



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 12:49 pm GMT

PDB ID : 4V74
EMDB ID: : EMD-1720
Title : 70S-fMetVal-tRNAVal-tRNAfMet complex in hybrid pre-translocation state (pre5b)
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 Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

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

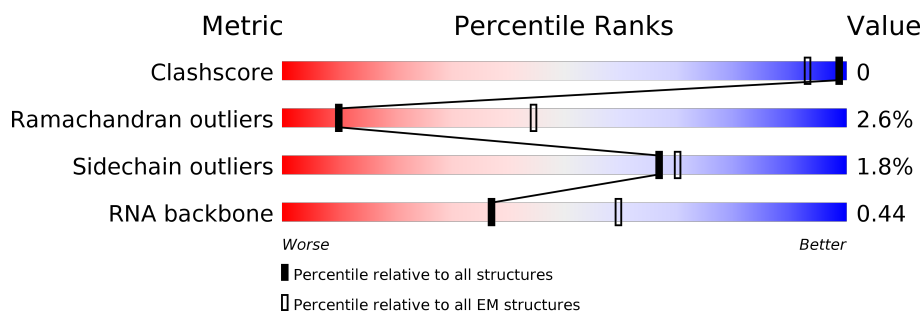
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.















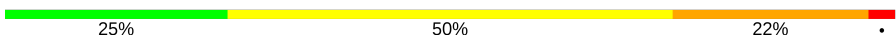
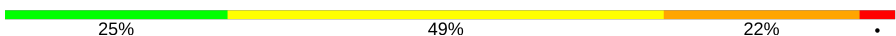
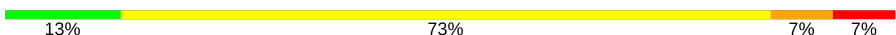










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AB	220	95% 5% •
2	AC	208	89% 10%
3	AD	206	88% 12%
4	AE	152	89% 11% •
5	AF	101	90% 9% •
6	AG	152	87% 13% •
7	AH	130	89% 10% •
8	AI	128	82% 16% •











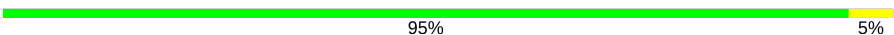





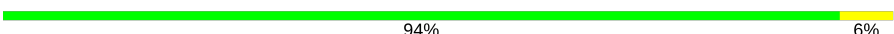



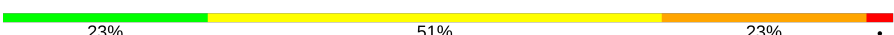
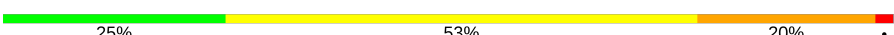

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Mol	Chain	Length	Quality of chain
9	AJ	100	 84% 15% .
10	AK	118	 92% 7% .
11	AL	124	 83% 15% ..
12	AM	115	 85% 14% .
13	AN	101	 86% 13% .
14	AO	89	 85% 13% .
15	AP	81	 84% 16%
16	AQ	82	 91% 9%
17	AR	57	 79% 21%
18	AS	81	 88% 11% .
19	AT	86	 93% 7%
20	AU	53	 79% 21%
21	AA	1533	 25% 50% 22% .
22	A1	76	 25% 49% 22% .
23	A2	15	 13% 73% 7% 7%
24	A3	77	 31% 45% 22% .
25	BC	273	 87% 12%
26	BD	209	 90% 9%
27	BE	201	 91% 9%
28	BF	179	 89% 11% .
29	BG	177	 89% 11% .
30	BH	149	 95% 5%
31	BI	142	 94% 5% .
32	BJ	142	 90% 10%
33	BK	123	 88% 11% ..

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Mol	Chain	Length	Quality of chain
34	BL	144	 85% 13% ..
35	BM	136	 85% 15%
36	BN	121	 87% 12% .
37	BO	117	 87% 11% ..
38	BP	115	 87% 12% .
39	BQ	118	 84% 15% .
40	BR	103	 90% 10%
41	BS	110	 89% 11%
42	BT	94	 85% 15%
43	BU	104	 89% 10% .
44	BV	94	 95% 5%
45	BW	80	 83% 14% ..
46	BX	79	 82% 14% ..
47	BY	63	 90% 10%
48	BZ	59	 83% 15% .
49	B0	57	 86% 12% .
50	B1	52	 94% 6%
51	B2	46	 78% 22%
52	B3	65	 85% 14% .
53	B4	38	 87% 13%
54	BA	2903	 23% 51% 23% .
55	BB	118	 25% 53% 20% ..
56	B5	234	 89% 6% 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		

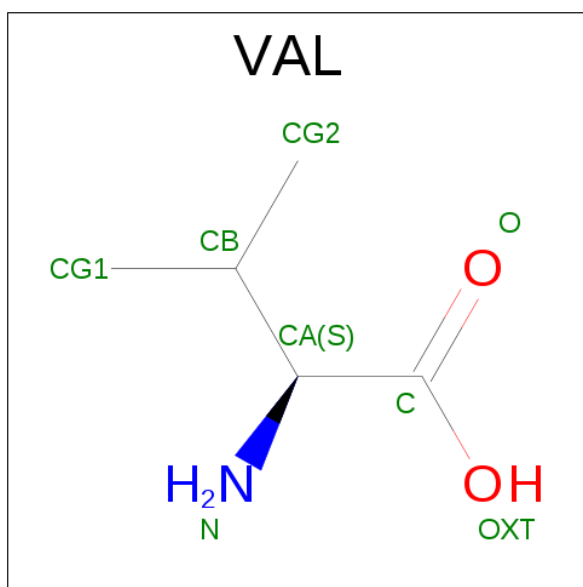
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

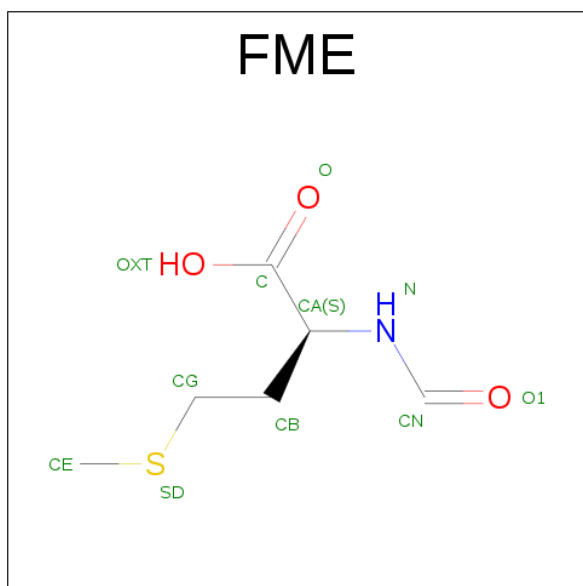
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- 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).

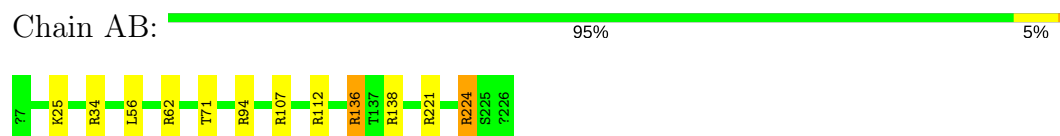


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

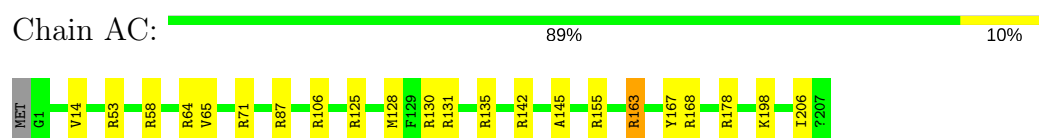
3 Residue-property plots [i](#)

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

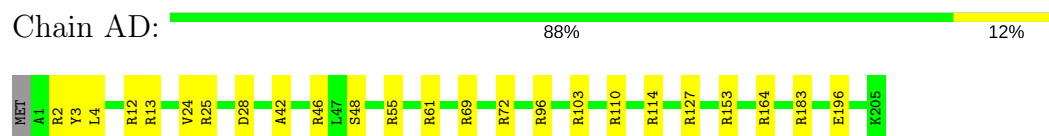
- Molecule 1: 30S ribosomal protein S2



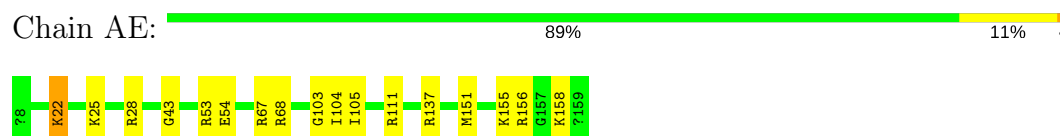
- Molecule 2: 30S ribosomal protein S3



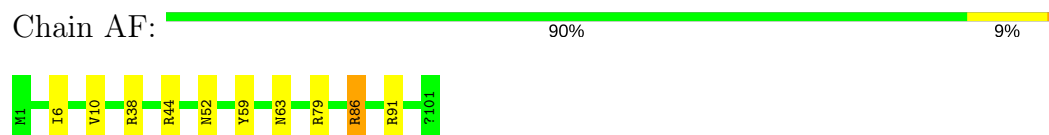
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



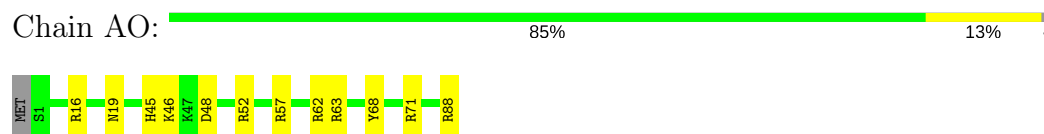
- Molecule 5: 30S ribosomal protein S6



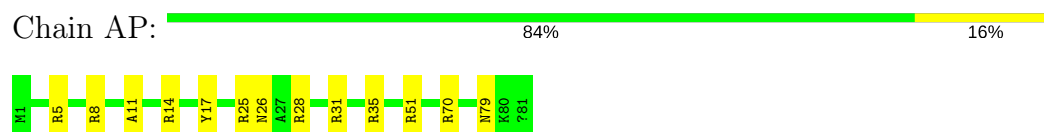
- Molecule 6: 30S ribosomal protein S7



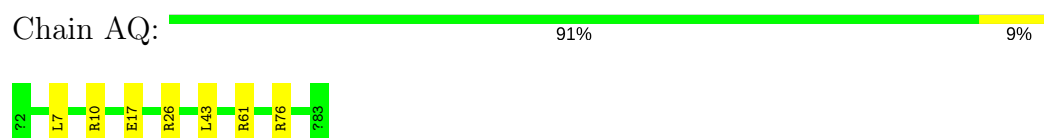
- Molecule 14: 30S ribosomal protein S15



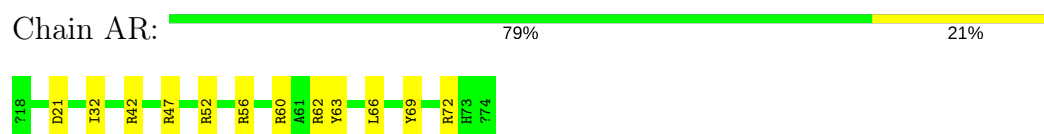
- Molecule 15: 30S ribosomal protein S16



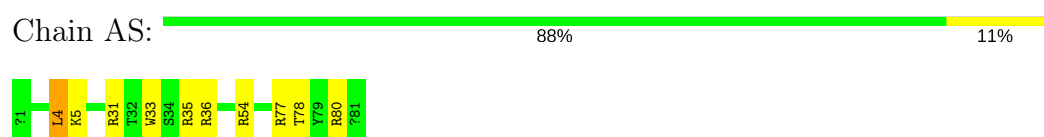
- Molecule 16: 30S ribosomal protein S17



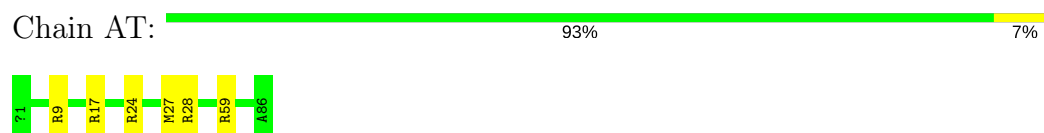
- Molecule 17: 30S ribosomal protein S18



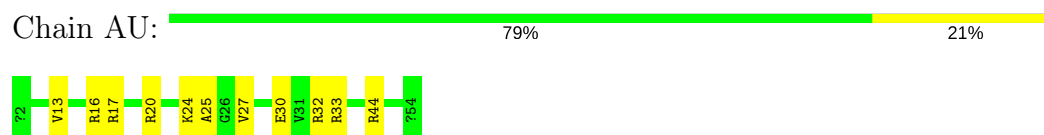
- Molecule 18: 30S ribosomal protein S19



- Molecule 19: 30S ribosomal protein S20



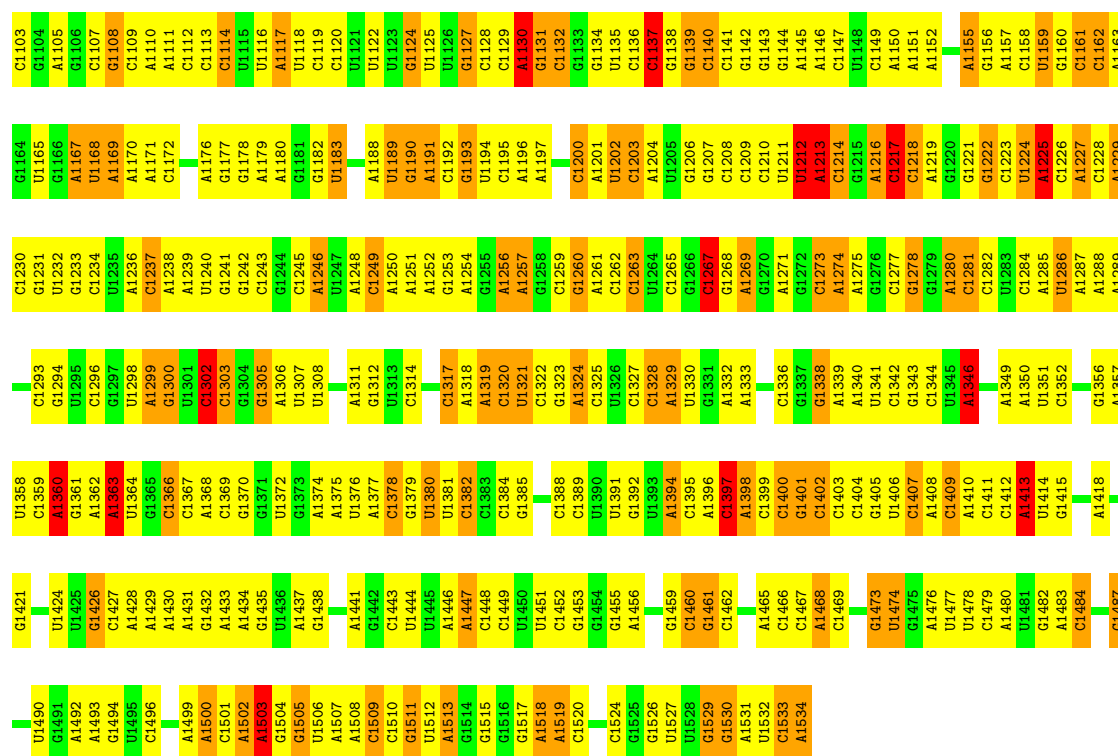
- Molecule 20: 30S ribosomal protein S21



- Molecule 21: 16S ribosomal RNA

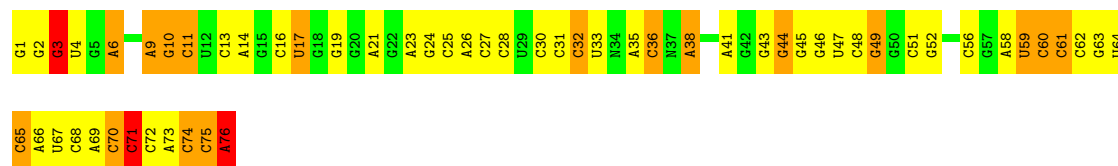


A1036	A1037	C1038	G1039	A1042	G1043	A1044	C1045	G1047	A1048	C1049	G1050	C1051	G1052	C1053	G1054	A1055	C1056	G1057	C1058	G1059	C1060	G1061	C1062	C1063	G1064	C1065	G1066	C1067	G1068	C1069	C1071	U1075	C1076	G1077	C1078	G1079	C1080	A1081	C1082	G1083	C1084	G1085	C1086	A1092	C1093	G1094	C1095	G1096	C1097	G1098	C1099	A1100	G1101	C1102	A1103																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
A908	A909	C910	G911	A912	G913	A914	C915	G917	A918	C919	G920	C921	G922	C923	G924	C925	G926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
A843	C844	A845	C846	G847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	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	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207	C1208	C1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379	C1380	C1381	C1382	C1383	C1384	C1385	C1386	C1387	C1388	C1389	C1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	C1470	C1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C17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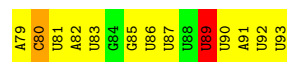
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 25% 49% 22%



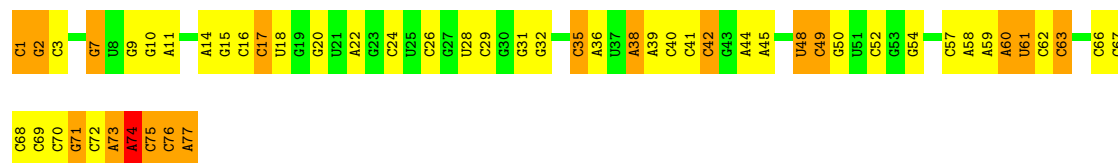
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

Chain A2: 13% 73% 7%



• Molecule 24: tRNA-fMet

Chain A3: 31% 45% 22%



• Molecule 25: 50S ribosomal protein L2

Chain BC: 87% 12%



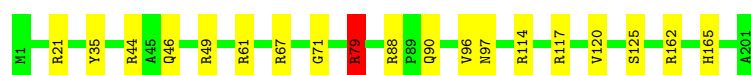
- Molecule 26: 50S ribosomal protein L3

Chain BD: 90% 9%



- Molecule 27: 50S ribosomal protein L4

Chain BE: 91% 9%



- Molecule 28: 50S ribosomal protein L5

Chain BF: 89% 11%



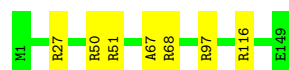
- Molecule 29: 50S ribosomal protein L6

Chain BG: 89% 11%



- Molecule 30: 50S ribosomal protein L9

Chain BH: 95% 5%



- Molecule 31: 50S ribosomal protein L11

Chain BI: 94% 5%



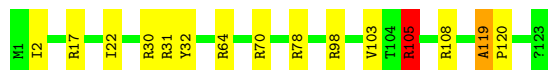
- Molecule 32: 50S ribosomal protein L13

Chain BJ: 90% 10%



- Molecule 33: 50S ribosomal protein L14

Chain BK: 88% 11% ..



- Molecule 34: 50S ribosomal protein L15

Chain BL: 85% 13% ..



- Molecule 35: 50S ribosomal protein L16

Chain BM: 85% 15%



- Molecule 36: 50S ribosomal protein L17

Chain BN: 87% 12% .



- Molecule 37: 50S ribosomal protein L18

Chain BO: 87% 11% ..



- Molecule 38: 50S ribosomal protein L19

Chain BP: 87% 12% .

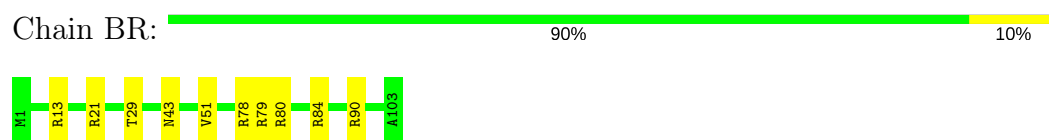


- Molecule 39: 50S ribosomal protein L20

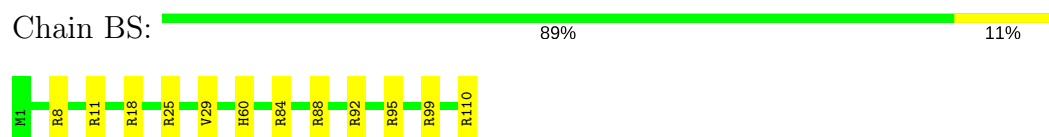
Chain BQ: 84% 15% .



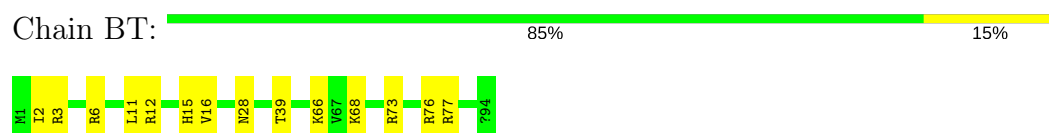
- Molecule 40: 50S ribosomal protein L21



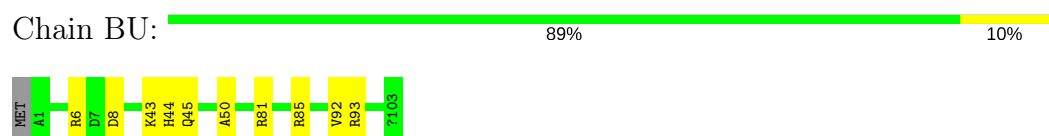
- Molecule 41: 50S ribosomal protein L22



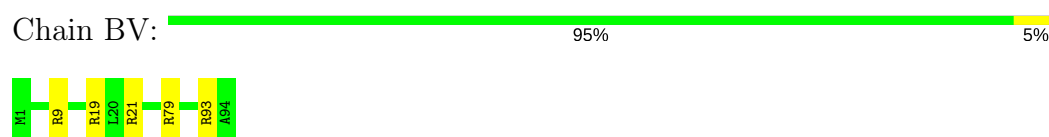
- Molecule 42: 50S ribosomal protein L23



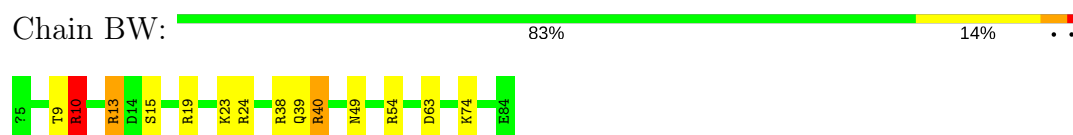
- Molecule 43: 50S ribosomal protein L24



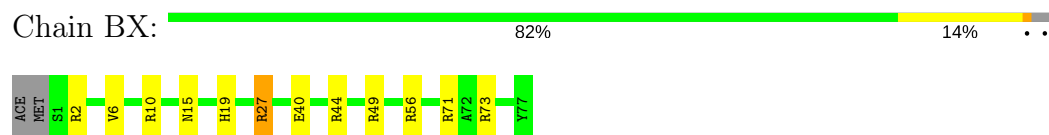
- Molecule 44: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L28




- Molecule 47: 50S ribosomal protein L29

Chain BY:  90% 10%




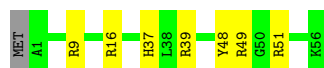
- Molecule 48: 50S ribosomal protein L30

Chain BZ:  83% 15%



- Molecule 49: 50S ribosomal protein L32

Chain B0:  86% 12%




- Molecule 50: 50S ribosomal protein L33

Chain B1:  94% 6%




- Molecule 51: 50S ribosomal protein L34

Chain B2:  78% 22%



- Molecule 52: 50S ribosomal protein L35

Chain B3:  85% 14%

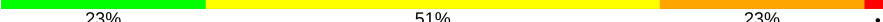


- Molecule 53: 50S ribosomal protein L36

Chain B4:  87% 13%

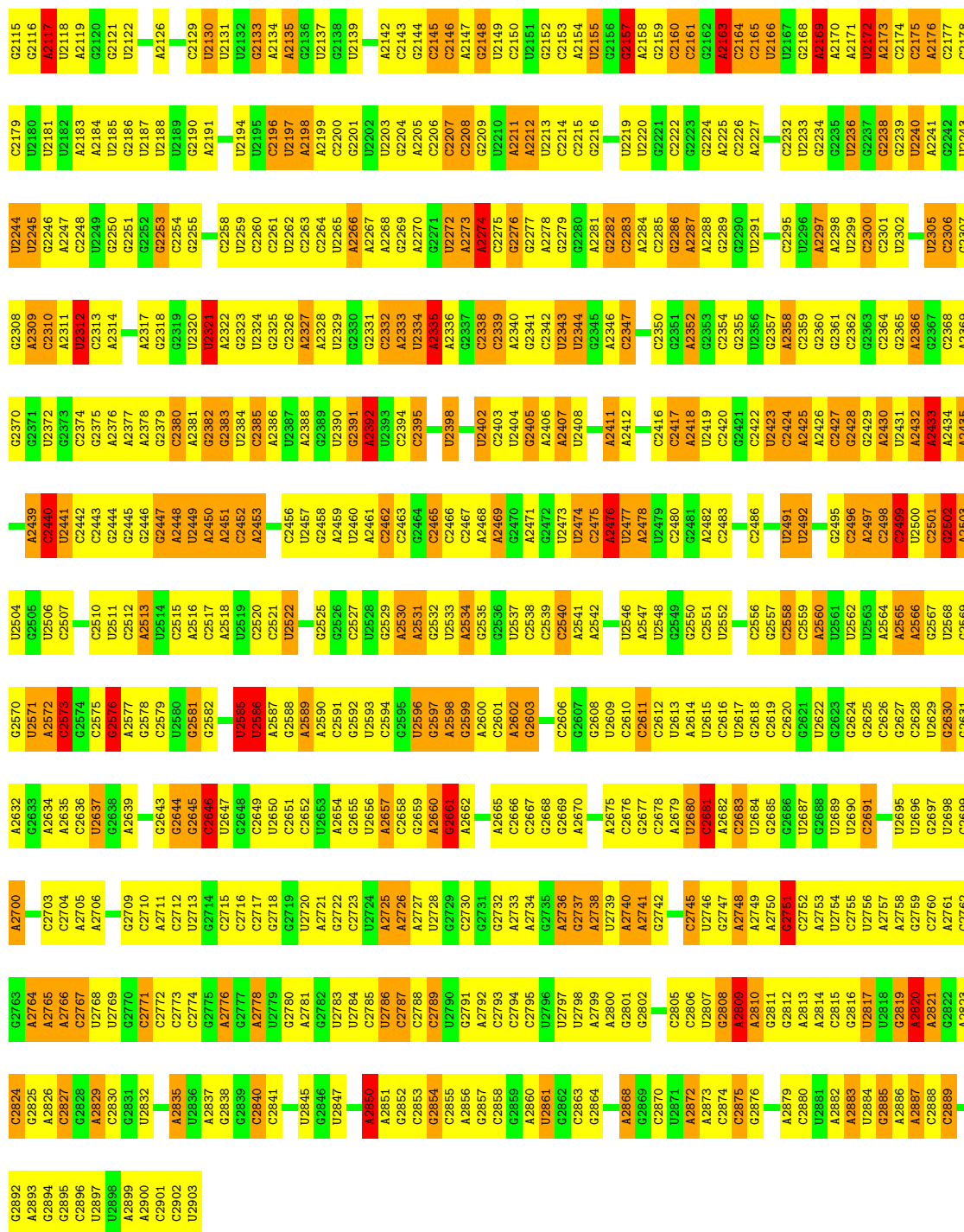


- Molecule 54: 23S ribosomal RNA

Chain BA:  23% 51% 23%

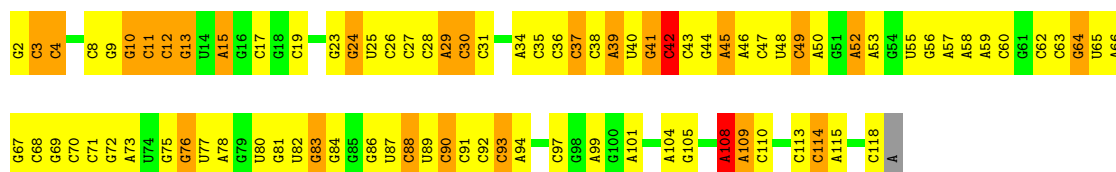
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G966	G967	C968	G969	C970	C971	A972	A973	G974	A975	A979	A980	A981	C982	A983	A984	C985	C986	C987	G988	A989	C990	C991	C992	C993	C994	C995	A996	G997	C998	U999	A1000	A1001	G1002	G1003	U1004	C1005	C1006	C1007	A1008	A1009	A1010	C1011	U1012	C1013	A1014	U1015	U1016	G1017	U1018	C1019	A1020	A1021	G1022	U1023	G1024	G1025	U1026	A1027																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
C840	C841	A844	A845	A846	U847	C848	A849	U850	C851	U852	C853	C854	A855	C856	C857	C858	C859	U860	A861	A862	A863	C864	C865	A866	C867	U868	C869	U870	C873	C874	C875	C876	A877	C878	C881	C882	C883	U884	C885	A886	U887	C888	C889	C890	C891	A892	C893	A896	C897	C898	A899	A900	C901	C902	C903	C904	C905																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G776	U779	G780	A781	A782	A783	G784	G785	C786	C787	A788	A789	U790	C791	A792	A793	A794	C795	C796	G799	A800	C801	C802	U803	A804	C805	C806	U807	C808	C809	U810	U811	C812	U813	C814	C815	C816	C817	C818	A819	A820	A821	C822	C823	U824	A825	U828	A829	C830	U831	U832	A833	C834	C835	C838	U839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549	A1550	A1551	A1552	A1553	A1554	A1555	A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	A1573	A1574	A1575	A1576	A1577	A1578	A1579	A1580	A1581	A1582	A1583	A1584	A1585	A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632	A1633	A1634	A1635	A1636	A1637	A1638	A1639	A1640	A1641	A1642	A1643	A1644	A1645	A1646	A1647	A1648	A1649	A1650	A1651	A1652	A1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G1288	C1289	U1290	A1291	G1292	C1293	U1294	C1295	G1296	C1297	U1298	G1299	G1300	A1301	G1302	U1303	A1304	C1305	C1306	A1307	A1308	U1312	U1313	C1314	G1315	U1316	G1317	U1318	C1319	A1320	A1321	C1322	G1323	C1324	U1325	G1326	A1327	A1328	U1329	C1330	G1331	G1332	U1333	G1334	C1335	A1336	G1337	U1338	C1339	U1340	A1341	U1342	G1345	U1346	A1347	C1348	U1349	C1350																																																																																																																																																																																																																																																																																																																															
C1351	U1352	A1353	U1354	G1355	C1356	C1357	G1358	A1359	U1360	G1361	C1362	U1363	G1364	A1365	A1366	A1367	C1370	G1371	A1372	A1373	C1376	G1377	A1378	U1379	G1382	A1383	A1384	A1385	C1386	G1387	G1388	C1389	U1390	U1391	A1392	A1393	U1394	A1395	U1396	U1397	C1398	C1399	A1403	C1404	G1407	G1408	U1409	G1410	U1411	U1412	A1413	G1414	U1415	G1416																																																																																																																																																																																																																																																																																																																																		
C1417	G1418	A1419	U1420	G1421	G1425	G1426	A1427	U1428	G1429	G1430	A1431	G1432	A1433	U1434	G1435	U1436	U1437	U1438	A1439	U1440	U1441	U1442	G1445	C1446	C1447	C1451	G1452	A1453	G1454	G1455	U1456	U1457	U1460	C1461	C1462	U1463	G1464	G1465	A1469	A1470	U1471	C1472	G1473	U1474	G1475	U1476	A1477	G1478	G1479	U1480	U1481	G1482	C1483	U1484																																																																																																																																																																																																																																																																																																																																		
U1487	C1488	A1489	U1490	G1491	G1492	C1493	A1494	U1495	A1496	U1497	A1498	A1499	G1500	G1501	A1502	C1503	A1504	A1505	U1506	C1507	A1508	A1509	G1510	G1511	C1512	U1513	G1514	C1515	U1516	U1517	C1518	U1519	G1520	G1521	A1522	U1523	G1524	A1525	G1526	G1527	A1528	C1531	A1532	C1533	U1534	C1535	A1536	C1537	U1538	U1539	A1540	C1541	U1542	G1543	A1544	U1545	G1546	C1547																																																																																																																																																																																																																																																																																																																														
A1548	A1549	C1550	A1551	U1552	A1553	G1554	G1555	U1556	C1557	U1558	G1559	C1560	A1561	U1562	U1563	C1564	G1565	A1566	G1567	G1568	A1569	A1570	A1571	A1572	G1573	C1574	U1575	U1576	C1577	U1578	A1579	U1580	G1581	C1582	A1583	U1584	C1585	A1586	A1590	A1591	C1592	A1593	U1594	C1595	A1596	U1597	A1598	U1599	C1600	G1601	U1602	A1603	C1604	G1605	C1606	U1607	A1608	A1609																																																																																																																																																																																																																																																																																																																														
A1610	C1611	G1612	G1613	A1614	C1615	G1616	C1617	A1618	G1619	G1620	U1621	G1622	G1623	C1624	U1625	A1626	G1627	G1628	U1629	A1630	G1631	A1632	G1633	A1634	A1635	U1636	A1637	C1638	C1639	A1640	A1641	G1642	G1643	A1644	G1645	C1646	U1647	U1648	A1650	G1651	A1652	G1653	A1654	C1655	C1656	U1657	C1658	G1659	A1664	A1665	G1666	G1667	A1668	A1669	C1670	U1671	A1672																																																																																																																																																																																																																																																																																																																															
G1673	G1674	C1675	A1676	U1677	A1678	C1679	U1680	G1681	G1682	U1683	G1684	C1685	C1686	A1689	A1690	G1691	U1692	G1693	C1694	G1695	G1696	G1697	A1698	G1699	A1700	C1701	U1702	G1703	C1704	A1705	U1706	U1707	C1708	A1711	U1712	U1713	G1714	U1715	U1716	A1717	G1718	G1719	U1720	G1721	U1722	G1723	U1724	U1725	C1726	U1727	C1728	U1729	C1730	G1731	C1732	U1733	G1734																																																																																																																																																																																																																																																																																																																															
A1735	U1736	G1737	C1738	A1739	U1740	C1741	U1742	G1743	A1744	U1745	A1746	U1747	C1748	A1749	C1752	G1753	C1754	A1755	G1756	A1757	U1758	A1759	C1760	C1761	A1762	G1763	U1764	U1765	G1766	G1767	C1768	U1769	G1770	C1771	A1772	U1773	C1774	U1775	A1780	U1781	U1782	A1783	A1784	A1785	U1786	A1787	C1788	A1789	C1790	U1791	A1792	C1793	A1794	C1795	U1796	G1797	U1798																																																																																																																																																																																																																																																																																																																															
G1799	C1800	A1801	U1802	A1803	C1804	A1805	C1806	G1807	A1808	C1809	A1810	G1811	U1812	G1813	A1814	U1815	C1816	G1817	U1818	A1819	U1820	A1821	G1822	C1823	G1824	U1825	A1826	U1827	G1828	A1829	C1830	G1831	C1832	U1833	U1834	G1835	A1836	C1837	U1838	G1839	G1840	U1841	U1842	C1843	C1844	A1847	A1848	U1852	A1853	U1854	U1855	C1856	U1857	A1858	U1861	G1862																																																																																																																																																																																																																																																																																																																																
G1863	U1864	U1865	A1866	G1867	C1868	G1869	C1870	A1871	A1872	C1873	C1874	G1875	A1876	A1877	G1878	C1879	U1880	C1881	G1884	A1885	U1886	C1887	G1888	A1889	A1890	C1891	C1892	C1893	G1894	U1895	C1896	G1897	U1898	A1899	A1900	A1901	C1902	C1905	G1906	G1907	C1908	C1909	U1910	U1911	U1912	A1913	C1914	U1915	A1916	U1917	A1918	U1919	C1920	G1921	U1922	U1923	C1924																																																																																																																																																																																																																																																																																																																															
C1925	U1926	A1927	U1928	G1929	C1930	U1931	A1932	U1933	C1934	G1935	A1936	U1937	A1938	U1939	A1940	C1941	G1942	U1943	U1944	G1945	C1946	G1948	G1949	G1950	U1951	A1952	A1953	G1954	U1955	U1956	C1957	G1958	C1959	A1960	C1961	C1962	U1963	G1964	C1965	A1966	C1967	G1968	A1969	U1970	U1971	G1972	C1973	C1974	U1975	U1976	A1977	U1978	A1981	U1982	C1983	U1984	C1985																																																																																																																																																																																																																																																																																																																															
C1986	A1987	C1990	U1991	G1992	U1993	U1994	U1995	C1996	C1997	A1998	C1999	C2000	C2001	G2002	A2003	G2004	A2005	C2006	U2007	C2008	A2009	A2013	A2014	U2015	A2016	U2017	G2018	A2019	U2020	C2021	U2022	C2023	G2024	C2025	A2030	A2031	G2032	A2033	U2034	G2035	C2036	A2037	U2038	G2039	C2100	G2101	G2102	A2103	C2104	U2105	A2108	U2111	G2112	A2114																																																																																																																																																																																																																																																																																																																																		
G2053	A2054	G2055	G2056	G2057	A2058	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	G2067	A2068	G2069	A2070	A2071	C2072	C2073	U2074	U2075	U2076	A2077	C2078	U2079	A2080	U2081	A2082	G2083	C2084	U2085	G2086	C2087	A2088	C2089	A2090	C2091	G2092	G2093	A2094	A2095	C2096	A2097	U2098	U2099	G2100	G2101	G2102	C2103	C2104	U2105	A2108	U2111	G2112	A2114																																																																																																																																																																																																																																																																																																																																
U2111	G2112	U2113	A2114	U2115	G2116	U2117	G2118	U2119	G2120	U2121	G2122	U2123	G2124	U2125	G2126	U2127	G2128	U2129	G2130	U2131	G2132	U2133	G2134	U2135	G2136	U2137	G2138	U2139	G2140	U2141	G2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	U2161	U2162	U2163	U2164	U2165	U2166	U2167	U2168	U2169	U2170	U2171	U2172	U2173	U2174	U2175	U2176	U2177	U2178	U2179	U2180	U2181	U2182	U2183	U2184	U2185	U2186	U2187	U2188	U2189	U2190	U2191	U2192	U2193	U2194	U2195	U2196	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230	U2231	U2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240	U2241	U2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2251	U2252	U2253	U2254	U2255	U2256	U2257	U2258	U2259	U2260	U2261	U2262	U2263	U2264	U2265	U2266	U2267	U2268	U2269	U2270	U2271	U2272	U2273	U2274	U2275	U2276	U2277	U2278	U2279	U2280	U2281	U2282	U2283	U2284	U2285	U2286	U2287	U2288	U2289	U2290	U2291	U2292	U2293	U2294	U2295	U2296	U2297	U2298	U2299	U2300	U2301	U2302	U2303	U2304	U2305	U2306	U2307	U2308	U2309	U2310	U2311	U2312	U2313	U2314	U2315	U2316	U2317	U2318	U2319	U2320	U2321	U2322	U2323	U2324	U2325	U2326	U2327	U2328	U2329	U2330	U2331	U2332	U2333	U2334	U2335	U2336	U2337	U2338	U2339	U2340	U2341	U2342	U2343	U2344	U2345	U2346	U2347	U2348	U2349	U2350	U2351	U2352	U2353	U2354	U2355	U2356	U2357	U2358	U2359	U2360	U2361	U2362	U2363	U2364	U2365	U2366	U2367	U2368	U2369	U2370	U2371	U2372	U2373	U2374	U2375	U2376	U2377	U2378	U2379	U2380	U2381	U2382	U2383	U2384	U2385	U2386	U2387	U2388	U2389	U2390	U2391	U2392	U2393	U2394	U2395	U2396	U2397	U2398	U2399	U2400	U2401	U2402	U2403	U2404	U2405	U2406	U2407	U2408	U2409	U2410	U2411	U2412	U2413	U2414	U2415	U2416	U2417	U2418	U2419	U2420	U2421	U2422	U2423	U2424	U2425	U2426	U2427	U2428	U2429	U2430	U2431	U2432	U2433	U2434	U2435	U2436	U2437	U2438	U2439	U2440	U2441	U2442	U2443	U2444	U2445	U2446	U2447	U2448	U2449	U2450	U2451	U2452	U2453	U2454	U2455	U2456	U2457	U2458	U2459	U2460	U2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471	U2472	U2473	U2474	U2475	U2476	U2477	U2478	U2479	U2480	U2481	U2482	U2483	U2484	U2485	U2486	U2



• Molecule 55: 5S ribosomal RNA

Chain BB: 25% 53% 20%



● Molecule 56: 50S ribosomal protein L1

Chain B5:

89%

6%

5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	3052	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	162740	Depositor
Image detector	4k CCD camera (TVIPS)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	AB	0.70	0/1736	1.07	11/2340 (0.5%)
10	AK	0.74	0/894	1.15	10/1207 (0.8%)
11	AL	0.76	0/969	1.23	15/1300 (1.2%)
12	AM	0.75	0/884	1.32	11/1181 (0.9%)
13	AN	0.77	0/817	1.26	12/1088 (1.1%)
14	AO	0.74	0/722	1.16	8/964 (0.8%)
15	AP	0.76	0/648	1.27	11/870 (1.3%)
16	AQ	0.70	0/658	1.06	4/883 (0.5%)
17	AR	0.81	0/463	1.29	10/623 (1.6%)
18	AS	0.76	0/653	1.13	7/879 (0.8%)
19	AT	0.68	0/672	1.05	5/890 (0.6%)
2	AC	0.72	0/1651	1.16	16/2225 (0.7%)
20	AU	0.83	0/431	1.44	8/572 (1.4%)
21	AA	1.53	1/36759 (0.0%)	2.22	1991/57346 (3.5%)
22	A1	1.53	0/1668	2.20	85/2595 (3.3%)
23	A2	1.47	0/343	2.25	15/531 (2.8%)
24	A3	1.53	0/1722	2.18	81/2685 (3.0%)
25	BC	0.74	0/2121	1.30	26/2852 (0.9%)
26	BD	0.68	0/1586	1.20	14/2134 (0.7%)
27	BE	0.67	0/1571	1.15	11/2113 (0.5%)
28	BF	0.74	0/1444	1.18	14/1937 (0.7%)
29	BG	0.69	0/1343	1.12	8/1816 (0.4%)
3	AD	0.77	0/1665	1.23	24/2227 (1.1%)
30	BH	0.65	0/1122	1.10	6/1515 (0.4%)
31	BI	0.65	0/1046	1.06	4/1410 (0.3%)
32	BJ	0.73	0/1152	1.16	8/1551 (0.5%)
33	BK	0.70	0/947	1.21	10/1268 (0.8%)
34	BL	0.73	0/1054	1.36	17/1403 (1.2%)
35	BM	0.74	0/1093	1.21	11/1460 (0.8%)
36	BN	0.77	0/973	1.36	15/1301 (1.2%)
37	BO	0.72	0/902	1.25	11/1209 (0.9%)
38	BP	0.75	0/929	1.27	8/1242 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.80	0/960	1.32	15/1278 (1.2%)
4	AE	0.70	0/1119	1.06	10/1506 (0.7%)
40	BR	0.70	0/829	1.22	7/1107 (0.6%)
41	BS	0.64	0/864	1.19	10/1156 (0.9%)
42	BT	0.65	0/744	1.19	7/994 (0.7%)
43	BU	0.68	0/787	1.10	4/1051 (0.4%)
44	BV	0.71	0/766	1.16	5/1025 (0.5%)
45	BW	0.77	0/604	1.36	9/799 (1.1%)
46	BX	0.75	0/635	1.28	10/848 (1.2%)
47	BY	0.65	0/510	1.17	5/677 (0.7%)
48	BZ	0.69	0/453	1.24	6/605 (1.0%)
49	B0	0.72	0/450	1.23	5/599 (0.8%)
5	AF	0.74	0/835	1.17	6/1128 (0.5%)
50	B1	0.73	0/417	1.05	2/556 (0.4%)
51	B2	0.81	0/380	1.49	11/498 (2.2%)
52	B3	0.72	0/513	1.23	5/676 (0.7%)
53	B4	0.68	0/303	1.24	4/397 (1.0%)
54	BA	1.41	2/69796 (0.0%)	2.21	4018/108888 (3.7%)
55	BB	1.42	0/2800	2.17	151/4367 (3.5%)
56	B5	0.64	0/1673	1.08	9/2255 (0.4%)
6	AG	0.74	0/1188	1.21	19/1593 (1.2%)
7	AH	0.70	0/989	1.08	5/1326 (0.4%)
8	AI	0.81	0/1035	1.34	20/1377 (1.5%)
9	AJ	0.69	0/797	1.23	13/1079 (1.2%)
All	All	1.28	3/160085 (0.0%)	2.00	6843/239402 (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
1	AB	0	1
14	AO	0	2
21	AA	0	368
22	A1	0	21
23	A2	0	4
24	A3	0	16
4	AE	0	1
43	BU	0	1
49	B0	0	1
54	BA	0	707

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	25
All	All	0	1147

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	6	G	C2-N2	-5.63	1.28	1.34
54	BA	1568	G	C2-N2	-5.08	1.29	1.34
54	BA	2627	G	C2-N2	-5.01	1.29	1.34

All (6843) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1301	A	O4'-C1'-N9	17.59	122.27	108.20
54	BA	2126	A	O4'-C1'-N9	13.48	118.98	108.20
21	AA	547	A	N1-C6-N6	-12.92	110.85	118.60
54	BA	323	C	O4'-C1'-N1	12.84	118.47	108.20
54	BA	2199	A	N1-C6-N6	-12.76	110.94	118.60
21	AA	1362	A	N1-C6-N6	-12.39	111.16	118.60
54	BA	1069	A	N1-C6-N6	-12.35	111.19	118.60
54	BA	2810	A	N1-C6-N6	-12.29	111.23	118.60
54	BA	614	A	N1-C6-N6	-11.99	111.40	118.60
54	BA	1981	A	N1-C6-N6	-11.97	111.42	118.60
54	BA	933	A	N1-C6-N6	-11.94	111.44	118.60
54	BA	1591	A	N1-C6-N6	-11.92	111.45	118.60
21	AA	190	A	N1-C6-N6	-11.78	111.53	118.60
54	BA	382	A	N1-C6-N6	-11.78	111.53	118.60
54	BA	1205	A	N1-C6-N6	-11.77	111.54	118.60
54	BA	2134	A	N1-C6-N6	-11.75	111.55	118.60
54	BA	1523	U	O4'-C1'-N1	11.61	117.49	108.20
5	AF	91	ARG	NE-CZ-NH1	11.58	126.09	120.30
21	AA	1251	A	N1-C6-N6	-11.57	111.66	118.60
54	BA	1010	A	N1-C6-N6	-11.54	111.67	118.60
21	AA	172	A	N1-C6-N6	-11.51	111.69	118.60
54	BA	2572	A	N1-C6-N6	-11.49	111.70	118.60
54	BA	99	U	O4'-C1'-N1	11.44	117.35	108.20
54	BA	1427	A	N1-C6-N6	-11.42	111.75	118.60
21	AA	466	A	N1-C6-N6	-11.42	111.75	118.60
21	AA	746	A	N1-C6-N6	-11.41	111.75	118.60
21	AA	228	A	N1-C6-N6	-11.39	111.77	118.60
54	BA	1698	A	N1-C6-N6	-11.38	111.77	118.60
54	BA	1301	A	C1'-O4'-C4'	-11.36	100.81	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	432	A	N1-C6-N6	-11.36	111.79	118.60
54	BA	1940	U	O4'-C1'-N1	11.32	117.25	108.20
55	BB	94	A	N1-C6-N6	-11.25	111.85	118.60
54	BA	2267	A	N1-C6-N6	-11.25	111.85	118.60
54	BA	800	A	N1-C6-N6	-11.24	111.85	118.60
54	BA	53	A	N1-C6-N6	-11.23	111.86	118.60
55	BB	78	A	N1-C6-N6	-11.23	111.86	118.60
54	BA	2851	A	N1-C6-N6	-11.22	111.87	118.60
54	BA	197	A	N1-C6-N6	-11.20	111.88	118.60
54	BA	2097	A	N1-C6-N6	-11.20	111.88	118.60
21	AA	1480	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	53	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	1503	A	N1-C6-N6	-11.17	111.90	118.60
54	BA	1241	A	N1-C6-N6	-11.17	111.90	118.60
54	BA	1580	A	N1-C6-N6	-11.14	111.92	118.60
7	AH	87	ARG	NE-CZ-NH2	11.13	125.87	120.30
54	BA	2705	A	N1-C6-N6	-11.12	111.93	118.60
54	BA	575	A	N1-C6-N6	-11.09	111.95	118.60
21	AA	389	A	N1-C6-N6	-11.07	111.96	118.60
54	BA	2726	A	N1-C6-N6	-11.02	111.99	118.60
54	BA	1808	A	N1-C6-N6	-10.99	112.01	118.60
54	BA	125	A	N1-C6-N6	-10.97	112.02	118.60
54	BA	152	A	N1-C6-N6	-10.96	112.02	118.60
21	AA	630	A	N1-C6-N6	-10.95	112.03	118.60
54	BA	1746	A	N1-C6-N6	-10.93	112.04	118.60
54	BA	626	A	N1-C6-N6	-10.93	112.04	118.60
54	BA	181	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	2376	A	N1-C6-N6	-10.87	112.08	118.60
54	BA	2358	A	N1-C6-N6	-10.86	112.08	118.60
54	BA	1784	A	N1-C6-N6	-10.86	112.09	118.60
21	AA	1329	A	N1-C6-N6	-10.85	112.09	118.60
54	BA	2750	A	N1-C6-N6	-10.84	112.10	118.60
21	AA	1014	A	N1-C6-N6	-10.83	112.10	118.60
21	AA	1518	A	N1-C6-N6	-10.82	112.11	118.60
52	B3	39	ARG	NE-CZ-NH2	10.82	125.71	120.30
54	BA	764	A	N1-C6-N6	-10.81	112.11	118.60
54	BA	1317	G	O4'-C1'-N9	10.81	116.85	108.20
54	BA	1000	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	432	A	N1-C6-N6	-10.79	112.13	118.60
21	AA	937	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	1095	A	N1-C6-N6	-10.75	112.15	118.60
54	BA	324	A	N1-C6-N6	-10.72	112.17	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2814	A	N1-C6-N6	-10.72	112.17	118.60
21	AA	749	A	N1-C6-N6	-10.69	112.19	118.60
21	AA	665	A	N1-C6-N6	-10.68	112.19	118.60
54	BA	2614	A	N1-C6-N6	-10.66	112.20	118.60
21	AA	520	A	N1-C6-N6	-10.66	112.21	118.60
54	BA	1352	U	O4'-C1'-N1	10.64	116.71	108.20
40	BR	84	ARG	NE-CZ-NH1	10.63	125.62	120.30
54	BA	2099	U	O4'-C1'-N1	10.63	116.71	108.20
54	BA	609	A	N1-C6-N6	-10.61	112.23	118.60
21	AA	1289	A	N1-C6-N6	-10.59	112.25	118.60
54	BA	1033	U	O4'-C1'-N1	10.59	116.67	108.20
54	BA	2320	U	O4'-C1'-N1	10.59	116.67	108.20
54	BA	928	A	N1-C6-N6	-10.59	112.25	118.60
44	BV	9	ARG	NE-CZ-NH1	10.58	125.59	120.30
54	BA	2130	U	O4'-C1'-N1	10.58	116.67	108.20
54	BA	1713	A	N1-C6-N6	-10.58	112.25	118.60
54	BA	1858	A	N1-C6-N6	-10.58	112.25	118.60
21	AA	729	A	N1-C6-N6	-10.57	112.26	118.60
21	AA	784	A	N1-C6-N6	-10.56	112.27	118.60
54	BA	1365	A	N1-C6-N6	-10.55	112.27	118.60
54	BA	1553	A	N1-C6-N6	-10.54	112.28	118.60
54	BA	2711	A	N1-C6-N6	-10.53	112.28	118.60
12	AM	106	ARG	NE-CZ-NH1	10.51	125.56	120.30
54	BA	716	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	936	A	N1-C6-N6	-10.49	112.30	118.60
54	BA	101	A	N1-C6-N6	-10.49	112.31	118.60
21	AA	1201	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	1327	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	1021	A	N1-C6-N6	-10.46	112.32	118.60
54	BA	2748	A	N1-C6-N6	-10.46	112.32	118.60
54	BA	1919	A	N1-C6-N6	-10.46	112.33	118.60
21	AA	819	A	N1-C6-N6	-10.43	112.34	118.60
21	AA	120	A	N1-C6-N6	-10.42	112.34	118.60
21	AA	1434	A	N1-C6-N6	-10.41	112.36	118.60
54	BA	1434	A	N1-C6-N6	-10.41	112.36	118.60
54	BA	1597	A	N1-C6-N6	-10.41	112.36	118.60
54	BA	1937	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	2070	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	1301	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	2434	A	N1-C6-N6	-10.36	112.38	118.60
54	BA	761	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	1635	A	N1-C6-N6	-10.34	112.40	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	943	A	N1-C6-N6	-10.34	112.40	118.60
21	AA	151	A	N1-C6-N6	-10.33	112.40	118.60
54	BA	1494	A	N1-C6-N6	-10.31	112.41	118.60
21	AA	978	A	N1-C6-N6	-10.29	112.42	118.60
54	BA	1439	A	N1-C6-N6	-10.30	112.42	118.60
31	BI	102	ARG	NE-CZ-NH1	10.29	125.44	120.30
21	AA	780	A	N1-C6-N6	-10.29	112.43	118.60
54	BA	1509	A	N1-C6-N6	-10.28	112.43	118.60
54	BA	1302	A	N1-C6-N6	-10.28	112.43	118.60
21	AA	873	A	N1-C6-N6	-10.28	112.43	118.60
54	BA	2809	A	N1-C6-N6	-10.28	112.43	118.60
21	AA	353	A	N1-C6-N6	-10.27	112.44	118.60
21	AA	415	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	782	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	821	A	N1-C6-N6	-10.26	112.45	118.60
54	BA	2287	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	643	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	2751	G	O4'-C1'-N9	10.25	116.40	108.20
21	AA	51	A	N1-C6-N6	-10.24	112.45	118.60
54	BA	1630	A	N1-C6-N6	-10.23	112.46	118.60
38	BP	52	ARG	NE-CZ-NH1	10.22	125.41	120.30
21	AA	412	A	N1-C6-N6	-10.22	112.47	118.60
21	AA	1082	A	N1-C6-N6	-10.21	112.47	118.60
8	AI	79	ARG	NE-CZ-NH1	10.21	125.40	120.30
54	BA	2577	A	N1-C6-N6	-10.18	112.49	118.60
21	AA	1431	A	N1-C6-N6	-10.17	112.50	118.60
21	AA	414	A	N1-C6-N6	-10.17	112.50	118.60
21	AA	1363	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	2534	A	N1-C6-N6	-10.16	112.50	118.60
21	AA	1248	A	N1-C6-N6	-10.16	112.50	118.60
55	BB	109	A	N1-C6-N6	-10.16	112.51	118.60
14	AO	71	ARG	NE-CZ-NH1	10.15	125.38	120.30
54	BA	1755	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	263	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	1336	C	N3-C2-O2	-10.15	114.79	121.90
21	AA	338	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	1046	A	N1-C6-N6	-10.15	112.51	118.60
54	BA	2297	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	2346	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	1815	A	N1-C6-N6	-10.13	112.52	118.60
54	BA	2887	A	N1-C6-N6	-10.13	112.52	118.60
54	BA	483	A	N1-C6-N6	-10.13	112.52	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1953	A	N1-C6-N6	-10.11	112.53	118.60
21	AA	288	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	1952	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	2654	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	845	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	66	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	1393	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	1668	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	1717	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	1618	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	1085	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	1129	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	1966	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	345	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	1803	A	N1-C6-N6	-10.06	112.56	118.60
21	AA	959	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	1496	A	N1-C6-N6	-10.05	112.57	118.60
24	A3	74	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	2799	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	1067	A	N1-C6-N6	-10.04	112.57	118.60
54	BA	1508	A	N1-C6-N6	-10.04	112.57	118.60
54	BA	1610	A	O4'-C1'-N9	10.04	116.23	108.20
54	BA	1126	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	1678	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	1360	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	1318	A	N1-C6-N6	-10.02	112.59	118.60
56	B5	60	ARG	NE-CZ-NH2	10.02	125.31	120.30
54	BA	354	A	N1-C6-N6	-10.01	112.59	118.60
21	AA	1280	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	10	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	629	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	139	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	1794	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	539	A	N1-C6-N6	-9.99	112.60	118.60
42	BT	3	ARG	NE-CZ-NH1	9.99	125.30	120.30
54	BA	2560	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	1783	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	1213	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	1288	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	2835	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	320	A	N1-C6-N6	-9.97	112.62	118.60
34	BL	2	ARG	NE-CZ-NH2	9.97	125.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2108	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	152	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	274	A	N1-C6-N6	-9.96	112.63	118.60
21	AA	1152	A	N1-C6-N6	-9.96	112.63	118.60
21	AA	1204	A	N1-C6-N6	-9.96	112.63	118.60
21	AA	1408	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	945	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	782	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	784	G	O4'-C1'-N9	9.94	116.16	108.20
54	BA	1230	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	181	A	N1-C6-N6	-9.91	112.65	118.60
54	BA	941	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	5	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1762	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1453	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1943	U	O4'-C1'-N1	9.89	116.11	108.20
54	BA	2886	A	O4'-C1'-N9	9.89	116.11	108.20
21	AA	223	A	N1-C6-N6	-9.89	112.67	118.60
54	BA	925	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	1610	A	N1-C6-N6	-9.86	112.68	118.60
54	BA	1916	A	N1-C6-N6	-9.86	112.68	118.60
21	AA	510	A	N1-C6-N6	-9.86	112.69	118.60
21	AA	1044	A	N1-C6-N6	-9.86	112.69	118.60
21	AA	579	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	947	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	1147	A	N1-C6-N6	-9.85	112.69	118.60
55	BB	39	A	N1-C6-N6	-9.85	112.69	118.60
55	BB	66	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	44	A	N1-C6-N6	-9.84	112.69	118.60
54	BA	849	A	N1-C6-N6	-9.84	112.69	118.60
54	BA	654	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	216	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	927	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	1134	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	1067	A	N1-C6-N6	-9.82	112.70	118.60
54	BA	2665	A	N1-C6-N6	-9.82	112.71	118.60
21	AA	1171	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	160	A	N1-C6-N6	-9.81	112.71	118.60
21	AA	716	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	282	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	1552	A	O4'-C1'-N9	9.79	116.03	108.20
54	BA	675	A	N1-C6-N6	-9.77	112.74	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	250	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	1346	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	2518	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	1005	A	N1-C6-N6	-9.76	112.75	118.60
54	BA	2765	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	1586	A	N1-C6-N6	-9.73	112.76	118.60
39	BQ	29	ARG	NE-CZ-NH1	9.73	125.17	120.30
38	BP	38	ARG	NE-CZ-NH1	9.73	125.17	120.30
21	AA	969	A	N1-C6-N6	-9.73	112.77	118.60
2	AC	64	ARG	NE-CZ-NH1	9.72	125.16	120.30
23	A2	91	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	165	A	N1-C6-N6	-9.72	112.77	118.60
21	AA	1019	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	2169	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	126	A	N1-C6-N6	-9.71	112.78	118.60
55	BB	50	A	N1-C6-N6	-9.71	112.78	118.60
54	BA	608	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	2052	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	845	A	C1'-O4'-C4'	-9.70	102.14	109.90
54	BA	905	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1739	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1098	A	N1-C6-N6	-9.69	112.78	118.60
21	AA	622	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	111	A	N1-C6-N6	-9.69	112.79	118.60
21	AA	1287	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	2198	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	1433	A	N1-C6-N6	-9.68	112.80	118.60
54	BA	1284	A	N1-C6-N6	-9.67	112.80	118.60
21	AA	78	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	1340	U	O4'-C1'-N1	9.67	115.93	108.20
54	BA	1900	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	481	G	O4'-C1'-N9	9.65	115.92	108.20
43	BU	81	ARG	NE-CZ-NH1	9.64	125.12	120.30
54	BA	2268	A	N1-C6-N6	-9.64	112.81	118.60
54	BA	2634	A	N1-C6-N6	-9.64	112.81	118.60
21	AA	80	A	N1-C6-N6	-9.63	112.82	118.60
21	AA	1196	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2451	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2639	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	767	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1144	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	825	A	N1-C6-N6	-9.61	112.83	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	303	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	1490	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	1333	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	349	A	N1-C6-N6	-9.61	112.84	118.60
54	BA	119	A	N1-C6-N6	-9.61	112.84	118.60
54	BA	1570	A	N1-C6-N6	-9.60	112.84	118.60
21	AA	1493	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	2369	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	586	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	631	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	1175	A	N1-C6-N6	-9.59	112.85	118.60
25	BC	12	ARG	NE-CZ-NH1	9.59	125.09	120.30
24	A3	77	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	238	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	696	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	918	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	918	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	504	A	O4'-C1'-N9	9.57	115.85	108.20
54	BA	1237	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	2761	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	227	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	507	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	196	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	431	A	N1-C6-N6	-9.54	112.87	118.60
26	BD	77	ARG	NE-CZ-NH1	9.54	125.07	120.30
54	BA	300	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	668	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	213	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	171	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2886	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2309	A	N1-C6-N6	-9.52	112.89	118.60
21	AA	915	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2225	A	N1-C6-N6	-9.52	112.89	118.60
13	AN	24	ARG	NE-CZ-NH1	9.52	125.06	120.30
54	BA	781	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	693	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	71	A	N1-C6-N6	-9.50	112.90	118.60
22	A1	66	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	322	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	751	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	1616	A	N1-C6-N6	-9.48	112.91	118.60
7	AH	12	ARG	NE-CZ-NH1	9.47	125.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1394	A	N1-C6-N6	-9.47	112.92	118.60
41	BS	84	ARG	NE-CZ-NH1	9.47	125.04	120.30
54	BA	38	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	1133	A	N1-C6-N6	-9.46	112.92	118.60
21	AA	676	A	N1-C6-N6	-9.46	112.92	118.60
49	B0	16	ARG	NE-CZ-NH1	9.45	125.03	120.30
54	BA	2478	A	N1-C6-N6	-9.45	112.93	118.60
11	AL	109	ARG	NE-CZ-NH1	9.44	125.02	120.30
25	BC	237	ARG	NE-CZ-NH1	9.44	125.02	120.30
21	AA	441	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	1086	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	2088	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	975	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	2095	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	689	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	59	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	877	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	583	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1866	A	N1-C6-N6	-9.42	112.95	118.60
23	A2	79	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	19	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	1476	A	N1-C6-N6	-9.40	112.96	118.60
44	BV	79	ARG	NE-CZ-NH1	9.40	125.00	120.30
25	BC	68	ARG	NE-CZ-NH1	9.40	125.00	120.30
7	AH	14	ARG	NE-CZ-NH1	9.39	125.00	120.30
21	AA	1130	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	528	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	2381	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	306	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	8	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	1101	A	N1-C6-N6	-9.38	112.97	118.60
46	BX	56	ARG	NE-CZ-NH1	9.38	124.99	120.30
21	AA	1150	A	N1-C6-N6	-9.38	112.97	118.60
55	BB	52	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	715	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1226	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1264	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	65	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	1163	A	N1-C6-N6	-9.37	112.98	118.60
36	BN	96	ARG	NE-CZ-NH1	9.37	124.98	120.30
54	BA	633	A	N1-C6-N6	-9.37	112.98	118.60
51	B2	34	ARG	NE-CZ-NH1	9.36	124.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1847	A	N1-C6-N6	-9.36	112.99	118.60
21	AA	1254	A	N1-C6-N6	-9.35	112.99	118.60
21	AA	1534	A	N1-C6-N6	-9.35	112.99	118.60
21	AA	523	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1918	A	N1-C6-N6	-9.34	112.99	118.60
21	AA	600	A	N1-C6-N6	-9.34	113.00	118.60
21	AA	1433	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1010	A	C5-C6-N1	9.34	122.37	117.70
54	BA	2899	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	346	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	752	A	O4'-C1'-N9	9.33	115.66	108.20
54	BA	2476	A	N1-C6-N6	-9.32	113.00	118.60
22	A1	38	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	2158	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	2412	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	560	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	742	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	1640	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	2530	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	977	A	N1-C6-N6	-9.31	113.02	118.60
54	BA	788	A	N1-C6-N6	-9.31	113.02	118.60
3	AD	72	ARG	NE-CZ-NH1	9.30	124.95	120.30
21	AA	706	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	2721	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1328	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1634	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	750	A	N1-C6-N6	-9.30	113.02	118.60
41	BS	25	ARG	NE-CZ-NH1	9.29	124.95	120.30
54	BA	2058	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	1275	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	1534	U	O4'-C1'-N1	9.28	115.62	108.20
54	BA	1885	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2135	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	1690	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2868	A	N1-C6-N6	-9.28	113.03	118.60
47	BY	52	ARG	NE-CZ-NH1	9.27	124.94	120.30
54	BA	900	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1057	A	N1-C6-N6	-9.27	113.04	118.60
24	A3	77	A	C4-C5-C6	-9.25	112.38	117.00
54	BA	2386	A	N1-C6-N6	-9.24	113.06	118.60
21	AA	131	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	2170	A	N1-C6-N6	-9.23	113.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	279	A	N1-C6-N6	-9.23	113.06	118.60
54	BA	2513	A	N1-C6-N6	-9.22	113.06	118.60
54	BA	677	A	N1-C6-N6	-9.21	113.08	118.60
54	BA	74	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	1016	A	N1-C6-N6	-9.20	113.08	118.60
55	BB	99	A	N1-C6-N6	-9.20	113.08	118.60
1	AB	112	ARG	NE-CZ-NH1	9.19	124.90	120.30
21	AA	1093	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	1700	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	411	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	919	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	1311	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	1515	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	183	C	N3-C2-O2	-9.18	115.47	121.90
21	AA	250	A	C5-C6-N1	9.17	122.29	117.70
21	AA	935	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	1004	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	1179	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	89	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	734	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	1077	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	863	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	466	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1960	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2171	A	N1-C6-N6	-9.15	113.11	118.60
46	BX	27	ARG	NE-CZ-NH1	9.15	124.88	120.30
21	AA	807	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2377	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	718	A	N1-C6-N6	-9.14	113.11	118.60
54	BA	1301	A	C5'-C4'-O4'	9.14	120.07	109.10
54	BA	504	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	753	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1142	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2430	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1366	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1665	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2423	U	O4'-C1'-N1	9.12	115.49	108.20
54	BA	1970	A	N1-C6-N6	-9.11	113.13	118.60
26	BD	13	ARG	NE-CZ-NH1	9.11	124.86	120.30
54	BA	2340	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	2278	A	N1-C6-N6	-9.11	113.14	118.60
55	BB	46	A	N1-C6-N6	-9.11	113.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AE	53	ARG	NE-CZ-NH1	9.10	124.85	120.30
21	AA	655	A	N1-C6-N6	-9.10	113.14	118.60
40	BR	90	ARG	NE-CZ-NH2	9.10	124.85	120.30
54	BA	1679	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	315	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	1871	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2657	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	1029	A	N1-C6-N6	-9.09	113.14	118.60
54	BA	195	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	1492	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	2565	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	352	A	N1-C6-N6	-9.08	113.16	118.60
54	BA	1287	A	N1-C6-N6	-9.08	113.15	118.60
3	AD	61	ARG	NE-CZ-NH1	9.07	124.84	120.30
21	AA	673	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	1169	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	1419	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	990	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	2212	A	O4'-C1'-N9	9.07	115.46	108.20
21	AA	1219	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	28	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	493	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	975	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	2547	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	156	A	N1-C6-N6	-9.04	113.17	118.60
21	AA	1447	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	522	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	125	A	O4'-C1'-N9	9.04	115.43	108.20
21	AA	493	A	C5-C6-N1	9.03	122.22	117.70
54	BA	2031	A	O4'-C1'-N9	9.04	115.43	108.20
21	AA	675	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	140	C	N3-C2-O2	-9.03	115.58	121.90
54	BA	2333	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1127	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	2037	A	N1-C6-N6	-9.03	113.19	118.60
54	BA	217	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	81	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2191	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	627	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	1722	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2288	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2015	A	N1-C6-N6	-9.01	113.19	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1336	C	N1-C2-O2	9.01	124.31	118.90
21	AA	1289	A	C5-C6-N1	9.01	122.20	117.70
54	BA	1913	A	N1-C6-N6	-9.01	113.20	118.60
21	AA	98	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	753	A	N1-C6-N6	-9.00	113.20	118.60
12	AM	69	ARG	NE-CZ-NH1	9.00	124.80	120.30
54	BA	457	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1569	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	2062	A	N1-C6-N6	-8.99	113.21	118.60
24	A3	22	A	N1-C6-N6	-8.99	113.21	118.60
24	A3	36	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2031	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2531	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	448	A	N1-C6-N6	-8.97	113.22	118.60
24	A3	44	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1912	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	2589	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	2781	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	1239	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	1468	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	26	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1672	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	2741	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	960	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	205	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	373	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1080	A	N1-C6-N6	-8.96	113.23	118.60
21	AA	74	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	2005	A	N1-C6-N6	-8.95	113.23	118.60
55	BB	58	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	309	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	64	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	844	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	1246	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1701	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	374	A	N1-C6-N6	-8.94	113.24	118.60
27	BE	49	ARG	NE-CZ-NH1	8.94	124.77	120.30
28	BF	109	ARG	NE-CZ-NH1	8.93	124.76	120.30
54	BA	2328	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	161	A	N1-C6-N6	-8.92	113.25	118.60
2	AC	58	ARG	NE-CZ-NH1	8.91	124.76	120.30
54	BA	1390	U	O4'-C1'-N1	8.91	115.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	792	A	N1-C6-N6	-8.91	113.26	118.60
54	BA	101	A	O4'-C1'-N9	8.90	115.32	108.20
54	BA	1061	U	O4'-C1'-N1	8.90	115.32	108.20
54	BA	1614	A	N1-C6-N6	-8.90	113.26	118.60
24	A3	73	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	864	A	N1-C6-N6	-8.90	113.26	118.60
41	BS	92	ARG	NE-CZ-NH1	8.90	124.75	120.30
54	BA	1420	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2482	A	N1-C6-N6	-8.89	113.26	118.60
21	AA	336	A	N1-C6-N6	-8.89	113.27	118.60
32	BJ	13	ARG	NE-CZ-NH1	8.89	124.74	120.30
54	BA	2503	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	1502	A	N1-C6-N6	-8.88	113.27	118.60
24	A3	45	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	909	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	1339	A	N1-C6-N6	-8.88	113.27	118.60
26	BD	124	ARG	NE-CZ-NH1	8.88	124.74	120.30
21	AA	1238	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	695	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1262	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	478	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	233	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	661	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	347	G	O4'-C1'-N9	8.86	115.29	108.20
21	AA	728	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	1377	A	N1-C6-N6	-8.86	113.29	118.60
54	BA	1073	A	N1-C6-N6	-8.86	113.29	118.60
54	BA	2227	A	N1-C6-N6	-8.86	113.29	118.60
54	BA	472	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	1349	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	502	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	747	A	N1-C6-N6	-8.85	113.29	118.60
34	BL	132	ARG	NE-CZ-NH1	8.85	124.72	120.30
17	AR	56	ARG	NE-CZ-NH1	8.84	124.72	120.30
54	BA	497	A	N1-C6-N6	-8.84	113.29	118.60
54	BA	603	A	N1-C6-N6	-8.84	113.30	118.60
21	AA	1105	A	N1-C6-N6	-8.84	113.30	118.60
24	A3	39	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	2432	A	N1-C6-N6	-8.84	113.30	118.60
21	AA	1227	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	1694	C	N3-C2-O2	-8.84	115.72	121.90
21	AA	1250	A	N1-C6-N6	-8.83	113.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2750	A	O4'-C1'-N9	8.83	115.27	108.20
21	AA	192	A	N1-C6-N6	-8.83	113.30	118.60
2	AC	87	ARG	NE-CZ-NH1	8.83	124.71	120.30
54	BA	1084	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	2418	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	1551	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	596	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	681	A	N1-C6-N6	-8.81	113.31	118.60
22	A1	73	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	994	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	2241	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	42	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	1229	A	C1'-O4'-C4'	-8.80	102.86	109.90
54	BA	404	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	162	A	N1-C6-N6	-8.79	113.32	118.60
21	AA	179	A	N1-C6-N6	-8.79	113.32	118.60
21	AA	459	A	N1-C6-N6	-8.79	113.33	118.60
49	B0	9	ARG	NE-CZ-NH1	8.79	124.70	120.30
39	BQ	49	ARG	NE-CZ-NH1	8.79	124.70	120.30
21	AA	958	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	1368	A	N1-C6-N6	-8.79	113.33	118.60
1	AB	221	ARG	NE-CZ-NH1	8.78	124.69	120.30
54	BA	1285	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	872	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	1254	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	246	A	N1-C6-N6	-8.77	113.34	118.60
22	A1	6	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1664	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	913	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1384	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	792	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	663	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	984	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	1495	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	207	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	2706	A	N1-C6-N6	-8.76	113.35	118.60
21	AA	996	A	N1-C6-N6	-8.75	113.35	118.60
55	BB	29	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	1280	A	C5-C6-N1	8.75	122.07	117.70
54	BA	73	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1268	A	N1-C6-N6	-8.74	113.35	118.60
21	AA	182	A	N1-C6-N6	-8.74	113.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1434	A	O4'-C1'-N9	8.74	115.19	108.20
54	BA	2461	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	602	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1705	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	313	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	509	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	253	A	N1-C6-N6	-8.72	113.36	118.60
54	BA	1535	A	N1-C6-N6	-8.72	113.36	118.60
54	BA	2352	A	N1-C6-N6	-8.72	113.36	118.60
54	BA	637	A	N1-C6-N6	-8.72	113.37	118.60
37	BO	16	ARG	NE-CZ-NH1	8.72	124.66	120.30
36	BN	30	ARG	NE-CZ-NH1	8.72	124.66	120.30
21	AA	914	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	1288	G	O4'-C1'-N9	8.72	115.17	108.20
54	BA	1609	A	C5-C6-N1	8.72	122.06	117.70
54	BA	2425	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	364	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	833	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	2142	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	1063	G	O4'-C1'-N9	8.70	115.16	108.20
54	BA	2469	A	N1-C6-N6	-8.69	113.38	118.60
21	AA	498	A	N1-C6-N6	-8.69	113.38	118.60
54	BA	2564	A	N1-C6-N6	-8.69	113.38	118.60
9	AJ	48	ARG	NE-CZ-NH1	8.69	124.65	120.30
55	BB	108	A	N1-C6-N6	-8.69	113.39	118.60
47	BY	29	ARG	NE-CZ-NH1	8.69	124.64	120.30
21	AA	393	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	776	G	O4'-C1'-N9	8.68	115.14	108.20
54	BA	1987	A	N1-C6-N6	-8.68	113.39	118.60
8	AI	105	ARG	NE-CZ-NH1	8.68	124.64	120.30
54	BA	2497	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	2776	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	815	A	N1-C6-N6	-8.67	113.40	118.60
24	A3	38	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	655	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	103	A	N1-C6-N6	-8.67	113.40	118.60
3	AD	2	ARG	NE-CZ-NH1	8.66	124.63	120.30
21	AA	814	A	N1-C6-N6	-8.66	113.40	118.60
21	AA	845	A	N1-C6-N6	-8.66	113.40	118.60
21	AA	1146	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	861	A	N1-C6-N6	-8.66	113.40	118.60
21	AA	1191	A	N1-C6-N6	-8.66	113.40	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1256	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	699	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	1571	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	172	A	C5-C6-N1	8.65	122.02	117.70
24	A3	77	A	C5-C6-N1	8.65	122.03	117.70
21	AA	913	A	C5-C6-N1	8.64	122.02	117.70
54	BA	1027	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	2092	U	O4'-C1'-N1	8.64	115.11	108.20
54	BA	2503	A	O4'-C1'-N9	8.64	115.11	108.20
54	BA	1276	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	515	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	937	A	C5-C6-N1	8.63	122.02	117.70
22	A1	26	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	460	A	N1-C6-N6	-8.63	113.42	118.60
34	BL	78	ARG	NE-CZ-NH1	8.63	124.61	120.30
21	AA	55	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	77	A	N1-C6-N6	-8.62	113.42	118.60
54	BA	1070	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	829	A	O4'-C1'-N9	8.62	115.10	108.20
15	AP	28	ARG	NE-CZ-NH1	8.62	124.61	120.30
54	BA	2030	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	2675	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	1430	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	2388	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	1467	C	N3-C2-O2	-8.61	115.87	121.90
54	BA	2727	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	1773	A	N1-C6-N6	-8.61	113.44	118.60
22	A1	69	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	221	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	1201	A	C5-C6-N1	8.60	122.00	117.70
54	BA	2749	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	2432	A	C5-C6-N1	8.60	122.00	117.70
21	AA	243	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1821	A	N1-C6-N6	-8.60	113.44	118.60
2	AC	135	ARG	NE-CZ-NH1	8.59	124.59	120.30
54	BA	1504	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	2077	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	2740	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	712	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	1493	A	C5-C6-N1	8.59	121.99	117.70
55	BB	34	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	428	A	N1-C6-N6	-8.58	113.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	977	A	C5-C6-N1	8.58	121.99	117.70
21	AA	1012	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	144	A	N1-C6-N6	-8.58	113.45	118.60
12	AM	86	ARG	NE-CZ-NH1	8.57	124.58	120.30
21	AA	909	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	592	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2335	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	715	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	1183	U	O4'-C1'-N1	8.56	115.05	108.20
21	AA	183	C	O4'-C1'-N1	8.56	115.05	108.20
21	AA	759	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	1603	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	2882	A	N1-C6-N6	-8.56	113.47	118.60
54	BA	2628	C	N3-C2-O2	-8.56	115.91	121.90
54	BA	146	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	787	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	752	A	C5-C6-N1	8.55	121.97	117.70
54	BA	1632	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2602	A	N1-C6-N6	-8.55	113.47	118.60
6	AG	110	ARG	NE-CZ-NH1	8.55	124.57	120.30
21	AA	1216	A	C5-C6-N1	8.55	121.97	117.70
54	BA	2158	A	C5-C6-N1	8.55	121.97	117.70
21	AA	547	A	C5-C6-N1	8.55	121.97	117.70
54	BA	959	A	C5-C6-N1	8.54	121.97	117.70
54	BA	2212	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	1398	A	N1-C6-N6	-8.54	113.48	118.60
28	BF	91	ARG	NE-CZ-NH1	8.54	124.57	120.30
54	BA	1854	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	2516	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	1180	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	294	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	1156	A	N1-C6-N6	-8.53	113.48	118.60
55	BB	45	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	323	C	N3-C2-O2	-8.52	115.94	121.90
21	AA	1197	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	1522	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	1111	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	1176	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	503	A	N1-C6-N6	-8.51	113.50	118.60
21	AA	1021	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	896	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1439	A	O4'-C1'-N9	8.50	115.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1035	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	10	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	560	A	C5-C6-N1	8.49	121.94	117.70
54	BA	478	A	N1-C6-N6	-8.49	113.50	118.60
24	A3	60	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	356	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	694	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	1304	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	2666	C	O4'-C1'-N1	8.48	114.98	108.20
21	AA	974	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	226	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	1552	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	199	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	320	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	1126	A	C5-C6-N1	8.47	121.94	117.70
54	BA	1654	A	N1-C6-N6	-8.47	113.52	118.60
12	AM	91	ARG	NE-CZ-NH1	8.47	124.53	120.30
21	AA	766	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	2448	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	309	A	N1-C6-N6	-8.46	113.53	118.60
22	A1	16	C	N3-C2-O2	-8.46	115.98	121.90
3	AD	114	ARG	NE-CZ-NH1	8.45	124.53	120.30
54	BA	735	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	1650	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	430	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	1525	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	532	A	N1-C6-N6	-8.44	113.53	118.60
21	AA	1022	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	670	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	973	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	979	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	1608	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	602	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	981	A	C5-C6-N1	8.44	121.92	117.70
10	AK	36	ARG	NE-CZ-NH1	8.43	124.51	120.30
54	BA	677	A	C5-C6-N1	8.43	121.91	117.70
21	AA	1216	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	195	A	C5-C6-N1	8.43	121.91	117.70
54	BA	1913	A	C5-C6-N1	8.43	121.91	117.70
54	BA	1791	A	N1-C6-N6	-8.43	113.55	118.60
9	AJ	72	ARG	NE-CZ-NH1	8.42	124.51	120.30
21	AA	1155	A	N1-C6-N6	-8.42	113.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	56	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2450	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	397	A	N1-C6-N6	-8.42	113.55	118.60
36	BN	4	ARG	NE-CZ-NH1	8.42	124.51	120.30
21	AA	33	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	298	A	N1-C6-N6	-8.41	113.55	118.60
32	BJ	116	ARG	NE-CZ-NH1	8.41	124.51	120.30
54	BA	13	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	1396	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	1928	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	1932	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	2825	G	O4'-C1'-N9	8.41	114.93	108.20
54	BA	2820	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2435	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	127	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2753	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	794	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2071	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	1566	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	1609	A	N1-C6-N6	-8.39	113.57	118.60
21	AA	129	A	N1-C6-N6	-8.39	113.57	118.60
21	AA	1151	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	131	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	2808	G	O4'-C1'-N9	8.38	114.91	108.20
54	BA	2033	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	1350	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	1253	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	1428	A	N1-C6-N6	-8.38	113.58	118.60
21	AA	7	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	44	A	N1-C6-N6	-8.38	113.58	118.60
54	BA	1819	A	N1-C6-N6	-8.38	113.58	118.60
54	BA	2541	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	2778	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	845	A	C5-C6-N1	8.37	121.89	117.70
54	BA	2266	A	N1-C6-N6	-8.37	113.58	118.60
31	BI	126	ARG	NE-CZ-NH1	8.37	124.48	120.30
36	BN	90	ARG	NE-CZ-NH1	8.37	124.48	120.30
54	BA	422	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	344	A	N1-C6-N6	-8.36	113.58	118.60
9	AJ	7	ARG	NE-CZ-NH1	8.36	124.48	120.30
54	BA	1420	A	C5-C6-N1	8.36	121.88	117.70
54	BA	621	A	N1-C6-N6	-8.35	113.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1042	A	N1-C6-N6	-8.35	113.59	118.60
48	BZ	15	ARG	NE-CZ-NH1	8.35	124.48	120.30
21	AA	363	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	968	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	1535	A	C5-C6-N1	8.35	121.87	117.70
36	BN	8	ARG	NE-CZ-NH1	8.34	124.47	120.30
54	BA	453	A	N1-C6-N6	-8.34	113.59	118.60
17	AR	52	ARG	NE-CZ-NH1	8.34	124.47	120.30
21	AA	321	A	N1-C6-N6	-8.34	113.60	118.60
40	BR	79	ARG	NE-CZ-NH1	8.33	124.47	120.30
54	BA	739	A	C5-C6-N1	8.33	121.86	117.70
54	BA	2051	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	1027	C	N3-C2-O2	-8.33	116.07	121.90
21	AA	1046	A	C5-C6-N1	8.33	121.86	117.70
54	BA	1566	A	C5-C6-N1	8.33	121.86	117.70
54	BA	1791	A	C5-C6-N1	8.33	121.86	117.70
21	AA	149	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	49	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	804	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	1244	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	125	A	C5-C6-N1	8.31	121.86	117.70
41	BS	88	ARG	NE-CZ-NH2	8.31	124.46	120.30
54	BA	1032	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	1780	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2267	A	C5-C6-N1	8.31	121.86	117.70
54	BA	2468	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	599	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	959	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2471	A	N1-C6-N6	-8.30	113.62	118.60
55	BB	109	A	C5-C6-N1	8.30	121.85	117.70
8	AI	94	ARG	NE-CZ-NH1	8.30	124.45	120.30
21	AA	109	A	N1-C6-N6	-8.30	113.62	118.60
21	AA	889	A	C5-C6-N1	8.30	121.85	117.70
54	BA	2163	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	1789	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	563	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	342	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	802	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1009	A	C5-C6-N1	8.29	121.84	117.70
54	BA	1205	A	C5-C6-N1	8.29	121.84	117.70
55	BB	53	A	C5-C6-N1	8.28	121.84	117.70
54	BA	1548	A	N1-C6-N6	-8.28	113.63	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	60	C	N3-C2-O2	-8.28	116.11	121.90
6	AG	108	ARG	NE-CZ-NH1	8.28	124.44	120.30
13	AN	69	ARG	NE-CZ-NH1	8.28	124.44	120.30
21	AA	371	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	91	A	C5-C6-N1	8.27	121.83	117.70
54	BA	1745	A	C5-C6-N1	8.27	121.83	117.70
21	AA	1246	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	547	A	C4-C5-C6	-8.26	112.87	117.00
54	BA	272	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	1652	A	N1-C6-N6	-8.26	113.64	118.60
8	AI	48	ARG	NE-CZ-NH1	8.26	124.43	120.30
21	AA	573	A	N1-C6-N6	-8.26	113.64	118.60
21	AA	967	C	N3-C2-O2	-8.26	116.12	121.90
54	BA	94	A	N1-C6-N6	-8.26	113.65	118.60
21	AA	72	A	N1-C6-N6	-8.25	113.65	118.60
37	BO	13	ARG	NE-CZ-NH1	8.25	124.43	120.30
54	BA	2042	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2850	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2450	A	C5-C6-N1	8.25	121.83	117.70
21	AA	1324	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2800	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	782	A	C5-C6-N1	8.24	121.82	117.70
54	BA	1641	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	1544	A	N1-C6-N6	-8.24	113.66	118.60
25	BC	220	ARG	NE-CZ-NH2	8.24	124.42	120.30
54	BA	2566	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	1321	A	C5-C6-N1	8.23	121.82	117.70
22	A1	41	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	1853	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	6	A	C5-C6-N1	8.23	121.81	117.70
54	BA	482	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2614	A	C4-C5-C6	-8.22	112.89	117.00
55	BB	15	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	152	A	C5-C6-N1	8.22	121.81	117.70
21	AA	704	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1390	U	C1'-O4'-C4'	-8.22	103.32	109.90
54	BA	176	A	C5-C6-N1	8.22	121.81	117.70
54	BA	1496	A	C5-C6-N1	8.22	121.81	117.70
54	BA	1552	A	C5-C6-N1	8.22	121.81	117.70
54	BA	2173	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	2070	A	C5-C6-N1	8.21	121.81	117.70
54	BA	2792	A	N1-C6-N6	-8.21	113.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2868	A	C5-C6-N1	8.21	121.81	117.70
21	AA	464	U	C1'-O4'-C4'	-8.21	103.33	109.90
21	AA	1500	A	N1-C6-N6	-8.21	113.68	118.60
36	BN	17	ARG	NE-CZ-NH1	8.20	124.40	120.30
54	BA	1522	A	C5-C6-N1	8.20	121.80	117.70
54	BA	2433	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1998	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1953	A	C5-C6-N1	8.20	121.80	117.70
21	AA	189	A	N1-C6-N6	-8.19	113.68	118.60
1	AB	34	ARG	NE-CZ-NH1	8.19	124.40	120.30
21	AA	325	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	1158	C	N3-C2-O2	-8.19	116.17	121.90
32	BJ	95	ARG	NE-CZ-NH2	8.19	124.40	120.30
54	BA	2646	C	N3-C2-O2	-8.19	116.17	121.90
54	BA	2879	A	C5-C6-N1	8.19	121.80	117.70
54	BA	705	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2199	A	C5-C6-N1	8.19	121.79	117.70
23	A2	91	A	C5-C6-N1	8.19	121.79	117.70
54	BA	2598	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	1200	C	N3-C2-O2	-8.19	116.17	121.90
54	BA	743	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1095	A	C5-C6-N1	8.18	121.79	117.70
54	BA	2406	A	N1-C6-N6	-8.18	113.69	118.60
19	AT	28	ARG	NE-CZ-NH1	8.18	124.39	120.30
21	AA	432	A	C5-C6-N1	8.17	121.79	117.70
54	BA	1028	A	C5-C6-N1	8.17	121.79	117.70
54	BA	299	A	C5-C6-N1	8.17	121.78	117.70
54	BA	1477	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	384	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	404	A	C5-C6-N1	8.16	121.78	117.70
54	BA	996	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1901	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	794	A	N1-C6-N6	-8.16	113.71	118.60
21	AA	1170	A	N1-C6-N6	-8.16	113.71	118.60
54	BA	1936	A	N1-C6-N6	-8.16	113.71	118.60
54	BA	526	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	2872	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1050	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	183	C	N1-C2-O2	8.15	123.79	118.90
54	BA	1378	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	626	A	C5-C6-N1	8.15	121.77	117.70
38	BP	112	ARG	NE-CZ-NH1	8.14	124.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1320	C	N3-C2-O2	-8.14	116.20	121.90
54	BA	6	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	983	A	N1-C6-N6	-8.14	113.72	118.60
52	B3	12	ARG	NE-CZ-NH1	8.13	124.37	120.30
21	AA	777	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	949	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	972	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	173	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1260	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	171	A	C5-C6-N1	8.13	121.76	117.70
54	BA	2094	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	222	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1442	U	O4'-C1'-N1	8.12	114.70	108.20
54	BA	2091	C	N3-C2-O2	-8.12	116.22	121.90
54	BA	1099	G	O4'-C1'-N9	8.12	114.69	108.20
21	AA	1317	C	N3-C2-O2	-8.11	116.22	121.90
54	BA	176	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	1110	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	1499	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	1054	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	1387	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	1146	A	C5-C6-N1	8.11	121.75	117.70
54	BA	514	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2205	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	648	A	N1-C6-N6	-8.11	113.74	118.60
21	AA	687	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	933	A	C5-C6-N1	8.10	121.75	117.70
54	BA	479	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1829	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	792	A	C5-C6-N1	8.10	121.75	117.70
21	AA	1067	A	C4-C5-C6	-8.10	112.95	117.00
25	BC	270	ARG	NE-CZ-NH1	8.10	124.35	120.30
21	AA	1252	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1383	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1847	A	O4'-C1'-N9	8.10	114.68	108.20
54	BA	1366	A	C5-C6-N1	8.10	121.75	117.70
54	BA	2635	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	468	A	N1-C6-N6	-8.09	113.74	118.60
21	AA	1117	A	N1-C6-N6	-8.09	113.75	118.60
21	AA	554	A	N1-C6-N6	-8.09	113.75	118.60
6	AG	78	ARG	NE-CZ-NH2	8.09	124.34	120.30
33	BK	31	ARG	NE-CZ-NH1	8.09	124.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1858	A	C5-C6-N1	8.09	121.74	117.70
21	AA	815	A	C5-C6-N1	8.09	121.74	117.70
55	BB	70	C	N3-C2-O2	-8.09	116.24	121.90
21	AA	1374	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	1700	A	C5-C6-N1	8.08	121.74	117.70
54	BA	1028	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	2541	A	C5-C6-N1	8.08	121.74	117.70
4	AE	111	ARG	NE-CZ-NH1	8.08	124.34	120.30
21	AA	167	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	728	A	C5-C6-N1	8.08	121.74	117.70
54	BA	2835	A	C5-C6-N1	8.08	121.74	117.70
21	AA	298	A	C5-C6-N1	8.07	121.74	117.70
54	BA	752	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2748	A	C5-C6-N1	8.07	121.74	117.70
54	BA	616	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	1089	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2154	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	1668	A	C5-C6-N1	8.07	121.73	117.70
3	AD	103	ARG	NE-CZ-NH1	8.07	124.33	120.30
21	AA	413	G	O4'-C1'-N9	8.07	114.65	108.20
54	BA	643	A	C5-C6-N1	8.07	121.73	117.70
54	BA	1809	A	C5-C6-N1	8.07	121.73	117.70
54	BA	2247	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2310	C	N3-C2-O2	-8.07	116.25	121.90
21	AA	602	A	C5-C6-N1	8.06	121.73	117.70
54	BA	1272	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	161	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	1009	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	1046	A	C5-C6-N1	8.06	121.73	117.70
21	AA	595	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	1698	A	C5-C6-N1	8.05	121.73	117.70
21	AA	878	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	199	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	609	A	C5-C6-N1	8.05	121.72	117.70
45	BW	19	ARG	NE-CZ-NH1	8.05	124.32	120.30
21	AA	702	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	1640	A	C5-C6-N1	8.05	121.72	117.70
54	BA	1308	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1981	A	O4'-C1'-N9	8.04	114.64	108.20
21	AA	155	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	1256	A	C5-C6-N1	8.04	121.72	117.70
21	AA	1157	A	N1-C6-N6	-8.04	113.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BG	34	ARG	NE-CZ-NH1	8.04	124.32	120.30
54	BA	1646	C	N3-C2-O2	-8.04	116.27	121.90
54	BA	2171	A	C5-C6-N1	8.04	121.72	117.70
54	BA	477	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	2725	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	328	C	N3-C2-O2	-8.03	116.28	121.90
54	BA	1759	A	C5-C6-N1	8.03	121.71	117.70
54	BA	1593	A	C5-C6-N1	8.03	121.71	117.70
21	AA	1418	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	14	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	1319	A	N1-C6-N6	-8.02	113.78	118.60
54	BA	718	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	60	A	N1-C6-N6	-8.02	113.79	118.60
43	BU	93	ARG	NE-CZ-NH1	8.02	124.31	120.30
54	BA	1772	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	101	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	2614	A	C5-C6-N1	8.01	121.71	117.70
21	AA	1225	A	C5-C6-N1	8.01	121.70	117.70
21	AA	238	A	C5-C6-N1	8.01	121.70	117.70
54	BA	63	A	N1-C6-N6	-8.00	113.80	118.60
45	BW	40	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	1503	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	1214	C	N3-C2-O2	-8.00	116.30	121.90
54	BA	1347	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1393	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2238	G	O4'-C1'-N9	8.00	114.60	108.20
54	BA	2281	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2176	A	C5-C6-N1	8.00	121.70	117.70
35	BM	114	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	1328	A	C5-C6-N1	8.00	121.70	117.70
21	AA	1286	U	O4'-C1'-N1	7.99	114.59	108.20
54	BA	689	A	C5-C6-N1	7.99	121.70	117.70
19	AT	24	ARG	NE-CZ-NH1	7.99	124.30	120.30
54	BA	1914	C	N3-C2-O2	-7.99	116.31	121.90
54	BA	2750	A	C5-C6-N1	7.99	121.69	117.70
1	AB	136	ARG	NE-CZ-NH1	7.99	124.29	120.30
21	AA	72	A	C5-C6-N1	7.99	121.69	117.70
21	AA	452	A	N1-C6-N6	-7.99	113.81	118.60
34	BL	21	ARG	NE-CZ-NH1	7.99	124.29	120.30
54	BA	685	A	C5-C6-N1	7.99	121.69	117.70
54	BA	1348	C	O4'-C1'-N1	7.99	114.59	108.20
54	BA	299	A	N1-C6-N6	-7.98	113.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AU	16	ARG	NE-CZ-NH1	7.98	124.29	120.30
54	BA	1336	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1490	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1583	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	2336	A	N1-C6-N6	-7.98	113.81	118.60
3	AD	46	ARG	NE-CZ-NH2	7.98	124.29	120.30
21	AA	607	A	C5-C6-N1	7.97	121.69	117.70
54	BA	118	A	N1-C6-N6	-7.97	113.81	118.60
54	BA	470	A	C5-C6-N1	7.97	121.69	117.70
21	AA	1081	A	N1-C6-N6	-7.97	113.82	118.60
36	BN	71	ARG	NE-CZ-NH1	7.97	124.28	120.30
54	BA	204	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	911	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	21	A	N1-C6-N6	-7.97	113.82	118.60
24	A3	58	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	845	A	O4'-C1'-N9	7.96	114.57	108.20
54	BA	1755	A	C4-C5-C6	-7.96	113.02	117.00
54	BA	2736	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	2899	A	C4-C5-C6	-7.96	113.02	117.00
38	BP	50	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	1286	A	N1-C6-N6	-7.96	113.83	118.60
54	BA	1509	A	C5-C6-N1	7.96	121.68	117.70
8	AI	11	ARG	NE-CZ-NH1	7.95	124.28	120.30
21	AA	1022	A	C5-C6-N1	7.95	121.68	117.70
21	AA	1229	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	303	A	C5-C6-N1	7.95	121.67	117.70
54	BA	83	A	N1-C6-N6	-7.95	113.83	118.60
45	BW	13	ARG	NE-CZ-NH1	7.95	124.27	120.30
54	BA	2660	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	1261	A	N1-C6-N6	-7.95	113.83	118.60
55	BB	78	A	C5-C6-N1	7.95	121.67	117.70
54	BA	781	A	C5-C6-N1	7.94	121.67	117.70
54	BA	945	A	C5-C6-N1	7.94	121.67	117.70
54	BA	1755	A	C5-C6-N1	7.94	121.67	117.70
55	BB	45	A	C5-C6-N1	7.94	121.67	117.70
54	BA	2829	A	N1-C6-N6	-7.94	113.84	118.60
24	A3	11	A	C5-C6-N1	7.93	121.67	117.70
54	BA	1744	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	332	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	983	A	C5-C6-N1	7.93	121.67	117.70
54	BA	2346	A	C5-C6-N1	7.93	121.67	117.70
21	AA	195	A	N1-C6-N6	-7.93	113.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	653	U	O4'-C1'-N1	7.93	114.54	108.20
54	BA	1532	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	676	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1143	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	2051	A	C5-C6-N1	7.93	121.66	117.70
21	AA	1257	A	N1-C6-N6	-7.92	113.84	118.60
54	BA	2883	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	1340	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	863	A	C5-C6-N1	7.92	121.66	117.70
54	BA	2758	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	1136	C	N3-C2-O2	-7.92	116.36	121.90
54	BA	415	A	N1-C6-N6	-7.92	113.85	118.60
22	A1	58	A	N1-C6-N6	-7.92	113.85	118.60
22	A1	66	A	C5-C6-N1	7.92	121.66	117.70
24	A3	45	A	C4-C5-C6	-7.92	113.04	117.00
22	A1	76	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	614	A	O4'-C1'-N9	7.91	114.53	108.20
54	BA	1307	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	1757	A	C5-C6-N1	7.91	121.66	117.70
54	BA	231	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	1553	A	C4-C5-C6	-7.91	113.05	117.00
54	BA	1745	A	N1-C6-N6	-7.91	113.85	118.60
55	BB	59	A	N1-C6-N6	-7.91	113.85	118.60
45	BW	10	ARG	NE-CZ-NH2	7.91	124.25	120.30
54	BA	645	C	N3-C2-O2	-7.91	116.36	121.90
54	BA	1204	A	C5-C6-N1	7.91	121.65	117.70
54	BA	482	A	C5-C6-N1	7.91	121.65	117.70
8	AI	32	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	265	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2632	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1195	C	N3-C2-O2	-7.90	116.37	121.90
55	BB	41	G	O4'-C1'-N9	7.90	114.52	108.20
25	BC	155	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	1847	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2358	A	C5-C6-N1	7.90	121.65	117.70
54	BA	574	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	2587	A	N1-C6-N6	-7.89	113.86	118.60
55	BB	88	C	N3-C2-O2	-7.89	116.37	121.90
54	BA	1336	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	647	G	N3-C2-N2	-7.89	114.38	119.90
54	BA	323	C	N1-C2-O2	7.89	123.63	118.90
54	BA	1505	A	N1-C6-N6	-7.89	113.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2198	A	C5-C6-N1	7.89	121.64	117.70
12	AM	56	ARG	NE-CZ-NH1	7.89	124.24	120.30
54	BA	368	A	N1-C6-N6	-7.89	113.87	118.60
54	BA	1253	A	C5-C6-N1	7.88	121.64	117.70
55	BB	73	A	N1-C6-N6	-7.88	113.87	118.60
21	AA	1302	C	N3-C2-O2	-7.88	116.38	121.90
21	AA	1434	A	C5-C6-N1	7.88	121.64	117.70
54	BA	158	U	O4'-C1'-N1	7.88	114.51	108.20
54	BA	522	A	C5-C6-N1	7.88	121.64	117.70
21	AA	300	A	N1-C6-N6	-7.88	113.87	118.60
51	B2	3	ARG	NE-CZ-NH2	7.88	124.24	120.30
54	BA	2826	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	382	A	C4-C5-C6	-7.88	113.06	117.00
54	BA	1579	A	C5-C6-N1	7.88	121.64	117.70
21	AA	85	U	N3-C2-O2	-7.87	116.69	122.20
54	BA	454	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	616	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1385	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	1437	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	1130	A	C5-C6-N1	7.87	121.64	117.70
21	AA	196	A	C5-C6-N1	7.87	121.63	117.70
21	AA	696	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1937	A	C5-C6-N1	7.87	121.63	117.70
54	BA	2451	A	C5-C6-N1	7.87	121.63	117.70
54	BA	2309	A	C5-C6-N1	7.87	121.63	117.70
54	BA	2598	A	C5-C6-N1	7.87	121.63	117.70
54	BA	1872	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	2307	G	O4'-C1'-N9	7.86	114.49	108.20
54	BA	2423	U	C1'-O4'-C4'	-7.86	103.61	109.90
54	BA	2873	A	N1-C6-N6	-7.86	113.88	118.60
21	AA	1036	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	504	A	C5-C6-N1	7.86	121.63	117.70
54	BA	783	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	1302	A	C5-C6-N1	7.86	121.63	117.70
54	BA	345	A	C5-C6-N1	7.86	121.63	117.70
24	A3	45	A	C5-C6-N1	7.86	121.63	117.70
54	BA	182	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	1669	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	981	A	N1-C6-N6	-7.85	113.89	118.60
21	AA	1376	U	O4'-C1'-N1	7.85	114.48	108.20
54	BA	2468	A	C5-C6-N1	7.85	121.63	117.70
25	BC	261	ARG	NE-CZ-NH2	7.85	124.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	975	A	C5-C6-N1	7.85	121.62	117.70
54	BA	1637	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2020	A	O4'-C1'-N9	7.85	114.48	108.20
54	BA	749	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2810	A	C5-C6-N1	7.85	121.62	117.70
21	AA	197	A	N1-C6-N6	-7.84	113.89	118.60
27	BE	117	ARG	NE-CZ-NH1	7.84	124.22	120.30
54	BA	362	A	C5-C6-N1	7.84	121.62	117.70
40	BR	78	ARG	NE-CZ-NH1	7.84	124.22	120.30
54	BA	1332	G	O4'-C1'-N9	7.84	114.47	108.20
54	BA	1314	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	1731	G	O4'-C1'-N9	7.83	114.47	108.20
21	AA	948	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	244	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1759	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	556	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1354	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	10	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1453	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1829	A	C5-C6-N1	7.83	121.61	117.70
20	AU	20	ARG	NE-CZ-NH1	7.83	124.21	120.30
21	AA	1219	A	C5-C6-N1	7.83	121.61	117.70
54	BA	280	U	O4'-C1'-N1	7.83	114.46	108.20
54	BA	2060	A	N1-C6-N6	-7.83	113.91	118.60
54	BA	2145	C	N3-C2-O2	-7.82	116.42	121.90
1	AB	107	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	1050	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1593	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	1383	A	C5-C6-N1	7.82	121.61	117.70
29	BG	152	ARG	NE-CZ-NH1	7.82	124.21	120.30
21	AA	914	A	C5-C6-N1	7.81	121.61	117.70
54	BA	2700	A	N1-C6-N6	-7.81	113.91	118.60
21	AA	906	A	C5-C6-N1	7.81	121.61	117.70
21	AA	1275	A	N1-C6-N6	-7.81	113.92	118.60
21	AA	1410	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	101	A	C5-C6-N1	7.81	121.61	117.70
21	AA	1109	C	N3-C2-O2	-7.81	116.44	121.90
54	BA	727	A	N1-C6-N6	-7.81	113.92	118.60
21	AA	262	A	C5-C6-N1	7.80	121.60	117.70
21	AA	704	A	C5-C6-N1	7.80	121.60	117.70
54	BA	2031	A	C5-C6-N1	7.80	121.60	117.70
54	BA	1069	A	C5-C6-N1	7.80	121.60	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	345	C	N3-C2-O2	-7.80	116.44	121.90
21	AA	353	A	C5-C6-N1	7.80	121.60	117.70
54	BA	1392	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	794	A	C5-C6-N1	7.80	121.60	117.70
21	AA	1285	A	N1-C6-N6	-7.80	113.92	118.60
22	A1	21	A	C5-C6-N1	7.80	121.60	117.70
54	BA	614	A	C5-C6-N1	7.80	121.60	117.70
54	BA	140	C	N1-C2-O2	7.79	123.58	118.90
15	AP	5	ARG	NE-CZ-NH1	7.79	124.20	120.30
21	AA	356	A	C5-C6-N1	7.79	121.59	117.70
54	BA	2369	A	C5-C6-N1	7.79	121.60	117.70
54	BA	2665	A	C5-C6-N1	7.79	121.59	117.70
21	AA	642	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	932	C	P-O3'-C3'	7.79	129.05	119.70
54	BA	620	G	O4'-C1'-N9	7.79	114.43	108.20
54	BA	2851	A	C4-C5-C6	-7.79	113.11	117.00
21	AA	50	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	729	A	C5-C6-N1	7.79	121.59	117.70
21	AA	795	C	N3-C2-O2	-7.79	116.45	121.90
21	AA	408	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	71	A	C5-C6-N1	7.79	121.59	117.70
54	BA	1359	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	2820	A	C5-C6-N1	7.79	121.59	117.70
21	AA	621	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	294	A	C5-C6-N1	7.78	121.59	117.70
54	BA	1067	A	C5-C6-N1	7.78	121.59	117.70
54	BA	1189	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	495	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	518	C	N3-C2-O2	-7.78	116.45	121.90
21	AA	1250	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1359	C	N3-C2-O2	-7.78	116.46	121.90
21	AA	1429	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	2670	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	160	A	N1-C6-N6	-7.78	113.94	118.60
48	BZ	29	ARG	NE-CZ-NH1	7.77	124.19	120.30
54	BA	1010	A	C4-C5-C6	-7.77	113.11	117.00
54	BA	2573	C	O4'-C1'-N1	7.77	114.42	108.20
54	BA	973	A	C5-C6-N1	7.77	121.59	117.70
54	BA	76	C	N3-C2-O2	-7.77	116.46	121.90
54	BA	972	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1876	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2164	C	N3-C2-O2	-7.77	116.46	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	466	A	C5-C6-N1	7.77	121.58	117.70
54	BA	52	A	N1-C6-N6	-7.77	113.94	118.60
55	BB	78	A	C4-C5-C6	-7.77	113.12	117.00
24	A3	60	A	C5-C6-N1	7.76	121.58	117.70
21	AA	676	A	C5-C6-N1	7.76	121.58	117.70
54	BA	910	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1762	A	C5-C6-N1	7.76	121.58	117.70
21	AA	160	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1048	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1871	A	C5-C6-N1	7.75	121.58	117.70
35	BM	59	ARG	NE-CZ-NH2	-7.75	116.42	120.30
54	BA	2823	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	764	A	C5-C6-N1	7.75	121.58	117.70
21	AA	1456	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	907	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1133	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1271	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	1413	A	N1-C6-N6	-7.74	113.95	118.60
37	BO	10	ARG	NE-CZ-NH1	7.74	124.17	120.30
54	BA	959	A	O4'-C1'-N9	7.74	114.39	108.20
54	BA	2781	A	C5-C6-N1	7.74	121.57	117.70
55	BB	92	C	O4'-C1'-N1	7.74	114.39	108.20
3	AD	69	ARG	NE-CZ-NH1	7.74	124.17	120.30
21	AA	48	C	N3-C2-O2	-7.74	116.49	121.90
21	AA	663	A	C5-C6-N1	7.74	121.57	117.70
54	BA	526	A	C5-C6-N1	7.74	121.57	117.70
21	AA	71	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	1403	C	N3-C2-O2	-7.73	116.49	121.90
24	A3	11	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	945	A	O4'-C1'-N9	7.73	114.39	108.20
54	BA	983	A	C5-C6-N1	7.73	121.57	117.70
2	AC	178	ARG	NE-CZ-NH1	7.73	124.17	120.30
21	AA	288	A	C5-C6-N1	7.73	121.57	117.70
54	BA	497	A	C5-C6-N1	7.73	121.56	117.70
54	BA	1652	A	C5-C6-N1	7.73	121.57	117.70
54	BA	1783	A	C5-C6-N1	7.73	121.56	117.70
54	BA	2786	U	O4'-C1'-N1	7.72	114.38	108.20
54	BA	2860	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2211	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2705	A	C5-C6-N1	7.72	121.56	117.70
21	AA	130	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	1054	C	N1-C2-O2	7.72	123.53	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1978	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2005	A	C5-C6-N1	7.72	121.56	117.70
55	BB	57	A	C5-C6-N1	7.72	121.56	117.70
21	AA	1004	A	C5-C6-N1	7.72	121.56	117.70
54	BA	984	A	C5-C6-N1	7.72	121.56	117.70
54	BA	50	U	O4'-C1'-N1	7.72	114.37	108.20
54	BA	1090	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	2474	U	O4'-C1'-N1	7.71	114.37	108.20
54	BA	73	A	C5-C6-N1	7.71	121.56	117.70
54	BA	626	A	C4-C5-C6	-7.71	113.14	117.00
54	BA	947	A	C5-C6-N1	7.71	121.56	117.70
54	BA	2130	U	N3-C2-O2	-7.71	116.80	122.20
21	AA	366	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	609	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	1301	A	C5-C6-N1	7.71	121.55	117.70
21	AA	129	A	C5-C6-N1	7.71	121.55	117.70
54	BA	91	A	O4'-C1'-N9	7.71	114.36	108.20
21	AA	865	A	N1-C6-N6	-7.71	113.98	118.60
24	A3	35	C	N3-C2-O2	-7.70	116.51	121.90
30	BH	68	ARG	NE-CZ-NH1	7.70	124.15	120.30
54	BA	1046	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1451	C	N3-C2-O2	-7.70	116.51	121.90
22	A1	38	A	C4-C5-C6	-7.70	113.15	117.00
54	BA	191	A	C5-C6-N1	7.70	121.55	117.70
54	BA	471	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	44	A	C4-C5-C6	-7.70	113.15	117.00
54	BA	666	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	16	A	N1-C6-N6	-7.69	113.98	118.60
21	AA	845	A	C5-C6-N1	7.69	121.55	117.70
54	BA	118	A	C5-C6-N1	7.69	121.55	117.70
54	BA	149	A	N1-C6-N6	-7.69	113.98	118.60
54	BA	1165	A	N1-C6-N6	-7.69	113.98	118.60
54	BA	382	A	C5-C6-N1	7.69	121.55	117.70
21	AA	274	A	C4-C5-C6	-7.69	113.16	117.00
54	BA	878	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	492	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	1615	C	N3-C2-O2	-7.69	116.52	121.90
21	AA	1225	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	1274	A	N1-C6-N6	-7.68	113.99	118.60
25	BC	51	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	219	A	N1-C6-N6	-7.68	113.99	118.60
11	AL	35	ARG	NE-CZ-NH1	7.68	124.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	432	A	C4-C5-C6	-7.68	113.16	117.00
54	BA	1590	A	N1-C6-N6	-7.68	113.99	118.60
9	AJ	16	ARG	NE-CZ-NH1	7.68	124.14	120.30
21	AA	982	U	P-O3'-C3'	7.68	128.91	119.70
8	AI	122	ARG	NE-CZ-NH2	7.68	124.14	120.30
54	BA	216	A	C5-C6-N1	7.68	121.54	117.70
54	BA	2682	A	N1-C6-N6	-7.68	113.99	118.60
14	AO	63	ARG	NE-CZ-NH1	7.67	124.14	120.30
21	AA	116	A	C5-C6-N1	7.67	121.54	117.70
54	BA	1395	A	C5-C6-N1	7.67	121.54	117.70
21	AA	720	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	2518	A	C5-C6-N1	7.67	121.54	117.70
22	A1	23	A	C5-C6-N1	7.67	121.53	117.70
21	AA	923	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1321	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	44	A	C5-C6-N1	7.67	121.53	117.70
21	AA	487	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	1969	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1229	A	C5-C6-N1	7.66	121.53	117.70
54	BA	1489	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	1991	U	O4'-C1'-N1	7.66	114.33	108.20
54	BA	2211	A	C5-C6-N1	7.66	121.53	117.70
21	AA	431	A	C5-C6-N1	7.66	121.53	117.70
54	BA	730	A	C5-C6-N1	7.66	121.53	117.70
48	BZ	37	ARG	NE-CZ-NH1	7.66	124.13	120.30
54	BA	196	A	C5-C6-N1	7.66	121.53	117.70
54	BA	889	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	1213	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	2191	A	C5-C6-N1	7.66	121.53	117.70
55	BB	12	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	1342	A	C5-C6-N1	7.65	121.53	117.70
21	AA	946	A	C5-C6-N1	7.65	121.53	117.70
2	AC	163	ARG	NE-CZ-NH1	7.65	124.12	120.30
21	AA	1101	A	C5-C6-N1	7.65	121.53	117.70
54	BA	514	A	C5-C6-N1	7.65	121.52	117.70
54	BA	547	A	N1-C6-N6	-7.65	114.01	118.60
21	AA	777	A	C5-C6-N1	7.65	121.52	117.70
54	BA	877	A	C5-C6-N1	7.65	121.52	117.70
54	BA	1927	A	N1-C6-N6	-7.65	114.01	118.60
3	AD	183	ARG	NE-CZ-NH1	7.64	124.12	120.30
54	BA	2823	A	C5-C6-N1	7.64	121.52	117.70
54	BA	513	A	N1-C6-N6	-7.64	114.01	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2814	A	C5-C6-N1	7.64	121.52	117.70
21	AA	978	A	C4-C5-C6	-7.64	113.18	117.00
54	BA	346	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2439	A	C5-C6-N1	7.64	121.52	117.70
54	BA	139	U	O4'-C1'-N1	7.64	114.31	108.20
54	BA	532	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	2059	A	C5-C6-N1	7.63	121.52	117.70
54	BA	181	A	C5-C6-N1	7.63	121.52	117.70
54	BA	2266	A	C5-C6-N1	7.63	121.52	117.70
21	AA	381	C	N3-C2-O2	-7.63	116.56	121.90
24	A3	73	A	C5-C6-N1	7.63	121.51	117.70
28	BF	29	ARG	NE-CZ-NH1	7.63	124.11	120.30
53	B4	24	ARG	NE-CZ-NH1	7.63	124.11	120.30
21	AA	501	C	N3-C2-O2	-7.63	116.56	121.90
54	BA	223	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	1363	A	C5-C6-N1	7.62	121.51	117.70
54	BA	374	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	753	A	C5-C6-N1	7.62	121.51	117.70
21	AA	790	A	C5-C6-N1	7.62	121.51	117.70
21	AA	961	U	O4'-C1'-N1	7.62	114.30	108.20
21	AA	1000	A	C5-C6-N1	7.62	121.51	117.70
21	AA	1236	A	C5-C6-N1	7.62	121.51	117.70
21	AA	89	U	O4'-C1'-N1	7.62	114.30	108.20
21	AA	747	A	C5-C6-N1	7.62	121.51	117.70
21	AA	1016	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1008	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1268	A	C5-C6-N1	7.62	121.51	117.70
21	AA	325	A	C5-C6-N1	7.61	121.51	117.70
54	BA	429	A	C5-C6-N1	7.61	121.51	117.70
54	BA	435	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	988	A	C5-C6-N1	7.61	121.51	117.70
54	BA	1705	A	C5-C6-N1	7.61	121.51	117.70
54	BA	2003	A	C5-C6-N1	7.61	121.51	117.70
27	BE	114	ARG	NE-CZ-NH1	7.61	124.11	120.30
54	BA	423	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	1022	G	O4'-C1'-N9	7.61	114.29	108.20
54	BA	2577	A	C5-C6-N1	7.61	121.51	117.70
6	AG	101	ARG	NE-CZ-NH1	7.61	124.11	120.30
54	BA	1129	A	C5-C6-N1	7.61	121.50	117.70
54	BA	2101	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	109	A	C1'-O4'-C4'	-7.61	103.82	109.90
54	BA	95	A	N1-C6-N6	-7.61	114.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2090	A	C5-C6-N1	7.61	121.50	117.70
54	BA	2394	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	2646	C	N1-C2-O2	7.60	123.46	118.90
21	AA	1394	A	C5-C6-N1	7.60	121.50	117.70
54	BA	1039	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	174	A	C5-C6-N1	7.60	121.50	117.70
21	AA	1492	A	C5-C6-N1	7.60	121.50	117.70
54	BA	2764	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	2766	A	C5-C6-N1	7.60	121.50	117.70
21	AA	205	A	C5-C6-N1	7.60	121.50	117.70
54	BA	179	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	1373	A	N1-C6-N6	-7.60	114.04	118.60
55	BB	39	A	C5-C6-N1	7.60	121.50	117.70
55	BB	115	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	1147	A	C5-C6-N1	7.60	121.50	117.70
54	BA	142	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	428	A	C5-C6-N1	7.59	121.50	117.70
21	AA	696	A	C4-C5-C6	-7.59	113.20	117.00
54	BA	1096	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	435	C	O4'-C1'-N1	7.59	114.27	108.20
54	BA	1711	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	1784	A	C5-C6-N1	7.59	121.49	117.70
21	AA	1519	A	C5-C6-N1	7.58	121.49	117.70
22	A1	38	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1007	C	N3-C2-O2	-7.58	116.59	121.90
21	AA	900	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1630	A	C4-C5-C6	-7.58	113.21	117.00
54	BA	1794	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1433	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1020	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	748	G	O4'-C1'-N9	7.58	114.26	108.20
54	BA	1211	C	N3-C2-O2	-7.58	116.59	121.90
21	AA	344	A	C5-C6-N1	7.58	121.49	117.70
21	AA	498	A	C5-C6-N1	7.58	121.49	117.70
21	AA	608	A	N1-C6-N6	-7.58	114.06	118.60
54	BA	2461	A	C5-C6-N1	7.58	121.49	117.70
9	AJ	9	ARG	NE-CZ-NH1	7.57	124.09	120.30
54	BA	685	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	751	A	O4'-C1'-N9	7.57	114.26	108.20
54	BA	1265	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1580	A	C5-C6-N1	7.57	121.49	117.70
54	BA	1872	A	C5-C6-N1	7.57	121.48	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2117	A	N1-C6-N6	-7.57	114.06	118.60
21	AA	7	A	C5-C6-N1	7.57	121.48	117.70
21	AA	80	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1528	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	1630	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1383	A	O4'-C1'-N9	7.56	114.25	108.20
21	AA	279	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2158	A	C4-C5-C6	-7.56	113.22	117.00
21	AA	280	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	457	A	C5-C6-N1	7.56	121.48	117.70
21	AA	1503	A	C5-C6-N1	7.56	121.48	117.70
54	BA	371	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	1549	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	2119	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	2451	A	C4-C5-C6	-7.56	113.22	117.00
54	BA	74	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2314	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2284	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	549	C	N3-C2-O2	-7.55	116.61	121.90
54	BA	1384	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2741	A	C5-C6-N1	7.55	121.47	117.70
2	AC	168	ARG	NE-CZ-NH1	7.55	124.07	120.30
21	AA	1269	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	706	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1145	A	C5-C6-N1	7.54	121.47	117.70
21	AA	1480	A	C4-C5-C6	-7.54	113.23	117.00
22	A1	26	A	C5-C6-N1	7.54	121.47	117.70
54	BA	119	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1352	U	N3-C2-O2	-7.54	116.92	122.20
54	BA	2117	A	C5-C6-N1	7.54	121.47	117.70
54	BA	2542	A	C5-C6-N1	7.54	121.47	117.70
22	A1	21	A	N1-C6-N6	-7.54	114.08	118.60
24	A3	74	A	C5-C6-N1	7.54	121.47	117.70
21	AA	574	A	C5-C6-N1	7.54	121.47	117.70
28	BF	149	ARG	NE-CZ-NH1	7.54	124.07	120.30
54	BA	1127	A	C5-C6-N1	7.54	121.47	117.70
54	BA	401	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	677	A	C4-C5-C6	-7.53	113.23	117.00
54	BA	2627	G	C1'-O4'-C4'	-7.53	103.87	109.90
54	BA	28	A	N1-C6-N6	-7.53	114.08	118.60
21	AA	1468	A	C5-C6-N1	7.53	121.47	117.70
54	BA	2060	A	C5-C6-N1	7.53	121.46	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	174	A	N1-C6-N6	-7.53	114.08	118.60
21	AA	1362	A	C5-C6-N1	7.53	121.46	117.70
21	AA	1102	A	N1-C6-N6	-7.53	114.08	118.60
24	A3	44	A	C5-C6-N1	7.53	121.46	117.70
54	BA	196	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	2893	A	C5-C6-N1	7.53	121.46	117.70
54	BA	1679	A	C5-C6-N1	7.52	121.46	117.70
54	BA	613	A	O4'-C1'-N9	7.52	114.22	108.20
54	BA	391	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1853	A	C5-C6-N1	7.52	121.46	117.70
54	BA	199	A	C5-C6-N1	7.52	121.46	117.70
54	BA	2392	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	665	A	C5-C6-N1	7.51	121.46	117.70
21	AA	1476	A	C5-C6-N1	7.51	121.46	117.70
35	BM	81	ARG	NE-CZ-NH2	7.51	124.06	120.30
21	AA	1226	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	505	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	892	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	130	A	C5-C6-N1	7.51	121.45	117.70
21	AA	151	A	C5-C6-N1	7.51	121.45	117.70
54	BA	1786	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2411	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2721	A	C5-C6-N1	7.51	121.45	117.70
21	AA	509	A	C5-C6-N1	7.51	121.45	117.70
44	BV	19	ARG	NE-CZ-NH1	7.51	124.05	120.30
54	BA	527	C	N3-C2-O2	-7.51	116.65	121.90
54	BA	538	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	157	C	O4'-C1'-N1	7.50	114.20	108.20
8	AI	118	ARG	NE-CZ-NH1	7.50	124.05	120.30
21	AA	263	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1518	A	C4-C5-C6	-7.50	113.25	117.00
30	BH	97	ARG	NE-CZ-NH1	7.50	124.05	120.30
21	AA	782	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1580	A	C4-C5-C6	-7.50	113.25	117.00
21	AA	320	A	C5-C6-N1	7.50	121.45	117.70
21	AA	909	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1054	C	N3-C2-O2	-7.50	116.65	121.90
54	BA	2611	C	N3-C2-O2	-7.50	116.65	121.90
6	AG	77	ARG	NE-CZ-NH1	7.49	124.05	120.30
21	AA	1019	A	C4-C5-C6	-7.49	113.25	117.00
21	AA	1163	A	C5-C6-N1	7.49	121.45	117.70
24	A3	38	A	C5-C6-N1	7.49	121.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1967	C	N3-C2-O2	-7.49	116.65	121.90
22	A1	56	C	N3-C2-O2	-7.49	116.66	121.90
54	BA	572	A	C5-C6-N1	7.49	121.45	117.70
21	AA	282	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	1134	A	C5-C6-N1	7.49	121.44	117.70
54	BA	563	A	C5-C6-N1	7.49	121.44	117.70
54	BA	654	A	C4-C5-C6	-7.49	113.26	117.00
54	BA	1244	A	C5-C6-N1	7.49	121.44	117.70
54	BA	927	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2733	A	C5-C6-N1	7.48	121.44	117.70
21	AA	313	A	C4-C5-C6	-7.48	113.26	117.00
21	AA	983	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	503	A	C5-C6-N1	7.48	121.44	117.70
54	BA	1496	A	C4-C5-C6	-7.48	113.26	117.00
54	BA	1000	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1353	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2126	A	N1-C6-N6	-7.47	114.11	118.60
54	BA	2270	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	941	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2288	A	C5-C6-N1	7.47	121.44	117.70
54	BA	631	A	C5-C6-N1	7.47	121.44	117.70
21	AA	546	A	C5-C6-N1	7.47	121.43	117.70
54	BA	163	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	1090	A	C5-C6-N1	7.47	121.44	117.70
21	AA	946	A	N1-C6-N6	-7.47	114.12	118.60
22	A1	14	A	N1-C6-N6	-7.47	114.12	118.60
35	BM	66	ARG	NE-CZ-NH1	7.47	124.03	120.30
54	BA	1194	A	C5-C6-N1	7.47	121.43	117.70
54	BA	947	A	C4-C5-C6	-7.46	113.27	117.00
54	BA	1005	C	N3-C2-O2	-7.46	116.67	121.90
54	BA	1544	A	C5-C6-N1	7.46	121.43	117.70
21	AA	8	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1938	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	2328	A	C5-C6-N1	7.46	121.43	117.70
12	AM	78	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	739	A	N1-C6-N6	-7.46	114.13	118.60
54	BA	229	C	N3-C2-O2	-7.45	116.68	121.90
54	BA	1933	G	O4'-C1'-N9	7.45	114.16	108.20
54	BA	1952	A	C5-C6-N1	7.45	121.43	117.70
54	BA	2666	C	N3-C2-O2	-7.45	116.68	121.90
21	AA	110	C	N3-C2-O2	-7.45	116.69	121.90
26	BD	169	ARG	NE-CZ-NH1	7.45	124.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2052	A	C4-C5-C6	-7.45	113.28	117.00
9	AJ	72	ARG	NE-CZ-NH2	-7.45	116.58	120.30
21	AA	1005	A	C5-C6-N1	7.45	121.42	117.70
21	AA	1362	A	C4-C5-C6	-7.45	113.28	117.00
21	AA	1447	A	C5-C6-N1	7.45	121.42	117.70
54	BA	998	C	N3-C2-O2	-7.45	116.69	121.90
21	AA	1534	A	C5-C6-N1	7.45	121.42	117.70
54	BA	362	A	N1-C6-N6	-7.45	114.13	118.60
5	AF	86	ARG	NE-CZ-NH1	7.45	124.02	120.30
15	AP	51	ARG	NE-CZ-NH1	7.45	124.02	120.30
21	AA	523	A	C5-C6-N1	7.45	121.42	117.70
21	AA	1200	C	N3-C2-O2	-7.45	116.69	121.90
29	BG	68	ARG	NE-CZ-NH1	7.45	124.02	120.30
54	BA	104	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	1137	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	918	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1021	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1142	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1735	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2499	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	2503	A	C5-C6-N1	7.44	121.42	117.70
54	BA	613	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2388	A	C5-C6-N1	7.44	121.42	117.70
21	AA	819	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	2900	A	C5-C6-N1	7.44	121.42	117.70
21	AA	831	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	131	A	C4-C5-C6	-7.43	113.28	117.00
21	AA	214	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	2183	A	C5-C6-N1	7.43	121.42	117.70
21	AA	430	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	814	A	C5-C6-N1	7.43	121.42	117.70
21	AA	938	A	N1-C6-N6	-7.43	114.14	118.60
34	BL	41	ARG	NE-CZ-NH1	-7.43	116.59	120.30
54	BA	460	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2407	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	2516	A	C5-C6-N1	7.43	121.42	117.70
54	BA	899	A	C5-C6-N1	7.43	121.41	117.70
54	BA	2856	A	C5-C6-N1	7.43	121.41	117.70
21	AA	864	A	C5-C6-N1	7.43	121.41	117.70
54	BA	1582	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	1722	A	C5-C6-N1	7.43	121.41	117.70
21	AA	55	A	C4-C5-C6	-7.42	113.29	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	414	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1111	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1513	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	730	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	222	A	C5-C6-N1	7.42	121.41	117.70
54	BA	347	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	1204	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	1460	U	O4'-C1'-N1	7.42	114.14	108.20
54	BA	1900	A	C5-C6-N1	7.42	121.41	117.70
21	AA	743	A	C5-C6-N1	7.42	121.41	117.70
54	BA	152	A	C4-C5-C6	-7.42	113.29	117.00
54	BA	776	G	N3-C2-N2	-7.42	114.71	119.90
21	AA	969	A	C5-C6-N1	7.42	121.41	117.70
23	A2	80	C	P-O3'-C3'	7.42	128.60	119.70
55	BB	52	A	C5-C6-N1	7.42	121.41	117.70
16	AQ	26	ARG	NE-CZ-NH1	7.42	124.01	120.30
25	BC	132	ARG	NE-CZ-NH2	-7.42	116.59	120.30
33	BK	30	ARG	NE-CZ-NH1	7.42	124.01	120.30
54	BA	2199	A	C4-C5-C6	-7.42	113.29	117.00
21	AA	535	A	C5-C6-N1	7.41	121.41	117.70
54	BA	2311	A	C5-C6-N1	7.41	121.41	117.70
33	BK	64	ARG	NE-CZ-NH1	7.41	124.01	120.30
3	AD	13	ARG	NE-CZ-NH1	7.41	124.00	120.30
18	AS	35	ARG	NE-CZ-NH1	7.41	124.00	120.30
21	AA	51	A	C5-C6-N1	7.41	121.41	117.70
21	AA	635	A	N1-C6-N6	-7.41	114.15	118.60
21	AA	1239	A	C5-C6-N1	7.41	121.41	117.70
54	BA	571	U	O4'-C1'-N1	7.41	114.13	108.20
54	BA	1962	C	N3-C2-O2	-7.41	116.71	121.90
54	BA	1241	A	C5-C6-N1	7.41	121.40	117.70
21	AA	718	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2711	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2765	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2809	A	C5-C6-N1	7.41	121.40	117.70
21	AA	119	A	N1-C6-N6	-7.41	114.16	118.60
21	AA	460	A	N1-C6-N6	-7.41	114.16	118.60
21	AA	640	A	C5-C6-N1	7.41	121.40	117.70
54	BA	1085	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2009	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	2887	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2317	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	81	A	C5-C6-N1	7.40	121.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	459	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1809	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	2213	U	O4'-C1'-N1	7.40	114.12	108.20
54	BA	2586	U	O4'-C1'-N1	7.40	114.12	108.20
54	BA	513	A	C5-C6-N1	7.40	121.40	117.70
21	AA	573	A	C5-C6-N1	7.40	121.40	117.70
54	BA	103	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2610	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	2639	A	C4-C5-C6	-7.40	113.30	117.00
55	BB	104	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	808	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	180	G	O4'-C1'-N9	7.40	114.12	108.20
54	BA	2602	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1105	A	C5-C6-N1	7.39	121.40	117.70
22	A1	9	A	C5-C6-N1	7.39	121.40	117.70
54	BA	602	A	C5-C6-N1	7.39	121.40	117.70
21	AA	78	A	C5-C6-N1	7.39	121.39	117.70
21	AA	532	A	C5-C6-N1	7.39	121.39	117.70
21	AA	630	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1545	A	N1-C6-N6	-7.39	114.17	118.60
21	AA	98	A	C5-C6-N1	7.39	121.39	117.70
54	BA	529	A	N1-C6-N6	-7.39	114.17	118.60
21	AA	702	A	C5-C6-N1	7.39	121.39	117.70
21	AA	1360	A	C5-C6-N1	7.39	121.39	117.70
54	BA	2497	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1655	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	1151	A	C5-C6-N1	7.38	121.39	117.70
54	BA	221	A	C5-C6-N1	7.38	121.39	117.70
54	BA	217	A	C5-C6-N1	7.38	121.39	117.70
21	AA	19	A	C5-C6-N1	7.38	121.39	117.70
21	AA	461	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1502	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	505	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	546	U	O4'-C1'-N1	7.38	114.10	108.20
54	BA	1754	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	2426	A	N1-C6-N6	-7.38	114.17	118.60
6	AG	118	ARG	NE-CZ-NH1	7.38	123.99	120.30
54	BA	1151	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	2251	G	O4'-C1'-N9	7.38	114.10	108.20
54	BA	1515	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1815	A	C4-C5-C6	-7.37	113.31	117.00
53	B4	12	ARG	NE-CZ-NH1	7.37	123.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	144	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1652	A	O4'-C1'-N9	7.37	114.10	108.20
54	BA	1689	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	2847	U	O4'-C1'-N1	7.37	114.10	108.20
6	AG	137	ARG	NE-CZ-NH1	7.37	123.98	120.30
54	BA	1590	A	C5-C6-N1	7.37	121.39	117.70
21	AA	1167	A	C5-C6-N1	7.37	121.38	117.70
54	BA	796	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	373	A	C5-C6-N1	7.37	121.38	117.70
21	AA	1333	A	C5-C6-N1	7.37	121.38	117.70
54	BA	740	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	2134	A	C4-C5-C6	-7.37	113.32	117.00
54	BA	2501	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	499	A	N1-C6-N6	-7.36	114.18	118.60
21	AA	975	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2449	U	O4'-C1'-N1	7.36	114.09	108.20
54	BA	2799	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2858	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	515	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2042	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1912	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2453	A	C5-C6-N1	7.36	121.38	117.70
3	AD	127	ARG	NE-CZ-NH1	7.36	123.98	120.30
21	AA	412	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1701	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2052	A	C5-C6-N1	7.36	121.38	117.70
21	AA	415	A	C5-C6-N1	7.35	121.38	117.70
24	A3	58	A	C5-C6-N1	7.35	121.38	117.70
32	BJ	34	ARG	NE-CZ-NH1	7.35	123.98	120.30
54	BA	156	A	C5-C6-N1	7.35	121.38	117.70
54	BA	1395	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1553	A	C5-C6-N1	7.35	121.38	117.70
54	BA	1717	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2856	A	N1-C6-N6	-7.35	114.19	118.60
17	AR	62	ARG	NE-CZ-NH1	7.35	123.97	120.30
21	AA	860	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1320	C	O4'-C1'-N1	7.35	114.08	108.20
21	AA	819	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1403	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1433	A	O4'-C1'-N9	7.34	114.08	108.20
54	BA	2062	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2883	A	C5-C6-N1	7.34	121.37	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	913	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	207	A	C5-C6-N1	7.34	121.37	117.70
24	A3	59	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	2310	C	O4'-C1'-N1	7.34	114.07	108.20
54	BA	2378	A	C5-C6-N1	7.34	121.37	117.70
54	BA	28	A	C5-C6-N1	7.34	121.37	117.70
21	AA	1280	A	O4'-C1'-N9	7.34	114.07	108.20
54	BA	706	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	1079	C	N3-C2-O2	-7.34	116.77	121.90
54	BA	2019	A	C5-C6-N1	7.34	121.37	117.70
54	BA	756	A	C5-C6-N1	7.33	121.37	117.70
54	BA	1088	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	2097	A	C4-C5-C6	-7.33	113.33	117.00
54	BA	2169	A	C5-C6-N1	7.33	121.37	117.70
21	AA	1394	A	C4-C5-C6	-7.33	113.33	117.00
54	BA	143	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	800	A	C4-C5-C6	-7.33	113.33	117.00
21	AA	364	A	C5-C6-N1	7.33	121.36	117.70
54	BA	878	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2551	C	N3-C2-O2	-7.33	116.77	121.90
14	AO	16	ARG	NE-CZ-NH1	7.33	123.96	120.30
21	AA	152	A	C4-C5-C6	-7.33	113.34	117.00
54	BA	197	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2054	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2340	A	C5-C6-N1	7.33	121.36	117.70
53	B4	19	ARG	NE-CZ-NH1	7.33	123.96	120.30
54	BA	443	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	1001	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	1322	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2639	A	C5-C6-N1	7.33	121.36	117.70
21	AA	235	C	N3-C2-O2	-7.32	116.77	121.90
54	BA	516	C	N3-C2-O2	-7.32	116.77	121.90
54	BA	1069	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	2147	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2670	A	C5-C6-N1	7.32	121.36	117.70
54	BA	603	A	C5-C6-N1	7.32	121.36	117.70
21	AA	1067	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1048	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	1070	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1531	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	255	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	1204	A	O4'-C1'-N9	7.32	114.06	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	473	U	P-O3'-C3'	7.32	128.48	119.70
21	AA	784	A	C4-C5-C6	-7.32	113.34	117.00
21	AA	915	A	C5-C6-N1	7.32	121.36	117.70
54	BA	69	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	311	A	C5-C6-N1	7.32	121.36	117.70
54	BA	789	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2212	A	C5-C6-N1	7.32	121.36	117.70
21	AA	807	A	C5-C6-N1	7.31	121.36	117.70
54	BA	1848	A	C5-C6-N1	7.31	121.36	117.70
21	AA	1219	A	C4-C5-C6	-7.31	113.34	117.00
54	BA	1000	A	C4-C5-C6	-7.31	113.34	117.00
54	BA	1175	A	C5-C6-N1	7.31	121.36	117.70
54	BA	402	A	C5-C6-N1	7.31	121.36	117.70
54	BA	541	A	C5-C6-N1	7.31	121.36	117.70
54	BA	721	A	N1-C6-N6	-7.31	114.22	118.60
54	BA	2459	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2725	A	C5-C6-N1	7.31	121.36	117.70
5	AF	44	ARG	NE-CZ-NH1	7.31	123.95	120.30
21	AA	1196	A	C5-C6-N1	7.31	121.35	117.70
54	BA	608	A	C5-C6-N1	7.31	121.35	117.70
54	BA	1246	A	C5-C6-N1	7.31	121.35	117.70
54	BA	1569	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1815	A	C5-C6-N1	7.30	121.35	117.70
54	BA	721	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2476	A	C5-C6-N1	7.30	121.35	117.70
37	BO	81	ARG	NE-CZ-NH1	7.30	123.95	120.30
54	BA	2114	A	N1-C6-N6	-7.30	114.22	118.60
21	AA	1014	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	829	A	C5-C6-N1	7.30	121.35	117.70
21	AA	441	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1346	A	C5-C6-N1	7.30	121.35	117.70
54	BA	34	U	O4'-C1'-N1	7.30	114.04	108.20
54	BA	1143	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1251	A	C5-C6-N1	7.29	121.35	117.70
21	AA	1507	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1398	C	N3-C2-O2	-7.29	116.79	121.90
20	AU	44	ARG	NE-CZ-NH1	7.29	123.95	120.30
54	BA	1532	A	C5-C6-N1	7.29	121.35	117.70
54	BA	2298	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	2358	A	C4-C5-C6	-7.29	113.35	117.00
54	BA	2667	C	N3-C2-O2	-7.29	116.80	121.90
21	AA	892	A	C5-C6-N1	7.29	121.35	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1378	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1801	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	2322	A	N1-C6-N6	-7.29	114.22	118.60
7	AH	113	ARG	NE-CZ-NH1	7.29	123.94	120.30
54	BA	2030	A	C5-C6-N1	7.29	121.34	117.70
54	BA	2899	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1180	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1431	A	C5-C6-N1	7.29	121.34	117.70
54	BA	896	A	C5-C6-N1	7.29	121.34	117.70
21	AA	978	A	C5-C6-N1	7.29	121.34	117.70
54	BA	2439	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	1470	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2721	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	582	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	1254	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	1322	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	1481	U	O4'-C1'-N1	7.28	114.02	108.20
54	BA	1505	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1918	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	590	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	750	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1375	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1775	U	O4'-C1'-N1	7.28	114.02	108.20
54	BA	155	A	N1-C6-N6	-7.27	114.24	118.60
54	BA	890	C	N3-C2-O2	-7.27	116.81	121.90
45	BW	54	ARG	NE-CZ-NH2	7.27	123.94	120.30
54	BA	654	A	C5-C6-N1	7.27	121.34	117.70
21	AA	919	A	C5-C6-N1	7.27	121.34	117.70
54	BA	613	A	N1-C6-N6	-7.27	114.24	118.60
12	AM	92	ARG	NE-CZ-NH1	7.27	123.94	120.30
54	BA	324	A	C5-C6-N1	7.27	121.33	117.70
54	BA	775	G	O4'-C1'-N9	7.27	114.02	108.20
54	BA	1938	A	C5-C6-N1	7.27	121.33	117.70
54	BA	2749	A	C5-C6-N1	7.27	121.33	117.70
3	AD	12	ARG	NE-CZ-NH1	7.27	123.93	120.30
54	BA	19	A	N1-C6-N6	-7.27	114.24	118.60
22	A1	35	A	C5-C6-N1	7.26	121.33	117.70
36	BN	86	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	1690	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2108	A	C5-C6-N1	7.26	121.33	117.70
21	AA	958	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1597	A	C5-C6-N1	7.26	121.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	109	A	C4-C5-C6	-7.26	113.37	117.00
21	AA	511	C	N3-C2-O2	-7.26	116.82	121.90
21	AA	243	A	C5-C6-N1	7.26	121.33	117.70
54	BA	472	A	C5-C6-N1	7.26	121.33	117.70
54	BA	866	A	N1-C6-N6	-7.26	114.25	118.60
54	BA	83	A	C5-C6-N1	7.25	121.33	117.70
21	AA	181	A	C5-C6-N1	7.25	121.33	117.70
21	AA	411	A	C5-C6-N1	7.25	121.33	117.70
22	A1	69	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1885	A	C5-C6-N1	7.25	121.33	117.70
21	AA	510	A	C5-C6-N1	7.25	121.33	117.70
21	AA	1500	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	1472	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	1413	A	N1-C6-N6	-7.25	114.25	118.60
21	AA	650	G	N3-C2-N2	-7.25	114.83	119.90
26	BD	128	ARG	NE-CZ-NH1	7.25	123.92	120.30
54	BA	2412	A	C5-C6-N1	7.25	121.32	117.70
54	BA	2565	A	C5-C6-N1	7.25	121.32	117.70
21	AA	1021	A	C5-C6-N1	7.25	121.32	117.70
54	BA	2070	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	2430	A	C5-C6-N1	7.25	121.32	117.70
10	AK	121	ARG	NE-CZ-NH1	7.24	123.92	120.30
54	BA	675	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1789	A	C5-C6-N1	7.24	121.32	117.70
25	BC	257	ARG	NE-CZ-NH1	7.24	123.92	120.30
54	BA	979	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1469	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1596	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	2660	A	C5-C6-N1	7.24	121.32	117.70
54	BA	845	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	637	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	161	A	C5-C6-N1	7.23	121.32	117.70
54	BA	2020	A	C1'-O4'-C4'	-7.23	104.11	109.90
54	BA	627	A	C5-C6-N1	7.23	121.31	117.70
54	BA	749	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1428	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	1549	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2893	A	N1-C6-N6	-7.23	114.26	118.60
21	AA	873	A	C5-C6-N1	7.23	121.31	117.70
54	BA	310	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	1894	C	O4'-C1'-N1	7.23	113.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2482	A	C5-C6-N1	7.23	121.31	117.70
12	AM	28	ARG	NE-CZ-NH1	7.23	123.91	120.30
21	AA	695	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1140	C	N3-C2-O2	-7.23	116.84	121.90
51	B2	28	ARG	NE-CZ-NH1	7.23	123.91	120.30
54	BA	522	A	C4-C5-C6	-7.23	113.39	117.00
21	AA	1377	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1469	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	480	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1103	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	1655	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1936	A	C5-C6-N1	7.22	121.31	117.70
21	AA	315	A	C5-C6-N1	7.22	121.31	117.70
21	AA	949	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1848	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	2434	A	C4-C5-C6	-7.22	113.39	117.00
55	BB	73	A	C5-C6-N1	7.22	121.31	117.70
21	AA	622	A	C5-C6-N1	7.22	121.31	117.70
39	BQ	10	ARG	NE-CZ-NH1	7.22	123.91	120.30
54	BA	279	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	53	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1609	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	149	A	C5-C6-N1	7.22	121.31	117.70
21	AA	780	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	311	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	1254	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2014	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2422	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	739	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	1014	A	C5-C6-N1	7.21	121.31	117.70
28	BF	132	ARG	NE-CZ-NH1	7.21	123.91	120.30
54	BA	490	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	899	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	5	A	C5-C6-N1	7.21	121.31	117.70
21	AA	228	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1035	A	C5-C6-N1	7.21	121.31	117.70
54	BA	371	A	C5-C6-N1	7.21	121.31	117.70
54	BA	886	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	1970	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2829	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1246	A	C4-C5-C6	-7.21	113.39	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2810	A	C4-C5-C6	-7.21	113.39	117.00
2	AC	130	ARG	NE-CZ-NH1	7.21	123.90	120.30
4	AE	156	ARG	NE-CZ-NH1	7.21	123.90	120.30
21	AA	1441	A	C5-C6-N1	7.21	121.31	117.70
54	BA	66	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	1634	A	C5-C6-N1	7.21	121.30	117.70
54	BA	2241	A	C4-C5-C6	-7.21	113.40	117.00
21	AA	285	C	N3-C2-O2	-7.21	116.86	121.90
21	AA	1352	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	420	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	572	A	N1-C6-N6	-7.21	114.28	118.60
21	AA	754	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	792	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1229	A	O4'-C1'-N9	7.20	113.96	108.20
54	BA	1427	A	C5-C6-N1	7.20	121.30	117.70
5	AF	79	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	104	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1877	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	2142	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1273	C	N3-C2-O2	-7.20	116.86	121.90
23	A2	82	A	C5-C6-N1	7.20	121.30	117.70
54	BA	804	A	C5-C6-N1	7.20	121.30	117.70
54	BA	838	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	1295	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	1326	U	O4'-C1'-N1	7.20	113.96	108.20
54	BA	1610	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2274	A	C5-C6-N1	7.20	121.30	117.70
21	AA	607	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	630	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	550	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	2003	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	2160	C	N3-C2-O2	-7.20	116.86	121.90
21	AA	1430	A	C5-C6-N1	7.19	121.30	117.70
54	BA	142	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2059	A	N1-C6-N6	-7.19	114.28	118.60
8	AI	40	ARG	NE-CZ-NH1	7.19	123.90	120.30
21	AA	729	A	C4-C5-C6	-7.19	113.41	117.00
54	BA	1434	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1572	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2478	A	C5-C6-N1	7.19	121.30	117.70
21	AA	370	C	N3-C2-O2	-7.19	116.87	121.90
21	AA	1357	A	C5-C6-N1	7.19	121.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	90	C	N3-C2-O2	-7.19	116.87	121.90
21	AA	397	A	C5-C6-N1	7.19	121.29	117.70
54	BA	272	A	C5-C6-N1	7.19	121.29	117.70
54	BA	344	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	401	A	C5-C6-N1	7.19	121.29	117.70
54	BA	901	C	N3-C2-O2	-7.19	116.87	121.90
54	BA	2327	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	2809	A	O4'-C1'-N9	7.19	113.95	108.20
21	AA	162	A	C5-C6-N1	7.18	121.29	117.70
56	B5	122	ARG	NE-CZ-NH1	7.18	123.89	120.30
54	BA	1977	A	N1-C6-N6	-7.18	114.29	118.60
21	AA	969	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	270	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	1340	U	N3-C2-O2	-7.18	117.17	122.20
54	BA	1889	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1899	A	N1-C6-N6	-7.18	114.29	118.60
21	AA	1239	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	322	A	C5-C6-N1	7.18	121.29	117.70
21	AA	487	A	C5-C6-N1	7.18	121.29	117.70
21	AA	927	G	C1'-O4'-C4'	-7.17	104.16	109.90
21	AA	1349	A	C5-C6-N1	7.17	121.29	117.70
54	BA	14	A	C5-C6-N1	7.17	121.29	117.70
21	AA	536	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	1130	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	960	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1013	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	2149	U	O4'-C1'-N1	7.17	113.94	108.20
21	AA	59	A	C5-C6-N1	7.17	121.28	117.70
21	AA	236	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2376	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2458	G	O4'-C1'-N9	7.17	113.94	108.20
54	BA	2682	A	C5-C6-N1	7.17	121.28	117.70
21	AA	199	A	C5-C6-N1	7.17	121.28	117.70
21	AA	363	A	C5-C6-N1	7.17	121.28	117.70
21	AA	1167	A	N1-C6-N6	-7.16	114.30	118.60
21	AA	1502	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2013	A	C5-C6-N1	7.16	121.28	117.70
21	AA	139	A	C5-C6-N1	7.16	121.28	117.70
54	BA	632	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2080	A	C5-C6-N1	7.16	121.28	117.70
21	AA	306	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	624	C	N3-C2-O2	-7.16	116.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	877	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	675	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2738	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2872	A	C5-C6-N1	7.16	121.28	117.70
21	AA	306	A	C5-C6-N1	7.16	121.28	117.70
21	AA	322	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	1286	A	C5-C6-N1	7.16	121.28	117.70
21	AA	768	A	N1-C6-N6	-7.15	114.31	118.60
1	AB	112	ARG	NE-CZ-NH2	-7.15	116.72	120.30
21	AA	857	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	693	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2054	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	2126	A	C5-C6-N1	7.15	121.28	117.70
55	BB	15	A	C5-C6-N1	7.15	121.28	117.70
21	AA	765	G	O4'-C1'-N9	7.15	113.92	108.20
24	A3	39	A	C5-C6-N1	7.15	121.28	117.70
54	BA	927	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	909	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1528	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2342	C	N3-C2-O2	-7.15	116.89	121.90
22	A1	76	A	C5-C6-N1	7.15	121.27	117.70
54	BA	131	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1156	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1342	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	1551	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1937	A	C4-C5-C6	-7.15	113.43	117.00
54	BA	126	A	C5-C6-N1	7.15	121.27	117.70
54	BA	911	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1694	C	N1-C2-O2	7.15	123.19	118.90
54	BA	1749	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	272	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	753	A	C5-C6-N1	7.14	121.27	117.70
21	AA	879	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	959	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1285	A	C5-C6-N1	7.14	121.27	117.70
54	BA	197	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	2566	A	C5-C6-N1	7.14	121.27	117.70
55	BB	57	A	N1-C6-N6	-7.14	114.31	118.60
21	AA	482	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1111	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	1135	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1598	A	N1-C6-N6	-7.14	114.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1616	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1785	A	N1-C6-N6	-7.14	114.31	118.60
21	AA	190	A	C5-C6-N1	7.14	121.27	117.70
45	BW	38	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	985	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1354	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2813	A	C5-C6-N1	7.14	121.27	117.70
21	AA	608	A	C5-C6-N1	7.14	121.27	117.70
54	BA	89	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2119	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2263	C	N3-C2-O2	-7.14	116.91	121.90
21	AA	1446	A	C5-C6-N1	7.13	121.27	117.70
21	AA	1465	A	C5-C6-N1	7.13	121.27	117.70
21	AA	559	A	C5-C6-N1	7.13	121.27	117.70
21	AA	802	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2734	A	C5-C6-N1	7.13	121.27	117.70
21	AA	533	A	C5-C6-N1	7.13	121.27	117.70
46	BX	49	ARG	NE-CZ-NH1	7.13	123.86	120.30
21	AA	768	A	C5-C6-N1	7.13	121.26	117.70
44	BV	21	ARG	NE-CZ-NH1	7.13	123.86	120.30
54	BA	1327	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2085	U	O4'-C1'-N1	7.13	113.90	108.20
22	A1	73	A	C5-C6-N1	7.13	121.26	117.70
28	BF	166	ARG	NE-CZ-NH1	7.13	123.86	120.30
54	BA	2776	A	C5-C6-N1	7.13	121.26	117.70
54	BA	2045	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	2541	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	2736	A	C5-C6-N1	7.12	121.26	117.70
54	BA	79	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	1607	C	O4'-C1'-N1	7.12	113.90	108.20
54	BA	1650	A	C5-C6-N1	7.12	121.26	117.70
21	AA	631	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	2377	A	C5-C6-N1	7.12	121.26	117.70
21	AA	435	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1150	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1408	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2297	A	C5-C6-N1	7.12	121.26	117.70
21	AA	994	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1155	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1916	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	499	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1299	A	N1-C6-N6	-7.12	114.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	160	A	C5-C6-N1	7.12	121.26	117.70
54	BA	866	A	C5-C6-N1	7.12	121.26	117.70
54	BA	982	C	N1-C2-O2	7.12	123.17	118.90
54	BA	1626	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1794	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	2716	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	109	A	C5-C6-N1	7.11	121.26	117.70
21	AA	315	A	C4-C5-C6	-7.11	113.44	117.00
54	BA	632	A	N1-C6-N6	-7.11	114.33	118.60
54	BA	2311	A	N1-C6-N6	-7.11	114.33	118.60
54	BA	2336	A	C5-C6-N1	7.11	121.26	117.70
54	BA	2058	A	C5-C6-N1	7.11	121.26	117.70
54	BA	1672	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2679	A	N1-C6-N6	-7.11	114.33	118.60
33	BK	108	ARG	NE-CZ-NH1	7.11	123.86	120.30
54	BA	1146	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	920	A	C5-C6-N1	7.11	121.25	117.70
54	BA	1086	A	C5-C6-N1	7.11	121.25	117.70
11	AL	82	ARG	NE-CZ-NH1	7.10	123.85	120.30
21	AA	1398	A	C5-C6-N1	7.10	121.25	117.70
54	BA	531	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	715	A	C5-C6-N1	7.10	121.25	117.70
54	BA	575	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	2134	A	C5-C6-N1	7.10	121.25	117.70
54	BA	816	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	1275	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2531	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2434	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2727	A	C5-C6-N1	7.10	121.25	117.70
21	AA	177	G	O4'-C1'-N9	7.10	113.88	108.20
21	AA	217	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	802	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	429	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	1155	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	866	C	N3-C2-O2	-7.09	116.93	121.90
21	AA	1093	A	C5-C6-N1	7.09	121.25	117.70
54	BA	449	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2814	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	203	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2227	A	C5-C6-N1	7.09	121.25	117.70
21	AA	55	A	C5-C6-N1	7.09	121.25	117.70
21	AA	746	A	C5-C6-N1	7.09	121.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	596	A	C5-C6-N1	7.09	121.25	117.70
21	AA	1170	A	C5-C6-N1	7.09	121.24	117.70
21	AA	1518	A	C5-C6-N1	7.09	121.24	117.70
54	BA	722	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1384	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2094	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2183	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	2418	A	C5-C6-N1	7.09	121.24	117.70
21	AA	1223	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	1364	U	O4'-C1'-N1	7.09	113.87	108.20
22	A1	58	A	C5-C6-N1	7.09	121.24	117.70
54	BA	218	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	1319	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	2632	A	C5-C6-N1	7.09	121.24	117.70
54	BA	2778	A	C5-C6-N1	7.09	121.24	117.70
55	BB	35	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	750	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	517	C	O4'-C1'-N1	7.08	113.87	108.20
21	AA	712	A	C5-C6-N1	7.08	121.24	117.70
21	AA	779	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	586	A	C5-C6-N1	7.08	121.24	117.70
54	BA	793	A	C5-C6-N1	7.08	121.24	117.70
54	BA	980	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	1916	A	C5-C6-N1	7.08	121.24	117.70
21	AA	26	A	C5-C6-N1	7.08	121.24	117.70
21	AA	382	A	C5-C6-N1	7.08	121.24	117.70
21	AA	572	A	N1-C6-N6	-7.08	114.35	118.60
21	AA	1192	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	1238	A	C5-C6-N1	7.08	121.24	117.70
25	BC	211	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	453	A	C5-C6-N1	7.08	121.24	117.70
54	BA	614	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	563	A	C5-C6-N1	7.08	121.24	117.70
21	AA	553	A	N1-C6-N6	-7.08	114.36	118.60
54	BA	10	A	C5-C6-N1	7.08	121.24	117.70
54	BA	49	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1800	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	1802	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1961	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	807	U	O4'-C1'-N1	7.07	113.86	108.20
54	BA	11	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1502	A	C5-C6-N1	7.07	121.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	886	A	C5-C6-N1	7.07	121.24	117.70
54	BA	1230	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	1243	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	496	A	C5-C6-N1	7.07	121.23	117.70
54	BA	915	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	1507	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	789	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	1366	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2761	A	C5-C6-N1	7.06	121.23	117.70
36	BN	2	ARG	NE-CZ-NH1	7.06	123.83	120.30
54	BA	213	A	C4-C5-C6	-7.06	113.47	117.00
10	AK	92	ARG	NE-CZ-NH1	7.06	123.83	120.30
21	AA	918	A	C5-C6-N1	7.06	121.23	117.70
21	AA	1382	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	1941	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	503	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2402	U	N3-C2-O2	-7.06	117.26	122.20
21	AA	74	A	C5-C6-N1	7.05	121.23	117.70
21	AA	456	A	C5-C6-N1	7.05	121.23	117.70
21	AA	600	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1029	A	C5-C6-N1	7.05	121.23	117.70
54	BA	204	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1302	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	1597	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	2314	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	2851	A	C5-C6-N1	7.05	121.23	117.70
21	AA	576	C	N3-C2-O2	-7.05	116.97	121.90
21	AA	1132	C	N3-C2-O2	-7.05	116.97	121.90
28	BF	79	ARG	NE-CZ-NH1	7.05	123.83	120.30
54	BA	262	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	903	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	2114	A	C5-C6-N1	7.05	121.22	117.70
21	AA	759	A	C5-C6-N1	7.05	121.22	117.70
54	BA	502	A	C5-C6-N1	7.05	121.22	117.70
54	BA	508	A	C5-C6-N1	7.05	121.22	117.70
54	BA	592	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2157	G	O4'-C1'-N9	7.05	113.84	108.20
55	BB	110	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	975	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	1508	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2471	A	C5-C6-N1	7.04	121.22	117.70
21	AA	143	A	C5-C6-N1	7.04	121.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1396	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1618	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2147	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	2748	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	2837	A	N1-C6-N6	-7.04	114.38	118.60
55	BB	39	A	C4-C5-C6	-7.04	113.48	117.00
16	AQ	61	ARG	NE-CZ-NH1	7.04	123.82	120.30
21	AA	998	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	681	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1513	A	C5-C6-N1	7.04	121.22	117.70
54	BA	279	A	C5-C6-N1	7.04	121.22	117.70
21	AA	737	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	255	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1092	C	N3-C2-O2	-7.04	116.97	121.90
55	BB	29	A	C5-C6-N1	7.04	121.22	117.70
21	AA	65	A	C5-C6-N1	7.04	121.22	117.70
21	AA	72	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	389	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2886	A	C5-C6-N1	7.04	121.22	117.70
21	AA	188	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	182	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1821	A	C4-C5-C6	-7.03	113.48	117.00
21	AA	814	A	C4-C5-C6	-7.03	113.48	117.00
21	AA	554	A	C5-C6-N1	7.03	121.22	117.70
21	AA	1080	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	631	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	2860	A	C5-C6-N1	7.03	121.22	117.70
11	AL	8	ARG	NE-CZ-NH1	7.03	123.81	120.30
21	AA	658	C	N3-C2-O2	-7.03	116.98	121.90
25	BC	101	ARG	NE-CZ-NH1	7.03	123.81	120.30
54	BA	241	A	C5-C6-N1	7.03	121.21	117.70
54	BA	1353	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	1757	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	2888	C	N3-C2-O2	-7.03	116.98	121.90
21	AA	327	A	N1-C6-N6	-7.03	114.39	118.60
54	BA	402	A	N1-C6-N6	-7.03	114.39	118.60
54	BA	477	A	C5-C6-N1	7.03	121.21	117.70
54	BA	2675	A	C5-C6-N1	7.03	121.21	117.70
21	AA	968	A	C5-C6-N1	7.02	121.21	117.70
23	A2	79	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1676	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	1805	A	N1-C6-N6	-7.02	114.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AP	35	ARG	NE-CZ-NH1	7.02	123.81	120.30
21	AA	468	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1092	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	853	C	N3-C2-O2	-7.02	116.99	121.90
21	AA	502	A	C5-C6-N1	7.02	121.21	117.70
54	BA	2309	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	2439	A	C1'-O4'-C4'	-7.02	104.29	109.90
5	AF	38	ARG	NE-CZ-NH1	7.02	123.81	120.30
21	AA	151	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	1470	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	340	A	C5-C6-N1	7.01	121.21	117.70
54	BA	456	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	1936	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2150	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	324	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2287	A	O4'-C1'-N9	7.01	113.81	108.20
21	AA	274	A	C5-C6-N1	7.01	121.20	117.70
21	AA	1306	A	C5-C6-N1	7.01	121.20	117.70
54	BA	302	C	N3-C2-O2	-7.01	116.99	121.90
37	BO	33	ARG	NE-CZ-NH2	7.01	123.80	120.30
54	BA	1669	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2835	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	382	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	1031	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	644	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	2542	A	N1-C6-N6	-7.00	114.40	118.60
22	A1	3	G	O4'-C1'-N9	7.00	113.80	108.20
21	AA	958	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	501	A	C5-C6-N1	7.00	121.20	117.70
54	BA	812	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2448	A	C5-C6-N1	7.00	121.20	117.70
55	BB	45	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	635	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1919	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2469	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2636	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	712	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	787	A	C5-C6-N1	7.00	121.20	117.70
21	AA	935	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	2097	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2711	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	539	A	C5-C6-N1	7.00	121.20	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2450	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	223	A	C5-C6-N1	6.99	121.20	117.70
54	BA	227	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	861	A	C5-C6-N1	6.99	121.20	117.70
54	BA	1403	A	N1-C6-N6	-6.99	114.40	118.60
54	BA	2095	A	C5-C6-N1	6.99	121.20	117.70
21	AA	1252	A	C5-C6-N1	6.99	121.20	117.70
54	BA	1678	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	1981	A	C5-C6-N1	6.99	121.20	117.70
55	BB	28	C	N3-C2-O2	-6.99	117.01	121.90
16	AQ	10	ARG	NE-CZ-NH1	6.99	123.80	120.30
54	BA	282	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	344	A	C5-C6-N1	6.99	121.19	117.70
54	BA	928	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	2706	A	C5-C6-N1	6.99	121.19	117.70
54	BA	111	A	C5-C6-N1	6.99	121.19	117.70
8	AI	121	ARG	NE-CZ-NH1	6.99	123.79	120.30
12	AM	108	ARG	NE-CZ-NH1	6.99	123.79	120.30
21	AA	221	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	364	A	C4-C5-C6	-6.99	113.51	117.00
21	AA	522	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	1574	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	329	A	C5-C6-N1	6.99	121.19	117.70
21	AA	1533	C	C1'-O4'-C4'	-6.99	104.31	109.90
34	BL	47	ARG	NE-CZ-NH1	6.99	123.79	120.30
54	BA	19	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1039	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2392	A	C5-C6-N1	6.99	121.19	117.70
21	AA	900	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	783	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2573	C	N3-C2-O2	-6.98	117.01	121.90
11	AL	49	ARG	NE-CZ-NH1	6.98	123.79	120.30
21	AA	620	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	751	A	C5-C6-N1	6.98	121.19	117.70
54	BA	920	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1237	A	C5-C6-N1	6.98	121.19	117.70
54	BA	564	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	1978	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2513	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2388	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	2813	A	N1-C6-N6	-6.98	114.41	118.60
21	AA	53	A	C4-C5-C6	-6.98	113.51	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	510	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	507	A	C5-C6-N1	6.98	121.19	117.70
21	AA	825	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	793	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	1833	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2572	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2757	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	1870	C	N3-C2-O2	-6.97	117.02	121.90
23	A2	89	U	O4'-C1'-N1	6.97	113.78	108.20
42	BT	12	ARG	NE-CZ-NH1	6.97	123.78	120.30
54	BA	1960	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	2333	A	C5-C6-N1	6.97	121.19	117.70
22	A1	69	A	C4-C5-C6	-6.97	113.52	117.00
14	AO	52	ARG	NE-CZ-NH1	6.97	123.78	120.30
21	AA	1499	A	C5-C6-N1	6.97	121.18	117.70
39	BQ	91	ARG	NE-CZ-NH1	6.97	123.78	120.30
54	BA	155	A	C5-C6-N1	6.97	121.18	117.70
54	BA	794	A	C5-C6-N1	6.97	121.18	117.70
54	BA	2019	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	2850	A	C5-C6-N1	6.97	121.18	117.70
21	AA	465	A	C5-C6-N1	6.96	121.18	117.70
54	BA	532	A	C5-C6-N1	6.96	121.18	117.70
54	BA	928	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1876	A	N1-C6-N6	-6.96	114.42	118.60
54	BA	2758	A	C5-C6-N1	6.96	121.18	117.70
22	A1	6	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2248	C	O4'-C1'-N1	6.96	113.77	108.20
54	BA	2547	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1093	A	C1'-O4'-C4'	-6.96	104.33	109.90
54	BA	1032	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1216	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	1395	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	716	A	C5-C6-N1	6.96	121.18	117.70
22	A1	28	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	1008	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1899	A	C5-C6-N1	6.96	121.18	117.70
54	BA	505	A	C5-C6-N1	6.96	121.18	117.70
54	BA	723	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	2215	C	N3-C2-O2	-6.96	117.03	121.90
13	AN	81	ARG	NE-CZ-NH1	6.96	123.78	120.30
54	BA	22	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	457	A	C4-C5-C6	-6.96	113.52	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1103	A	C5-C6-N1	6.96	121.18	117.70
20	AU	17	ARG	NE-CZ-NH1	6.95	123.78	120.30
21	AA	251	G	P-O3'-C3'	6.95	128.04	119.70
21	AA	383	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	1966	A	C5-C6-N1	6.95	121.18	117.70
21	AA	621	A	C5-C6-N1	6.95	121.18	117.70
21	AA	1357	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	1365	A	C4-C5-C6	-6.95	113.52	117.00
21	AA	321	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	732	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	599	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1754	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2108	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	456	A	N1-C6-N6	-6.95	114.43	118.60
46	BX	44	ARG	NE-CZ-NH1	6.95	123.77	120.30
54	BA	1251	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	835	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	2268	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2682	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	1092	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1264	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1504	A	C5-C6-N1	6.95	121.17	117.70
21	AA	1269	A	C5-C6-N1	6.94	121.17	117.70
54	BA	219	A	C5-C6-N1	6.94	121.17	117.70
21	AA	559	A	N1-C6-N6	-6.94	114.43	118.60
21	AA	66	A	C5-C6-N1	6.94	121.17	117.70
54	BA	802	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1111	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1365	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1300	G	P-O3'-C3'	6.94	128.03	119.70
54	BA	429	A	N1-C6-N6	-6.94	114.44	118.60
54	BA	673	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	2284	A	C5-C6-N1	6.94	121.17	117.70
21	AA	32	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1082	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	1735	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	209	U	O4'-C1'-N1	6.93	113.75	108.20
21	AA	451	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	758	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	1332	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1428	A	C5-C6-N1	6.93	121.17	117.70
21	AA	651	C	N3-C2-O2	-6.93	117.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1508	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	1096	A	C5-C6-N1	6.93	121.17	117.70
21	AA	195	A	C5-C6-N1	6.93	121.17	117.70
21	AA	1251	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	1428	A	C4-C5-C6	-6.93	113.54	117.00
24	A3	42	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	1986	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	1089	A	C5-C6-N1	6.93	121.16	117.70
21	AA	120	A	C5-C6-N1	6.93	121.16	117.70
54	BA	2090	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	2096	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	2627	G	O4'-C1'-N9	6.93	113.74	108.20
54	BA	2815	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	366	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2171	A	C4-C5-C6	-6.92	113.54	117.00
5	AF	79	ARG	NE-CZ-NH2	-6.92	116.84	120.30
54	BA	42	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2340	A	C4-C5-C6	-6.92	113.54	117.00
55	BB	11	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	146	A	C5-C6-N1	6.92	121.16	117.70
54	BA	348	A	N1-C6-N6	-6.92	114.45	118.60
21	AA	167	A	C5-C6-N1	6.92	121.16	117.70
21	AA	563	A	N1-C6-N6	-6.92	114.45	118.60
49	B0	51	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	144	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	746	A	C4-C5-C6	-6.91	113.54	117.00
21	AA	1287	A	C5-C6-N1	6.91	121.16	117.70
54	BA	506	G	O4'-C1'-N9	6.91	113.73	108.20
54	BA	1877	A	C5-C6-N1	6.91	121.16	117.70
21	AA	1110	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1953	A	C4-C5-C6	-6.91	113.54	117.00
21	AA	640	A	N1-C6-N6	-6.91	114.45	118.60
21	AA	1151	A	C5-C6-N1	6.91	121.16	117.70
24	A3	22	A	C5-C6-N1	6.91	121.16	117.70
54	BA	920	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1942	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	2880	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	841	C	N3-C2-O2	-6.91	117.06	121.90
34	BL	41	ARG	NE-CZ-NH2	6.91	123.75	120.30
54	BA	1427	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2298	A	C5-C6-N1	6.91	121.15	117.70
55	BB	99	A	C5-C6-N1	6.91	121.15	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	106	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	910	C	N3-C2-O2	-6.91	117.07	121.90
21	AA	1339	A	C4-C5-C6	-6.91	113.55	117.00
27	BE	44	ARG	NE-CZ-NH1	6.91	123.75	120.30
54	BA	825	A	N1-C6-N6	-6.91	114.46	118.60
54	BA	1732	C	N3-C2-O2	-6.91	117.07	121.90
54	BA	2281	A	C5-C6-N1	6.91	121.15	117.70
54	BA	2666	C	N1-C2-O2	6.91	123.04	118.90
21	AA	321	A	C5-C6-N1	6.90	121.15	117.70
21	AA	706	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	1448	C	N3-C2-O2	-6.90	117.07	121.90
22	A1	66	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	192	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	1780	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2082	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2343	U	O4'-C1'-N1	6.90	113.72	108.20
54	BA	2418	A	C4-C5-C6	-6.90	113.55	117.00
24	A3	1	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	602	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	1019	A	C5-C6-N1	6.90	121.15	117.70
54	BA	643	A	O4'-C1'-N9	6.90	113.72	108.20
54	BA	2008	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2513	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	934	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	764	C	N3-C2-O2	-6.89	117.07	121.90
21	AA	1096	C	N3-C2-O2	-6.89	117.07	121.90
54	BA	1616	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	2427	C	N3-C2-O2	-6.89	117.07	121.90
21	AA	316	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	794	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	172	A	N1-C6-N6	-6.89	114.47	118.60
54	BA	727	A	C5-C6-N1	6.89	121.15	117.70
54	BA	944	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	982	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1040	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1894	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	300	A	C5-C6-N1	6.89	121.14	117.70
34	BL	123	ARG	NE-CZ-NH1	6.89	123.75	120.30
54	BA	1165	A	C5-C6-N1	6.89	121.15	117.70
21	AA	223	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	623	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1614	A	C5-C6-N1	6.89	121.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	44	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	2440	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1367	A	C5-C6-N1	6.89	121.14	117.70
54	BA	1866	A	C5-C6-N1	6.89	121.14	117.70
54	BA	1632	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2705	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	996	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1890	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	583	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1879	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	2635	A	C5-C6-N1	6.88	121.14	117.70
9	AJ	5	ARG	NE-CZ-NH1	6.88	123.74	120.30
21	AA	665	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2546	U	O4'-C1'-N1	6.88	113.70	108.20
54	BA	2868	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	878	A	C5-C6-N1	6.88	121.14	117.70
54	BA	146	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1895	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	338	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1201	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	71	A	O4'-C1'-N9	6.88	113.70	108.20
54	BA	103	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	541	A	N1-C6-N6	-6.88	114.47	118.60
54	BA	621	A	C5-C6-N1	6.88	121.14	117.70
56	B5	9	ARG	NE-CZ-NH1	6.88	123.74	120.30
21	AA	461	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	1375	A	N1-C6-N6	-6.88	114.47	118.60
54	BA	787	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1808	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1874	C	N3-C2-O2	-6.87	117.09	121.90
56	B5	7	ARG	NE-CZ-NH1	6.87	123.74	120.30
21	AA	339	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1088	A	C5-C6-N1	6.87	121.14	117.70
21	AA	298	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	386	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	695	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	1157	A	C5-C6-N1	6.87	121.14	117.70
21	AA	649	A	C5-C6-N1	6.87	121.13	117.70
54	BA	547	A	C5-C6-N1	6.87	121.14	117.70
54	BA	782	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	1676	A	C5-C6-N1	6.87	121.13	117.70
55	BB	29	A	C4-C5-C6	-6.87	113.57	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1496	C	N3-C2-O2	-6.87	117.09	121.90
22	A1	75	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1965	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	1476	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	2082	A	N1-C6-N6	-6.86	114.48	118.60
21	AA	533	A	N1-C6-N6	-6.86	114.48	118.60
32	BJ	37	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	1881	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2652	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	907	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1489	C	O4'-C1'-N1	6.86	113.69	108.20
54	BA	1566	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	1650	A	C4-C5-C6	-6.86	113.57	117.00
55	BB	58	A	C5-C6-N1	6.86	121.13	117.70
21	AA	13	U	C1'-O4'-C4'	-6.86	104.41	109.90
21	AA	496	A	N1-C6-N6	-6.86	114.48	118.60
21	AA	1046	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	910	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1247	A	C5-C6-N1	6.86	121.13	117.70
21	AA	228	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	612	C	N3-C2-O2	-6.86	117.10	121.90
22	A1	26	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	1350	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	839	U	O4'-C1'-N1	6.85	113.68	108.20
54	BA	1610	A	C1'-O4'-C4'	-6.85	104.42	109.90
54	BA	2386	A	C5-C6-N1	6.85	121.13	117.70
21	AA	192	A	C4-C5-C6	-6.85	113.57	117.00
21	AA	197	A	C5-C6-N1	6.85	121.13	117.70
54	BA	1746	A	C5-C6-N1	6.85	121.13	117.70
54	BA	1746	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	2015	A	C5-C6-N1	6.85	121.13	117.70
54	BA	2900	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	78	A	C4-C5-C6	-6.85	113.58	117.00
13	AN	61	ARG	NE-CZ-NH1	6.85	123.72	120.30
54	BA	1027	A	C5-C6-N1	6.85	121.12	117.70
54	BA	2327	A	C5-C6-N1	6.85	121.12	117.70
54	BA	2755	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	59	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	460	A	C5-C6-N1	6.85	121.12	117.70
54	BA	1918	A	C5-C6-N1	6.85	121.12	117.70
54	BA	2715	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	99	C	N3-C2-O2	-6.85	117.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	177	ARG	NE-CZ-NH1	6.85	123.72	120.30
54	BA	764	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	101	A	C5-C6-N1	6.84	121.12	117.70
21	AA	178	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	460	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1100	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1678	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1322	C	N3-C2-O2	-6.84	117.11	121.90
56	B5	12	ARG	NE-CZ-NH1	6.84	123.72	120.30
54	BA	270	A	C5-C6-N1	6.84	121.12	117.70
54	BA	951	C	O4'-C1'-N1	6.84	113.67	108.20
54	BA	1272	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2117	A	O4'-C1'-N9	6.84	113.67	108.20
21	AA	246	A	C5-C6-N1	6.84	121.12	117.70
21	AA	972	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	432	A	C5-C6-N1	6.84	121.12	117.70
55	BB	27	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	156	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	2535	G	N3-C2-N2	-6.84	115.11	119.90
9	AJ	45	ARG	NE-CZ-NH1	6.83	123.72	120.30
54	BA	497	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	637	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	1226	A	C5-C6-N1	6.83	121.12	117.70
21	AA	466	A	C4-C5-C6	-6.83	113.58	117.00
21	AA	860	A	C5-C6-N1	6.83	121.12	117.70
21	AA	932	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1081	A	C5-C6-N1	6.83	121.12	117.70
54	BA	905	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	2424	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	238	A	P-O3'-C3'	6.83	127.90	119.70
21	AA	347	G	C1'-O4'-C4'	-6.83	104.43	109.90
54	BA	2035	G	O4'-C1'-N9	6.83	113.67	108.20
21	AA	131	A	C5-C6-N1	6.83	121.11	117.70
54	BA	487	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	1020	A	C5-C6-N1	6.83	121.11	117.70
54	BA	1526	C	O4'-C1'-N1	6.83	113.66	108.20
54	BA	1677	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	435	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	1288	A	C5-C6-N1	6.83	121.11	117.70
54	BA	1393	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	1572	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	172	A	C4-C5-C6	-6.83	113.59	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	648	A	C5-C6-N1	6.83	121.11	117.70
54	BA	821	A	C5-C6-N1	6.83	121.11	117.70
54	BA	2433	A	C5-C6-N1	6.83	121.11	117.70
21	AA	408	A	C5-C6-N1	6.82	121.11	117.70
21	AA	583	A	C5-C6-N1	6.82	121.11	117.70
21	AA	1163	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	925	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1155	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2241	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2740	A	C5-C6-N1	6.82	121.11	117.70
21	AA	994	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1188	A	N1-C6-N6	-6.82	114.51	118.60
21	AA	1218	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	13	A	C5-C6-N1	6.82	121.11	117.70
55	BB	34	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	507	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	1194	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	2560	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	98	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	384	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1213	A	C5-C6-N1	6.82	121.11	117.70
21	AA	1299	A	C5-C6-N1	6.81	121.11	117.70
54	BA	2634	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	1439	A	C5-C6-N1	6.81	121.11	117.70
55	BB	52	A	C4-C5-C6	-6.81	113.59	117.00
21	AA	738	C	N3-C2-O2	-6.81	117.13	121.90
34	BL	48	ARG	NE-CZ-NH1	6.81	123.70	120.30
3	AD	164	ARG	NE-CZ-NH1	6.81	123.70	120.30
54	BA	1826	G	O4'-C1'-N9	6.81	113.65	108.20
54	BA	2507	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	16	A	C5-C6-N1	6.81	121.10	117.70
54	BA	1090	A	C4-C5-C6	-6.81	113.60	117.00
54	BA	2527	C	N3-C2-O2	-6.81	117.14	121.90
15	AP	5	ARG	NE-CZ-NH2	-6.81	116.90	120.30
54	BA	2716	C	O4'-C1'-N1	6.81	113.64	108.20
21	AA	974	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1169	A	N1-C6-N6	-6.80	114.52	118.60
21	AA	1410	A	C5-C6-N1	6.80	121.10	117.70
54	BA	10	A	C4-C5-C6	-6.80	113.60	117.00
2	AC	64	ARG	NE-CZ-NH2	-6.80	116.90	120.30
21	AA	1378	C	N3-C2-O2	-6.80	117.14	121.90
40	BR	13	ARG	NE-CZ-NH1	6.80	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	433	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	655	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1787	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2267	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	47	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	223	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1433	A	C5-C6-N1	6.80	121.10	117.70
55	BB	46	A	C5-C6-N1	6.80	121.10	117.70
54	BA	221	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	715	A	C4-C5-C6	-6.80	113.60	117.00
55	BB	59	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	781	A	C5-C6-N1	6.79	121.10	117.70
21	AA	1369	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	32	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	482	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	2403	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	2726	A	C5-C6-N1	6.79	121.10	117.70
21	AA	80	A	C4-C5-C6	-6.79	113.60	117.00
21	AA	472	U	C1'-O4'-C4'	-6.79	104.47	109.90
25	BC	176	ARG	NE-CZ-NH1	6.79	123.70	120.30
54	BA	1001	A	C5-C6-N1	6.79	121.10	117.70
54	BA	1064	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	1392	A	C5-C6-N1	6.79	121.10	117.70
54	BA	1584	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	2887	A	C4-C5-C6	-6.79	113.60	117.00
21	AA	1080	A	C5-C6-N1	6.79	121.09	117.70
54	BA	849	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	2281	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	1357	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	823	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	1433	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	2273	A	C5-C6-N1	6.79	121.09	117.70
21	AA	175	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	288	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	84	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1889	A	N1-C6-N6	-6.78	114.53	118.60
56	B5	134	ARG	NE-CZ-NH1	6.78	123.69	120.30
21	AA	906	A	N1-C6-N6	-6.78	114.53	118.60
21	AA	1374	A	C5-C6-N1	6.78	121.09	117.70
54	BA	466	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1244	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2752	C	N3-C2-O2	-6.78	117.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1169	A	C5-C6-N1	6.78	121.09	117.70
54	BA	705	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2335	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2602	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1004	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1051	C	N3-C2-O2	-6.78	117.15	121.90
24	A3	67	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	211	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	749	A	C5-C6-N1	6.78	121.09	117.70
21	AA	1066	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	1339	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2080	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	249	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	2014	A	N1-C6-N6	-6.78	114.53	118.60
21	AA	532	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	990	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2328	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	796	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	1500	A	C5-C6-N1	6.77	121.09	117.70
54	BA	650	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	900	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2510	C	O4'-C1'-N1	6.77	113.62	108.20
21	AA	1287	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	1494	A	C5-C6-N1	6.77	121.09	117.70
54	BA	1504	A	C4-C5-C6	-6.77	113.61	117.00
17	AR	72	ARG	NE-CZ-NH2	6.77	123.69	120.30
54	BA	1625	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	1635	A	C5-C6-N1	6.77	121.08	117.70
21	AA	345	C	N1-C2-O2	6.77	122.96	118.90
54	BA	278	A	C5-C6-N1	6.77	121.08	117.70
54	BA	706	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1700	A	C4-C5-C6	-6.77	113.62	117.00
54	BA	1912	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	1055	A	N1-C6-N6	-6.77	114.54	118.60
21	AA	1227	A	C5-C6-N1	6.77	121.08	117.70
21	AA	371	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	629	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	1102	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1276	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1772	A	C4-C5-C6	-6.76	113.62	117.00
55	BB	97	C	N3-C2-O2	-6.76	117.17	121.90
9	AJ	48	ARG	NE-CZ-NH2	-6.76	116.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2362	C	O4'-C1'-N1	6.76	113.61	108.20
21	AA	1257	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1437	A	C5-C6-N1	6.76	121.08	117.70
54	BA	423	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1359	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1509	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	334	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	694	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1012	A	C5-C6-N1	6.76	121.08	117.70
54	BA	320	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1054	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1200	C	O4'-C1'-N1	6.76	113.61	108.20
54	BA	1269	A	N1-C6-N6	-6.76	114.54	118.60
54	BA	1664	A	C5-C6-N1	6.76	121.08	117.70
21	AA	139	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	806	C	N3-C2-O2	-6.76	117.17	121.90
27	BE	21	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	2600	A	N1-C6-N6	-6.76	114.55	118.60
21	AA	374	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	893	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	817	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1114	C	N3-C2-O2	-6.76	117.17	121.90
55	BB	94	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1120	C	N3-C2-O2	-6.75	117.17	121.90
33	BK	78	ARG	NE-CZ-NH1	6.75	123.68	120.30
21	AA	451	A	C5-C6-N1	6.75	121.08	117.70
21	AA	968	A	O4'-C1'-N9	6.75	113.60	108.20
21	AA	578	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	579	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	1350	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1400	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	136	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	426	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	67	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	155	A	C5-C6-N1	6.75	121.07	117.70
54	BA	167	A	C5-C6-N1	6.75	121.07	117.70
54	BA	578	G	N3-C2-N2	-6.75	115.17	119.90
54	BA	917	A	C5-C6-N1	6.75	121.07	117.70
21	AA	25	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	192	A	C5-C6-N1	6.75	121.07	117.70
54	BA	21	A	C5-C6-N1	6.75	121.07	117.70
54	BA	439	A	N1-C6-N6	-6.75	114.55	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1987	A	C5-C6-N1	6.75	121.07	117.70
21	AA	81	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	1318	A	C5-C6-N1	6.74	121.07	117.70
54	BA	56	A	C5-C6-N1	6.74	121.07	117.70
54	BA	343	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1431	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1786	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2376	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2883	A	O4'-C1'-N9	6.74	113.59	108.20
8	AI	129	ARG	NE-CZ-NH2	6.74	123.67	120.30
21	AA	71	A	C5-C6-N1	6.74	121.07	117.70
21	AA	554	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1042	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1480	A	C5-C6-N1	6.74	121.07	117.70
24	A3	76	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	896	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2691	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	655	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1503	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	742	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1591	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2232	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	2577	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1285	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1632	A	C4-C5-C6	-6.74	113.63	117.00
23	A2	89	U	P-O3'-C3'	6.74	127.78	119.70
54	BA	544	C	N3-C2-O2	-6.74	117.19	121.90
54	BA	1868	C	N3-C2-O2	-6.74	117.19	121.90
24	A3	59	A	C5-C6-N1	6.73	121.07	117.70
21	AA	513	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	152	A	C5-C6-N1	6.73	121.07	117.70
21	AA	865	A	C5-C6-N1	6.73	121.06	117.70
39	BQ	32	ARG	NE-CZ-NH2	6.73	123.67	120.30
54	BA	2589	A	C4-C5-C6	-6.73	113.64	117.00
21	AA	349	A	C5-C6-N1	6.73	121.06	117.70
54	BA	99	U	N3-C2-O2	-6.73	117.49	122.20
54	BA	176	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	955	U	O4'-C1'-N1	6.73	113.58	108.20
54	BA	1591	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	2530	A	C5-C6-N1	6.73	121.06	117.70
21	AA	816	A	C5-C6-N1	6.73	121.06	117.70
54	BA	1276	A	C5-C6-N1	6.73	121.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	673	A	C5-C6-N1	6.72	121.06	117.70
21	AA	880	C	N3-C2-O2	-6.72	117.19	121.90
37	BO	25	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	586	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1465	G	N1-C6-O6	-6.72	115.87	119.90
54	BA	2366	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	2634	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2808	G	N3-C2-N2	-6.72	115.19	119.90
55	BB	101	A	C5-C6-N1	6.72	121.06	117.70
21	AA	944	G	P-O3'-C3'	6.72	127.77	119.70
54	BA	95	A	C5-C6-N1	6.72	121.06	117.70
54	BA	374	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2766	A	N1-C6-N6	-6.72	114.57	118.60
21	AA	270	A	C5-C6-N1	6.72	121.06	117.70
21	AA	313	A	C5-C6-N1	6.72	121.06	117.70
54	BA	644	A	C5-C6-N1	6.72	121.06	117.70
54	BA	1284	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2417	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	718	A	C5-C6-N1	6.72	121.06	117.70
54	BA	1070	A	O4'-C1'-N9	6.72	113.57	108.20
54	BA	1265	A	N1-C6-N6	-6.72	114.57	118.60
21	AA	1384	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	2291	U	O4'-C1'-N1	6.72	113.57	108.20
28	BF	111	ARG	NE-CZ-NH1	6.71	123.66	120.30
25	BC	132	ARG	NE-CZ-NH1	6.71	123.66	120.30
54	BA	1167	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	816	A	N1-C6-N6	-6.71	114.57	118.60
21	AA	1188	A	C5-C6-N1	6.71	121.06	117.70
54	BA	53	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1858	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2468	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	399	U	O4'-C1'-N1	6.71	113.57	108.20
54	BA	415	A	C5-C6-N1	6.71	121.06	117.70
54	BA	765	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1532	A	C4-C5-C6	-6.71	113.64	117.00
21	AA	1176	A	C5-C6-N1	6.71	121.05	117.70
54	BA	428	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	584	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1073	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1169	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	1919	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2179	C	N3-C2-O2	-6.71	117.20	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2243	U	O4'-C1'-N1	6.71	113.57	108.20
55	BB	89	U	O4'-C1'-N1	6.71	113.57	108.20
13	AN	65	ARG	NE-CZ-NH1	6.71	123.65	120.30
54	BA	422	A	C5-C6-N1	6.71	121.05	117.70
54	BA	575	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1006	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1802	A	N1-C6-N6	-6.71	114.58	118.60
54	BA	2590	A	N1-C6-N6	-6.71	114.58	118.60
22	A1	6	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	1350	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	1376	U	C1'-O4'-C4'	-6.70	104.54	109.90
54	BA	515	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1095	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1363	C	N3-C2-O2	-6.70	117.21	121.90
55	BB	43	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	574	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1664	A	C4-C5-C6	-6.70	113.65	117.00
32	BJ	27	ARG	NE-CZ-NH1	6.70	123.65	120.30
54	BA	1966	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	648	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	1069	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	1082	A	C5-C6-N1	6.70	121.05	117.70
44	BV	93	ARG	NE-CZ-NH1	6.70	123.65	120.30
47	BY	23	ARG	NE-CZ-NH1	6.70	123.65	120.30
54	BA	609	A	C5-C6-N1	6.70	121.05	117.70
54	BA	821	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2733	A	N1-C6-N6	-6.70	114.58	118.60
51	B2	33	ARG	NE-CZ-NH1	6.70	123.65	120.30
54	BA	281	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	1282	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1598	A	C5-C6-N1	6.70	121.05	117.70
21	AA	896	C	N3-C2-O2	-6.69	117.21	121.90
21	AA	253	A	C4-C5-C6	-6.69	113.65	117.00
21	AA	936	C	O4'-C1'-N1	6.69	113.55	108.20
21	AA	1413	A	C5-C6-N1	6.69	121.05	117.70
54	BA	352	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	668	A	C5-C6-N1	6.69	121.05	117.70
54	BA	2377	A	C4-C5-C6	-6.69	113.65	117.00
55	BB	8	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	238	A	C4-C5-C6	-6.69	113.66	117.00
22	A1	76	A	O4'-C1'-N9	6.69	113.55	108.20
54	BA	2207	C	N3-C2-O2	-6.69	117.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2486	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	92	U	O4'-C1'-N1	6.69	113.55	108.20
54	BA	1556	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	629	A	C5-C6-N1	6.69	121.04	117.70
21	AA	1502	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	201	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2025	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2675	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	2723	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2170	A	C5-C6-N1	6.69	121.04	117.70
54	BA	2234	G	O4'-C1'-N9	6.69	113.55	108.20
55	BB	42	C	N3-C2-O2	-6.69	117.22	121.90
55	BB	94	A	C4-C5-C6	-6.69	113.66	117.00
23	A2	91	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	2654	A	C5-C6-N1	6.68	121.04	117.70
21	AA	40	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	815	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	517	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1522	A	C4-C5-C6	-6.68	113.66	117.00
24	A3	14	A	C5-C6-N1	6.68	121.04	117.70
54	BA	795	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	1100	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1077	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	2840	C	N3-C2-O2	-6.68	117.22	121.90
8	AI	11	ARG	NE-CZ-NH2	-6.68	116.96	120.30
54	BA	1028	A	C4-C5-C6	-6.68	113.66	117.00
21	AA	681	A	C4-C5-C6	-6.68	113.66	117.00
21	AA	825	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1816	C	N3-C2-O2	-6.68	117.23	121.90
54	BA	2020	A	N1-C6-N6	-6.68	114.59	118.60
21	AA	1534	A	O4'-C1'-N9	6.67	113.54	108.20
36	BN	30	ARG	NE-CZ-NH2	-6.67	116.96	120.30
54	BA	737	C	O4'-C1'-N1	6.67	113.54	108.20
21	AA	564	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	687	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	1152	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	1314	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2594	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	459	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	790	A	N1-C6-N6	-6.67	114.60	118.60
26	BD	59	ARG	NE-CZ-NH1	6.67	123.63	120.30
54	BA	849	A	C5-C6-N1	6.67	121.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1209	U	C5'-C4'-O4'	6.67	117.10	109.10
54	BA	1382	G	C5'-C4'-C3'	-6.67	105.33	116.00
54	BA	2225	A	C5-C6-N1	6.67	121.03	117.70
54	BA	1513	U	O4'-C1'-N1	6.67	113.53	108.20
54	BA	1784	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	580	C	N3-C2-O2	-6.67	117.23	121.90
25	BC	181	ARG	NE-CZ-NH1	6.67	123.63	120.30
21	AA	130	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	256	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1385	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1477	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1535	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1890	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2088	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2411	A	C5-C6-N1	6.66	121.03	117.70
21	AA	649	A	N1-C6-N6	-6.66	114.60	118.60
21	AA	1210	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1447	A	O4'-C1'-N9	6.66	113.53	108.20
21	AA	58	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	129	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	1197	A	C5-C6-N1	6.66	121.03	117.70
54	BA	5	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	678	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1144	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2565	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	672	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1985	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	371	A	C5-C6-N1	6.66	121.03	117.70
21	AA	1063	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1389	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	56	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	634	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1708	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	2131	U	O4'-C1'-N1	6.66	113.53	108.20
54	BA	2628	C	N1-C2-O2	6.66	122.89	118.90
55	BB	62	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	309	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1583	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1837	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	2510	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	766	A	C5-C6-N1	6.65	121.03	117.70
54	BA	716	A	C5-C6-N1	6.65	121.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1080	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	2558	C	N3-C2-O2	-6.65	117.24	121.90
55	BB	50	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	520	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	1204	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	1076	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1305	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1612	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	634	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1172	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1173	U	O4'-C1'-N1	6.65	113.52	108.20
54	BA	2101	A	C5-C6-N1	6.65	121.03	117.70
54	BA	296	U	O4'-C1'-N1	6.65	113.52	108.20
54	BA	1175	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	1178	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	2173	A	C5-C6-N1	6.65	121.02	117.70
21	AA	1368	A	C5-C6-N1	6.65	121.02	117.70
54	BA	1677	A	C5-C6-N1	6.65	121.02	117.70
21	AA	336	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	1093	A	C4-C5-C6	-6.64	113.68	117.00
51	B2	39	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	1611	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	189	A	C5-C6-N1	6.64	121.02	117.70
21	AA	280	C	N1-C2-O2	6.64	122.89	118.90
21	AA	330	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	519	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	1183	U	C1'-O4'-C4'	-6.64	104.59	109.90
21	AA	1329	A	C5-C6-N1	6.64	121.02	117.70
21	AA	1510	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	48	C	N1-C2-O2	6.64	122.88	118.90
21	AA	156	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	1413	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1698	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	432	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1893	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2166	U	O4'-C1'-N1	6.64	113.51	108.20
54	BA	2359	C	N3-C2-O2	-6.64	117.25	121.90
25	BC	47	ARG	NE-CZ-NH1	6.63	123.62	120.30
54	BA	451	U	C1'-O4'-C4'	-6.63	104.59	109.90
54	BA	1048	A	C4-C5-C6	-6.63	113.68	117.00
54	BA	1773	A	C5-C6-N1	6.63	121.02	117.70
21	AA	419	C	N3-C2-O2	-6.63	117.26	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	937	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	1306	A	N1-C6-N6	-6.63	114.62	118.60
45	BW	24	ARG	NE-CZ-NH1	6.63	123.62	120.30
54	BA	97	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1039	A	C4-C5-C6	-6.63	113.68	117.00
54	BA	1417	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1793	C	N3-C2-O2	-6.63	117.26	121.90
19	AT	59	ARG	NE-CZ-NH2	6.63	123.61	120.30
35	BM	6	ARG	NE-CZ-NH2	6.63	123.61	120.30
54	BA	173	A	C4-C5-C6	-6.63	113.69	117.00
24	A3	3	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	231	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	767	U	O4'-C1'-N1	6.63	113.50	108.20
54	BA	1548	A	C5-C6-N1	6.63	121.01	117.70
54	BA	1892	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	2278	A	C5-C6-N1	6.63	121.01	117.70
54	BA	2601	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	1150	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	2154	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	478	A	C5-C6-N1	6.62	121.01	117.70
54	BA	19	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1738	G	O4'-C1'-N9	6.62	113.50	108.20
54	BA	2088	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	2135	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2471	A	C4-C5-C6	-6.62	113.69	117.00
8	AI	10	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	53	A	C5-C6-N1	6.62	121.01	117.70
22	A1	31	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	565	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1293	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1805	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1810	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1854	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2600	A	C5-C6-N1	6.62	121.01	117.70
21	AA	574	A	N1-C6-N6	-6.62	114.63	118.60
21	AA	1466	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	57	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1247	A	N1-C6-N6	-6.62	114.63	118.60
54	BA	1764	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	115	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1508	A	C5-C6-N1	6.61	121.01	117.70
54	BA	1541	C	N3-C2-O2	-6.61	117.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2077	A	C5-C6-N1	6.61	121.01	117.70
54	BA	661	A	C5-C6-N1	6.61	121.01	117.70
54	BA	666	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1836	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	310	A	C5-C6-N1	6.61	121.00	117.70
54	BA	540	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1067	A	C4-C5-C6	-6.61	113.69	117.00
21	AA	1277	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	352	A	C5-C6-N1	6.61	121.00	117.70
54	BA	501	A	N1-C6-N6	-6.61	114.64	118.60
54	BA	1713	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	32	A	N1-C6-N6	-6.60	114.64	118.60
21	AA	478	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1605	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	309	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1932	A	C5-C6-N1	6.60	121.00	117.70
54	BA	38	A	C5-C6-N1	6.60	121.00	117.70
54	BA	264	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1241	A	O4'-C1'-N9	6.60	113.48	108.20
54	BA	2054	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	2650	U	O4'-C1'-N1	6.60	113.48	108.20
21	AA	1261	A	C5-C6-N1	6.60	121.00	117.70
54	BA	270	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	825	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1274	A	N1-C6-N6	-6.59	114.64	118.60
54	BA	1606	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	1670	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	2261	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	1290	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	2879	A	O4'-C1'-N9	6.59	113.47	108.20
21	AA	179	A	C5-C6-N1	6.59	121.00	117.70
54	BA	47	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	52	A	C5-C6-N1	6.59	121.00	117.70
54	BA	299	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	735	A	C5-C6-N1	6.59	121.00	117.70
54	BA	945	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1127	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	1456	A	C5-C6-N1	6.59	121.00	117.70
54	BA	351	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1593	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1981	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	2717	C	N3-C2-O2	-6.59	117.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	373	A	C4-C5-C6	-6.59	113.71	117.00
54	BA	1416	G	O4'-C1'-N9	6.59	113.47	108.20
54	BA	2198	A	O4'-C1'-N9	6.59	113.47	108.20
54	BA	2774	C	O4'-C1'-N1	6.59	113.47	108.20
55	BB	115	A	C5-C6-N1	6.59	120.99	117.70
54	BA	1214	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	2432	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1363	A	C4-C5-C6	-6.58	113.71	117.00
35	BM	51	ARG	NE-CZ-NH1	6.58	123.59	120.30
51	B2	14	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	2632	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	171	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1022	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2227	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	264	C	N3-C2-O2	-6.58	117.30	121.90
21	AA	600	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	964	A	C5-C6-N1	6.58	120.99	117.70
54	BA	671	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	2283	C	O4'-C1'-N1	6.58	113.46	108.20
21	AA	279	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	936	C	N3-C2-O2	-6.58	117.30	121.90
24	A3	39	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	792	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1404	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1803	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2326	C	N3-C2-O2	-6.58	117.30	121.90
40	BR	80	ARG	NE-CZ-NH1	6.57	123.59	120.30
54	BA	1549	A	C4-C5-C6	-6.57	113.71	117.00
17	AR	63	TYR	CB-CG-CD1	-6.57	117.06	121.00
21	AA	77	A	C5-C6-N1	6.57	120.98	117.70
24	A3	36	A	C5-C6-N1	6.57	120.98	117.70
24	A3	63	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	596	U	O4'-C1'-N1	6.57	113.46	108.20
54	BA	1084	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2738	A	N1-C6-N6	-6.57	114.66	118.60
21	AA	83	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	60	A	C5-C6-N1	6.57	120.98	117.70
21	AA	329	A	N1-C6-N6	-6.57	114.66	118.60
21	AA	784	A	C5-C6-N1	6.57	120.98	117.70
21	AA	908	A	C5-C6-N1	6.57	120.98	117.70
21	AA	1511	G	N1-C6-O6	-6.57	115.96	119.90
54	BA	127	A	C5-C6-N1	6.57	120.98	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	635	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1084	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	1104	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1925	C	N3-C2-O2	-6.57	117.30	121.90
55	BB	34	A	C5-C6-N1	6.57	120.98	117.70
54	BA	1788	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2322	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2368	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	1228	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2000	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	23	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	193	C	N3-C2-O2	-6.56	117.31	121.90
42	BT	77	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	1051	G	O4'-C1'-N9	6.56	113.45	108.20
54	BA	2073	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	613	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2332	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2374	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2753	A	C5-C6-N1	6.56	120.98	117.70
25	BC	79	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	183	C	O4'-C1'-N1	6.56	113.45	108.20
54	BA	1246	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	1960	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2581	G	O4'-C1'-N9	6.56	113.45	108.20
54	BA	2764	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1944	U	O4'-C1'-N1	6.56	113.44	108.20
21	AA	489	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1281	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1341	U	O4'-C1'-N1	6.55	113.44	108.20
54	BA	748	G	C1'-O4'-C4'	-6.55	104.66	109.90
54	BA	1057	A	C5-C6-N1	6.55	120.98	117.70
54	BA	2589	A	C5-C6-N1	6.55	120.98	117.70
54	BA	2522	U	O4'-C1'-N1	6.55	113.44	108.20
21	AA	206	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	422	C	N3-C2-O2	-6.55	117.32	121.90
21	AA	1289	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	1360	A	C4-C5-C6	-6.55	113.73	117.00
48	BZ	30	ARG	NE-CZ-NH1	6.55	123.58	120.30
54	BA	346	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	1121	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2362	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2827	C	N3-C2-O2	-6.55	117.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1262	A	C5-C6-N1	6.55	120.97	117.70
54	BA	1796	U	O4'-C1'-N1	6.55	113.44	108.20
54	BA	2566	A	C4-C5-C6	-6.55	113.73	117.00
21	AA	338	A	C5-C6-N1	6.55	120.97	117.70
24	A3	70	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	216	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	2517	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	680	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	728	A	C4-C5-C6	-6.54	113.73	117.00
37	BO	25	ARG	NE-CZ-NH2	-6.54	117.03	120.30
54	BA	1085	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1819	A	C5-C6-N1	6.54	120.97	117.70
21	AA	1042	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1233	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1739	A	C5-C6-N1	6.54	120.97	117.70
54	BA	791	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1752	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	715	A	C5-C6-N1	6.54	120.97	117.70
21	AA	1113	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1914	C	N1-C2-O2	6.54	122.82	118.90
54	BA	2050	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	523	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	655	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	840	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	1634	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1652	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	119	A	C5-C6-N1	6.53	120.97	117.70
21	AA	234	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1155	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	251	A	C5-C6-N1	6.53	120.97	117.70
54	BA	854	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	675	A	C4-C5-C6	-6.53	113.73	117.00
21	AA	844	G	N3-C2-N2	-6.53	115.33	119.90
21	AA	1161	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1519	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	345	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	1260	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	1347	A	C5-C6-N1	6.53	120.97	117.70
54	BA	2119	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	177	G	O4'-C1'-N9	6.53	113.42	108.20
54	BA	471	A	C5-C6-N1	6.53	120.96	117.70
54	BA	925	A	C4-C5-C6	-6.53	113.74	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1745	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	2381	A	C5-C6-N1	6.53	120.96	117.70
54	BA	2738	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	936	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	2369	A	C4-C5-C6	-6.53	113.74	117.00
21	AA	1434	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2837	A	C5-C6-N1	6.52	120.96	117.70
11	AL	113	ARG	NE-CZ-NH1	6.52	123.56	120.30
54	BA	492	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1825	U	O4'-C1'-N1	6.52	113.42	108.20
54	BA	2343	U	C3'-C2'-C1'	6.52	106.72	101.50
54	BA	2534	A	C5-C6-N1	6.52	120.96	117.70
54	BA	2699	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	1771	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	647	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	1285	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1327	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	1055	A	C5-C6-N1	6.52	120.96	117.70
21	AA	1479	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	743	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1313	U	N3-C2-O2	-6.52	117.64	122.20
54	BA	1438	U	O4'-C1'-N1	6.52	113.42	108.20
54	BA	2829	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	633	A	C5-C6-N1	6.52	120.96	117.70
41	BS	95	ARG	NE-CZ-NH1	6.51	123.56	120.30
54	BA	1575	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	2095	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	393	A	C5-C6-N1	6.51	120.96	117.70
11	AL	53	ARG	NE-CZ-NH1	6.51	123.56	120.30
54	BA	398	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	640	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	116	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	167	A	N1-C6-N6	-6.51	114.69	118.60
54	BA	439	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1205	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	2560	A	C5-C6-N1	6.51	120.95	117.70
54	BA	2882	A	C4-C5-C6	-6.51	113.75	117.00
21	AA	1418	A	C5-C6-N1	6.51	120.95	117.70
54	BA	274	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	2009	A	C5-C6-N1	6.51	120.95	117.70
21	AA	1158	C	N1-C2-O2	6.51	122.80	118.90
54	BA	943	A	C5-C6-N1	6.51	120.95	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	430	A	C5-C6-N1	6.50	120.95	117.70
22	A1	25	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2163	A	C5-C6-N1	6.50	120.95	117.70
21	AA	614	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	649	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1011	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1156	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2726	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	553	A	C5-C6-N1	6.50	120.95	117.70
21	AA	559	A	O4'-C1'-N9	6.50	113.40	108.20
54	BA	968	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1123	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	959	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1271	A	C5-C6-N1	6.50	120.95	117.70
54	BA	64	A	C5-C6-N1	6.50	120.95	117.70
54	BA	340	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	980	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2635	A	C4-C5-C6	-6.50	113.75	117.00
55	BB	59	A	C5-C6-N1	6.50	120.95	117.70
11	AL	30	ARG	NE-CZ-NH1	6.50	123.55	120.30
21	AA	475	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1490	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1561	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1901	A	C5-C6-N1	6.50	120.95	117.70
55	BB	66	A	C5-C6-N1	6.50	120.95	117.70
54	BA	447	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	595	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2767	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	63	C	N3-C2-O2	-6.49	117.35	121.90
54	BA	1304	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1526	C	N3-C2-O2	-6.49	117.35	121.90
54	BA	2020	A	C5-C6-N1	6.49	120.95	117.70
55	BB	101	A	N1-C6-N6	-6.49	114.70	118.60
21	AA	85	U	O4'-C1'-N1	6.49	113.39	108.20
22	A1	35	A	N1-C6-N6	-6.49	114.70	118.60
54	BA	1413	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1414	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1689	A	C5-C6-N1	6.49	120.95	117.70
21	AA	190	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	1236	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	898	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1165	A	C4-C5-C6	-6.49	113.75	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AD	110	ARG	NE-CZ-NH1	6.49	123.54	120.30
18	AS	4	LEU	C-N-CA	6.49	137.92	121.70
21	AA	353	A	O4'-C1'-N9	6.49	113.39	108.20
54	BA	6	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	1608	A	C5-C6-N1	6.49	120.94	117.70
54	BA	2071	A	C5-C6-N1	6.49	120.94	117.70
54	BA	2649	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	915	A	C4-C5-C6	-6.49	113.76	117.00
21	AA	1160	G	O4'-C1'-N9	6.49	113.39	108.20
54	BA	1134	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	1262	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	1711	A	C5-C6-N1	6.49	120.94	117.70
21	AA	10	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	327	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1571	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2700	A	C5-C6-N1	6.48	120.94	117.70
21	AA	694	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	1036	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1259	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1614	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2191	A	C4-C5-C6	-6.48	113.76	117.00
2	AC	142	ARG	NE-CZ-NH1	6.48	123.54	120.30
54	BA	1768	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1974	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1656	C	N3-C2-O2	-6.48	117.37	121.90
54	BA	1669	A	C4-C5-C6	-6.48	113.76	117.00
24	A3	14	A	N1-C6-N6	-6.48	114.71	118.60
21	AA	349	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	335	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	637	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	718	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	1032	G	O4'-C1'-N9	6.47	113.38	108.20
54	BA	528	A	C5-C6-N1	6.47	120.94	117.70
54	BA	959	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1617	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1947	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2020	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1005	C	C3'-C2'-C1'	6.47	106.68	101.50
54	BA	1461	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1502	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	2154	A	C5-C6-N1	6.47	120.94	117.70
54	BA	2681	C	N3-C2-O2	-6.47	117.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	609	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	402	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1040	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	2753	A	C4-C5-C6	-6.47	113.77	117.00
55	BB	104	A	C5-C6-N1	6.47	120.94	117.70
21	AA	18	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1150	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	412	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	366	C	O4'-C1'-N1	6.47	113.37	108.20
54	BA	449	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	1603	A	C5-C6-N1	6.47	120.93	117.70
54	BA	1639	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1926	U	O4'-C1'-N1	6.47	113.37	108.20
54	BA	2768	U	O4'-C1'-N1	6.47	113.37	108.20
55	BB	108	A	C5-C6-N1	6.47	120.93	117.70
21	AA	795	C	N1-C2-O2	6.46	122.78	118.90
49	B0	49	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	693	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1203	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1443	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	72	U	O4'-C1'-N1	6.46	113.37	108.20
54	BA	1385	A	O4'-C1'-N9	6.46	113.37	108.20
54	BA	2175	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1214	A	C5-C6-N1	6.46	120.93	117.70
21	AA	495	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1128	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1713	A	C5-C6-N1	6.46	120.93	117.70
21	AA	411	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1208	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1399	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	608	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	2047	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2266	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	2407	A	C5-C6-N1	6.46	120.93	117.70
55	BB	36	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	820	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1373	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1152	A	C5-C6-N1	6.45	120.93	117.70
21	AA	1180	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	655	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	1654	A	C5-C6-N1	6.45	120.93	117.70
55	BB	17	C	N3-C2-O2	-6.45	117.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	29	A	O4'-C1'-N9	6.45	113.36	108.20
15	AP	14	ARG	NE-CZ-NH1	6.45	123.53	120.30
21	AA	1274	A	C5-C6-N1	6.45	120.92	117.70
54	BA	244	A	C5-C6-N1	6.45	120.92	117.70
54	BA	645	C	N1-C2-O2	6.45	122.77	118.90
54	BA	661	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1291	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1821	A	C5-C6-N1	6.45	120.93	117.70
21	AA	28	A	C5-C6-N1	6.45	120.92	117.70
54	BA	992	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1928	A	C5-C6-N1	6.45	120.92	117.70
54	BA	394	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1531	A	N1-C6-N6	-6.45	114.73	118.60
54	BA	734	A	C5-C6-N1	6.45	120.92	117.70
54	BA	2021	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	2539	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	435	A	C4-C5-C6	-6.44	113.78	117.00
55	BB	71	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	197	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	1213	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1404	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	383	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1078	U	N3-C2-O2	-6.44	117.69	122.20
54	BA	892	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1754	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2564	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	899	C	N3-C2-O2	-6.44	117.39	121.90
22	A1	11	C	N3-C2-O2	-6.44	117.39	121.90
34	BL	18	ARG	NE-CZ-NH1	6.44	123.52	120.30
21	AA	831	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	742	A	C4-C5-C6	-6.44	113.78	117.00
37	BO	94	ARG	NE-CZ-NH1	6.43	123.52	120.30
39	BQ	12	ARG	NE-CZ-NH2	6.43	123.52	120.30
21	AA	251	G	O4'-C1'-N9	6.43	113.34	108.20
21	AA	1045	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1307	A	C5-C6-N1	6.43	120.92	117.70
54	BA	2068	U	C1'-O4'-C4'	-6.43	104.75	109.90
54	BA	2205	A	C5-C6-N1	6.43	120.92	117.70
55	BB	15	A	O4'-C1'-N9	6.43	113.35	108.20
1	AB	62	ARG	NE-CZ-NH1	6.43	123.52	120.30
54	BA	357	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	668	A	C4-C5-C6	-6.43	113.78	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1452	G	N1-C6-O6	-6.43	116.04	119.90
54	BA	2273	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	2521	C	N3-C2-O2	-6.43	117.40	121.90
19	AT	17	ARG	NE-CZ-NH1	6.43	123.52	120.30
21	AA	54	C	N3-C2-O2	-6.43	117.40	121.90
27	BE	79	ARG	NE-CZ-NH1	6.43	123.52	120.30
54	BA	1888	G	O4'-C1'-N9	6.43	113.34	108.20
21	AA	560	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	595	A	C5-C6-N1	6.43	120.91	117.70
21	AA	1286	U	N3-C2-O2	-6.43	117.70	122.20
54	BA	1045	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	739	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	181	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	627	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2006	C	N3-C2-O2	-6.42	117.40	121.90
54	BA	1772	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2196	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	215	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1524	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1569	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1675	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	767	A	C5-C6-N1	6.42	120.91	117.70
21	AA	316	C	O4'-C1'-N1	6.42	113.33	108.20
21	AA	768	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	62	U	C1'-O4'-C4'	-6.41	104.77	109.90
54	BA	157	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1044	C	O4'-C1'-N1	6.41	113.33	108.20
54	BA	1571	A	C4-C5-C6	-6.41	113.79	117.00
55	BB	15	A	C4-C5-C6	-6.41	113.79	117.00
21	AA	743	A	N1-C6-N6	-6.41	114.75	118.60
21	AA	143	A	N1-C6-N6	-6.41	114.75	118.60
54	BA	227	A	C5-C6-N1	6.41	120.91	117.70
54	BA	1674	G	C3'-C2'-C1'	6.41	106.63	101.50
54	BA	404	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2033	A	C5-C6-N1	6.41	120.90	117.70
21	AA	44	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	431	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1674	G	N1-C6-O6	-6.41	116.06	119.90
21	AA	1117	A	C5-C6-N1	6.41	120.90	117.70
54	BA	1404	C	O4'-C1'-N1	6.41	113.33	108.20
54	BA	2170	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2703	C	O4'-C1'-N1	6.41	113.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	941	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1446	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1998	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	2403	C	O4'-C1'-N1	6.40	113.32	108.20
21	AA	421	U	O4'-C1'-N1	6.40	113.32	108.20
54	BA	109	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	354	A	C5-C6-N1	6.40	120.90	117.70
21	AA	952	U	O4'-C1'-N1	6.40	113.32	108.20
54	BA	322	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	74	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	1327	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	173	A	C5-C6-N1	6.40	120.90	117.70
54	BA	1330	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2795	C	N3-C2-O2	-6.40	117.42	121.90
24	A3	74	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1169	A	C5-C6-N1	6.40	120.90	117.70
54	BA	1287	A	C5-C6-N1	6.40	120.90	117.70
24	A3	17	C	N3-C2-O2	-6.39	117.42	121.90
24	A3	36	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	888	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	1385	A	C5-C6-N1	6.39	120.90	117.70
54	BA	2176	A	N1-C6-N6	-6.39	114.76	118.60
54	BA	2534	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	1296	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	603	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	1399	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	2761	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	1274	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	2443	C	N3-C2-O2	-6.39	117.43	121.90
3	AD	55	ARG	NE-CZ-NH1	6.39	123.49	120.30
54	BA	833	A	C5-C6-N1	6.39	120.89	117.70
54	BA	1396	U	O4'-C1'-N1	6.39	113.31	108.20
54	BA	1759	A	C4-C5-C6	-6.39	113.81	117.00
37	BO	111	ARG	NE-CZ-NH1	6.39	123.49	120.30
54	BA	182	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	240	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	692	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1140	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2287	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2406	A	C5-C6-N1	6.39	120.89	117.70
55	BB	73	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	111	A	C4-C5-C6	-6.38	113.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2453	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	2646	C	O4'-C1'-N1	6.38	113.31	108.20
21	AA	708	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	328	U	O4'-C1'-N1	6.38	113.31	108.20
54	BA	1548	A	C4-C5-C6	-6.38	113.81	117.00
24	A3	48	U	O4'-C1'-N1	6.38	113.31	108.20
39	BQ	27	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BA	118	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	529	A	C5-C6-N1	6.38	120.89	117.70
54	BA	610	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2350	C	O4'-C1'-N1	6.38	113.30	108.20
21	AA	448	A	C5-C6-N1	6.38	120.89	117.70
21	AA	883	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	1035	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	861	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1264	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1729	U	N3-C2-O2	-6.38	117.73	122.20
54	BA	1744	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2456	C	N3-C2-O2	-6.38	117.44	121.90
20	AU	32	ARG	NE-CZ-NH1	6.38	123.49	120.30
21	AA	873	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	278	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	716	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	621	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	226	A	C5-C6-N1	6.38	120.89	117.70
54	BA	125	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	183	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	209	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1349	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2051	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2462	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2547	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2800	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	572	A	C5-C6-N1	6.37	120.89	117.70
54	BA	1284	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2019	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	393	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	1367	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2425	A	C5-C6-N1	6.37	120.89	117.70
21	AA	176	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1171	A	C4-C5-C6	-6.37	113.82	117.00
26	BD	179	ARG	NE-CZ-NH1	6.37	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	301	G	O4'-C1'-N9	6.37	113.30	108.20
54	BA	675	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	685	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	1014	A	N1-C6-N6	-6.37	114.78	118.60
54	BA	1668	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	1760	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	412	A	N1-C6-N6	-6.37	114.78	118.60
54	BA	680	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1126	A	C4-C5-C6	-6.37	113.82	117.00
21	AA	1427	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	699	A	C5-C6-N1	6.36	120.88	117.70
54	BA	761	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1920	C	N3-C2-O2	-6.36	117.44	121.90
54	BA	418	C	O4'-C1'-N1	6.36	113.29	108.20
54	BA	1952	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2712	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	248	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	1246	A	C5-C6-N1	6.36	120.88	117.70
54	BA	676	A	C5-C6-N1	6.36	120.88	117.70
54	BA	819	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1392	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1419	A	C5-C6-N1	6.36	120.88	117.70
54	BA	73	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2037	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2103	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	507	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	623	C	N3-C2-O2	-6.36	117.45	121.90
22	A1	71	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1289	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1437	C	O4'-C1'-N1	6.36	113.28	108.20
54	BA	2590	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	917	A	N1-C6-N6	-6.36	114.79	118.60
54	BA	1987	A	C4-C5-C6	-6.36	113.82	117.00
56	B5	71	ARG	NE-CZ-NH1	6.36	123.48	120.30
24	A3	72	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	1810	A	N1-C6-N6	-6.35	114.79	118.60
54	BA	2099	U	N3-C2-O2	-6.35	117.75	122.20
54	BA	2469	A	C4-C5-C6	-6.35	113.82	117.00
55	BB	77	U	O4'-C1'-N1	6.35	113.28	108.20
24	A3	58	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	2476	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	2874	C	N3-C2-O2	-6.35	117.45	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	781	A	N1-C6-N6	-6.35	114.79	118.60
22	A1	73	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	145	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	653	U	N3-C2-O2	-6.35	117.75	122.20
54	BA	788	A	C5-C6-N1	6.35	120.87	117.70
21	AA	186	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	282	A	C5-C6-N1	6.35	120.87	117.70
21	AA	1179	A	C5-C6-N1	6.35	120.87	117.70
54	BA	2564	A	C5-C6-N1	6.35	120.87	117.70
21	AA	1248	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	1531	A	C5-C6-N1	6.35	120.87	117.70
54	BA	1428	C	O4'-C1'-N1	6.35	113.28	108.20
21	AA	132	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	236	A	N1-C6-N6	-6.34	114.79	118.60
21	AA	263	A	C4-C5-C6	-6.34	113.83	117.00
38	BP	102	ARG	NE-CZ-NH1	6.34	123.47	120.30
54	BA	1197	G	O4'-C1'-N9	6.34	113.28	108.20
54	BA	1208	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	478	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1142	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	1303	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1536	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1801	A	C5-C6-N1	6.34	120.87	117.70
54	BA	63	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	265	A	O4'-C1'-N9	6.34	113.27	108.20
54	BA	2077	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	1146	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	462	C	N3-C2-O2	-6.34	117.47	121.90
54	BA	504	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1278	C	O4'-C1'-N1	6.34	113.27	108.20
54	BA	1395	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	831	A	C5-C6-N1	6.33	120.87	117.70
21	AA	1329	A	C4-C5-C6	-6.33	113.83	117.00
25	BC	176	ARG	NE-CZ-NH2	-6.33	117.13	120.30
54	BA	1626	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	882	C	N3-C2-O2	-6.33	117.47	121.90
22	A1	48	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	233	A	C5-C6-N1	6.33	120.87	117.70
54	BA	2381	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	1143	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	1189	A	C5-C6-N1	6.33	120.86	117.70
54	BA	1268	A	C4-C5-C6	-6.33	113.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2902	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	328	C	N1-C2-O2	6.33	122.70	118.90
21	AA	374	A	C5-C6-N1	6.33	120.86	117.70
54	BA	105	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	582	A	C5-C6-N1	6.33	120.86	117.70
54	BA	2435	A	C5-C6-N1	6.33	120.86	117.70
21	AA	676	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	914	G	O4'-C1'-N9	6.33	113.26	108.20
54	BA	1285	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	2270	A	C5-C6-N1	6.33	120.86	117.70
55	BB	108	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	1462	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1889	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	2442	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	719	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1749	A	C5-C6-N1	6.33	120.86	117.70
54	BA	1843	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1977	A	C5-C6-N1	6.33	120.86	117.70
54	BA	2873	A	C5-C6-N1	6.33	120.86	117.70
2	AC	155	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	1172	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	510	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	670	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1288	G	N1-C6-O6	-6.32	116.11	119.90
54	BA	1565	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	1785	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2420	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	2459	A	N1-C6-N6	-6.32	114.81	118.60
54	BA	2497	A	C4-C5-C6	-6.32	113.84	117.00
10	AK	68	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	50	A	C5-C6-N1	6.32	120.86	117.70
24	A3	16	C	N3-C2-O2	-6.32	117.47	121.90
21	AA	207	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	624	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	844	A	C5-C6-N1	6.32	120.86	117.70
17	AR	62	ARG	NE-CZ-NH2	-6.32	117.14	120.30
54	BA	190	A	C5-C6-N1	6.32	120.86	117.70
21	AA	1110	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	353	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1769	U	O4'-C1'-N1	6.31	113.25	108.20
21	AA	498	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	1429	A	C5-C6-N1	6.31	120.86	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	21	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1044	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1353	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	31	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	418	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	539	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	557	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	599	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2197	U	O4'-C1'-N1	6.31	113.25	108.20
54	BA	1128	G	N3-C2-N2	-6.30	115.49	119.90
54	BA	1267	U	O4'-C1'-N1	6.30	113.24	108.20
21	AA	162	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1152	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2038	G	N1-C6-O6	-6.30	116.12	119.90
54	BA	2766	A	C4-C5-C6	-6.30	113.85	117.00
19	AT	9	ARG	NE-CZ-NH1	6.30	123.45	120.30
21	AA	1346	A	C4-C5-C6	-6.30	113.85	117.00
24	A3	11	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2163	A	O4'-C1'-N9	6.30	113.24	108.20
54	BA	2264	C	N3-C2-O2	-6.30	117.49	121.90
22	A1	27	C	N3-C2-O2	-6.30	117.49	121.90
41	BS	8	ARG	NE-CZ-NH1	6.30	123.45	120.30
54	BA	353	C	O4'-C1'-N1	6.30	113.24	108.20
54	BA	414	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	995	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	309	A	C5-C6-N1	6.30	120.85	117.70
21	AA	1502	A	O4'-C1'-N9	6.30	113.24	108.20
54	BA	2725	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	436	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1221	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1665	A	C5-C6-N1	6.30	120.85	117.70
21	AA	1317	C	N1-C2-O2	6.29	122.68	118.90
54	BA	1398	C	C3'-C2'-C1'	6.29	106.54	101.50
54	BA	1347	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	1871	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	1927	A	C5-C6-N1	6.29	120.85	117.70
22	A1	14	A	C5-C6-N1	6.29	120.84	117.70
54	BA	262	A	C5-C6-N1	6.29	120.85	117.70
54	BA	973	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	13	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	2031	A	C1'-O4'-C4'	-6.29	104.87	109.90
21	AA	179	A	C4-C5-C6	-6.29	113.86	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	262	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	356	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	126	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1388	G	O4'-C1'-N9	6.29	113.23	108.20
54	BA	1692	U	O4'-C1'-N1	6.29	113.23	108.20
55	BB	113	C	N3-C2-O2	-6.29	117.50	121.90
1	AB	94	ARG	NE-CZ-NH1	6.29	123.44	120.30
21	AA	1325	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	8	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	270	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1226	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	2288	A	C4-C5-C6	-6.29	113.86	117.00
22	A1	23	A	C4-C5-C6	-6.28	113.86	117.00
34	BL	60	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	265	A	N1-C6-N6	-6.28	114.83	118.60
54	BA	601	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	362	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	804	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1321	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2354	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1408	A	C4-C5-C6	-6.28	113.86	117.00
39	BQ	63	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	918	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1362	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1934	C	O4'-C1'-N1	6.28	113.22	108.20
18	AS	31	ARG	NE-CZ-NH1	6.28	123.44	120.30
26	BD	46	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	41	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	61	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	1117	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	1905	C	N3-C2-O2	-6.28	117.51	121.90
21	AA	573	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	779	C	N1-C2-O2	6.28	122.67	118.90
21	AA	1109	C	N1-C2-O2	6.28	122.67	118.90
31	BI	133	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	1686	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	780	A	C4-C5-C6	-6.27	113.86	117.00
39	BQ	52	ARG	NE-CZ-NH1	6.27	123.44	120.30
54	BA	2226	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	395	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1032	G	N1-C6-O6	-6.27	116.14	119.90
54	BA	1427	A	P-O3'-C3'	6.27	127.22	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2385	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	549	C	N1-C2-O2	6.27	122.66	118.90
21	AA	635	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	1260	A	C5-C6-N1	6.27	120.83	117.70
54	BA	1320	C	N1-C2-O2	6.27	122.66	118.90
54	BA	1706	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2657	A	C5-C6-N1	6.27	120.83	117.70
21	AA	545	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1451	C	N1-C2-O2	6.27	122.66	118.90
54	BA	2332	C	O4'-C1'-N1	6.27	113.21	108.20
54	BA	2395	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	645	C	O4'-C1'-N1	6.27	113.21	108.20
54	BA	2467	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1162	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	556	A	C5-C6-N1	6.26	120.83	117.70
54	BA	1370	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	308	C	N3-C2-O2	-6.26	117.52	121.90
50	B1	43	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	1158	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1940	U	C1'-O4'-C4'	-6.26	104.89	109.90
54	BA	1304	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2794	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2301	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2364	C	O4'-C1'-N1	6.26	113.21	108.20
54	BA	2480	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	1237	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	602	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1990	C	N3-C2-O2	-6.26	117.52	121.90
18	AS	80	ARG	NE-CZ-NH1	6.25	123.43	120.30
54	BA	199	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	213	A	C5-C6-N1	6.25	120.83	117.70
54	BA	1503	A	C5-C6-N1	6.25	120.83	117.70
54	BA	2787	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	312	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	414	A	C4-C5-C6	-6.25	113.88	117.00
22	A1	70	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	225	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1545	A	C5-C6-N1	6.25	120.83	117.70
54	BA	1943	U	N3-C2-O2	-6.25	117.82	122.20
54	BA	2001	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	1433	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	1507	A	C4-C5-C6	-6.25	113.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1525	A	C5-C6-N1	6.25	120.83	117.70
54	BA	1728	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	262	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	11	C	O4'-C1'-N1	6.25	113.20	108.20
54	BA	670	A	P-O3'-C3'	6.25	127.20	119.70
54	BA	2870	C	N3-C2-O2	-6.25	117.53	121.90
1	AB	138	ARG	NE-CZ-NH1	6.25	123.42	120.30
21	AA	756	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	439	A	C5-C6-N1	6.25	120.82	117.70
54	BA	479	A	C5-C6-N1	6.25	120.82	117.70
54	BA	508	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	620	G	N3-C4-C5	-6.25	125.48	128.60
54	BA	897	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1515	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1806	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	236	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	401	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	34	U	N3-C2-O2	-6.24	117.83	122.20
54	BA	348	A	C5-C6-N1	6.24	120.82	117.70
54	BA	454	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1382	G	O4'-C1'-N9	6.24	113.19	108.20
54	BA	1583	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	172	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1494	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1591	A	C1'-O4'-C4'	-6.24	104.91	109.90
54	BA	2300	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	6	G	N3-C2-N2	-6.24	115.53	119.90
21	AA	1407	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2178	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2188	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	2710	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	423	G	O4'-C1'-N9	6.24	113.19	108.20
21	AA	509	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1214	C	N1-C2-O2	6.24	122.64	118.90
54	BA	2439	A	O4'-C1'-N9	6.24	113.19	108.20
21	AA	1398	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1014	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1472	C	O4'-C1'-N1	6.24	113.19	108.20
54	BA	1998	A	C5-C6-N1	6.24	120.82	117.70
54	BA	2064	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1735	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2089	C	N3-C2-O2	-6.23	117.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	34	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	286	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	864	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	1059	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	525	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	807	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	1320	C	N3-C2-O2	-6.23	117.54	121.90
24	A3	29	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1415	U	O4'-C1'-N1	6.23	113.18	108.20
54	BA	1507	C	N3-C2-O2	-6.23	117.54	121.90
10	AK	12	ARG	NE-CZ-NH1	-6.23	117.19	120.30
54	BA	483	A	C5-C6-N1	6.23	120.81	117.70
54	BA	779	U	O4'-C1'-N1	6.23	113.18	108.20
54	BA	996	A	C4-C5-C6	-6.23	113.89	117.00
51	B2	12	ARG	NE-CZ-NH1	6.23	123.41	120.30
54	BA	523	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1069	C	O4'-C1'-N1	6.22	113.18	108.20
54	BA	238	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	330	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1312	U	P-O3'-C3'	6.22	127.17	119.70
54	BA	1585	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	1762	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	792	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1529	G	O4'-C1'-N9	6.22	113.18	108.20
54	BA	1866	A	C4-C5-C6	-6.22	113.89	117.00
24	A3	49	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2616	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	127	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	815	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1237	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1597	A	O4'-C1'-N9	6.22	113.18	108.20
54	BA	1908	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	267	C	N3-C2-O2	-6.22	117.55	121.90
25	BC	268	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	820	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	2883	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	167	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1250	A	C4-C5-C6	-6.22	113.89	117.00
28	BF	147	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	418	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2799	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1234	C	N3-C2-O2	-6.21	117.55	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1446	A	N1-C6-N6	-6.21	114.87	118.60
54	BA	89	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1705	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2347	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1012	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	933	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	972	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2222	C	O4'-C1'-N1	6.21	113.17	108.20
21	AA	744	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	846	G	C1'-O4'-C4'	-6.21	104.93	109.90
22	A1	70	C	P-O3'-C3'	6.21	127.15	119.70
54	BA	840	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	16	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	1105	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	461	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	679	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1027	C	N1-C2-O2	6.21	122.62	118.90
21	AA	1101	A	P-O3'-C3'	6.21	127.15	119.70
21	AA	1101	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	1429	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	124	G	N3-C2-N2	-6.21	115.55	119.90
54	BA	1447	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2352	A	C5-C6-N1	6.21	120.80	117.70
54	BA	2538	C	N3-C2-O2	-6.21	117.55	121.90
2	AC	125	ARG	NE-CZ-NH1	6.21	123.40	120.30
21	AA	817	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	314	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	964	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	1157	G	O4'-C1'-N9	6.21	113.17	108.20
54	BA	1983	G	N3-C2-N2	-6.21	115.56	119.90
12	AM	112	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	AA	1201	A	P-O3'-C3'	6.20	127.14	119.70
21	AA	1262	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1311	A	C5-C6-N1	6.20	120.80	117.70
21	AA	1501	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	604	G	C5'-C4'-O4'	6.20	116.55	109.10
54	BA	2059	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2426	A	C5-C6-N1	6.20	120.80	117.70
10	AK	127	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	BA	165	A	C5-C6-N1	6.20	120.80	117.70
54	BA	902	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1520	C	N3-C2-O2	-6.20	117.56	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1275	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1818	U	O4'-C1'-N1	6.20	113.16	108.20
21	AA	95	C	N3-C2-O2	-6.20	117.56	121.90
35	BM	59	ARG	NE-CZ-NH1	6.20	123.40	120.30
41	BS	18	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	BA	184	C	O4'-C1'-N1	6.20	113.16	108.20
54	BA	246	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	666	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1075	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1080	A	C5-C6-N1	6.20	120.80	117.70
54	BA	1969	A	C5-C6-N1	6.20	120.80	117.70
21	AA	1167	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1453	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	501	C	N1-C2-O2	6.20	122.62	118.90
21	AA	1319	A	C5-C6-N1	6.20	120.80	117.70
41	BS	11	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	BA	670	A	C5-C6-N1	6.20	120.80	117.70
54	BA	994	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	119	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	119	A	O4'-C1'-N9	6.19	113.16	108.20
54	BA	480	A	N1-C6-N6	-6.19	114.88	118.60
54	BA	2169	A	O4'-C1'-N9	6.19	113.16	108.20
21	AA	1248	A	C1'-O4'-C4'	-6.19	104.94	109.90
29	BG	169	ARG	NE-CZ-NH1	6.19	123.40	120.30
21	AA	1141	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1111	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	1970	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	1618	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	443	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1071	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1468	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	935	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	2558	C	O4'-C1'-N1	6.19	113.15	108.20
45	BW	74	LYS	C-N-CA	6.19	137.17	121.70
21	AA	1229	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	62	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	1978	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	123	U	C5'-C4'-C3'	-6.18	106.11	116.00
54	BA	269	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	758	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	761	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1070	A	C4-C5-C6	-6.18	113.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1240	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	1306	C	N3-C2-O2	-6.18	117.57	121.90
15	AP	70	ARG	NE-CZ-NH1	6.18	123.39	120.30
54	BA	609	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	735	C	N3-C2-O2	-6.18	117.57	121.90
22	A1	32	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	886	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2334	U	O4'-C1'-N1	6.18	113.14	108.20
22	A1	68	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	726	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1253	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	155	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	878	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	36	C	N3-C2-O2	-6.17	117.58	121.90
22	A1	41	A	C5-C6-N1	6.17	120.79	117.70
54	BA	282	A	C5-C6-N1	6.17	120.79	117.70
21	AA	52	C	N3-C2-O2	-6.17	117.58	121.90
39	BQ	2	ARG	NE-CZ-NH2	6.17	123.39	120.30
54	BA	957	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2165	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	893	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1996	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	272	C	N1-C2-O2	6.17	122.60	118.90
21	AA	1016	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	1196	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	384	A	C4-C5-C6	-6.17	113.92	117.00
55	BB	11	C	N1-C2-O2	6.17	122.60	118.90
21	AA	673	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	749	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	933	A	O4'-C1'-N9	6.17	113.13	108.20
29	BG	2	ARG	NE-CZ-NH1	6.17	123.38	120.30
54	BA	50	U	N3-C2-O2	-6.17	117.88	122.20
54	BA	2662	A	N1-C6-N6	-6.17	114.90	118.60
54	BA	1550	C	N3-C2-O2	-6.16	117.58	121.90
54	BA	873	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2478	A	C4-C5-C6	-6.16	113.92	117.00
10	AK	12	ARG	NE-CZ-NH2	6.16	123.38	120.30
54	BA	1378	A	O4'-C1'-N9	6.16	113.13	108.20
21	AA	961	U	C1'-O4'-C4'	-6.16	104.97	109.90
54	BA	1269	A	C5-C6-N1	6.16	120.78	117.70
54	BA	1582	C	N1-C2-O2	6.16	122.59	118.90
6	AG	52	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1832	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2005	A	C4-C5-C6	-6.16	113.92	117.00
24	A3	68	C	N3-C2-O2	-6.16	117.59	121.90
55	BB	87	U	O4'-C1'-N1	6.16	113.12	108.20
21	AA	1197	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	163	C	N1-C2-O2	6.15	122.59	118.90
54	BA	1261	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	135	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	719	C	N3-C2-O2	-6.15	117.59	121.90
43	BU	85	ARG	NE-CZ-NH1	6.15	123.38	120.30
54	BA	486	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2483	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1665	A	C4-C5-C6	-6.15	113.92	117.00
30	BH	51	ARG	NE-CZ-NH1	6.15	123.37	120.30
47	BY	48	ARG	NE-CZ-NH1	6.15	123.38	120.30
21	AA	1388	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	908	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	1367	A	N1-C6-N6	-6.15	114.91	118.60
54	BA	2626	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	2745	C	N3-C2-O2	-6.15	117.60	121.90
21	AA	1103	C	N3-C2-O2	-6.15	117.60	121.90
21	AA	1275	A	C5-C6-N1	6.14	120.77	117.70
54	BA	198	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	300	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1323	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1463	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1814	G	N1-C6-O6	-6.14	116.21	119.90
54	BA	2114	A	O4'-C1'-N9	6.14	113.11	108.20
21	AA	6	G	C1'-O4'-C4'	-6.14	104.99	109.90
8	AI	84	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	1780	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1924	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2425	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1248	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1972	G	N1-C6-O6	-6.14	116.22	119.90
21	AA	320	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1280	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	509	C	C1'-O4'-C4'	-6.14	104.99	109.90
54	BA	983	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1902	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	60	A	C4-C5-C6	-6.13	113.93	117.00
21	AA	663	A	C4-C5-C6	-6.13	113.93	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1412	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	582	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	587	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1808	A	O4'-C1'-N9	6.13	113.11	108.20
21	AA	87	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	579	A	C5-C6-N1	6.13	120.77	117.70
21	AA	1508	A	C4-C5-C6	-6.13	113.93	117.00
22	A1	30	C	N3-C2-O2	-6.13	117.61	121.90
22	A1	60	C	N1-C2-O2	6.13	122.58	118.90
54	BA	2283	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2781	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	233	A	C4-C5-C6	-6.13	113.94	117.00
55	BB	56	G	N1-C6-O6	-6.13	116.22	119.90
21	AA	33	A	C5-C6-N1	6.13	120.76	117.70
54	BA	36	G	N3-C2-N2	-6.13	115.61	119.90
54	BA	1999	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2320	U	N3-C2-O2	-6.13	117.91	122.20
54	BA	2452	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2591	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	1431	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	943	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	528	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	38	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2247	A	C5-C6-N1	6.12	120.76	117.70
54	BA	2875	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	120	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	1151	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2496	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	844	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	970	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	1050	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2366	A	C5-C6-N1	6.12	120.76	117.70
21	AA	1195	C	N1-C2-O2	6.12	122.57	118.90
54	BA	1166	G	N1-C6-O6	-6.12	116.23	119.90
54	BA	1994	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2416	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	147	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	633	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1351	C	O4'-C1'-N1	6.12	113.09	108.20
54	BA	1909	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2774	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	273	G	C1'-O4'-C4'	-6.11	105.01	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2176	A	C4-C5-C6	-6.11	113.94	117.00
21	AA	400	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	1044	A	C5-C6-N1	6.11	120.76	117.70
27	BE	61	ARG	NE-CZ-NH2	-6.11	117.25	120.30
54	BA	2466	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2901	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	94	A	C5-C6-N1	6.11	120.75	117.70
54	BA	378	C	N3-C2-O2	-6.11	117.62	121.90
55	BB	50	A	C5-C6-N1	6.11	120.75	117.70
21	AA	368	U	O4'-C1'-N1	6.11	113.08	108.20
21	AA	243	A	C4-C5-C6	-6.11	113.95	117.00
21	AA	415	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	241	A	N1-C6-N6	-6.11	114.94	118.60
54	BA	277	G	O4'-C1'-N9	6.11	113.08	108.20
54	BA	1021	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	1376	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	1957	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	2377	A	O4'-C1'-N9	6.11	113.08	108.20
54	BA	95	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	730	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	422	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	789	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1372	U	O4'-C1'-N1	6.10	113.08	108.20
21	AA	1238	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2030	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2321	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	478	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1049	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1761	C	N3-C2-O2	-6.10	117.63	121.90
49	B0	39	ARG	NE-CZ-NH2	6.09	123.35	120.30
54	BA	453	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	643	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	979	A	C4-C5-C6	-6.09	113.95	117.00
55	BB	70	C	N1-C2-O2	6.09	122.56	118.90
21	AA	607	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	1057	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	1098	A	C5-C6-N1	6.09	120.75	117.70
54	BA	2637	U	O4'-C1'-N1	6.09	113.07	108.20
22	A1	72	C	N3-C2-O2	-6.09	117.64	121.90
40	BR	21	ARG	NE-CZ-NH1	6.09	123.34	120.30
54	BA	63	A	C5-C6-N1	6.09	120.75	117.70
54	BA	1257	C	N3-C2-O2	-6.09	117.64	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	44	A	C5-C6-N1	6.09	120.74	117.70
6	AG	94	ARG	NE-CZ-NH1	6.09	123.34	120.30
21	AA	1245	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	932	U	O4'-C1'-N1	6.09	113.07	108.20
54	BA	1291	C	N1-C2-O2	6.09	122.55	118.90
55	BB	63	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	1398	C	N1-C2-O2	6.08	122.55	118.90
21	AA	1204	A	C5-C6-N1	6.08	120.74	117.70
21	AA	1318	A	C4-C5-C6	-6.08	113.96	117.00
26	BD	141	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	218	A	C5-C6-N1	6.08	120.74	117.70
54	BA	96	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	342	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2606	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	275	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	1161	C	O4'-C1'-N1	6.08	113.06	108.20
54	BA	2447	G	O4'-C1'-N9	6.08	113.06	108.20
54	BA	2463	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2695	U	O4'-C1'-N1	6.08	113.06	108.20
21	AA	35	G	P-O3'-C3'	6.08	126.99	119.70
21	AA	1136	C	N1-C2-O2	6.08	122.55	118.90
26	BD	83	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	1031	G	O4'-C1'-N9	6.08	113.06	108.20
54	BA	2037	A	C5-C6-N1	6.08	120.74	117.70
54	BA	2143	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2474	U	N3-C2-O2	-6.08	117.94	122.20
21	AA	379	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	788	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1469	A	N1-C6-N6	-6.08	114.95	118.60
54	BA	1787	A	N1-C6-N6	-6.08	114.95	118.60
54	BA	2559	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	101	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	490	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	922	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	2800	A	C5-C6-N1	6.08	120.74	117.70
21	AA	611	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	412	A	C5-C6-N1	6.07	120.74	117.70
54	BA	1547	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1801	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	382	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	853	C	N3-C2-O2	-6.07	117.65	121.90
55	BB	31	C	N3-C2-O2	-6.07	117.65	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	458	G	O4'-C1'-N9	6.07	113.06	108.20
54	BA	652	U	O4'-C1'-N1	6.07	113.06	108.20
54	BA	689	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	911	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	948	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1641	A	C5-C6-N1	6.07	120.73	117.70
54	BA	2161	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	520	A	C5-C6-N1	6.07	120.73	117.70
54	BA	2327	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	699	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	756	A	N1-C6-N6	-6.07	114.96	118.60
21	AA	1452	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	106	C	N3-C2-O2	-6.07	117.66	121.90
54	BA	1641	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	436	C	N3-C2-O2	-6.06	117.66	121.90
23	A2	82	A	N1-C6-N6	-6.06	114.96	118.60
54	BA	1230	A	C5-C6-N1	6.06	120.73	117.70
54	BA	2531	A	C4-C5-C6	-6.06	113.97	117.00
13	AN	85	ARG	NE-CZ-NH1	6.06	123.33	120.30
21	AA	1176	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1640	A	C4-C5-C6	-6.06	113.97	117.00
22	A1	65	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	988	A	N1-C6-N6	-6.06	114.96	118.60
54	BA	2587	A	C5-C6-N1	6.06	120.73	117.70
21	AA	8	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	307	C	C3'-C2'-C1'	6.06	106.35	101.50
21	AA	465	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1335	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1893	C	O4'-C1'-N1	6.06	113.05	108.20
54	BA	2058	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2407	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2651	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	935	A	C5-C6-N1	6.06	120.73	117.70
21	AA	946	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	1157	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	502	A	N1-C6-N6	-6.06	114.97	118.60
54	BA	1658	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	196	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	503	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	16	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	1161	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	325	A	C4-C5-C6	-6.05	113.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2435	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	687	A	C5-C6-N1	6.05	120.72	117.70
54	BA	430	A	C5-C6-N1	6.05	120.72	117.70
21	AA	1513	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	195	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1058	U	O4'-C1'-N1	6.05	113.04	108.20
54	BA	1387	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	2830	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	743	A	C4-C5-C6	-6.05	113.98	117.00
55	BB	30	C	N3-C2-O2	-6.05	117.67	121.90
41	BS	110	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	257	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	461	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1439	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1685	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2155	U	O4'-C1'-N1	6.04	113.03	108.20
1	AB	25	LYS	C-N-CA	6.04	136.81	121.70
54	BA	937	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1387	A	C5-C6-N1	6.04	120.72	117.70
3	AD	96	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	772	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1495	A	C4-C5-C6	-6.04	113.98	117.00
55	BB	91	C	N3-C2-O2	-6.04	117.67	121.90
6	AG	91	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	417	C	O4'-C1'-N1	6.04	113.03	108.20
54	BA	470	A	N1-C6-N6	-6.04	114.98	118.60
23	A2	87	U	O4'-C1'-N1	6.04	113.03	108.20
54	BA	1077	A	C5-C6-N1	6.04	120.72	117.70
21	AA	750	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	823	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1118	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2078	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2477	U	O4'-C1'-N1	6.03	113.03	108.20
54	BA	2773	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2811	G	O4'-C1'-N9	6.03	113.03	108.20
54	BA	2821	A	C5-C6-N1	6.03	120.72	117.70
54	BA	2174	C	N3-C2-O2	-6.03	117.68	121.90
10	AK	55	ARG	NE-CZ-NH2	6.03	123.32	120.30
21	AA	452	A	C5-C6-N1	6.03	120.72	117.70
54	BA	105	C	O4'-C1'-N1	6.03	113.02	108.20
21	AA	73	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	913	A	O4'-C1'-N9	6.03	113.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1822	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	271	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	763	G	N3-C2-N2	-6.03	115.68	119.90
54	BA	800	A	C5-C6-N1	6.03	120.71	117.70
54	BA	1072	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1552	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	427	U	O4'-C1'-N1	6.03	113.02	108.20
21	AA	1396	A	C4-C5-C6	-6.03	113.99	117.00
27	BE	88	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	851	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1270	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1577	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	253	C	N3-C2-O2	-6.02	117.68	121.90
54	BA	2313	C	N3-C2-O2	-6.02	117.68	121.90
21	AA	1032	G	N3-C4-C5	-6.02	125.59	128.60
54	BA	946	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	2498	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	2512	C	O4'-C1'-N1	6.02	113.02	108.20
21	AA	938	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	1044	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	596	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	1449	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1885	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2129	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	2338	C	N3-C2-O2	-6.02	117.69	121.90
22	A1	9	A	N1-C6-N6	-6.02	114.99	118.60
54	BA	380	G	O4'-C1'-N9	6.02	113.02	108.20
54	BA	1336	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1606	C	N1-C2-O2	6.02	122.51	118.90
54	BA	1900	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	819	A	N1-C6-N6	-6.02	114.99	118.60
55	BB	38	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	441	A	C4-C5-C6	-6.01	113.99	117.00
46	BX	10	ARG	NE-CZ-NH1	6.01	123.31	120.30
54	BA	553	G	N1-C6-O6	-6.01	116.29	119.90
54	BA	1694	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	753	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	488	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	979	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	66	C	N1-C2-O2	6.01	122.51	118.90
54	BA	423	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	477	A	C4-C5-C6	-6.01	113.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1595	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1638	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	766	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	972	C	O4'-C1'-N1	6.01	113.01	108.20
21	AA	996	A	C5-C6-N1	6.01	120.70	117.70
21	AA	1359	C	N1-C2-O2	6.01	122.51	118.90
22	A1	35	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	161	A	C5-C6-N1	6.01	120.70	117.70
54	BA	2636	C	O4'-C1'-N1	6.01	113.01	108.20
20	AU	30	GLU	C-N-CA	6.01	136.72	121.70
54	BA	447	A	C5-C6-N1	6.01	120.70	117.70
54	BA	531	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	1207	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1470	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2665	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	1477	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2190	G	N3-C2-N2	-6.01	115.70	119.90
54	BA	2386	A	C4-C5-C6	-6.01	114.00	117.00
24	A3	75	C	N3-C2-O2	-6.00	117.70	121.90
55	BB	87	U	C1'-O4'-C4'	-6.00	105.10	109.90
21	AA	65	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	845	A	C4-C5-C6	-6.00	114.00	117.00
22	A1	61	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1490	A	O4'-C1'-N9	6.00	113.00	108.20
54	BA	1715	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	2826	A	O4'-C1'-N9	6.00	113.00	108.20
54	BA	151	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1557	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2061	G	N3-C2-N2	-6.00	115.70	119.90
54	BA	2380	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2734	A	N1-C6-N6	-6.00	115.00	118.60
21	AA	422	C	O4'-C1'-N1	6.00	113.00	108.20
21	AA	1037	C	N3-C2-O2	-6.00	117.70	121.90
24	A3	26	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	981	A	C4-C5-C6	-6.00	114.00	117.00
13	AN	90	ARG	NE-CZ-NH1	6.00	123.30	120.30
21	AA	295	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1465	A	N1-C6-N6	-6.00	115.00	118.60
54	BA	2183	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2619	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	673	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	2103	C	O4'-C1'-N1	6.00	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2540	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2792	A	C5-C6-N1	6.00	120.70	117.70
55	BB	68	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2826	A	C5-C6-N1	6.00	120.70	117.70
21	AA	1209	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	1553	A	O4'-C1'-N9	5.99	113.00	108.20
54	BA	1627	G	C5'-C4'-O4'	5.99	116.29	109.10
21	AA	182	A	C5-C6-N1	5.99	120.70	117.70
54	BA	541	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1505	A	C4-C5-C6	-5.99	114.00	117.00
11	AL	13	ARG	NE-CZ-NH1	5.99	123.30	120.30
21	AA	502	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	918	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	528	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1354	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1528	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	2003	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	2084	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	721	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	199	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	767	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	781	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	872	A	C5-C6-N1	5.98	120.69	117.70
54	BA	1315	C	N3-C2-O2	-5.98	117.71	121.90
2	AC	53	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	26	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	546	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1499	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	315	G	N1-C6-O6	-5.98	116.31	119.90
21	AA	440	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	878	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1887	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	2187	U	O4'-C1'-N1	5.98	112.98	108.20
55	BB	53	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1179	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	787	C	N1-C2-O2	5.98	122.49	118.90
54	BA	892	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	15	G	N3-C2-N2	-5.98	115.72	119.90
21	AA	839	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	1243	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	563	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1144	A	C4-C5-C6	-5.98	114.01	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1378	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2206	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	1210	C	N1-C2-O2	5.98	122.49	118.90
54	BA	2101	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	747	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	481	G	C1'-O4'-C4'	-5.97	105.12	109.90
54	BA	1341	G	O4'-C1'-N9	5.97	112.98	108.20
54	BA	2262	U	O4'-C1'-N1	5.97	112.98	108.20
55	BB	12	C	N1-C2-O2	5.97	122.48	118.90
21	AA	1263	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	37	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1637	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	42	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	948	C	O4'-C1'-N1	5.97	112.97	108.20
55	BB	88	C	N1-C2-O2	5.97	122.48	118.90
21	AA	810	C	O4'-C1'-N1	5.97	112.97	108.20
54	BA	2142	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2612	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	552	U	O4'-C1'-N1	5.96	112.97	108.20
54	BA	1655	A	C4-C5-C6	-5.96	114.02	117.00
55	BB	66	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	1129	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	493	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	790	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	900	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1413	A	C5-C6-N1	5.96	120.68	117.70
54	BA	2205	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1717	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1783	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	940	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	1086	U	N3-C2-O2	-5.96	118.03	122.20
30	BH	116	ARG	NE-CZ-NH1	5.96	123.28	120.30
24	A3	22	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1056	G	N1-C6-O6	-5.96	116.33	119.90
55	BB	4	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2758	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	1040	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	2740	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	749	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	1411	C	N3-C2-O2	-5.95	117.73	121.90
25	BC	202	ARG	NE-CZ-NH1	5.95	123.28	120.30
21	AA	452	A	C4-C5-C6	-5.95	114.03	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	892	A	N1-C6-N6	-5.95	115.03	118.60
54	BA	1145	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1254	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	492	C	N3-C2-O2	-5.95	117.74	121.90
15	AP	31	ARG	NE-CZ-NH1	5.95	123.27	120.30
21	AA	110	C	N1-C2-O2	5.95	122.47	118.90
21	AA	535	A	N1-C6-N6	-5.95	115.03	118.60
21	AA	1112	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	28	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	2044	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1231	U	O4'-C1'-N1	5.94	112.95	108.20
54	BA	1564	C	N3-C2-O2	-5.94	117.74	121.90
9	AJ	68	ARG	NE-CZ-NH1	5.94	123.27	120.30
22	A1	23	A	N1-C6-N6	-5.94	115.03	118.60
54	BA	737	C	N3-C2-O2	-5.94	117.74	121.90
8	AI	112	ARG	NE-CZ-NH1	5.94	123.27	120.30
21	AA	341	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	766	A	C1'-O4'-C4'	-5.94	105.15	109.90
21	AA	1223	C	N1-C2-O2	5.94	122.46	118.90
54	BA	364	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	382	A	C6-C5-N7	5.94	136.46	132.30
54	BA	524	G	N1-C6-O6	-5.94	116.34	119.90
54	BA	1495	A	C5-C6-N1	5.94	120.67	117.70
21	AA	389	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	610	U	C1'-O4'-C4'	-5.94	105.15	109.90
54	BA	1809	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	34	C	P-O3'-C3'	5.94	126.82	119.70
21	AA	923	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	574	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	926	G	P-O3'-C3'	5.93	126.82	119.70
54	BA	2461	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2785	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	739	C	N1-C2-O2	5.93	122.46	118.90
21	AA	900	A	C4-C5-C6	-5.93	114.03	117.00
24	A3	59	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2789	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1225	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	1484	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1340	A	C5-C6-N1	5.93	120.67	117.70
24	A3	40	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	987	C	N3-C2-O2	-5.93	117.75	121.90
4	AE	68	ARG	NE-CZ-NH1	5.93	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	169	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	786	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	1554	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	2652	C	N1-C2-O2	5.93	122.46	118.90
6	AG	4	ARG	NE-CZ-NH1	5.93	123.26	120.30
33	BK	98	ARG	NE-CZ-NH1	5.93	123.26	120.30
54	BA	890	C	N1-C2-O2	5.93	122.46	118.90
21	AA	1293	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	2821	A	N1-C6-N6	-5.92	115.05	118.60
54	BA	1765	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2502	G	N1-C6-O6	-5.92	116.35	119.90
54	BA	1013	C	N1-C2-O2	5.92	122.45	118.90
54	BA	1099	G	N1-C6-O6	-5.92	116.35	119.90
54	BA	1493	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1730	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1784	A	O4'-C1'-N9	5.92	112.94	108.20
54	BA	2412	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2068	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2258	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	1191	A	C5-C6-N1	5.92	120.66	117.70
54	BA	936	A	C5-C6-N1	5.92	120.66	117.70
54	BA	1113	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	1790	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	2117	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	161	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	991	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	1518	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	2042	A	C4-C5-C6	-5.92	114.04	117.00
55	BB	108	A	O4'-C1'-N9	5.92	112.93	108.20
21	AA	865	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	965	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	526	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	962	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2658	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2679	A	C5-C6-N1	5.91	120.66	117.70
54	BA	960	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	2225	A	C4-C5-C6	-5.91	114.04	117.00
21	AA	960	U	O4'-C1'-N1	5.91	112.93	108.20
46	BX	27	ARG	NE-CZ-NH2	-5.91	117.34	120.30
54	BA	33	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1420	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1938	A	C4-C5-C6	-5.91	114.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	66	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	156	C	N3-C4-N4	-5.91	113.86	118.00
21	AA	316	C	C3'-C2'-C1'	5.91	106.23	101.50
54	BA	1551	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1592	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	465	A	N1-C6-N6	-5.91	115.06	118.60
54	BA	2070	A	O4'-C1'-N9	5.91	112.93	108.20
54	BA	2250	G	N1-C6-O6	-5.91	116.36	119.90
21	AA	469	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	1308	A	N1-C6-N6	-5.91	115.06	118.60
54	BA	1546	G	O4'-C1'-N9	5.91	112.92	108.20
54	BA	2590	A	C5-C6-N1	5.91	120.65	117.70
55	BB	58	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	71	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1437	C	N3-C2-O2	-5.90	117.77	121.90
13	AN	53	ARG	NE-CZ-NH1	5.90	123.25	120.30
54	BA	172	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	984	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1420	A	O4'-C1'-N9	5.90	112.92	108.20
21	AA	222	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	901	A	C5-C6-N1	5.90	120.65	117.70
21	AA	985	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1575	C	O4'-C1'-N1	5.90	112.92	108.20
21	AA	1418	A	C4-C5-C6	-5.90	114.05	117.00
15	AP	25	ARG	NE-CZ-NH1	5.90	123.25	120.30
21	AA	653	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	909	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	1114	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	219	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	611	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	253	A	C5-C6-N1	5.89	120.65	117.70
54	BA	79	C	N1-C2-O2	5.89	122.44	118.90
54	BA	703	U	O4'-C1'-N1	5.89	112.92	108.20
54	BA	912	C	N3-C2-O2	-5.89	117.77	121.90
54	BA	1795	C	N3-C2-O2	-5.89	117.77	121.90
54	BA	2579	C	N3-C2-O2	-5.89	117.77	121.90
21	AA	805	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	1302	C	N1-C2-O2	5.89	122.44	118.90
54	BA	679	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1271	G	O4'-C1'-N9	5.89	112.91	108.20
54	BA	1480	C	N3-C2-O2	-5.89	117.78	121.90
55	BB	60	C	N3-C2-O2	-5.89	117.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	315	A	C3'-C2'-C1'	5.89	106.21	101.50
21	AA	1368	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	806	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1933	G	N3-C4-C5	-5.89	125.65	128.60
9	AJ	31	ARG	NE-CZ-NH1	5.89	123.24	120.30
21	AA	19	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	811	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	949	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	162	U	N3-C2-O2	-5.89	118.08	122.20
54	BA	980	A	P-O3'-C3'	5.89	126.77	119.70
54	BA	1063	G	C1'-O4'-C4'	-5.89	105.19	109.90
54	BA	1073	A	O4'-C1'-N9	5.89	112.91	108.20
54	BA	2433	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	2654	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	1492	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	2184	A	C5-C6-N1	5.89	120.64	117.70
21	AA	51	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	626	A	C6-C5-N7	5.89	136.42	132.30
21	AA	1509	C	N3-C2-O2	-5.88	117.78	121.90
24	A3	24	C	N3-C2-O2	-5.88	117.78	121.90
39	BQ	47	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	1164	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	2772	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1288	G	C1'-O4'-C4'	-5.88	105.19	109.90
4	AE	137	ARG	NE-CZ-NH2	-5.88	117.36	120.30
21	AA	1379	G	N1-C6-O6	-5.88	116.37	119.90
24	A3	35	C	N1-C2-O2	5.88	122.43	118.90
54	BA	94	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1382	G	N3-C4-C5	-5.88	125.66	128.60
31	BI	64	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	1414	C	O4'-C1'-N1	5.88	112.90	108.20
21	AA	1028	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	1009	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2380	C	O4'-C1'-N1	5.88	112.90	108.20
54	BA	2645	G	O4'-C1'-N9	5.88	112.90	108.20
21	AA	610	U	N3-C2-O2	-5.88	118.09	122.20
21	AA	1271	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2793	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	83	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	546	U	C1'-O4'-C4'	-5.88	105.20	109.90
54	BA	660	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	1475	G	O4'-C1'-N9	5.88	112.90	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1704	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	1802	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2211	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2683	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	64	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	1512	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1646	C	N1-C2-O2	5.87	122.42	118.90
54	BA	2184	A	N1-C6-N6	-5.87	115.08	118.60
54	BA	2285	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	174	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	202	G	N1-C6-O6	-5.87	116.38	119.90
21	AA	866	C	N1-C2-O2	5.87	122.42	118.90
21	AA	1145	A	N1-C6-N6	-5.87	115.08	118.60
21	AA	1338	G	N1-C6-O6	-5.87	116.38	119.90
54	BA	2055	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	914	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2760	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1230	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	443	A	C5-C6-N1	5.87	120.63	117.70
54	BA	2825	G	N3-C4-C5	-5.87	125.67	128.60
52	B3	7	ARG	NE-CZ-NH1	5.87	123.23	120.30
21	AA	868	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1097	C	N3-C2-O2	-5.87	117.80	121.90
21	AA	1352	C	N1-C2-O2	5.87	122.42	118.90
24	A3	38	A	C4-C5-C6	-5.87	114.07	117.00
21	AA	334	C	N1-C2-O2	5.86	122.42	118.90
54	BA	2841	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	205	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1920	C	O4'-C1'-N1	5.86	112.89	108.20
21	AA	124	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	466	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	885	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2163	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1462	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1508	A	C4-C5-C6	-5.86	114.07	117.00
24	A3	66	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1830	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1167	C	O4'-C1'-N1	5.86	112.89	108.20
54	BA	2639	A	O4'-C1'-N9	5.86	112.88	108.20
54	BA	2741	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	1111	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	398	C	O4'-C1'-N1	5.85	112.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	717	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	2181	U	O4'-C1'-N1	5.85	112.88	108.20
21	AA	116	A	N1-C6-N6	-5.85	115.09	118.60
21	AA	1081	A	C4-C5-C6	-5.85	114.07	117.00
22	A1	16	C	N1-C2-O2	5.85	122.41	118.90
39	BQ	69	ARG	NE-CZ-NH1	5.85	123.23	120.30
54	BA	1170	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	2614	A	C6-C5-N7	5.85	136.40	132.30
33	BK	70	ARG	NE-CZ-NH1	5.85	123.22	120.30
54	BA	2260	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	1133	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1417	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	1774	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2274	A	N1-C6-N6	-5.85	115.09	118.60
21	AA	1067	A	C6-C5-N7	5.85	136.39	132.30
54	BA	1206	G	N3-C2-N2	-5.85	115.81	119.90
54	BA	1654	A	C4-C5-C6	-5.85	114.08	117.00
21	AA	608	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	474	G	O4'-C1'-N9	5.85	112.88	108.20
54	BA	590	A	C5-C6-N1	5.85	120.62	117.70
54	BA	1634	A	O4'-C1'-N9	5.85	112.88	108.20
54	BA	1829	A	C4-C5-C6	-5.85	114.08	117.00
55	BB	92	C	N3-C2-O2	-5.85	117.81	121.90
21	AA	931	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1552	A	C1'-O4'-C4'	-5.84	105.22	109.90
54	BA	1603	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1644	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2096	C	O4'-C1'-N1	5.84	112.88	108.20
54	BA	2778	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	879	C	N1-C2-O2	5.84	122.41	118.90
54	BA	395	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	550	C	N1-C2-O2	5.84	122.41	118.90
54	BA	2194	U	O4'-C1'-N1	5.84	112.87	108.20
17	AR	47	ARG	NE-CZ-NH1	5.84	123.22	120.30
54	BA	251	A	N1-C6-N6	-5.84	115.10	118.60
18	AS	36	ARG	NE-CZ-NH2	5.84	123.22	120.30
21	AA	783	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	826	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	1145	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	1333	A	C4-C5-C6	-5.84	114.08	117.00
22	A1	59	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	184	C	N3-C2-O2	-5.84	117.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	930	G	O4'-C1'-N9	5.84	112.87	108.20
54	BA	2575	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	2670	A	C4-C5-C6	-5.84	114.08	117.00
6	AG	142	ARG	NE-CZ-NH1	5.84	123.22	120.30
54	BA	334	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	957	C	N1-C2-O2	5.84	122.40	118.90
54	BA	1789	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1054	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	2333	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	20	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2339	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2441	U	O4'-C1'-N1	5.83	112.87	108.20
21	AA	977	A	C4-C5-C6	-5.83	114.08	117.00
24	A3	60	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	905	A	C5-C6-N1	5.83	120.62	117.70
54	BA	1003	G	N1-C6-O6	-5.83	116.40	119.90
54	BA	2662	A	C5-C6-N1	5.83	120.62	117.70
55	BB	78	A	C6-C5-N7	5.83	136.38	132.30
54	BA	53	A	O4'-C1'-N9	5.83	112.86	108.20
54	BA	2173	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	487	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	459	U	O4'-C1'-N1	5.83	112.86	108.20
54	BA	527	C	N1-C2-O2	5.83	122.40	118.90
54	BA	1328	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	1431	A	N1-C6-N6	-5.83	115.10	118.60
54	BA	1741	C	N3-C2-O2	-5.83	117.82	121.90
22	A1	36	C	N3-C2-O2	-5.83	117.82	121.90
37	BO	9	ARG	NE-CZ-NH1	5.83	123.21	120.30
54	BA	2518	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	1311	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	222	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	231	A	C5-C6-N1	5.82	120.61	117.70
54	BA	434	U	O4'-C1'-N1	5.82	112.86	108.20
54	BA	2254	C	N3-C2-O2	-5.82	117.82	121.90
21	AA	770	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1507	C	O4'-C1'-N1	5.82	112.86	108.20
55	BB	52	A	O4'-C1'-N9	5.82	112.86	108.20
54	BA	210	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1600	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2788	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	277	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	368	A	C5-C6-N1	5.82	120.61	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2746	U	O4'-C1'-N1	5.82	112.86	108.20
21	AA	269	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1098	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1288	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1562	U	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2072	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	470	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1540	G	O4'-C1'-N9	5.82	112.85	108.20
54	BA	2060	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2146	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2882	A	C5-C6-N1	5.82	120.61	117.70
21	AA	381	C	O4'-C1'-N1	5.81	112.85	108.20
21	AA	990	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	1430	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	526	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1503	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1525	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2754	U	O4'-C1'-N1	5.81	112.85	108.20
21	AA	862	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	852	G	N1-C6-O6	-5.81	116.42	119.90
26	BD	169	ARG	NE-CZ-NH2	-5.81	117.40	120.30
54	BA	369	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	538	A	C5-C6-N1	5.81	120.60	117.70
54	BA	581	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2679	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	2720	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	2750	A	C4-C5-C6	-5.81	114.10	117.00
55	BB	64	G	N1-C6-O6	-5.81	116.42	119.90
54	BA	542	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1146	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2757	A	C5-C6-N1	5.80	120.60	117.70
21	AA	906	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	77	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	978	A	C6-C5-N7	5.80	136.36	132.30
21	AA	1217	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	1298	U	N3-C2-O2	-5.80	118.14	122.20
54	BA	267	C	N3-C2-O2	-5.80	117.84	121.90
27	BE	67	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	866	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2015	A	O4'-C1'-N9	5.80	112.84	108.20
54	BA	2458	G	N3-C4-C5	-5.80	125.70	128.60
55	BB	118	C	N3-C2-O2	-5.80	117.84	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2043	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	2222	C	N3-C2-O2	-5.80	117.84	121.90
28	BF	70	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	1690	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1447	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	829	A	N1-C6-N6	-5.79	115.12	118.60
54	BA	2177	C	N3-C2-O2	-5.79	117.84	121.90
55	BB	49	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	1117	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	698	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	1243	C	N1-C2-O2	5.79	122.38	118.90
54	BA	2312	U	N3-C2-O2	-5.79	118.14	122.20
54	BA	2556	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	816	A	C4-C5-C6	-5.79	114.10	117.00
21	AA	970	C	N3-C4-C5	5.79	124.22	121.90
54	BA	268	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	472	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	889	A	N1-C6-N6	-5.79	115.13	118.60
21	AA	927	G	O4'-C1'-N9	5.79	112.83	108.20
21	AA	460	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	167	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	990	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	704	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	894	G	N1-C6-O6	-5.78	116.43	119.90
21	AA	923	A	N1-C6-N6	-5.78	115.13	118.60
54	BA	1498	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	1758	U	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2651	C	O4'-C1'-N1	5.78	112.83	108.20
21	AA	1254	A	C5-C6-N1	5.78	120.59	117.70
54	BA	445	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2297	A	O4'-C1'-N9	5.78	112.83	108.20
21	AA	307	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	1005	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1469	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1894	C	N1-C2-O2	5.78	122.37	118.90
54	BA	2247	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2364	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2482	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	514	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	1913	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	844	G	N3-C4-C5	-5.78	125.71	128.60
54	BA	572	A	C4-C5-C6	-5.78	114.11	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1570	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1483	A	C5-C6-N1	5.78	120.59	117.70
54	BA	909	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2094	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2597	G	N1-C6-O6	-5.78	116.44	119.90
55	BB	115	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	131	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	426	C	O4'-C1'-N1	5.77	112.82	108.20
54	BA	994	C	N1-C2-O2	5.77	122.36	118.90
54	BA	1056	G	C5-C6-N1	5.77	114.39	111.50
54	BA	915	C	N1-C2-O2	5.77	122.36	118.90
54	BA	2512	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	975	A	C4-C5-C6	-5.77	114.11	117.00
21	AA	1188	A	C4-C5-C6	-5.77	114.11	117.00
24	A3	72	C	N1-C2-O2	5.77	122.36	118.90
34	BL	32	GLY	C-N-CA	5.77	136.13	121.70
54	BA	421	C	N3-C2-O2	-5.77	117.86	121.90
55	BB	93	C	N3-C2-O2	-5.77	117.86	121.90
51	B2	35	ARG	NE-CZ-NH1	5.77	123.18	120.30
54	BA	966	G	N1-C6-O6	-5.77	116.44	119.90
54	BA	1791	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	2314	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	339	C	N1-C2-O2	5.77	122.36	118.90
54	BA	160	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	592	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	2678	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	448	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	1170	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	1518	A	C6-C5-N7	5.76	136.34	132.30
54	BA	2036	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	2730	C	N3-C2-O2	-5.76	117.86	121.90
21	AA	177	G	N3-C4-C5	-5.76	125.72	128.60
21	AA	1001	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	164	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	980	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2853	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	876	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	1322	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2706	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2806	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	833	A	O4'-C1'-N9	5.76	112.81	108.20
21	AA	787	A	C4-C5-C6	-5.76	114.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	228	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	330	A	O4'-C1'-N9	5.76	112.81	108.20
54	BA	599	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	616	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1586	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	368	U	N3-C2-O2	-5.75	118.17	122.20
54	BA	1637	A	C5-C6-N1	5.75	120.58	117.70
21	AA	1031	C	N1-C2-O2	5.75	122.35	118.90
21	AA	1131	G	N3-C2-N2	-5.75	115.87	119.90
54	BA	272	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	320	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	1278	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	2411	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2483	C	O4'-C1'-N1	5.75	112.80	108.20
2	AC	131	ARG	NE-CZ-NH1	5.75	123.17	120.30
21	AA	919	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	336	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	433	C	N1-C2-O2	5.75	122.35	118.90
54	BA	678	C	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2091	C	N1-C2-O2	5.75	122.35	118.90
21	AA	980	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	41	G	N1-C6-O6	-5.75	116.45	119.90
21	AA	374	A	O4'-C1'-N9	5.75	112.80	108.20
21	AA	810	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	1214	C	C1'-O4'-C4'	-5.75	105.30	109.90
21	AA	1366	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	1804	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	702	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	999	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	1171	A	C5-C6-N1	5.75	120.57	117.70
54	BA	1848	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	547	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	2837	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	181	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	363	A	C4-C5-C6	-5.74	114.13	117.00
24	A3	73	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	191	A	N1-C6-N6	-5.74	115.15	118.60
54	BA	1147	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1351	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	2733	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	8	A	O4'-C1'-N9	5.74	112.79	108.20
54	BA	1030	C	N3-C2-O2	-5.74	117.88	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1176	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1487	U	O4'-C1'-N1	5.74	112.79	108.20
21	AA	35	G	O4'-C1'-N9	5.74	112.79	108.20
21	AA	385	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	1319	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	554	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1141	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1194	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	1342	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	1410	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	226	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2066	C	N3-C2-O2	-5.74	117.88	121.90
23	A2	80	C	N3-C2-O2	-5.74	117.89	121.90
54	BA	203	A	N1-C6-N6	-5.74	115.16	118.60
54	BA	1362	C	N1-C2-O2	5.74	122.34	118.90
54	BA	1379	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1153	C	N3-C2-O2	-5.73	117.89	121.90
55	BB	97	C	N1-C2-O2	5.73	122.34	118.90
21	AA	967	C	N1-C2-O2	5.73	122.34	118.90
54	BA	203	A	C4-C5-C6	-5.73	114.13	117.00
52	B3	39	ARG	NH1-CZ-NH2	-5.73	113.10	119.40
54	BA	921	C	N3-C2-O2	-5.73	117.89	121.90
17	AR	42	ARG	NE-CZ-NH1	5.73	123.16	120.30
54	BA	415	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1043	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2518	A	O4'-C1'-N9	5.73	112.78	108.20
13	AN	9	ARG	NE-CZ-NH1	5.73	123.16	120.30
21	AA	160	A	C4-C5-C6	-5.73	114.14	117.00
26	BD	15	PHE	CB-CG-CD1	-5.73	116.79	120.80
21	AA	482	A	N1-C6-N6	-5.72	115.17	118.60
21	AA	622	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	501	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1151	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	352	C	N3-C2-O2	-5.72	117.89	121.90
21	AA	979	C	N3-C2-O2	-5.72	117.89	121.90
22	A1	21	A	C4-C5-C6	-5.72	114.14	117.00
22	A1	62	C	N3-C2-O2	-5.72	117.89	121.90
39	BQ	49	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
54	BA	217	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1844	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	2305	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	1127	G	N1-C6-O6	-5.72	116.47	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2889	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	536	C	N1-C2-O2	5.72	122.33	118.90
54	BA	1686	C	O4'-C1'-N1	5.72	112.78	108.20
15	AP	8	ARG	NE-CZ-NH1	5.71	123.16	120.30
54	BA	1274	A	C5-C6-N1	5.71	120.56	117.70
21	AA	1284	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	910	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2762	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1456	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1155	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1241	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2771	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	944	G	N1-C6-O6	-5.71	116.47	119.90
55	BB	19	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	633	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1884	G	C3'-C2'-C1'	5.71	106.07	101.50
21	AA	582	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	14	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	1574	C	N3-C4-C5	5.71	124.18	121.90
54	BA	2039	U	O4'-C1'-N1	5.71	112.77	108.20
21	AA	309	A	C4-C5-C6	-5.71	114.15	117.00
21	AA	1102	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	2208	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	2900	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	347	A	C4-C5-C6	-5.70	114.15	117.00
23	A2	79	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	802	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1838	C	O4'-C1'-N1	5.70	112.76	108.20
21	AA	214	C	N1-C2-O2	5.70	122.32	118.90
29	BG	54	ARG	NE-CZ-NH1	5.70	123.15	120.30
54	BA	1847	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2715	C	N1-C2-O2	5.70	122.32	118.90
21	AA	642	A	C5-C6-N1	5.70	120.55	117.70
21	AA	1324	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	311	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	989	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1928	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2737	G	N1-C6-O6	-5.70	116.48	119.90
54	BA	2860	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1438	U	P-O3'-C3'	5.69	126.53	119.70
54	BA	2792	A	C4-C5-C6	-5.69	114.15	117.00
21	AA	285	C	N1-C2-O2	5.69	122.31	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	336	A	C5-C6-N1	5.69	120.55	117.70
21	AA	782	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2295	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	1261	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	687	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1434	A	C4-C5-C6	-5.69	114.16	117.00
21	AA	556	C	N3-C2-O2	-5.69	117.92	121.90
27	BE	61	ARG	NE-CZ-NH1	5.69	123.14	120.30
54	BA	1591	A	O4'-C1'-N9	5.69	112.75	108.20
54	BA	2600	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	740	C	N1-C2-O2	5.69	122.31	118.90
54	BA	794	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1565	C	O4'-C1'-N1	5.68	112.75	108.20
54	BA	2617	U	O4'-C1'-N1	5.68	112.75	108.20
21	AA	1182	G	N3-C2-N2	-5.68	115.92	119.90
21	AA	1369	C	N1-C2-O2	5.68	122.31	118.90
21	AA	1409	C	N3-C2-O2	-5.68	117.92	121.90
25	BC	216	ARG	NE-CZ-NH2	5.68	123.14	120.30
41	BS	99	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	277	G	N3-C4-C5	-5.68	125.76	128.60
21	AA	512	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	2850	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1596	A	C5-C6-N1	5.68	120.54	117.70
48	BZ	10	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	838	C	C5'-C4'-O4'	5.68	115.91	109.10
21	AA	625	U	O4'-C1'-N1	5.67	112.74	108.20
21	AA	1460	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	1500	A	C6-C5-N7	5.67	136.27	132.30
54	BA	337	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	347	A	C5-C6-N1	5.67	120.54	117.70
54	BA	2598	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	471	U	C1'-O4'-C4'	-5.67	105.36	109.90
22	A1	70	C	C5'-C4'-C3'	-5.67	106.92	116.00
54	BA	223	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1773	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1987	A	O4'-C1'-N9	5.67	112.74	108.20
54	BA	2317	A	C5-C6-N1	5.67	120.54	117.70
21	AA	28	A	C4-C5-C6	-5.67	114.17	117.00
32	BJ	99	ARG	NE-CZ-NH1	5.67	123.14	120.30
6	AG	95	ARG	NE-CZ-NH1	5.67	123.13	120.30
21	AA	897	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	140	C	N3-C4-N4	-5.67	114.03	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	285	G	O4'-C1'-N9	5.67	112.73	108.20
54	BA	558	U	O4'-C1'-N1	5.67	112.73	108.20
54	BA	731	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1075	C	O4'-C1'-N1	5.67	112.73	108.20
54	BA	1934	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2515	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	353	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2448	A	C4-C5-C6	-5.67	114.17	117.00
21	AA	392	C	N3-C2-O2	-5.67	117.94	121.90
54	BA	1001	A	C4-C5-C6	-5.67	114.17	117.00
39	BQ	54	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	161	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	440	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	752	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	884	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	2277	G	N1-C6-O6	-5.66	116.50	119.90
54	BA	2630	G	O4'-C1'-N9	5.66	112.73	108.20
54	BA	341	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	646	U	O4'-C1'-N1	5.66	112.73	108.20
21	AA	1397	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1441	A	N1-C6-N6	-5.66	115.20	118.60
22	A1	51	C	N3-C2-O2	-5.66	117.94	121.90
24	A3	52	C	N3-C2-O2	-5.66	117.94	121.90
30	BH	50	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	417	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1292	G	O4'-C1'-N9	5.66	112.73	108.20
54	BA	1570	A	C5-C6-N1	5.66	120.53	117.70
21	AA	89	U	N3-C2-O2	-5.66	118.24	122.20
21	AA	703	G	C3'-C2'-C1'	5.66	106.03	101.50
21	AA	716	A	C4-C5-C6	-5.66	114.17	117.00
46	BX	2	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	1027	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1086	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	348	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2465	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	35	G	C5'-C4'-C3'	-5.66	106.95	116.00
21	AA	1119	C	N3-C2-O2	-5.66	117.94	121.90
22	A1	51	C	O4'-C1'-N1	5.66	112.72	108.20
34	BL	48	ARG	NH1-CZ-NH2	-5.66	113.18	119.40
54	BA	147	C	O4'-C1'-N1	5.66	112.72	108.20
54	BA	149	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	475	C	O4'-C1'-N1	5.66	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	479	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1032	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1196	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1359	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1731	G	N3-C4-C5	-5.66	125.77	128.60
54	BA	1824	G	N1-C6-O6	-5.66	116.51	119.90
21	AA	250	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	863	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1585	C	O4'-C1'-N1	5.65	112.72	108.20
21	AA	403	C	N3-C2-O2	-5.65	117.94	121.90
22	A1	38	A	C6-C5-N7	5.65	136.25	132.30
54	BA	22	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1204	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1899	A	C4-C5-C6	-5.65	114.17	117.00
55	BB	37	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	838	C	N1-C2-O2	5.65	122.29	118.90
21	AA	233	C	N3-C2-O2	-5.65	117.95	121.90
54	BA	2261	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	835	C	N1-C2-O2	5.65	122.29	118.90
21	AA	467	U	N3-C2-O2	-5.64	118.25	122.20
21	AA	1305	G	N1-C6-O6	-5.64	116.51	119.90
54	BA	601	C	O4'-C1'-N1	5.64	112.72	108.20
21	AA	722	G	C5-C6-N1	5.64	114.32	111.50
54	BA	722	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	961	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2287	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1325	U	C1'-O4'-C4'	-5.64	105.39	109.90
21	AA	225	C	N3-C2-O2	-5.64	117.95	121.90
8	AI	44	ARG	NE-CZ-NH1	5.64	123.12	120.30
8	AI	17	ARG	NE-CZ-NH1	5.64	123.12	120.30
21	AA	777	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	76	C	N1-C2-O2	5.64	122.28	118.90
54	BA	2727	A	C4-C5-C6	-5.64	114.18	117.00
6	AG	101	ARG	NE-CZ-NH2	-5.63	117.48	120.30
7	AH	83	ARG	NE-CZ-NH1	5.63	123.12	120.30
21	AA	1533	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	1792	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	2024	G	N3-C2-N2	-5.63	115.96	119.90
22	A1	2	G	O4'-C1'-N9	5.63	112.71	108.20
54	BA	529	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	951	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	1064	C	N1-C2-O2	5.63	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2443	C	C4'-C3'-C2'	-5.63	96.97	102.60
54	BA	2530	A	C4-C5-C6	-5.63	114.18	117.00
56	B5	162	ARG	NE-CZ-NH1	5.63	123.12	120.30
21	AA	998	C	N1-C2-O2	5.63	122.28	118.90
54	BA	84	A	N1-C6-N6	-5.63	115.22	118.60
54	BA	2704	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	563	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1236	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1340	A	C4-C5-C6	-5.63	114.19	117.00
22	A1	56	C	N1-C2-O2	5.63	122.28	118.90
34	BL	48	ARG	NE-CZ-NH2	5.63	123.11	120.30
54	BA	1640	A	O4'-C1'-N9	5.63	112.70	108.20
54	BA	2378	A	N1-C6-N6	-5.63	115.22	118.60
54	BA	2749	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	270	A	C5'-C4'-C3'	-5.62	107.00	116.00
21	AA	270	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	303	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	239	C	N3-C2-O2	-5.62	117.96	121.90
21	AA	715	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2765	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1275	A	C4-C5-C6	-5.62	114.19	117.00
25	BC	174	ARG	NE-CZ-NH1	5.62	123.11	120.30
54	BA	1544	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2248	C	N3-C2-O2	-5.62	117.97	121.90
4	AE	67	ARG	NE-CZ-NH1	5.62	123.11	120.30
6	AG	3	ARG	NE-CZ-NH1	5.62	123.11	120.30
21	AA	856	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1718	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	2571	U	O4'-C1'-N1	5.62	112.69	108.20
21	AA	322	C	N1-C2-O2	5.61	122.27	118.90
54	BA	318	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1129	A	O4'-C1'-N9	5.61	112.69	108.20
21	AA	948	C	N1-C2-O2	5.61	122.27	118.90
54	BA	2268	A	C4-C5-C6	-5.61	114.19	117.00
21	AA	257	G	N1-C6-O6	-5.61	116.53	119.90
21	AA	483	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1888	G	N3-C4-C5	-5.61	125.80	128.60
54	BA	2306	C	N3-C2-O2	-5.61	117.97	121.90
55	BB	91	C	O4'-C1'-N1	5.61	112.69	108.20
21	AA	1107	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1538	G	N3-C2-N2	-5.61	115.97	119.90
21	AA	33	A	C4-C5-C6	-5.61	114.20	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	193	C	N1-C2-O2	5.61	122.26	118.90
21	AA	366	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	483	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	848	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	947	A	C6-C5-N7	5.61	136.22	132.30
54	BA	1645	G	C5-C6-N1	5.61	114.30	111.50
54	BA	1672	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	1827	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2270	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	423	G	N3-C4-C5	-5.61	125.80	128.60
54	BA	1061	U	N3-C2-O2	-5.61	118.28	122.20
54	BA	1295	C	N1-C2-O2	5.61	122.26	118.90
54	BA	1647	U	O4'-C1'-N1	5.61	112.68	108.20
54	BA	1747	U	O4'-C1'-N1	5.61	112.68	108.20
54	BA	2071	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	629	A	C6-C5-N7	5.60	136.22	132.30
54	BA	1774	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	2275	C	N3-C2-O2	-5.60	117.98	121.90
21	AA	643	C	N3-C2-O2	-5.60	117.98	121.90
22	A1	13	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	107	G	C5'-C4'-O4'	5.60	115.82	109.10
54	BA	1961	C	N1-C2-O2	5.60	122.26	118.90
54	BA	2302	U	O4'-C1'-N1	5.60	112.68	108.20
3	AD	25	ARG	NE-CZ-NH1	5.60	123.10	120.30
52	B3	7	ARG	NE-CZ-NH2	-5.60	117.50	120.30
54	BA	237	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	812	C	N1-C2-O2	5.60	122.26	118.90
54	BA	1052	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1598	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	2851	A	C6-C5-N7	5.60	136.22	132.30
54	BA	1729	U	O4'-C1'-N1	5.60	112.68	108.20
21	AA	984	C	N3-C2-O2	-5.60	117.98	121.90
21	AA	641	U	N3-C2-O2	-5.59	118.28	122.20
21	AA	1032	G	C8-N9-C4	-5.59	104.16	106.40
21	AA	1212	U	C1'-O4'-C4'	-5.59	105.42	109.90
54	BA	1236	G	O4'-C1'-N9	5.59	112.68	108.20
54	BA	581	C	O4'-C1'-N1	5.59	112.67	108.20
21	AA	1478	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	148	U	C3'-C2'-C1'	5.59	105.97	101.50
54	BA	1863	G	N1-C6-O6	-5.59	116.55	119.90
21	AA	419	C	N1-C2-O2	5.59	122.25	118.90
21	AA	1227	A	C4-C5-C6	-5.59	114.20	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BN	69	ARG	NE-CZ-NH1	5.59	123.09	120.30
54	BA	91	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	1088	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	2854	G	O4'-C1'-N9	5.59	112.67	108.20
21	AA	736	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1213	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	1265	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1448	C	C6-N1-C2	-5.59	118.06	120.30
54	BA	305	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2422	C	N1-C2-O2	5.59	122.25	118.90
54	BA	2453	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	329	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	1301	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	1360	G	N1-C6-O6	-5.59	116.55	119.90
54	BA	1679	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	2279	G	N1-C6-O6	-5.59	116.55	119.90
54	BA	1648	U	C5-C6-N1	-5.58	119.91	122.70
21	AA	508	U	N3-C2-O2	-5.58	118.29	122.20
54	BA	193	U	N3-C2-O2	-5.58	118.29	122.20
54	BA	731	C	C3'-C2'-C1'	5.58	105.97	101.50
54	BA	2687	U	O4'-C1'-N1	5.58	112.67	108.20
21	AA	428	G	O4'-C1'-N9	5.58	112.67	108.20
54	BA	237	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	998	C	N1-C2-O2	5.58	122.25	118.90
54	BA	1553	A	C6-C5-N7	5.58	136.21	132.30
54	BA	2215	C	N1-C2-O2	5.58	122.25	118.90
54	BA	2440	C	O4'-C1'-N1	5.58	112.66	108.20
54	BA	130	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	413	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	1342	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2419	U	O4'-C1'-N1	5.58	112.66	108.20
55	BB	35	C	N1-C2-O2	5.58	122.25	118.90
55	BB	47	C	N3-C2-O2	-5.58	118.00	121.90
22	A1	76	A	C4-C5-C6	-5.58	114.21	117.00
3	AD	69	ARG	NH1-CZ-NH2	-5.58	113.27	119.40
21	AA	106	C	C5'-C4'-O4'	5.58	115.79	109.10
21	AA	689	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	1102	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	2169	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	331	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1116	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	1608	A	C4-C5-C6	-5.57	114.21	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1741	C	N1-C2-O2	5.57	122.24	118.90
54	BA	2322	A	C4-C5-C6	-5.57	114.21	117.00
21	AA	703	G	O4'-C1'-N9	5.57	112.66	108.20
54	BA	1574	C	N1-C2-O2	5.57	122.24	118.90
21	AA	549	C	N3-C4-N4	-5.57	114.10	118.00
54	BA	2382	G	O4'-C1'-N9	5.57	112.66	108.20
21	AA	163	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	432	A	C6-C5-N7	5.57	136.20	132.30
21	AA	1108	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	2408	U	O4'-C1'-N1	5.57	112.66	108.20
21	AA	271	C	O4'-C1'-N1	5.57	112.65	108.20
21	AA	1124	G	O4'-C1'-N9	5.57	112.65	108.20
54	BA	1297	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1853	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	2656	U	O4'-C1'-N1	5.57	112.65	108.20
54	BA	2823	A	C3'-C2'-C1'	5.57	105.95	101.50
54	BA	1223	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	2838	G	O4'-C1'-N9	5.57	112.65	108.20
43	BU	81	ARG	NE-CZ-NH2	-5.56	117.52	120.30
21	AA	300	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	330	A	N1-C6-N6	-5.56	115.26	118.60
54	BA	1348	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1720	U	O4'-C1'-N1	5.56	112.65	108.20
54	BA	271	G	O4'-C1'-N9	5.56	112.65	108.20
54	BA	1005	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	2820	A	C4-C5-C6	-5.56	114.22	117.00
55	BB	43	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	1701	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1870	C	N1-C2-O2	5.56	122.23	118.90
21	AA	964	A	N1-C6-N6	-5.56	115.27	118.60
21	AA	1467	C	N1-C2-O2	5.56	122.23	118.90
54	BA	401	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1087	G	C3'-C2'-C1'	5.56	105.94	101.50
55	BB	86	G	N1-C6-O6	-5.56	116.57	119.90
21	AA	731	G	N3-C2-N2	-5.55	116.01	119.90
51	B2	21	ARG	NE-CZ-NH1	5.55	123.08	120.30
54	BA	560	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	876	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1200	C	N1-C2-O2	5.55	122.23	118.90
54	BA	1590	A	C4-C5-C6	-5.55	114.22	117.00
56	B5	74	ARG	NE-CZ-NH1	5.55	123.08	120.30
21	AA	1480	A	C6-C5-N7	5.55	136.19	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2232	C	N1-C2-O2	5.55	122.23	118.90
3	AD	153	ARG	NE-CZ-NH1	5.55	123.08	120.30
35	BM	55	ARG	NE-CZ-NH2	5.55	123.08	120.30
48	BZ	44	ARG	NE-CZ-NH1	5.55	123.08	120.30
54	BA	7	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	294	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	509	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	1306	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1967	C	N1-C2-O2	5.55	122.23	118.90
54	BA	2879	A	N1-C6-N6	-5.55	115.27	118.60
54	BA	2311	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	2475	C	N3-C2-O2	-5.55	118.02	121.90
21	AA	1349	A	C4-C5-C6	-5.55	114.23	117.00
33	BK	105	ARG	NE-CZ-NH1	5.55	123.07	120.30
54	BA	2014	A	C4-C5-C6	-5.55	114.23	117.00
21	AA	759	A	C4-C5-C6	-5.55	114.23	117.00
21	AA	1137	C	N1-C2-O2	5.55	122.23	118.90
54	BA	1534	U	N3-C2-O2	-5.55	118.32	122.20
2	AC	71	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	504	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	357	G	C3'-C2'-C1'	5.54	105.94	101.50
21	AA	653	U	N3-C2-O2	-5.54	118.32	122.20
54	BA	1955	U	O4'-C1'-N1	5.54	112.64	108.20
54	BA	2200	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	7	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	1296	C	N1-C2-O2	5.54	122.22	118.90
54	BA	2346	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2872	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1757	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2122	U	O4'-C1'-N1	5.54	112.63	108.20
54	BA	776	G	N9-C4-C5	5.54	107.61	105.40
50	B1	27	ARG	NE-CZ-NH1	5.54	123.07	120.30
54	BA	2214	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	1165	U	O4'-C1'-N1	5.54	112.63	108.20
24	A3	41	C	N3-C2-O2	-5.54	118.03	121.90
54	BA	244	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	119	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	212	G	O4'-C1'-N9	5.53	112.63	108.20
54	BA	632	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	722	A	O4'-C1'-N9	5.53	112.63	108.20
54	BA	2795	C	O4'-C1'-N1	5.53	112.63	108.20
21	AA	227	G	N1-C6-O6	-5.53	116.58	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1540	G	C5'-C4'-O4'	5.53	115.74	109.10
54	BA	2581	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	2153	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2520	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2717	C	N1-C2-O2	5.53	122.22	118.90
21	AA	660	C	N3-C2-O2	-5.53	118.03	121.90
47	BY	7	ARG	NE-CZ-NH1	5.53	123.06	120.30
54	BA	332	A	C5-C6-N1	5.53	120.46	117.70
54	BA	566	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	671	C	N1-C2-O2	5.53	122.22	118.90
54	BA	890	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	1239	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	1872	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	1881	C	N1-C2-O2	5.53	122.22	118.90
54	BA	2699	C	N1-C2-O2	5.53	122.22	118.90
21	AA	200	G	O4'-C1'-N9	5.53	112.62	108.20
54	BA	1630	A	C6-C5-N7	5.53	136.17	132.30
54	BA	2713	U	O4'-C1'-N1	5.52	112.62	108.20
54	BA	2784	U	O4'-C1'-N1	5.52	112.62	108.20
54	BA	876	C	N3-C2-O2	-5.52	118.03	121.90
54	BA	1073	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1123	C	O4'-C1'-N1	5.52	112.62	108.20
17	AR	56	ARG	NE-CZ-NH2	-5.52	117.54	120.30
21	AA	1534	A	C5'-C4'-C3'	-5.52	107.17	116.00
21	AA	945	G	C5-C6-N1	5.52	114.26	111.50
22	A1	41	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	166	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	824	U	C4'-C3'-C2'	-5.52	97.08	102.60
54	BA	1744	A	C4-C5-C6	-5.52	114.24	117.00
14	AO	88	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	AA	133	U	N3-C2-O2	-5.52	118.34	122.20
54	BA	606	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	785	G	N1-C6-O6	-5.52	116.59	119.90
54	BA	1591	A	C6-C5-N7	5.52	136.16	132.30
54	BA	2145	C	N1-C2-O2	5.52	122.21	118.90
54	BA	2562	U	O4'-C1'-N1	5.52	112.61	108.20
10	AK	52	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	AA	34	C	O4'-C1'-N1	5.52	112.61	108.20
21	AA	1000	A	N1-C6-N6	-5.52	115.29	118.60
21	AA	1021	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	1376	U	N3-C2-O2	-5.52	118.34	122.20
54	BA	1299	G	C3'-C2'-C1'	5.52	105.91	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	128	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	404	A	O4'-C1'-N9	5.51	112.61	108.20
54	BA	1371	G	N3-C2-N2	-5.51	116.04	119.90
54	BA	1722	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	2398	U	O4'-C1'-N1	5.51	112.61	108.20
21	AA	305	G	C3'-C2'-C1'	5.51	105.91	101.50
21	AA	595	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	2899	A	C6-C5-N7	5.51	136.16	132.30
4	AE	25	LYS	C-N-CA	5.51	133.87	122.30
21	AA	108	G	O4'-C1'-N9	5.51	112.61	108.20
21	AA	417	G	N1-C6-O6	-5.51	116.59	119.90
21	AA	760	G	N1-C6-O6	-5.51	116.59	119.90
21	AA	1534	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	455	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	1046	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	1070	A	C1'-O4'-C4'	-5.51	105.49	109.90
21	AA	848	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	279	A	C3'-C2'-C1'	5.51	105.91	101.50
54	BA	2278	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	1755	A	C6-C5-N7	5.51	136.16	132.30
21	AA	546	A	N1-C6-N6	-5.51	115.30	118.60
21	AA	1400	C	N1-C2-O2	5.51	122.20	118.90
54	BA	537	G	N1-C6-O6	-5.51	116.60	119.90
54	BA	1808	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	1862	G	N3-C2-N2	-5.51	116.05	119.90
54	BA	2723	C	N1-C2-O2	5.51	122.20	118.90
21	AA	85	U	C3'-C2'-C1'	5.50	105.90	101.50
54	BA	419	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	621	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1533	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1554	U	C3'-C2'-C1'	5.50	105.90	101.50
54	BA	1737	G	N3-C2-N2	-5.50	116.05	119.90
54	BA	1762	A	O4'-C1'-N9	5.50	112.60	108.20
21	AA	108	G	N3-C2-N2	-5.50	116.05	119.90
21	AA	151	A	C6-C5-N7	5.50	136.15	132.30
21	AA	714	G	N3-C4-C5	-5.50	125.85	128.60
21	AA	1269	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	84	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	120	U	N3-C2-O2	-5.50	118.35	122.20
54	BA	1876	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1961	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	243	U	O4'-C1'-N1	5.50	112.60	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2116	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	586	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	2272	U	N3-C2-O2	-5.50	118.35	122.20
21	AA	99	C	N1-C2-O2	5.50	122.20	118.90
21	AA	1344	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1109	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	2164	C	N1-C2-O2	5.50	122.20	118.90
21	AA	36	C	C5'-C4'-C3'	-5.50	107.21	116.00
21	AA	693	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	1266	G	C1'-O4'-C4'	-5.50	105.50	109.90
21	AA	869	G	C3'-C2'-C1'	5.49	105.89	101.50
54	BA	190	A	N1-C6-N6	-5.49	115.30	118.60
54	BA	1176	U	N3-C2-O2	-5.49	118.35	122.20
54	BA	1345	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	1489	C	N1-C2-O2	5.49	122.20	118.90
54	BA	355	U	O4'-C1'-N1	5.49	112.59	108.20
21	AA	912	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	970	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	337	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	1294	U	O4'-C1'-N1	5.49	112.59	108.20
21	AA	732	C	N1-C2-O2	5.49	122.19	118.90
21	AA	1249	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	1267	C	N3-C2-O2	-5.49	118.06	121.90
34	BL	33	ARG	NE-CZ-NH1	5.49	123.04	120.30
36	BN	71	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
54	BA	342	A	C5-C6-N1	5.49	120.44	117.70
54	BA	931	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	2033	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	2255	G	N3-C2-N2	-5.49	116.06	119.90
21	AA	1382	C	N1-C2-O2	5.49	122.19	118.90
26	BD	58	ASN	C-N-CA	5.49	135.42	121.70
54	BA	281	C	N1-C2-O2	5.49	122.19	118.90
21	AA	415	A	O4'-C1'-N9	5.49	112.59	108.20
21	AA	941	G	N9-C1'-C2'	-5.49	105.97	112.00
54	BA	823	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1213	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	2420	C	N1-C2-O2	5.49	122.19	118.90
54	BA	2537	U	C4'-C3'-C2'	-5.49	97.11	102.60
54	BA	2573	C	C1'-O4'-C4'	-5.49	105.51	109.90
54	BA	1877	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	13	U	O4'-C1'-N1	5.48	112.59	108.20
21	AA	760	G	O4'-C1'-N9	5.48	112.59	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	17	U	N3-C2-O2	-5.48	118.36	122.20
24	A3	62	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	339	U	O4'-C1'-N1	5.48	112.59	108.20
54	BA	393	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	1602	U	P-O3'-C3'	5.48	126.28	119.70
21	AA	857	C	N1-C2-O2	5.48	122.19	118.90
54	BA	1007	C	N1-C2-O2	5.48	122.19	118.90
54	BA	2447	G	C1'-O4'-C4'	-5.48	105.52	109.90
21	AA	143	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	982	C	O4'-C1'-N1	5.48	112.58	108.20
55	BB	69	G	N1-C6-O6	-5.48	116.61	119.90
21	AA	43	C	N3-C2-O2	-5.48	118.07	121.90
54	BA	1594	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	1898	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2426	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1781	U	N3-C2-O2	-5.48	118.37	122.20
54	BA	1967	C	O4'-C1'-N1	5.48	112.58	108.20
55	BB	104	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	96	U	O4'-C1'-N1	5.47	112.58	108.20
21	AA	1257	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	66	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	732	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	1272	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	92	U	O4'-C1'-N1	5.47	112.58	108.20
21	AA	520	A	C6-C5-N7	5.47	136.13	132.30
54	BA	168	G	N3-C2-N2	-5.47	116.07	119.90
54	BA	205	G	C5-C6-N1	5.47	114.24	111.50
54	BA	1794	A	C6-C5-N7	5.47	136.13	132.30
54	BA	2465	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	2596	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	2610	C	N1-C2-O2	5.47	122.18	118.90
21	AA	164	G	C1'-O4'-C4'	-5.47	105.53	109.90
54	BA	1386	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	832	G	N3-C2-N2	-5.47	116.07	119.90
54	BA	371	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	1509	A	O4'-C1'-N9	5.47	112.57	108.20
54	BA	1895	C	N1-C2-O2	5.47	122.18	118.90
54	BA	1895	C	O4'-C1'-N1	5.47	112.57	108.20
54	BA	2896	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	58	G	O4'-C1'-N9	5.46	112.57	108.20
54	BA	1129	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1152	C	O4'-C1'-N1	5.46	112.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2310	C	N1-C2-O2	5.46	122.18	118.90
54	BA	2527	C	N1-C2-O2	5.46	122.18	118.90
54	BA	2903	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1627	G	N3-C4-C5	-5.46	125.87	128.60
54	BA	2769	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	614	A	C1'-O4'-C4'	-5.46	105.53	109.90
54	BA	706	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	229	C	N1-C2-O2	5.46	122.18	118.90
54	BA	1936	A	P-O3'-C3'	5.46	126.25	119.70
13	AN	13	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	179	C	N1-C2-O2	5.46	122.17	118.90
54	BA	525	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1933	G	C8-N9-C4	-5.46	104.22	106.40
54	BA	2676	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	2885	G	N1-C6-O6	-5.46	116.62	119.90
21	AA	282	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	396	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	640	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	1039	G	N1-C6-O6	-5.46	116.63	119.90
21	AA	1531	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2434	A	C6-C5-N7	5.46	136.12	132.30
54	BA	676	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2212	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	429	U	C5-C6-N1	-5.45	119.97	122.70
25	BC	269	ARG	NE-CZ-NH1	5.45	123.03	120.30
54	BA	1020	A	C4-C5-C6	-5.45	114.27	117.00
6	AG	69	ARG	NE-CZ-NH1	5.45	123.03	120.30
16	AQ	76	ARG	NE-CZ-NH1	5.45	123.03	120.30
54	BA	364	C	N1-C2-O2	5.45	122.17	118.90
54	BA	1162	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	1409	U	O4'-C1'-N1	5.45	112.56	108.20
54	BA	2660	A	O4'-C1'-N9	5.45	112.56	108.20
54	BA	1854	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	923	G	N1-C6-O6	-5.45	116.63	119.90
11	AL	85	ARG	NE-CZ-NH1	5.45	123.02	120.30
21	AA	686	U	N3-C2-O2	-5.45	118.39	122.20
54	BA	881	G	N3-C2-N2	-5.45	116.09	119.90
54	BA	1580	A	C6-C5-N7	5.45	136.11	132.30
54	BA	1743	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	1799	G	N3-C4-C5	-5.45	125.88	128.60
54	BA	2734	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	1092	A	C4-C5-C6	-5.44	114.28	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	192	C	N1-C2-O2	5.44	122.17	118.90
54	BA	1291	C	N3-C4-C5	5.44	124.08	121.90
21	AA	37	U	N3-C2-O2	-5.44	118.39	122.20
21	AA	1000	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	1437	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1799	G	C8-N9-C4	-5.44	104.22	106.40
54	BA	2286	G	N1-C6-O6	-5.44	116.63	119.90
21	AA	156	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	503	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	372	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	2220	U	O4'-C1'-N1	5.44	112.55	108.20
21	AA	313	A	C6-C5-N7	5.44	136.11	132.30
21	AA	720	C	N1-C2-O2	5.44	122.16	118.90
21	AA	1099	G	C5-C6-N1	5.44	114.22	111.50
53	B4	4	ARG	NE-CZ-NH1	5.44	123.02	120.30
54	BA	882	G	N3-C2-N2	-5.44	116.09	119.90
54	BA	1012	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	1958	C	N3-C2-O2	-5.44	118.09	121.90
3	AD	42	ALA	C-N-CA	5.44	135.29	121.70
54	BA	492	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	831	G	C5-C6-N1	5.44	114.22	111.50
54	BA	1211	C	N1-C2-O2	5.44	122.16	118.90
21	AA	1251	A	C6-C5-N7	5.43	136.10	132.30
54	BA	175	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	2430	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	1194	U	N3-C2-O2	-5.43	118.40	122.20
21	AA	1324	A	C5-C6-N1	5.43	120.42	117.70
54	BA	443	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	2838	G	C4'-C3'-C2'	-5.43	97.17	102.60
18	AS	77	ARG	NE-CZ-NH1	5.43	123.02	120.30
21	AA	209	U	N3-C2-O2	-5.43	118.40	122.20
24	A3	42	C	N1-C2-O2	5.43	122.16	118.90
54	BA	1089	A	C3'-C2'-C1'	5.43	105.84	101.50
54	BA	1317	G	C1'-O4'-C4'	-5.43	105.56	109.90
54	BA	1519	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	2785	C	O4'-C1'-N1	5.43	112.55	108.20
21	AA	818	G	C5-C6-N1	5.43	114.22	111.50
54	BA	2459	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	274	A	C6-C5-N7	5.43	136.10	132.30
54	BA	1857	G	O4'-C1'-N9	5.43	112.54	108.20
21	AA	517	G	O4'-C1'-N9	5.43	112.54	108.20
21	AA	722	G	N3-C4-C5	-5.43	125.89	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	765	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	1020	G	N1-C6-O6	-5.43	116.64	119.90
22	A1	74	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	1748	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	2776	A	O4'-C1'-N9	5.43	112.54	108.20
54	BA	2838	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	1036	A	C4-C5-C6	-5.42	114.29	117.00
28	BF	94	ARG	NE-CZ-NH1	5.42	123.01	120.30
54	BA	1000	A	C1'-O4'-C4'	-5.42	105.56	109.90
54	BA	1367	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1542	U	O4'-C1'-N1	5.42	112.54	108.20
54	BA	2065	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	2889	C	O4'-C1'-N1	5.42	112.54	108.20
21	AA	845	A	C5'-C4'-O4'	5.42	115.61	109.10
54	BA	574	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2040	G	N3-C2-N2	-5.42	116.10	119.90
21	AA	560	A	C3'-C2'-C1'	5.42	105.84	101.50
21	AA	765	G	N3-C4-C5	-5.42	125.89	128.60
42	BT	73	ARG	NE-CZ-NH1	5.42	123.01	120.30
54	BA	81	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	556	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2066	C	O4'-C1'-N1	5.42	112.54	108.20
21	AA	108	G	N3-C4-C5	-5.42	125.89	128.60
21	AA	993	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	484	C	N3-C2-O2	-5.42	118.11	121.90
9	AJ	72	ARG	CD-NE-CZ	5.42	131.19	123.60
21	AA	1183	U	N3-C2-O2	-5.42	118.41	122.20
24	A3	16	C	C3'-C2'-C1'	5.42	105.84	101.50
54	BA	1101	U	O4'-C1'-N1	5.42	112.53	108.20
54	BA	1259	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	2700	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1377	A	C4-C5-C6	-5.42	114.29	117.00
35	BM	40	ARG	NE-CZ-NH1	5.42	123.01	120.30
54	BA	899	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2516	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2805	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	1794	A	O4'-C1'-N9	5.42	112.53	108.20
54	BA	2342	C	N1-C2-O2	5.41	122.15	118.90
54	BA	2760	C	N3-C4-C5	5.41	124.07	121.90
21	AA	430	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	300	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1233	C	O4'-C1'-N1	5.41	112.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1555	G	N3-C4-C5	-5.41	125.89	128.60
54	BA	1944	U	P-O3'-C3'	5.41	126.19	119.70
54	BA	1865	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2432	A	O4'-C1'-N9	5.41	112.53	108.20
55	BB	53	A	N1-C6-N6	-5.41	115.36	118.60
21	AA	1519	A	C4-C5-C6	-5.41	114.30	117.00
24	A3	67	C	N1-C2-O2	5.41	122.14	118.90
21	AA	575	G	P-O3'-C3'	5.41	126.19	119.70
21	AA	1080	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	1218	C	N1-C2-O2	5.41	122.14	118.90
54	BA	1089	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1398	C	O4'-C1'-N1	5.41	112.52	108.20
54	BA	1862	G	C8-N9-C4	-5.41	104.24	106.40
54	BA	2070	A	C6-C5-N7	5.41	136.08	132.30
54	BA	2080	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	818	G	N3-C4-C5	-5.40	125.90	128.60
21	AA	1129	C	C3'-C2'-C1'	5.40	105.82	101.50
28	BF	114	ARG	NE-CZ-NH1	5.40	123.00	120.30
54	BA	1786	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1832	C	C3'-C2'-C1'	5.40	105.82	101.50
55	BB	4	C	O4'-C1'-N1	5.40	112.52	108.20
13	AN	63	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	995	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	1226	C	N1-C2-O2	5.40	122.14	118.90
54	BA	503	A	C3'-C2'-C1'	5.40	105.82	101.50
54	BA	2134	A	C6-C5-N7	5.40	136.08	132.30
18	AS	54	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	124	C	C1'-O4'-C4'	-5.40	105.58	109.90
54	BA	615	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	1189	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1363	C	N1-C2-O2	5.40	122.14	118.90
4	AE	28	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	477	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	569	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	1579	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	1229	A	C5'-C4'-O4'	5.40	115.58	109.10
29	BG	94	ARG	NE-CZ-NH1	5.40	123.00	120.30
54	BA	1086	A	O4'-C1'-N9	5.40	112.52	108.20
54	BA	1536	C	N1-C2-O2	5.40	122.14	118.90
54	BA	1726	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	122	G	N3-C2-N2	-5.40	116.12	119.90
21	AA	924	C	N3-C2-O2	-5.40	118.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	827	U	N3-C2-O2	-5.39	118.42	122.20
21	AA	1192	C	N1-C2-O2	5.39	122.14	118.90
21	AA	1268	G	C5-C6-N1	5.39	114.20	111.50
54	BA	57	C	O4'-C1'-N1	5.39	112.52	108.20
54	BA	490	C	N1-C2-O2	5.39	122.14	118.90
54	BA	665	U	O4'-C1'-N1	5.39	112.52	108.20
54	BA	2499	C	O4'-C1'-N1	5.39	112.52	108.20
3	AD	153	ARG	NE-CZ-NH2	-5.39	117.60	120.30
21	AA	1453	G	N3-C4-C5	-5.39	125.90	128.60
54	BA	2511	U	O4'-C1'-N1	5.39	112.51	108.20
24	A3	57	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	33	C	O4'-C4'-C3'	5.39	110.41	106.10
54	BA	351	C	N1-C2-O2	5.39	122.14	118.90
54	BA	2112	G	N1-C6-O6	-5.39	116.67	119.90
8	AI	108	ARG	NE-CZ-NH1	5.39	122.99	120.30
21	AA	1099	G	N1-C6-O6	-5.39	116.67	119.90
21	AA	1156	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	2813	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	1812	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	2762	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1325	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1828	G	O4'-C1'-N9	5.39	112.51	108.20
21	AA	1224	U	N3-C2-O2	-5.38	118.43	122.20
21	AA	1259	C	N1-C2-O2	5.38	122.13	118.90
54	BA	2198	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	365	U	C1'-O4'-C4'	-5.38	105.59	109.90
54	BA	262	A	C4-C5-C6	-5.38	114.31	117.00
25	BC	100	ARG	NE-CZ-NH1	5.38	122.99	120.30
21	AA	118	U	N3-C2-O2	-5.38	118.43	122.20
54	BA	2667	C	N1-C2-O2	5.38	122.13	118.90
21	AA	372	C	N3-C2-O2	-5.38	118.14	121.90
21	AA	981	U	O4'-C1'-N1	5.38	112.50	108.20
24	A3	71	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	97	C	O4'-C1'-N1	5.38	112.50	108.20
54	BA	1121	C	O4'-C1'-N1	5.38	112.50	108.20
54	BA	2350	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	2611	C	N1-C2-O2	5.38	122.13	118.90
14	AO	57	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BA	143	C	N1-C2-O2	5.38	122.12	118.90
54	BA	420	C	N1-C2-O2	5.38	122.13	118.90
21	AA	1200	C	N1-C2-O2	5.38	122.12	118.90
21	AA	1487	G	C5-C6-N1	5.38	114.19	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1521	G	C5-C6-N1	5.38	114.19	111.50
54	BA	2856	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	726	G	N3-C4-C5	-5.37	125.91	128.60
54	BA	2062	A	C4-C5-C6	-5.37	114.31	117.00
55	BB	90	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	149	A	C4-C5-C6	-5.37	114.31	117.00
21	AA	907	A	C4-C5-C6	-5.37	114.31	117.00
24	A3	69	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	249	C	O4'-C1'-N1	5.37	112.50	108.20
21	AA	1150	A	C6-C5-N7	5.37	136.06	132.30
54	BA	2009	A	C4-C5-C6	-5.37	114.31	117.00
21	AA	171	A	C6-C5-N7	5.37	136.06	132.30
54	BA	1563	U	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2100	G	N3-C2-N2	-5.37	116.14	119.90
21	AA	35	G	N3-C4-C5	-5.37	125.92	128.60
21	AA	251	G	N3-C4-C5	-5.37	125.92	128.60
21	AA	1474	U	O4'-C1'-N1	5.37	112.49	108.20
32	BJ	69	ARG	NE-CZ-NH1	5.37	122.98	120.30
54	BA	1615	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2486	C	N1-C2-O2	5.37	122.12	118.90
54	BA	1628	G	N3-C2-N2	-5.36	116.15	119.90
54	BA	1644	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2680	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2861	U	O4'-C1'-N1	5.36	112.49	108.20
55	BB	89	U	N3-C2-O2	-5.36	118.45	122.20
21	AA	153	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	1532	U	C1'-O4'-C4'	-5.36	105.61	109.90
54	BA	2135	A	C4-C5-C6	-5.36	114.32	117.00
3	AD	103	ARG	CD-NE-CZ	5.36	131.10	123.60
21	AA	347	G	N3-C4-C5	-5.36	125.92	128.60
21	AA	1055	A	P-O3'-C3'	5.36	126.13	119.70
55	BB	41	G	N3-C4-C5	-5.36	125.92	128.60
21	AA	189	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2209	G	N1-C6-O6	-5.36	116.69	119.90
55	BB	101	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	456	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	1202	U	O4'-C1'-N1	5.36	112.49	108.20
21	AA	1346	A	C1'-O4'-C4'	-5.36	105.61	109.90
54	BA	141	G	N1-C6-O6	-5.36	116.69	119.90
54	BA	575	A	C6-C5-N7	5.36	136.05	132.30
54	BA	1969	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2458	G	C5-C6-N1	5.36	114.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	46	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	784	A	C6-C5-N7	5.36	136.05	132.30
21	AA	1294	G	N1-C6-O6	-5.36	116.69	119.90
21	AA	1403	C	N1-C2-O2	5.36	122.11	118.90
21	AA	1461	G	N1-C6-O6	-5.36	116.69	119.90
42	BT	6	ARG	NE-CZ-NH2	5.36	122.98	120.30
54	BA	1752	C	N1-C2-O2	5.36	122.11	118.90
54	BA	2711	A	C6-C5-N7	5.36	136.05	132.30
54	BA	2824	C	N3-C2-O2	-5.36	118.15	121.90
51	B2	34	ARG	NE-CZ-NH2	-5.35	117.62	120.30
21	AA	463	U	N3-C2-O2	-5.35	118.45	122.20
21	AA	806	C	C1'-O4'-C4'	-5.35	105.62	109.90
21	AA	1151	A	C5'-C4'-C3'	-5.35	107.44	116.00
54	BA	1053	C	N3-C2-O2	-5.35	118.15	121.90
54	BA	2286	G	C1'-O4'-C4'	-5.35	105.62	109.90
54	BA	2517	C	N1-C2-O2	5.35	122.11	118.90
21	AA	627	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	457	A	C6-C5-N7	5.35	136.05	132.30
54	BA	1011	G	O4'-C1'-N9	5.35	112.48	108.20
54	BA	1905	C	N1-C2-O2	5.35	122.11	118.90
21	AA	999	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	31	C	N1-C2-O2	5.35	122.11	118.90
54	BA	207	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	227	A	C6-C5-N7	5.35	136.04	132.30
54	BA	368	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	1175	A	C6-C5-N7	5.35	136.04	132.30
54	BA	1884	G	O4'-C1'-N9	5.35	112.48	108.20
21	AA	302	G	N1-C6-O6	-5.35	116.69	119.90
21	AA	512	U	C5-C6-N1	-5.35	120.03	122.70
21	AA	1169	A	C4-C5-C6	-5.35	114.33	117.00
28	BF	29	ARG	CD-NE-CZ	5.35	131.09	123.60
54	BA	74	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	502	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	787	C	N3-C4-C5	5.35	124.04	121.90
54	BA	2395	C	O4'-C1'-N1	5.35	112.48	108.20
55	BB	26	C	O4'-C1'-N1	5.35	112.48	108.20
14	AO	62	ARG	NE-CZ-NH1	5.35	122.97	120.30
21	AA	1048	G	N1-C6-O6	-5.35	116.69	119.90
34	BL	69	ARG	NE-CZ-NH1	5.35	122.97	120.30
21	AA	499	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	703	G	C8-N9-C4	-5.34	104.26	106.40
21	AA	1287	A	C6-C5-N7	5.34	136.04	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2321	U	N3-C2-O2	-5.34	118.46	122.20
21	AA	758	C	N1-C2-O2	5.34	122.11	118.90
24	A3	54	G	N3-C2-N2	-5.34	116.16	119.90
54	BA	12	U	O4'-C1'-N1	5.34	112.47	108.20
11	AL	55	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BA	724	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1122	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	2172	U	C1'-O4'-C4'	-5.34	105.63	109.90
54	BA	2620	C	N3-C2-O2	-5.34	118.16	121.90
55	BB	80	U	O4'-C1'-N1	5.34	112.47	108.20
21	AA	518	C	N1-C2-O2	5.34	122.10	118.90
54	BA	109	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	986	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1103	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	560	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1332	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	2394	C	N1-C2-O2	5.34	122.10	118.90
54	BA	2612	C	N1-C2-O2	5.34	122.10	118.90
21	AA	1216	A	O4'-C1'-N9	5.34	112.47	108.20
22	A1	4	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	441	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	783	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	901	C	N1-C2-O2	5.34	122.10	118.90
54	BA	336	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	2480	C	N1-C2-O2	5.33	122.10	118.90
21	AA	697	U	O4'-C1'-N1	5.33	112.47	108.20
21	AA	1190	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	49	A	O4'-C1'-N9	5.33	112.47	108.20
54	BA	338	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	1760	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	2275	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	2297	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	1217	C	C1'-O4'-C4'	-5.33	105.64	109.90
54	BA	2639	A	C6-C5-N7	5.33	136.03	132.30
54	BA	354	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	440	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	572	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	753	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	890	G	O4'-C1'-N9	5.33	112.46	108.20
54	BA	1604	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	1055	A	C4-C5-C6	-5.33	114.34	117.00
38	BP	97	TYR	CB-CG-CD2	-5.33	117.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	808	C	N1-C2-O2	5.33	122.10	118.90
54	BA	576	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	962	G	N3-C2-N2	-5.33	116.17	119.90
21	AA	86	G	N3-C4-C5	-5.32	125.94	128.60
21	AA	618	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	444	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	2439	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	355	C	N3-C2-O2	-5.32	118.17	121.90
21	AA	588	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	1046	A	C6-C5-N7	5.32	136.03	132.30
24	A3	77	A	C6-C5-N7	5.32	136.03	132.30
55	BB	19	C	O4'-C1'-N1	5.32	112.46	108.20
21	AA	654	G	N3-C2-N2	-5.32	116.18	119.90
21	AA	890	G	N3-C4-C5	-5.32	125.94	128.60
54	BA	1691	C	N3-C2-O2	-5.32	118.18	121.90
54	BA	2179	C	N1-C2-O2	5.32	122.09	118.90
22	A1	75	C	N1-C2-O2	5.32	122.09	118.90
20	AU	33	ARG	NE-CZ-NH1	5.32	122.96	120.30
39	BQ	57	ARG	NE-CZ-NH1	5.32	122.96	120.30
54	BA	544	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1217	U	O4'-C1'-N1	5.32	112.45	108.20
54	BA	2390	U	O4'-C1'-N1	5.32	112.45	108.20
54	BA	2826	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	149	A	C5'-C4'-O4'	5.32	115.48	109.10
54	BA	218	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	1245	G	N3-C2-N2	-5.32	116.18	119.90
54	BA	2880	C	N1-C2-O2	5.32	122.09	118.90
21	AA	316	C	N1-C2-O2	5.31	122.09	118.90
54	BA	2424	C	N1-C2-O2	5.31	122.09	118.90
21	AA	641	U	C3'-C2'-C1'	5.31	105.75	101.50
54	BA	672	C	N1-C2-O2	5.31	122.09	118.90
54	BA	1499	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	1819	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	2443	C	C5'-C4'-O4'	5.31	115.47	109.10
21	AA	5	U	N1-C2-N3	5.31	118.09	114.90
21	AA	559	A	C4-C5-C6	-5.31	114.34	117.00
33	BK	32	TYR	CB-CG-CD1	-5.31	117.81	121.00
54	BA	405	U	N3-C2-O2	-5.31	118.48	122.20
54	BA	1317	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	705	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	734	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	1098	A	C4-C5-C6	-5.31	114.34	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1967	C	N3-C4-C5	5.31	124.02	121.90
54	BA	1985	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	493	A	O4'-C1'-N9	5.31	112.45	108.20
21	AA	934	C	N1-C2-O2	5.31	122.08	118.90
54	BA	580	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1612	C	N1-C2-O2	5.31	122.08	118.90
54	BA	2457	U	O4'-C1'-N1	5.31	112.44	108.20
21	AA	1237	C	N1-C2-O2	5.31	122.08	118.90
54	BA	2284	A	C4-C5-C6	-5.31	114.35	117.00
21	AA	454	G	N3-C2-N2	-5.30	116.19	119.90
21	AA	535	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	922	G	N3-C4-C5	-5.30	125.95	128.60
54	BA	1488	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	2685	G	N3-C2-N2	-5.30	116.19	119.90
54	BA	1104	C	C5'-C4'-O4'	5.30	115.46	109.10
21	AA	438	U	N3-C2-O2	-5.30	118.49	122.20
21	AA	1222	G	N3-C2-N2	-5.30	116.19	119.90
46	BX	44	ARG	NE-CZ-NH2	-5.30	117.65	120.30
54	BA	2090	A	C4-C5-C6	-5.30	114.35	117.00
3	AD	48	SER	C-N-CA	5.30	134.95	121.70
21	AA	258	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	496	A	O4'-C1'-N9	5.30	112.44	108.20
54	BA	344	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1597	A	C6-C5-N7	5.30	136.01	132.30
21	AA	269	C	O4'-C1'-N1	5.30	112.44	108.20
21	AA	1446	A	O4'-C1'-N9	5.30	112.44	108.20
21	AA	1490	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	129	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	1286	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	1361	G	N1-C6-O6	-5.29	116.72	119.90
54	BA	324	A	C6-C5-N7	5.29	136.01	132.30
54	BA	2160	C	N1-C2-O2	5.29	122.08	118.90
21	AA	416	G	O4'-C1'-N9	5.29	112.44	108.20
54	BA	508	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	631	A	C6-C5-N7	5.29	136.01	132.30
54	BA	2776	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	2863	C	N3-C2-O2	-5.29	118.19	121.90
55	BB	13	G	N1-C6-O6	-5.29	116.72	119.90
9	AJ	16	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
21	AA	871	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1457	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2503	A	C4-C5-C6	-5.29	114.35	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2568	U	O4'-C1'-N1	5.29	112.43	108.20
21	AA	53	A	C6-C5-N7	5.29	136.00	132.30
21	AA	83	C	N1-C2-O2	5.29	122.07	118.90
21	AA	188	C	N1-C2-O2	5.29	122.07	118.90
54	BA	1977	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	480	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	601	C	N1-C2-O2	5.29	122.07	118.90
54	BA	1035	U	N3-C2-O2	-5.29	118.50	122.20
55	BB	28	C	N1-C2-O2	5.29	122.07	118.90
21	AA	236	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	790	U	C5-C6-N1	-5.29	120.06	122.70
54	BA	1014	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	1293	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1446	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1615	C	N1-C2-O2	5.29	122.07	118.90
54	BA	2240	U	O4'-C1'-N1	5.29	112.43	108.20
24	A3	74	A	O4'-C1'-N9	5.28	112.43	108.20
54	BA	359	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	2431	U	C5-C6-N1	-5.28	120.06	122.70
21	AA	1084	G	N1-C6-O6	-5.28	116.73	119.90
21	AA	1096	C	N1-C2-O2	5.28	122.07	118.90
54	BA	1227	G	O4'-C1'-N9	5.28	112.43	108.20
54	BA	1993	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2144	G	N1-C6-O6	-5.28	116.73	119.90
55	BB	44	G	N1-C6-O6	-5.28	116.73	119.90
21	AA	195	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	383	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	706	A	C6-C5-N7	5.28	136.00	132.30
21	AA	1190	G	P-O3'-C3'	5.28	126.04	119.70
54	BA	265	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	447	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	634	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	1288	G	N3-C4-C5	-5.28	125.96	128.60
54	BA	2443	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2601	C	N1-C2-O2	5.28	122.07	118.90
54	BA	405	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2155	U	N3-C2-O2	-5.28	118.50	122.20
54	BA	2627	G	N9-C4-C5	5.28	107.51	105.40
54	BA	2691	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2703	C	N3-C2-O2	-5.28	118.21	121.90
21	AA	216	U	N3-C2-O2	-5.28	118.51	122.20
21	AA	575	G	N1-C6-O6	-5.28	116.73	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1135	U	O4'-C1'-N1	5.28	112.42	108.20
21	AA	1479	C	C3'-C2'-C1'	5.28	105.72	101.50
35	BM	50	ARG	NE-CZ-NH1	5.28	122.94	120.30
54	BA	1157	G	N1-C6-O6	-5.28	116.73	119.90
21	AA	1132	C	N1-C2-O2	5.27	122.06	118.90
21	AA	57	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	391	A	N1-C6-N6	-5.27	115.44	118.60
54	BA	664	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	1000	A	C6-C5-N7	5.27	135.99	132.30
54	BA	1436	G	O4'-C1'-N9	5.27	112.42	108.20
54	BA	1659	G	N1-C6-O6	-5.27	116.74	119.90
21	AA	988	G	N3-C4-C5	-5.27	125.96	128.60
6	AG	110	ARG	NE-CZ-NH2	-5.27	117.67	120.30
21	AA	432	A	O4'-C1'-N9	5.27	112.42	108.20
21	AA	586	C	O4'-C1'-N1	5.27	112.42	108.20
21	AA	612	C	N1-C2-O2	5.27	122.06	118.90
21	AA	860	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	4	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	310	A	C4-C5-C6	-5.27	114.37	117.00
54	BA	430	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	516	C	N1-C2-O2	5.27	122.06	118.90
54	BA	1051	G	C1'-O4'-C4'	-5.27	105.69	109.90
54	BA	1412	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2023	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2530	A	C5'-C4'-C3'	-5.27	107.57	116.00
21	AA	699	C	N1-C2-O2	5.27	122.06	118.90
21	AA	1469	C	N1-C2-O2	5.27	122.06	118.90
54	BA	639	U	N3-C2-O2	-5.27	118.51	122.20
54	BA	1681	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	288	U	O4'-C1'-N1	5.27	112.41	108.20
11	AL	93	ARG	NE-CZ-NH1	5.26	122.93	120.30
21	AA	1033	G	O4'-C1'-N9	5.26	112.41	108.20
21	AA	1076	U	C5-C6-N1	-5.26	120.07	122.70
36	BN	22	ARG	NE-CZ-NH1	5.26	122.93	120.30
54	BA	251	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1433	A	C6-C5-N7	5.26	135.99	132.30
54	BA	2265	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	1412	C	O4'-C1'-N1	5.26	112.41	108.20
25	BC	62	ARG	NE-CZ-NH1	5.26	122.93	120.30
54	BA	1202	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	1500	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	751	A	C4-C5-C6	-5.26	114.37	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	932	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	1071	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	1478	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	1677	A	C4-C5-C6	-5.26	114.37	117.00
55	BB	69	G	O4'-C1'-N9	5.26	112.41	108.20
21	AA	1455	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	47	C	N1-C2-O2	5.26	122.06	118.90
54	BA	335	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	242	G	N1-C6-O6	-5.26	116.75	119.90
54	BA	1395	A	C1'-O4'-C4'	-5.26	105.69	109.90
54	BA	1558	C	N3-C2-O2	-5.26	118.22	121.90
54	BA	2097	A	C6-C5-N7	5.26	135.98	132.30
54	BA	2576	G	N3-C4-C5	-5.26	125.97	128.60
21	AA	593	U	C5-C6-N1	-5.26	120.07	122.70
21	AA	616	G	N3-C2-N2	-5.26	116.22	119.90
21	AA	1336	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	360	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	727	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1308	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2147	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	449	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	817	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2307	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	1054	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	1256	A	C4-C5-C6	-5.25	114.37	117.00
22	A1	25	C	N1-C2-O2	5.25	122.05	118.90
54	BA	759	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	1419	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	2491	U	N3-C2-O2	-5.25	118.52	122.20
54	BA	2576	G	C5-C6-N1	5.25	114.13	111.50
30	BH	27	ARG	NE-CZ-NH1	5.25	122.93	120.30
54	BA	1029	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	1269	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	2501	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2644	G	O4'-C1'-N9	5.25	112.40	108.20
21	AA	584	G	N3-C4-C5	-5.25	125.98	128.60
23	A2	87	U	C5-C6-N1	-5.25	120.08	122.70
54	BA	75	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	1524	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	547	A	C6-C5-N7	5.25	135.97	132.30
21	AA	665	A	C6-C5-N7	5.25	135.97	132.30
21	AA	797	C	N3-C2-O2	-5.25	118.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BO	102	ARG	NE-CZ-NH1	5.25	122.92	120.30
54	BA	888	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1625	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2214	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2329	U	N3-C2-O2	-5.25	118.53	122.20
54	BA	22	C	N1-C2-O2	5.25	122.05	118.90
54	BA	350	G	C5-C6-N1	5.25	114.12	111.50
54	BA	2627	G	N3-C2-N2	-5.25	116.23	119.90
21	AA	299	G	N1-C6-O6	-5.24	116.75	119.90
54	BA	1193	G	O4'-C4'-C3'	5.24	110.30	106.10
54	BA	814	C	N3-C2-O2	-5.24	118.23	121.90
54	BA	1768	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2391	G	O4'-C1'-N9	5.24	112.39	108.20
21	AA	792	A	C1'-O4'-C4'	-5.24	105.71	109.90
21	AA	1082	A	C6-C5-N7	5.24	135.97	132.30
21	AA	1284	C	N1-C2-O2	5.24	122.04	118.90
54	BA	445	C	N3-C4-C5	5.24	124.00	121.90
21	AA	531	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	818	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	1811	G	O4'-C1'-N9	5.24	112.39	108.20
54	BA	1815	A	C6-C5-N7	5.24	135.97	132.30
21	AA	1159	U	C1'-O4'-C4'	-5.23	105.71	109.90
12	AM	108	ARG	NE-CZ-NH2	-5.23	117.68	120.30
21	AA	148	G	C5-C6-N1	5.23	114.12	111.50
21	AA	935	A	C6-C5-N7	5.23	135.96	132.30
21	AA	1038	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	660	C	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2057	G	C5-C6-N1	5.23	114.12	111.50
54	BA	2105	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2807	U	C5-C6-N1	-5.23	120.08	122.70
21	AA	248	C	N1-C2-O2	5.23	122.04	118.90
21	AA	950	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	471	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	1298	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	2185	U	O4'-C1'-N1	5.23	112.38	108.20
54	BA	2318	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	306	A	C6-C5-N7	5.23	135.96	132.30
21	AA	381	C	N1-C2-O2	5.23	122.04	118.90
36	BN	46	ARG	NE-CZ-NH1	5.23	122.92	120.30
54	BA	456	C	N1-C2-O2	5.23	122.04	118.90
54	BA	1763	G	N3-C4-C5	-5.23	125.98	128.60
21	AA	385	C	O4'-C1'-N1	5.23	112.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	398	U	O4'-C1'-N1	5.23	112.38	108.20
21	AA	1250	A	C1'-O4'-C4'	-5.23	105.72	109.90
54	BA	1183	U	O4'-C1'-N1	5.23	112.38	108.20
21	AA	534	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	904	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	2575	C	N3-C2-O2	-5.23	118.24	121.90
55	BB	118	C	O4'-C1'-N1	5.23	112.38	108.20
21	AA	651	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1727	C	N3-C2-O2	-5.22	118.24	121.90
54	BA	2013	A	N1-C6-N6	-5.22	115.47	118.60
54	BA	2539	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2807	U	O4'-C1'-N1	5.22	112.38	108.20
55	BB	27	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	367	G	N3-C4-C5	-5.22	125.99	128.60
54	BA	849	A	C6-C5-N7	5.22	135.96	132.30
54	BA	1263	U	N3-C2-O2	-5.22	118.54	122.20
54	BA	2219	U	O4'-C1'-N1	5.22	112.38	108.20
55	BB	83	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	482	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	935	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2133	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	2551	C	N1-C2-O2	5.22	122.03	118.90
54	BA	681	G	N3-C4-C5	-5.22	125.99	128.60
54	BA	1595	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2418	A	C6-C5-N7	5.22	135.95	132.30
54	BA	2533	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	58	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	2599	G	N3-C4-C5	-5.22	125.99	128.60
11	AL	86	VAL	C-N-CA	5.22	134.74	121.70
21	AA	47	C	N1-C2-O2	5.22	122.03	118.90
54	BA	421	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1376	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1713	A	P-O3'-C3'	5.22	125.96	119.70
54	BA	2823	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	1395	C	N1-C2-O2	5.21	122.03	118.90
54	BA	331	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2024	G	O4'-C1'-N9	5.21	112.37	108.20
54	BA	2102	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	2144	G	C5-C6-N1	5.21	114.11	111.50
55	BB	24	G	O4'-C1'-N9	5.21	112.37	108.20
55	BB	76	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	1451	C	C2'-C3'-O3'	5.21	122.04	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1476	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2864	G	N1-C6-O6	-5.21	116.77	119.90
21	AA	405	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	529	A	C1'-O4'-C4'	-5.21	105.73	109.90
54	BA	530	G	O4'-C4'-C3'	5.21	110.27	106.10
54	BA	898	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2104	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2716	C	N1-C2-O2	5.21	122.03	118.90
11	AL	109	ARG	NE-CZ-NH2	-5.21	117.69	120.30
21	AA	246	A	C4-C5-C6	-5.21	114.39	117.00
21	AA	505	G	C5'-C4'-O4'	5.21	115.35	109.10
54	BA	1676	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	316	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	975	A	C6-C5-N7	5.21	135.95	132.30
54	BA	1572	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	1873	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	1881	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1994	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2092	U	N3-C2-O2	-5.21	118.55	122.20
35	BM	38	ARG	NE-CZ-NH1	5.21	122.90	120.30
54	BA	435	C	N1-C2-O2	5.21	122.02	118.90
54	BA	736	C	N3-C2-O2	-5.21	118.26	121.90
54	BA	855	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	885	C	O4'-C1'-N1	5.21	112.36	108.20
54	BA	919	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1670	C	N1-C2-O2	5.21	122.02	118.90
54	BA	2213	U	N3-C2-O2	-5.21	118.56	122.20
54	BA	1428	C	N1-C2-O2	5.21	122.02	118.90
54	BA	1694	C	N3-C4-N4	-5.21	114.36	118.00
54	BA	2814	A	C6-C5-N7	5.21	135.94	132.30
6	AG	125	ASP	CB-CG-OD2	5.20	122.98	118.30
21	AA	357	G	O4'-C1'-N9	5.20	112.36	108.20
54	BA	391	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	1454	C	N3-C2-O2	-5.20	118.26	121.90
54	BA	1574	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1997	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2245	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2652	C	O4'-C1'-N1	5.20	112.36	108.20
21	AA	1242	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	2697	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	342	C	N3-C2-O2	-5.20	118.26	121.90
21	AA	610	U	O4'-C1'-N1	5.20	112.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	31	C	N1-C2-O2	5.20	122.02	118.90
54	BA	452	G	C4'-C3'-C2'	-5.20	97.40	102.60
54	BA	2008	C	N1-C2-O2	5.20	122.02	118.90
21	AA	315	A	C6-C5-N7	5.20	135.94	132.30
54	BA	784	G	C1'-O4'-C4'	-5.20	105.74	109.90
54	BA	928	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1305	C	N1-C2-O2	5.20	122.02	118.90
54	BA	2658	C	O4'-C1'-N1	5.20	112.36	108.20
21	AA	1059	C	N1-C2-O2	5.19	122.02	118.90
22	A1	10	G	N1-C6-O6	-5.19	116.78	119.90
54	BA	15	G	O4'-C1'-N9	5.19	112.36	108.20
54	BA	692	C	N1-C2-O2	5.19	122.02	118.90
54	BA	49	A	C4-C5-C6	-5.19	114.40	117.00
55	BB	24	G	C3'-C2'-C1'	5.19	105.65	101.50
21	AA	1389	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1059	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	1803	A	C4-C5-C6	-5.19	114.40	117.00
21	AA	379	C	N1-C2-O2	5.19	122.01	118.90
34	BL	132	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
54	BA	2752	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	2812	G	C5'-C4'-C3'	-5.19	107.70	116.00
21	AA	597	G	N1-C6-O6	-5.19	116.79	119.90
46	BX	71	ARG	NE-CZ-NH1	5.19	122.89	120.30
54	BA	104	A	C4-C5-C6	-5.19	114.41	117.00
55	BB	99	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	208	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	452	G	N3-C4-C5	-5.19	126.01	128.60
54	BA	1473	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	1545	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	1564	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1704	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1600	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	1646	C	N3-C4-C5	5.18	123.97	121.90
54	BA	2114	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2333	A	C3'-C2'-C1'	5.18	105.65	101.50
54	BA	2657	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	237	G	C8-N9-C4	-5.18	104.33	106.40
21	AA	680	C	O4'-C1'-N1	5.18	112.34	108.20
21	AA	1064	G	N3-C4-C5	-5.18	126.01	128.60
21	AA	1379	G	N3-C2-N2	-5.18	116.27	119.90
54	BA	129	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	564	C	N1-C2-O2	5.18	122.01	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	793	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2696	U	O4'-C1'-N1	5.18	112.35	108.20
21	AA	1217	C	N3-C4-C5	5.18	123.97	121.90
26	BD	15	PHE	CB-CG-CD2	5.18	124.43	120.80
54	BA	114	U	N3-C2-O2	-5.18	118.57	122.20
54	BA	882	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	959	A	C4'-C3'-C2'	-5.18	97.42	102.60
24	A3	3	C	N1-C2-O2	5.18	122.01	118.90
54	BA	1675	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	2809	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	1066	C	N1-C2-O2	5.18	122.01	118.90
54	BA	100	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	191	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	196	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2040	G	N9-C4-C5	5.18	107.47	105.40
54	BA	2331	G	O4'-C1'-N9	5.18	112.34	108.20
21	AA	916	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	624	C	N1-C2-O2	5.18	122.01	118.90
54	BA	644	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	722	A	N1-C6-N6	-5.18	115.49	118.60
54	BA	2378	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	634	C	N1-C2-O2	5.17	122.00	118.90
21	AA	1487	G	N3-C2-N2	-5.17	116.28	119.90
54	BA	349	U	O4'-C1'-N1	5.17	112.34	108.20
54	BA	2015	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	2055	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	2362	C	C4'-C3'-C2'	-5.17	97.42	102.60
14	AO	71	ARG	NE-CZ-NH2	-5.17	117.71	120.30
21	AA	722	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	475	C	O4'-C1'-N1	5.17	112.34	108.20
21	AA	953	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	974	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	1350	C	N1-C2-O2	5.17	122.00	118.90
54	BA	67	U	O4'-C1'-N1	5.17	112.34	108.20
21	AA	187	G	C5-C6-N1	5.17	114.08	111.50
54	BA	1732	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1769	U	C4'-C3'-C2'	-5.17	97.43	102.60
55	BB	42	C	N1-C2-O2	5.17	122.00	118.90
21	AA	123	U	C3'-C2'-C1'	5.17	105.63	101.50
21	AA	182	A	C4-C5-C6	-5.17	114.42	117.00
21	AA	1042	A	C6-C5-N7	5.17	135.92	132.30
21	AA	1332	A	N1-C6-N6	-5.17	115.50	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2025	C	N1-C2-O2	5.17	122.00	118.90
54	BA	2137	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	2570	G	N3-C2-N2	-5.17	116.28	119.90
55	BB	12	C	O4'-C1'-N1	5.17	112.33	108.20
21	AA	733	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	1100	C	N1-C2-O2	5.17	122.00	118.90
54	BA	101	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1463	C	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1626	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	2384	U	C5'-C4'-C3'	-5.16	107.74	116.00
54	BA	2643	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	2661	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	2808	G	C1'-O4'-C4'	-5.16	105.77	109.90
54	BA	490	C	N3-C4-C5	5.16	123.97	121.90
23	A2	92	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	2585	U	N3-C2-O2	-5.16	118.59	122.20
8	AI	11	ARG	CD-NE-CZ	5.16	130.82	123.60
54	BA	10	A	O4'-C1'-N9	5.16	112.33	108.20
54	BA	43	G	N3-C2-N2	-5.16	116.29	119.90
54	BA	1680	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1749	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	2873	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	297	G	C5'-C4'-C3'	-5.16	107.75	116.00
54	BA	1893	C	N1-C2-O2	5.16	121.99	118.90
21	AA	1147	C	N3-C2-O2	-5.16	118.29	121.90
51	B2	19	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BA	211	C	O4'-C1'-N1	5.16	112.32	108.20
54	BA	297	G	O4'-C1'-N9	5.16	112.32	108.20
54	BA	514	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1079	C	O4'-C1'-N1	5.16	112.32	108.20
54	BA	1229	C	N3-C2-O2	-5.16	118.29	121.90
54	BA	2428	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	289	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	587	C	N1-C2-O2	5.15	121.99	118.90
3	AD	103	ARG	NE-CZ-NH2	-5.15	117.72	120.30
54	BA	1605	C	N1-C2-O2	5.15	121.99	118.90
54	BA	2199	A	O4'-C1'-N9	5.15	112.32	108.20
20	AU	30	GLU	CA-C-N	5.15	128.53	117.20
21	AA	250	A	C2-N3-C4	5.15	113.17	110.60
21	AA	1328	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	1399	C	N1-C2-O2	5.15	121.99	118.90
54	BA	1018	U	O4'-C1'-N1	5.15	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1051	C	N1-C2-O2	5.15	121.99	118.90
54	BA	69	C	N1-C2-O2	5.15	121.99	118.90
54	BA	834	G	N7-C8-N9	5.15	115.67	113.10
54	BA	2148	G	N3-C2-N2	-5.15	116.30	119.90
21	AA	749	A	C6-C5-N7	5.15	135.90	132.30
21	AA	1214	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	95	A	O4'-C1'-N9	5.15	112.32	108.20
54	BA	1576	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	1579	A	N1-C6-N6	-5.15	115.51	118.60
54	BA	1668	A	C6-C5-N7	5.15	135.90	132.30
54	BA	2456	C	C5'-C4'-O4'	5.15	115.28	109.10
21	AA	584	G	C5-C6-N1	5.15	114.07	111.50
21	AA	1233	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	70	G	C5-C6-N1	5.15	114.07	111.50
46	BX	73	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	394	C	N1-C2-O2	5.14	121.99	118.90
54	BA	1233	C	N1-C2-O2	5.14	121.99	118.90
54	BA	1411	U	O4'-C1'-N1	5.14	112.32	108.20
54	BA	1461	C	N1-C2-O2	5.14	121.99	118.90
54	BA	2462	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2619	C	N3-C2-O2	-5.14	118.30	121.90
55	BB	87	U	C5'-C4'-O4'	5.14	115.27	109.10
6	AG	4	ARG	C-N-CA	5.14	134.56	121.70
21	AA	126	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	242	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	1639	C	N1-C2-O2	5.14	121.99	118.90
54	BA	2041	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	32	C	N1-C2-O2	5.14	121.98	118.90
54	BA	250	G	N3-C2-N2	-5.14	116.30	119.90
55	BB	3	C	N3-C2-O2	-5.14	118.30	121.90
21	AA	86	G	O4'-C1'-N9	5.14	112.31	108.20
21	AA	163	C	P-O3'-C3'	5.14	125.87	119.70
21	AA	284	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	687	C	C4'-C3'-C2'	-5.14	97.46	102.60
54	BA	2298	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2608	G	C5-C6-N1	5.14	114.07	111.50
54	BA	2888	C	N1-C2-O2	5.14	121.98	118.90
21	AA	275	G	N3-C2-N2	-5.14	116.30	119.90
21	AA	1314	C	N1-C2-O2	5.14	121.98	118.90
54	BA	1078	U	O4'-C4'-C3'	5.14	110.21	106.10
54	BA	1666	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	1962	C	N1-C2-O2	5.14	121.98	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2618	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	2649	C	N1-C2-O2	5.14	121.98	118.90
21	AA	881	G	N3-C2-N2	-5.14	116.30	119.90
8	AI	48	ARG	NE-CZ-NH2	-5.13	117.73	120.30
54	BA	155	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	165	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	2052	A	C6-C5-N7	5.13	135.89	132.30
54	BA	2572	A	C4-C5-C6	-5.13	114.43	117.00
55	BB	55	U	O4'-C1'-N1	5.13	112.31	108.20
21	AA	453	G	C5-C6-N1	5.13	114.07	111.50
21	AA	631	C	N1-C2-O2	5.13	121.98	118.90
21	AA	1380	U	C5'-C4'-C3'	-5.13	107.79	116.00
54	BA	53	A	C6-C5-N7	5.13	135.89	132.30
54	BA	105	C	N1-C2-O2	5.13	121.98	118.90
54	BA	530	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1921	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2186	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2542	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	13	U	N3-C2-O2	-5.13	118.61	122.20
21	AA	510	A	C6-C5-N7	5.13	135.89	132.30
54	BA	530	G	N3-C4-C5	-5.13	126.03	128.60
54	BA	595	C	N1-C2-O2	5.13	121.98	118.90
54	BA	1005	C	N1-C2-O2	5.13	121.98	118.90
54	BA	1624	U	C5'-C4'-O4'	5.13	115.26	109.10
54	BA	1874	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2883	A	C1'-O4'-C4'	-5.13	105.80	109.90
21	AA	1191	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	1254	A	C6-C5-N7	5.13	135.89	132.30
54	BA	1006	C	C5'-C4'-O4'	5.13	115.25	109.10
54	BA	1357	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	1884	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2207	C	N1-C2-O2	5.13	121.98	118.90
21	AA	657	U	C5'-C4'-O4'	5.13	115.25	109.10
54	BA	1666	G	O4'-C1'-N9	5.13	112.30	108.20
54	BA	2581	G	N3-C4-C5	-5.13	126.04	128.60
21	AA	394	G	N3-C2-N2	-5.12	116.31	119.90
21	AA	1360	A	C6-C5-N7	5.12	135.89	132.30
29	BG	162	ARG	NE-CZ-NH1	5.12	122.86	120.30
54	BA	590	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1805	A	C4-C5-C6	-5.12	114.44	117.00
55	BB	114	C	N3-C2-O2	-5.12	118.31	121.90
4	AE	104	ILE	C-N-CA	5.12	134.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	350	G	N1-C6-O6	-5.12	116.83	119.90
22	A1	66	A	C6-C5-N7	5.12	135.89	132.30
54	BA	1115	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2603	G	N3-C4-C5	-5.12	126.04	128.60
21	AA	50	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	292	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1724	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1781	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	2805	C	O4'-C1'-N1	5.12	112.30	108.20
21	AA	338	A	C6-C5-N7	5.12	135.88	132.30
21	AA	669	G	O4'-C1'-N9	5.12	112.30	108.20
21	AA	1362	A	O4'-C1'-N9	5.12	112.29	108.20
21	AA	1364	U	N3-C2-O2	-5.12	118.62	122.20
22	A1	3	G	N1-C6-O6	-5.12	116.83	119.90
42	BT	3	ARG	NE-CZ-NH2	-5.12	117.74	120.30
54	BA	540	C	C4'-C3'-C2'	-5.12	97.48	102.60
54	BA	744	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	1950	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1997	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	2406	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2845	U	C5-C6-N1	-5.12	120.14	122.70
21	AA	861	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	144	A	C6-C5-N7	5.12	135.88	132.30
54	BA	758	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	810	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	1219	U	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2115	G	C8-N9-C4	-5.12	104.35	106.40
54	BA	2593	U	O4'-C1'-N1	5.12	112.29	108.20
21	AA	428	G	N3-C2-N2	-5.11	116.32	119.90
54	BA	1926	U	N3-C2-O2	-5.11	118.62	122.20
21	AA	1459	G	C5-C6-N1	5.11	114.06	111.50
54	BA	858	G	N3-C4-C5	-5.11	126.04	128.60
21	AA	883	C	N3-C4-N4	-5.11	114.42	118.00
21	AA	988	G	C8-N9-C4	-5.11	104.36	106.40
21	AA	1473	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	164	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	2062	A	O4'-C1'-N9	5.11	112.29	108.20
21	AA	1239	A	C6-C5-N7	5.11	135.88	132.30
21	AA	1406	U	C1'-O4'-C4'	-5.11	105.81	109.90
54	BA	686	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	955	U	C1'-O4'-C4'	-5.11	105.81	109.90
54	BA	1861	G	C4'-C3'-C2'	-5.11	97.49	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2238	G	N3-C4-C5	-5.11	126.05	128.60
21	AA	730	G	N1-C6-O6	-5.11	116.84	119.90
21	AA	1300	G	C5-C6-N1	5.11	114.05	111.50
22	A1	9	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	1407	G	N1-C6-O6	-5.11	116.84	119.90
54	BA	1715	G	C5-C6-N1	5.11	114.05	111.50
54	BA	732	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	828	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	1480	C	O4'-C1'-N1	5.10	112.28	108.20
3	AD	183	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
15	AP	79	ASN	C-N-CA	5.10	134.46	121.70
21	AA	605	U	C5-C6-N1	-5.10	120.15	122.70
21	AA	1108	G	C5-C6-N1	5.10	114.05	111.50
54	BA	903	C	N1-C2-O2	5.10	121.96	118.90
54	BA	927	A	C6-C5-N7	5.10	135.87	132.30
54	BA	1313	U	C3'-C2'-C1'	5.10	105.58	101.50
54	BA	1388	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	1861	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	2004	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	1474	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	201	G	N3-C2-N2	-5.10	116.33	119.90
21	AA	251	G	C3'-C2'-C1'	5.10	105.58	101.50
21	AA	370	C	N1-C2-O2	5.10	121.96	118.90
21	AA	485	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	764	C	N1-C2-O2	5.10	121.96	118.90
21	AA	872	A	C4-C5-C6	-5.10	114.45	117.00
38	BP	87	ARG	NE-CZ-NH1	5.10	122.85	120.30
54	BA	168	G	O4'-C1'-N9	5.10	112.28	108.20
54	BA	2795	C	N1-C2-O2	5.10	121.96	118.90
21	AA	310	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	1465	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	143	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2317	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2764	A	C4-C5-C6	-5.10	114.45	117.00
25	BC	47	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
54	BA	44	A	O4'-C1'-N9	5.10	112.28	108.20
54	BA	2748	A	C6-C5-N7	5.10	135.87	132.30
21	AA	25	C	N1-C2-O2	5.09	121.96	118.90
21	AA	271	C	C3'-C2'-C1'	5.09	105.58	101.50
21	AA	799	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	1856	U	N3-C2-O2	-5.09	118.63	122.20
54	BA	2855	C	N3-C2-O2	-5.09	118.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1331	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	1695	G	C3'-C2'-C1'	5.09	105.57	101.50
21	AA	46	G	N3-C2-N2	-5.09	116.34	119.90
21	AA	220	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	1787	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	2000	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2558	C	N1-C2-O2	5.09	121.95	118.90
54	BA	747	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	796	C	N1-C2-O2	5.09	121.95	118.90
54	BA	803	U	N1-C2-N3	5.09	117.95	114.90
54	BA	2239	G	C5-C6-N1	5.09	114.05	111.50
54	BA	2683	C	O4'-C1'-N1	5.09	112.27	108.20
10	AK	92	ARG	NE-CZ-NH2	-5.09	117.76	120.30
54	BA	1606	C	N3-C4-C5	5.09	123.94	121.90
54	BA	2072	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2594	C	N1-C2-O2	5.09	121.95	118.90
55	BB	8	C	N1-C2-O2	5.09	121.95	118.90
33	BK	17	ARG	NE-CZ-NH1	5.09	122.84	120.30
54	BA	816	C	N1-C2-O2	5.09	121.95	118.90
54	BA	1852	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1879	C	N1-C2-O2	5.09	121.95	118.90
55	BB	28	C	O4'-C1'-N1	5.09	112.27	108.20
21	AA	553	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1339	G	N3-C2-N2	-5.08	116.34	119.90
54	BA	2305	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	242	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1195	G	N7-C8-N9	5.08	115.64	113.10
54	BA	1599	U	O4'-C1'-N1	5.08	112.27	108.20
54	BA	2063	C	N3-C4-C5	5.08	123.93	121.90
54	BA	2858	C	N1-C2-O2	5.08	121.95	118.90
13	AN	81	ARG	NE-CZ-NH2	-5.08	117.76	120.30
38	BP	71	ARG	NE-CZ-NH1	5.08	122.84	120.30
54	BA	633	A	O4'-C1'-N9	5.08	112.26	108.20
54	BA	679	C	O4'-C1'-N1	5.08	112.27	108.20
54	BA	771	G	O4'-C1'-N9	5.08	112.26	108.20
54	BA	1123	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2466	C	N3-C4-N4	-5.08	114.44	118.00
54	BA	1833	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	239	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	301	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1050	A	O4'-C1'-N9	5.08	112.26	108.20
54	BA	2355	G	C5'-C4'-O4'	5.08	115.19	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	525	U	N3-C2-O2	-5.08	118.65	122.20
54	BA	1901	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1909	C	O4'-C1'-N1	5.08	112.26	108.20
17	AR	60	ARG	NE-CZ-NH1	5.08	122.84	120.30
21	AA	290	C	N3-C2-O2	-5.08	118.35	121.90
21	AA	1057	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	1223	C	N3-C4-C5	5.08	123.93	121.90
54	BA	1230	A	C6-C5-N7	5.08	135.85	132.30
4	AE	137	ARG	NE-CZ-NH1	5.07	122.84	120.30
21	AA	744	C	O4'-C1'-N1	5.07	112.26	108.20
54	BA	531	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1096	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	1120	G	C5-C6-N1	5.07	114.04	111.50
54	BA	1985	C	N1-C2-O2	5.07	121.94	118.90
54	BA	2199	A	C6-C5-N7	5.07	135.85	132.30
54	BA	2570	G	O4'-C1'-N9	5.07	112.26	108.20
54	BA	2819	G	C8-N9-C4	-5.07	104.37	106.40
55	BB	94	A	C6-C5-N7	5.07	135.85	132.30
21	AA	711	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2405	G	C5-C6-N1	5.07	114.04	111.50
21	AA	349	A	C6-C5-N7	5.07	135.85	132.30
21	AA	1303	C	N1-C2-O2	5.07	121.94	118.90
54	BA	974	G	N3-C2-N2	-5.07	116.35	119.90
54	BA	1483	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2506	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	672	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1340	U	P-O3'-C3'	5.07	125.78	119.70
21	AA	124	C	N1-C2-O2	5.07	121.94	118.90
54	BA	269	C	N1-C2-O2	5.07	121.94	118.90
54	BA	2063	C	O4'-C1'-N1	5.07	112.25	108.20
21	AA	1426	G	N3-C2-N2	-5.07	116.35	119.90
42	BT	76	ARG	NE-CZ-NH1	5.07	122.83	120.30
54	BA	181	A	C6-C5-N7	5.07	135.84	132.30
54	BA	678	C	N1-C2-O2	5.07	121.94	118.90
54	BA	865	C	N3-C4-C5	5.07	123.93	121.90
54	BA	939	G	C5-C6-N1	5.07	114.03	111.50
54	BA	2197	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	2622	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	2845	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2022	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	2736	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	131	A	C6-C5-N7	5.06	135.84	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	468	A	C1'-O4'-C4'	-5.06	105.85	109.90
21	AA	593	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1104	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2236	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2870	C	N1-C2-O2	5.06	121.94	118.90
21	AA	173	U	C1'-O4'-C4'	-5.06	105.85	109.90
21	AA	882	C	O4'-C1'-N1	5.06	112.25	108.20
21	AA	965	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	1378	C	N1-C2-O2	5.06	121.94	118.90
54	BA	179	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1864	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	2499	C	N3-C4-C5	5.06	123.92	121.90
55	BB	70	C	C5'-C4'-O4'	5.06	115.17	109.10
21	AA	1162	C	N1-C2-O2	5.06	121.93	118.90
21	AA	1512	U	N3-C2-O2	-5.06	118.66	122.20
45	BW	19	ARG	NE-CZ-NH2	-5.06	117.77	120.30
54	BA	1990	C	N1-C2-O2	5.06	121.93	118.90
21	AA	427	U	N3-C2-O2	-5.05	118.66	122.20
21	AA	948	C	C5'-C4'-O4'	5.05	115.17	109.10
24	A3	45	A	O4'-C1'-N9	5.05	112.24	108.20
54	BA	1227	G	C5-C6-N1	5.05	114.03	111.50
54	BA	2085	U	C5-C6-N1	-5.05	120.17	122.70
54	BA	2282	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	281	G	C3'-C2'-C1'	5.05	105.54	101.50
21	AA	493	A	C2-N3-C4	5.05	113.13	110.60
21	AA	1504	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	875	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	2372	U	C3'-C2'-C1'	-5.05	97.46	101.50
21	AA	200	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	545	C	N1-C2-O2	5.05	121.93	118.90
54	BA	364	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2250	G	C5-C6-N1	5.05	114.03	111.50
55	BB	71	C	O4'-C1'-N1	5.05	112.24	108.20
21	AA	526	C	N1-C2-O2	5.05	121.93	118.90
54	BA	640	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1140	C	C5'-C4'-O4'	5.05	115.16	109.10
54	BA	2385	C	N1-C2-O2	5.05	121.93	118.90
54	BA	497	A	C6-C5-N7	5.05	135.83	132.30
54	BA	1892	C	C6-N1-C2	-5.05	118.28	120.30
54	BA	2263	C	N1-C2-O2	5.05	121.93	118.90
54	BA	2759	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	1228	C	O4'-C1'-N1	5.04	112.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	14	A	C4-C5-C6	-5.04	114.48	117.00
24	A3	45	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1133	A	O4'-C1'-N9	5.04	112.24	108.20
21	AA	278	G	N1-C6-O6	-5.04	116.87	119.90
54	BA	197	A	C6-C5-N7	5.04	135.83	132.30
54	BA	988	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	2677	G	N1-C6-O6	-5.04	116.87	119.90
21	AA	40	C	N1-C2-O2	5.04	121.92	118.90
21	AA	495	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	538	G	N1-C6-O6	-5.04	116.88	119.90
21	AA	680	C	C1'-O4'-C4'	-5.04	105.87	109.90
21	AA	905	U	N3-C2-O2	-5.04	118.67	122.20
21	AA	1362	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1678	A	C6-C5-N7	5.04	135.83	132.30
21	AA	1231	G	N3-C2-N2	-5.04	116.37	119.90
21	AA	1443	C	N1-C2-O2	5.04	121.92	118.90
21	AA	429	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	819	A	C6-C5-N7	5.04	135.83	132.30
21	AA	923	A	C5'-C4'-C3'	-5.04	107.94	116.00
54	BA	552	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	765	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	295	C	N1-C2-O2	5.04	121.92	118.90
21	AA	583	A	C6-C5-N7	5.04	135.82	132.30
21	AA	821	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	772	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	1455	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	1531	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	1643	G	O4'-C1'-N9	5.04	112.23	108.20
11	AL	94	TYR	CB-CG-CD2	-5.03	117.98	121.00
21	AA	814	A	C6-C5-N7	5.03	135.82	132.30
21	AA	1494	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	522	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1366	A	C6-C5-N7	5.03	135.82	132.30
54	BA	646	U	N1-C2-N3	5.03	117.92	114.90
21	AA	927	G	C5'-C4'-O4'	5.03	115.14	109.10
21	AA	1161	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	188	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	691	C	N3-C2-O2	-5.03	118.38	121.90
54	BA	1992	G	N3-C2-N2	-5.03	116.38	119.90
54	BA	2417	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	2739	U	O4'-C1'-N1	5.03	112.22	108.20
21	AA	217	C	N1-C2-O2	5.03	121.92	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	318	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	1880	U	O4'-C1'-N1	5.03	112.22	108.20
2	AC	106	ARG	NE-CZ-NH1	5.03	122.81	120.30
24	A3	10	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	211	C	N1-C2-O2	5.03	121.92	118.90
54	BA	374	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	773	U	C5-C6-N1	-5.03	120.19	122.70
54	BA	1296	G	N3-C2-N2	-5.03	116.38	119.90
54	BA	1404	C	N1-C2-O2	5.03	121.92	118.90
21	AA	5	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	213	G	O4'-C1'-N9	5.03	112.22	108.20
21	AA	858	G	N1-C6-O6	-5.03	116.89	119.90
22	A1	43	G	C5-C6-N1	5.03	114.01	111.50
54	BA	461	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1119	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1352	U	C5'-C4'-O4'	5.03	115.13	109.10
54	BA	2682	A	C6-C5-N7	5.03	135.82	132.30
21	AA	78	A	C6-C5-N7	5.02	135.82	132.30
21	AA	796	C	N1-C2-O2	5.02	121.92	118.90
54	BA	479	A	C3'-C2'-C1'	-5.02	97.48	101.50
54	BA	1274	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	1351	C	N3-C4-N4	-5.02	114.48	118.00
21	AA	426	U	C5-C6-N1	-5.02	120.19	122.70
21	AA	920	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	588	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	970	U	C5'-C4'-O4'	5.02	115.13	109.10
54	BA	1209	U	N3-C2-O2	-5.02	118.68	122.20
21	AA	35	G	O3'-P-O5'	-5.02	94.46	104.00
22	A1	17	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	68	G	C5-C6-N1	5.02	114.01	111.50
21	AA	658	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1069	A	C6-C5-N7	5.02	135.81	132.30
54	BA	1191	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	1197	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	1585	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1818	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	2226	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	2244	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	108	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	869	G	C5-C6-N1	5.02	114.01	111.50
21	AA	982	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	81	G	O4'-C1'-N9	5.02	112.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	389	G	P-O3'-C3'	5.02	125.72	119.70
54	BA	787	C	N3-C4-N4	-5.02	114.49	118.00
21	AA	501	C	N3-C4-C5	5.02	123.91	121.90
21	AA	729	A	C6-C5-N7	5.02	135.81	132.30
54	BA	867	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	1305	C	N3-C4-C5	5.02	123.91	121.90
55	BB	2	G	N3-C4-C5	-5.02	126.09	128.60
1	AB	112	ARG	CD-NE-CZ	5.01	130.62	123.60
21	AA	637	C	N1-C2-O2	5.01	121.91	118.90
21	AA	800	G	N1-C6-O6	-5.01	116.89	119.90
27	BE	162	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	398	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1005	C	C6-N1-C2	-5.01	118.29	120.30
21	AA	561	U	C5-C6-N1	-5.01	120.19	122.70
54	BA	800	A	C6-C5-N7	5.01	135.81	132.30
54	BA	2365	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	1300	G	C1'-O4'-C4'	-5.01	105.89	109.90
54	BA	1068	G	N3-C4-C5	-5.01	126.09	128.60
54	BA	1974	C	O4'-C1'-N1	5.01	112.21	108.20
21	AA	961	U	N3-C2-O2	-5.01	118.69	122.20
21	AA	1405	G	N1-C6-O6	-5.01	116.89	119.90
36	BN	63	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	1832	C	N1-C2-O2	5.01	121.91	118.90
54	BA	2902	C	O4'-C1'-N1	5.01	112.21	108.20
21	AA	567	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	840	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1247	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	2018	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	122	G	O4'-C1'-N9	5.01	112.20	108.20
21	AA	149	A	C5-C6-N1	5.01	120.20	117.70
21	AA	802	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	639	U	C3'-C2'-C1'	5.01	105.50	101.50
54	BA	2370	G	N1-C6-O6	-5.01	116.90	119.90
55	BB	10	G	O4'-C1'-N9	5.01	112.21	108.20
54	BA	295	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	1307	A	C4-C5-C6	-5.00	114.50	117.00
54	BA	2601	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	206	C	N1-C2-O2	5.00	121.90	118.90
21	AA	1168	U	N3-C2-O2	-5.00	118.70	122.20
21	AA	1299	A	C4-C5-C6	-5.00	114.50	117.00
54	BA	1357	C	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1798	U	O4'-C1'-N1	5.00	112.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2525	G	N3-C2-N2	-5.00	116.40	119.90
21	AA	224	U	N3-C2-O2	-5.00	118.70	122.20
21	AA	1503	A	C6-C5-N7	5.00	135.80	132.30
22	A1	76	A	C8-N9-C4	-5.00	103.80	105.80
24	A3	7	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	408	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	481	G	C3'-C2'-C1'	5.00	105.50	101.50
54	BA	2115	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	2269	G	C5-C6-N1	5.00	114.00	111.50
55	BB	67	G	N3-C4-C5	-5.00	126.10	128.60

There are no chirality outliers.

All (1147) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	1	G	Sidechain
22	A1	11	C	Sidechain
22	A1	24	G	Sidechain
22	A1	3	G	Sidechain
22	A1	32	C	Sidechain
22	A1	33	U	Sidechain
22	A1	36	C	Sidechain
22	A1	38	A	Sidechain
22	A1	44	G	Sidechain
22	A1	49	G	Sidechain
22	A1	52	G	Sidechain
22	A1	6	A	Sidechain
22	A1	60	C	Sidechain
22	A1	63	G	Sidechain
22	A1	64	U	Sidechain
22	A1	65	C	Sidechain
22	A1	67	U	Sidechain
22	A1	71	C	Sidechain
22	A1	75	C	Sidechain
22	A1	76	A	Sidechain
22	A1	9	A	Sidechain
23	A2	80	C	Sidechain
23	A2	83	U	Sidechain
23	A2	86	U	Sidechain
23	A2	89	U	Sidechain
24	A3	1	C	Sidechain
24	A3	15	G	Sidechain

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Mol	Chain	Res	Type	Group
24	A3	17	C	Sidechain
24	A3	2	G	Sidechain
24	A3	28	U	Sidechain
24	A3	32	G	Sidechain
24	A3	35	C	Sidechain
24	A3	38	A	Sidechain
24	A3	42	C	Sidechain
24	A3	50	G	Sidechain
24	A3	61	U	Sidechain
24	A3	7	G	Sidechain
24	A3	71	G	Sidechain
24	A3	74	A	Sidechain
24	A3	75	C	Sidechain
24	A3	76	C	Sidechain
21	AA	100	G	Sidechain
21	AA	1010	U	Sidechain
21	AA	1013	G	Sidechain
21	AA	1025	U	Sidechain
21	AA	1028	C	Sidechain
21	AA	1029	U	Sidechain
21	AA	1038	C	Sidechain
21	AA	1044	A	Sidechain
21	AA	1046	A	Sidechain
21	AA	1048	G	Sidechain
21	AA	1053	G	Sidechain
21	AA	1054	C	Sidechain
21	AA	1066	C	Sidechain
21	AA	1075	U	Sidechain
21	AA	109	A	Sidechain
21	AA	1093	A	Sidechain
21	AA	1097	C	Sidechain
21	AA	110	C	Sidechain
21	AA	1108	G	Sidechain
21	AA	111	G	Sidechain
21	AA	1114	C	Sidechain
21	AA	1116	U	Sidechain
21	AA	1117	A	Sidechain
21	AA	1118	U	Sidechain
21	AA	1122	U	Sidechain
21	AA	1127	G	Sidechain
21	AA	1130	A	Sidechain
21	AA	1131	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1132	C	Sidechain
21	AA	1134	G	Sidechain
21	AA	1137	C	Sidechain
21	AA	1138	G	Sidechain
21	AA	1139	G	Sidechain
21	AA	114	U	Sidechain
21	AA	1140	C	Sidechain
21	AA	1142	G	Sidechain
21	AA	1144	G	Sidechain
21	AA	1149	C	Sidechain
21	AA	1155	A	Sidechain
21	AA	1162	C	Sidechain
21	AA	1177	G	Sidechain
21	AA	1178	G	Sidechain
21	AA	1189	U	Sidechain
21	AA	1193	G	Sidechain
21	AA	1200	C	Sidechain
21	AA	1206	G	Sidechain
21	AA	1207	G	Sidechain
21	AA	1211	U	Sidechain
21	AA	1212	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1214	C	Sidechain
21	AA	1216	A	Sidechain
21	AA	1217	C	Sidechain
21	AA	1218	C	Sidechain
21	AA	122	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1225	A	Sidechain
21	AA	1229	A	Sidechain
21	AA	1237	C	Sidechain
21	AA	1246	A	Sidechain
21	AA	1249	C	Sidechain
21	AA	1253	G	Sidechain
21	AA	126	G	Sidechain
21	AA	1260	G	Sidechain
21	AA	1263	C	Sidechain
21	AA	1267	C	Sidechain
21	AA	1269	A	Sidechain
21	AA	1273	C	Sidechain
21	AA	1274	A	Sidechain
21	AA	1278	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1299	A	Sidechain
21	AA	1300	G	Sidechain
21	AA	1302	C	Sidechain
21	AA	1305	G	Sidechain
21	AA	1312	G	Sidechain
21	AA	1321	U	Sidechain
21	AA	1324	A	Sidechain
21	AA	1328	C	Sidechain
21	AA	133	U	Sidechain
21	AA	1330	U	Sidechain
21	AA	1343	G	Sidechain
21	AA	1346	A	Sidechain
21	AA	1351	U	Sidechain
21	AA	1356	G	Sidechain
21	AA	1358	U	Sidechain
21	AA	1360	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	1366	C	Sidechain
21	AA	1370	G	Sidechain
21	AA	1372	U	Sidechain
21	AA	1380	U	Sidechain
21	AA	1381	U	Sidechain
21	AA	1382	C	Sidechain
21	AA	1385	G	Sidechain
21	AA	1391	U	Sidechain
21	AA	1392	G	Sidechain
21	AA	1397	C	Sidechain
21	AA	1398	A	Sidechain
21	AA	14	U	Sidechain
21	AA	1400	C	Sidechain
21	AA	1401	G	Sidechain
21	AA	1402	C	Sidechain
21	AA	1407	C	Sidechain
21	AA	1409	C	Sidechain
21	AA	1413	A	Sidechain
21	AA	1414	U	Sidechain
21	AA	1415	G	Sidechain
21	AA	1421	G	Sidechain
21	AA	1424	U	Sidechain
21	AA	1426	G	Sidechain
21	AA	1435	G	Sidechain
21	AA	1438	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	144	G	Sidechain
21	AA	1444	U	Sidechain
21	AA	1451	U	Sidechain
21	AA	1461	G	Sidechain
21	AA	1468	A	Sidechain
21	AA	1473	G	Sidechain
21	AA	1474	U	Sidechain
21	AA	1477	U	Sidechain
21	AA	1482	G	Sidechain
21	AA	1484	C	Sidechain
21	AA	1487	G	Sidechain
21	AA	15	G	Sidechain
21	AA	1500	A	Sidechain
21	AA	1502	A	Sidechain
21	AA	1503	A	Sidechain
21	AA	1505	G	Sidechain
21	AA	1509	C	Sidechain
21	AA	1511	G	Sidechain
21	AA	1513	A	Sidechain
21	AA	1515	G	Sidechain
21	AA	1519	A	Sidechain
21	AA	1526	G	Sidechain
21	AA	1527	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1530	G	Sidechain
21	AA	1533	C	Sidechain
21	AA	1534	A	Sidechain
21	AA	159	G	Sidechain
21	AA	161	A	Sidechain
21	AA	162	A	Sidechain
21	AA	164	G	Sidechain
21	AA	167	A	Sidechain
21	AA	17	U	Sidechain
21	AA	172	A	Sidechain
21	AA	173	U	Sidechain
21	AA	186	C	Sidechain
21	AA	187	G	Sidechain
21	AA	190	A	Sidechain
21	AA	198	G	Sidechain
21	AA	200	G	Sidechain
21	AA	207	C	Sidechain
21	AA	208	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	210	C	Sidechain
21	AA	215	C	Sidechain
21	AA	217	C	Sidechain
21	AA	220	G	Sidechain
21	AA	225	C	Sidechain
21	AA	233	C	Sidechain
21	AA	234	C	Sidechain
21	AA	235	C	Sidechain
21	AA	237	G	Sidechain
21	AA	241	G	Sidechain
21	AA	242	G	Sidechain
21	AA	244	U	Sidechain
21	AA	25	C	Sidechain
21	AA	250	A	Sidechain
21	AA	255	G	Sidechain
21	AA	265	G	Sidechain
21	AA	269	C	Sidechain
21	AA	273	U	Sidechain
21	AA	280	C	Sidechain
21	AA	281	G	Sidechain
21	AA	29	U	Sidechain
21	AA	292	G	Sidechain
21	AA	295	C	Sidechain
21	AA	298	A	Sidechain
21	AA	299	G	Sidechain
21	AA	305	G	Sidechain
21	AA	307	C	Sidechain
21	AA	310	G	Sidechain
21	AA	312	C	Sidechain
21	AA	317	U	Sidechain
21	AA	324	G	Sidechain
21	AA	33	A	Sidechain
21	AA	336	A	Sidechain
21	AA	337	G	Sidechain
21	AA	343	U	Sidechain
21	AA	347	G	Sidechain
21	AA	35	G	Sidechain
21	AA	350	G	Sidechain
21	AA	356	A	Sidechain
21	AA	359	G	Sidechain
21	AA	36	C	Sidechain
21	AA	361	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	367	U	Sidechain
21	AA	370	C	Sidechain
21	AA	372	C	Sidechain
21	AA	375	U	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	387	U	Sidechain
21	AA	388	G	Sidechain
21	AA	391	G	Sidechain
21	AA	398	U	Sidechain
21	AA	399	G	Sidechain
21	AA	404	G	Sidechain
21	AA	407	U	Sidechain
21	AA	413	G	Sidechain
21	AA	414	A	Sidechain
21	AA	419	C	Sidechain
21	AA	430	A	Sidechain
21	AA	436	C	Sidechain
21	AA	443	C	Sidechain
21	AA	446	G	Sidechain
21	AA	451	A	Sidechain
21	AA	455	G	Sidechain
21	AA	472	U	Sidechain
21	AA	478	A	Sidechain
21	AA	479	U	Sidechain
21	AA	481	G	Sidechain
21	AA	484	G	Sidechain
21	AA	485	U	Sidechain
21	AA	487	A	Sidechain
21	AA	491	G	Sidechain
21	AA	492	C	Sidechain
21	AA	493	A	Sidechain
21	AA	5	U	Sidechain
21	AA	506	G	Sidechain
21	AA	51	A	Sidechain
21	AA	513	C	Sidechain
21	AA	517	G	Sidechain
21	AA	519	C	Sidechain
21	AA	525	C	Sidechain
21	AA	529	G	Sidechain
21	AA	532	A	Sidechain
21	AA	546	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	55	A	Sidechain
21	AA	550	G	Sidechain
21	AA	554	A	Sidechain
21	AA	555	U	Sidechain
21	AA	558	G	Sidechain
21	AA	561	U	Sidechain
21	AA	565	U	Sidechain
21	AA	571	U	Sidechain
21	AA	572	A	Sidechain
21	AA	573	A	Sidechain
21	AA	581	G	Sidechain
21	AA	585	G	Sidechain
21	AA	595	A	Sidechain
21	AA	600	A	Sidechain
21	AA	604	G	Sidechain
21	AA	610	U	Sidechain
21	AA	611	C	Sidechain
21	AA	612	C	Sidechain
21	AA	622	A	Sidechain
21	AA	627	G	Sidechain
21	AA	628	G	Sidechain
21	AA	630	A	Sidechain
21	AA	635	A	Sidechain
21	AA	641	U	Sidechain
21	AA	642	A	Sidechain
21	AA	646	G	Sidechain
21	AA	650	G	Sidechain
21	AA	660	C	Sidechain
21	AA	661	G	Sidechain
21	AA	663	A	Sidechain
21	AA	666	G	Sidechain
21	AA	670	G	Sidechain
21	AA	675	A	Sidechain
21	AA	678	U	Sidechain
21	AA	682	G	Sidechain
21	AA	684	U	Sidechain
21	AA	685	G	Sidechain
21	AA	687	A	Sidechain
21	AA	689	C	Sidechain
21	AA	691	G	Sidechain
21	AA	693	G	Sidechain
21	AA	699	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	7	A	Sidechain
21	AA	701	U	Sidechain
21	AA	703	G	Sidechain
21	AA	704	A	Sidechain
21	AA	71	A	Sidechain
21	AA	712	A	Sidechain
21	AA	719	C	Sidechain
21	AA	720	C	Sidechain
21	AA	721	G	Sidechain
21	AA	732	C	Sidechain
21	AA	740	U	Sidechain
21	AA	741	G	Sidechain
21	AA	745	G	Sidechain
21	AA	750	C	Sidechain
21	AA	751	U	Sidechain
21	AA	752	G	Sidechain
21	AA	76	G	Sidechain
21	AA	760	G	Sidechain
21	AA	762	U	Sidechain
21	AA	765	G	Sidechain
21	AA	768	A	Sidechain
21	AA	769	G	Sidechain
21	AA	770	C	Sidechain
21	AA	771	G	Sidechain
21	AA	787	A	Sidechain
21	AA	791	G	Sidechain
21	AA	797	C	Sidechain
21	AA	8	A	Sidechain
21	AA	800	G	Sidechain
21	AA	802	A	Sidechain
21	AA	81	A	Sidechain
21	AA	812	G	Sidechain
21	AA	821	G	Sidechain
21	AA	822	U	Sidechain
21	AA	827	U	Sidechain
21	AA	828	U	Sidechain
21	AA	829	G	Sidechain
21	AA	83	C	Sidechain
21	AA	832	G	Sidechain
21	AA	833	G	Sidechain
21	AA	843	U	Sidechain
21	AA	852	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	86	G	Sidechain
21	AA	863	U	Sidechain
21	AA	869	G	Sidechain
21	AA	87	C	Sidechain
21	AA	870	U	Sidechain
21	AA	871	U	Sidechain
21	AA	873	A	Sidechain
21	AA	880	C	Sidechain
21	AA	887	G	Sidechain
21	AA	888	G	Sidechain
21	AA	898	G	Sidechain
21	AA	900	A	Sidechain
21	AA	907	A	Sidechain
21	AA	909	A	Sidechain
21	AA	913	A	Sidechain
21	AA	914	A	Sidechain
21	AA	917	G	Sidechain
21	AA	918	A	Sidechain
21	AA	920	U	Sidechain
21	AA	923	A	Sidechain
21	AA	927	G	Sidechain
21	AA	93	U	Sidechain
21	AA	932	C	Sidechain
21	AA	933	G	Sidechain
21	AA	938	A	Sidechain
21	AA	939	G	Sidechain
21	AA	94	G	Sidechain
21	AA	941	G	Sidechain
21	AA	944	G	Sidechain
21	AA	948	C	Sidechain
21	AA	949	A	Sidechain
21	AA	954	G	Sidechain
21	AA	956	U	Sidechain
21	AA	960	U	Sidechain
21	AA	970	C	Sidechain
21	AA	973	G	Sidechain
21	AA	976	G	Sidechain
21	AA	978	A	Sidechain
21	AA	982	U	Sidechain
21	AA	983	A	Sidechain
21	AA	984	C	Sidechain
21	AA	988	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	989	U	Sidechain
21	AA	99	C	Sidechain
21	AA	990	C	Sidechain
21	AA	998	C	Sidechain
1	AB	224	ARG	Sidechain
4	AE	22	LYS	Peptide
14	AO	48	ASP	Peptide
14	AO	68	TYR	Sidechain
49	B0	48	TYR	Sidechain
54	BA	100	U	Sidechain
54	BA	1000	A	Sidechain
54	BA	1009	A	Sidechain
54	BA	1013	C	Sidechain
54	BA	1016	G	Sidechain
54	BA	1022	G	Sidechain
54	BA	1026	G	Sidechain
54	BA	1027	A	Sidechain
54	BA	1028	A	Sidechain
54	BA	1030	C	Sidechain
54	BA	104	A	Sidechain
54	BA	1044	C	Sidechain
54	BA	1045	C	Sidechain
54	BA	1046	A	Sidechain
54	BA	1047	G	Sidechain
54	BA	1051	G	Sidechain
54	BA	1052	C	Sidechain
54	BA	1053	C	Sidechain
54	BA	1054	A	Sidechain
54	BA	1056	G	Sidechain
54	BA	1063	G	Sidechain
54	BA	1068	G	Sidechain
54	BA	107	G	Sidechain
54	BA	1071	G	Sidechain
54	BA	1074	G	Sidechain
54	BA	1075	C	Sidechain
54	BA	1076	C	Sidechain
54	BA	1083	U	Sidechain
54	BA	1090	A	Sidechain
54	BA	1093	G	Sidechain
54	BA	1099	G	Sidechain
54	BA	1108	U	Sidechain
54	BA	1111	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1115	G	Sidechain
54	BA	1121	C	Sidechain
54	BA	1129	A	Sidechain
54	BA	1135	C	Sidechain
54	BA	1139	G	Sidechain
54	BA	1142	A	Sidechain
54	BA	115	C	Sidechain
54	BA	1151	A	Sidechain
54	BA	1152	C	Sidechain
54	BA	1163	G	Sidechain
54	BA	1170	C	Sidechain
54	BA	1175	A	Sidechain
54	BA	1177	G	Sidechain
54	BA	1179	G	Sidechain
54	BA	1184	U	Sidechain
54	BA	1185	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1188	U	Sidechain
54	BA	1192	G	Sidechain
54	BA	1195	G	Sidechain
54	BA	1198	U	Sidechain
54	BA	1200	C	Sidechain
54	BA	1221	C	Sidechain
54	BA	1223	G	Sidechain
54	BA	1236	G	Sidechain
54	BA	124	G	Sidechain
54	BA	1244	A	Sidechain
54	BA	1254	A	Sidechain
54	BA	126	A	Sidechain
54	BA	1264	A	Sidechain
54	BA	1269	A	Sidechain
54	BA	1270	C	Sidechain
54	BA	1271	G	Sidechain
54	BA	1272	A	Sidechain
54	BA	1273	U	Sidechain
54	BA	1277	G	Sidechain
54	BA	1281	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	1287	A	Sidechain
54	BA	1299	G	Sidechain
54	BA	130	C	Sidechain
54	BA	1303	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1307	A	Sidechain
54	BA	1308	A	Sidechain
54	BA	1312	U	Sidechain
54	BA	1315	C	Sidechain
54	BA	1317	G	Sidechain
54	BA	1319	C	Sidechain
54	BA	1320	C	Sidechain
54	BA	1323	C	Sidechain
54	BA	1326	U	Sidechain
54	BA	1329	U	Sidechain
54	BA	1330	C	Sidechain
54	BA	1332	G	Sidechain
54	BA	1336	A	Sidechain
54	BA	1338	G	Sidechain
54	BA	1345	C	Sidechain
54	BA	1346	G	Sidechain
54	BA	1356	G	Sidechain
54	BA	1359	A	Sidechain
54	BA	136	G	Sidechain
54	BA	1360	G	Sidechain
54	BA	1361	G	Sidechain
54	BA	1362	C	Sidechain
54	BA	1366	A	Sidechain
54	BA	1373	A	Sidechain
54	BA	1376	C	Sidechain
54	BA	1388	G	Sidechain
54	BA	1392	A	Sidechain
54	BA	1393	A	Sidechain
54	BA	1399	C	Sidechain
54	BA	1410	G	Sidechain
54	BA	1416	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1429	G	Sidechain
54	BA	1435	G	Sidechain
54	BA	1438	U	Sidechain
54	BA	1445	G	Sidechain
54	BA	1457	U	Sidechain
54	BA	146	A	Sidechain
54	BA	1460	U	Sidechain
54	BA	1465	G	Sidechain
54	BA	1471	G	Sidechain
54	BA	1477	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1484	U	Sidechain
54	BA	1488	C	Sidechain
54	BA	1489	C	Sidechain
54	BA	1490	A	Sidechain
54	BA	1492	G	Sidechain
54	BA	1498	C	Sidechain
54	BA	15	G	Sidechain
54	BA	150	U	Sidechain
54	BA	1502	A	Sidechain
54	BA	1504	A	Sidechain
54	BA	1505	A	Sidechain
54	BA	1508	A	Sidechain
54	BA	1510	G	Sidechain
54	BA	152	A	Sidechain
54	BA	1522	A	Sidechain
54	BA	1525	A	Sidechain
54	BA	1535	A	Sidechain
54	BA	1543	G	Sidechain
54	BA	1546	G	Sidechain
54	BA	1548	A	Sidechain
54	BA	1551	A	Sidechain
54	BA	1553	A	Sidechain
54	BA	1555	G	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1565	C	Sidechain
54	BA	1567	G	Sidechain
54	BA	1569	A	Sidechain
54	BA	1573	G	Sidechain
54	BA	1580	A	Sidechain
54	BA	1584	U	Sidechain
54	BA	1595	C	Sidechain
54	BA	1599	U	Sidechain
54	BA	1600	C	Sidechain
54	BA	1601	G	Sidechain
54	BA	1606	C	Sidechain
54	BA	1612	C	Sidechain
54	BA	1615	C	Sidechain
54	BA	1616	A	Sidechain
54	BA	1620	G	Sidechain
54	BA	1621	U	Sidechain
54	BA	1622	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1623	G	Sidechain
54	BA	1627	G	Sidechain
54	BA	1628	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1633	G	Sidechain
54	BA	1634	A	Sidechain
54	BA	1635	A	Sidechain
54	BA	164	C	Sidechain
54	BA	1644	C	Sidechain
54	BA	1651	G	Sidechain
54	BA	1653	G	Sidechain
54	BA	1654	A	Sidechain
54	BA	1657	U	Sidechain
54	BA	1659	G	Sidechain
54	BA	1672	A	Sidechain
54	BA	1673	G	Sidechain
54	BA	1674	G	Sidechain
54	BA	168	G	Sidechain
54	BA	1680	U	Sidechain
54	BA	1682	G	Sidechain
54	BA	1683	U	Sidechain
54	BA	1686	C	Sidechain
54	BA	1697	G	Sidechain
54	BA	1699	G	Sidechain
54	BA	1703	G	Sidechain
54	BA	1705	A	Sidechain
54	BA	1707	G	Sidechain
54	BA	1708	C	Sidechain
54	BA	1713	A	Sidechain
54	BA	1716	U	Sidechain
54	BA	1719	G	Sidechain
54	BA	1721	G	Sidechain
54	BA	1724	G	Sidechain
54	BA	1725	U	Sidechain
54	BA	1729	U	Sidechain
54	BA	1735	A	Sidechain
54	BA	1736	U	Sidechain
54	BA	1737	G	Sidechain
54	BA	1738	G	Sidechain
54	BA	1740	G	Sidechain
54	BA	1743	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1746	A	Sidechain
54	BA	1748	C	Sidechain
54	BA	1753	G	Sidechain
54	BA	1758	U	Sidechain
54	BA	1762	A	Sidechain
54	BA	1767	G	Sidechain
54	BA	1774	C	Sidechain
54	BA	1781	U	Sidechain
54	BA	1790	C	Sidechain
54	BA	1796	U	Sidechain
54	BA	180	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1803	A	Sidechain
54	BA	1804	C	Sidechain
54	BA	1809	A	Sidechain
54	BA	1823	G	Sidechain
54	BA	1828	G	Sidechain
54	BA	1835	G	Sidechain
54	BA	1837	C	Sidechain
54	BA	1840	G	Sidechain
54	BA	1841	U	Sidechain
54	BA	1842	G	Sidechain
54	BA	1847	A	Sidechain
54	BA	1854	A	Sidechain
54	BA	1857	G	Sidechain
54	BA	1865	U	Sidechain
54	BA	1869	G	Sidechain
54	BA	1876	A	Sidechain
54	BA	1884	G	Sidechain
54	BA	1886	U	Sidechain
54	BA	1889	A	Sidechain
54	BA	189	G	Sidechain
54	BA	1890	A	Sidechain
54	BA	1891	G	Sidechain
54	BA	19	A	Sidechain
54	BA	190	A	Sidechain
54	BA	1908	C	Sidechain
54	BA	191	A	Sidechain
54	BA	1910	G	Sidechain
54	BA	1918	A	Sidechain
54	BA	1922	G	Sidechain
54	BA	1927	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1928	A	Sidechain
54	BA	1931	U	Sidechain
54	BA	1932	A	Sidechain
54	BA	1939	U	Sidechain
54	BA	1940	U	Sidechain
54	BA	1944	U	Sidechain
54	BA	1948	G	Sidechain
54	BA	1950	G	Sidechain
54	BA	1958	C	Sidechain
54	BA	1959	G	Sidechain
54	BA	1962	C	Sidechain
54	BA	197	A	Sidechain
54	BA	1973	G	Sidechain
54	BA	1976	U	Sidechain
54	BA	198	C	Sidechain
54	BA	1982	U	Sidechain
54	BA	1983	G	Sidechain
54	BA	1993	U	Sidechain
54	BA	1995	U	Sidechain
54	BA	1996	C	Sidechain
54	BA	20	C	Sidechain
54	BA	200	U	Sidechain
54	BA	2005	A	Sidechain
54	BA	2007	U	Sidechain
54	BA	2014	A	Sidechain
54	BA	2015	A	Sidechain
54	BA	2019	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2022	U	Sidechain
54	BA	2031	A	Sidechain
54	BA	2033	A	Sidechain
54	BA	2034	U	Sidechain
54	BA	2037	A	Sidechain
54	BA	2040	G	Sidechain
54	BA	2041	U	Sidechain
54	BA	2052	A	Sidechain
54	BA	206	U	Sidechain
54	BA	2061	G	Sidechain
54	BA	2064	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	2069	G	Sidechain
54	BA	2073	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2075	U	Sidechain
54	BA	2083	G	Sidechain
54	BA	2087	G	Sidechain
54	BA	2092	U	Sidechain
54	BA	210	C	Sidechain
54	BA	2103	C	Sidechain
54	BA	2104	C	Sidechain
54	BA	2113	U	Sidechain
54	BA	2114	A	Sidechain
54	BA	2117	A	Sidechain
54	BA	2121	G	Sidechain
54	BA	2130	U	Sidechain
54	BA	2135	A	Sidechain
54	BA	2139	U	Sidechain
54	BA	214	G	Sidechain
54	BA	215	G	Sidechain
54	BA	2152	G	Sidechain
54	BA	2155	U	Sidechain
54	BA	2157	G	Sidechain
54	BA	2161	C	Sidechain
54	BA	2163	A	Sidechain
54	BA	2165	C	Sidechain
54	BA	2166	U	Sidechain
54	BA	2168	G	Sidechain
54	BA	2169	A	Sidechain
54	BA	217	A	Sidechain
54	BA	2172	U	Sidechain
54	BA	2175	C	Sidechain
54	BA	2176	A	Sidechain
54	BA	218	A	Sidechain
54	BA	2196	C	Sidechain
54	BA	2197	U	Sidechain
54	BA	22	C	Sidechain
54	BA	2201	G	Sidechain
54	BA	2204	G	Sidechain
54	BA	2207	C	Sidechain
54	BA	2208	C	Sidechain
54	BA	2224	G	Sidechain
54	BA	2233	U	Sidechain
54	BA	2236	U	Sidechain
54	BA	2240	U	Sidechain
54	BA	2244	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2245	U	Sidechain
54	BA	2253	G	Sidechain
54	BA	2259	U	Sidechain
54	BA	2272	U	Sidechain
54	BA	2273	A	Sidechain
54	BA	2274	A	Sidechain
54	BA	2276	G	Sidechain
54	BA	228	C	Sidechain
54	BA	2282	G	Sidechain
54	BA	2289	G	Sidechain
54	BA	2299	U	Sidechain
54	BA	2300	C	Sidechain
54	BA	2306	C	Sidechain
54	BA	2308	G	Sidechain
54	BA	2310	C	Sidechain
54	BA	2312	U	Sidechain
54	BA	2321	U	Sidechain
54	BA	2323	G	Sidechain
54	BA	2324	U	Sidechain
54	BA	2327	A	Sidechain
54	BA	2332	C	Sidechain
54	BA	2335	A	Sidechain
54	BA	2338	C	Sidechain
54	BA	2341	G	Sidechain
54	BA	2344	U	Sidechain
54	BA	2352	A	Sidechain
54	BA	2357	G	Sidechain
54	BA	2358	A	Sidechain
54	BA	2360	G	Sidechain
54	BA	2361	G	Sidechain
54	BA	2366	A	Sidechain
54	BA	2375	G	Sidechain
54	BA	2379	G	Sidechain
54	BA	2380	C	Sidechain
54	BA	2382	G	Sidechain
54	BA	2383	G	Sidechain
54	BA	2391	G	Sidechain
54	BA	2392	A	Sidechain
54	BA	2395	C	Sidechain
54	BA	2398	U	Sidechain
54	BA	2404	U	Sidechain
54	BA	2405	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2411	A	Sidechain
54	BA	2417	C	Sidechain
54	BA	2418	A	Sidechain
54	BA	2423	U	Sidechain
54	BA	2424	C	Sidechain
54	BA	2427	C	Sidechain
54	BA	2433	A	Sidechain
54	BA	244	A	Sidechain
54	BA	2440	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2445	G	Sidechain
54	BA	2446	G	Sidechain
54	BA	2451	A	Sidechain
54	BA	2453	A	Sidechain
54	BA	2460	U	Sidechain
54	BA	2462	C	Sidechain
54	BA	2465	C	Sidechain
54	BA	2469	A	Sidechain
54	BA	2475	C	Sidechain
54	BA	2476	A	Sidechain
54	BA	2477	U	Sidechain
54	BA	2478	A	Sidechain
54	BA	248	G	Sidechain
54	BA	2492	U	Sidechain
54	BA	2495	G	Sidechain
54	BA	2496	C	Sidechain
54	BA	2497	A	Sidechain
54	BA	2498	C	Sidechain
54	BA	2499	C	Sidechain
54	BA	250	G	Sidechain
54	BA	2502	G	Sidechain
54	BA	2504	U	Sidechain
54	BA	2522	U	Sidechain
54	BA	2529	G	Sidechain
54	BA	2530	A	Sidechain
54	BA	2534	A	Sidechain
54	BA	254	G	Sidechain
54	BA	2540	C	Sidechain
54	BA	2548	U	Sidechain
54	BA	2550	G	Sidechain
54	BA	2552	U	Sidechain
54	BA	2557	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	256	A	Sidechain
54	BA	2560	A	Sidechain
54	BA	2569	G	Sidechain
54	BA	2571	U	Sidechain
54	BA	2573	C	Sidechain
54	BA	2576	G	Sidechain
54	BA	2581	G	Sidechain
54	BA	2582	G	Sidechain
54	BA	2585	U	Sidechain
54	BA	2586	U	Sidechain
54	BA	2588	G	Sidechain
54	BA	2589	A	Sidechain
54	BA	2597	G	Sidechain
54	BA	2598	A	Sidechain
54	BA	2611	C	Sidechain
54	BA	2615	U	Sidechain
54	BA	2624	G	Sidechain
54	BA	2625	G	Sidechain
54	BA	2629	U	Sidechain
54	BA	263	G	Sidechain
54	BA	2631	G	Sidechain
54	BA	2637	U	Sidechain
54	BA	264	C	Sidechain
54	BA	2646	C	Sidechain
54	BA	2647	U	Sidechain
54	BA	2657	A	Sidechain
54	BA	2659	G	Sidechain
54	BA	2661	G	Sidechain
54	BA	2668	G	Sidechain
54	BA	2680	U	Sidechain
54	BA	2681	C	Sidechain
54	BA	2683	C	Sidechain
54	BA	269	C	Sidechain
54	BA	2698	U	Sidechain
54	BA	270	A	Sidechain
54	BA	2700	A	Sidechain
54	BA	2709	G	Sidechain
54	BA	2722	G	Sidechain
54	BA	2725	A	Sidechain
54	BA	2726	A	Sidechain
54	BA	2728	U	Sidechain
54	BA	2732	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2737	G	Sidechain
54	BA	2738	A	Sidechain
54	BA	2740	A	Sidechain
54	BA	2741	A	Sidechain
54	BA	2742	G	Sidechain
54	BA	2745	C	Sidechain
54	BA	2747	G	Sidechain
54	BA	2748	A	Sidechain
54	BA	2751	G	Sidechain
54	BA	2756	U	Sidechain
54	BA	276	U	Sidechain
54	BA	2764	A	Sidechain
54	BA	2767	C	Sidechain
54	BA	277	G	Sidechain
54	BA	2771	C	Sidechain
54	BA	2776	A	Sidechain
54	BA	278	A	Sidechain
54	BA	2783	U	Sidechain
54	BA	2786	U	Sidechain
54	BA	2787	C	Sidechain
54	BA	2789	C	Sidechain
54	BA	2797	U	Sidechain
54	BA	2801	G	Sidechain
54	BA	2802	G	Sidechain
54	BA	2808	G	Sidechain
54	BA	2809	A	Sidechain
54	BA	2810	A	Sidechain
54	BA	2816	G	Sidechain
54	BA	2817	U	Sidechain
54	BA	2819	G	Sidechain
54	BA	2820	A	Sidechain
54	BA	2824	C	Sidechain
54	BA	2827	C	Sidechain
54	BA	2829	A	Sidechain
54	BA	283	G	Sidechain
54	BA	2832	U	Sidechain
54	BA	2835	A	Sidechain
54	BA	2840	C	Sidechain
54	BA	2850	A	Sidechain
54	BA	2852	G	Sidechain
54	BA	2854	G	Sidechain
54	BA	2857	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2868	A	Sidechain
54	BA	2872	A	Sidechain
54	BA	2875	C	Sidechain
54	BA	2883	A	Sidechain
54	BA	2884	U	Sidechain
54	BA	2885	G	Sidechain
54	BA	2887	A	Sidechain
54	BA	2889	C	Sidechain
54	BA	289	G	Sidechain
54	BA	2892	G	Sidechain
54	BA	2897	U	Sidechain
54	BA	291	G	Sidechain
54	BA	297	G	Sidechain
54	BA	3	U	Sidechain
54	BA	303	G	Sidechain
54	BA	305	C	Sidechain
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	31	C	Sidechain
54	BA	311	A	Sidechain
54	BA	313	G	Sidechain
54	BA	314	C	Sidechain
54	BA	317	G	Sidechain
54	BA	322	A	Sidechain
54	BA	323	C	Sidechain
54	BA	329	G	Sidechain
54	BA	33	C	Sidechain
54	BA	333	G	Sidechain
54	BA	356	G	Sidechain
54	BA	358	U	Sidechain
54	BA	359	G	Sidechain
54	BA	361	G	Sidechain
54	BA	363	G	Sidechain
54	BA	364	C	Sidechain
54	BA	365	U	Sidechain
54	BA	371	A	Sidechain
54	BA	373	U	Sidechain
54	BA	374	A	Sidechain
54	BA	376	G	Sidechain
54	BA	377	G	Sidechain
54	BA	379	G	Sidechain
54	BA	384	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	386	G	Sidechain
54	BA	39	G	Sidechain
54	BA	390	U	Sidechain
54	BA	394	C	Sidechain
54	BA	395	U	Sidechain
54	BA	40	U	Sidechain
54	BA	401	A	Sidechain
54	BA	402	A	Sidechain
54	BA	403	U	Sidechain
54	BA	405	U	Sidechain
54	BA	409	G	Sidechain
54	BA	418	C	Sidechain
54	BA	420	C	Sidechain
54	BA	423	A	Sidechain
54	BA	428	A	Sidechain
54	BA	43	G	Sidechain
54	BA	436	C	Sidechain
54	BA	439	A	Sidechain
54	BA	44	A	Sidechain
54	BA	440	C	Sidechain
54	BA	446	G	Sidechain
54	BA	449	A	Sidechain
54	BA	451	U	Sidechain
54	BA	452	G	Sidechain
54	BA	454	A	Sidechain
54	BA	458	G	Sidechain
54	BA	460	A	Sidechain
54	BA	463	G	Sidechain
54	BA	473	G	Sidechain
54	BA	476	G	Sidechain
54	BA	479	A	Sidechain
54	BA	48	G	Sidechain
54	BA	481	G	Sidechain
54	BA	484	C	Sidechain
54	BA	485	C	Sidechain
54	BA	491	G	Sidechain
54	BA	492	A	Sidechain
54	BA	493	G	Sidechain
54	BA	495	G	Sidechain
54	BA	496	G	Sidechain
54	BA	500	G	Sidechain
54	BA	517	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	521	U	Sidechain
54	BA	523	C	Sidechain
54	BA	524	G	Sidechain
54	BA	525	U	Sidechain
54	BA	526	A	Sidechain
54	BA	527	C	Sidechain
54	BA	528	A	Sidechain
54	BA	530	G	Sidechain
54	BA	551	G	Sidechain
54	BA	561	G	Sidechain
54	BA	568	U	Sidechain
54	BA	571	U	Sidechain
54	BA	572	A	Sidechain
54	BA	578	G	Sidechain
54	BA	579	G	Sidechain
54	BA	580	U	Sidechain
54	BA	582	A	Sidechain
54	BA	583	G	Sidechain
54	BA	587	C	Sidechain
54	BA	588	U	Sidechain
54	BA	590	A	Sidechain
54	BA	593	U	Sidechain
54	BA	606	U	Sidechain
54	BA	611	C	Sidechain
54	BA	614	A	Sidechain
54	BA	616	A	Sidechain
54	BA	617	G	Sidechain
54	BA	621	A	Sidechain
54	BA	630	G	Sidechain
54	BA	632	A	Sidechain
54	BA	633	A	Sidechain
54	BA	635	C	Sidechain
54	BA	636	G	Sidechain
54	BA	641	U	Sidechain
54	BA	645	C	Sidechain
54	BA	650	C	Sidechain
54	BA	652	U	Sidechain
54	BA	655	A	Sidechain
54	BA	656	G	Sidechain
54	BA	657	U	Sidechain
54	BA	669	G	Sidechain
54	BA	670	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	687	C	Sidechain
54	BA	690	G	Sidechain
54	BA	695	G	Sidechain
54	BA	700	G	Sidechain
54	BA	706	A	Sidechain
54	BA	707	G	Sidechain
54	BA	709	U	Sidechain
54	BA	718	A	Sidechain
54	BA	72	U	Sidechain
54	BA	724	U	Sidechain
54	BA	726	G	Sidechain
54	BA	727	A	Sidechain
54	BA	736	C	Sidechain
54	BA	738	G	Sidechain
54	BA	739	A	Sidechain
54	BA	74	A	Sidechain
54	BA	749	A	Sidechain
54	BA	75	G	Sidechain
54	BA	750	A	Sidechain
54	BA	754	U	Sidechain
54	BA	76	C	Sidechain
54	BA	761	A	Sidechain
54	BA	763	G	Sidechain
54	BA	765	C	Sidechain
54	BA	770	G	Sidechain
54	BA	772	C	Sidechain
54	BA	773	U	Sidechain
54	BA	775	G	Sidechain
54	BA	788	A	Sidechain
54	BA	790	U	Sidechain
54	BA	800	A	Sidechain
54	BA	808	G	Sidechain
54	BA	816	C	Sidechain
54	BA	829	A	Sidechain
54	BA	830	G	Sidechain
54	BA	835	C	Sidechain
54	BA	840	C	Sidechain
54	BA	841	G	Sidechain
54	BA	845	A	Sidechain
54	BA	846	U	Sidechain
54	BA	848	C	Sidechain
54	BA	850	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	851	C	Sidechain
54	BA	852	U	Sidechain
54	BA	855	G	Sidechain
54	BA	857	G	Sidechain
54	BA	859	G	Sidechain
54	BA	862	G	Sidechain
54	BA	864	G	Sidechain
54	BA	865	C	Sidechain
54	BA	869	G	Sidechain
54	BA	870	U	Sidechain
54	BA	875	G	Sidechain
54	BA	881	G	Sidechain
54	BA	882	G	Sidechain
54	BA	899	A	Sidechain
54	BA	905	A	Sidechain
54	BA	906	U	Sidechain
54	BA	907	G	Sidechain
54	BA	908	C	Sidechain
54	BA	912	C	Sidechain
54	BA	914	G	Sidechain
54	BA	92	U	Sidechain
54	BA	921	C	Sidechain
54	BA	922	C	Sidechain
54	BA	925	A	Sidechain
54	BA	926	G	Sidechain
54	BA	930	G	Sidechain
54	BA	932	U	Sidechain
54	BA	933	A	Sidechain
54	BA	934	U	Sidechain
54	BA	942	G	Sidechain
54	BA	954	G	Sidechain
54	BA	958	U	Sidechain
54	BA	960	A	Sidechain
54	BA	961	C	Sidechain
54	BA	962	G	Sidechain
54	BA	963	U	Sidechain
54	BA	969	G	Sidechain
54	BA	971	G	Sidechain
54	BA	979	A	Sidechain
54	BA	984	A	Sidechain
54	BA	986	C	Sidechain
54	BA	993	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	995	C	Sidechain
54	BA	998	C	Sidechain
55	BB	10	G	Sidechain
55	BB	105	G	Sidechain
55	BB	108	A	Sidechain
55	BB	114	C	Sidechain
55	BB	13	G	Sidechain
55	BB	23	G	Sidechain
55	BB	24	G	Sidechain
55	BB	29	A	Sidechain
55	BB	37	C	Sidechain
55	BB	39	A	Sidechain
55	BB	4	C	Sidechain
55	BB	40	U	Sidechain
55	BB	41	G	Sidechain
55	BB	42	C	Sidechain
55	BB	48	U	Sidechain
55	BB	49	C	Sidechain
55	BB	52	A	Sidechain
55	BB	64	G	Sidechain
55	BB	65	U	Sidechain
55	BB	72	G	Sidechain
55	BB	75	G	Sidechain
55	BB	76	G	Sidechain
55	BB	84	G	Sidechain
55	BB	9	G	Sidechain
55	BB	93	C	Sidechain
43	BU	6	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	1	0
5	AF	818	0	808	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	2	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	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	1	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	3	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	2	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	0
38	BP	917	0	965	1	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	1	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	31341	4	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99659	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)
34:BL:30:THR:HG21	34:BL:36:LYS:H	1.72	0.54
54:BA:388:G:H2'	54:BA:389:G:H3'	1.91	0.52
42:BT:15:HIS:CG	42:BT:16:VAL:H	2.29	0.50
21:AA:1054:C:C6	23:A2:89:U:H1'	2.48	0.48
37:BO:53:THR:HG21	37:BO:70:ALA:HB1	1.98	0.46
38:BP:95:LYS:HE2	54:BA:2718:G:O3'	2.17	0.45
35:BM:34:LYS:HE3	35:BM:131:VAL:HG11	1.99	0.44
33:BK:119:ALA:H	33:BK:120:PRO:CD	2.31	0.44
21:AA:865:A:H2'	21:AA:866:C:C6	2.55	0.42
7:AH:60:LEU:H	7:AH:60:LEU:HD23	1.84	0.41
21:AA:1517:G:H2'	21:AA:1518:A:C8	2.56	0.41
4:AE:155:LYS:HE3	7:AH:44:PHE:CE1	2.56	0.41
35:BM:14:LYS:HE3	54:BA:958:U:C2	2.56	0.41
45:BW:9:THR:HB	45:BW:10:ARG:HA	2.02	0.41
54:BA:833:A:H2'	54:BA:834:G:C8	2.56	0.41
33:BK:105:ARG:NE	33:BK:105:ARG:H	2.20	0.40
33:BK:119:ALA:H	33:BK:120:PRO:HD2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	200 (92%)	17 (8%)	1 (0%)	32	74
2	AC	205/208 (99%)	184 (90%)	15 (7%)	6 (3%)	5	38
3	AD	203/206 (98%)	185 (91%)	14 (7%)	4 (2%)	9	46
4	AE	150/152 (99%)	134 (89%)	10 (7%)	6 (4%)	3	31
5	AF	99/101 (98%)	80 (81%)	13 (13%)	6 (6%)	2	22
6	AG	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	6	40
7	AH	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	7	42
8	AI	126/128 (98%)	107 (85%)	15 (12%)	4 (3%)	5	36
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	2	26
10	AK	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	11	50
11	AL	121/124 (98%)	107 (88%)	8 (7%)	6 (5%)	2	27
12	AM	112/115 (97%)	94 (84%)	13 (12%)	5 (4%)	3	29
13	AN	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
14	AO	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	15	57
15	AP	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	4	32
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	AR	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	10	49
18	AS	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	4	32
19	AT	84/86 (98%)	76 (90%)	8 (10%)	0	100	100
20	AU	51/53 (96%)	32 (63%)	15 (29%)	4 (8%)	1	18
25	BC	270/273 (99%)	238 (88%)	25 (9%)	7 (3%)	6	40
26	BD	207/209 (99%)	185 (89%)	17 (8%)	5 (2%)	7	42
27	BE	199/201 (99%)	171 (86%)	20 (10%)	8 (4%)	3	31
28	BF	176/179 (98%)	155 (88%)	17 (10%)	4 (2%)	7	43
29	BG	174/177 (98%)	155 (89%)	12 (7%)	7 (4%)	3	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BH	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	25	68
31	BI	139/142 (98%)	125 (90%)	12 (9%)	2 (1%)	13	54
32	BJ	140/142 (99%)	126 (90%)	11 (8%)	3 (2%)	8	45
33	BK	121/123 (98%)	107 (88%)	10 (8%)	4 (3%)	4	35
34	BL	141/144 (98%)	124 (88%)	11 (8%)	6 (4%)	3	29
35	BM	134/136 (98%)	115 (86%)	14 (10%)	5 (4%)	4	33
36	BN	119/121 (98%)	105 (88%)	11 (9%)	3 (2%)	6	41
37	BO	114/117 (97%)	108 (95%)	3 (3%)	3 (3%)	6	40
38	BP	112/115 (97%)	92 (82%)	17 (15%)	3 (3%)	6	40
39	BQ	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	11	50
40	BR	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	5	37
41	BS	108/110 (98%)	105 (97%)	2 (2%)	1 (1%)	20	63
42	BT	92/94 (98%)	80 (87%)	6 (6%)	6 (6%)	1	22
43	BU	101/104 (97%)	83 (82%)	14 (14%)	4 (4%)	3	31
44	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
45	BW	78/80 (98%)	59 (76%)	17 (22%)	2 (3%)	6	40
46	BX	75/79 (95%)	68 (91%)	3 (4%)	4 (5%)	2	26
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	49 (88%)	4 (7%)	3 (5%)	2	25
49	B0	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
50	B1	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
51	B2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
52	B3	62/65 (95%)	54 (87%)	5 (8%)	3 (5%)	2	28
53	B4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	6	39
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	32	74
All	All	5876/6008 (98%)	5245 (89%)	476 (8%)	155 (3%)	10	40

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	224	ARG
2	AC	14	VAL
5	AF	86	ARG

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Mol	Chain	Res	Type
15	AP	11	ALA
15	AP	17	TYR
18	AS	4	LEU
25	BC	191	LEU
26	BD	2	ILE
27	BE	96	VAL
28	BF	12	VAL
29	BG	8	VAL
33	BK	103	VAL
33	BK	119	ALA
34	BL	29	LYS
43	BU	45	GLN
56	B5	50	ILE
2	AC	65	VAL
3	AD	24	VAL
4	AE	158	LYS
5	AF	10	VAL
5	AF	52	ASN
5	AF	63	ASN
6	AG	9	ARG
6	AG	56	SER
8	AI	115	VAL
8	AI	120	ALA
9	AJ	75	ASP
11	AL	33	CYS
11	AL	78	VAL
11	AL	108	ASP
14	AO	45	HIS
18	AS	5	LYS
20	AU	25	ALA
25	BC	36	ASN
29	BG	16	VAL
29	BG	22	VAL
29	BG	59	ASP
30	BH	67	ALA
31	BI	135	MET
32	BJ	48	VAL
32	BJ	72	LYS
32	BJ	81	ILE
34	BL	33	ARG
34	BL	34	GLY
34	BL	36	LYS

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Mol	Chain	Res	Type
34	BL	94	THR
35	BM	36	VAL
35	BM	70	ASP
35	BM	123	LYS
36	BN	110	MET
37	BO	89	ASP
39	BQ	87	VAL
42	BT	11	LEU
42	BT	39	THR
42	BT	66	LYS
42	BT	68	LYS
43	BU	50	ALA
43	BU	92	VAL
46	BX	27	ARG
52	B3	3	ILE
3	AD	3	TYR
3	AD	4	LEU
4	AE	43	GLY
4	AE	54	GLU
6	AG	60	ALA
7	AH	53	ASP
7	AH	69	ALA
9	AJ	102	LEU
10	AK	117	HIS
12	AM	21	ILE
17	AR	21	ASP
18	AS	33	TRP
20	AU	27	VAL
25	BC	189	ALA
25	BC	196	ASN
26	BD	60	VAL
26	BD	112	THR
26	BD	119	ALA
27	BE	46	GLN
27	BE	71	GLY
27	BE	97	ASN
27	BE	120	VAL
28	BF	46	LYS
28	BF	116	LEU
33	BK	22	ILE
35	BM	21	ALA
35	BM	58	LYS

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Mol	Chain	Res	Type
36	BN	2	ARG
37	BO	23	ALA
37	BO	102	ARG
38	BP	31	VAL
40	BR	43	ASN
42	BT	2	ILE
43	BU	43	LYS
45	BW	15	SER
52	B3	25	HIS
2	AC	145	ALA
2	AC	163	ARG
2	AC	167	TYR
3	AD	28	ASP
4	AE	105	ILE
5	AF	59	TYR
8	AI	42	THR
8	AI	55	ASP
11	AL	87	LYS
11	AL	122	LYS
12	AM	22	TYR
20	AU	24	LYS
25	BC	109	LEU
27	BE	165	HIS
33	BK	2	ILE
38	BP	86	LYS
40	BR	51	VAL
45	BW	23	LYS
2	AC	206	ILE
4	AE	22	LYS
5	AF	6	ILE
6	AG	5	VAL
10	AK	12	ARG
12	AM	11	HIS
15	AP	26	ASN
27	BE	79	ARG
27	BE	90	GLN
36	BN	66	ALA
39	BQ	4	LYS
42	BT	28	ASN
48	BZ	3	THR
48	BZ	4	ILE
52	B3	35	LYS

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Mol	Chain	Res	Type
29	BG	164	ALA
31	BI	31	GLY
40	BR	29	THR
46	BX	19	HIS
46	BX	40	GLU
48	BZ	9	THR
4	AE	103	GLY
9	AJ	57	VAL
26	BD	73	VAL
29	BG	9	VAL
7	AH	77	VAL
25	BC	136	VAL
28	BF	136	ILE
34	BL	55	MET
46	BX	6	VAL
9	AJ	38	GLY
12	AM	66	GLY
20	AU	13	VAL
29	BG	116	LEU
53	B4	16	ILE
9	AJ	42	LEU
12	AM	3	ILE
25	BC	53	ILE
41	BS	29	VAL
11	AL	43	LYS
38	BP	32	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%)	177 (98%)	3 (2%)	66	84
2	AC	170/171 (99%)	168 (99%)	2 (1%)	75	88
3	AD	172/173 (99%)	171 (99%)	1 (1%)	89	94
4	AE	113/113 (100%)	112 (99%)	1 (1%)	82	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	85	92
7	AH	104/105 (99%)	101 (97%)	3 (3%)	48	73
8	AI	105/105 (100%)	101 (96%)	4 (4%)	38	67
9	AJ	86/86 (100%)	83 (96%)	3 (4%)	41	69
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	102 (99%)	1 (1%)	80	90
12	AM	91/92 (99%)	90 (99%)	1 (1%)	78	89
13	AN	83/84 (99%)	81 (98%)	2 (2%)	54	78
14	AO	76/77 (99%)	74 (97%)	2 (3%)	51	75
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	71 (96%)	3 (4%)	35	65
17	AR	48/48 (100%)	45 (94%)	3 (6%)	21	53
18	AS	70/70 (100%)	69 (99%)	1 (1%)	71	86
19	AT	65/65 (100%)	64 (98%)	1 (2%)	70	85
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	49	74
26	BD	164/164 (100%)	160 (98%)	4 (2%)	54	78
27	BE	165/165 (100%)	162 (98%)	3 (2%)	64	84
28	BF	149/150 (99%)	147 (99%)	2 (1%)	73	87
29	BG	137/138 (99%)	133 (97%)	4 (3%)	48	73
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	108 (99%)	1 (1%)	82	91
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	51	75
33	BK	103/103 (100%)	102 (99%)	1 (1%)	80	90
34	BL	102/103 (99%)	100 (98%)	2 (2%)	60	82
35	BM	109/109 (100%)	107 (98%)	2 (2%)	64	84
36	BN	100/100 (100%)	99 (99%)	1 (1%)	80	90
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	97 (98%)	2 (2%)	60	82
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	57	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BR	84/84 (100%)	84 (100%)	0	100	100
41	BS	93/93 (100%)	92 (99%)	1 (1%)	78	89
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	54	78
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	53 (90%)	6 (10%)	8	33
46	BX	67/68 (98%)	66 (98%)	1 (2%)	70	85
47	BY	55/55 (100%)	54 (98%)	1 (2%)	64	84
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	59	80
50	B1	45/45 (100%)	44 (98%)	1 (2%)	57	79
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	48 (94%)	3 (6%)	23	55
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	169 (98%)	4 (2%)	56	79
All	All	4842/4870 (99%)	4757 (98%)	85 (2%)	67	84

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	56	LEU
1	AB	71	THR
1	AB	136	ARG
2	AC	128	MET
2	AC	198	LYS
3	AD	196	GLU
4	AE	151	MET
6	AG	56	SER
7	AH	40	LYS
7	AH	66	GLN
7	AH	104	SER
8	AI	41	GLU
8	AI	42	THR
8	AI	105	ARG
8	AI	125	GLN
9	AJ	19	ASP
9	AJ	44	THR

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Mol	Chain	Res	Type
9	AJ	102	LEU
11	AL	8	ARG
12	AM	81	ASP
13	AN	41	ARG
13	AN	42	TRP
14	AO	19	ASN
14	AO	46	LYS
16	AQ	7	LEU
16	AQ	17	GLU
16	AQ	43	LEU
17	AR	32	ILE
17	AR	66	LEU
17	AR	69	TYR
18	AS	78	THR
19	AT	27	MET
25	BC	47	ARG
25	BC	50	THR
25	BC	86	ARG
25	BC	123	ILE
25	BC	194	VAL
25	BC	229	HIS
26	BD	15	PHE
26	BD	33	ARG
26	BD	154	LYS
26	BD	200	ASP
27	BE	35	TYR
27	BE	79	ARG
27	BE	125	SER
28	BF	80	GLN
28	BF	124	ARG
29	BG	148	ARG
29	BG	163	TYR
29	BG	165	ASP
29	BG	166	GLU
31	BI	110	GLN
32	BJ	9	GLU
32	BJ	14	ASP
32	BJ	24	THR
33	BK	105	ARG
34	BL	4	ASN
34	BL	93	ASN
35	BM	1	MET

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Mol	Chain	Res	Type
35	BM	97	GLN
36	BN	37	THR
38	BP	105	LYS
38	BP	108	ARG
39	BQ	50	ARG
39	BQ	56	PHE
41	BS	60	HIS
43	BU	8	ASP
43	BU	44	HIS
45	BW	10	ARG
45	BW	13	ARG
45	BW	39	GLN
45	BW	40	ARG
45	BW	49	ASN
45	BW	63	ASP
46	BX	15	ASN
47	BY	26	PHE
49	B0	37	HIS
50	B1	20	TYR
52	B3	37	THR
52	B3	38	LYS
52	B3	53	ASP
56	B5	126	GLN
56	B5	129	GLN
56	B5	164	ARG
56	B5	165	ASN

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

Mol	Chain	Res	Type
12	AM	104	ASN
44	BV	88	HIS
46	BX	15	ASN
49	B0	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	248 (16%)	0
22	A1	73/76 (96%)	15 (20%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	A2	14/15 (93%)	5 (35%)	0
24	A3	76/77 (98%)	13 (17%)	0
54	BA	2902/2903 (99%)	464 (15%)	0
55	BB	116/118 (98%)	15 (12%)	0
All	All	4710/4722 (99%)	760 (16%)	0

All (760) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	16	A
21	AA	28	A
21	AA	32	A
21	AA	35	G
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	56	U
21	AA	66	A
21	AA	67	C
21	AA	71	A
21	AA	81	A
21	AA	86	G
21	AA	90	C
21	AA	91	U
21	AA	95	C
21	AA	110	C
21	AA	121	U
21	AA	124	C
21	AA	131	A
21	AA	144	G
21	AA	163	C
21	AA	164	G
21	AA	168	G
21	AA	198	G
21	AA	207	C

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Mol	Chain	Res	Type
21	AA	212	G
21	AA	213	G
21	AA	214	C
21	AA	236	A
21	AA	238	A
21	AA	239	U
21	AA	240	G
21	AA	244	U
21	AA	245	U
21	AA	247	G
21	AA	250	A
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	267	C
21	AA	272	C
21	AA	279	A
21	AA	289	G
21	AA	293	G
21	AA	307	C
21	AA	308	C
21	AA	315	A
21	AA	316	C
21	AA	317	U
21	AA	328	C
21	AA	329	A
21	AA	344	A
21	AA	345	C
21	AA	347	G
21	AA	352	C
21	AA	353	A
21	AA	354	G
21	AA	358	U
21	AA	361	G
21	AA	367	U
21	AA	372	C
21	AA	381	C
21	AA	384	G
21	AA	389	A
21	AA	397	A
21	AA	412	A
21	AA	413	G

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Mol	Chain	Res	Type
21	AA	414	A
21	AA	415	A
21	AA	422	C
21	AA	424	G
21	AA	428	G
21	AA	429	U
21	AA	458	U
21	AA	461	A
21	AA	462	G
21	AA	464	U
21	AA	472	U
21	AA	474	G
21	AA	484	G
21	AA	496	A
21	AA	499	A
21	AA	511	C
21	AA	527	G
21	AA	533	A
21	AA	547	A
21	AA	559	A
21	AA	560	A
21	AA	561	U
21	AA	562	U
21	AA	564	C
21	AA	566	G
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	577	G
21	AA	607	A
21	AA	608	A
21	AA	618	C
21	AA	619	U
21	AA	620	C
21	AA	626	G
21	AA	632	U
21	AA	633	G
21	AA	653	U
21	AA	659	U
21	AA	663	A
21	AA	664	G

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Mol	Chain	Res	Type
21	AA	714	G
21	AA	718	A
21	AA	731	G
21	AA	755	G
21	AA	777	A
21	AA	794	A
21	AA	812	G
21	AA	815	A
21	AA	816	A
21	AA	817	C
21	AA	819	A
21	AA	822	U
21	AA	828	U
21	AA	841	C
21	AA	843	U
21	AA	845	A
21	AA	846	G
21	AA	872	A
21	AA	885	G
21	AA	890	G
21	AA	902	G
21	AA	918	A
21	AA	927	G
21	AA	933	G
21	AA	934	C
21	AA	935	A
21	AA	939	G
21	AA	942	G
21	AA	945	G
21	AA	958	A
21	AA	959	A
21	AA	960	U
21	AA	961	U
21	AA	962	C
21	AA	964	A
21	AA	965	U
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	972	C
21	AA	975	A
21	AA	977	A

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Mol	Chain	Res	Type
21	AA	980	C
21	AA	983	A
21	AA	992	U
21	AA	993	G
21	AA	994	A
21	AA	996	A
21	AA	1004	A
21	AA	1006	G
21	AA	1026	G
21	AA	1028	C
21	AA	1032	G
21	AA	1033	G
21	AA	1049	U
21	AA	1053	G
21	AA	1054	C
21	AA	1055	A
21	AA	1056	U
21	AA	1061	G
21	AA	1065	U
21	AA	1068	G
21	AA	1081	A
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1124	G
21	AA	1125	U
21	AA	1130	A
21	AA	1137	C
21	AA	1139	G
21	AA	1143	G
21	AA	1159	U
21	AA	1161	C
21	AA	1167	A
21	AA	1168	U
21	AA	1169	A
21	AA	1183	U
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1193	G
21	AA	1202	U

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Mol	Chain	Res	Type
21	AA	1203	C
21	AA	1212	U
21	AA	1213	A
21	AA	1217	C
21	AA	1221	G
21	AA	1224	U
21	AA	1225	A
21	AA	1227	A
21	AA	1232	U
21	AA	1240	U
21	AA	1241	G
21	AA	1256	A
21	AA	1257	A
21	AA	1260	G
21	AA	1267	C
21	AA	1278	G
21	AA	1280	A
21	AA	1281	C
21	AA	1286	U
21	AA	1302	C
21	AA	1303	C
21	AA	1307	U
21	AA	1308	U
21	AA	1317	C
21	AA	1319	A
21	AA	1320	C
21	AA	1321	U
21	AA	1323	G
21	AA	1329	A
21	AA	1338	G
21	AA	1346	A
21	AA	1360	A
21	AA	1363	A
21	AA	1378	C
21	AA	1394	A
21	AA	1397	C
21	AA	1401	G
21	AA	1402	C
21	AA	1413	A
21	AA	1432	G
21	AA	1447	A
21	AA	1460	C

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Mol	Chain	Res	Type
21	AA	1503	A
21	AA	1505	G
21	AA	1506	U
21	AA	1529	G
21	AA	1530	G
22	A1	3	G
22	A1	10	G
22	A1	17	U
22	A1	19	G
22	A1	44	G
22	A1	45	G
22	A1	46	7MG
22	A1	47	U
22	A1	49	G
22	A1	59	U
22	A1	61	C
22	A1	70	C
22	A1	71	C
22	A1	74	C
22	A1	76	A
23	A2	81	U
23	A2	85	G
23	A2	89	U
23	A2	90	U
23	A2	93	U
24	A3	2	G
24	A3	9	G
24	A3	18	U
24	A3	20	G
24	A3	31	G
24	A3	48	U
24	A3	49	C
24	A3	60	A
24	A3	61	U
24	A3	63	C
24	A3	73	A
24	A3	74	A
24	A3	77	A
54	BA	15	G
54	BA	29	U
54	BA	34	U
54	BA	45	G

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Mol	Chain	Res	Type
54	BA	60	G
54	BA	62	U
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	77	G
54	BA	100	U
54	BA	101	A
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	128	C
54	BA	139	U
54	BA	141	G
54	BA	142	A
54	BA	143	C
54	BA	165	A
54	BA	180	G
54	BA	181	A
54	BA	196	A
54	BA	199	A
54	BA	200	U
54	BA	205	G
54	BA	206	U
54	BA	216	A
54	BA	221	A
54	BA	222	A
54	BA	230	G
54	BA	233	A
54	BA	245	G
54	BA	248	G
54	BA	271	G
54	BA	272	A
54	BA	273	G
54	BA	275	C
54	BA	278	A
54	BA	279	A
54	BA	283	G
54	BA	297	G
54	BA	316	C

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Mol	Chain	Res	Type
54	BA	323	C
54	BA	324	A
54	BA	325	G
54	BA	330	A
54	BA	331	C
54	BA	333	G
54	BA	346	A
54	BA	365	U
54	BA	372	G
54	BA	373	U
54	BA	374	A
54	BA	389	G
54	BA	390	U
54	BA	403	U
54	BA	404	A
54	BA	405	U
54	BA	406	G
54	BA	411	G
54	BA	413	C
54	BA	430	A
54	BA	436	C
54	BA	443	A
54	BA	444	C
54	BA	450	G
54	BA	451	U
54	BA	453	A
54	BA	457	A
54	BA	475	C
54	BA	481	G
54	BA	482	A
54	BA	491	G
54	BA	504	A
54	BA	505	A
54	BA	507	A
54	BA	518	G
54	BA	527	C
54	BA	529	A
54	BA	530	G
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	546	U

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Mol	Chain	Res	Type
54	BA	547	A
54	BA	548	G
54	BA	563	A
54	BA	571	U
54	BA	572	A
54	BA	573	U
54	BA	587	C
54	BA	603	A
54	BA	615	U
54	BA	616	A
54	BA	620	G
54	BA	621	A
54	BA	628	G
54	BA	637	A
54	BA	644	A
54	BA	653	U
54	BA	654	A
54	BA	671	C
54	BA	672	C
54	BA	686	U
54	BA	706	A
54	BA	719	C
54	BA	732	C
54	BA	736	C
54	BA	747	U
54	BA	748	G
54	BA	751	A
54	BA	752	A
54	BA	775	G
54	BA	776	G
54	BA	781	A
54	BA	782	A
54	BA	784	G
54	BA	788	A
54	BA	789	A
54	BA	791	C
54	BA	793	A
54	BA	799	G
54	BA	800	A
54	BA	805	G
54	BA	830	G
54	BA	846	U

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Mol	Chain	Res	Type
54	BA	847	U
54	BA	848	C
54	BA	853	C
54	BA	854	C
54	BA	888	C
54	BA	889	C
54	BA	890	C
54	BA	891	G
54	BA	910	A
54	BA	912	C
54	BA	915	C
54	BA	931	U
54	BA	932	U
54	BA	933	A
54	BA	941	A
54	BA	945	A
54	BA	946	C
54	BA	955	U
54	BA	958	U
54	BA	959	A
54	BA	981	A
54	BA	983	A
54	BA	984	A
54	BA	996	A
54	BA	999	U
54	BA	1000	A
54	BA	1005	C
54	BA	1006	C
54	BA	1012	U
54	BA	1024	G
54	BA	1026	G
54	BA	1033	U
54	BA	1044	C
54	BA	1046	A
54	BA	1047	G
54	BA	1051	G
54	BA	1057	A
54	BA	1063	G
54	BA	1067	A
54	BA	1070	A
54	BA	1072	C
54	BA	1073	A

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Mol	Chain	Res	Type
54	BA	1076	C
54	BA	1087	G
54	BA	1088	A
54	BA	1089	A
54	BA	1094	U
54	BA	1096	A
54	BA	1109	C
54	BA	1110	G
54	BA	1129	A
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1142	A
54	BA	1148	U
54	BA	1155	A
54	BA	1157	G
54	BA	1158	C
54	BA	1175	A
54	BA	1176	U
54	BA	1186	G
54	BA	1204	A
54	BA	1206	G
54	BA	1227	G
54	BA	1237	A
54	BA	1238	G
54	BA	1242	U
54	BA	1245	G
54	BA	1256	G
54	BA	1265	A
54	BA	1275	A
54	BA	1276	A
54	BA	1287	A
54	BA	1288	G
54	BA	1289	C
54	BA	1292	G
54	BA	1293	C
54	BA	1300	G
54	BA	1301	A
54	BA	1302	A
54	BA	1313	U
54	BA	1317	G
54	BA	1322	A

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Mol	Chain	Res	Type
54	BA	1325	U
54	BA	1329	U
54	BA	1330	C
54	BA	1333	G
54	BA	1341	G
54	BA	1365	A
54	BA	1378	A
54	BA	1379	U
54	BA	1383	A
54	BA	1385	A
54	BA	1389	G
54	BA	1390	U
54	BA	1398	C
54	BA	1399	C
54	BA	1416	G
54	BA	1417	C
54	BA	1420	A
54	BA	1421	G
54	BA	1428	C
54	BA	1439	A
54	BA	1440	U
54	BA	1452	G
54	BA	1455	G
54	BA	1482	G
54	BA	1490	A
54	BA	1491	G
54	BA	1493	C
54	BA	1523	U
54	BA	1524	G
54	BA	1532	A
54	BA	1535	A
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1540	G
54	BA	1555	G
54	BA	1568	G
54	BA	1578	U
54	BA	1591	A
54	BA	1598	A
54	BA	1603	A
54	BA	1607	C

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Mol	Chain	Res	Type
54	BA	1610	A
54	BA	1611	C
54	BA	1616	A
54	BA	1618	A
54	BA	1627	G
54	BA	1647	U
54	BA	1648	U
54	BA	1651	G
54	BA	1652	A
54	BA	1654	A
54	BA	1655	A
54	BA	1664	A
54	BA	1670	C
54	BA	1674	G
54	BA	1675	C
54	BA	1693	U
54	BA	1696	G
54	BA	1699	G
54	BA	1700	A
54	BA	1701	A
54	BA	1707	G
54	BA	1713	A
54	BA	1714	U
54	BA	1730	C
54	BA	1731	G
54	BA	1733	G
54	BA	1763	G
54	BA	1764	C
54	BA	1773	A
54	BA	1775	U
54	BA	1780	A
54	BA	1782	U
54	BA	1783	A
54	BA	1784	A
54	BA	1791	A
54	BA	1797	G
54	BA	1800	C
54	BA	1808	A
54	BA	1809	A
54	BA	1815	A
54	BA	1816	C
54	BA	1817	G

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Mol	Chain	Res	Type
54	BA	1821	A
54	BA	1835	G
54	BA	1858	A
54	BA	1870	C
54	BA	1871	A
54	BA	1873	G
54	BA	1877	A
54	BA	1886	U
54	BA	1896	G
54	BA	1906	G
54	BA	1916	A
54	BA	1919	A
54	BA	1926	U
54	BA	1929	G
54	BA	1930	G
54	BA	1937	A
54	BA	1938	A
54	BA	1945	G
54	BA	1955	U
54	BA	1963	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	1997	C
54	BA	2016	U
54	BA	2023	C
54	BA	2030	A
54	BA	2043	C
54	BA	2047	C
54	BA	2052	A
54	BA	2055	C
54	BA	2061	G
54	BA	2062	A
54	BA	2069	G
54	BA	2076	U
54	BA	2077	A
54	BA	2090	A
54	BA	2092	U

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Mol	Chain	Res	Type
54	BA	2093	G
54	BA	2111	U
54	BA	2113	U
54	BA	2117	A
54	BA	2118	U
54	BA	2133	G
54	BA	2145	C
54	BA	2146	C
54	BA	2148	G
54	BA	2157	G
54	BA	2159	G
54	BA	2160	C
54	BA	2163	A
54	BA	2164	C
54	BA	2169	A
54	BA	2172	U
54	BA	2173	A
54	BA	2198	A
54	BA	2203	U
54	BA	2211	A
54	BA	2212	A
54	BA	2216	G
54	BA	2238	G
54	BA	2246	G
54	BA	2253	G
54	BA	2266	A
54	BA	2274	A
54	BA	2276	G
54	BA	2283	C
54	BA	2286	G
54	BA	2287	A
54	BA	2297	A
54	BA	2305	U
54	BA	2309	A
54	BA	2312	U
54	BA	2321	U
54	BA	2325	G
54	BA	2333	A
54	BA	2334	U
54	BA	2335	A
54	BA	2339	C
54	BA	2343	U

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Mol	Chain	Res	Type
54	BA	2344	U
54	BA	2347	C
54	BA	2383	G
54	BA	2385	C
54	BA	2392	A
54	BA	2402	U
54	BA	2407	A
54	BA	2425	A
54	BA	2428	G
54	BA	2429	G
54	BA	2430	A
54	BA	2432	A
54	BA	2433	A
54	BA	2435	A
54	BA	2439	A
54	BA	2440	C
54	BA	2441	U
54	BA	2447	G
54	BA	2448	A
54	BA	2449	U
54	BA	2450	A
54	BA	2452	C
54	BA	2473	U
54	BA	2474	U
54	BA	2476	A
54	BA	2491	U
54	BA	2492	U
54	BA	2499	C
54	BA	2500	U
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2513	A
54	BA	2531	A
54	BA	2532	G
54	BA	2558	C
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2572	A
54	BA	2573	C
54	BA	2576	G

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Mol	Chain	Res	Type
54	BA	2578	G
54	BA	2585	U
54	BA	2586	U
54	BA	2592	G
54	BA	2596	U
54	BA	2599	G
54	BA	2602	A
54	BA	2603	G
54	BA	2609	U
54	BA	2613	U
54	BA	2630	G
54	BA	2644	G
54	BA	2645	G
54	BA	2646	C
54	BA	2655	G
54	BA	2660	A
54	BA	2661	G
54	BA	2669	G
54	BA	2681	C
54	BA	2684	U
54	BA	2689	U
54	BA	2690	U
54	BA	2691	C
54	BA	2736	A
54	BA	2751	G
54	BA	2765	A
54	BA	2766	A
54	BA	2778	A
54	BA	2780	G
54	BA	2791	G
54	BA	2798	U
54	BA	2809	A
54	BA	2817	U
54	BA	2820	A
54	BA	2821	A
54	BA	2850	A
54	BA	2861	U
54	BA	2876	G
54	BA	2894	G
54	BA	2895	G
55	BB	3	C
55	BB	11	C

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Mol	Chain	Res	Type
55	BB	12	C
55	BB	15	A
55	BB	25	U
55	BB	30	C
55	BB	42	C
55	BB	45	A
55	BB	81	G
55	BB	82	U
55	BB	83	G
55	BB	88	C
55	BB	90	C
55	BB	108	A
55	BB	109	A

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	CM0	A1	34	21,22	16,26,27	1.90	3 (18%)	14,37,40	3.35	3 (21%)
22	6MZ	A1	37	22	18,25,26	1.05	1 (5%)	16,36,39	1.68	2 (12%)
22	7MG	A1	46	22	20,26,27	2.19	3 (15%)	22,39,42	1.92	2 (9%)
22	5MU	A1	54	22	14,22,23	1.29	2 (14%)	16,32,35	4.09	2 (12%)
22	PSU	A1	55	22	16,21,22	1.11	1 (6%)	20,30,33	5.31	7 (35%)
22	4SU	A1	7	22	14,21,22	1.19	1 (7%)	15,30,33	2.77	4 (26%)
24	H2U	A3	21	24	17,21,22	1.51	2 (11%)	21,30,33	1.32	4 (19%)
24	OMC	A3	33	24	15,22,23	1.24	0	19,31,34	1.05	1 (5%)
24	5MU	A3	55	24	14,22,23	1.09	1 (7%)	16,32,35	3.86	3 (18%)
24	PSU	A3	56	24	16,21,22	1.36	2 (12%)	20,30,33	5.54	7 (35%)
24	4SU	A3	8	24	14,21,22	1.32	3 (21%)	15,30,33	2.80	2 (13%)

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

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.13	1.33	1.45
22	A1	34	CM0	O5-C5	-6.13	1.25	1.37
24	A3	21	H2U	C4-N3	-3.60	1.31	1.37
24	A3	21	H2U	C2-N3	-3.45	1.31	1.38
22	A1	46	7MG	C8-N7	-2.76	1.31	1.43
22	A1	37	6MZ	C8-N7	-2.43	1.30	1.34
24	A3	8	4SU	O5'-C5'	-2.33	1.41	1.44
24	A3	56	PSU	O4'-C1'	-2.09	1.41	1.44
22	A1	7	4SU	C6-N1	2.12	1.38	1.35
22	A1	34	CM0	C4-N3	2.13	1.36	1.33
24	A3	8	4SU	C6-N1	2.22	1.38	1.35
24	A3	8	4SU	O4'-C1'	2.22	1.44	1.41
22	A1	55	PSU	C4-N3	2.38	1.37	1.33
22	A1	54	5MU	C4-N3	2.45	1.37	1.33
22	A1	54	5MU	O4'-C1'	2.50	1.44	1.41
24	A3	55	5MU	C4-N3	2.58	1.37	1.33
22	A1	34	CM0	C4-C5	2.59	1.47	1.41
22	A1	46	7MG	C6-N1	2.67	1.37	1.33
24	A3	56	PSU	C4-N3	2.74	1.38	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	56	PSU	N1-C2-N3	-16.31	116.67	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	55	PSU	N1-C2-N3	-15.43	117.30	128.40
24	A3	56	PSU	C5-C4-N3	-12.61	115.08	125.43
22	A1	55	PSU	C5-C4-N3	-12.19	115.43	125.43
22	A1	54	5MU	C5-C4-N3	-9.96	114.26	125.24
24	A3	55	5MU	C5-C4-N3	-9.30	114.98	125.24
24	A3	8	4SU	C5-C4-N3	-6.69	115.28	123.73
22	A1	46	7MG	C5-C6-N1	-6.52	113.14	123.37
22	A1	7	4SU	C5-C4-N3	-6.10	116.02	123.73
22	A1	55	PSU	C5-C1'-C2'	-3.75	109.07	115.55
22	A1	7	4SU	C4'-O4'-C1'	-3.38	106.17	109.77
22	A1	55	PSU	C5-C6-N1	-3.19	120.25	124.39
24	A3	56	PSU	C5-C6-N1	-3.17	120.28	124.39
24	A3	33	OMC	C4'-O4'-C1'	-2.96	106.62	109.77
22	A1	34	CM0	C4'-O4'-C1'	-2.44	107.17	109.77
24	A3	56	PSU	O2'-C2'-C1'	-2.28	107.06	112.21
24	A3	55	5MU	C4'-O4'-C1'	-2.08	107.56	109.77
24	A3	21	H2U	C5-C4-N3	2.04	118.75	116.72
22	A1	55	PSU	O4'-C1'-C2'	2.10	107.82	104.45
22	A1	7	4SU	O4'-C4'-C3'	2.15	109.43	105.17
24	A3	21	H2U	C4-N3-C2	2.52	127.97	125.81
24	A3	21	H2U	C5-C6-N1	2.67	113.47	110.70
22	A1	34	CM0	O5-C5-C4	2.68	118.75	115.20
24	A3	56	PSU	O4'-C1'-C2'	2.82	108.98	104.45
24	A3	21	H2U	N3-C2-N1	2.96	119.68	116.73
22	A1	37	6MZ	C2-N1-C6	3.15	118.58	116.53
22	A1	55	PSU	C6-N1-C2	4.11	121.93	115.36
24	A3	56	PSU	C6-N1-C2	4.51	122.57	115.36
22	A1	37	6MZ	C9-N6-C6	4.98	127.12	122.85
22	A1	46	7MG	C6-N1-C2	5.40	123.82	116.06
22	A1	7	4SU	C2-N3-C4	7.28	125.85	115.11
24	A3	8	4SU	C2-N3-C4	7.85	126.69	115.11
22	A1	55	PSU	C4-N3-C2	10.94	124.73	115.16
22	A1	34	CM0	C4-N3-C2	11.71	125.40	115.16
24	A3	55	5MU	C4-N3-C2	11.75	125.44	115.16
24	A3	56	PSU	C4-N3-C2	11.79	125.47	115.16
22	A1	54	5MU	C4-N3-C2	12.45	126.05	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	VAL	A1	101	58,22	6,6,7	1.45	1 (16%)	6,7,9	2.30	2 (33%)
58	FME	BA	3001	57	9,9,10	1.31	1 (11%)	7,9,11	0.99	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	VAL	A1	101	58,22	-	0/5/6/8	0/0/0/0
58	FME	BA	3001	57	-	1/6/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	A1	101	VAL	CA-C	3.21	1.54	1.50
58	BA	3001	FME	CA-C	3.54	1.54	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A1	101	VAL	O-C-CA	-4.27	115.18	125.15
57	A1	101	VAL	C-CA-N	3.62	117.17	109.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.