C4-C5-C6	-5.87	114.07	117.00
21	AA	76	G	C5-C6-N1	5.87	114.43	111.50
54	BA	1096	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	2147	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	2160	C	N1-C2-O2	5.87	122.42	118.90
18	AS	54	ARG	NE-CZ-NH1	5.86	123.23	120.30
21	AA	282	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1524	C	N3-C2-O2	-5.86	117.80	121.90
55	BB	43	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	569	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	459	U	O4'-C1'-N1	5.86	112.89	108.20
54	BA	1351	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2285	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	194	C	O4'-C1'-N1	5.86	112.89	108.20
21	AA	1150	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	361	G	O4'-C1'-N9	5.86	112.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	912	C	N1-C2-O2	5.86	122.42	118.90
54	BA	2287	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	739	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	1437	A	C4-C5-C6	-5.86	114.07	117.00
37	BO	81	ARG	NE-CZ-NH1	5.86	123.23	120.30
21	AA	599	C	N3-C2-O2	-5.86	117.80	121.90
53	B4	12	ARG	NE-CZ-NH1	5.86	123.23	120.30
54	BA	480	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1796	U	O4'-C1'-N1	5.86	112.89	108.20
3	AD	187	ARG	NE-CZ-NH1	5.85	123.23	120.30
21	AA	1447	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	89	A	C5-C6-N1	5.85	120.63	117.70
54	BA	1247	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	1499	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	2657	A	C4-C5-C6	-5.85	114.07	117.00
55	BB	59	A	C5-C6-N1	5.85	120.63	117.70
21	AA	996	A	N1-C6-N6	-5.85	115.09	118.60
21	AA	1507	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	347	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	2496	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	2586	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2752	C	O4'-C1'-N1	5.85	112.88	108.20
21	AA	1214	C	C1'-O4'-C4'	-5.85	105.22	109.90
54	BA	146	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	277	G	N3-C4-C5	-5.85	125.67	128.60
54	BA	402	A	N1-C6-N6	-5.85	115.09	118.60
54	BA	531	C	O4'-C1'-N1	5.85	112.88	108.20
21	AA	465	A	O4'-C1'-N9	5.85	112.88	108.20
21	AA	1375	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1596	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	2070	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	2263	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	2736	A	C4-C5-C6	-5.85	114.08	117.00
55	BB	108	A	C4-C5-C6	-5.85	114.08	117.00
22	A1	66	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1006	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	1503	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1558	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2084	C	N1-C2-O2	5.84	122.41	118.90
54	BA	2103	C	O4'-C1'-N1	5.84	112.88	108.20
54	BA	2541	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	307	C	N1-C2-O2	5.84	122.41	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1244	G	N1-C6-O6	-5.84	116.39	119.90
54	BA	130	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	986	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2793	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2900	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	263	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	1382	C	N1-C2-O2	5.84	122.41	118.90
54	BA	578	G	N1-C6-O6	-5.84	116.39	119.90
54	BA	1193	G	N1-C6-O6	-5.84	116.39	119.90
12	AM	112	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	AA	1466	C	N1-C2-O2	5.84	122.40	118.90
54	BA	2071	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	116	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	418	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2647	U	O4'-C1'-N1	5.84	112.87	108.20
21	AA	816	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	448	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	610	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1060	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	1133	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	2496	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	2899	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1559	U	N3-C2-O2	-5.83	118.12	122.20
54	BA	2432	A	O4'-C1'-N9	5.83	112.87	108.20
54	BA	2783	U	O4'-C1'-N1	5.83	112.87	108.20
21	AA	735	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	1202	U	O4'-C1'-N1	5.83	112.87	108.20
54	BA	2300	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	250	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	752	G	N3-C2-N2	-5.83	115.82	119.90
38	BP	92	ARG	NE-CZ-NH1	5.83	123.22	120.30
54	BA	249	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2143	C	O4'-C1'-N1	5.83	112.87	108.20
54	BA	1686	C	O4'-C1'-N1	5.83	112.86	108.20
54	BA	1297	C	N3-C2-O2	-5.83	117.82	121.90
55	BB	70	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	990	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	1521	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1431	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	851	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2792	A	C4-C5-C6	-5.83	114.09	117.00
24	A3	45	A	C4-C5-C6	-5.82	114.09	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	71	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	197	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	860	U	O4'-C1'-N1	5.82	112.86	108.20
54	BA	1836	C	N3-C2-O2	-5.82	117.82	121.90
21	AA	1112	C	N1-C2-O2	5.82	122.39	118.90
21	AA	370	C	N1-C2-O2	5.82	122.39	118.90
21	AA	1273	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2868	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	1237	C	N1-C2-O2	5.82	122.39	118.90
54	BA	818	G	C4'-C3'-O3'	5.82	124.64	113.00
54	BA	1373	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1978	A	C5-C6-N1	5.82	120.61	117.70
54	BA	2311	A	C4-C5-C6	-5.82	114.09	117.00
55	BB	49	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	756	C	N1-C2-O2	5.82	122.39	118.90
21	AA	1172	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	168	G	N3-C2-N2	-5.82	115.83	119.90
54	BA	2304	G	N3-C2-N2	-5.82	115.83	119.90
54	BA	2581	G	O4'-C1'-N9	5.82	112.85	108.20
54	BA	2784	U	C5-C6-N1	-5.82	119.79	122.70
21	AA	168	G	C5'-C4'-C3'	-5.82	106.69	116.00
21	AA	441	A	N1-C6-N6	-5.82	115.11	118.60
21	AA	554	A	C5-C6-N1	5.82	120.61	117.70
54	BA	873	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2196	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	156	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1144	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1593	A	C5-C6-N1	5.81	120.61	117.70
54	BA	2502	G	N1-C6-O6	-5.81	116.41	119.90
21	AA	321	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	1236	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	179	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	901	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2123	G	O4'-C1'-N9	5.81	112.85	108.20
54	BA	224	U	O4'-C1'-N1	5.81	112.85	108.20
21	AA	706	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	825	A	C6-C5-N7	5.81	136.37	132.30
21	AA	840	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	1332	A	N1-C6-N6	-5.81	115.11	118.60
22	A1	9	A	O4'-C1'-N9	5.81	112.85	108.20
54	BA	2486	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2842	G	N1-C6-O6	-5.81	116.41	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	68	ARG	NE-CZ-NH1	5.81	123.20	120.30
21	AA	719	C	N1-C2-O2	5.81	122.38	118.90
21	AA	806	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	541	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	581	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1749	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	988	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	503	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	525	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	516	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	2222	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2416	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1101	U	O4'-C1'-N1	5.80	112.84	108.20
21	AA	221	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	756	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1520	U	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2388	A	C5-C6-N1	5.80	120.60	117.70
21	AA	1423	G	C1'-O4'-C4'	-5.80	105.26	109.90
32	BJ	69	ARG	NE-CZ-NH1	5.80	123.20	120.30
44	BV	18	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	1187	G	N3-C4-C5	-5.80	125.70	128.60
54	BA	1792	G	C5'-C4'-C3'	-5.80	106.72	116.00
54	BA	1890	A	C4-C5-C6	-5.80	114.10	117.00
5	AF	45	ARG	NE-CZ-NH1	5.80	123.20	120.30
21	AA	876	C	C3'-C2'-C1'	-5.80	96.86	101.50
54	BA	1100	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1105	U	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2043	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2200	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	2403	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1398	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	99	U	N3-C2-O2	-5.79	118.14	122.20
54	BA	995	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	2807	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1837	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	1145	A	C4-C5-C6	-5.79	114.11	117.00
41	BS	88	ARG	NE-CZ-NH1	5.79	123.19	120.30
54	BA	83	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	1726	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	2393	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	719	C	N1-C2-O2	5.79	122.37	118.90
54	BA	2233	U	O4'-C1'-N1	5.79	112.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	166	ARG	NE-CZ-NH1	5.79	123.19	120.30
21	AA	1027	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	1799	G	O4'-C1'-N9	5.78	112.83	108.20
54	BA	1913	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2610	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2638	G	N1-C6-O6	-5.78	116.43	119.90
21	AA	53	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	443	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	864	A	C5-C6-N1	5.78	120.59	117.70
21	AA	1403	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	1612	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	364	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1254	A	C4-C5-C6	-5.78	114.11	117.00
55	BB	73	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1465	A	C4-C5-C6	-5.78	114.11	117.00
24	A3	40	C	N1-C2-O2	5.78	122.37	118.90
54	BA	503	A	O4'-C1'-N9	5.78	112.82	108.20
54	BA	621	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	968	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	2512	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	121	G	O4'-C1'-N9	5.78	112.82	108.20
54	BA	1028	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1417	C	N1-C2-O2	5.78	122.37	118.90
21	AA	13	U	O4'-C1'-N1	5.77	112.82	108.20
21	AA	20	U	O4'-C1'-N1	5.77	112.82	108.20
49	B0	49	ARG	NE-CZ-NH1	5.77	123.19	120.30
54	BA	1924	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	1004	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	2572	A	C4-C5-C6	-5.77	114.11	117.00
53	B4	4	ARG	NE-CZ-NH1	5.77	123.19	120.30
22	A1	10	G	N1-C6-O6	-5.77	116.44	119.90
54	BA	1170	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1583	A	O4'-C1'-N9	5.77	112.82	108.20
54	BA	804	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	2594	C	O4'-C1'-N1	5.77	112.81	108.20
3	AD	103	ARG	NE-CZ-NH1	5.77	123.18	120.30
21	AA	269	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	379	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	2450	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	85	U	N3-C2-O2	-5.76	118.17	122.20
21	AA	1411	C	N1-C2-O2	5.76	122.36	118.90
54	BA	96	C	O4'-C1'-N1	5.76	112.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1209	U	C5-C6-N1	-5.76	119.82	122.70
54	BA	2465	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	900	A	N1-C6-N6	-5.76	115.14	118.60
9	AJ	68	ARG	NE-CZ-NH1	5.76	123.18	120.30
21	AA	631	C	O4'-C1'-N1	5.76	112.81	108.20
21	AA	1063	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	1227	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	1437	A	C5-C6-N1	5.76	120.58	117.70
54	BA	2245	U	O4'-C1'-N1	5.76	112.81	108.20
24	A3	77	A	C1'-O4'-C4'	-5.76	105.29	109.90
54	BA	191	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	253	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	634	C	N1-C2-O2	5.76	122.36	118.90
54	BA	1967	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2466	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2683	C	N1-C2-O2	5.76	122.36	118.90
21	AA	1319	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1336	A	C5-C6-N1	5.76	120.58	117.70
55	BB	62	C	N3-C2-O2	-5.76	117.87	121.90
24	A3	19	G	C3'-C2'-C1'	5.76	106.11	101.50
54	BA	975	A	C6-C5-N7	5.76	136.33	132.30
54	BA	1237	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1669	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2426	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2432	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	277	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	564	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	465	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	532	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2690	U	O4'-C1'-N1	5.75	112.80	108.20
21	AA	430	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	655	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	749	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	915	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	1118	C	N1-C2-O2	5.75	122.35	118.90
21	AA	211	G	N3-C2-N2	-5.75	115.88	119.90
54	BA	1832	C	N1-C2-O2	5.75	122.35	118.90
21	AA	1183	U	N3-C2-O2	-5.75	118.18	122.20
54	BA	1330	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	2097	A	C4-C5-C6	-5.75	114.12	117.00
24	A3	12	G	N1-C6-O6	-5.75	116.45	119.90
24	A3	75	C	N1-C2-O2	5.75	122.35	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	237	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	336	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	1376	C	O4'-C1'-N1	5.75	112.80	108.20
54	BA	1463	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	2866	U	O4'-C1'-N1	5.75	112.80	108.20
21	AA	635	A	C5-C6-N1	5.75	120.57	117.70
21	AA	469	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	203	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2551	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	418	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1655	A	N1-C6-N6	-5.74	115.16	118.60
54	BA	1695	G	N3-C2-N2	-5.74	115.88	119.90
21	AA	235	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	1190	G	P-O3'-C3'	5.74	126.59	119.70
54	BA	762	U	P-O3'-C3'	5.74	126.59	119.70
54	BA	1711	A	O4'-C1'-N9	5.74	112.79	108.20
21	AA	681	A	C4-C5-C6	-5.74	114.13	117.00
39	BQ	10	ARG	NE-CZ-NH2	-5.74	117.43	120.30
54	BA	246	C	O4'-C1'-N1	5.74	112.79	108.20
54	BA	2282	G	N1-C6-O6	-5.74	116.46	119.90
54	BA	2625	G	N1-C6-O6	-5.74	116.46	119.90
55	BB	35	C	N1-C2-O2	5.74	122.34	118.90
54	BA	346	A	O4'-C1'-N9	5.74	112.79	108.20
54	BA	1284	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	765	G	O4'-C1'-N9	5.74	112.79	108.20
54	BA	1010	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	130	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	837	U	O4'-C1'-N1	5.73	112.78	108.20
35	BM	44	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	893	C	N3-C2-O2	-5.73	117.89	121.90
55	BB	91	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	909	A	C4-C5-C6	-5.73	114.13	117.00
21	AA	1102	A	C5-C6-N1	5.73	120.56	117.70
21	AA	1176	A	C4-C5-C6	-5.73	114.14	117.00
50	B1	5	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	233	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	456	C	C6-N1-C2	-5.73	118.01	120.30
3	AD	187	ARG	NE-CZ-NH2	-5.73	117.44	120.30
21	AA	489	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	1278	G	C8-N9-C4	-5.73	104.11	106.40
25	BC	261	ARG	NE-CZ-NH1	5.73	123.16	120.30
54	BA	535	G	N3-C2-N2	-5.73	115.89	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1121	C	O4'-C1'-N1	5.73	112.78	108.20
54	BA	1970	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	2547	A	C1'-O4'-C4'	-5.73	105.32	109.90
24	A3	49	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	671	C	N1-C2-O2	5.73	122.34	118.90
54	BA	2095	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	2723	C	N1-C2-O2	5.73	122.34	118.90
22	A1	48	C	N1-C2-O2	5.72	122.33	118.90
54	BA	2743	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	199	A	C4-C5-C6	-5.72	114.14	117.00
49	B0	51	ARG	NE-CZ-NH1	5.72	123.16	120.30
54	BA	1746	A	O4'-C1'-N9	5.72	112.78	108.20
54	BA	1268	A	C5-C6-N1	5.72	120.56	117.70
21	AA	183	C	N1-C2-O2	5.72	122.33	118.90
21	AA	553	A	C5-C6-N1	5.72	120.56	117.70
54	BA	108	G	N1-C6-O6	-5.72	116.47	119.90
54	BA	109	C	O4'-C1'-N1	5.72	112.78	108.20
54	BA	432	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	468	A	O4'-C1'-N9	5.72	112.77	108.20
54	BA	21	A	C5-C6-N1	5.72	120.56	117.70
54	BA	149	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1821	A	C5-C6-N1	5.72	120.56	117.70
21	AA	63	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	1163	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	865	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	2260	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	2738	A	C4-C5-C6	-5.72	114.14	117.00
7	AH	79	ARG	NE-CZ-NH1	5.71	123.16	120.30
21	AA	975	A	C4-C5-C6	-5.71	114.14	117.00
34	BL	132	ARG	NE-CZ-NH1	5.71	123.16	120.30
54	BA	413	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	503	A	C3'-C2'-C1'	5.71	106.07	101.50
54	BA	2055	C	O4'-C1'-N1	5.71	112.77	108.20
12	AM	70	ARG	NE-CZ-NH1	5.71	123.16	120.30
21	AA	647	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1449	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1171	A	C5-C6-N1	5.71	120.55	117.70
54	BA	1214	A	C4-C5-C6	-5.71	114.15	117.00
9	AJ	37	ARG	NE-CZ-NH1	5.71	123.15	120.30
21	AA	519	C	N3-C2-O2	-5.71	117.91	121.90
26	BD	124	ARG	NE-CZ-NH2	-5.71	117.45	120.30
54	BA	257	C	N1-C2-O2	5.71	122.32	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	444	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	829	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	1691	C	C4'-C3'-C2'	-5.71	96.89	102.60
54	BA	1754	A	C5-C6-N1	5.71	120.55	117.70
54	BA	1874	C	O4'-C1'-N1	5.71	112.77	108.20
54	BA	1211	C	N3-C2-O2	-5.71	117.91	121.90
21	AA	504	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	595	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1033	U	N3-C2-O2	-5.70	118.21	122.20
54	BA	2040	G	N1-C6-O6	-5.70	116.48	119.90
54	BA	855	G	N1-C6-O6	-5.70	116.48	119.90
54	BA	2212	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	477	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	1829	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2329	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	2552	U	N3-C2-O2	-5.70	118.21	122.20
21	AA	675	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	765	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	732	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1030	C	N1-C2-O2	5.70	122.32	118.90
54	BA	1698	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2264	C	C4'-C3'-C2'	-5.70	96.90	102.60
54	BA	379	G	N1-C6-O6	-5.69	116.48	119.90
23	A2	89	U	N3-C2-O2	-5.69	118.22	122.20
54	BA	674	G	O4'-C1'-N9	5.69	112.75	108.20
54	BA	1301	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	1637	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2225	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2264	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	2333	A	C4-C5-C6	-5.69	114.15	117.00
21	AA	415	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	2515	C	O4'-C1'-N1	5.69	112.75	108.20
21	AA	596	A	C4-C5-C6	-5.69	114.16	117.00
21	AA	1021	A	C4-C5-C6	-5.69	114.16	117.00
22	A1	70	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	576	U	O4'-C1'-N1	5.69	112.75	108.20
54	BA	584	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	1254	A	C5-C6-N1	5.68	120.54	117.70
32	BJ	120	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	194	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	1053	C	N1-C2-O2	5.68	122.31	118.90
54	BA	2612	C	O4'-C1'-N1	5.68	112.75	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	570	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	1201	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1325	U	N3-C2-O2	-5.68	118.22	122.20
54	BA	1802	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	2022	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	2417	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	2581	G	N1-C6-O6	-5.68	116.49	119.90
32	BJ	35	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	1908	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	542	C	O4'-C1'-N1	5.68	112.74	108.20
54	BA	774	G	O4'-C1'-N9	5.68	112.74	108.20
54	BA	984	A	C6-C5-N7	5.68	136.28	132.30
54	BA	1528	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	2182	U	C5'-C4'-O4'	5.68	115.92	109.10
54	BA	2875	C	N3-C2-O2	-5.68	117.92	121.90
24	A3	41	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	853	C	N3-C2-O2	-5.68	117.92	121.90
21	AA	178	C	N3-C2-O2	-5.68	117.93	121.90
54	BA	422	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	2679	A	C5-C6-N1	5.68	120.54	117.70
54	BA	2757	A	C4-C5-C6	-5.68	114.16	117.00
55	BB	93	C	N3-C2-O2	-5.68	117.93	121.90
21	AA	1502	A	O4'-C1'-N9	5.67	112.74	108.20
54	BA	892	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1210	G	N1-C6-O6	-5.67	116.50	119.90
54	BA	1353	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1472	C	N1-C2-O2	5.67	122.31	118.90
54	BA	1881	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2025	C	O4'-C1'-N1	5.67	112.74	108.20
21	AA	856	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2001	C	N3-C2-O2	-5.67	117.93	121.90
11	AL	109	ARG	NE-CZ-NH1	5.67	123.14	120.30
21	AA	66	A	C4-C5-C6	-5.67	114.17	117.00
21	AA	800	G	N3-C4-C5	-5.67	125.76	128.60
54	BA	128	C	N3-C4-N4	-5.67	114.03	118.00
54	BA	969	G	O4'-C1'-N9	5.67	112.74	108.20
54	BA	2314	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	743	A	O4'-C1'-N9	5.67	112.74	108.20
54	BA	1209	U	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2740	A	N1-C6-N6	-5.67	115.20	118.60
24	A3	38	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	57	C	N3-C2-O2	-5.67	117.93	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1302	A	N1-C6-N6	-5.67	115.20	118.60
54	BA	1940	U	N3-C2-O2	-5.67	118.23	122.20
21	AA	60	A	C4-C5-C6	-5.67	114.17	117.00
21	AA	1102	A	N1-C6-N6	-5.67	115.20	118.60
54	BA	278	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	610	C	O4'-C1'-N1	5.67	112.73	108.20
54	BA	796	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1012	U	N3-C2-O2	-5.67	118.23	122.20
54	BA	1985	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2342	C	O4'-C1'-N1	5.67	112.73	108.20
54	BA	319	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	459	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	592	G	N1-C6-O6	-5.66	116.50	119.90
21	AA	998	C	N3-C2-O2	-5.66	117.94	121.90
24	A3	57	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	723	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1629	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1763	G	C5-C6-N1	5.66	114.33	111.50
21	AA	689	C	O4'-C1'-N1	5.66	112.73	108.20
21	AA	896	C	N3-C2-O2	-5.66	117.94	121.90
22	A1	56	C	N1-C2-O2	5.66	122.30	118.90
54	BA	138	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	838	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	2645	G	O4'-C1'-N9	5.66	112.73	108.20
54	BA	255	A	C5-C6-N1	5.66	120.53	117.70
54	BA	435	C	N3-C4-C5	5.66	124.16	121.90
54	BA	979	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1809	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2232	C	N1-C2-O2	5.66	122.30	118.90
54	BA	2301	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	2467	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	43	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	16	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	520	G	O4'-C1'-N9	5.66	112.73	108.20
54	BA	1557	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1773	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2310	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	661	G	N1-C6-O6	-5.66	116.51	119.90
54	BA	208	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1658	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1700	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2601	C	N3-C2-O2	-5.66	117.94	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	167	A	C5-C6-N1	5.65	120.53	117.70
54	BA	2274	A	C4-C5-C6	-5.65	114.17	117.00
21	AA	68	G	N3-C2-N2	-5.65	115.94	119.90
21	AA	575	G	N1-C6-O6	-5.65	116.51	119.90
21	AA	1369	C	N1-C2-O2	5.65	122.29	118.90
54	BA	2678	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	743	A	C4-C5-C6	-5.65	114.17	117.00
21	AA	1263	C	O4'-C1'-N1	5.65	112.72	108.20
24	A3	17	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	772	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	818	G	P-O3'-C3'	5.65	126.48	119.70
54	BA	1934	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	2624	G	C5'-C4'-C3'	-5.65	106.96	116.00
55	BB	69	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	1141	U	C3'-C2'-C1'	5.65	106.02	101.50
54	BA	2671	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	724	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	787	C	N1-C2-O2	5.65	122.29	118.90
54	BA	2802	G	O4'-C1'-N9	5.65	112.72	108.20
21	AA	559	A	C4-C5-C6	-5.65	114.18	117.00
28	BF	70	ARG	NE-CZ-NH1	5.65	123.12	120.30
54	BA	816	C	N1-C2-O2	5.65	122.29	118.90
54	BA	2065	C	N3-C2-O2	-5.65	117.95	121.90
54	BA	2295	C	N3-C2-O2	-5.65	117.95	121.90
24	A3	35	C	N1-C2-O2	5.64	122.29	118.90
54	BA	565	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	831	G	O4'-C1'-N9	5.64	112.72	108.20
54	BA	847	U	N3-C2-O2	-5.64	118.25	122.20
35	BM	50	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	47	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	709	U	O4'-C1'-N1	5.64	112.71	108.20
54	BA	1130	U	O4'-C1'-N1	5.64	112.72	108.20
54	BA	1625	C	N1-C2-O2	5.64	122.29	118.90
54	BA	2047	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2374	C	N1-C2-O2	5.64	122.28	118.90
54	BA	210	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	527	C	P-O3'-C3'	5.64	126.47	119.70
54	BA	1531	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2354	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2495	G	O4'-C1'-N9	5.64	112.71	108.20
21	AA	1388	C	N3-C2-O2	-5.64	117.95	121.90
24	A3	76	C	N3-C2-O2	-5.64	117.95	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	948	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	1818	U	O4'-C1'-N1	5.64	112.71	108.20
54	BA	1936	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2384	U	O4'-C1'-N1	5.64	112.71	108.20
54	BA	2721	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	974	G	N1-C6-O6	-5.64	116.52	119.90
54	BA	2440	C	N1-C2-O2	5.64	122.28	118.90
13	AN	61	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	517	C	N1-C2-O2	5.64	122.28	118.90
55	BB	12	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	426	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	746	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	2463	C	O4'-C1'-N1	5.63	112.71	108.20
54	BA	2870	C	N1-C2-O2	5.63	122.28	118.90
23	A2	79	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	1415	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	1658	C	O4'-C1'-N1	5.63	112.71	108.20
54	BA	2737	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	1289	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	2261	C	N1-C2-O2	5.63	122.28	118.90
21	AA	795	C	N1-C2-O2	5.63	122.28	118.90
25	BC	13	ARG	NE-CZ-NH1	5.63	123.11	120.30
25	BC	174	ARG	NE-CZ-NH1	5.63	123.11	120.30
54	BA	2538	C	O4'-C1'-N1	5.63	112.70	108.20
21	AA	300	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1271	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	2082	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	2740	A	C4-C5-C6	-5.63	114.19	117.00
55	BB	80	U	O4'-C1'-N1	5.63	112.70	108.20
24	A3	66	C	N1-C2-O2	5.62	122.28	118.90
54	BA	979	A	C5'-C4'-O4'	5.62	115.85	109.10
21	AA	422	C	N1-C2-O2	5.62	122.27	118.90
54	BA	542	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	717	C	N1-C2-O2	5.62	122.27	118.90
6	AG	108	ARG	NE-CZ-NH2	-5.62	117.49	120.30
21	AA	1394	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	899	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1050	A	N1-C6-N6	-5.62	115.23	118.60
54	BA	1526	C	O4'-C1'-N1	5.62	112.70	108.20
54	BA	322	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	671	G	N9-C4-C5	5.62	107.65	105.40
21	AA	129	A	C4-C5-C6	-5.62	114.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	546	U	N3-C2-O2	-5.62	118.27	122.20
54	BA	770	G	O4'-C1'-N9	5.62	112.69	108.20
21	AA	383	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1448	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	2117	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2861	U	O4'-C1'-N1	5.62	112.69	108.20
55	BB	71	C	N3-C2-O2	-5.62	117.97	121.90
11	AL	13	ARG	NE-CZ-NH1	5.61	123.11	120.30
21	AA	44	A	C4-C5-C6	-5.61	114.19	117.00
22	A1	35	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	2091	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	2656	U	C1'-O4'-C4'	-5.61	105.41	109.90
54	BA	2822	G	N3-C4-C5	-5.61	125.79	128.60
2	AC	58	ARG	NE-CZ-NH2	-5.61	117.49	120.30
21	AA	121	U	C3'-C2'-C1'	5.61	105.99	101.50
21	AA	941	G	N9-C4-C5	5.61	107.64	105.40
54	BA	1585	C	O4'-C1'-N1	5.61	112.69	108.20
21	AA	1460	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	343	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	894	U	C5-C6-N1	-5.61	119.89	122.70
54	BA	990	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	1367	A	N1-C6-N6	-5.61	115.23	118.60
54	BA	2710	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	845	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	316	C	O4'-C1'-N1	5.61	112.69	108.20
21	AA	576	C	C1'-O4'-C4'	-5.61	105.41	109.90
26	BD	59	ARG	NE-CZ-NH1	5.61	123.10	120.30
54	BA	105	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	134	G	N1-C6-O6	-5.61	116.54	119.90
54	BA	1545	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	2018	G	N1-C6-O6	-5.61	116.53	119.90
21	AA	251	G	N3-C4-C5	-5.61	125.80	128.60
21	AA	1347	G	O4'-C1'-N9	5.61	112.69	108.20
54	BA	1354	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	1638	C	N1-C2-O2	5.61	122.26	118.90
21	AA	105	G	N3-C2-N2	-5.60	115.98	119.90
21	AA	1128	C	N1-C2-O2	5.60	122.26	118.90
54	BA	191	A	O4'-C1'-N9	5.60	112.68	108.20
54	BA	418	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	1180	U	O4'-C1'-N1	5.60	112.68	108.20
54	BA	1443	U	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2795	C	N1-C2-O2	5.60	122.26	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AH	53	ASP	C-N-CA	5.60	135.71	121.70
45	BW	13	ARG	NE-CZ-NH1	5.60	123.10	120.30
54	BA	274	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	467	G	O4'-C1'-N9	5.60	112.68	108.20
54	BA	643	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	741	U	C5'-C4'-O4'	5.60	115.82	109.10
54	BA	2670	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	17	U	C1'-O4'-C4'	-5.60	105.42	109.90
21	AA	1251	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	431	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	658	C	N3-C2-O2	-5.60	117.98	121.90
21	AA	697	U	O4'-C1'-N1	5.60	112.68	108.20
54	BA	447	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1103	A	C4-C5-C6	-5.60	114.20	117.00
22	A1	6	A	C4-C5-C6	-5.60	114.20	117.00
25	BC	237	ARG	NE-CZ-NH1	5.60	123.10	120.30
54	BA	54	G	N3-C2-N2	-5.60	115.98	119.90
54	BA	1365	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1543	G	C5-C6-N1	5.60	114.30	111.50
21	AA	205	A	N1-C6-N6	-5.59	115.24	118.60
21	AA	892	A	C4-C5-C6	-5.59	114.20	117.00
22	A1	72	C	N3-C2-O2	-5.59	117.98	121.90
54	BA	1887	C	N1-C2-O2	5.59	122.26	118.90
54	BA	2243	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	1147	A	O4'-C1'-N9	5.59	112.67	108.20
54	BA	1150	C	N3-C2-O2	-5.59	117.99	121.90
2	AC	125	ARG	NE-CZ-NH1	5.59	123.09	120.30
15	AP	14	ARG	NE-CZ-NH1	5.59	123.09	120.30
21	AA	753	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	781	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	1342	C	N3-C2-O2	-5.59	117.99	121.90
22	A1	17	U	N3-C2-O2	-5.59	118.29	122.20
54	BA	52	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	273	G	N1-C6-O6	-5.59	116.55	119.90
54	BA	353	C	N1-C2-O2	5.59	122.25	118.90
54	BA	758	C	O4'-C1'-N1	5.59	112.67	108.20
54	BA	1559	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	1689	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	1980	G	N3-C4-C5	-5.59	125.81	128.60
54	BA	2273	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	2510	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2368	C	O4'-C1'-N1	5.59	112.67	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	152	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	160	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	1895	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2774	C	O4'-C1'-N1	5.59	112.67	108.20
6	AG	77	ARG	NE-CZ-NH1	5.58	123.09	120.30
54	BA	787	C	N3-C4-C5	5.58	124.13	121.90
54	BA	2308	G	N3-C4-C5	-5.58	125.81	128.60
54	BA	2346	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	302	G	C5-C6-N1	5.58	114.29	111.50
21	AA	288	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	640	C	O4'-C1'-N1	5.58	112.67	108.20
54	BA	686	U	O4'-C1'-N1	5.58	112.67	108.20
55	BB	116	G	N1-C6-O6	-5.58	116.55	119.90
54	BA	2303	G	N1-C6-O6	-5.58	116.55	119.90
55	BB	41	G	N1-C6-O6	-5.58	116.55	119.90
55	BB	77	U	O4'-C1'-N1	5.58	112.66	108.20
11	AL	120	ARG	NE-CZ-NH1	5.58	123.09	120.30
25	BC	188	ARG	NE-CZ-NH1	5.58	123.09	120.30
54	BA	1620	G	C8-N9-C4	-5.58	104.17	106.40
54	BA	1888	G	O4'-C1'-N9	5.58	112.66	108.20
54	BA	2039	U	O4'-C1'-N1	5.58	112.66	108.20
24	A3	40	C	C1'-O4'-C4'	-5.58	105.44	109.90
54	BA	1793	C	N1-C2-O2	5.58	122.25	118.90
21	AA	414	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	986	U	O4'-C1'-N1	5.58	112.66	108.20
21	AA	1201	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	736	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	1216	G	N1-C6-O6	-5.58	116.56	119.90
54	BA	2547	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2826	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	77	A	C4-C5-C6	-5.57	114.21	117.00
21	AA	1360	A	C4-C5-C6	-5.57	114.21	117.00
54	BA	2068	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	2720	U	O4'-C1'-N1	5.57	112.66	108.20
49	B0	51	ARG	NE-CZ-NH2	-5.57	117.52	120.30
54	BA	2356	U	N3-C2-O2	-5.57	118.30	122.20
21	AA	1476	A	C5-C6-N1	5.57	120.48	117.70
54	BA	1782	U	N3-C2-O2	-5.57	118.30	122.20
21	AA	914	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	1447	A	O4'-C1'-N9	5.57	112.66	108.20
24	A3	13	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	484	C	N1-C2-O2	5.57	122.24	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	678	C	N1-C2-O2	5.57	122.24	118.90
54	BA	759	G	C4'-C3'-C2'	-5.57	97.03	102.60
54	BA	1702	G	N1-C6-O6	-5.57	116.56	119.90
4	AE	156	ARG	NE-CZ-NH2	5.57	123.08	120.30
21	AA	1381	U	C1'-O4'-C4'	-5.57	105.45	109.90
21	AA	1496	C	N1-C2-O2	5.57	122.24	118.90
39	BQ	52	ARG	NE-CZ-NH1	5.57	123.08	120.30
54	BA	236	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	802	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	2736	A	C5-C6-N1	5.57	120.48	117.70
22	A1	60	C	N1-C2-O2	5.56	122.24	118.90
54	BA	1150	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	1809	A	O3'-P-O5'	-5.56	93.43	104.00
21	AA	416	G	C5'-C4'-C3'	-5.56	107.10	116.00
21	AA	573	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	1340	A	C6-C5-N7	5.56	136.19	132.30
22	A1	11	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	2542	A	C4-C5-C6	-5.56	114.22	117.00
34	BL	78	ARG	NE-CZ-NH1	5.56	123.08	120.30
54	BA	1008	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	209	U	O4'-C4'-C3'	5.56	110.55	106.10
54	BA	421	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	597	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	1164	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1437	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1714	U	N3-C2-O2	-5.56	118.31	122.20
54	BA	2586	U	N3-C2-O2	-5.56	118.31	122.20
54	BA	2800	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	2827	C	O4'-C1'-N1	5.56	112.65	108.20
21	AA	1051	C	N1-C2-O2	5.56	122.23	118.90
54	BA	126	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	2055	C	N1-C2-O2	5.56	122.23	118.90
54	BA	2129	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	257	C	C6-N1-C2	-5.56	118.08	120.30
54	BA	1508	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	2101	A	C4-C5-C6	-5.56	114.22	117.00
55	BB	57	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	499	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1076	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	2420	C	N1-C2-O2	5.55	122.23	118.90
46	BX	49	ARG	NE-CZ-NH2	-5.55	117.52	120.30
21	AA	1441	A	C4-C5-C6	-5.55	114.22	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	BP	52	ARG	NE-CZ-NH2	-5.55	117.52	120.30
54	BA	659	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	1552	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	2209	G	C5-C6-N1	5.55	114.28	111.50
54	BA	1054	A	C6-C5-N7	5.55	136.18	132.30
54	BA	1787	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	2338	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	2462	C	O4'-C1'-N1	5.55	112.64	108.20
21	AA	96	U	O4'-C1'-N1	5.55	112.64	108.20
21	AA	148	G	N3-C2-N2	-5.55	116.02	119.90
21	AA	332	G	N1-C6-O6	-5.55	116.57	119.90
21	AA	554	A	C4-C5-C6	-5.55	114.23	117.00
21	AA	1113	C	N1-C2-O2	5.55	122.23	118.90
54	BA	2035	G	O4'-C1'-N9	5.55	112.64	108.20
21	AA	855	U	C1'-O4'-C4'	-5.55	105.46	109.90
21	AA	1073	U	O4'-C1'-N1	5.55	112.64	108.20
21	AA	1305	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	1681	G	N3-C4-C5	-5.55	125.83	128.60
54	BA	2428	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	2327	A	C6-C5-N7	5.54	136.18	132.30
21	AA	421	U	N3-C2-O2	-5.54	118.32	122.20
21	AA	809	G	N1-C6-O6	-5.54	116.57	119.90
21	AA	1041	G	N1-C6-O6	-5.54	116.58	119.90
21	AA	1287	A	C6-C5-N7	5.54	136.18	132.30
54	BA	314	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	1451	C	P-O3'-C3'	5.54	126.35	119.70
21	AA	151	A	C6-C5-N7	5.54	136.18	132.30
21	AA	1055	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	670	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2178	C	N3-C2-O2	-5.54	118.02	121.90
37	BO	33	ARG	NE-CZ-NH1	5.54	123.07	120.30
54	BA	69	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1127	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1166	G	N9-C4-C5	5.54	107.61	105.40
54	BA	2175	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	2560	A	C4-C5-C6	-5.54	114.23	117.00
12	AM	100	ARG	NE-CZ-NH1	5.54	123.07	120.30
20	AU	20	ARG	CD-NE-CZ	5.54	131.35	123.60
21	AA	23	C	O4'-C1'-N1	5.54	112.63	108.20
21	AA	1516	G	O4'-C1'-N9	5.54	112.63	108.20
38	BP	108	ARG	NE-CZ-NH1	5.54	123.07	120.30
54	BA	267	C	O4'-C1'-N1	5.54	112.63	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2281	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2771	C	N1-C2-O2	5.54	122.22	118.90
21	AA	219	U	O4'-C1'-N1	5.53	112.63	108.20
54	BA	928	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1442	U	O4'-C1'-N1	5.53	112.63	108.20
54	BA	1790	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	488	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	1741	C	O4'-C1'-N1	5.53	112.62	108.20
45	BW	54	ARG	NE-CZ-NH1	5.53	123.06	120.30
54	BA	34	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	1542	U	O4'-C1'-N1	5.53	112.62	108.20
12	AM	28	ARG	NE-CZ-NH1	5.53	123.06	120.30
54	BA	1352	U	C4'-C3'-C2'	-5.53	97.07	102.60
54	BA	1598	A	C4-C5-C6	-5.53	114.24	117.00
21	AA	207	C	N3-C2-O2	-5.53	118.03	121.90
22	A1	9	A	C4-C5-C6	-5.53	114.24	117.00
21	AA	39	G	N1-C6-O6	-5.52	116.59	119.90
54	BA	2006	C	O4'-C1'-N1	5.52	112.62	108.20
21	AA	967	C	C1'-O4'-C4'	-5.52	105.48	109.90
21	AA	1070	U	O4'-C1'-N1	5.52	112.62	108.20
21	AA	54	C	N1-C2-O2	5.52	122.21	118.90
54	BA	209	C	O4'-C1'-N1	5.52	112.62	108.20
21	AA	311	C	N1-C2-O2	5.52	122.21	118.90
41	BS	110	ARG	NE-CZ-NH2	5.52	123.06	120.30
54	BA	453	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1050	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1205	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2070	A	C5-C6-N1	5.52	120.46	117.70
17	AR	72	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	AA	360	G	C5-C6-N1	5.52	114.26	111.50
21	AA	980	C	N3-C2-O2	-5.52	118.04	121.90
24	A3	14	A	N1-C6-N6	-5.52	115.29	118.60
54	BA	270	A	N1-C6-N6	-5.52	115.29	118.60
54	BA	957	C	N1-C2-O2	5.52	122.21	118.90
54	BA	1287	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1367	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2268	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2705	A	C4-C5-C6	-5.52	114.24	117.00
36	BN	69	ARG	NE-CZ-NH2	-5.52	117.54	120.30
54	BA	350	G	N3-C2-N2	-5.52	116.04	119.90
54	BA	647	G	O4'-C1'-N9	5.51	112.61	108.20
54	BA	2715	C	N3-C2-O2	-5.51	118.04	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AB	34	ARG	NE-CZ-NH1	5.51	123.06	120.30
12	AM	112	ARG	NE-CZ-NH2	-5.51	117.54	120.30
24	A3	11	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	152	A	C5-C6-N1	5.51	120.46	117.70
54	BA	2520	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	2183	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	2656	U	O4'-C1'-N1	5.51	112.61	108.20
24	A3	24	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	989	G	N3-C2-N2	-5.51	116.04	119.90
54	BA	1328	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	1326	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	51	G	O4'-C1'-N9	5.51	112.61	108.20
54	BA	213	A	N1-C6-N6	-5.51	115.30	118.60
54	BA	1406	U	C1'-O4'-C4'	-5.51	105.50	109.90
54	BA	1936	A	P-O3'-C3'	5.51	126.31	119.70
54	BA	2104	C	N3-C4-C5	5.51	124.10	121.90
21	AA	996	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	107	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	2238	G	O4'-C1'-N9	5.50	112.60	108.20
21	AA	545	C	N1-C2-O2	5.50	122.20	118.90
54	BA	971	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	2611	C	O4'-C1'-N1	5.50	112.60	108.20
21	AA	422	C	N3-C4-C5	5.50	124.10	121.90
51	B2	21	ARG	NE-CZ-NH1	5.50	123.05	120.30
54	BA	296	U	O4'-C1'-N1	5.50	112.60	108.20
21	AA	699	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1081	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	2332	C	N3-C4-N4	-5.50	114.15	118.00
54	BA	2772	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	328	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	513	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	830	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	54	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	789	A	O4'-C1'-N9	5.50	112.60	108.20
54	BA	1276	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1784	A	N1-C6-N6	-5.50	115.30	118.60
54	BA	2527	C	N1-C2-O2	5.50	122.20	118.90
21	AA	1093	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	606	U	C5-C6-N1	-5.49	119.95	122.70
54	BA	912	C	O4'-C1'-N1	5.49	112.60	108.20
54	BA	1345	C	N3-C2-O2	-5.49	118.05	121.90
21	AA	1072	G	N1-C6-O6	-5.49	116.61	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BE	170	ARG	NE-CZ-NH1	5.49	123.05	120.30
54	BA	2540	C	O4'-C1'-N1	5.49	112.59	108.20
23	A2	79	A	O4'-C1'-N9	5.49	112.59	108.20
24	A3	67	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	791	C	N1-C2-O2	5.49	122.19	118.90
54	BA	122	G	O4'-C1'-N9	5.49	112.59	108.20
54	BA	881	G	N3-C4-C5	-5.49	125.86	128.60
21	AA	702	A	C6-C5-N7	5.49	136.14	132.30
54	BA	1000	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	1788	C	N3-C4-C5	5.49	124.09	121.90
21	AA	428	G	N3-C4-C5	-5.49	125.86	128.60
21	AA	1030	U	N3-C2-O2	-5.49	118.36	122.20
21	AA	1295	U	O4'-C1'-N1	5.49	112.59	108.20
24	A3	22	A	N1-C6-N6	-5.49	115.31	118.60
54	BA	965	C	O4'-C1'-N1	5.49	112.59	108.20
54	BA	1664	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	2095	A	C5-C6-N1	5.49	120.44	117.70
54	BA	2766	A	C6-C5-N7	5.49	136.14	132.30
54	BA	2171	A	P-O3'-C3'	5.48	126.28	119.70
21	AA	607	A	C4-C5-C6	-5.48	114.26	117.00
24	A3	74	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	691	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	2189	U	O4'-C1'-N1	5.48	112.59	108.20
21	AA	385	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	967	C	N1-C2-O2	5.48	122.19	118.90
54	BA	748	G	C1'-O4'-C4'	-5.48	105.52	109.90
54	BA	835	C	N3-C2-O2	-5.48	118.06	121.90
6	AG	52	ARG	NE-CZ-NH1	5.48	123.04	120.30
54	BA	471	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1837	C	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2576	G	N3-C4-C5	-5.48	125.86	128.60
21	AA	898	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	1946	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2227	A	C4'-C3'-C2'	-5.48	97.12	102.60
21	AA	1479	C	N1-C2-O2	5.48	122.19	118.90
54	BA	144	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1530	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	2248	C	N1-C2-O2	5.47	122.19	118.90
11	AL	11	ARG	NE-CZ-NH1	5.47	123.04	120.30
21	AA	306	A	C4-C5-C6	-5.47	114.26	117.00
44	BV	9	ARG	NE-CZ-NH1	5.47	123.04	120.30
52	B3	1	PRO	CA-N-CD	-5.47	103.84	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1347	A	C4-C5-C6	-5.47	114.26	117.00
54	BA	1612	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	1724	G	C5'-C4'-O4'	5.47	115.67	109.10
54	BA	1868	C	N3-C2-O2	-5.47	118.07	121.90
2	AC	142	ARG	NE-CZ-NH1	5.47	123.04	120.30
54	BA	1322	A	C4-C5-C6	-5.47	114.26	117.00
54	BA	2050	C	N1-C2-O2	5.47	122.18	118.90
54	BA	2669	G	C4'-C3'-C2'	-5.47	97.13	102.60
21	AA	21	G	N1-C6-O6	-5.47	116.62	119.90
21	AA	188	C	N1-C2-O2	5.47	122.18	118.90
54	BA	1418	G	N1-C6-O6	-5.47	116.62	119.90
21	AA	100	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	1608	A	N1-C6-N6	-5.47	115.32	118.60
54	BA	1975	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	2060	A	N1-C6-N6	-5.47	115.32	118.60
55	BB	96	G	N1-C6-O6	-5.47	116.62	119.90
21	AA	1284	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	1156	A	O4'-C1'-N9	5.47	112.57	108.20
54	BA	1565	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	1145	C	N1-C2-O2	5.46	122.18	118.90
54	BA	2267	A	C4-C5-C6	-5.46	114.27	117.00
55	BB	99	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	919	A	C6-C5-N7	5.46	136.12	132.30
8	AI	128	LYS	C-N-CA	5.46	135.35	121.70
21	AA	475	C	N3-C4-N4	-5.46	114.18	118.00
21	AA	751	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	105	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	1192	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	198	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	226	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2358	A	C6-C5-N7	5.46	136.12	132.30
21	AA	687	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1791	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2858	C	C3'-C2'-C1'	5.46	105.87	101.50
21	AA	363	A	C6-C5-N7	5.46	136.12	132.30
54	BA	331	C	O4'-C1'-N1	5.46	112.57	108.20
54	BA	886	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1229	C	N1-C2-O2	5.46	122.17	118.90
24	A3	22	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	171	U	O4'-C1'-N1	5.46	112.56	108.20
54	BA	2595	G	C4'-C3'-C2'	-5.46	97.14	102.60
21	AA	268	U	C5-C6-N1	-5.45	119.97	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	872	A	C4-C5-C6	-5.45	114.27	117.00
22	A1	68	C	N3-C2-O2	-5.45	118.08	121.90
24	A3	58	A	C4-C5-C6	-5.45	114.27	117.00
37	BO	111	ARG	NE-CZ-NH1	5.45	123.03	120.30
54	BA	95	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	698	C	N1-C2-O2	5.45	122.17	118.90
54	BA	894	U	O4'-C1'-N1	5.45	112.56	108.20
54	BA	1966	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	2663	G	C5-C6-N1	5.45	114.23	111.50
54	BA	1092	C	N3-C2-O2	-5.45	118.08	121.90
54	BA	1102	C	O4'-C1'-N1	5.45	112.56	108.20
54	BA	819	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	450	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	1996	C	N1-C2-O2	5.45	122.17	118.90
54	BA	2566	A	C4-C5-C6	-5.45	114.28	117.00
55	BB	64	G	O4'-C1'-N9	5.45	112.56	108.20
21	AA	721	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	1254	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	1929	G	O4'-C1'-N9	5.45	112.56	108.20
54	BA	2191	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	145	G	N3-C2-N2	-5.45	116.09	119.90
54	BA	1301	A	O4'-C1'-N9	5.45	112.56	108.20
21	AA	18	C	N3-C2-O2	-5.44	118.09	121.90
21	AA	1489	G	N1-C6-O6	-5.44	116.63	119.90
55	BB	37	C	O4'-C1'-N1	5.44	112.56	108.20
33	BK	49	ARG	NE-CZ-NH1	5.44	123.02	120.30
54	BA	1783	A	P-O3'-C3'	5.44	126.23	119.70
54	BA	1859	U	O4'-C1'-N1	5.44	112.56	108.20
21	AA	408	A	C6-C5-N7	5.44	136.11	132.30
21	AA	913	A	C6-C5-N7	5.44	136.11	132.30
54	BA	2648	G	N3-C2-N2	-5.44	116.09	119.90
54	BA	2716	C	N1-C2-O2	5.44	122.16	118.90
21	AA	1228	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	1152	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	1845	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	10	A	C6-C5-N7	5.44	136.10	132.30
54	BA	45	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	2806	C	N1-C2-O2	5.44	122.16	118.90
54	BA	221	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	440	C	O4'-C1'-N1	5.43	112.55	108.20
54	BA	1254	A	C3'-C2'-C1'	5.43	105.85	101.50
54	BA	1579	A	C4-C5-C6	-5.43	114.28	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1617	C	N3-C2-O2	-5.43	118.09	121.90
54	BA	2855	C	N3-C4-C5	5.43	124.07	121.90
21	AA	492	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	1357	A	C6-C5-N7	5.43	136.10	132.30
54	BA	634	C	O4'-C1'-N1	5.43	112.55	108.20
54	BA	2733	A	C6-C5-N7	5.43	136.10	132.30
21	AA	8	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	285	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	1126	U	O4'-C1'-N1	5.43	112.54	108.20
54	BA	506	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1158	C	N1-C2-O2	5.43	122.16	118.90
54	BA	1602	U	O4'-C1'-N1	5.43	112.54	108.20
21	AA	308	C	N1-C2-O2	5.43	122.16	118.90
21	AA	643	C	N3-C2-O2	-5.43	118.10	121.90
34	BL	123	ARG	NE-CZ-NH1	5.43	123.01	120.30
54	BA	342	A	C6-C5-N7	5.43	136.10	132.30
54	BA	947	A	C6-C5-N7	5.43	136.10	132.30
54	BA	2021	C	N1-C2-O2	5.43	122.16	118.90
1	AB	62	ARG	NE-CZ-NH1	5.42	123.01	120.30
21	AA	1462	C	N1-C2-O2	5.42	122.16	118.90
21	AA	1521	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	2821	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	349	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2233	U	C5'-C4'-O4'	5.42	115.61	109.10
21	AA	392	C	N1-C2-O2	5.42	122.15	118.90
54	BA	1022	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	2226	C	O4'-C1'-N1	5.42	112.54	108.20
21	AA	130	A	C2-N3-C4	5.42	113.31	110.60
21	AA	575	G	C5-C6-N1	5.42	114.21	111.50
55	BB	92	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	108	G	C5-C6-N1	5.42	114.21	111.50
54	BA	364	C	N1-C2-O2	5.42	122.15	118.90
54	BA	410	G	C8-N9-C4	-5.42	104.23	106.40
21	AA	713	G	O4'-C1'-N9	5.42	112.53	108.20
21	AA	938	A	C6-C5-N7	5.42	136.09	132.30
54	BA	1072	C	O4'-C1'-N1	5.42	112.53	108.20
54	BA	1617	C	O4'-C1'-N1	5.42	112.53	108.20
54	BA	1964	G	N3-C4-N9	5.42	129.25	126.00
22	A1	58	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	218	A	C6-C5-N7	5.42	136.09	132.30
54	BA	2652	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	1428	A	C4-C5-C6	-5.41	114.29	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	76	A	C8-N9-C4	-5.41	103.63	105.80
54	BA	549	G	N1-C6-O6	-5.41	116.65	119.90
54	BA	941	A	O4'-C1'-N9	5.41	112.53	108.20
54	BA	446	G	C3'-C2'-C1'	5.41	105.83	101.50
54	BA	479	A	P-O3'-C3'	5.41	126.19	119.70
24	A3	36	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1762	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	462	G	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	1300	G	N3-C4-C5	-5.41	125.90	128.60
24	A3	77	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	345	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	885	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	1266	G	N3-C4-C5	-5.41	125.90	128.60
54	BA	1728	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1778	U	N3-C2-O2	-5.41	118.41	122.20
54	BA	2079	U	O4'-C1'-N1	5.41	112.53	108.20
21	AA	1182	G	N3-C4-C5	-5.41	125.90	128.60
21	AA	171	A	C6-C5-N7	5.41	136.08	132.30
22	A1	18	G	N1-C6-O6	-5.41	116.66	119.90
54	BA	493	G	N1-C6-O6	-5.41	116.66	119.90
54	BA	510	C	N1-C2-O2	5.41	122.14	118.90
54	BA	1575	C	N1-C2-O2	5.41	122.14	118.90
54	BA	2178	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2503	A	C4-C5-C6	-5.41	114.30	117.00
55	BB	89	U	N3-C2-O2	-5.41	118.42	122.20
54	BA	2326	C	N3-C4-C5	5.40	124.06	121.90
21	AA	917	G	C8-N9-C4	-5.40	104.24	106.40
24	A3	59	A	C4-C5-C6	-5.40	114.30	117.00
34	BL	126	ARG	NE-CZ-NH1	5.40	123.00	120.30
54	BA	800	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1901	A	C5-C6-N1	5.40	120.40	117.70
55	BB	47	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	868	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	1137	C	N3-C4-C5	5.40	124.06	121.90
54	BA	927	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1089	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2208	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	195	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	839	C	N1-C2-O2	5.40	122.14	118.90
23	A2	90	U	O4'-C4'-C3'	-5.40	98.60	104.00
37	BO	9	ARG	NE-CZ-NH1	5.40	123.00	120.30
54	BA	470	A	C4-C5-C6	-5.40	114.30	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	611	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	829	A	O4'-C1'-N9	5.40	112.52	108.20
21	AA	885	G	N1-C6-O6	-5.40	116.66	119.90
21	AA	1005	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2000	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	1354	U	O4'-C1'-N1	5.40	112.52	108.20
55	BB	80	U	C5-C6-N1	-5.40	120.00	122.70
21	AA	754	C	N1-C2-O2	5.39	122.14	118.90
51	B2	39	ARG	NE-CZ-NH1	5.39	123.00	120.30
54	BA	457	A	C6-C5-N7	5.39	136.08	132.30
54	BA	554	U	C5-C6-N1	-5.39	120.00	122.70
54	BA	735	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	815	C	N3-C2-O2	-5.39	118.12	121.90
54	BA	893	C	C4'-C3'-C2'	-5.39	97.21	102.60
54	BA	1339	G	O4'-C1'-N9	5.39	112.52	108.20
54	BA	1675	C	N3-C4-C5	5.39	124.06	121.90
21	AA	217	C	N1-C2-O2	5.39	122.14	118.90
21	AA	1137	C	N1-C2-O2	5.39	122.14	118.90
21	AA	1227	A	O4'-C1'-N9	5.39	112.51	108.20
21	AA	1502	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	205	G	N3-C4-C5	-5.39	125.90	128.60
54	BA	1423	G	O4'-C1'-N9	5.39	112.52	108.20
54	BA	1709	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1711	A	C6-C5-N7	5.39	136.07	132.30
54	BA	2031	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	2150	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	358	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1739	A	N1-C6-N6	-5.39	115.37	118.60
54	BA	1990	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	2527	C	C5'-C4'-O4'	5.39	115.57	109.10
54	BA	1362	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	2276	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	1828	G	P-O3'-C3'	5.39	126.17	119.70
54	BA	1833	C	N1-C2-O2	5.39	122.13	118.90
19	AT	17	ARG	NE-CZ-NH1	5.39	122.99	120.30
21	AA	249	U	N3-C2-O2	-5.39	118.43	122.20
54	BA	2480	C	O4'-C1'-N1	5.39	112.51	108.20
21	AA	121	U	N3-C2-O2	-5.38	118.43	122.20
54	BA	917	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1091	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1393	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1620	G	N3-C4-C5	-5.38	125.91	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1640	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1808	A	O4'-C1'-N9	5.38	112.51	108.20
54	BA	2606	C	N1-C2-O2	5.38	122.13	118.90
54	BA	2893	A	N1-C6-N6	-5.38	115.37	118.60
21	AA	820	U	N3-C2-O2	-5.38	118.43	122.20
21	AA	1119	C	O4'-C1'-N1	5.38	112.51	108.20
21	AA	1196	A	C1'-O4'-C4'	-5.38	105.59	109.90
24	A3	7	G	O4'-C1'-N9	5.38	112.51	108.20
54	BA	16	C	P-O3'-C3'	5.38	126.16	119.70
54	BA	544	C	N3-C4-C5	5.38	124.05	121.90
54	BA	850	U	N3-C2-O2	-5.38	118.43	122.20
54	BA	1985	C	O4'-C1'-N1	5.38	112.51	108.20
54	BA	2539	C	O4'-C1'-N1	5.38	112.51	108.20
21	AA	1337	G	N3-C4-C5	-5.38	125.91	128.60
21	AA	7	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	563	A	C6-C5-N7	5.38	136.07	132.30
54	BA	983	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1488	C	N3-C2-O2	-5.38	118.13	121.90
54	BA	878	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1141	U	N1-C2-N3	5.38	118.13	114.90
54	BA	1526	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	2003	A	C6-C5-N7	5.38	136.06	132.30
54	BA	2188	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	2317	A	C6-C5-N7	5.38	136.06	132.30
54	BA	2850	A	O4'-C1'-N9	5.38	112.50	108.20
55	BB	68	C	N3-C2-O2	-5.38	118.14	121.90
21	AA	114	U	O4'-C1'-N1	5.38	112.50	108.20
21	AA	292	G	C3'-C2'-C1'	5.38	105.80	101.50
21	AA	784	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1537	G	C5'-C4'-O4'	5.38	115.55	109.10
54	BA	2096	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	2104	C	N1-C2-O2	5.38	122.12	118.90
17	AR	62	ARG	NE-CZ-NH2	5.37	122.99	120.30
54	BA	672	C	C1'-O4'-C4'	-5.37	105.60	109.90
54	BA	2517	C	N1-C2-O2	5.37	122.12	118.90
21	AA	819	A	C4-C5-C6	-5.37	114.31	117.00
21	AA	970	C	N1-C2-O2	5.37	122.12	118.90
54	BA	856	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	808	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2429	G	N1-C6-O6	-5.37	116.68	119.90
16	AQ	61	ARG	NE-CZ-NH1	5.37	122.98	120.30
25	BC	176	ARG	NE-CZ-NH1	5.37	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BI	64	ARG	NE-CZ-NH2	-5.37	117.62	120.30
54	BA	835	C	O4'-C1'-N1	5.37	112.49	108.20
21	AA	85	U	O4'-C1'-N1	5.37	112.49	108.20
21	AA	196	A	C4-C5-C6	-5.37	114.32	117.00
54	BA	84	A	C6-C5-N7	5.37	136.06	132.30
54	BA	2045	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2153	C	N1-C2-O2	5.37	122.12	118.90
21	AA	940	C	N3-C2-O2	-5.36	118.15	121.90
32	BJ	37	ARG	NE-CZ-NH2	-5.36	117.62	120.30
54	BA	621	A	C5'-C4'-C3'	-5.36	107.42	116.00
54	BA	989	G	N9-C4-C5	5.36	107.55	105.40
54	BA	2023	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2538	C	N1-C2-O2	5.36	122.12	118.90
55	BB	94	A	C6-C5-N7	5.36	136.06	132.30
21	AA	746	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	826	C	N1-C2-O2	5.36	122.12	118.90
24	A3	60	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	13	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	561	G	C5-C6-N1	5.36	114.18	111.50
54	BA	2739	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1969	A	N1-C6-N6	-5.36	115.39	118.60
54	BA	2146	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	239	U	C5'-C4'-C3'	-5.36	107.43	116.00
21	AA	665	A	C6-C5-N7	5.36	136.05	132.30
51	B2	41	ARG	NE-CZ-NH1	5.36	122.98	120.30
54	BA	349	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	404	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	1519	A	C6-C5-N7	5.36	136.05	132.30
54	BA	1114	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	1739	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1758	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	1768	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	765	G	C5-C6-N1	5.35	114.18	111.50
21	AA	1239	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	1490	U	N3-C2-O2	-5.35	118.45	122.20
54	BA	369	U	C5-C6-N1	-5.35	120.02	122.70
54	BA	1522	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	17	U	O4'-C1'-N1	5.35	112.48	108.20
21	AA	1185	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	942	G	O4'-C1'-N9	5.35	112.48	108.20
21	AA	448	A	C4-C5-C6	-5.35	114.33	117.00
21	AA	1490	U	C1'-O4'-C4'	-5.35	105.62	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	917	G	N7-C8-N9	5.35	115.78	113.10
54	BA	6	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	1218	G	C5-C6-N1	5.35	114.17	111.50
54	BA	1478	G	N3-C2-N2	-5.35	116.16	119.90
54	BA	1962	C	N1-C2-O2	5.35	122.11	118.90
54	BA	2089	C	N1-C2-O2	5.35	122.11	118.90
21	AA	208	U	N3-C2-O2	-5.35	118.46	122.20
22	A1	72	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	1433	A	N1-C6-N6	-5.35	115.39	118.60
54	BA	1724	G	C5-C6-N1	5.35	114.17	111.50
54	BA	1882	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2421	G	N3-C4-C5	-5.35	125.93	128.60
21	AA	792	A	O4'-C1'-N9	5.35	112.48	108.20
22	A1	73	A	O4'-C1'-N9	5.35	112.48	108.20
54	BA	1421	G	P-O3'-C3'	5.34	126.11	119.70
54	BA	2734	A	C6-C5-N7	5.34	136.04	132.30
54	BA	661	A	C5'-C4'-O4'	5.34	115.51	109.10
21	AA	101	A	C6-C5-N7	5.34	136.04	132.30
21	AA	837	U	N1-C2-N3	5.34	118.11	114.90
21	AA	1069	C	N1-C2-O2	5.34	122.11	118.90
39	BQ	54	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BA	1349	C	N3-C4-C5	5.34	124.04	121.90
54	BA	1894	C	N1-C2-O2	5.34	122.11	118.90
21	AA	647	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	207	A	N1-C6-N6	-5.34	115.40	118.60
54	BA	492	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	1300	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	1853	A	C6-C5-N7	5.34	136.04	132.30
54	BA	1267	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2565	A	O4'-C1'-N9	5.34	112.47	108.20
21	AA	742	G	C5-C6-N1	5.34	114.17	111.50
21	AA	1383	C	N1-C2-O2	5.34	122.10	118.90
54	BA	1189	A	C4-C5-C6	-5.34	114.33	117.00
9	AJ	7	ARG	NE-CZ-NH1	5.33	122.97	120.30
29	BG	162	ARG	NE-CZ-NH2	-5.33	117.63	120.30
54	BA	752	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	724	G	C5'-C4'-C3'	-5.33	107.47	116.00
54	BA	280	U	N3-C2-O2	-5.33	118.47	122.20
54	BA	1893	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	2202	U	C4'-C3'-C2'	-5.33	97.27	102.60
54	BA	2297	A	C5-C6-N1	5.33	120.37	117.70
24	A3	6	G	O4'-C1'-N9	5.33	112.47	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	11	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	2535	G	N3-C2-N2	-5.33	116.17	119.90
54	BA	1132	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	1766	G	C5-C6-N1	5.33	114.17	111.50
55	BB	33	G	N1-C6-O6	-5.33	116.70	119.90
3	AD	114	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
54	BA	785	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	801	G	C5-C6-N1	5.33	114.16	111.50
54	BA	1807	G	N3-C2-N2	-5.33	116.17	119.90
22	A1	44	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	1332	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	612	C	N1-C2-O2	5.33	122.09	118.90
54	BA	553	G	C5'-C4'-O4'	5.33	115.49	109.10
54	BA	902	C	N3-C2-O2	-5.33	118.17	121.90
55	BB	45	A	C6-C5-N7	5.33	136.03	132.30
21	AA	528	C	N1-C2-O2	5.32	122.09	118.90
54	BA	121	G	N3-C2-N2	-5.32	116.17	119.90
21	AA	495	A	C4-C5-C6	-5.32	114.34	117.00
51	B2	14	ARG	NE-CZ-NH1	5.32	122.96	120.30
54	BA	435	C	N1-C2-O2	5.32	122.09	118.90
54	BA	935	C	C3'-C2'-C1'	-5.32	97.24	101.50
54	BA	2394	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	715	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	1224	U	C5-C6-N1	-5.32	120.04	122.70
21	AA	1230	C	O4'-C1'-N1	5.32	112.45	108.20
21	AA	1498	U	N3-C2-O2	-5.32	118.48	122.20
9	AJ	62	ARG	CD-NE-CZ	5.32	131.04	123.60
21	AA	1017	U	O4'-C1'-N1	5.32	112.45	108.20
21	AA	1277	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1272	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	1366	C	N1-C2-O2	5.32	122.09	118.90
54	BA	220	G	N3-C4-C5	-5.32	125.94	128.60
54	BA	2044	C	N3-C4-C5	5.32	124.03	121.90
54	BA	2649	C	O4'-C1'-N1	5.32	112.45	108.20
21	AA	40	C	O4'-C1'-N1	5.31	112.45	108.20
54	BA	563	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	1708	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	173	U	C1'-O4'-C4'	-5.31	105.65	109.90
21	AA	331	G	O4'-C4'-C3'	5.31	110.35	106.10
38	BP	112	ARG	NE-CZ-NH2	-5.31	117.64	120.30
54	BA	1569	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	2872	A	C4-C5-C6	-5.31	114.34	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AK	92	ARG	NE-CZ-NH2	-5.31	117.64	120.30
24	A3	1	C	N1-C2-O2	5.31	122.09	118.90
54	BA	1082	U	N3-C2-O2	-5.31	118.48	122.20
54	BA	2815	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	395	C	N1-C2-O2	5.31	122.09	118.90
21	AA	992	U	N3-C2-O2	-5.31	118.48	122.20
54	BA	182	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	1742	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	2443	C	C5'-C4'-O4'	5.31	115.47	109.10
24	A3	29	C	N3-C4-N4	-5.31	114.28	118.00
54	BA	401	A	C6-C5-N7	5.31	136.02	132.30
54	BA	974	G	C5-C6-N1	5.31	114.15	111.50
54	BA	1308	A	O4'-C1'-N9	5.31	112.45	108.20
54	BA	1521	G	N1-C6-O6	-5.31	116.72	119.90
54	BA	2115	G	N3-C4-C5	-5.31	125.95	128.60
54	BA	2171	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	2011	U	O4'-C1'-N1	5.31	112.44	108.20
54	BA	771	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	1021	A	C6-C5-N7	5.30	136.01	132.30
54	BA	1376	C	N3-C4-N4	-5.30	114.29	118.00
55	BB	69	G	O4'-C1'-N9	5.30	112.44	108.20
22	A1	26	A	C6-C5-N7	5.30	136.01	132.30
54	BA	213	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1386	C	N1-C2-O2	5.30	122.08	118.90
23	A2	93	U	N3-C2-O2	-5.30	118.49	122.20
35	BM	40	ARG	NE-CZ-NH1	5.30	122.95	120.30
54	BA	720	U	C5-C6-N1	-5.30	120.05	122.70
54	BA	1137	G	C5'-C4'-O4'	5.30	115.46	109.10
54	BA	1253	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1403	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	2130	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	2500	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	163	C	N3-C4-C5	5.30	124.02	121.90
21	AA	305	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	372	C	N3-C4-C5	5.30	124.02	121.90
21	AA	475	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2073	C	O4'-C1'-N1	5.30	112.44	108.20
55	BB	110	C	N1-C2-O2	5.30	122.08	118.90
54	BA	1667	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	1151	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	74	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1885	A	C4-C5-C6	-5.30	114.35	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1096	C	N1-C2-O2	5.29	122.08	118.90
54	BA	1385	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	1424	G	C3'-C2'-C1'	5.29	105.74	101.50
54	BA	1759	A	C4-C5-C6	-5.29	114.35	117.00
21	AA	883	C	N1-C2-O2	5.29	122.08	118.90
30	BH	68	ARG	NE-CZ-NH1	5.29	122.95	120.30
54	BA	462	C	N3-C2-O2	-5.29	118.19	121.90
54	BA	1881	C	N1-C2-O2	5.29	122.08	118.90
54	BA	2411	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	2773	C	N3-C2-O2	-5.29	118.19	121.90
54	BA	863	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	1732	C	N1-C2-O2	5.29	122.07	118.90
54	BA	2516	A	C6-C5-N7	5.29	136.00	132.30
21	AA	176	C	N1-C2-O2	5.29	122.07	118.90
54	BA	60	G	C1'-O4'-C4'	-5.29	105.67	109.90
54	BA	877	A	C6-C5-N7	5.29	136.00	132.30
54	BA	1171	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	1371	G	O4'-C1'-N9	5.29	112.43	108.20
54	BA	2269	G	N1-C6-O6	-5.29	116.73	119.90
21	AA	907	A	C4-C5-C6	-5.29	114.36	117.00
21	AA	966	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	806	C	N3-C4-C5	5.29	124.01	121.90
54	BA	810	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	915	C	O4'-C1'-N1	5.28	112.43	108.20
54	BA	1334	G	C5-C6-N1	5.28	114.14	111.50
54	BA	1518	C	N1-C2-O2	5.28	122.07	118.90
54	BA	1537	G	N3-C4-C5	-5.28	125.96	128.60
54	BA	2133	G	N3-C2-N2	-5.28	116.20	119.90
54	BA	2142	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	2702	G	N3-C2-N2	-5.28	116.20	119.90
21	AA	1231	G	N3-C4-C5	-5.28	125.96	128.60
54	BA	514	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1562	U	C5-C6-N1	-5.28	120.06	122.70
54	BA	2645	G	C5-C6-N1	5.28	114.14	111.50
54	BA	115	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2844	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	821	A	O4'-C1'-N9	5.28	112.42	108.20
54	BA	1541	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	1641	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	2491	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	256	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	732	C	N3-C4-N4	-5.28	114.31	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1442	U	C5-C6-N1	-5.28	120.06	122.70
54	BA	2811	G	N1-C6-O6	-5.28	116.73	119.90
21	AA	95	C	N1-C2-O2	5.28	122.06	118.90
21	AA	330	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	1583	A	C4-C5-C6	-5.28	114.36	117.00
55	BB	41	G	N3-C4-C5	-5.28	125.96	128.60
55	BB	63	C	O4'-C1'-N1	5.28	112.42	108.20
21	AA	1234	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	1054	C	N1-C2-O2	5.27	122.06	118.90
23	A2	88	U	N3-C2-O2	-5.27	118.51	122.20
54	BA	1942	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	2058	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	2501	C	C1'-O4'-C4'	-5.27	105.68	109.90
54	BA	2835	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	998	C	N1-C2-O2	5.27	122.06	118.90
54	BA	1024	G	C5-C6-N1	5.27	114.14	111.50
17	AR	60	ARG	NE-CZ-NH1	5.27	122.94	120.30
21	AA	1374	A	C4-C5-C6	-5.27	114.37	117.00
54	BA	481	G	C8-N9-C4	-5.27	104.29	106.40
54	BA	1092	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	1505	A	C6-C5-N7	5.27	135.99	132.30
54	BA	1602	U	C5-C6-N1	-5.27	120.06	122.70
54	BA	1644	C	N1-C2-O2	5.27	122.06	118.90
21	AA	765	G	N3-C4-C5	-5.27	125.97	128.60
54	BA	481	G	N3-C4-C5	-5.27	125.97	128.60
54	BA	527	C	N3-C4-N4	-5.27	114.31	118.00
54	BA	1816	C	N1-C2-O2	5.27	122.06	118.90
54	BA	1872	A	N1-C6-N6	-5.27	115.44	118.60
54	BA	2488	G	N1-C6-O6	-5.27	116.74	119.90
21	AA	862	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	931	U	N3-C2-O2	-5.27	118.51	122.20
54	BA	2416	C	O4'-C1'-N1	5.27	112.41	108.20
21	AA	930	C	N1-C2-O2	5.26	122.06	118.90
21	AA	1509	C	N1-C2-O2	5.26	122.06	118.90
54	BA	1601	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	2887	A	O4'-C1'-N9	5.26	112.41	108.20
21	AA	576	C	N1-C2-O2	5.26	122.06	118.90
54	BA	103	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1071	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	991	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	1014	A	C6-C5-N7	5.26	135.98	132.30
21	AA	1278	G	N3-C4-C5	-5.26	125.97	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1093	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	1990	C	N1-C2-O2	5.26	122.06	118.90
54	BA	2043	C	N3-C4-C5	5.26	124.00	121.90
54	BA	2498	C	O4'-C1'-N1	5.26	112.41	108.20
14	AO	62	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
21	AA	210	C	N1-C2-O2	5.26	122.06	118.90
21	AA	1129	C	N1-C2-O2	5.26	122.06	118.90
24	A3	42	C	N3-C2-O2	-5.26	118.22	121.90
54	BA	402	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	718	A	C6-C5-N7	5.26	135.98	132.30
21	AA	94	G	N1-C6-O6	-5.26	116.75	119.90
21	AA	802	A	C4-C5-C6	-5.26	114.37	117.00
22	A1	73	A	C5-C6-N6	5.26	127.90	123.70
54	BA	351	C	N3-C2-O2	-5.26	118.22	121.90
54	BA	383	C	N3-C2-O2	-5.26	118.22	121.90
54	BA	1467	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	2573	C	N1-C2-O2	5.26	122.05	118.90
21	AA	593	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1439	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	2296	U	N3-C2-O2	-5.25	118.52	122.20
21	AA	111	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	582	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	147	C	C1'-O4'-C4'	-5.25	105.70	109.90
54	BA	468	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	1193	G	C4'-C3'-C2'	-5.25	97.35	102.60
54	BA	1262	A	C4-C5-C6	-5.25	114.37	117.00
55	BB	53	A	N1-C6-N6	-5.25	115.45	118.60
8	AI	123	ARG	NE-CZ-NH1	5.25	122.93	120.30
21	AA	87	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	179	A	C4-C5-C6	-5.25	114.38	117.00
21	AA	948	C	O4'-C1'-N1	5.25	112.40	108.20
22	A1	30	C	O4'-C1'-N1	5.25	112.40	108.20
28	BF	114	ARG	NE-CZ-NH1	5.25	122.93	120.30
54	BA	66	C	N3-C2-O2	-5.25	118.22	121.90
54	BA	760	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	1523	U	N3-C2-O2	-5.25	118.52	122.20
54	BA	2352	A	C4-C5-C6	-5.25	114.37	117.00
21	AA	1035	A	C6-C5-N7	5.25	135.97	132.30
21	AA	1498	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	192	C	N3-C4-C5	5.25	124.00	121.90
54	BA	736	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	147	G	N1-C6-O6	-5.25	116.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	366	A	C3'-C2'-C1'	5.25	105.70	101.50
21	AA	853	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	1226	C	N1-C2-O2	5.25	122.05	118.90
21	AA	1299	A	C2-N3-C4	5.25	113.22	110.60
21	AA	1368	A	C6-C5-N7	5.25	135.97	132.30
54	BA	3	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	319	G	C5'-C4'-O4'	5.25	115.40	109.10
54	BA	1350	C	N1-C2-O2	5.25	122.05	118.90
21	AA	936	C	N3-C2-O2	-5.25	118.23	121.90
54	BA	211	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	538	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	1748	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1846	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	1949	G	C5'-C4'-O4'	5.25	115.39	109.10
54	BA	2276	G	C5-C6-N1	5.25	114.12	111.50
54	BA	2459	A	C4-C5-C6	-5.25	114.38	117.00
21	AA	1517	G	C3'-C2'-C1'	5.25	105.70	101.50
54	BA	969	G	C8-N9-C4	-5.25	104.30	106.40
54	BA	1517	G	N3-C2-N2	-5.25	116.23	119.90
54	BA	2510	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	865	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	1123	U	N3-C2-O2	-5.24	118.53	122.20
54	BA	179	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	244	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1123	C	C6-N1-C2	-5.24	118.20	120.30
54	BA	620	G	N3-C4-C5	-5.24	125.98	128.60
6	AG	108	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BA	1335	C	N1-C2-O2	5.24	122.04	118.90
54	BA	1599	U	N3-C2-O2	-5.24	118.53	122.20
54	BA	2396	G	N3-C4-C5	-5.24	125.98	128.60
21	AA	211	G	N3-C4-C5	-5.24	125.98	128.60
21	AA	1345	U	C1'-O4'-C4'	-5.24	105.71	109.90
39	BQ	47	ARG	NE-CZ-NH2	-5.24	117.68	120.30
54	BA	429	A	N1-C6-N6	-5.24	115.46	118.60
54	BA	719	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1175	A	O4'-C1'-N9	5.24	112.39	108.20
55	BB	76	G	N3-C4-C5	-5.24	125.98	128.60
21	AA	261	U	O4'-C1'-N1	5.24	112.39	108.20
21	AA	1233	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	316	C	N1-C2-O2	5.24	122.04	118.90
54	BA	2663	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	2889	C	N1-C2-O2	5.24	122.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	68	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	662	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	546	A	C6-C5-N7	5.23	135.96	132.30
21	AA	1098	C	N1-C2-O2	5.23	122.04	118.90
54	BA	1315	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	1507	C	N1-C2-O2	5.23	122.04	118.90
54	BA	2652	C	N1-C2-O2	5.23	122.04	118.90
21	AA	105	G	O4'-C1'-N9	5.23	112.38	108.20
21	AA	1532	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	1982	U	C5-C6-N1	-5.23	120.08	122.70
54	BA	2891	U	N3-C2-O2	-5.23	118.54	122.20
21	AA	488	C	O4'-C1'-N1	5.23	112.38	108.20
21	AA	977	A	C3'-C2'-C1'	5.23	105.68	101.50
38	BP	52	ARG	NE-CZ-NH1	5.23	122.91	120.30
54	BA	670	A	P-O3'-C3'	5.23	125.97	119.70
54	BA	2179	C	C6-N1-C2	-5.23	118.21	120.30
54	BA	2644	G	N3-C4-C5	-5.23	125.99	128.60
54	BA	1684	G	N1-C6-O6	-5.23	116.77	119.90
21	AA	318	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	737	C	N3-C2-O2	-5.22	118.24	121.90
26	BD	33	ARG	NE-CZ-NH1	5.22	122.91	120.30
54	BA	37	C	N1-C2-O2	5.22	122.03	118.90
54	BA	450	G	N3-C4-C5	-5.22	125.99	128.60
54	BA	841	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	903	C	N3-C2-O2	-5.22	118.24	121.90
54	BA	2060	A	C6-N1-C2	-5.22	115.47	118.60
54	BA	2762	C	N1-C2-O2	5.22	122.03	118.90
55	BB	104	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	609	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	1426	G	N7-C8-N9	5.22	115.71	113.10
54	BA	2187	U	O4'-C1'-N1	5.22	112.38	108.20
21	AA	206	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	976	G	N3-C4-C5	-5.22	125.99	128.60
54	BA	2167	U	O4'-C1'-N1	5.22	112.38	108.20
21	AA	153	C	N3-C2-O2	-5.22	118.25	121.90
21	AA	759	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	346	A	C2-N3-C4	5.22	113.21	110.60
54	BA	501	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	731	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	846	U	C3'-C2'-C1'	5.22	105.68	101.50
54	BA	936	A	C5'-C4'-O4'	5.22	115.36	109.10
54	BA	1015	U	O4'-C1'-N1	5.22	112.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2359	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2478	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	351	G	N3-C2-N2	-5.22	116.25	119.90
54	BA	57	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1306	C	O4'-C1'-N1	5.22	112.37	108.20
54	BA	2088	A	C6-C5-N7	5.22	135.95	132.30
54	BA	2091	C	O4'-C1'-N1	5.22	112.37	108.20
19	AT	59	ARG	NE-CZ-NH1	5.21	122.91	120.30
21	AA	58	C	N1-C2-O2	5.21	122.03	118.90
21	AA	649	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	573	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1413	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	2902	C	N3-C4-N4	-5.21	114.35	118.00
55	BB	34	A	C6-C5-N7	5.21	135.95	132.30
54	BA	509	C	N1-C2-O2	5.21	122.03	118.90
54	BA	556	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	1426	G	C8-N9-C4	-5.21	104.31	106.40
54	BA	1864	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2150	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2203	U	C5-C6-N1	-5.21	120.09	122.70
54	BA	2261	C	O4'-C1'-N1	5.21	112.37	108.20
21	AA	136	C	N1-C2-O2	5.21	122.03	118.90
21	AA	924	C	N1-C2-O2	5.21	122.03	118.90
54	BA	346	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	560	C	N1-C2-O2	5.21	122.03	118.90
54	BA	564	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2537	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2679	A	C6-C5-N7	5.21	135.95	132.30
54	BA	2777	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	417	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	1854	A	C4-C5-C6	-5.21	114.39	117.00
21	AA	148	G	O4'-C1'-N9	5.21	112.37	108.20
21	AA	184	G	N1-C6-O6	-5.21	116.78	119.90
21	AA	192	A	C6-C5-N7	5.21	135.94	132.30
21	AA	1476	A	C4-C5-C6	-5.21	114.40	117.00
54	BA	69	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2348	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2757	A	C5'-C4'-C3'	-5.21	107.67	116.00
21	AA	1119	C	N3-C2-O2	-5.21	118.25	121.90
24	A3	2	G	N3-C2-N2	-5.21	116.26	119.90
54	BA	1507	C	O4'-C1'-N1	5.21	112.36	108.20
54	BA	1920	C	N1-C2-O2	5.21	122.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2338	C	N1-C2-O2	5.21	122.02	118.90
54	BA	2460	U	O4'-C1'-N1	5.21	112.36	108.20
21	AA	466	A	C2-N3-C4	5.20	113.20	110.60
21	AA	814	A	C4-C5-C6	-5.20	114.40	117.00
24	A3	53	G	N1-C6-O6	-5.20	116.78	119.90
24	A3	69	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	390	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	633	A	C6-C5-N7	5.20	135.94	132.30
54	BA	2238	G	C5-C6-N1	5.20	114.10	111.50
54	BA	2828	G	N3-C4-C5	-5.20	126.00	128.60
21	AA	1358	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	1797	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	1198	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	1427	A	C6-C5-N7	5.20	135.94	132.30
54	BA	2169	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2699	C	N1-C2-O2	5.20	122.02	118.90
21	AA	1379	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	890	C	N1-C2-O2	5.20	122.02	118.90
54	BA	1771	C	N1-C2-O2	5.20	122.02	118.90
54	BA	2000	C	N1-C2-O2	5.20	122.02	118.90
54	BA	2066	C	N1-C2-O2	5.20	122.02	118.90
21	AA	722	G	C5-C6-N1	5.20	114.10	111.50
21	AA	1264	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	195	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	472	A	N1-C6-N6	-5.20	115.48	118.60
54	BA	1677	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	1910	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	2123	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	2657	A	O4'-C1'-N9	5.20	112.36	108.20
54	BA	2825	G	C5-C6-N1	5.20	114.10	111.50
21	AA	443	C	O4'-C1'-N1	5.19	112.36	108.20
54	BA	1506	U	O4'-C1'-N1	5.19	112.36	108.20
21	AA	417	G	N3-C2-N2	-5.19	116.27	119.90
54	BA	363	G	N3-C4-C5	-5.19	126.00	128.60
54	BA	601	C	N1-C2-O2	5.19	122.02	118.90
54	BA	723	C	N1-C2-O2	5.19	122.02	118.90
54	BA	1063	G	N1-C6-O6	-5.19	116.78	119.90
54	BA	1702	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	1930	G	N3-C4-C5	-5.19	126.00	128.60
21	AA	1076	U	C5-C6-N1	-5.19	120.10	122.70
54	BA	1611	C	C5'-C4'-O4'	5.19	115.33	109.10
54	BA	1714	U	O4'-C1'-N1	5.19	112.35	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1773	A	O4'-C1'-N9	5.19	112.35	108.20
20	AU	51	ALA	C-N-CA	5.19	134.67	121.70
21	AA	26	A	C4-C5-C6	-5.19	114.41	117.00
21	AA	451	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	465	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	2672	U	O4'-C1'-N1	5.19	112.35	108.20
21	AA	1212	U	N3-C2-O2	-5.19	118.57	122.20
54	BA	532	A	O4'-C1'-N9	5.19	112.35	108.20
54	BA	1418	G	N3-C2-N2	-5.19	116.27	119.90
54	BA	2102	G	N1-C6-O6	-5.19	116.79	119.90
13	AN	69	ARG	NE-CZ-NH1	5.18	122.89	120.30
21	AA	765	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	1115	U	N3-C2-O2	-5.18	118.57	122.20
21	AA	1423	G	C6-C5-N7	5.18	133.51	130.40
54	BA	29	U	N3-C2-O2	-5.18	118.57	122.20
54	BA	816	C	N3-C4-C5	5.18	123.97	121.90
54	BA	876	C	N1-C2-O2	5.18	122.01	118.90
54	BA	2166	U	C5-C6-N1	-5.18	120.11	122.70
54	BA	2683	C	N3-C4-C5	5.18	123.97	121.90
21	AA	1337	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	857	G	C8-N9-C4	-5.18	104.33	106.40
54	BA	1273	U	N3-C2-O2	-5.18	118.57	122.20
54	BA	1370	C	N1-C2-O2	5.18	122.01	118.90
21	AA	476	U	C5'-C4'-C3'	-5.18	107.71	116.00
24	A3	26	C	N1-C2-O2	5.18	122.01	118.90
54	BA	391	A	C4-C5-C6	-5.18	114.41	117.00
1	AB	221	ARG	NE-CZ-NH1	5.18	122.89	120.30
21	AA	334	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1141	C	N1-C2-O2	5.18	122.01	118.90
24	A3	3	C	N1-C2-O2	5.18	122.01	118.90
54	BA	21	A	C6-C5-N7	5.18	135.93	132.30
54	BA	1333	G	C5'-C4'-O4'	5.18	115.31	109.10
54	BA	1465	G	O4'-C1'-N9	5.18	112.34	108.20
54	BA	1764	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	2499	C	N3-C2-O2	-5.18	118.28	121.90
21	AA	99	C	N1-C2-O2	5.18	122.01	118.90
36	BN	94	TYR	CB-CG-CD2	-5.18	117.89	121.00
54	BA	366	C	N3-C2-O2	-5.18	118.28	121.90
21	AA	1111	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	1371	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	177	G	C2-N3-C4	5.17	114.49	111.90
54	BA	32	C	N3-C2-O2	-5.17	118.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	400	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	740	C	C6-N1-C2	-5.17	118.23	120.30
54	BA	1112	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1537	G	N9-C1'-C2'	-5.17	106.31	112.00
54	BA	1600	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1642	G	O4'-C1'-N9	5.17	112.34	108.20
54	BA	1824	G	C5-C6-N1	5.17	114.09	111.50
54	BA	2336	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	2425	A	O4'-C1'-N9	5.17	112.34	108.20
54	BA	2714	G	C5'-C4'-O4'	5.17	115.31	109.10
54	BA	1798	U	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1889	A	C4-C5-C6	-5.17	114.41	117.00
32	BJ	34	ARG	NE-CZ-NH1	5.17	122.89	120.30
54	BA	243	U	O4'-C1'-N1	5.17	112.34	108.20
54	BA	855	G	N3-C2-N2	-5.17	116.28	119.90
54	BA	1432	G	C5-C6-N1	5.17	114.09	111.50
54	BA	1919	A	C4-C5-C6	-5.17	114.41	117.00
21	AA	1280	A	O4'-C1'-N9	5.17	112.34	108.20
54	BA	305	C	N1-C2-O2	5.17	122.00	118.90
54	BA	905	A	C6-C5-N7	5.17	135.92	132.30
54	BA	1626	A	O4'-C1'-N9	5.17	112.34	108.20
54	BA	37	C	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	187	G	C8-N9-C4	-5.17	104.33	106.40
54	BA	802	A	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	1596	A	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	2160	C	O4'-C1'-N1	5.17	112.33	108.20
54	BA	2232	C	N3-C4-C5	5.17	123.97	121.90
55	BB	101	A	C4-C5-C6	-5.17	114.42	117.00
21	AA	995	C	N1-C2-O2	5.17	122.00	118.90
21	AA	1298	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	140	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1308	A	C6-C5-N7	5.17	135.92	132.30
21	AA	1141	C	N3-C4-C5	5.17	123.97	121.90
54	BA	1893	C	N1-C2-O2	5.17	122.00	118.90
54	BA	272	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1432	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	1487	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1681	G	C8-N9-C4	-5.16	104.33	106.40
54	BA	1764	C	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	2704	C	N1-C2-O2	5.16	122.00	118.90
54	BA	2418	A	C6-C5-N7	5.16	135.91	132.30
54	BA	2813	A	C6-C5-N7	5.16	135.91	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	25	C	N3-C2-O2	-5.16	118.29	121.90
24	A3	64	G	N3-C4-C5	-5.16	126.02	128.60
54	BA	196	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	275	C	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1022	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	1493	C	N1-C2-O2	5.16	122.00	118.90
54	BA	2573	C	N3-C4-N4	-5.16	114.39	118.00
21	AA	618	C	N1-C2-O2	5.16	122.00	118.90
21	AA	1131	G	N3-C2-N2	-5.16	116.29	119.90
27	BE	69	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BA	211	C	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	1838	C	N3-C2-O2	-5.16	118.29	121.90
54	BA	1966	A	N1-C6-N6	-5.16	115.50	118.60
54	BA	2083	G	N3-C4-C5	-5.16	126.02	128.60
54	BA	2638	G	C5-C6-N1	5.16	114.08	111.50
54	BA	2658	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	175	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	301	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	265	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	784	G	N3-C4-C5	-5.16	126.02	128.60
54	BA	1842	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	2285	C	N1-C2-O2	5.16	121.99	118.90
54	BA	2726	A	O4'-C1'-N9	5.16	112.33	108.20
21	AA	1350	A	C6-C5-N7	5.16	135.91	132.30
21	AA	1484	C	N1-C2-O2	5.16	121.99	118.90
22	A1	73	A	C6-C5-N7	5.16	135.91	132.30
25	BC	268	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BA	479	A	C6-C5-N7	5.16	135.91	132.30
54	BA	657	U	N1-C2-N3	5.16	117.99	114.90
54	BA	937	C	N1-C2-O2	5.16	121.99	118.90
54	BA	1948	G	O4'-C1'-N9	5.16	112.33	108.20
21	AA	73	C	N1-C2-O2	5.15	121.99	118.90
21	AA	244	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2593	U	O4'-C1'-N1	5.15	112.32	108.20
21	AA	629	A	C6-C5-N7	5.15	135.91	132.30
21	AA	1457	G	N3-C4-C5	-5.15	126.02	128.60
54	BA	31	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	1378	A	O4'-C1'-N9	5.15	112.32	108.20
54	BA	1646	C	N1-C2-O2	5.15	121.99	118.90
54	BA	1711	A	C1'-O4'-C4'	-5.15	105.78	109.90
54	BA	1951	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2475	C	N3-C4-C5	5.15	123.96	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	157	U	O4'-C1'-N1	5.15	112.32	108.20
21	AA	918	A	C6-C5-N7	5.15	135.91	132.30
21	AA	1320	C	N1-C2-O2	5.15	121.99	118.90
54	BA	616	A	C5-C6-N1	5.15	120.28	117.70
54	BA	2580	U	C5-C6-N1	-5.15	120.12	122.70
21	AA	1037	C	N1-C2-O2	5.15	121.99	118.90
54	BA	740	C	O4'-C1'-N1	5.15	112.32	108.20
4	AE	44	ARG	NE-CZ-NH2	-5.15	117.73	120.30
54	BA	23	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1544	A	C4-C5-C6	-5.15	114.43	117.00
54	BA	1564	C	N1-C2-O2	5.15	121.99	118.90
54	BA	2121	G	N9-C4-C5	5.15	107.46	105.40
54	BA	2206	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	2567	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	2686	G	N3-C4-C5	-5.15	126.03	128.60
21	AA	418	C	N1-C2-O2	5.15	121.99	118.90
21	AA	984	C	N1-C2-O2	5.15	121.99	118.90
21	AA	1352	C	N1-C2-O2	5.15	121.99	118.90
54	BA	158	U	N1-C2-N3	5.15	117.99	114.90
54	BA	726	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1095	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	37	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	1121	U	O4'-C1'-N1	5.14	112.32	108.20
54	BA	1210	G	P-O3'-C3'	5.14	125.87	119.70
54	BA	2793	C	O4'-C1'-N1	5.14	112.32	108.20
21	AA	623	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	1172	C	N1-C2-O2	5.14	121.99	118.90
54	BA	1406	U	C5'-C4'-O4'	5.14	115.27	109.10
54	BA	2049	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	2667	C	N1-C2-O2	5.14	121.99	118.90
21	AA	793	U	N3-C2-O2	-5.14	118.60	122.20
54	BA	1323	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	2851	A	C6-C5-N7	5.14	135.90	132.30
21	AA	139	A	C6-C5-N7	5.14	135.90	132.30
25	BC	68	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	1925	C	N1-C2-O2	5.14	121.98	118.90
54	BA	2562	U	C5'-C4'-C3'	-5.14	107.78	116.00
54	BA	2789	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2815	C	N1-C2-O2	5.14	121.98	118.90
54	BA	2297	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2902	C	N3-C4-C5	5.14	123.95	121.90
23	A2	82	A	C3'-C2'-C1'	5.14	105.61	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	61	U	O4'-C4'-C3'	5.14	110.21	106.10
26	BD	141	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	489	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	1115	G	N3-C2-N2	-5.14	116.31	119.90
55	BB	81	G	C5-C6-N1	5.14	114.07	111.50
54	BA	1170	C	N3-C4-C5	5.13	123.95	121.90
54	BA	1293	C	O4'-C1'-N1	5.13	112.31	108.20
54	BA	1761	C	N1-C2-O2	5.13	121.98	118.90
55	BB	78	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	630	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1929	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2375	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	707	U	O4'-C1'-N1	5.13	112.31	108.20
24	A3	14	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	1319	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2045	C	N3-C4-C5	5.13	123.95	121.90
54	BA	2223	G	N3-C2-N2	-5.13	116.31	119.90
54	BA	2532	G	N3-C4-C5	-5.13	126.03	128.60
54	BA	583	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1451	C	C2'-C3'-O3'	5.13	121.91	113.70
54	BA	2414	G	C8-N9-C4	-5.13	104.35	106.40
54	BA	2502	G	O4'-C1'-N9	5.13	112.30	108.20
22	A1	62	C	N1-C2-O2	5.13	121.98	118.90
54	BA	254	G	C4'-C3'-C2'	-5.13	97.47	102.60
54	BA	496	G	C5-C6-N1	5.13	114.06	111.50
54	BA	607	U	C5-C6-N1	-5.13	120.14	122.70
54	BA	641	U	C5-C6-N1	-5.13	120.14	122.70
54	BA	820	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	989	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1918	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	2691	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2882	A	C6-C5-N7	5.13	135.89	132.30
21	AA	972	C	N1-C2-O2	5.13	121.97	118.90
33	BK	31	ARG	NE-CZ-NH1	5.13	122.86	120.30
54	BA	301	G	O4'-C1'-N9	5.13	112.30	108.20
54	BA	455	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2154	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	2479	U	O4'-C1'-N1	5.13	112.30	108.20
36	BN	103	ARG	NE-CZ-NH1	5.12	122.86	120.30
54	BA	1200	C	N1-C2-O2	5.12	121.97	118.90
54	BA	2687	U	O4'-C1'-N1	5.12	112.30	108.20
21	AA	1204	A	C6-C5-N7	5.12	135.89	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	540	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1301	A	O4'-C1'-C2'	-5.12	100.68	105.80
54	BA	1769	U	C4'-C3'-C2'	-5.12	97.48	102.60
54	BA	200	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	616	A	O4'-C1'-N9	5.12	112.30	108.20
54	BA	1080	A	C6-C5-N7	5.12	135.88	132.30
55	BB	51	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	398	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1612	C	N1-C2-O2	5.12	121.97	118.90
54	BA	2204	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	382	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	501	C	N1-C2-O2	5.12	121.97	118.90
21	AA	704	A	C6-C5-N7	5.12	135.88	132.30
21	AA	1292	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	1397	C	N1-C2-O2	5.12	121.97	118.90
54	BA	375	G	C5-C6-N1	5.12	114.06	111.50
54	BA	522	A	C6-C5-N7	5.12	135.88	132.30
54	BA	721	A	C6-C5-N7	5.12	135.88	132.30
54	BA	726	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1004	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1428	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1713	A	C6-C5-N7	5.12	135.88	132.30
54	BA	2378	A	C6-C5-N7	5.12	135.88	132.30
54	BA	2458	G	N3-C2-N2	-5.12	116.32	119.90
54	BA	2879	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	134	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	590	U	O4'-C1'-N1	5.12	112.29	108.20
21	AA	609	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1639	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2179	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2703	C	O4'-C1'-N1	5.12	112.29	108.20
21	AA	338	A	C6-C5-N7	5.11	135.88	132.30
21	AA	934	C	C1'-O4'-C4'	-5.11	105.81	109.90
54	BA	77	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	1630	A	C6-C5-N7	5.11	135.88	132.30
54	BA	1954	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	1980	G	C5-C6-N1	5.11	114.06	111.50
54	BA	2118	U	N3-C2-O2	-5.11	118.62	122.20
54	BA	2685	G	C4'-C3'-C2'	-5.11	97.49	102.60
54	BA	154	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	705	G	N3-C2-N2	-5.11	116.32	119.90
21	AA	803	G	N1-C6-O6	-5.11	116.83	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	410	G	O4'-C1'-N9	5.11	112.29	108.20
54	BA	432	A	C6-C5-N7	5.11	135.88	132.30
54	BA	441	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	518	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	2247	A	C6-C5-N7	5.11	135.88	132.30
54	BA	2395	C	O4'-C1'-N1	5.11	112.29	108.20
3	AD	80	ARG	NE-CZ-NH1	5.11	122.86	120.30
54	BA	946	C	C5'-C4'-O4'	5.11	115.23	109.10
54	BA	2198	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	2828	G	C5'-C4'-O4'	5.11	115.23	109.10
21	AA	391	G	C5-C6-N1	5.11	114.05	111.50
54	BA	864	G	N3-C4-C5	-5.11	126.05	128.60
54	BA	998	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	1489	C	N1-C2-O2	5.11	121.97	118.90
54	BA	1706	C	N3-C2-O2	-5.11	118.33	121.90
54	BA	2656	U	C4'-C3'-C2'	-5.11	97.49	102.60
21	AA	973	G	C8-N9-C4	-5.11	104.36	106.40
54	BA	31	C	N1-C2-O2	5.11	121.96	118.90
54	BA	882	G	N3-C2-N2	-5.11	116.33	119.90
54	BA	1556	C	N3-C2-O2	-5.11	118.33	121.90
54	BA	1604	C	N1-C2-O2	5.11	121.96	118.90
54	BA	2127	G	O4'-C1'-N9	5.11	112.28	108.20
54	BA	2477	U	O4'-C1'-N1	5.11	112.28	108.20
21	AA	525	C	N1-C2-O2	5.10	121.96	118.90
54	BA	119	A	C5'-C4'-C3'	-5.10	107.83	116.00
54	BA	242	G	N3-C4-C5	-5.10	126.05	128.60
54	BA	961	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1230	C	N1-C2-O2	5.10	121.96	118.90
54	BA	216	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	551	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	1035	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	1252	G	C5-C6-N1	5.10	114.05	111.50
21	AA	83	C	N1-C2-O2	5.10	121.96	118.90
54	BA	1498	C	N1-C2-O2	5.10	121.96	118.90
5	AF	2	ARG	NE-CZ-NH2	-5.10	117.75	120.30
21	AA	912	C	N1-C2-O2	5.10	121.96	118.90
54	BA	2421	G	C5-C6-N1	5.10	114.05	111.50
54	BA	2706	A	C6-C5-N7	5.10	135.87	132.30
11	AL	49	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
55	BB	81	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	2295	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2861	U	C4'-C3'-C2'	-5.10	97.50	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	757	U	N3-C2-O2	-5.09	118.63	122.20
21	AA	1023	U	C5-C6-N1	-5.09	120.15	122.70
44	BV	21	ARG	CD-NE-CZ	5.09	130.73	123.60
54	BA	1378	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	2055	C	N3-C4-C5	5.09	123.94	121.90
54	BA	2458	G	C8-N9-C4	-5.09	104.36	106.40
54	BA	2524	G	C5'-C4'-O4'	5.09	115.21	109.10
21	AA	1298	U	C1'-O4'-C4'	-5.09	105.83	109.90
21	AA	345	C	N3-C4-N4	-5.09	114.44	118.00
21	AA	396	C	N1-C2-O2	5.09	121.95	118.90
21	AA	840	C	N1-C2-O2	5.09	121.95	118.90
22	A1	33	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	2725	A	C4-C5-C6	-5.09	114.45	117.00
1	AB	206	ILE	C-N-CA	5.09	134.42	121.70
21	AA	933	G	N1-C6-O6	-5.09	116.85	119.90
21	AA	1434	A	C6-C5-N7	5.09	135.86	132.30
54	BA	1359	A	O4'-C1'-N9	5.09	112.27	108.20
54	BA	1593	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	1731	G	N1-C6-O6	-5.09	116.85	119.90
54	BA	2364	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	429	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	811	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	1196	C	N1-C2-O2	5.09	121.95	118.90
54	BA	2483	C	N1-C2-O2	5.09	121.95	118.90
54	BA	2751	G	N3-C4-C5	-5.09	126.06	128.60
21	AA	968	A	C2-N3-C4	5.09	113.14	110.60
21	AA	1214	C	O4'-C1'-N1	5.09	112.27	108.20
21	AA	1469	C	N1-C2-O2	5.09	121.95	118.90
54	BA	55	G	N1-C6-O6	-5.09	116.85	119.90
54	BA	1134	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	1836	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2047	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2048	G	N1-C6-O6	-5.09	116.85	119.90
54	BA	217	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	2816	G	C8-N9-C4	-5.08	104.37	106.40
21	AA	1493	A	C4-C5-C6	-5.08	114.46	117.00
23	A2	83	U	C1'-O4'-C4'	-5.08	105.83	109.90
54	BA	102	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	1537	G	C8-N9-C4	-5.08	104.37	106.40
54	BA	1570	A	C6-C5-N7	5.08	135.86	132.30
54	BA	2438	U	O4'-C1'-N1	5.08	112.27	108.20
2	AC	171	ARG	NE-CZ-NH1	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	858	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	990	C	N1-C2-O2	5.08	121.95	118.90
54	BA	653	U	O4'-C1'-N1	5.08	112.27	108.20
54	BA	1204	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1342	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1909	C	N3-C4-N4	-5.08	114.44	118.00
54	BA	1952	A	O4'-C1'-C2'	-5.08	100.72	105.80
21	AA	1511	G	N3-C2-N2	-5.08	116.34	119.90
54	BA	987	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2017	U	C3'-C2'-C1'	5.08	105.56	101.50
54	BA	1	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	1167	C	N1-C2-O2	5.08	121.95	118.90
54	BA	1314	C	N1-C1'-C2'	5.08	120.60	114.00
54	BA	2451	A	C6-C5-N7	5.08	135.85	132.30
21	AA	635	A	C6-C5-N7	5.08	135.85	132.30
21	AA	818	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2874	C	N3-C2-O2	-5.08	118.35	121.90
3	AD	61	ARG	CD-NE-CZ	5.08	130.71	123.60
21	AA	870	U	O4'-C1'-N1	5.08	112.26	108.20
21	AA	1121	U	N3-C2-O2	-5.08	118.65	122.20
21	AA	1177	G	N3-C2-N2	-5.08	116.35	119.90
21	AA	1458	G	N3-C2-N2	-5.08	116.35	119.90
54	BA	805	G	N3-C2-N2	-5.08	116.35	119.90
54	BA	1708	C	N3-C2-O2	-5.08	118.35	121.90
54	BA	2562	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	2841	C	O4'-C1'-N1	5.08	112.26	108.20
21	AA	641	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	1383	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	1613	G	N3-C2-N2	-5.07	116.35	119.90
54	BA	1921	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2769	U	O4'-C1'-N1	5.07	112.26	108.20
21	AA	641	U	N3-C2-O2	-5.07	118.65	122.20
21	AA	1161	C	N3-C2-O2	-5.07	118.35	121.90
23	A2	91	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	177	G	C8-N9-C4	-5.07	104.37	106.40
54	BA	260	G	C8-N9-C4	-5.07	104.37	106.40
54	BA	428	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	1370	C	O4'-C1'-N1	5.07	112.26	108.20
54	BA	1754	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	2167	U	C5-C6-N1	-5.07	120.17	122.70
7	AH	12	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
21	AA	1449	C	O4'-C1'-N1	5.07	112.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	895	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	1731	G	N3-C4-C5	-5.07	126.07	128.60
54	BA	2591	C	O4'-C1'-N1	5.07	112.25	108.20
21	AA	429	U	C5-C6-N1	-5.07	120.17	122.70
22	A1	39	G	N3-C4-C5	-5.07	126.07	128.60
54	BA	806	C	C2-N3-C4	-5.07	117.37	119.90
54	BA	825	A	C6-C5-N7	5.07	135.84	132.30
54	BA	2489	U	C3'-C2'-C1'	5.07	105.55	101.50
21	AA	340	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	812	C	N3-C2-O2	-5.06	118.36	121.90
54	BA	1852	U	O4'-C1'-N1	5.06	112.25	108.20
21	AA	1168	U	N1-C2-N3	5.06	117.94	114.90
54	BA	129	C	N1-C2-O2	5.06	121.94	118.90
54	BA	192	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	654	A	C6-C5-N7	5.06	135.84	132.30
54	BA	686	U	C5-C6-N1	-5.06	120.17	122.70
54	BA	2006	C	C5'-C4'-O4'	5.06	115.18	109.10
21	AA	1423	G	N3-C2-N2	-5.06	116.36	119.90
54	BA	1032	A	O4'-C1'-N9	5.06	112.25	108.20
54	BA	1187	G	N7-C8-N9	5.06	115.63	113.10
54	BA	1285	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	2052	A	C5-C6-N1	5.06	120.23	117.70
21	AA	520	A	C5-C6-N1	5.06	120.23	117.70
22	A1	16	C	C1'-O4'-C4'	-5.06	105.85	109.90
54	BA	615	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	2298	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	2556	C	N1-C2-O2	5.06	121.94	118.90
54	BA	2695	U	O4'-C1'-N1	5.06	112.25	108.20
21	AA	625	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	903	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	167	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	193	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1128	G	N1-C6-O6	-5.06	116.87	119.90
54	BA	2747	G	N7-C8-N9	5.06	115.63	113.10
54	BA	2818	U	C5-C6-N1	-5.06	120.17	122.70
21	AA	297	G	N1-C6-O6	-5.06	116.87	119.90
54	BA	368	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	493	A	O4'-C1'-N9	5.05	112.24	108.20
54	BA	316	C	N3-C4-N4	-5.05	114.46	118.00
54	BA	395	U	N3-C2-O2	-5.05	118.66	122.20
54	BA	1025	G	N3-C2-N2	-5.05	116.36	119.90
54	BA	1031	G	N1-C6-O6	-5.05	116.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AN	81	ARG	NE-CZ-NH1	5.05	122.83	120.30
21	AA	1191	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	510	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	997	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1609	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	1775	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2822	G	C5-C6-N1	5.05	114.03	111.50
21	AA	257	G	O4'-C1'-N9	5.05	112.24	108.20
21	AA	968	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	394	C	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	436	C	N1-C2-O2	5.05	121.93	118.90
54	BA	611	C	N1-C2-O2	5.05	121.93	118.90
54	BA	644	A	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	2114	A	C6-C5-N7	5.05	135.84	132.30
21	AA	1231	G	N1-C6-O6	-5.05	116.87	119.90
33	BK	70	ARG	NE-CZ-NH1	5.05	122.83	120.30
54	BA	1458	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2114	A	C5-C6-N6	5.05	127.74	123.70
54	BA	2149	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2264	C	C5'-C4'-O4'	5.05	115.16	109.10
54	BA	2775	G	C5-C6-N1	5.05	114.03	111.50
21	AA	911	U	C5-C6-N1	-5.05	120.18	122.70
54	BA	533	G	N1-C6-O6	-5.05	116.87	119.90
55	BB	44	G	N3-C4-C5	-5.05	126.08	128.60
21	AA	1126	U	N3-C2-O2	-5.05	118.67	122.20
24	A3	7	G	C1'-O4'-C4'	-5.05	105.86	109.90
54	BA	64	A	C6-C5-N7	5.05	135.83	132.30
54	BA	89	A	C4-C5-C6	-5.05	114.48	117.00
54	BA	240	C	N1-C2-O2	5.05	121.93	118.90
54	BA	2448	A	C4-C5-C6	-5.05	114.48	117.00
54	BA	2578	G	N3-C2-N2	-5.05	116.37	119.90
55	BB	82	U	O4'-C1'-N1	5.05	112.24	108.20
21	AA	436	C	N1-C2-O2	5.04	121.93	118.90
21	AA	504	C	N1-C2-O2	5.04	121.93	118.90
54	BA	1108	U	O4'-C1'-N1	5.04	112.24	108.20
54	BA	1499	C	O4'-C1'-N1	5.04	112.24	108.20
21	AA	616	G	N1-C6-O6	-5.04	116.87	119.90
21	AA	1478	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	431	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	746	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	863	A	C3'-C2'-C1'	5.04	105.53	101.50
21	AA	74	A	C6-C5-N7	5.04	135.83	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1220	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	155	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1159	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	1295	C	N3-C2-O2	-5.04	118.37	121.90
54	BA	1424	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	1784	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	1899	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	2222	C	C3'-C2'-C1'	5.04	105.53	101.50
54	BA	2650	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	1376	C	N1-C2-O2	5.04	121.92	118.90
54	BA	2787	C	N3-C2-O2	-5.04	118.37	121.90
21	AA	962	C	N3-C4-C5	5.04	123.92	121.90
21	AA	1501	C	N1-C2-O2	5.04	121.92	118.90
54	BA	53	A	C6-C5-N7	5.04	135.83	132.30
54	BA	152	A	O4'-C1'-N9	5.04	112.23	108.20
54	BA	382	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	750	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1195	G	C8-N9-C4	-5.04	104.39	106.40
54	BA	1339	G	N1-C6-O6	-5.04	116.88	119.90
21	AA	1028	C	N1-C2-O2	5.04	121.92	118.90
54	BA	2035	G	C1'-O4'-C4'	-5.04	105.87	109.90
1	AB	207	ARG	NE-CZ-NH2	-5.04	117.78	120.30
54	BA	430	A	C6-C5-N7	5.04	135.82	132.30
54	BA	435	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2356	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2444	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	2452	C	N3-C2-O2	-5.04	118.38	121.90
54	BA	2458	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2543	G	C5-C6-N1	5.04	114.02	111.50
55	BB	113	C	N3-C4-C5	5.04	123.92	121.90
21	AA	427	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	1105	A	C6-C5-N7	5.03	135.82	132.30
54	BA	746	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	950	G	C5-C6-N1	5.03	114.02	111.50
54	BA	2449	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	2559	C	O4'-C1'-N1	5.03	112.23	108.20
21	AA	419	C	O4'-C1'-N1	5.03	112.23	108.20
24	A3	52	C	N1-C2-O2	5.03	121.92	118.90
54	BA	783	A	C6-C5-N7	5.03	135.82	132.30
54	BA	784	G	C5-C6-N1	5.03	114.02	111.50
54	BA	918	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	961	C	N3-C4-N4	-5.03	114.48	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1030	C	O4'-C1'-N1	5.03	112.22	108.20
21	AA	578	C	N1-C2-O2	5.03	121.92	118.90
21	AA	880	C	O4'-C1'-N1	5.03	112.22	108.20
27	BE	40	ARG	NE-CZ-NH1	5.03	122.81	120.30
54	BA	784	G	C1'-O4'-C4'	-5.03	105.88	109.90
54	BA	952	G	C3'-C2'-C1'	5.03	105.52	101.50
54	BA	1079	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2124	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	2368	C	N3-C4-N4	-5.03	114.48	118.00
54	BA	2504	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	2582	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	48	C	N1-C2-O2	5.03	121.92	118.90
21	AA	590	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	1374	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	406	G	N3-C4-C5	-5.03	126.09	128.60
21	AA	1423	G	C5-C6-N1	5.03	114.01	111.50
39	BQ	50	ARG	NE-CZ-NH1	5.03	122.81	120.30
54	BA	339	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1236	G	N3-C2-N2	-5.03	116.38	119.90
54	BA	1521	G	C5-C6-N1	5.03	114.01	111.50
54	BA	2350	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2533	U	C5-C6-N1	-5.03	120.19	122.70
12	AM	97	ARG	NE-CZ-NH2	-5.03	117.79	120.30
21	AA	453	G	N1-C6-O6	-5.03	116.89	119.90
21	AA	1400	C	N1-C2-O2	5.03	121.92	118.90
54	BA	1252	G	N3-C4-C5	-5.03	126.09	128.60
54	BA	1455	G	C5-C6-N1	5.03	114.01	111.50
54	BA	2495	G	N1-C6-O6	-5.03	116.89	119.90
54	BA	2846	G	N3-C4-C5	-5.03	126.09	128.60
55	BB	3	C	O4'-C1'-N1	5.03	112.22	108.20
21	AA	1299	A	C4-C5-C6	-5.02	114.49	117.00
23	A2	91	A	C2-N3-C4	5.02	113.11	110.60
54	BA	1122	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2891	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	474	G	N3-C2-N2	-5.02	116.38	119.90
21	AA	1152	A	C6-C5-N7	5.02	135.82	132.30
21	AA	1341	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	234	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1191	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	2827	C	N1-C2-O2	5.02	121.91	118.90
54	BA	24	G	O4'-C1'-N9	5.02	112.22	108.20
54	BA	616	A	P-O3'-C3'	5.02	125.72	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1278	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1929	G	N3-C2-N2	-5.02	116.39	119.90
54	BA	2090	A	C6-C5-N7	5.02	135.81	132.30
54	BA	2282	G	O4'-C1'-N9	5.02	112.22	108.20
21	AA	1333	A	C4-C5-C6	-5.02	114.49	117.00
21	AA	1419	G	N3-C2-N2	-5.02	116.39	119.90
22	A1	70	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	515	A	C6-C5-N7	5.02	135.81	132.30
54	BA	1697	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	1804	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1824	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2060	A	O4'-C1'-N9	5.02	112.22	108.20
54	BA	2659	G	C5-C6-N1	5.02	114.01	111.50
21	AA	342	C	N1-C2-O2	5.02	121.91	118.90
21	AA	817	C	N1-C2-O2	5.02	121.91	118.90
54	BA	828	U	C5'-C4'-C3'	-5.02	107.97	116.00
54	BA	1303	G	C5-C6-N1	5.02	114.01	111.50
54	BA	1766	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	2219	U	O4'-C1'-N1	5.02	112.21	108.20
55	BB	24	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	895	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	120	U	O4'-C1'-N1	5.02	112.21	108.20
54	BA	1755	A	C6-C5-N7	5.02	135.81	132.30
21	AA	191	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	328	C	C5'-C4'-C3'	-5.01	107.98	116.00
21	AA	520	A	C4-C5-C6	-5.01	114.49	117.00
21	AA	855	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	1508	A	C6-C5-N7	5.01	135.81	132.30
54	BA	243	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	574	A	C4-C5-C6	-5.01	114.49	117.00
54	BA	729	G	N3-C4-C5	-5.01	126.09	128.60
54	BA	737	C	O4'-C1'-N1	5.01	112.21	108.20
54	BA	2873	A	C4-C5-C6	-5.01	114.49	117.00
54	BA	970	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	1830	C	C6-N1-C2	-5.01	118.30	120.30
54	BA	1911	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	1178	G	O4'-C1'-N9	5.01	112.21	108.20
26	BD	179	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	450	G	C5-C6-N1	5.01	114.01	111.50
54	BA	590	A	C6-C5-N7	5.01	135.81	132.30
54	BA	855	G	C6-C5-N7	5.01	133.41	130.40
54	BA	1317	G	N1-C6-O6	-5.01	116.89	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1935	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	2251	G	C5-C6-N1	5.01	114.01	111.50
54	BA	2517	C	O4'-C1'-N1	5.01	112.21	108.20
54	BA	2577	A	C4-C5-C6	-5.01	114.50	117.00
55	BB	64	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	177	G	C5-C6-N1	5.01	114.00	111.50
27	BE	61	ARG	NE-CZ-NH1	5.01	122.80	120.30
54	BA	242	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	1286	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	2883	A	C6-C5-N7	5.01	135.81	132.30
24	A3	4	G	N9-C4-C5	5.01	107.40	105.40
54	BA	3	U	C5-C6-N1	-5.01	120.20	122.70
54	BA	1018	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	2463	C	N1-C2-O2	5.01	121.91	118.90
21	AA	595	A	O4'-C1'-N9	5.01	112.21	108.20
21	AA	1139	G	C5-C6-N1	5.01	114.00	111.50
22	A1	27	C	N1-C2-O2	5.01	121.90	118.90
54	BA	630	G	C5-C6-N1	5.01	114.00	111.50
54	BA	642	U	C5-C6-N1	-5.01	120.20	122.70
54	BA	1109	C	N3-C4-C5	5.01	123.90	121.90
54	BA	1457	U	O4'-C4'-C3'	5.01	110.11	106.10
54	BA	1757	A	C4-C5-C6	-5.01	114.50	117.00
21	AA	123	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	223	A	C4-C5-C6	-5.00	114.50	117.00
55	BB	44	G	C5-C6-N1	5.00	114.00	111.50
21	AA	1284	C	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1585	C	N1-C2-O2	5.00	121.90	118.90
54	BA	1603	A	C6-C5-N7	5.00	135.80	132.30
54	BA	2718	G	N1-C6-O6	-5.00	116.90	119.90
21	AA	98	A	C6-C5-N7	5.00	135.80	132.30
21	AA	444	G	N1-C6-O6	-5.00	116.90	119.90
21	AA	1182	G	C3'-C2'-C1'	5.00	105.50	101.50
21	AA	1184	G	N3-C2-N2	-5.00	116.40	119.90
21	AA	1512	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	950	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	1480	C	N1-C2-O2	5.00	121.90	118.90
54	BA	1677	A	C4'-C3'-C2'	-5.00	97.60	102.60

There are no chirality outliers.

All (1051) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	1	G	Sidechain
22	A1	24	G	Sidechain
22	A1	36	C	Sidechain
22	A1	40	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	59	U	Sidechain
22	A1	72	C	Sidechain
22	A1	76	A	Sidechain
23	A2	81	U	Sidechain
23	A2	83	U	Sidechain
23	A2	85	G	Sidechain
23	A2	90	U	Sidechain
24	A3	24	C	Sidechain
24	A3	32	G	Sidechain
24	A3	34	U	Sidechain
24	A3	44	A	Sidechain
24	A3	49	C	Sidechain
24	A3	50	G	Sidechain
24	A3	57	C	Sidechain
24	A3	6	G	Sidechain
24	A3	62	C	Sidechain
24	A3	65	G	Sidechain
24	A3	7	G	Sidechain
24	A3	72	C	Sidechain
24	A3	75	C	Sidechain
21	AA	1002	G	Sidechain
21	AA	1003	G	Sidechain
21	AA	1010	U	Sidechain
21	AA	1020	G	Sidechain
21	AA	1021	A	Sidechain
21	AA	1026	G	Sidechain
21	AA	1027	C	Sidechain
21	AA	1029	U	Sidechain
21	AA	1034	G	Sidechain
21	AA	1046	A	Sidechain
21	AA	1048	G	Sidechain
21	AA	1054	C	Sidechain
21	AA	1055	A	Sidechain
21	AA	1061	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1063	C	Sidechain
21	AA	1065	U	Sidechain
21	AA	1075	U	Sidechain
21	AA	1076	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	1080	A	Sidechain
21	AA	1083	U	Sidechain
21	AA	109	A	Sidechain
21	AA	1092	A	Sidechain
21	AA	1099	G	Sidechain
21	AA	11	G	Sidechain
21	AA	110	C	Sidechain
21	AA	1107	C	Sidechain
21	AA	1108	G	Sidechain
21	AA	111	G	Sidechain
21	AA	1110	A	Sidechain
21	AA	1112	C	Sidechain
21	AA	1113	C	Sidechain
21	AA	1118	U	Sidechain
21	AA	112	G	Sidechain
21	AA	1120	C	Sidechain
21	AA	1128	C	Sidechain
21	AA	1131	G	Sidechain
21	AA	1139	G	Sidechain
21	AA	1141	C	Sidechain
21	AA	1144	G	Sidechain
21	AA	115	G	Sidechain
21	AA	1150	A	Sidechain
21	AA	1151	A	Sidechain
21	AA	1152	A	Sidechain
21	AA	1153	G	Sidechain
21	AA	1155	A	Sidechain
21	AA	1157	A	Sidechain
21	AA	1164	G	Sidechain
21	AA	1166	G	Sidechain
21	AA	117	G	Sidechain
21	AA	1175	G	Sidechain
21	AA	118	U	Sidechain
21	AA	1180	A	Sidechain
21	AA	1181	G	Sidechain
21	AA	1192	C	Sidechain
21	AA	1195	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1196	A	Sidechain
21	AA	1200	C	Sidechain
21	AA	121	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1217	C	Sidechain
21	AA	1218	C	Sidechain
21	AA	1222	G	Sidechain
21	AA	1225	A	Sidechain
21	AA	1228	C	Sidechain
21	AA	123	U	Sidechain
21	AA	1230	C	Sidechain
21	AA	1234	C	Sidechain
21	AA	1235	U	Sidechain
21	AA	1238	A	Sidechain
21	AA	1239	A	Sidechain
21	AA	1248	A	Sidechain
21	AA	1249	C	Sidechain
21	AA	1266	G	Sidechain
21	AA	1277	C	Sidechain
21	AA	1279	G	Sidechain
21	AA	1282	C	Sidechain
21	AA	1289	A	Sidechain
21	AA	1290	G	Sidechain
21	AA	1292	G	Sidechain
21	AA	1294	G	Sidechain
21	AA	130	A	Sidechain
21	AA	1306	A	Sidechain
21	AA	1308	U	Sidechain
21	AA	131	A	Sidechain
21	AA	1313	U	Sidechain
21	AA	1314	C	Sidechain
21	AA	1316	G	Sidechain
21	AA	1317	C	Sidechain
21	AA	1324	A	Sidechain
21	AA	1330	U	Sidechain
21	AA	1331	G	Sidechain
21	AA	1332	A	Sidechain
21	AA	1333	A	Sidechain
21	AA	1336	C	Sidechain
21	AA	1339	A	Sidechain
21	AA	1351	U	Sidechain
21	AA	1355	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1356	G	Sidechain
21	AA	1359	C	Sidechain
21	AA	1360	A	Sidechain
21	AA	1362	A	Sidechain
21	AA	1372	U	Sidechain
21	AA	1376	U	Sidechain
21	AA	1377	A	Sidechain
21	AA	1378	C	Sidechain
21	AA	1389	C	Sidechain
21	AA	1397	C	Sidechain
21	AA	1402	C	Sidechain
21	AA	1412	C	Sidechain
21	AA	1414	U	Sidechain
21	AA	1415	G	Sidechain
21	AA	1432	G	Sidechain
21	AA	1444	U	Sidechain
21	AA	1474	U	Sidechain
21	AA	148	G	Sidechain
21	AA	1480	A	Sidechain
21	AA	1482	G	Sidechain
21	AA	1494	G	Sidechain
21	AA	150	U	Sidechain
21	AA	1516	G	Sidechain
21	AA	1517	G	Sidechain
21	AA	152	A	Sidechain
21	AA	1524	C	Sidechain
21	AA	1527	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1533	C	Sidechain
21	AA	156	C	Sidechain
21	AA	157	U	Sidechain
21	AA	159	G	Sidechain
21	AA	163	C	Sidechain
21	AA	167	A	Sidechain
21	AA	180	U	Sidechain
21	AA	182	A	Sidechain
21	AA	184	G	Sidechain
21	AA	187	G	Sidechain
21	AA	197	A	Sidechain
21	AA	200	G	Sidechain
21	AA	217	C	Sidechain
21	AA	23	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	234	C	Sidechain
21	AA	236	A	Sidechain
21	AA	24	U	Sidechain
21	AA	242	G	Sidechain
21	AA	251	G	Sidechain
21	AA	258	G	Sidechain
21	AA	26	A	Sidechain
21	AA	260	G	Sidechain
21	AA	264	C	Sidechain
21	AA	267	C	Sidechain
21	AA	273	U	Sidechain
21	AA	274	A	Sidechain
21	AA	278	G	Sidechain
21	AA	285	C	Sidechain
21	AA	287	U	Sidechain
21	AA	289	G	Sidechain
21	AA	296	U	Sidechain
21	AA	297	G	Sidechain
21	AA	298	A	Sidechain
21	AA	30	U	Sidechain
21	AA	300	A	Sidechain
21	AA	306	A	Sidechain
21	AA	309	A	Sidechain
21	AA	312	C	Sidechain
21	AA	313	A	Sidechain
21	AA	315	A	Sidechain
21	AA	323	U	Sidechain
21	AA	324	G	Sidechain
21	AA	330	C	Sidechain
21	AA	334	C	Sidechain
21	AA	340	U	Sidechain
21	AA	345	C	Sidechain
21	AA	349	A	Sidechain
21	AA	35	G	Sidechain
21	AA	353	A	Sidechain
21	AA	354	G	Sidechain
21	AA	356	A	Sidechain
21	AA	361	G	Sidechain
21	AA	362	G	Sidechain
21	AA	366	A	Sidechain
21	AA	376	G	Sidechain
21	AA	377	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	387	U	Sidechain
21	AA	388	G	Sidechain
21	AA	39	G	Sidechain
21	AA	400	C	Sidechain
21	AA	415	A	Sidechain
21	AA	416	G	Sidechain
21	AA	417	G	Sidechain
21	AA	420	U	Sidechain
21	AA	423	G	Sidechain
21	AA	429	U	Sidechain
21	AA	431	A	Sidechain
21	AA	44	A	Sidechain
21	AA	442	G	Sidechain
21	AA	444	G	Sidechain
21	AA	446	G	Sidechain
21	AA	447	G	Sidechain
21	AA	448	A	Sidechain
21	AA	450	G	Sidechain
21	AA	456	A	Sidechain
21	AA	458	U	Sidechain
21	AA	462	G	Sidechain
21	AA	467	U	Sidechain
21	AA	469	C	Sidechain
21	AA	473	U	Sidechain
21	AA	474	G	Sidechain
21	AA	478	A	Sidechain
21	AA	48	C	Sidechain
21	AA	481	G	Sidechain
21	AA	484	G	Sidechain
21	AA	489	C	Sidechain
21	AA	491	G	Sidechain
21	AA	492	C	Sidechain
21	AA	494	G	Sidechain
21	AA	496	A	Sidechain
21	AA	497	G	Sidechain
21	AA	50	A	Sidechain
21	AA	505	G	Sidechain
21	AA	506	G	Sidechain
21	AA	507	C	Sidechain
21	AA	508	U	Sidechain
21	AA	511	C	Sidechain
21	AA	515	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	516	U	Sidechain
21	AA	517	G	Sidechain
21	AA	518	C	Sidechain
21	AA	519	C	Sidechain
21	AA	526	C	Sidechain
21	AA	530	G	Sidechain
21	AA	533	A	Sidechain
21	AA	536	C	Sidechain
21	AA	537	G	Sidechain
21	AA	538	G	Sidechain
21	AA	54	C	Sidechain
21	AA	549	C	Sidechain
21	AA	55	A	Sidechain
21	AA	557	G	Sidechain
21	AA	558	G	Sidechain
21	AA	559	A	Sidechain
21	AA	570	G	Sidechain
21	AA	571	U	Sidechain
21	AA	572	A	Sidechain
21	AA	573	A	Sidechain
21	AA	576	C	Sidechain
21	AA	581	G	Sidechain
21	AA	585	G	Sidechain
21	AA	588	G	Sidechain
21	AA	59	A	Sidechain
21	AA	592	G	Sidechain
21	AA	595	A	Sidechain
21	AA	602	A	Sidechain
21	AA	605	U	Sidechain
21	AA	610	U	Sidechain
21	AA	611	C	Sidechain
21	AA	618	C	Sidechain
21	AA	622	A	Sidechain
21	AA	629	A	Sidechain
21	AA	633	G	Sidechain
21	AA	641	U	Sidechain
21	AA	643	C	Sidechain
21	AA	653	U	Sidechain
21	AA	662	U	Sidechain
21	AA	663	A	Sidechain
21	AA	669	G	Sidechain
21	AA	670	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	671	G	Sidechain
21	AA	673	A	Sidechain
21	AA	675	A	Sidechain
21	AA	690	G	Sidechain
21	AA	691	G	Sidechain
21	AA	697	U	Sidechain
21	AA	700	G	Sidechain
21	AA	710	G	Sidechain
21	AA	72	A	Sidechain
21	AA	722	G	Sidechain
21	AA	725	G	Sidechain
21	AA	728	A	Sidechain
21	AA	741	G	Sidechain
21	AA	751	U	Sidechain
21	AA	752	G	Sidechain
21	AA	754	C	Sidechain
21	AA	760	G	Sidechain
21	AA	765	G	Sidechain
21	AA	769	G	Sidechain
21	AA	774	G	Sidechain
21	AA	778	G	Sidechain
21	AA	779	C	Sidechain
21	AA	786	G	Sidechain
21	AA	788	U	Sidechain
21	AA	789	U	Sidechain
21	AA	792	A	Sidechain
21	AA	8	A	Sidechain
21	AA	800	G	Sidechain
21	AA	806	C	Sidechain
21	AA	81	A	Sidechain
21	AA	813	U	Sidechain
21	AA	818	G	Sidechain
21	AA	82	G	Sidechain
21	AA	820	U	Sidechain
21	AA	824	G	Sidechain
21	AA	827	U	Sidechain
21	AA	83	C	Sidechain
21	AA	832	G	Sidechain
21	AA	837	U	Sidechain
21	AA	838	G	Sidechain
21	AA	859	G	Sidechain
21	AA	86	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	862	C	Sidechain
21	AA	865	A	Sidechain
21	AA	869	G	Sidechain
21	AA	874	G	Sidechain
21	AA	877	G	Sidechain
21	AA	878	A	Sidechain
21	AA	88	U	Sidechain
21	AA	884	U	Sidechain
21	AA	885	G	Sidechain
21	AA	886	G	Sidechain
21	AA	887	G	Sidechain
21	AA	888	G	Sidechain
21	AA	898	G	Sidechain
21	AA	905	U	Sidechain
21	AA	909	A	Sidechain
21	AA	915	A	Sidechain
21	AA	916	U	Sidechain
21	AA	919	A	Sidechain
21	AA	921	U	Sidechain
21	AA	924	C	Sidechain
21	AA	925	G	Sidechain
21	AA	926	G	Sidechain
21	AA	931	C	Sidechain
21	AA	932	C	Sidechain
21	AA	933	G	Sidechain
21	AA	944	G	Sidechain
21	AA	949	A	Sidechain
21	AA	954	G	Sidechain
21	AA	957	U	Sidechain
21	AA	974	A	Sidechain
21	AA	978	A	Sidechain
21	AA	989	U	Sidechain
21	AA	99	C	Sidechain
21	AA	991	U	Sidechain
21	AA	992	U	Sidechain
21	AA	994	A	Sidechain
21	AA	996	A	Sidechain
21	AA	998	C	Sidechain
3	AD	75	TYR	Sidechain
3	AD	96	ARG	Sidechain
4	AE	53	ARG	Sidechain
8	AI	129	ARG	Sidechain

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Mol	Chain	Res	Type	Group
9	AJ	72	ARG	Sidechain
11	AL	26	CYS	Peptide
18	AS	79	TYR	Sidechain
50	B1	5	ARG	Sidechain
56	B5	223	ALA	Mainchain
54	BA	1	G	Sidechain
54	BA	10	A	Sidechain
54	BA	1005	C	Sidechain
54	BA	1014	A	Sidechain
54	BA	1019	U	Sidechain
54	BA	1020	A	Sidechain
54	BA	1022	G	Sidechain
54	BA	1029	A	Sidechain
54	BA	1038	G	Sidechain
54	BA	1056	G	Sidechain
54	BA	1057	A	Sidechain
54	BA	1062	G	Sidechain
54	BA	1065	U	Sidechain
54	BA	1070	A	Sidechain
54	BA	1074	G	Sidechain
54	BA	1080	A	Sidechain
54	BA	1085	A	Sidechain
54	BA	1090	A	Sidechain
54	BA	1091	G	Sidechain
54	BA	1095	A	Sidechain
54	BA	11	C	Sidechain
54	BA	1101	U	Sidechain
54	BA	1106	G	Sidechain
54	BA	111	A	Sidechain
54	BA	1124	G	Sidechain
54	BA	1133	A	Sidechain
54	BA	1135	C	Sidechain
54	BA	1142	A	Sidechain
54	BA	1143	A	Sidechain
54	BA	1151	A	Sidechain
54	BA	1159	U	Sidechain
54	BA	1160	G	Sidechain
54	BA	1162	G	Sidechain
54	BA	1166	G	Sidechain
54	BA	1167	C	Sidechain
54	BA	1175	A	Sidechain
54	BA	1179	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1185	G	Sidechain
54	BA	1186	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1190	G	Sidechain
54	BA	1199	U	Sidechain
54	BA	12	U	Sidechain
54	BA	1208	C	Sidechain
54	BA	1209	U	Sidechain
54	BA	1211	C	Sidechain
54	BA	1212	G	Sidechain
54	BA	123	G	Sidechain
54	BA	1231	U	Sidechain
54	BA	1234	U	Sidechain
54	BA	1236	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	1238	G	Sidechain
54	BA	1239	G	Sidechain
54	BA	124	G	Sidechain
54	BA	1241	A	Sidechain
54	BA	1245	G	Sidechain
54	BA	1248	G	Sidechain
54	BA	1251	C	Sidechain
54	BA	1254	A	Sidechain
54	BA	1256	G	Sidechain
54	BA	1263	U	Sidechain
54	BA	1269	A	Sidechain
54	BA	1275	A	Sidechain
54	BA	1283	G	Sidechain
54	BA	1284	A	Sidechain
54	BA	129	C	Sidechain
54	BA	1291	C	Sidechain
54	BA	1292	G	Sidechain
54	BA	1298	C	Sidechain
54	BA	1311	G	Sidechain
54	BA	1315	C	Sidechain
54	BA	132	G	Sidechain
54	BA	1320	C	Sidechain
54	BA	1322	A	Sidechain
54	BA	1324	G	Sidechain
54	BA	1327	A	Sidechain
54	BA	1330	C	Sidechain
54	BA	1332	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1334	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1343	G	Sidechain
54	BA	1344	U	Sidechain
54	BA	1346	G	Sidechain
54	BA	1350	C	Sidechain
54	BA	1355	G	Sidechain
54	BA	1362	C	Sidechain
54	BA	1364	G	Sidechain
54	BA	1366	A	Sidechain
54	BA	1368	G	Sidechain
54	BA	1371	G	Sidechain
54	BA	1387	A	Sidechain
54	BA	1396	U	Sidechain
54	BA	142	A	Sidechain
54	BA	1420	A	Sidechain
54	BA	1424	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1427	A	Sidechain
54	BA	1433	A	Sidechain
54	BA	1434	A	Sidechain
54	BA	1435	G	Sidechain
54	BA	1436	G	Sidechain
54	BA	1439	A	Sidechain
54	BA	1444	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1446	C	Sidechain
54	BA	1448	G	Sidechain
54	BA	1451	C	Sidechain
54	BA	1457	U	Sidechain
54	BA	1460	U	Sidechain
54	BA	1462	C	Sidechain
54	BA	1463	C	Sidechain
54	BA	1465	G	Sidechain
54	BA	1469	A	Sidechain
54	BA	1475	G	Sidechain
54	BA	1477	A	Sidechain
54	BA	1478	G	Sidechain
54	BA	1485	U	Sidechain
54	BA	1487	U	Sidechain
54	BA	1492	G	Sidechain
54	BA	1497	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1499	C	Sidechain
54	BA	15	G	Sidechain
54	BA	152	A	Sidechain
54	BA	1524	G	Sidechain
54	BA	1529	G	Sidechain
54	BA	153	U	Sidechain
54	BA	1531	C	Sidechain
54	BA	1535	A	Sidechain
54	BA	1536	C	Sidechain
54	BA	1537	G	Sidechain
54	BA	154	U	Sidechain
54	BA	1540	G	Sidechain
54	BA	1546	G	Sidechain
54	BA	1554	U	Sidechain
54	BA	1555	G	Sidechain
54	BA	1556	C	Sidechain
54	BA	1559	U	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1570	A	Sidechain
54	BA	1573	G	Sidechain
54	BA	1580	A	Sidechain
54	BA	1581	G	Sidechain
54	BA	1582	C	Sidechain
54	BA	1583	A	Sidechain
54	BA	1591	A	Sidechain
54	BA	1593	A	Sidechain
54	BA	1594	U	Sidechain
54	BA	1601	G	Sidechain
54	BA	1604	C	Sidechain
54	BA	1607	C	Sidechain
54	BA	1609	A	Sidechain
54	BA	161	A	Sidechain
54	BA	1610	A	Sidechain
54	BA	1614	A	Sidechain
54	BA	1619	G	Sidechain
54	BA	1624	U	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1635	A	Sidechain
54	BA	1640	A	Sidechain
54	BA	1641	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1646	C	Sidechain
54	BA	1656	C	Sidechain
54	BA	1660	G	Sidechain
54	BA	1666	G	Sidechain
54	BA	1671	U	Sidechain
54	BA	1674	G	Sidechain
54	BA	1676	A	Sidechain
54	BA	168	G	Sidechain
54	BA	1681	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1683	U	Sidechain
54	BA	1684	G	Sidechain
54	BA	169	G	Sidechain
54	BA	1695	G	Sidechain
54	BA	1696	G	Sidechain
54	BA	17	G	Sidechain
54	BA	1706	C	Sidechain
54	BA	1709	U	Sidechain
54	BA	1711	A	Sidechain
54	BA	1719	G	Sidechain
54	BA	1723	G	Sidechain
54	BA	1727	C	Sidechain
54	BA	1729	U	Sidechain
54	BA	1734	G	Sidechain
54	BA	1737	G	Sidechain
54	BA	1738	G	Sidechain
54	BA	175	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1758	U	Sidechain
54	BA	1759	A	Sidechain
54	BA	177	G	Sidechain
54	BA	1779	U	Sidechain
54	BA	1788	C	Sidechain
54	BA	1797	G	Sidechain
54	BA	1801	A	Sidechain
54	BA	1802	A	Sidechain
54	BA	1807	G	Sidechain
54	BA	1808	A	Sidechain
54	BA	1817	G	Sidechain
54	BA	1818	U	Sidechain
54	BA	1821	A	Sidechain
54	BA	183	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1830	C	Sidechain
54	BA	1831	G	Sidechain
54	BA	1840	G	Sidechain
54	BA	1845	G	Sidechain
54	BA	1856	U	Sidechain
54	BA	1857	G	Sidechain
54	BA	1866	A	Sidechain
54	BA	1869	G	Sidechain
54	BA	187	G	Sidechain
54	BA	1871	A	Sidechain
54	BA	1879	C	Sidechain
54	BA	1884	G	Sidechain
54	BA	189	G	Sidechain
54	BA	1892	C	Sidechain
54	BA	190	A	Sidechain
54	BA	1929	G	Sidechain
54	BA	1931	U	Sidechain
54	BA	1932	A	Sidechain
54	BA	1937	A	Sidechain
54	BA	1940	U	Sidechain
54	BA	1951	U	Sidechain
54	BA	1953	A	Sidechain
54	BA	197	A	Sidechain
54	BA	1972	G	Sidechain
54	BA	1973	G	Sidechain
54	BA	1978	A	Sidechain
54	BA	1982	U	Sidechain
54	BA	1987	A	Sidechain
54	BA	1996	C	Sidechain
54	BA	2	G	Sidechain
54	BA	200	U	Sidechain
54	BA	2012	G	Sidechain
54	BA	2013	A	Sidechain
54	BA	2015	A	Sidechain
54	BA	2016	U	Sidechain
54	BA	2018	G	Sidechain
54	BA	2019	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2020	A	Sidechain
54	BA	2021	C	Sidechain
54	BA	2022	U	Sidechain
54	BA	2025	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2034	U	Sidechain
54	BA	2036	C	Sidechain
54	BA	2040	G	Sidechain
54	BA	2041	U	Sidechain
54	BA	2046	G	Sidechain
54	BA	205	G	Sidechain
54	BA	2050	C	Sidechain
54	BA	2052	A	Sidechain
54	BA	2053	G	Sidechain
54	BA	2059	A	Sidechain
54	BA	206	U	Sidechain
54	BA	2064	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	2067	G	Sidechain
54	BA	2073	C	Sidechain
54	BA	2075	U	Sidechain
54	BA	2076	U	Sidechain
54	BA	2077	A	Sidechain
54	BA	2078	C	Sidechain
54	BA	208	C	Sidechain
54	BA	2083	G	Sidechain
54	BA	2086	U	Sidechain
54	BA	2090	A	Sidechain
54	BA	2095	A	Sidechain
54	BA	2100	G	Sidechain
54	BA	2103	C	Sidechain
54	BA	2104	C	Sidechain
54	BA	2109	U	Sidechain
54	BA	2116	G	Sidechain
54	BA	2121	G	Sidechain
54	BA	2132	U	Sidechain
54	BA	2134	A	Sidechain
54	BA	2142	A	Sidechain
54	BA	2146	C	Sidechain
54	BA	2149	U	Sidechain
54	BA	2153	C	Sidechain
54	BA	2154	A	Sidechain
54	BA	2156	G	Sidechain
54	BA	2157	G	Sidechain
54	BA	2163	A	Sidechain
54	BA	2165	C	Sidechain
54	BA	2168	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2179	C	Sidechain
54	BA	2186	G	Sidechain
54	BA	2187	U	Sidechain
54	BA	2201	G	Sidechain
54	BA	2206	C	Sidechain
54	BA	2215	C	Sidechain
54	BA	2225	A	Sidechain
54	BA	2228	G	Sidechain
54	BA	2232	C	Sidechain
54	BA	2233	U	Sidechain
54	BA	2236	U	Sidechain
54	BA	2238	G	Sidechain
54	BA	227	A	Sidechain
54	BA	2271	G	Sidechain
54	BA	2273	A	Sidechain
54	BA	2274	A	Sidechain
54	BA	2284	A	Sidechain
54	BA	2285	C	Sidechain
54	BA	2286	G	Sidechain
54	BA	2287	A	Sidechain
54	BA	2293	G	Sidechain
54	BA	2294	G	Sidechain
54	BA	2295	C	Sidechain
54	BA	2297	A	Sidechain
54	BA	2299	U	Sidechain
54	BA	2300	C	Sidechain
54	BA	2301	C	Sidechain
54	BA	2305	U	Sidechain
54	BA	2307	G	Sidechain
54	BA	2315	G	Sidechain
54	BA	2316	G	Sidechain
54	BA	2318	G	Sidechain
54	BA	2319	G	Sidechain
54	BA	2324	U	Sidechain
54	BA	2327	A	Sidechain
54	BA	2333	A	Sidechain
54	BA	2337	G	Sidechain
54	BA	2341	G	Sidechain
54	BA	2345	G	Sidechain
54	BA	2354	C	Sidechain
54	BA	2356	U	Sidechain
54	BA	2357	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2358	A	Sidechain
54	BA	2360	G	Sidechain
54	BA	2363	G	Sidechain
54	BA	2366	A	Sidechain
54	BA	2375	G	Sidechain
54	BA	2383	G	Sidechain
54	BA	2386	A	Sidechain
54	BA	2392	A	Sidechain
54	BA	2398	U	Sidechain
54	BA	2399	G	Sidechain
54	BA	2421	G	Sidechain
54	BA	2425	A	Sidechain
54	BA	2427	C	Sidechain
54	BA	2428	G	Sidechain
54	BA	2429	G	Sidechain
54	BA	2433	A	Sidechain
54	BA	2434	A	Sidechain
54	BA	2436	G	Sidechain
54	BA	244	A	Sidechain
54	BA	2442	C	Sidechain
54	BA	2443	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2445	G	Sidechain
54	BA	2448	A	Sidechain
54	BA	2453	A	Sidechain
54	BA	2457	U	Sidechain
54	BA	2461	A	Sidechain
54	BA	247	G	Sidechain
54	BA	2475	C	Sidechain
54	BA	2478	A	Sidechain
54	BA	2488	G	Sidechain
54	BA	2495	G	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2500	U	Sidechain
54	BA	2501	C	Sidechain
54	BA	2515	C	Sidechain
54	BA	2516	A	Sidechain
54	BA	2517	C	Sidechain
54	BA	2538	C	Sidechain
54	BA	2543	G	Sidechain
54	BA	2555	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	256	A	Sidechain
54	BA	2562	U	Sidechain
54	BA	257	C	Sidechain
54	BA	2573	C	Sidechain
54	BA	2574	G	Sidechain
54	BA	2582	G	Sidechain
54	BA	2595	G	Sidechain
54	BA	2596	U	Sidechain
54	BA	2598	A	Sidechain
54	BA	2601	C	Sidechain
54	BA	2602	A	Sidechain
54	BA	2609	U	Sidechain
54	BA	2615	U	Sidechain
54	BA	2621	G	Sidechain
54	BA	2627	G	Sidechain
54	BA	263	G	Sidechain
54	BA	2636	C	Sidechain
54	BA	2637	U	Sidechain
54	BA	2638	G	Sidechain
54	BA	2639	A	Sidechain
54	BA	2645	G	Sidechain
54	BA	265	A	Sidechain
54	BA	2650	U	Sidechain
54	BA	2654	A	Sidechain
54	BA	2659	G	Sidechain
54	BA	2660	A	Sidechain
54	BA	2663	G	Sidechain
54	BA	2664	G	Sidechain
54	BA	2668	G	Sidechain
54	BA	2680	U	Sidechain
54	BA	2690	U	Sidechain
54	BA	2699	C	Sidechain
54	BA	27	G	Sidechain
54	BA	2700	A	Sidechain
54	BA	2709	G	Sidechain
54	BA	271	G	Sidechain
54	BA	2712	C	Sidechain
54	BA	2716	C	Sidechain
54	BA	2721	A	Sidechain
54	BA	2729	G	Sidechain
54	BA	273	G	Sidechain
54	BA	2732	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2736	A	Sidechain
54	BA	274	C	Sidechain
54	BA	2749	A	Sidechain
54	BA	2752	C	Sidechain
54	BA	2757	A	Sidechain
54	BA	2765	A	Sidechain
54	BA	2775	G	Sidechain
54	BA	2779	U	Sidechain
54	BA	278	A	Sidechain
54	BA	2781	A	Sidechain
54	BA	2786	U	Sidechain
54	BA	28	A	Sidechain
54	BA	2801	G	Sidechain
54	BA	2802	G	Sidechain
54	BA	2805	C	Sidechain
54	BA	2809	A	Sidechain
54	BA	2816	G	Sidechain
54	BA	2818	U	Sidechain
54	BA	2819	G	Sidechain
54	BA	2834	G	Sidechain
54	BA	2838	G	Sidechain
54	BA	2839	G	Sidechain
54	BA	2852	G	Sidechain
54	BA	2856	A	Sidechain
54	BA	2857	G	Sidechain
54	BA	2862	G	Sidechain
54	BA	2863	C	Sidechain
54	BA	2866	U	Sidechain
54	BA	2868	A	Sidechain
54	BA	2873	A	Sidechain
54	BA	2875	C	Sidechain
54	BA	2885	G	Sidechain
54	BA	2888	C	Sidechain
54	BA	2891	U	Sidechain
54	BA	2893	A	Sidechain
54	BA	2894	G	Sidechain
54	BA	2895	G	Sidechain
54	BA	290	U	Sidechain
54	BA	2902	C	Sidechain
54	BA	2903	U	Sidechain
54	BA	296	U	Sidechain
54	BA	307	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	308	G	Sidechain
54	BA	311	A	Sidechain
54	BA	314	C	Sidechain
54	BA	317	G	Sidechain
54	BA	321	U	Sidechain
54	BA	323	C	Sidechain
54	BA	327	G	Sidechain
54	BA	329	G	Sidechain
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	340	A	Sidechain
54	BA	345	A	Sidechain
54	BA	347	A	Sidechain
54	BA	350	G	Sidechain
54	BA	354	A	Sidechain
54	BA	361	G	Sidechain
54	BA	362	A	Sidechain
54	BA	370	G	Sidechain
54	BA	371	A	Sidechain
54	BA	375	G	Sidechain
54	BA	38	A	Sidechain
54	BA	383	C	Sidechain
54	BA	384	A	Sidechain
54	BA	385	C	Sidechain
54	BA	390	U	Sidechain
54	BA	392	U	Sidechain
54	BA	393	C	Sidechain
54	BA	395	U	Sidechain
54	BA	399	U	Sidechain
54	BA	40	U	Sidechain
54	BA	400	G	Sidechain
54	BA	403	U	Sidechain
54	BA	416	U	Sidechain
54	BA	417	C	Sidechain
54	BA	418	C	Sidechain
54	BA	420	C	Sidechain
54	BA	422	A	Sidechain
54	BA	427	U	Sidechain
54	BA	428	A	Sidechain
54	BA	43	G	Sidechain
54	BA	431	U	Sidechain
54	BA	434	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	437	U	Sidechain
54	BA	442	G	Sidechain
54	BA	446	G	Sidechain
54	BA	448	U	Sidechain
54	BA	449	A	Sidechain
54	BA	45	G	Sidechain
54	BA	452	G	Sidechain
54	BA	453	A	Sidechain
54	BA	457	A	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	476	G	Sidechain
54	BA	477	A	Sidechain
54	BA	479	A	Sidechain
54	BA	480	A	Sidechain
54	BA	484	C	Sidechain
54	BA	489	G	Sidechain
54	BA	49	A	Sidechain
54	BA	490	C	Sidechain
54	BA	492	A	Sidechain
54	BA	493	G	Sidechain
54	BA	497	A	Sidechain
54	BA	500	G	Sidechain
54	BA	505	A	Sidechain
54	BA	507	A	Sidechain
54	BA	51	G	Sidechain
54	BA	515	A	Sidechain
54	BA	520	G	Sidechain
54	BA	528	A	Sidechain
54	BA	530	G	Sidechain
54	BA	531	C	Sidechain
54	BA	545	U	Sidechain
54	BA	546	U	Sidechain
54	BA	551	G	Sidechain
54	BA	56	A	Sidechain
54	BA	562	U	Sidechain
54	BA	563	A	Sidechain
54	BA	569	U	Sidechain
54	BA	571	U	Sidechain
54	BA	579	G	Sidechain
54	BA	58	G	Sidechain
54	BA	580	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	584	C	Sidechain
54	BA	59	U	Sidechain
54	BA	602	A	Sidechain
54	BA	606	U	Sidechain
54	BA	607	U	Sidechain
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	619	G	Sidechain
54	BA	621	A	Sidechain
54	BA	626	A	Sidechain
54	BA	628	G	Sidechain
54	BA	63	A	Sidechain
54	BA	630	G	Sidechain
54	BA	631	A	Sidechain
54	BA	637	A	Sidechain
54	BA	642	U	Sidechain
54	BA	644	A	Sidechain
54	BA	646	U	Sidechain
54	BA	647	G	Sidechain
54	BA	65	U	Sidechain
54	BA	670	A	Sidechain
54	BA	671	C	Sidechain
54	BA	674	G	Sidechain
54	BA	675	A	Sidechain
54	BA	68	G	Sidechain
54	BA	69	C	Sidechain
54	BA	691	C	Sidechain
54	BA	698	C	Sidechain
54	BA	703	U	Sidechain
54	BA	709	U	Sidechain
54	BA	711	G	Sidechain
54	BA	714	U	Sidechain
54	BA	717	C	Sidechain
54	BA	720	U	Sidechain
54	BA	725	G	Sidechain
54	BA	726	G	Sidechain
54	BA	727	A	Sidechain
54	BA	728	G	Sidechain
54	BA	730	A	Sidechain
54	BA	734	A	Sidechain
54	BA	741	U	Sidechain
54	BA	744	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	760	G	Sidechain
54	BA	763	G	Sidechain
54	BA	767	U	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain
54	BA	784	G	Sidechain
54	BA	793	A	Sidechain
54	BA	800	A	Sidechain
54	BA	801	G	Sidechain
54	BA	803	U	Sidechain
54	BA	804	A	Sidechain
54	BA	805	G	Sidechain
54	BA	829	A	Sidechain
54	BA	833	A	Sidechain
54	BA	835	C	Sidechain
54	BA	838	C	Sidechain
54	BA	84	A	Sidechain
54	BA	840	C	Sidechain
54	BA	841	G	Sidechain
54	BA	844	A	Sidechain
54	BA	849	A	Sidechain
54	BA	852	U	Sidechain
54	BA	858	G	Sidechain
54	BA	86	G	Sidechain
54	BA	861	A	Sidechain
54	BA	864	G	Sidechain
54	BA	873	C	Sidechain
54	BA	874	G	Sidechain
54	BA	875	G	Sidechain
54	BA	879	G	Sidechain
54	BA	882	G	Sidechain
54	BA	891	G	Sidechain
54	BA	893	C	Sidechain
54	BA	895	U	Sidechain
54	BA	897	C	Sidechain
54	BA	912	C	Sidechain
54	BA	914	G	Sidechain
54	BA	919	U	Sidechain
54	BA	920	A	Sidechain
54	BA	923	G	Sidechain
54	BA	927	A	Sidechain
54	BA	930	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	932	U	Sidechain
54	BA	933	A	Sidechain
54	BA	934	U	Sidechain
54	BA	936	A	Sidechain
54	BA	941	A	Sidechain
54	BA	946	C	Sidechain
54	BA	947	A	Sidechain
54	BA	949	G	Sidechain
54	BA	950	G	Sidechain
54	BA	952	G	Sidechain
54	BA	954	G	Sidechain
54	BA	956	G	Sidechain
54	BA	968	C	Sidechain
54	BA	969	G	Sidechain
54	BA	979	A	Sidechain
54	BA	980	A	Sidechain
54	BA	981	A	Sidechain
54	BA	982	C	Sidechain
54	BA	983	A	Sidechain
54	BA	989	G	Sidechain
54	BA	99	U	Sidechain
54	BA	993	G	Sidechain
55	BB	105	G	Sidechain
55	BB	106	G	Sidechain
55	BB	107	G	Sidechain
55	BB	112	G	Sidechain
55	BB	13	G	Sidechain
55	BB	26	C	Sidechain
55	BB	32	U	Sidechain
55	BB	38	C	Sidechain
55	BB	41	G	Sidechain
55	BB	47	C	Sidechain
55	BB	48	U	Sidechain
55	BB	54	G	Sidechain
55	BB	57	A	Sidechain
55	BB	61	G	Sidechain
55	BB	62	C	Sidechain
55	BB	64	G	Sidechain
55	BB	75	G	Sidechain
55	BB	83	G	Sidechain
55	BB	96	G	Sidechain
38	BP	98	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	1	0
4	AE	1109	0	1152	1	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	3	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16520	3	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	841	0	0
25	BC	2083	0	2157	1	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	1	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	1	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	1	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	1	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31298	6	0
55	BB	2504	0	1269	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99612	17	0

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

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AL:69:GLU:H	11:AL:106:VAL:HG13	1.75	0.52
54:BA:1349:C:N4	54:BA:1383:A:H61	2.11	0.49
54:BA:1324:G:H3'	54:BA:1325:U:H5''	1.97	0.46
4:AE:88:HIS:CG	4:AE:89:THR:H	2.32	0.45
33:BK:111:LYS:HE3	33:BK:112:PHE:CZ	2.52	0.45
47:BY:41:HIS:CG	54:BA:96:C:H4'	2.51	0.45
21:AA:1191:A:C8	21:AA:1191:A:C5'	3.01	0.44
54:BA:441:U:H2'	54:BA:442:G:C8	2.52	0.44
11:AL:15:VAL:HG21	11:AL:17:LYS:HE3	2.01	0.43
11:AL:49:ARG:CZ	21:AA:523:A:H61	2.31	0.43
34:BL:13:LYS:HE3	54:BA:661:A:H4'	2.03	0.41
3:AD:191:SER:HA	3:AD:192:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BI:27:LEU:HD12	31:BI:28:GLY:N	2.36	0.41
43:BU:42:LYS:HZ3	43:BU:44:HIS:CG	2.38	0.41
54:BA:1364:G:H2'	54:BA:1365:A:H5'	2.03	0.41
21:AA:1191:A:C8	21:AA:1191:A:H5'	2.57	0.40
25:BC:239:PHE:CE2	25:BC:241:LYS:HE3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	201 (92%)	15 (7%)	2 (1%)	21	67
2	AC	205/208 (99%)	190 (93%)	9 (4%)	6 (3%)	6	43
3	AD	203/206 (98%)	191 (94%)	9 (4%)	3 (2%)	13	57
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	9	51
5	AF	99/101 (98%)	87 (88%)	7 (7%)	5 (5%)	2	30
6	AG	150/152 (99%)	136 (91%)	8 (5%)	6 (4%)	4	35
7	AH	127/130 (98%)	118 (93%)	8 (6%)	1 (1%)	24	69
8	AI	126/128 (98%)	110 (87%)	15 (12%)	1 (1%)	24	69
9	AJ	98/100 (98%)	86 (88%)	8 (8%)	4 (4%)	3	35
10	AK	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	21	67
11	AL	121/124 (98%)	110 (91%)	9 (7%)	2 (2%)	11	55
12	AM	112/115 (97%)	92 (82%)	16 (14%)	4 (4%)	4	38
13	AN	98/101 (97%)	92 (94%)	4 (4%)	2 (2%)	9	51
14	AO	86/89 (97%)	76 (88%)	5 (6%)	5 (6%)	2	27
15	AP	79/81 (98%)	69 (87%)	6 (8%)	4 (5%)	2	30
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AR	55/57 (96%)	52 (94%)	2 (4%)	1 (2%)	11	53
18	AS	79/81 (98%)	69 (87%)	7 (9%)	3 (4%)	4	37
19	AT	84/86 (98%)	80 (95%)	3 (4%)	1 (1%)	16	61
20	AU	51/53 (96%)	38 (74%)	9 (18%)	4 (8%)	1	20
25	BC	270/273 (99%)	235 (87%)	27 (10%)	8 (3%)	5	42
26	BD	207/209 (99%)	185 (89%)	16 (8%)	6 (3%)	6	43
27	BE	199/201 (99%)	180 (90%)	11 (6%)	8 (4%)	4	35
28	BF	176/179 (98%)	157 (89%)	13 (7%)	6 (3%)	5	40
29	BG	174/177 (98%)	155 (89%)	18 (10%)	1 (1%)	30	74
30	BH	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	9	51
31	BI	139/142 (98%)	129 (93%)	9 (6%)	1 (1%)	26	71
32	BJ	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	6	43
33	BK	121/123 (98%)	103 (85%)	13 (11%)	5 (4%)	3	35
34	BL	141/144 (98%)	109 (77%)	24 (17%)	8 (6%)	2	28
35	BM	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	13	57
36	BN	119/121 (98%)	105 (88%)	13 (11%)	1 (1%)	24	69
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	21	67
38	BP	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	4	38
39	BQ	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	7	45
40	BR	101/103 (98%)	94 (93%)	5 (5%)	2 (2%)	9	51
41	BS	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	10	52
42	BT	92/94 (98%)	79 (86%)	9 (10%)	4 (4%)	3	34
43	BU	101/104 (97%)	87 (86%)	9 (9%)	5 (5%)	3	31
44	BV	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
45	BW	78/80 (98%)	54 (69%)	15 (19%)	9 (12%)	0	9
46	BX	75/79 (95%)	64 (85%)	8 (11%)	3 (4%)	4	35
47	BY	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	12	56
48	BZ	56/59 (95%)	52 (93%)	1 (2%)	3 (5%)	2	29
49	B0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2	28
50	B1	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
51	B2	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	8	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	B3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	5	41
53	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	6	44
56	B5	221/234 (94%)	210 (95%)	8 (4%)	3 (1%)	14	58
All	All	5876/6008 (98%)	5259 (90%)	459 (8%)	158 (3%)	10	45

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AM	107	THR
14	AO	45	HIS
20	AU	9	GLU
20	AU	37	TYR
25	BC	181	ARG
25	BC	191	LEU
26	BD	2	ILE
27	BE	70	SER
28	BF	136	ILE
29	BG	112	VAL
34	BL	101	ILE
43	BU	70	ALA
45	BW	18	LYS
45	BW	23	LYS
48	BZ	30	ARG
49	B0	5	ASN
49	B0	54	ILE
2	AC	14	VAL
4	AE	105	ILE
5	AF	6	ILE
5	AF	63	ASN
6	AG	3	ARG
9	AJ	57	VAL
13	AN	99	ALA
14	AO	48	ASP
15	AP	17	TYR
25	BC	36	ASN
25	BC	187	CYS
26	BD	60	VAL
27	BE	188	MET
30	BH	10	ALA
31	BI	93	ASN
33	BK	92	GLU

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Mol	Chain	Res	Type
33	BK	103	VAL
34	BL	29	LYS
34	BL	46	VAL
36	BN	102	PHE
41	BS	74	ILE
41	BS	90	LYS
42	BT	63	VAL
42	BT	91	GLN
43	BU	43	LYS
51	B2	4	THR
52	B3	3	ILE
56	B5	46	VAL
56	B5	213	SER
1	AB	18	GLN
1	AB	21	TYR
2	AC	171	ARG
3	AD	47	LEU
4	AE	25	LYS
5	AF	90	MET
5	AF	93	LYS
6	AG	114	SER
18	AS	6	LYS
19	AT	3	ILE
26	BD	43	ASP
27	BE	80	SER
27	BE	120	VAL
28	BF	77	LYS
30	BH	121	VAL
32	BJ	15	TRP
32	BJ	80	HIS
32	BJ	128	ASN
33	BK	46	ALA
34	BL	36	LYS
39	BQ	4	LYS
39	BQ	91	ARG
40	BR	82	HIS
42	BT	2	ILE
42	BT	11	LEU
45	BW	10	ARG
45	BW	19	ARG
45	BW	20	LEU
45	BW	56	HIS

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Mol	Chain	Res	Type
46	BX	27	ARG
46	BX	32	LEU
48	BZ	9	THR
52	B3	46	LYS
3	AD	187	ARG
4	AE	43	GLY
6	AG	43	TYR
6	AG	134	VAL
7	AH	105	THR
9	AJ	42	LEU
10	AK	16	SER
12	AM	4	ALA
12	AM	42	VAL
13	AN	60	GLN
14	AO	18	ALA
14	AO	43	ALA
15	AP	24	SER
15	AP	49	GLY
15	AP	63	GLN
18	AS	45	GLY
20	AU	12	ASP
20	AU	52	VAL
25	BC	96	LYS
25	BC	161	VAL
25	BC	196	ASN
26	BD	119	ALA
27	BE	96	VAL
28	BF	46	LYS
32	BJ	53	TYR
34	BL	15	ALA
40	BR	53	PHE
43	BU	45	GLN
43	BU	59	GLU
45	BW	11	ASN
45	BW	16	GLU
49	B0	27	LEU
56	B5	91	GLY
2	AC	3	LYS
3	AD	192	ALA
5	AF	92	THR
6	AG	7	GLY
9	AJ	68	ARG

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Mol	Chain	Res	Type
11	AL	78	VAL
14	AO	23	SER
25	BC	153	LEU
26	BD	75	ALA
27	BE	165	HIS
28	BF	120	SER
33	BK	2	ILE
34	BL	30	THR
35	BM	6	ARG
35	BM	20	LEU
38	BP	26	GLU
38	BP	69	VAL
38	BP	79	VAL
39	BQ	87	VAL
45	BW	35	ILE
47	BY	46	VAL
11	AL	33	CYS
26	BD	134	HIS
28	BF	41	GLU
34	BL	5	THR
34	BL	55	MET
37	BO	23	ALA
46	BX	34	SER
48	BZ	31	ILE
53	B4	37	GLN
2	AC	4	VAL
6	AG	81	GLY
12	AM	23	GLY
17	AR	20	ILE
18	AS	39	ILE
30	BH	130	VAL
38	BP	20	ARG
2	AC	144	GLY
28	BF	103	ILE
9	AJ	41	PRO
43	BU	12	VAL
2	AC	206	ILE
8	AI	57	VAL
27	BE	83	VAL
33	BK	47	ILE
27	BE	31	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	175 (97%)	5 (3%)	51	78
2	AC	170/171 (99%)	169 (99%)	1 (1%)	90	95
3	AD	172/173 (99%)	172 (100%)	0	100	100
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	86 (99%)	1 (1%)	80	91
6	AG	123/123 (100%)	119 (97%)	4 (3%)	45	76
7	AH	104/105 (99%)	103 (99%)	1 (1%)	82	92
8	AI	105/105 (100%)	103 (98%)	2 (2%)	65	86
9	AJ	86/86 (100%)	85 (99%)	1 (1%)	78	90
10	AK	90/90 (100%)	85 (94%)	5 (6%)	26	62
11	AL	103/104 (99%)	102 (99%)	1 (1%)	82	92
12	AM	91/92 (99%)	89 (98%)	2 (2%)	60	83
13	AN	83/84 (99%)	82 (99%)	1 (1%)	78	90
14	AO	76/77 (99%)	75 (99%)	1 (1%)	76	89
15	AP	65/65 (100%)	64 (98%)	1 (2%)	72	88
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	52	79
17	AR	48/48 (100%)	47 (98%)	1 (2%)	61	84
18	AS	70/70 (100%)	68 (97%)	2 (3%)	50	78
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	41 (93%)	3 (7%)	20	57
25	BC	216/217 (100%)	211 (98%)	5 (2%)	58	83
26	BD	164/164 (100%)	161 (98%)	3 (2%)	66	87
27	BE	165/165 (100%)	163 (99%)	2 (1%)	78	90
28	BF	149/150 (99%)	145 (97%)	4 (3%)	52	79
29	BG	137/138 (99%)	134 (98%)	3 (2%)	60	83
30	BH	114/114 (100%)	113 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	68	87
33	BK	103/103 (100%)	100 (97%)	3 (3%)	50	78
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	108 (99%)	1 (1%)	84	93
36	BN	100/100 (100%)	99 (99%)	1 (1%)	82	92
37	BO	86/87 (99%)	84 (98%)	2 (2%)	58	83
38	BP	99/100 (99%)	97 (98%)	2 (2%)	63	85
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	80	91
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	91 (98%)	2 (2%)	60	83
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	80 (96%)	3 (4%)	42	74
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	54 (92%)	5 (8%)	13	48
46	BX	67/68 (98%)	66 (98%)	1 (2%)	72	88
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%)	47 (100%)	0	100	100
50	B1	45/45 (100%)	43 (96%)	2 (4%)	35	69
51	B2	38/38 (100%)	37 (97%)	1 (3%)	54	80
52	B3	51/52 (98%)	47 (92%)	4 (8%)	16	51
53	B4	34/34 (100%)	33 (97%)	1 (3%)	50	78
56	B5	173/181 (96%)	171 (99%)	2 (1%)	78	90
All	All	4842/4870 (99%)	4755 (98%)	87 (2%)	69	87

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	14	HIS
1	AB	71	THR
1	AB	88	GLN
1	AB	189	ASN
1	AB	204	ASP

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Mol	Chain	Res	Type
2	AC	66	THR
5	AF	42	TRP
6	AG	2	ARG
6	AG	3	ARG
6	AG	58	LEU
6	AG	100	MET
7	AH	54	THR
8	AI	56	MET
8	AI	129	ARG
9	AJ	49	PHE
10	AK	35	ASP
10	AK	36	ARG
10	AK	81	LEU
10	AK	118	ASN
10	AK	127	ARG
11	AL	120	ARG
12	AM	41	ASP
12	AM	71	GLU
13	AN	101	TRP
14	AO	24	THR
15	AP	1	MET
16	AQ	19	SER
16	AQ	43	LEU
17	AR	30	ASN
18	AS	13	HIS
18	AS	46	LEU
20	AU	13	VAL
20	AU	34	ARG
20	AU	52	VAL
25	BC	179	GLU
25	BC	184	GLU
25	BC	200	MET
25	BC	222	THR
25	BC	227	VAL
26	BD	2	ILE
26	BD	70	LYS
26	BD	164	GLN
27	BE	79	ARG
27	BE	176	ASP
28	BF	6	TYR
28	BF	70	ARG
28	BF	124	ARG

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Mol	Chain	Res	Type
28	BF	142	TYR
29	BG	2	ARG
29	BG	71	LEU
29	BG	154	GLU
30	BH	82	SER
32	BJ	116	ARG
32	BJ	130	HIS
33	BK	70	ARG
33	BK	97	THR
33	BK	105	ARG
35	BM	126	ILE
36	BN	98	LEU
37	BO	30	ARG
37	BO	31	THR
38	BP	23	ASP
38	BP	50	ARG
39	BQ	5	ARG
40	BR	19	THR
41	BS	1	MET
41	BS	94	ASP
43	BU	8	ASP
43	BU	13	LEU
43	BU	44	HIS
45	BW	9	THR
45	BW	11	ASN
45	BW	39	GLN
45	BW	54	ARG
45	BW	80	SER
46	BX	32	LEU
48	BZ	37	ARG
50	B1	20	TYR
50	B1	45	HIS
51	B2	4	THR
52	B3	23	HIS
52	B3	27	ASN
52	B3	48	MET
52	B3	61	LEU
53	B4	32	LYS
56	B5	24	ASN
56	B5	165	ASN

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

Mol	Chain	Res	Type
26	BD	173	GLN
27	BE	165	HIS
50	B1	18	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	244 (15%)	92 (6%)
22	A1	73/76 (96%)	11 (15%)	2 (2%)
23	A2	14/15 (93%)	6 (42%)	3 (21%)
24	A3	77/77 (100%)	18 (23%)	8 (10%)
54	BA	2902/2903 (99%)	468 (16%)	130 (4%)
55	BB	116/118 (98%)	17 (14%)	3 (2%)
All	All	4711/4722 (99%)	764 (16%)	238 (5%)

All (764) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	8	A
21	AA	9	G
21	AA	10	A
21	AA	13	U
21	AA	14	U
21	AA	25	C
21	AA	31	G
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	52	C
21	AA	54	C
21	AA	55	A
21	AA	84	U
21	AA	85	U
21	AA	86	G
21	AA	87	C
21	AA	109	A
21	AA	120	A
21	AA	121	U
21	AA	122	G
21	AA	131	A

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Mol	Chain	Res	Type
21	AA	144	G
21	AA	149	A
21	AA	153	C
21	AA	184	G
21	AA	185	U
21	AA	188	C
21	AA	190	A
21	AA	198	G
21	AA	240	G
21	AA	244	U
21	AA	245	U
21	AA	247	G
21	AA	251	G
21	AA	252	U
21	AA	253	A
21	AA	266	G
21	AA	274	A
21	AA	281	G
21	AA	287	U
21	AA	289	G
21	AA	293	G
21	AA	298	A
21	AA	299	G
21	AA	309	A
21	AA	310	G
21	AA	317	U
21	AA	328	C
21	AA	329	A
21	AA	332	G
21	AA	344	A
21	AA	346	G
21	AA	347	G
21	AA	350	G
21	AA	351	G
21	AA	352	C
21	AA	354	G
21	AA	362	G
21	AA	363	A
21	AA	367	U
21	AA	369	G
21	AA	373	A
21	AA	381	C

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Mol	Chain	Res	Type
21	AA	384	G
21	AA	389	A
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	409	U
21	AA	412	A
21	AA	416	G
21	AA	420	U
21	AA	421	U
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	461	A
21	AA	462	G
21	AA	463	U
21	AA	464	U
21	AA	466	A
21	AA	467	U
21	AA	468	A
21	AA	469	C
21	AA	474	G
21	AA	477	C
21	AA	484	G
21	AA	496	A
21	AA	509	A
21	AA	511	C
21	AA	525	C
21	AA	547	A
21	AA	559	A
21	AA	562	U
21	AA	564	C
21	AA	565	U
21	AA	566	G
21	AA	567	G
21	AA	572	A
21	AA	575	G
21	AA	576	C
21	AA	577	G
21	AA	607	A
21	AA	608	A
21	AA	610	U

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Mol	Chain	Res	Type
21	AA	620	C
21	AA	648	A
21	AA	649	A
21	AA	653	U
21	AA	665	A
21	AA	700	G
21	AA	724	G
21	AA	754	C
21	AA	755	G
21	AA	777	A
21	AA	778	G
21	AA	779	C
21	AA	812	G
21	AA	817	C
21	AA	819	A
21	AA	827	U
21	AA	841	C
21	AA	843	U
21	AA	845	A
21	AA	846	G
21	AA	847	G
21	AA	877	G
21	AA	884	U
21	AA	885	G
21	AA	887	G
21	AA	890	G
21	AA	914	A
21	AA	920	U
21	AA	931	C
21	AA	934	C
21	AA	935	A
21	AA	939	G
21	AA	958	A
21	AA	959	A
21	AA	960	U
21	AA	966	G
21	AA	967	C
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	972	C
21	AA	974	A

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Mol	Chain	Res	Type
21	AA	975	A
21	AA	976	G
21	AA	978	A
21	AA	992	U
21	AA	993	G
21	AA	994	A
21	AA	1004	A
21	AA	1017	U
21	AA	1020	G
21	AA	1026	G
21	AA	1027	C
21	AA	1031	C
21	AA	1032	G
21	AA	1035	A
21	AA	1045	C
21	AA	1049	U
21	AA	1050	G
21	AA	1056	U
21	AA	1065	U
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1126	U
21	AA	1130	A
21	AA	1137	C
21	AA	1139	G
21	AA	1146	A
21	AA	1147	C
21	AA	1152	A
21	AA	1156	G
21	AA	1157	A
21	AA	1159	U
21	AA	1160	G
21	AA	1167	A
21	AA	1169	A
21	AA	1178	G
21	AA	1179	A
21	AA	1181	G
21	AA	1183	U
21	AA	1184	G
21	AA	1189	U

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Mol	Chain	Res	Type
21	AA	1190	G
21	AA	1191	A
21	AA	1196	A
21	AA	1201	A
21	AA	1202	U
21	AA	1212	U
21	AA	1213	A
21	AA	1218	C
21	AA	1222	G
21	AA	1224	U
21	AA	1225	A
21	AA	1227	A
21	AA	1231	G
21	AA	1238	A
21	AA	1256	A
21	AA	1257	A
21	AA	1279	G
21	AA	1285	A
21	AA	1286	U
21	AA	1298	U
21	AA	1299	A
21	AA	1300	G
21	AA	1301	U
21	AA	1303	C
21	AA	1305	G
21	AA	1317	C
21	AA	1319	A
21	AA	1332	A
21	AA	1335	U
21	AA	1336	C
21	AA	1337	G
21	AA	1340	A
21	AA	1363	A
21	AA	1364	U
21	AA	1365	G
21	AA	1379	G
21	AA	1381	U
21	AA	1382	C
21	AA	1398	A
21	AA	1411	C
21	AA	1419	G
21	AA	1426	G

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Mol	Chain	Res	Type
21	AA	1432	G
21	AA	1447	A
21	AA	1492	A
21	AA	1493	A
21	AA	1494	G
21	AA	1506	U
21	AA	1517	G
21	AA	1524	C
21	AA	1529	G
21	AA	1530	G
22	A1	9	A
22	A1	16	C
22	A1	17	U
22	A1	20	G
22	A1	21	A
22	A1	46	7MG
22	A1	48	C
22	A1	59	U
22	A1	73	A
22	A1	74	C
22	A1	76	A
23	A2	82	A
23	A2	83	U
23	A2	88	U
23	A2	90	U
23	A2	91	A
23	A2	92	U
24	A3	2	G
24	A3	9	G
24	A3	20	G
24	A3	21	H2U
24	A3	22	A
24	A3	23	G
24	A3	30	G
24	A3	40	C
24	A3	48	U
24	A3	49	C
24	A3	51	U
24	A3	59	A
24	A3	61	U
24	A3	62	C
24	A3	71	G

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Mol	Chain	Res	Type
24	A3	72	C
24	A3	76	C
24	A3	77	A
54	BA	6	A
54	BA	12	U
54	BA	17	G
54	BA	20	C
54	BA	29	U
54	BA	30	G
54	BA	34	U
54	BA	38	A
54	BA	60	G
54	BA	61	C
54	BA	64	A
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	100	U
54	BA	101	A
54	BA	102	U
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	125	A
54	BA	126	A
54	BA	139	U
54	BA	145	C
54	BA	147	C
54	BA	149	A
54	BA	150	U
54	BA	155	A
54	BA	172	A
54	BA	196	A
54	BA	199	A
54	BA	200	U
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	224	U
54	BA	248	G

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Mol	Chain	Res	Type
54	BA	249	C
54	BA	265	A
54	BA	266	G
54	BA	271	G
54	BA	272	A
54	BA	277	G
54	BA	278	A
54	BA	279	A
54	BA	297	G
54	BA	316	C
54	BA	323	C
54	BA	324	A
54	BA	327	G
54	BA	330	A
54	BA	331	C
54	BA	332	A
54	BA	335	C
54	BA	338	G
54	BA	370	G
54	BA	372	G
54	BA	373	U
54	BA	374	A
54	BA	377	G
54	BA	378	C
54	BA	386	G
54	BA	387	U
54	BA	390	U
54	BA	404	A
54	BA	428	A
54	BA	451	U
54	BA	454	A
54	BA	455	C
54	BA	457	A
54	BA	458	G
54	BA	459	U
54	BA	473	G
54	BA	481	G
54	BA	484	C
54	BA	490	C
54	BA	504	A
54	BA	505	A
54	BA	509	C

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Mol	Chain	Res	Type
54	BA	510	C
54	BA	528	A
54	BA	529	A
54	BA	530	G
54	BA	532	A
54	BA	533	G
54	BA	546	U
54	BA	547	A
54	BA	548	G
54	BA	563	A
54	BA	569	U
54	BA	570	G
54	BA	573	U
54	BA	574	A
54	BA	575	A
54	BA	587	C
54	BA	590	A
54	BA	603	A
54	BA	614	A
54	BA	615	U
54	BA	617	G
54	BA	620	G
54	BA	627	A
54	BA	630	G
54	BA	637	A
54	BA	643	A
54	BA	645	C
54	BA	655	A
54	BA	671	C
54	BA	672	C
54	BA	686	U
54	BA	716	A
54	BA	717	C
54	BA	724	U
54	BA	730	A
54	BA	748	G
54	BA	752	A
54	BA	763	G
54	BA	764	A
54	BA	775	G
54	BA	782	A
54	BA	784	G

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Mol	Chain	Res	Type
54	BA	791	C
54	BA	792	A
54	BA	805	G
54	BA	812	C
54	BA	815	C
54	BA	819	A
54	BA	827	U
54	BA	846	U
54	BA	847	U
54	BA	858	G
54	BA	860	U
54	BA	866	A
54	BA	867	C
54	BA	871	U
54	BA	885	C
54	BA	889	C
54	BA	890	C
54	BA	910	A
54	BA	915	C
54	BA	931	U
54	BA	932	U
54	BA	934	U
54	BA	936	A
54	BA	938	G
54	BA	945	A
54	BA	946	C
54	BA	958	U
54	BA	961	C
54	BA	974	G
54	BA	981	A
54	BA	982	C
54	BA	983	A
54	BA	1005	C
54	BA	1006	C
54	BA	1008	A
54	BA	1009	A
54	BA	1011	G
54	BA	1012	U
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	1063	G
54	BA	1067	A
54	BA	1068	G
54	BA	1070	A
54	BA	1073	A
54	BA	1076	C
54	BA	1087	G
54	BA	1088	A
54	BA	1092	C
54	BA	1094	U
54	BA	1095	A
54	BA	1112	G
54	BA	1124	G
54	BA	1129	A
54	BA	1131	G
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1141	U
54	BA	1142	A
54	BA	1144	A
54	BA	1155	A
54	BA	1175	A
54	BA	1176	U
54	BA	1188	U
54	BA	1204	A
54	BA	1205	A
54	BA	1211	C
54	BA	1212	G
54	BA	1229	C
54	BA	1236	G
54	BA	1237	A
54	BA	1238	G
54	BA	1247	A
54	BA	1252	G
54	BA	1253	A
54	BA	1254	A
54	BA	1266	G
54	BA	1269	A

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Mol	Chain	Res	Type
54	BA	1288	G
54	BA	1289	C
54	BA	1300	G
54	BA	1301	A
54	BA	1311	G
54	BA	1313	U
54	BA	1314	C
54	BA	1325	U
54	BA	1332	G
54	BA	1337	G
54	BA	1341	G
54	BA	1343	G
54	BA	1344	U
54	BA	1365	A
54	BA	1368	G
54	BA	1374	G
54	BA	1378	A
54	BA	1379	U
54	BA	1383	A
54	BA	1385	A
54	BA	1391	U
54	BA	1393	A
54	BA	1396	U
54	BA	1416	G
54	BA	1420	A
54	BA	1422	G
54	BA	1427	A
54	BA	1428	C
54	BA	1429	G
54	BA	1434	A
54	BA	1435	G
54	BA	1440	U
54	BA	1452	G
54	BA	1453	A
54	BA	1454	C
54	BA	1455	G
54	BA	1457	U
54	BA	1458	U
54	BA	1459	G
54	BA	1482	G
54	BA	1490	A
54	BA	1491	G

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Mol	Chain	Res	Type
54	BA	1495	A
54	BA	1510	G
54	BA	1535	A
54	BA	1536	C
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1540	G
54	BA	1558	C
54	BA	1559	U
54	BA	1568	G
54	BA	1569	A
54	BA	1598	A
54	BA	1607	C
54	BA	1608	A
54	BA	1610	A
54	BA	1611	C
54	BA	1618	A
54	BA	1634	A
54	BA	1635	A
54	BA	1639	C
54	BA	1647	U
54	BA	1648	U
54	BA	1656	C
54	BA	1664	A
54	BA	1668	A
54	BA	1669	A
54	BA	1674	G
54	BA	1675	C
54	BA	1701	A
54	BA	1707	G
54	BA	1711	A
54	BA	1729	U
54	BA	1730	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	1780	A

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Mol	Chain	Res	Type
54	BA	1784	A
54	BA	1800	C
54	BA	1802	A
54	BA	1808	A
54	BA	1810	A
54	BA	1815	A
54	BA	1816	C
54	BA	1900	A
54	BA	1901	A
54	BA	1914	C
54	BA	1919	A
54	BA	1937	A
54	BA	1938	A
54	BA	1939	U
54	BA	1940	U
54	BA	1943	U
54	BA	1944	U
54	BA	1945	G
54	BA	1952	A
54	BA	1955	U
54	BA	1956	U
54	BA	1964	G
54	BA	1967	C
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1982	U
54	BA	1993	U
54	BA	1996	C
54	BA	2002	G
54	BA	2006	C
54	BA	2023	C
54	BA	2031	A
54	BA	2032	G
54	BA	2034	U
54	BA	2043	C
54	BA	2051	A
54	BA	2055	C
54	BA	2060	A
54	BA	2061	G
54	BA	2062	A
54	BA	2068	U

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Mol	Chain	Res	Type
54	BA	2069	G
54	BA	2092	U
54	BA	2093	G
54	BA	2113	U
54	BA	2126	A
54	BA	2127	G
54	BA	2131	U
54	BA	2132	U
54	BA	2138	G
54	BA	2155	U
54	BA	2159	G
54	BA	2163	A
54	BA	2164	C
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2198	A
54	BA	2203	U
54	BA	2211	A
54	BA	2212	A
54	BA	2213	U
54	BA	2214	C
54	BA	2216	G
54	BA	2227	A
54	BA	2232	C
54	BA	2238	G
54	BA	2251	G
54	BA	2262	U
54	BA	2266	A
54	BA	2268	A
54	BA	2275	C
54	BA	2276	G
54	BA	2283	C
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2312	U
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2326	C

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Mol	Chain	Res	Type
54	BA	2333	A
54	BA	2334	U
54	BA	2339	C
54	BA	2346	A
54	BA	2347	C
54	BA	2350	C
54	BA	2353	G
54	BA	2379	G
54	BA	2383	G
54	BA	2385	C
54	BA	2388	A
54	BA	2403	C
54	BA	2406	A
54	BA	2407	A
54	BA	2409	G
54	BA	2422	C
54	BA	2424	C
54	BA	2425	A
54	BA	2428	G
54	BA	2431	U
54	BA	2441	U
54	BA	2447	G
54	BA	2448	A
54	BA	2450	A
54	BA	2451	A
54	BA	2474	U
54	BA	2475	C
54	BA	2476	A
54	BA	2491	U
54	BA	2498	C
54	BA	2499	C
54	BA	2500	U
54	BA	2502	G
54	BA	2504	U
54	BA	2505	G
54	BA	2518	A
54	BA	2519	U
54	BA	2533	U
54	BA	2539	C
54	BA	2547	A
54	BA	2554	U
54	BA	2555	U

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Mol	Chain	Res	Type
54	BA	2564	A
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2573	C
54	BA	2576	G
54	BA	2581	G
54	BA	2582	G
54	BA	2585	U
54	BA	2586	U
54	BA	2596	U
54	BA	2602	A
54	BA	2603	G
54	BA	2609	U
54	BA	2610	C
54	BA	2613	U
54	BA	2614	A
54	BA	2629	U
54	BA	2639	A
54	BA	2640	G
54	BA	2646	C
54	BA	2654	A
54	BA	2656	U
54	BA	2663	G
54	BA	2665	A
54	BA	2669	G
54	BA	2683	C
54	BA	2684	U
54	BA	2689	U
54	BA	2690	U
54	BA	2714	G
54	BA	2717	C
54	BA	2732	G
54	BA	2733	A
54	BA	2765	A
54	BA	2766	A
54	BA	2778	A
54	BA	2798	U
54	BA	2801	G
54	BA	2816	G
54	BA	2821	A
54	BA	2823	A

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Mol	Chain	Res	Type
54	BA	2834	G
54	BA	2835	A
54	BA	2850	A
54	BA	2868	A
54	BA	2876	G
54	BA	2879	A
54	BA	2884	U
54	BA	2886	A
54	BA	2895	G
55	BB	13	G
55	BB	14	U
55	BB	15	A
55	BB	16	G
55	BB	25	U
55	BB	31	C
55	BB	36	C
55	BB	37	C
55	BB	41	G
55	BB	42	C
55	BB	44	G
55	BB	45	A
55	BB	61	G
55	BB	84	G
55	BB	87	U
55	BB	90	C
55	BB	109	A

All (238) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	13	U
21	AA	51	A
21	AA	54	C
21	AA	85	U
21	AA	120	A
21	AA	184	G
21	AA	189	A
21	AA	251	G
21	AA	274	A
21	AA	281	G
21	AA	298	A

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Mol	Chain	Res	Type
21	AA	309	A
21	AA	327	A
21	AA	328	C
21	AA	346	G
21	AA	351	G
21	AA	362	G
21	AA	366	A
21	AA	368	U
21	AA	408	A
21	AA	420	U
21	AA	461	A
21	AA	462	G
21	AA	463	U
21	AA	465	A
21	AA	496	A
21	AA	538	G
21	AA	563	A
21	AA	567	G
21	AA	572	A
21	AA	575	G
21	AA	576	C
21	AA	607	A
21	AA	609	A
21	AA	648	A
21	AA	671	G
21	AA	753	A
21	AA	777	A
21	AA	778	G
21	AA	826	C
21	AA	843	U
21	AA	845	A
21	AA	876	C
21	AA	884	U
21	AA	890	G
21	AA	913	A
21	AA	958	A
21	AA	960	U
21	AA	970	C
21	AA	971	G
21	AA	978	A
21	AA	983	A
21	AA	992	U

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Mol	Chain	Res	Type
21	AA	1026	G
21	AA	1030	U
21	AA	1049	U
21	AA	1053	G
21	AA	1101	A
21	AA	1124	G
21	AA	1139	G
21	AA	1146	A
21	AA	1151	A
21	AA	1156	G
21	AA	1159	U
21	AA	1178	G
21	AA	1179	A
21	AA	1183	U
21	AA	1190	G
21	AA	1191	A
21	AA	1196	A
21	AA	1200	C
21	AA	1201	A
21	AA	1212	U
21	AA	1214	C
21	AA	1217	C
21	AA	1222	G
21	AA	1225	A
21	AA	1227	A
21	AA	1298	U
21	AA	1318	A
21	AA	1335	U
21	AA	1337	G
21	AA	1363	A
21	AA	1364	U
21	AA	1381	U
21	AA	1425	U
21	AA	1440	U
21	AA	1452	C
21	AA	1492	A
21	AA	1523	G
21	AA	1529	G
22	A1	72	C
22	A1	75	C
23	A2	82	A
23	A2	87	U

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Mol	Chain	Res	Type
23	A2	90	U
24	A3	1	C
24	A3	22	A
24	A3	47	G
24	A3	50	G
24	A3	58	A
24	A3	61	U
24	A3	71	G
24	A3	74	A
54	BA	16	C
54	BA	29	U
54	BA	60	G
54	BA	91	A
54	BA	99	U
54	BA	101	A
54	BA	149	A
54	BA	199	A
54	BA	221	A
54	BA	265	A
54	BA	271	G
54	BA	277	G
54	BA	278	A
54	BA	330	A
54	BA	372	G
54	BA	374	A
54	BA	377	G
54	BA	446	G
54	BA	451	U
54	BA	458	G
54	BA	479	A
54	BA	481	G
54	BA	510	C
54	BA	527	C
54	BA	530	G
54	BA	569	U
54	BA	587	C
54	BA	614	A
54	BA	625	G
54	BA	670	A
54	BA	751	A
54	BA	762	U
54	BA	764	A

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Mol	Chain	Res	Type
54	BA	818	G
54	BA	931	U
54	BA	958	U
54	BA	962	G
54	BA	974	G
54	BA	980	A
54	BA	981	A
54	BA	982	C
54	BA	983	A
54	BA	1019	U
54	BA	1073	A
54	BA	1089	A
54	BA	1123	C
54	BA	1128	G
54	BA	1130	U
54	BA	1133	A
54	BA	1141	U
54	BA	1142	A
54	BA	1187	G
54	BA	1210	G
54	BA	1228	G
54	BA	1236	G
54	BA	1238	G
54	BA	1240	U
54	BA	1252	G
54	BA	1253	A
54	BA	1289	C
54	BA	1300	G
54	BA	1312	U
54	BA	1313	U
54	BA	1329	U
54	BA	1343	G
54	BA	1379	U
54	BA	1419	A
54	BA	1420	A
54	BA	1421	G
54	BA	1427	A
54	BA	1428	C
54	BA	1433	A
54	BA	1434	A
54	BA	1451	C
54	BA	1453	A

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Mol	Chain	Res	Type
54	BA	1454	C
54	BA	1457	U
54	BA	1508	A
54	BA	1539	U
54	BA	1568	G
54	BA	1597	A
54	BA	1615	C
54	BA	1616	A
54	BA	1634	A
54	BA	1655	A
54	BA	1668	A
54	BA	1706	C
54	BA	1733	G
54	BA	1757	A
54	BA	1760	C
54	BA	1783	A
54	BA	1799	G
54	BA	1847	A
54	BA	1900	A
54	BA	1913	A
54	BA	1914	C
54	BA	1936	A
54	BA	1938	A
54	BA	1943	U
54	BA	1955	U
54	BA	1970	A
54	BA	2017	U
54	BA	2035	G
54	BA	2131	U
54	BA	2163	A
54	BA	2172	U
54	BA	2213	U
54	BA	2233	U
54	BA	2267	A
54	BA	2275	C
54	BA	2282	G
54	BA	2286	G
54	BA	2312	U
54	BA	2352	A
54	BA	2373	G
54	BA	2430	A
54	BA	2450	A

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Mol	Chain	Res	Type
54	BA	2499	C
54	BA	2500	U
54	BA	2528	U
54	BA	2532	G
54	BA	2566	A
54	BA	2581	G
54	BA	2585	U
54	BA	2669	G
54	BA	2689	U
54	BA	2780	G
54	BA	2833	U
54	BA	2858	C
54	BA	2879	A
55	BB	12	C
55	BB	15	A
55	BB	56	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CM0	A1	34	22,23	15,26,27	1.84	3 (20%)	18,37,40	3.28	3 (16%)
22	6MZ	A1	37	22	17,25,26	0.89	0	15,36,39	1.08	1 (6%)
22	7MG	A1	46	22	20,26,27	2.17	3 (15%)	23,39,42	2.01	2 (8%)
22	5MU	A1	54	22	13,22,23	1.13	1 (7%)	16,32,35	4.60	2 (12%)
22	PSU	A1	55	22	15,21,22	0.99	0	16,30,33	3.28	4 (25%)
22	4SU	A1	7	22	12,21,22	0.91	0	15,30,33	2.18	2 (13%)
24	H2U	A3	21	24	17,21,22	1.40	2 (11%)	23,30,33	1.30	3 (13%)
24	OMC	A3	33	24	15,22,23	1.07	0	20,31,34	0.70	0
24	5MU	A3	55	24	13,22,23	1.07	1 (7%)	16,32,35	4.73	2 (12%)
24	PSU	A3	56	24	15,21,22	1.07	0	16,30,33	3.38	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	4SU	A3	8	24	12,21,22	1.06	1 (8%)	15,30,33	2.23	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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.15	1.33	1.45
22	A1	34	CM0	O5-C5	-6.00	1.25	1.37
24	A3	21	H2U	C4-N3	-3.41	1.32	1.37
24	A3	21	H2U	C2-N3	-3.01	1.32	1.38
22	A1	46	7MG	C8-N7	-2.80	1.30	1.43
22	A1	34	CM0	C4-N3	2.15	1.36	1.33
24	A3	8	4SU	C6-N1	2.17	1.38	1.35
22	A1	34	CM0	C4-C5	2.36	1.46	1.40
22	A1	54	5MU	C4-N3	2.63	1.37	1.33
24	A3	55	5MU	C4-N3	2.68	1.37	1.33
22	A1	46	7MG	C6-N1	2.77	1.38	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	55	5MU	C5-C4-N3	-12.88	114.54	125.35
22	A1	54	5MU	C5-C4-N3	-12.70	114.69	125.35
24	A3	8	4SU	C5-C4-N3	-7.86	115.23	123.56
22	A1	7	4SU	C5-C4-N3	-7.48	115.62	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	46	7MG	C5-C6-N1	-6.47	113.75	123.39
24	A3	56	PSU	C5-C6-N1	-3.25	119.84	124.38
22	A1	55	PSU	C5-C6-N1	-2.54	120.84	124.38
22	A1	55	PSU	C5-C1'-C2'	-2.43	111.30	115.44
24	A3	56	PSU	C4'-O4'-C1'	-2.21	107.27	109.54
22	A1	34	CM0	O4'-C4'-C3'	2.16	109.53	105.16
22	A1	7	4SU	O4'-C4'-C3'	2.22	109.67	105.16
24	A3	21	H2U	C5-C6-N1	2.32	113.30	110.76
24	A3	21	H2U	C5-C4-N3	2.34	119.09	116.62
22	A1	55	PSU	O4'-C1'-C2'	2.71	107.62	104.69
22	A1	37	6MZ	C2-N1-C6	3.08	118.68	116.47
24	A3	21	H2U	N3-C2-N1	3.22	119.62	116.64
22	A1	34	CM0	C7-O5-C5	3.71	124.65	117.83
24	A3	56	PSU	O4'-C1'-C2'	3.94	108.95	104.69
22	A1	46	7MG	C6-N1-C2	6.22	123.17	115.88
22	A1	55	PSU	C4-N3-C2	11.92	125.10	115.16
24	A3	56	PSU	C4-N3-C2	12.00	125.17	115.16
22	A1	34	CM0	C4-N3-C2	12.84	125.87	115.16
22	A1	54	5MU	C4-N3-C2	12.85	125.88	115.16
24	A3	55	5MU	C4-N3-C2	13.41	126.35	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	VAL	A1	101	58,22	5,6,7	0.51	0	5,7,9	1.13	0
58	FME	BA	3001	57	8,9,10	0.81	0	5,9,11	1.52	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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	O1-CN-N	-2.49	120.98	124.80
58	BA	3001	FME	O-C-CA	-2.14	119.84	125.69

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.