

## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:00 PM BST

PDB ID : 4V6V  
EMDB ID: : EMD-5562  
Title : Tetracycline resistance protein Tet(O) bound to the ribosome  
Authors : Li, W.; Atkinson, G.C.; Thakor, N.S.; Allas, U.; Lu, C.; Chan, K.Y.; Tenson, T.; Schulten, K.; Wilson, K.S.; Hauryliuk, V.; Frank, J.  
Deposited on : 2013-02-25  
Resolution : 9.80 Å(reported)  
Based on PDB ID : 2I2U, 2I2V

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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

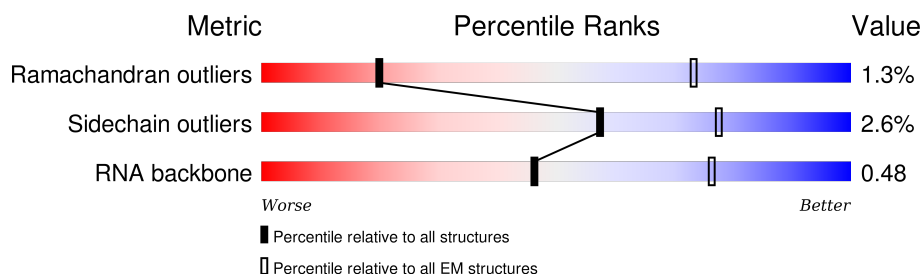
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 9.80 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.




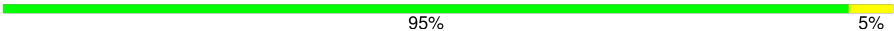







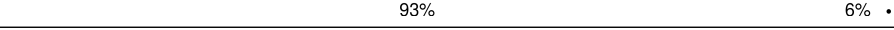

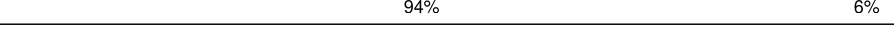

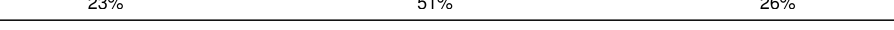

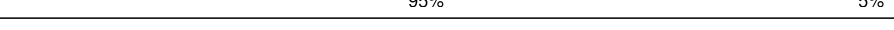
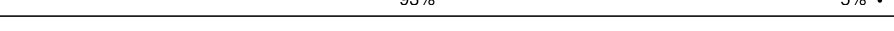
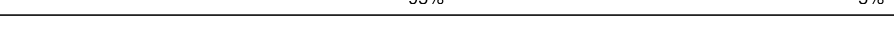

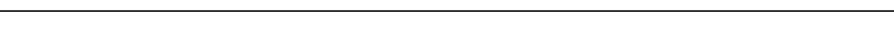

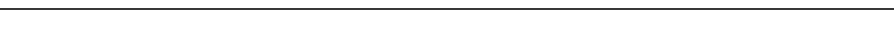
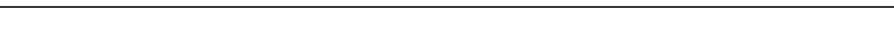


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	AJ	103	
2	AK	128	
3	AL	123	
4	AM	117	
5	AN	100	
6	AO	88	
7	AP	82	
8	AQ	83	
9	AR	74	





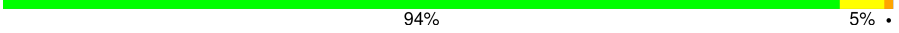
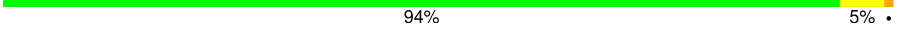
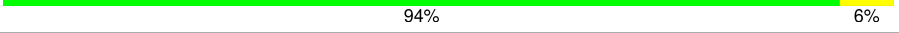





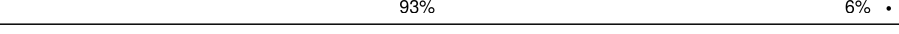
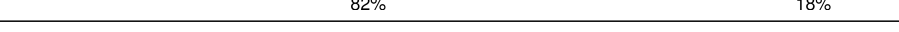
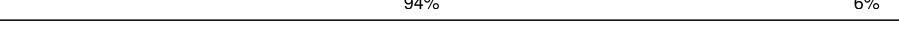
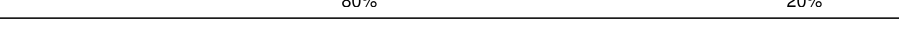



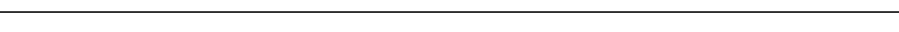




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Mol	Chain	Length	Quality of chain
10	AS	91	 87% 13%
11	AB	240	 95% 5%
12	AT	86	 93% 7%
13	AU	70	 77% 20% .
14	AC	232	 91% 9%
15	AD	205	 90% 9% .
16	AE	166	 92% 8% .
17	AF	135	 90% 9% .
18	AG	178	 90% 9% .
19	AH	129	 93% 6% .
20	AI	129	 87% 12% .
21	A1	639	 94% 6%
22	AA	1542	 16% 57% 24% .
23	A2	47	 23% 51% 26%
24	A3	77	 17% 57% 26%
25	BC	234	 95% 5%
26	BJ	164	 93% 5% .
27	BK	141	 95% 5%
28	BN	142	 87% 12% .
29	BO	123	 84% 13% ..
30	BP	144	 88% 10% .
31	BQ	136	 87% 13%
32	BR	127	 84% 15% .
33	BS	117	 91% 9%
34	BT	114	 89% 11% .

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Mol	Chain	Length	Quality of chain
35	BD	272	 88% 11% .
36	BU	117	 85% 13% .
37	BV	103	 88% 12%
38	BW	110	 90% 8% .
39	BX	100	 94% 5% .
40	BY	103	 94% 5% .
41	BZ	94	 94% 6%
42	B0	84	 85% 12% .
43	B1	77	 87% 10% .
44	B2	63	 92% 6% .
45	BE	209	 92% 7%
46	B3	58	 90% 10%
47	B4	70	 93% 6% .
48	B5	56	 82% 18%
49	B6	54	 94% 6%
50	B7	46	 80% 20%
51	B8	64	 89% 9% .
52	B9	38	 87% 13%
53	BF	201	 92% 7% .
54	BG	178	 88% 11% .
55	BH	176	 92% 6% .
56	BL	149	 95% 5%
57	BA	2904	 15% 57% 24% .
58	Ba	120	 18% 64% 17% .

## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 154956 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 S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AJ	103	Total	C	N	O	S	0	0
			794	483	158	151	2		

- Molecule 2 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AK	128	Total	C	N	O	S	0	0
			923	553	196	171	3		

- Molecule 3 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AL	123	Total	C	N	O	S	0	0
			923	558	196	165	4		

- Molecule 4 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AM	117	Total	C	N	O	S	0	0
			876	530	183	160	3		

- Molecule 5 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AN	100	Total	C	N	O	S	0	0
			771	465	164	139	3		

- Molecule 6 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AO	88	Total	C	N	O	S	0	0
			690	414	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	79	ARG	GLN	CONFLICT	UNP P0ADZ4

- Molecule 7 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AP	82	Total	C	N	O	S	0	0
			620	377	128	114	1		

- Molecule 8 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AQ	83	Total	C	N	O	S	0	0
			657	410	124	120	3		

- Molecule 9 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AR	74	Total	C	N	O	S	0	0
			603	372	123	107	1		

- Molecule 10 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AS	91	Total	C	N	O	S	0	0
			708	445	139	122	2		

- Molecule 11 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AB	240	Total	C	N	O	S	0	0
			1805	1113	332	352	8		

- Molecule 12 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AT	86	Total	C	N	O	S	0	0
			636	380	138	115	3		

- Molecule 13 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AU	70	Total	C	N	O	S	0	0
			564	340	125	98	1		

- Molecule 14 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AC	232	Total	C	N	O	S	0	0
			1761	1088	346	323	4		

- Molecule 15 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AD	205	Total	C	N	O	S	0	0
			1587	970	315	298	4		

- Molecule 16 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AE	166	Total	C	N	O	S	0	0
			1182	718	232	226	6		

- Molecule 17 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AF	135	Total	C	N	O	S	0	0
			1061	637	198	219	7		

- Molecule 18 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AG	178	Total	C	N	O	S	0	0
			1347	821	269	253	4		

- Molecule 19 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AH	129	Total	C	N	O	S	0	0
			948	585	173	184	6		

- Molecule 20 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AI	129	Total	C	N	O	S	0	0
			1000	606	208	183	3		

- Molecule 21 is a protein called Tetracycline resistance protein TetO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A1	639	Total	C	N	O	S	0	0
			4989	3146	850	966	27		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	227	ILE	THR	CONFLICT	UNP P10952

- Molecule 22 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AA	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	47	Total	C	N	O	P	0	0
			993	445	167	335	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	A3	77	Total	C	N	O	P	S	0	0
			1640	734	297	533	75	1		

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BC	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 26 is a protein called 50S ribosomal protein L10.



Mol	Chain	Residues	Atoms					AltConf	Trace
26	BJ	164	Total	C	N	O	S	0	0
			1233	776	220	231	6		

- Molecule 27 is a protein called 50S ribosomal protein L11.

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

- Molecule 28 is a protein called 50S ribosomal protein L13.

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

- Molecule 29 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BO	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 30 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BP	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 31 is a protein called 50S ribosomal protein L16.

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

- Molecule 32 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BR	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 33 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BS	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 34 is a protein called 50S ribosomal protein L19.

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

- Molecule 35 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BD	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 36 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BU	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 37 is a protein called 50S ribosomal protein L21.

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

- Molecule 38 is a protein called 50S ribosomal protein L22.

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

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BX	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BY	103	Total	C	N	O		
			789	498	148	143	0	0

- Molecule 41 is a protein called 50S ribosomal protein L25.

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

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	B0	84	Total	C	N	O	S	
			634	391	129	113	1	0

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	B1	77	Total	C	N	O	S	
			625	388	129	106	2	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	B2	63	Total	C	N	O	S	
			509	313	99	95	2	0

- Molecule 45 is a protein called 50S ribosomal protein L3.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	B3	58	Total	C	N	O	S	
			449	281	87	79	2	0

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	B4	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B6	54	Total	C	N	O	S	0	0
			441	284	81	76			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called 50S ribosomal protein L4.

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

- Molecule 54 is a protein called 50S ribosomal protein L5.

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

- Molecule 55 is a protein called 50S ribosomal protein L6.

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

- Molecule 56 is a protein called 50S ribosomal protein L9.

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

- Molecule 57 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BA	2904	Total	C	N	O	P	0	0
			62351	27824	11469	20155	2903		

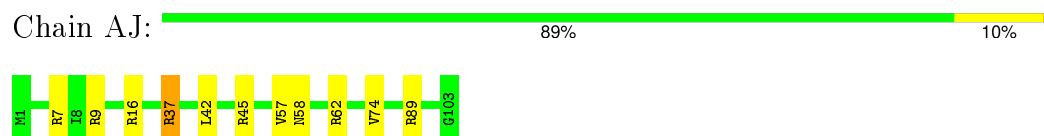
- Molecule 58 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Ba	120	Total	C	N	O	P	0	0
			2566	1144	468	835	119		

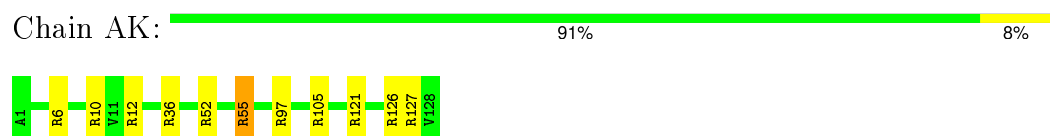
### 3 Residue-property plots [i](#)

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

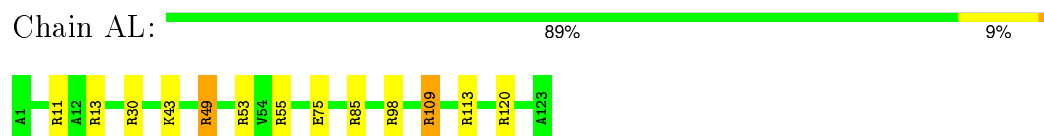
- Molecule 1: 30S ribosomal protein S10



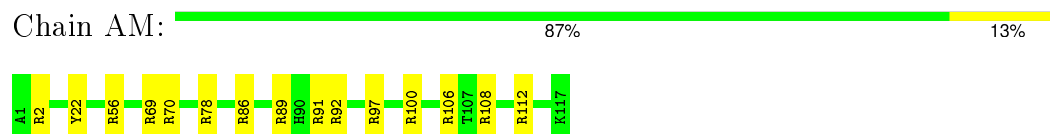
- Molecule 2: 30S ribosomal protein S11



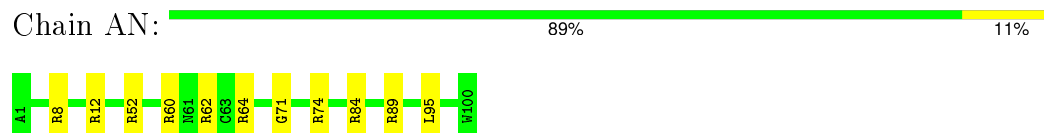
- Molecule 3: 30S ribosomal protein S12



- Molecule 4: 30S ribosomal protein S13



- Molecule 5: 30S ribosomal protein S14



- Molecule 6: 30S ribosomal protein S15





- Molecule 7: 30S ribosomal protein S16

Chain AP: 88% 11%



- Molecule 8: 30S ribosomal protein S17

Chain AQ: 93% 6%



- Molecule 9: 30S ribosomal protein S18

Chain AR: 82% 16%



- Molecule 10: 30S ribosomal protein S19

Chain AS: 87% 13%



- Molecule 11: 30S ribosomal protein S2

Chain AB: 95% 5%



- Molecule 12: 30S ribosomal protein S20

Chain AT: 93% 7%

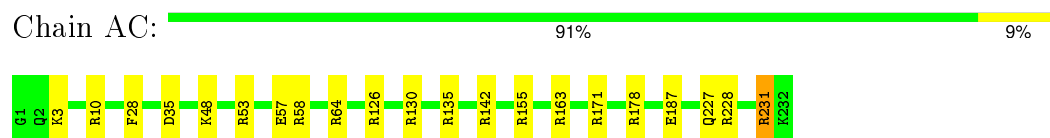


- Molecule 13: 30S ribosomal protein S21

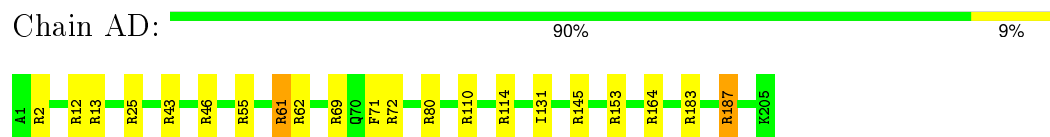
Chain AU: 77% 20%



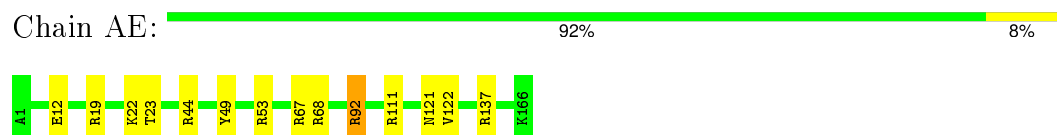
- Molecule 14: 30S ribosomal protein S3



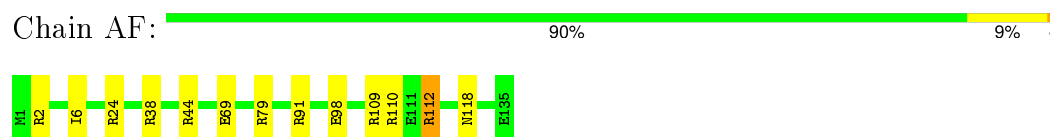
- Molecule 15: 30S ribosomal protein S4



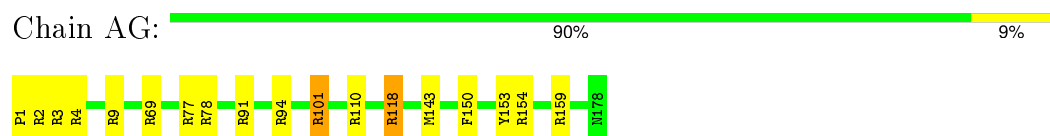
- Molecule 16: 30S ribosomal protein S5



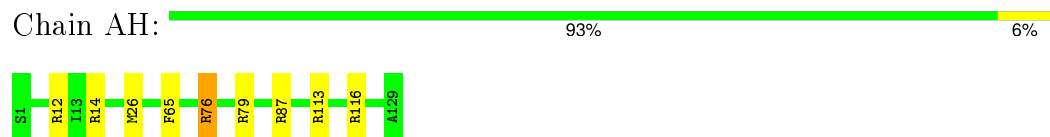
- Molecule 17: 30S ribosomal protein S6



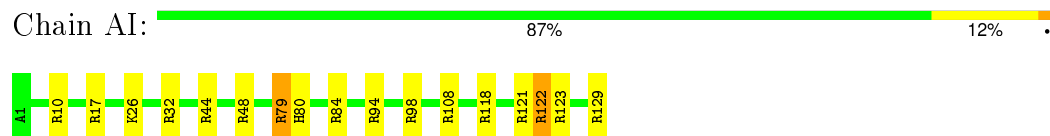
- Molecule 18: 30S ribosomal protein S7



- Molecule 19: 30S ribosomal protein S8

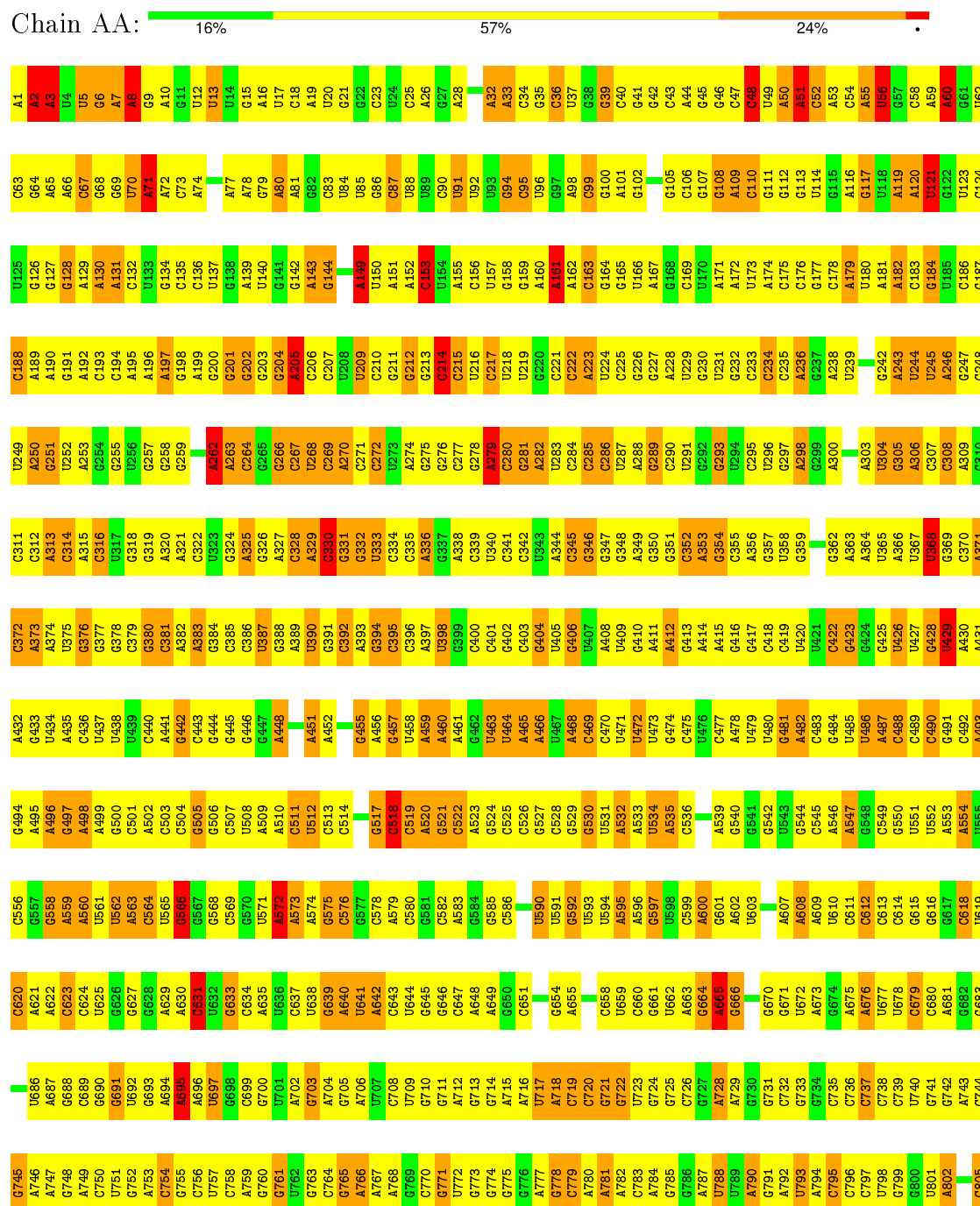


- Molecule 20: 30S ribosomal protein S9



- Molecule 21: Tetracycline resistance protein TetO



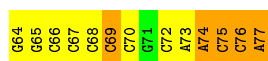


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• Molecule 23: mRNA



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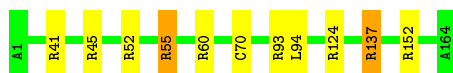
- Molecule 25: 50S ribosomal protein L1

Chain BC: 95% 5%



- Molecule 26: 50S ribosomal protein L10

Chain BJ: 93% 5%



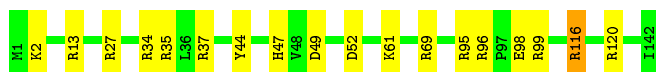
- Molecule 27: 50S ribosomal protein L11

Chain BK: 95% 5%



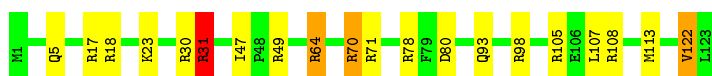
- Molecule 28: 50S ribosomal protein L13

Chain BN: 87% 12%



- Molecule 29: 50S ribosomal protein L14

Chain BO: 84% 13%



- Molecule 30: 50S ribosomal protein L15

Chain BP: 88% 10%




- Molecule 31: 50S ribosomal protein L16

Chain BQ: 87% 13%



## • Molecule 32: 50S ribosomal protein L17

Chain BR:  84% 15%


## • Molecule 33: 50S ribosomal protein L18

Chain BS:  91% 9%


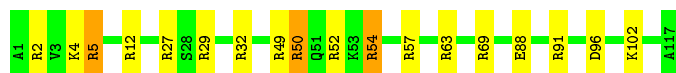
## • Molecule 34: 50S ribosomal protein L19

Chain BT:  89% 11%


## • Molecule 35: 50S ribosomal protein L2

Chain BD:  88% 11%

## • Molecule 36: 50S ribosomal protein L20

Chain BU:  85% 13%

## • Molecule 37: 50S ribosomal protein L21

Chain BV:  88% 12%

## • Molecule 38: 50S ribosomal protein L22

Chain BW:  90% 8%

- Molecule 39: 50S ribosomal protein L23

Chain BX:  94% 5%



- Molecule 40: 50S ribosomal protein L24

Chain BY:  94% 5%




- Molecule 41: 50S ribosomal protein L25

Chain BZ:  94% 6%




- Molecule 42: 50S ribosomal protein L27

Chain B0:  85% 12%



- Molecule 43: 50S ribosomal protein L28

Chain B1:  87% 10%



- Molecule 44: 50S ribosomal protein L29

Chain B2:  92% 6%



- Molecule 45: 50S ribosomal protein L3

Chain BE:  92% 7%



- Molecule 46: 50S ribosomal protein L30

Chain B3:  90% 10%




- Molecule 47: 50S ribosomal protein L31

Chain B4:  93% 6%



- Molecule 48: 50S ribosomal protein L32

Chain B5:  82% 18%




- Molecule 49: 50S ribosomal protein L33

Chain B6:  94% 6%



- Molecule 50: 50S ribosomal protein L34

Chain B7:  80% 20%




- Molecule 51: 50S ribosomal protein L35

Chain B8:  89% 9%



- Molecule 52: 50S ribosomal protein L36

Chain B9:  87% 13%



- Molecule 53: 50S ribosomal protein L4

Chain BF:  92% 7%



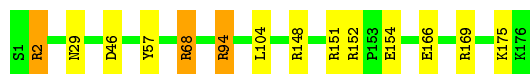
- Molecule 54: 50S ribosomal protein L5

Chain BG: 88% 11%



- Molecule 55: 50S ribosomal protein L6

Chain BH: 92% 6%



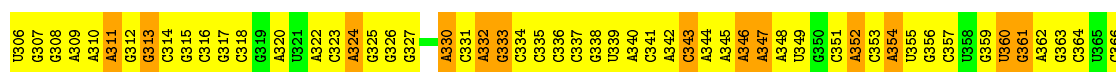
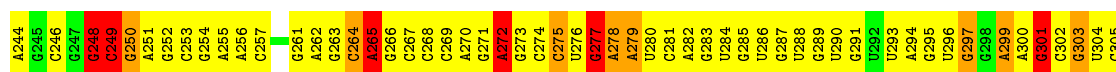
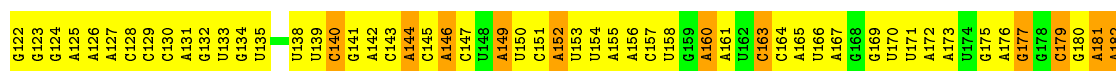
- Molecule 56: 50S ribosomal protein L9

Chain BL: 95% 5%



- Molecule 57: 23S ribosomal RNA

Chain BA: 15% 57% 24%



U1412	C1348	A1287	U1224	C1164	C1104	C1044	A983	A920	U860	A800	C732	A670	A608	G548	C487
A1413	C1349	G1288	G1225	A1165	U1105	C1045	A984	C921	A861	G801	G733	C671	A609	G549	G488
C1414	C1350	C1289	A1226	G1166	G1106	A1046	C985	C922	G862	A802	A734	C672	A610	C550	G489
U1415	C1351	C1290	G1227	G1167	G1107	G1047	C986	G923	A863	U803	A735	C673	C611	G551	C490
G1416	U1352	G1291	G1228	G1168	U1108	A1048	C987	G924	G864	A804	C736	G674	G612	U552	G491
C1417	A1353	G1292	G1229	A1169	C1049	C1049	C988	A925	C565	G805	C737	A675	G613	G553	A492
G1418	A1354	C1293	A1230	C1170	G1110	A1050	C989	G926	A866	C806	G738	A676	A614	U554	A493
A1419	G1355	U1294	U1231	G1171	A1111	G1051	A990	A927	C867	U807	A739	A677	U615	G555	
A1420	G1356	C1295	G1232	C1172	G1112	C1052	C991	A928	U868	G808	C740	C678	A616	G496	
G1421	C1357	G1296	C1233	U1173	U1113	A1053	C992	U929	G869	G809	U741	C679	G617	A556	A497
G1422	G1358	C1297	U1174	U1174	C1114	A1054	C993	G930	U870	U810	U742	C680	G618	U557	G498
G1423	A1359	C1298	G1235	A1175	G1115	G1055	C994	U931	U871	U811	U743		G619	U499	
G1424	G1360	C1299	U1236	U1176	G1116	G1056	C995	U932	U872	C812	U744		G620	C560	G500
G1425	G1361	G1300	A1237	G1177	C1117	A1057	A996	A933	C873	U813		U683	A621	G561	A501
G1426	C1362	A1301	G1238	C1178	C1118	U1058	C997	U934	G874	C814	U747	A685	A622	U562	A502
A1427	C1363	G1302		G1179	U1119	U1059	C998	C935	G875	C815	G748	U686	C623	A563	A503
C1428	G1364	A1303	A1241	U1180	G1120	U1060	U999	A936	C876	C816	A749	U687	C624	C564	A504
	A1365	G1304	U1242	U1181	C1121	G1062	A1001	C937	A878	C817	A750	U688	G625	C565	A505
A1431	A1366	C1305	C1243	G1182	G1122	G1063	G1002		G879	A819	A752	G689	A626	U566	G506
G1432	A1367	C1306	U1184	U1183	C1123	C1064	G1003	G940	G890	A820	A753	G690	A627	U567	A507
A1433	G1368	A1307	G1245	U1184	G1124	U1065	U1004	G942	G881	A821	U754	C692	G629	U568	A508
A1434	G1369	A1308	G1185	G1185	G1125	U1066	C1005	G943	G882	G822	U755	C693	G630	G570	C510
G1435	C1370	G1309	G1186	A1247	A1126	G1067	C1006	G944	G883	C823	U756	U694	A631	U571	U511
G1436		G1310	G1248	G1187	A1127	A1067	C1007	A945	U884	U824	G757		A632	A572	G512
C1437	A1373	G1311		U1188	G1128	G1068	A1008	C946	C885	A825	C758		A633	U573	A513
U1438	G1374	U1312	C1251	A1189	A1129	A1069	A1009	A947	A886	U826		C698	C634	A574	A514
A1439	U1375	U1313	G1190	G1190	U1130	A1070	A1010	C948	U887	U827	A761	A699	C635	A575	A515
U1440	C1376	C1314	A1253	A1253	G1131	G1071	A1010		G888	A828		G700	C636	U576	C516
G1441	A1377	C1315	G1192	G1192	U1132	C1072	U1012	G949	C889	U829	A764	G701	A637	G577	C517
A1442	A1378	G1316	U1255	G1193	A1133	A1073	G1013	G950	U895	A830	U765	U702	G638	G578	G518
U1443	U1379	U1317	G1256	A1194	A1134	G1074	C1013	C951	C890	G830	C766	U703	G639	G579	U519
		G1318	C1257	G1195	C1135	C1075	A1014	G952	G891	G831	U767	U704	U639	U580	G520
C1446	G1382	C1319	U1258	C1196	G1136	C1076	U1015	G953	A892	U832	U768	G705	U641	C581	U521
C1447	A1383	G1320	U1259	G1197	G1137	A1077	G1016	G954	C993	A833	G769	A705	U642	A522	A522
G1448	A1384	A1321	A1260	U1198	G1138	U1078	G1017	U955	U894	G834	U769	A706	G643	G583	C523
G1449	A1385	C1322	C1261	U1199	G1139	C1079	U1018	G956	U895	C835	G770	G707	A643	G584	G524
G1450	G1386	C1323	A1262	G1200	C1140	A1080	U1019	C957	A896	G836	G771	G708	A644	C585	U525
C1451	A1387	G1324	U1263	U1201	U1141	U1081	A1020	U958	C997	C837	C772	U709	C645	G586	A526
G1452	G1388		U1264	U1202	A1142	U1082	A1021	A959	C998	C838		U710	U646	A586	C527
A1453		U1326	A1265	G1203	A1143	U1083	G1022	A960	A899	U839	G776	G712		C587	C527
C1454	A1392	A1327	G1266	A1204	A1144	A1084	U1023	C961	A900	C840	U779	G713	C650	U588	A528
G1455	A1393	G1328	U1267	A1205	C1145	A1085	G1024	G962	C901	G841	U780	U714	G651	A590	A529
U1456	U1394	U1329	A1268	G1206	C1146	A1086	G1025	U963	C902	U842	G780	U715	G652	A591	C531
U1457	A1395	C1330	C1269	C1207	A1147	G1087	G1026	C964	C903	G843	A781	A716	U653	A592	A532
U1458	U1396	C1331	C1270	C1208	U1148	A1088	A1027	C965	G904	A844	A782	C717	U654	U593	G533
G1459	G1397	G1332	G1271	U1209	G1149	A1089	A1028	U966	A905	A845	A783	C718	A655	U594	U534
U1460	C1398	C1333	G1272	G1210	C1150	A1090	A1029	U967	U906	U846	G784	A718	A656	C595	G535
C1461	C1399	G1334	U1273	A1205	A1151	G1091	C1030	C968	G907	U847	G785	C719	G656	U596	G536
C1462	U1400	C1335	A1274	G1212	C1152	C1092	G1031	G969	C908	C848	G786	U720	U657	U597	G537
C1463	G1401	A1336	A1275	A1213	C1153	G1093	A1032	U970	A909	A849	C787	A721	U658	G597	A538
G1464	G1402	G1337	A1276	A1214	G1154	U1094	U1033	G971	A910	U850	A788	A722	G659	U598	
G1465	A1403		G1277	G1215	A1155	A1095	G1034	A972	A911	C851	A789	C723	C660	A599	G539
U1466	C1404	C1340	C1278	G1216	A1156	A1096	U1035	A973	C912	U852	U790	U724	A661	G600	C540
U1467	U1405	G1341	U1217	U1217	G1157	U1097	G1036	G974	U913	C853	C791	G725		C601	A541
U1468	U1406	A1342	G1218	A1218	C1158	A1098	G1037	A975	G914	C854	A792	G726	G664	A602	C542
A1469	G1407	G1343	U1219	U1159	C1159	G1099	G1038		C915	G855	A793	A727	U665	A603	G543
G1470	G1408	U1344	G1283	G1220	G1160	C1100	A1039	A979	G916	G856	A794	G728	A866	G604	G544
G1471	U1409	C1345	A1284	C1221	C1161	U1101	A1040	A980	A917	G857	A795	G729	U667	G605	U545
C1472	G1410	G1346	U1222	U1102	G1162	U1101		A981	A918	G858	C796	A730	A668	U606	U546
G1473		A1347	G1223	A1103	G1163	A1103	C1043	C982	U919	G859		C731	G669	U607	A547



U2398	A2385	G2272	G2209	G2148	U2086	C2025	U1963	A1900	G1840	U1779	G1718	U1657	A1597	C1536	U1474
G2399	A2386	A2273	U2210	U2149	G2087	U2026	G1964	A1901	U1841	A1780	G1719	C1658	A1598	G1537	G1475
G2400	G2337	C2274	A2211	C2150	A2088	G2027	G1965	G1902	G1842	U1781	G1720	G1659	U1599	G1538	U1476
U2401	C2338	C2275	A2212	U2151	C2089	U2028	A1966	G1903	G1843	U1782	G1721	G1660	C1600	U1539	A1477
U2402	C2339	G2276	G2213	G2152	C2090	A2031	G1967	G1904	G1844	A1784	G1722	G1661	U1602	G1540	G1478
C2403	C2340	C2214	C2214	C2153	C2091	G2032	G1968	G1905	G1845	U1785	G1723	U1662	A1603	C1541	G1479
U2404	G2341	C2215	G2216	A2154	U2092	G2033	A1969	G1906	G1846	A1786	G1724	G1663	A1604	U1542	C1480
G2405	G2342	G2216	U2219	U2155	G2093	U2034	A1970	G1907	A1847	U1787	U1725	A1664	G1543	U1481	U1480
A2406	U2345	G2280	A2281	A2158	A2094	U2034	U1971	C1908	A1848	A1788	G1726	A1665	A1544	G1482	
A2407	A2346	G2282	U2220	G2159	A2095	G2035	G1972	C1909	G1850	C1788	C1727	G1666	C1606	A1545	A1483
U2408	G2347	C2283	G2221	C2160	C2096	G2036	G1973	C1910	G1851	U1789	G1728	G1667	G1607	G1546	U1484
G2409	U2348	A2284	C2222	C2161	A2097	G2037	G1974	A1912	U1851	C1790	U1729	A1668	A1608	U1547	U1485
A2411	G2349	G2285	G2223	G2162	U2098	U2038	G1975	C1914	U1852	A1791	C1730	A1669	A1609	U1548	U1486
A2412	C2350	G2286	G2224	A2163	G2100	G2039	U1976	C1915	A1853	G1792	G1731	C1670	A1610	A1549	U1487
G2413	G2351	A2287	C2225	C2164	A2101	U2040	A1977	G1916	A1854	C1793	G1732	A1671	C1611	C1550	C1488
G2414	A2352	G2288	C2226	C2165	G2102	A2042	A1978	A1917	U1855	A1794	G1733	A1672	A1551	A1552	C1489
G2415	G2353	G2289	A2227	U2166	C2103	C2043	A1981	A1918	U1856	C1795	G1734	G1673	A1614	A1553	G1491
C2416	C2354	G2290	G2228	U2167	C2104	C2045	U1982	A1919	U1857	G1797	U1736	C1675	C1615	U1554	G1492
C2417	G2355	U2291	U2229	G2168	U2105	C2046	C1983	C1920	U1858	U1798	G1737	A1676	A1616	G1555	C1493
U2418	U2356	G2292	G2230	A2169	U2106	G2046	C1985	G1921	G1860	G1799	G1738	A1677	C1556	C1557	A1494
U2419	G2357	C2293	U2231	A2170	G2107	C2047	A1986	U1922	G1861	A1800	A1739	A1678	G1618	C1557	A1495
C2420	A2358	C2295	G2232	A2171	A2108	G2048	A1987	U1923	G1862	A1801	G1740	A1679	G1619	C1558	A1496
G2421	C2359	U2296	U2233	U2172	U2109	G2049	G1988	C1924	G1863	A1802	C1741	U1680	G1620	U1559	U1497
C2422	G2360	A2297	G2234	A2173	G2110	C2050	G1989	C1925	U1864	A1803	U1742	G1681	G1621	G1560	C1498
U2423	G2361	A2298	G2235	C2174	U2111	A2051	C1990	U1926	U1865	C1804	G1743	G1682	G1622	C1561	C1499
C2424	C2362	C2299	U2236	C2175	G2112	A2052	U1991	A1927	A1866	A1805	A1744	U1683	U1623	C1564	A1502
A2425	G2363	G2300	G2237	A2176	U2113	G2053	G1992	A1928	G1867	A1745	U1624	U1684	U1624	C1565	A1503
A2426	C2364	C2301	G2238	C2177	A2114	A2054	U1993	G1929	C1868	G1807	A1746	C1685	C1625	A1566	A1504
G2427	G2365	U2302	G2239	C2178	G2115	C2055	C1994	G1930	G1869	A1808	U1747	C1686	A1626	G1567	A1505
G2428	A2366	G2303	U2240	C2179	G2116	G2056	U1995	U1931	C1870	A1809	C1748	G1687	G1627	U1506	
G2429	G2367	G2304	A2241	U2180	A2117	G2057	C1996	A1932	A1871	A1810	A1749	U1688	G1628	G1568	
C2430	C2368	U2305	G2242	U2181	U2118	A2058	C1997	G1933	A1872	G1750	U1629	A1689	U1629	A1569	C1507
U2431	A2369	G2306	U2243	A2182	A2119	A2059	A1998	C1934	C1873	A1811	G1751	A1690	A1630	A1570	A1508
A2432	G2370	C2307	U2244	A2183	G2120	A2060	G1999	G1935	C1874	G1813	G1752	C1691	A1631	A1571	
A2433	U2371	G2308	U2245	A2184	G2121	G2061	C2000	A1936	G1875	G1814	G1753	U1692	A1632	A1572	
A2434	G2373	C2310	G2246	U2185	U2122	C2063	C2001	A1937	A1876	A1754	A1755	U1693	G1633	G1573	G1512
A2435	G2375	G2311	A2247	G2186	U2123	C2064	G2002	A1938	A1877	C1816	C1756	C1694	A1634	C1574	U1513
G2436	A2376	U2312	C2248	U2187	A2126	C2065	A2003	C1939	G1878	G1817	G1757	G1695	A1635	C1575	G1514
G2437	C2377	G2313	U2249	U2188	G2127	C2066	G2004	U1940	C1879	U1818	A1758	G1696	U1636	U1576	A1515
A2438	A2378	C2314	G2250	U2189	G2128	C2067	A2005	C1941	U1880	A1819	U1759	G1697	A1637	C1577	G1516
A2439	G2379	U2315	G2251	G2190	C2129	U2068	C2006	C1942	C1881	U1820	A1759	A1698	C1638	U1578	G1517
C2440	C2380	A2317	G2252	A2191	U2130	U2069	U2007	U1943	U1882	A1821	G1760	G1699	C1639	A1579	G1518
U2441	A2381	G2317	G2253	U2192	U2131	G2069	C2008	U1944	U1883	C1822	G1761	A1700	A1640	A1580	G1519
C2442	G2382	U2320	G2254	G2193	U2132	A2070	A2009	G1945	G1884	G1823	A1762	A1701	A1641	G1581	U1520
C2443	G2383	U2321	C2255	U2194	G2133	A2071	G2010	U1946	A1885	G1824	G1763	G1702	G1642	C1582	G1521
G2444	U2384	C2322	C2256	U2195	A2134	C2072	U2011	C1947	U1886	U1825	C1764	G1703	G1643	U1583	U1522
G2445	C2385	A2327	U2259	C2196	A2135	G2073	G2012	U1948	C1887	G1826	U1765	A1704	C1644	G1584	U1523
G2446	A2386	G2323	C2260	U2197	G2136	U2074	A2013	G1948	G1888	U1827	U1766	A1705	G1645	G1585	G1524
A2448	U2387	U2324	C2261	A2198	U2137	U2075	A2014	A1952	A1889	G1828	G1768	C1706	C1646	A1586	A1525
U2449	A2388	G2325	U2262	A2199	G2138	U2076	A2015	A1953	A1890	A1829	U1769	G1707	U1647	G1587	C1526
A2450	G2389	C2326	C2263	C2200	U2139	A2077	U2016	G1954	G1891	C1830	G1770	G1708	U1648	G1588	G1527
A2451	U2390	A2327	C2264	G2201	G2140	C2078	U2017	U1955	C1892	G1831	C1771	U1709	G1649	U1589	A1528
C2452	G2391	U2328	U2265	U2202	G2141	U2079	G2018	U1956	C1893	A1832	A1772	G1710	A1650	A1590	G1529
A2453	A2392	G2329	A2266	U2203	A2142	A2080	A2019	C1957	C1894	A1773	A1711	C1957	G1651	A1591	G1530
U2454	U2393	G2330	A2267	G2204	C2143	U2081	A2020	C1958	C1895	U1712	C1774	A1652	A1592	C1592	G1531
C2456	C2394	G2331	A2268	A2205	G2144	A2082	C2021	G1959	G1896	C1836	U1775	A1713	G1653	A1593	A1532
G2457	U2395	C2332	G2269	C2206	C2145	G2083	U2022	A1960	G1897	C1837	G1776	U1716	A1654	U1594	U1533
G2458	G2396	A2333	A2270	C2207	C2146	G2084	C2023	C1961	U1898	A1655	U1777	C1778	A1655	C1595	U1534
A2459	C2397	U2334	G2271	C2208	A2147	U2085	G2024	C1962	A1899	G1839			C1656	A1596	



## 4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	98000	Depositor
Resolution determination method	FSC	Depositor
CTF correction method	group defocus	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	10	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 3TD, OMG, 5MC, MA6, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, 4SU, 7MG, 5MU, 1MG, 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	AJ	0.75	0/742	1.26	7/941 (0.7%)
10	AS	0.77	0/687	1.27	10/880 (1.1%)
11	AB	0.74	0/1703	1.07	9/2161 (0.4%)
12	AT	0.75	0/574	1.25	12/694 (1.7%)
13	AU	0.94	0/520	1.61	15/636 (2.4%)
14	AC	0.75	0/1669	1.15	16/2122 (0.8%)
15	AD	0.80	0/1497	1.29	19/1890 (1.0%)
16	AE	0.73	0/1110	1.14	9/1405 (0.6%)
17	AF	0.79	0/1001	1.23	11/1268 (0.9%)
18	AG	0.79	0/1263	1.33	16/1590 (1.0%)
19	AH	0.72	0/896	1.11	7/1141 (0.6%)
2	AK	0.79	0/856	1.39	14/1069 (1.3%)
20	AI	0.85	0/940	1.37	19/1180 (1.6%)
21	A1	0.76	0/4864	1.12	24/6363 (0.4%)
22	AA	1.47	6/36769 (0.0%)	2.38	2673/57354 (4.7%)
23	A2	1.48	0/1108	2.31	71/1724 (4.1%)
24	A3	1.49	0/1717	2.41	129/2675 (4.8%)
25	BC	0.68	0/1748	0.98	4/2355 (0.2%)
26	BJ	0.73	0/1247	1.15	10/1679 (0.6%)
27	BK	0.67	0/1046	1.00	4/1410 (0.3%)
28	BN	0.75	0/1152	1.11	11/1551 (0.7%)
29	BO	0.74	0/956	1.20	13/1279 (1.0%)
3	AL	0.79	0/873	1.30	12/1110 (1.1%)
30	BP	0.79	0/1062	1.36	15/1413 (1.1%)
31	BQ	0.78	0/1093	1.24	13/1460 (0.9%)
32	BR	0.79	0/1021	1.35	17/1364 (1.2%)
33	BS	0.76	0/910	1.23	14/1219 (1.1%)
34	BT	0.77	0/929	1.25	10/1242 (0.8%)
35	BD	0.75	0/2131	1.25	32/2863 (1.1%)
36	BU	0.80	0/960	1.29	15/1278 (1.2%)
37	BV	0.76	0/829	1.18	9/1107 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	BW	0.67	0/864	1.10	12/1156 (1.0%)
39	BX	0.69	0/794	1.10	3/1060 (0.3%)
4	AM	0.79	0/817	1.45	20/1022 (2.0%)
40	BY	0.69	0/797	1.04	4/1062 (0.4%)
41	BZ	0.73	0/766	1.11	6/1025 (0.6%)
42	B0	0.79	0/642	1.25	8/848 (0.9%)
43	B1	0.79	0/635	1.37	13/848 (1.5%)
44	B2	0.71	0/510	1.17	6/677 (0.9%)
45	BE	0.72	0/1586	1.14	15/2134 (0.7%)
46	B3	0.72	0/453	1.29	9/605 (1.5%)
47	B4	0.75	0/559	1.06	5/745 (0.7%)
48	B5	0.79	0/450	1.38	9/599 (1.5%)
49	B6	0.73	0/448	1.02	3/594 (0.5%)
5	AN	0.82	0/715	1.37	10/883 (1.1%)
50	B7	0.84	0/380	1.47	10/498 (2.0%)
51	B8	0.76	0/513	1.28	9/676 (1.3%)
52	B9	0.71	0/303	1.16	3/397 (0.8%)
53	BF	0.71	0/1571	1.09	13/2113 (0.6%)
54	BG	0.77	0/1444	1.18	10/1937 (0.5%)
55	BH	0.72	0/1343	1.08	7/1816 (0.4%)
56	BL	0.70	0/1122	1.05	8/1515 (0.5%)
57	BA	1.47	5/69280 (0.0%)	2.39	5083/108078 (4.7%)
58	Ba	1.46	0/2869	2.35	208/4474 (4.6%)
6	AO	0.76	0/646	1.22	8/813 (1.0%)
7	AP	0.83	0/572	1.39	11/711 (1.5%)
8	AQ	0.72	0/636	1.16	6/822 (0.7%)
9	AR	0.92	0/568	1.46	12/713 (1.7%)
All	All	1.28	11/165156 (0.0%)	2.11	8751/244244 (3.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	AS	0	1
15	AD	0	1
18	AG	0	2
21	A1	0	2
22	AA	0	350
23	A2	0	5
24	A3	0	15

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	BJ	0	1
28	BN	0	2
29	BO	0	1
3	AL	0	1
32	BR	0	1
34	BT	0	1
35	BD	0	1
36	BU	0	2
38	BW	0	1
40	BY	0	1
42	B0	0	1
51	B8	0	1
55	BH	0	2
57	BA	0	660
58	Ba	0	15
6	AO	0	1
7	AP	0	1
9	AR	0	1
All	All	0	1070

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AA	1223	C	C4-N4	-5.72	1.28	1.33
22	AA	1226	C	O3'-P	-5.66	1.54	1.61
22	AA	1432	G	C2-N2	-5.45	1.29	1.34
57	BA	823	C	C4-N4	-5.35	1.29	1.33
22	AA	1497	G	C2-N2	-5.32	1.29	1.34
57	BA	1568	G	C2-N2	-5.22	1.29	1.34
57	BA	750	A	P-O5'	5.17	1.65	1.59
22	AA	326	G	C2-N2	-5.16	1.29	1.34
57	BA	2500	U	P-O5'	5.12	1.64	1.59
57	BA	2667	C	C4-N4	-5.11	1.29	1.33
22	AA	566	G	C2-N2	-5.02	1.29	1.34

All (8751) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AE	111	ARG	NE-CZ-NH1	15.27	127.93	120.30
57	BA	1073	A	N1-C6-N6	-14.45	109.93	118.60
26	BJ	55	ARG	NE-CZ-NH1	14.31	127.46	120.30
57	BA	423	A	N1-C6-N6	-14.03	110.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AP	70	ARG	NE-CZ-NH1	13.34	126.97	120.30
13	AU	34	ARG	NE-CZ-NH1	13.01	126.81	120.30
57	BA	346	A	O4'-C1'-N9	12.88	118.50	108.20
30	BP	33	ARG	NE-CZ-NH1	12.79	126.69	120.30
31	BQ	81	ARG	NE-CZ-NH1	12.79	126.69	120.30
57	BA	2882	A	N1-C6-N6	-12.70	110.98	118.60
22	AA	573	A	N1-C6-N6	-12.56	111.06	118.60
22	AA	983	A	N1-C6-N6	-12.53	111.08	118.60
22	AA	704	A	N1-C6-N6	-12.52	111.09	118.60
57	BA	877	A	N1-C6-N6	-12.32	111.21	118.60
22	AA	1513	A	N1-C6-N6	-12.20	111.28	118.60
58	Ba	46	A	N1-C6-N6	-12.20	111.28	118.60
22	AA	793	U	O4'-C1'-N1	12.17	117.93	108.20
22	AA	325	A	N1-C6-N6	-12.12	111.33	118.60
18	AG	101	ARG	NE-CZ-NH1	12.09	126.34	120.30
22	AA	523	A	N1-C6-N6	-12.07	111.36	118.60
57	BA	219	A	N1-C6-N6	-12.07	111.36	118.60
22	AA	815	A	N1-C6-N6	-12.03	111.39	118.60
57	BA	99	U	O4'-C1'-N1	12.02	117.81	108.20
57	BA	1204	A	N1-C6-N6	-11.98	111.41	118.60
22	AA	622	A	N1-C6-N6	-11.92	111.45	118.60
57	BA	1515	A	N1-C6-N6	-11.87	111.48	118.60
57	BA	84	A	N1-C6-N6	-11.83	111.50	118.60
57	BA	299	A	N1-C6-N6	-11.81	111.51	118.60
57	BA	2476	A	N1-C6-N6	-11.79	111.52	118.60
22	AA	563	A	N1-C6-N6	-11.79	111.53	118.60
57	BA	1672	A	N1-C6-N6	-11.79	111.53	118.60
30	BP	18	ARG	NE-CZ-NH1	11.76	126.18	120.30
36	BU	57	ARG	NE-CZ-NH1	11.75	126.18	120.30
22	AA	415	A	O4'-C1'-N9	11.74	117.59	108.20
57	BA	1427	A	N1-C6-N6	-11.71	111.57	118.60
57	BA	278	A	N1-C6-N6	-11.70	111.58	118.60
57	BA	1284	A	N1-C6-N6	-11.69	111.59	118.60
20	AI	129	ARG	NE-CZ-NH1	11.68	126.14	120.30
57	BA	1943	U	O4'-C1'-N1	11.68	117.54	108.20
22	AA	1191	A	N1-C6-N6	-11.63	111.62	118.60
22	AA	160	A	N1-C6-N6	-11.62	111.63	118.60
57	BA	2576	G	O4'-C1'-N9	11.62	117.50	108.20
24	A3	9	G	O4'-C1'-N9	11.61	117.49	108.20
22	AA	765	G	O4'-C1'-N9	11.61	117.49	108.20
57	BA	74	A	N1-C6-N6	-11.59	111.65	118.60
22	AA	899	C	O4'-C1'-N1	11.57	117.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Ba	15	A	O4'-C1'-N9	11.55	117.44	108.20
22	AA	448	A	N1-C6-N6	-11.53	111.68	118.60
48	B5	9	ARG	NE-CZ-NH2	11.53	126.06	120.30
57	BA	1552	A	O4'-C1'-N9	11.51	117.40	108.20
22	AA	728	A	N1-C6-N6	-11.50	111.70	118.60
22	AA	108	G	O4'-C1'-N9	11.47	117.38	108.20
22	AA	1204	A	N1-C6-N6	-11.45	111.73	118.60
57	BA	294	A	N1-C6-N6	-11.42	111.75	118.60
21	A1	87	ARG	NE-CZ-NH1	11.41	126.01	120.30
22	AA	422	C	O4'-C1'-N1	11.40	117.32	108.20
22	AA	151	A	N1-C6-N6	-11.40	111.76	118.60
57	BA	1127	A	N1-C6-N6	-11.38	111.78	118.60
2	AK	121	ARG	NE-CZ-NH1	11.37	125.98	120.30
23	A2	24	A	N1-C6-N6	-11.35	111.79	118.60
22	AA	498	A	N1-C6-N6	-11.35	111.79	118.60
22	AA	766	A	N1-C6-N6	-11.33	111.80	118.60
57	BA	404	A	N1-C6-N6	-11.31	111.81	118.60
57	BA	479	A	N1-C6-N6	-11.30	111.82	118.60
22	AA	1286	U	O4'-C1'-N1	11.25	117.20	108.20
57	BA	13	A	N1-C6-N6	-11.24	111.85	118.60
57	BA	1155	A	N1-C6-N6	-11.24	111.85	118.60
22	AA	171	A	N1-C6-N6	-11.23	111.86	118.60
57	BA	2241	A	N1-C6-N6	-11.22	111.86	118.60
57	BA	1755	A	N1-C6-N6	-11.19	111.89	118.60
57	BA	1783	A	N1-C6-N6	-11.18	111.89	118.60
57	BA	1378	A	N1-C6-N6	-11.12	111.93	118.60
18	AG	4	ARG	NE-CZ-NH1	11.12	125.86	120.30
22	AA	493	A	N1-C6-N6	-11.12	111.93	118.60
34	BT	112	ARG	NE-CZ-NH1	11.11	125.86	120.30
2	AK	126	ARG	NE-CZ-NH1	11.11	125.85	120.30
22	AA	665	A	N1-C6-N6	-11.09	111.95	118.60
57	BA	2054	A	N1-C6-N6	-11.08	111.95	118.60
57	BA	896	A	N1-C6-N6	-11.08	111.95	118.60
22	AA	1238	A	N1-C6-N6	-11.07	111.96	118.60
57	BA	508	A	N1-C6-N6	-11.06	111.96	118.60
57	BA	2425	A	N1-C6-N6	-11.06	111.96	118.60
57	BA	119	A	N1-C6-N6	-11.06	111.97	118.60
57	BA	217	A	N1-C6-N6	-11.05	111.97	118.60
57	BA	196	A	N1-C6-N6	-11.04	111.97	118.60
22	AA	532	A	N1-C6-N6	-11.03	111.98	118.60
22	AA	610	U	O4'-C1'-N1	11.03	117.02	108.20
22	AA	1433	A	N1-C6-N6	-11.01	111.99	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2600	A	N1-C6-N6	-11.00	112.00	118.60
57	BA	910	A	N1-C6-N6	-10.99	112.00	118.60
57	BA	2274	A	N1-C6-N6	-10.96	112.02	118.60
57	BA	1580	A	N1-C6-N6	-10.93	112.04	118.60
57	BA	2450	A	N1-C6-N6	-10.92	112.05	118.60
57	BA	1739	A	N1-C6-N6	-10.91	112.05	118.60
57	BA	1569	A	N1-C6-N6	-10.88	112.07	118.60
57	BA	1129	A	N1-C6-N6	-10.86	112.08	118.60
57	BA	2266	A	N1-C6-N6	-10.84	112.09	118.60
4	AM	89	ARG	NE-CZ-NH1	10.83	125.72	120.30
57	BA	2750	A	N1-C6-N6	-10.83	112.10	118.60
57	BA	1853	A	N1-C6-N6	-10.83	112.10	118.60
22	AA	152	A	N1-C6-N6	-10.81	112.11	118.60
57	BA	1635	A	N1-C6-N6	-10.78	112.13	118.60
57	BA	990	A	N1-C6-N6	-10.77	112.14	118.60
57	BA	2733	A	N1-C6-N6	-10.76	112.14	118.60
57	BA	575	A	N1-C6-N6	-10.76	112.14	118.60
57	BA	2851	A	N1-C6-N6	-10.74	112.16	118.60
57	BA	2327	A	N1-C6-N6	-10.73	112.16	118.60
57	BA	1096	A	N1-C6-N6	-10.72	112.17	118.60
57	BA	1952	A	N1-C6-N6	-10.71	112.17	118.60
2	AK	127	ARG	NE-CZ-NH1	10.71	125.66	120.30
22	AA	274	A	N1-C6-N6	-10.71	112.17	118.60
57	BA	2062	A	N1-C6-N6	-10.70	112.18	118.60
57	BA	91	A	N1-C6-N6	-10.70	112.18	118.60
57	BA	1566	A	O4'-C1'-N9	10.69	116.75	108.20
22	AA	195	A	N1-C6-N6	-10.69	112.19	118.60
22	AA	196	A	N1-C6-N6	-10.69	112.19	118.60
57	BA	2386	A	N1-C6-N6	-10.65	112.21	118.60
57	BA	2675	A	N1-C6-N6	-10.64	112.21	118.60
57	BA	1918	A	N1-C6-N6	-10.64	112.22	118.60
22	AA	262	A	N1-C6-N6	-10.63	112.22	118.60
57	BA	1650	A	N1-C6-N6	-10.63	112.22	118.60
22	AA	1502	A	O4'-C1'-N9	10.63	116.70	108.20
22	AA	109	A	N1-C6-N6	-10.62	112.23	118.60
36	BU	5	ARG	NE-CZ-NH2	10.62	125.61	120.30
57	BA	1353	A	N1-C6-N6	-10.61	112.23	118.60
57	BA	1566	A	N1-C6-N6	-10.61	112.23	118.60
22	AA	1349	A	N1-C6-N6	-10.61	112.24	118.60
57	BA	1801	A	N1-C6-N6	-10.60	112.24	118.60
22	AA	1362	A	N1-C6-N6	-10.59	112.24	118.60
22	AA	465	A	O4'-C1'-N9	10.58	116.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	790	U	O4'-C1'-N1	10.58	116.66	108.20
22	AA	423	G	O4'-C1'-N9	10.55	116.64	108.20
22	AA	315	A	N1-C6-N6	-10.55	112.27	118.60
22	AA	977	A	N1-C6-N6	-10.55	112.27	118.60
57	BA	1494	A	N1-C6-N6	-10.54	112.28	118.60
57	BA	1665	A	N1-C6-N6	-10.54	112.28	118.60
57	BA	941	A	N1-C6-N6	-10.51	112.30	118.60
22	AA	608	A	N1-C6-N6	-10.51	112.30	118.60
57	BA	2054	A	C5-C6-N1	10.51	122.95	117.70
57	BA	1579	A	N1-C6-N6	-10.50	112.30	118.60
2	AK	10	ARG	NE-CZ-NH1	10.49	125.55	120.30
22	AA	16	A	N1-C6-N6	-10.47	112.32	118.60
57	BA	603	A	N1-C6-N6	-10.47	112.32	118.60
57	BA	71	A	N1-C6-N6	-10.45	112.33	118.60
57	BA	1205	A	N1-C6-N6	-10.45	112.33	118.60
57	BA	197	A	N1-C6-N6	-10.45	112.33	118.60
22	AA	1067	A	N1-C6-N6	-10.44	112.34	118.60
22	AA	1111	A	N1-C6-N6	-10.44	112.34	118.60
22	AA	139	A	N1-C6-N6	-10.43	112.34	118.60
57	BA	428	A	N1-C6-N6	-10.41	112.35	118.60
54	BG	29	ARG	NE-CZ-NH1	10.40	125.50	120.30
22	AA	465	A	C5-C6-N1	10.39	122.90	117.70
51	B8	44	ARG	NE-CZ-NH1	10.39	125.50	120.30
57	BA	2799	A	N1-C6-N6	-10.39	112.36	118.60
57	BA	2439	A	N1-C6-N6	-10.39	112.37	118.60
57	BA	1301	A	N1-C6-N6	-10.38	112.37	118.60
22	AA	161	A	N1-C6-N6	-10.37	112.38	118.60
22	AA	938	A	N1-C6-N6	-10.36	112.38	118.60
57	BA	1327	A	N1-C6-N6	-10.36	112.38	118.60
57	BA	38	A	N1-C6-N6	-10.36	112.38	118.60
57	BA	1000	A	N1-C6-N6	-10.36	112.38	118.60
22	AA	129	A	N1-C6-N6	-10.36	112.39	118.60
15	AD	12	ARG	NE-CZ-NH1	10.35	125.48	120.30
57	BA	2726	A	N1-C6-N6	-10.35	112.39	118.60
57	BA	1640	A	N1-C6-N6	-10.35	112.39	118.60
57	BA	1419	A	N1-C6-N6	-10.34	112.39	118.60
57	BA	592	A	N1-C6-N6	-10.33	112.40	118.60
57	BA	2108	A	N1-C6-N6	-10.32	112.41	118.60
57	BA	825	A	N1-C6-N6	-10.31	112.41	118.60
22	AA	1105	A	N1-C6-N6	-10.31	112.42	118.60
20	AI	17	ARG	NE-CZ-NH1	10.30	125.45	120.30
22	AA	1441	A	N1-C6-N6	-10.28	112.43	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	BZ	18	ARG	NE-CZ-NH1	10.28	125.44	120.30
22	AA	353	A	N1-C6-N6	-10.27	112.44	118.60
57	BA	788	A	N1-C6-N6	-10.27	112.44	118.60
57	BA	781	A	N1-C6-N6	-10.26	112.44	118.60
57	BA	1490	A	N1-C6-N6	-10.25	112.45	118.60
22	AA	559	A	N1-C6-N6	-10.25	112.45	118.60
57	BA	95	A	N1-C6-N6	-10.24	112.46	118.60
22	AA	1213	A	N1-C6-N6	-10.24	112.46	118.60
57	BA	2764	A	N1-C6-N6	-10.23	112.46	118.60
57	BA	631	A	N1-C6-N6	-10.23	112.47	118.60
22	AA	389	A	N1-C6-N6	-10.22	112.47	118.60
22	AA	864	A	N1-C6-N6	-10.22	112.47	118.60
57	BA	529	A	N1-C6-N6	-10.21	112.47	118.60
57	BA	1664	A	N1-C6-N6	-10.21	112.47	118.60
57	BA	2080	A	N1-C6-N6	-10.21	112.47	118.60
57	BA	1142	A	N1-C6-N6	-10.20	112.48	118.60
57	BA	1717	A	N1-C6-N6	-10.19	112.48	118.60
57	BA	2287	A	N1-C6-N6	-10.19	112.49	118.60
22	AA	872	A	N1-C6-N6	-10.19	112.49	118.60
57	BA	2872	A	N1-C6-N6	-10.18	112.49	118.60
57	BA	2225	A	N1-C6-N6	-10.18	112.49	118.60
57	BA	2478	A	N1-C6-N6	-10.18	112.49	118.60
57	BA	2433	A	N1-C6-N6	-10.17	112.50	118.60
22	AA	414	A	N1-C6-N6	-10.17	112.50	118.60
24	A3	39	A	N1-C6-N6	-10.17	112.50	118.60
58	Ba	78	A	N1-C6-N6	-10.17	112.50	118.60
57	BA	412	A	N1-C6-N6	-10.16	112.50	118.60
57	BA	1133	A	N1-C6-N6	-10.16	112.50	118.60
57	BA	2253	G	O4'-C1'-N9	10.16	116.33	108.20
5	AN	84	ARG	NE-CZ-NH1	10.15	125.38	120.30
24	A3	22	A	N1-C6-N6	-10.14	112.52	118.60
57	BA	685	A	N1-C6-N6	-10.14	112.52	118.60
57	BA	1614	A	N1-C6-N6	-10.14	112.52	118.60
57	BA	1913	A	N1-C6-N6	-10.13	112.52	118.60
57	BA	2134	A	O4'-C1'-N9	10.13	116.31	108.20
32	BR	12	ARG	NE-CZ-NH1	10.12	125.36	120.30
22	AA	1311	A	N1-C6-N6	-10.12	112.53	118.60
22	AA	1269	A	N1-C6-N6	-10.12	112.53	118.60
57	BA	2721	A	N1-C6-N6	-10.12	112.53	118.60
57	BA	1175	A	N1-C6-N6	-10.11	112.53	118.60
22	AA	1329	A	N1-C6-N6	-10.11	112.54	118.60
57	BA	2335	A	N1-C6-N6	-10.10	112.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2198	A	N1-C6-N6	-10.09	112.55	118.60
57	BA	2309	A	N1-C6-N6	-10.08	112.55	118.60
22	AA	572	A	N1-C6-N6	-10.08	112.55	118.60
57	BA	1285	A	N1-C6-N6	-10.08	112.55	118.60
57	BA	666	A	N1-C6-N6	-10.08	112.55	118.60
57	BA	905	A	N1-C6-N6	-10.08	112.55	118.60
57	BA	829	A	N1-C6-N6	-10.08	112.56	118.60
22	AA	547	A	N1-C6-N6	-10.07	112.56	118.60
9	AR	42	ARG	NE-CZ-NH1	10.07	125.34	120.30
57	BA	2311	A	N1-C6-N6	-10.07	112.56	118.60
57	BA	1103	A	N1-C6-N6	-10.06	112.56	118.60
57	BA	2711	A	N1-C6-N6	-10.06	112.56	118.60
22	AA	1248	A	N1-C6-N6	-10.06	112.57	118.60
32	BR	4	ARG	NE-CZ-NH1	10.06	125.33	120.30
57	BA	2886	A	N1-C6-N6	-10.05	112.57	118.60
57	BA	1553	A	N1-C6-N6	-10.05	112.57	118.60
22	AA	101	A	N1-C6-N6	-10.04	112.58	118.60
22	AA	1271	A	N1-C6-N6	-10.04	112.58	118.60
57	BA	1810	A	N1-C6-N6	-10.03	112.58	118.60
57	BA	2541	A	N1-C6-N6	-10.03	112.58	118.60
1	AJ	37	ARG	NE-CZ-NH1	10.03	125.31	120.30
57	BA	1048	A	N1-C6-N6	-10.03	112.58	118.60
57	BA	223	A	N1-C6-N6	-10.02	112.59	118.60
57	BA	1307	A	N1-C6-N6	-10.02	112.59	118.60
57	BA	1508	A	O4'-C1'-N9	10.02	116.21	108.20
57	BA	2661	G	C1'-O4'-C4'	-10.02	101.89	109.90
57	BA	2471	A	N1-C6-N6	-10.01	112.59	118.60
22	AA	460	A	N1-C6-N6	-10.01	112.59	118.60
57	BA	2059	A	N1-C6-N6	-10.01	112.59	118.60
22	AA	451	A	N1-C6-N6	-10.00	112.60	118.60
57	BA	382	A	N1-C6-N6	-10.00	112.60	118.60
22	AA	459	A	N1-C6-N6	-9.99	112.61	118.60
24	A3	16	C	O4'-C1'-N1	9.99	116.19	108.20
22	AA	1346	A	N1-C6-N6	-9.98	112.61	118.60
57	BA	430	A	N1-C6-N6	-9.98	112.61	118.60
22	AA	381	C	O4'-C1'-N1	9.98	116.18	108.20
22	AA	716	A	N1-C6-N6	-9.97	112.62	118.60
57	BA	1067	A	N1-C6-N6	-9.96	112.62	118.60
58	Ba	104	A	N1-C6-N6	-9.96	112.62	118.60
22	AA	1289	A	N1-C6-N6	-9.95	112.63	118.60
57	BA	492	A	N1-C6-N6	-9.95	112.63	118.60
22	AA	899	C	N3-C2-O2	-9.95	114.94	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2448	A	N1-C6-N6	-9.94	112.63	118.60
57	BA	1247	A	N1-C6-N6	-9.94	112.64	118.60
22	AA	965	U	O4'-C1'-N1	9.94	116.15	108.20
57	BA	716	A	N1-C6-N6	-9.93	112.64	118.60
57	BA	945	A	N1-C6-N6	-9.92	112.65	118.60
57	BA	2451	A	N1-C6-N6	-9.92	112.65	118.60
22	AA	900	A	N1-C6-N6	-9.91	112.65	118.60
22	AA	718	A	N1-C6-N6	-9.90	112.66	118.60
57	BA	900	A	N1-C6-N6	-9.90	112.66	118.60
22	AA	251	G	O4'-C1'-N9	9.90	116.12	108.20
57	BA	309	A	N1-C6-N6	-9.90	112.66	118.60
57	BA	2432	A	N1-C6-N6	-9.88	112.67	118.60
32	BR	17	ARG	NE-CZ-NH1	9.88	125.24	120.30
57	BA	2278	A	N1-C6-N6	-9.88	112.67	118.60
57	BA	2434	A	N1-C6-N6	-9.88	112.67	118.60
57	BA	190	A	N1-C6-N6	-9.87	112.68	118.60
57	BA	454	A	N1-C6-N6	-9.87	112.68	118.60
57	BA	1509	A	N1-C6-N6	-9.87	112.68	118.60
22	AA	918	A	N1-C6-N6	-9.86	112.68	118.60
23	A2	19	A	N1-C6-N6	-9.86	112.68	118.60
57	BA	1495	A	N1-C6-N6	-9.86	112.68	118.60
15	AD	114	ARG	NE-CZ-NH1	9.86	125.23	120.30
22	AA	309	A	N1-C6-N6	-9.86	112.68	118.60
22	AA	792	A	N1-C6-N6	-9.86	112.69	118.60
5	AN	74	ARG	NE-CZ-NH1	9.86	125.23	120.30
6	AO	53	ARG	NE-CZ-NH1	9.85	125.23	120.30
22	AA	499	A	N1-C6-N6	-9.85	112.69	118.60
22	AA	1285	A	N1-C6-N6	-9.85	112.69	118.60
22	AA	155	A	N1-C6-N6	-9.84	112.69	118.60
22	AA	915	A	N1-C6-N6	-9.84	112.69	118.60
57	BA	532	A	N1-C6-N6	-9.84	112.69	118.60
34	BT	87	ARG	NE-CZ-NH1	9.84	125.22	120.30
22	AA	74	A	N1-C6-N6	-9.84	112.70	118.60
57	BA	42	A	N1-C6-N6	-9.84	112.70	118.60
57	BA	64	A	N1-C6-N6	-9.84	112.70	118.60
22	AA	1288	A	N1-C6-N6	-9.83	112.70	118.60
57	BA	2654	A	N1-C6-N6	-9.83	112.70	118.60
9	AR	56	ARG	NE-CZ-NH1	9.82	125.21	120.30
37	BV	68	ARG	NE-CZ-NH2	9.82	125.21	120.30
22	AA	781	A	N1-C6-N6	-9.81	112.71	118.60
57	BA	2577	A	N1-C6-N6	-9.81	112.71	118.60
57	BA	161	A	N1-C6-N6	-9.81	112.71	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1010	A	N1-C6-N6	-9.80	112.72	118.60
57	BA	1735	A	N1-C6-N6	-9.80	112.72	118.60
57	BA	1194	A	N1-C6-N6	-9.80	112.72	118.60
57	BA	582	A	N1-C6-N6	-9.80	112.72	118.60
57	BA	2531	A	N1-C6-N6	-9.80	112.72	118.60
22	AA	958	A	N1-C6-N6	-9.79	112.72	118.60
4	AM	70	ARG	NE-CZ-NH1	9.79	125.19	120.30
57	BA	590	A	N1-C6-N6	-9.78	112.73	118.60
58	Ba	15	A	N1-C6-N6	-9.78	112.73	118.60
57	BA	126	A	N1-C6-N6	-9.78	112.73	118.60
22	AA	364	A	N1-C6-N6	-9.77	112.74	118.60
22	AA	675	A	N1-C6-N6	-9.77	112.74	118.60
22	AA	1363	A	N1-C6-N6	-9.76	112.74	118.60
57	BA	270	A	N1-C6-N6	-9.76	112.74	118.60
22	AA	1170	A	N1-C6-N6	-9.76	112.75	118.60
57	BA	1395	A	N1-C6-N6	-9.76	112.75	118.60
57	BA	216	A	N1-C6-N6	-9.75	112.75	118.60
22	AA	1021	A	N1-C6-N6	-9.74	112.75	118.60
57	BA	2270	A	N1-C6-N6	-9.74	112.76	118.60
57	BA	2879	A	N1-C6-N6	-9.73	112.76	118.60
26	BJ	137	ARG	NE-CZ-NH1	9.73	125.16	120.30
24	A3	38	A	N1-C6-N6	-9.72	112.77	118.60
57	BA	1262	A	N1-C6-N6	-9.72	112.77	118.60
12	AT	24	ARG	NE-CZ-NH1	9.72	125.16	120.30
22	AA	431	A	N1-C6-N6	-9.72	112.77	118.60
22	AA	746	A	N1-C6-N6	-9.71	112.77	118.60
35	BD	220	ARG	NE-CZ-NH1	9.71	125.15	120.30
57	BA	1877	A	N1-C6-N6	-9.70	112.78	118.60
22	AA	937	A	N1-C6-N6	-9.70	112.78	118.60
57	BA	1237	A	N1-C6-N6	-9.70	112.78	118.60
57	BA	2031	A	N1-C6-N6	-9.70	112.78	118.60
57	BA	2033	A	N1-C6-N6	-9.70	112.78	118.60
57	BA	2530	A	N1-C6-N6	-9.70	112.78	118.60
1	AJ	16	ARG	NE-CZ-NH1	9.69	125.15	120.30
35	BD	51	ARG	NE-CZ-NH1	9.69	125.15	120.30
22	AA	1227	A	N1-C6-N6	-9.68	112.79	118.60
57	BA	1321	A	N1-C6-N6	-9.68	112.79	118.60
57	BA	975	A	N1-C6-N6	-9.68	112.79	118.60
57	BA	2781	A	N1-C6-N6	-9.68	112.79	118.60
22	AA	1322	C	O4'-C1'-N1	9.68	115.94	108.20
10	AS	77	ARG	NE-CZ-NH1	9.67	125.14	120.30
57	BA	1932	A	N1-C6-N6	-9.67	112.80	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2388	A	N1-C6-N6	-9.67	112.80	118.60
5	AN	52	ARG	NE-CZ-NH1	9.67	125.13	120.30
57	BA	1632	A	N1-C6-N6	-9.66	112.80	118.60
57	BA	2212	A	N1-C6-N6	-9.66	112.81	118.60
22	AA	1117	A	N1-C6-N6	-9.66	112.81	118.60
57	BA	1786	A	N1-C6-N6	-9.65	112.81	118.60
10	AS	80	ARG	NE-CZ-NH1	9.65	125.12	120.30
22	AA	452	A	N1-C6-N6	-9.65	112.81	118.60
22	AA	842	U	O4'-C1'-N1	9.65	115.92	108.20
57	BA	1746	A	N1-C6-N6	-9.64	112.81	118.60
22	AA	640	A	N1-C6-N6	-9.64	112.82	118.60
22	AA	1036	A	N1-C6-N6	-9.63	112.82	118.60
57	BA	2682	A	N1-C6-N6	-9.64	112.82	118.60
22	AA	807	A	N1-C6-N6	-9.63	112.82	118.60
57	BA	74	A	C5-C6-N1	9.63	122.52	117.70
57	BA	925	A	N1-C6-N6	-9.63	112.82	118.60
22	AA	816	A	N1-C6-N6	-9.63	112.82	118.60
57	BA	2418	A	N1-C6-N6	-9.63	112.82	118.60
22	AA	533	A	C5-C6-N1	9.62	122.51	117.70
57	BA	2662	A	N1-C6-N6	-9.62	112.83	118.60
4	AM	86	ARG	NE-CZ-NH1	9.62	125.11	120.30
22	AA	843	U	O4'-C1'-N1	9.62	115.89	108.20
57	BA	718	A	N1-C6-N6	-9.62	112.83	118.60
41	BZ	19	ARG	NE-CZ-NH1	9.62	125.11	120.30
57	BA	1829	A	N1-C6-N6	-9.61	112.83	118.60
57	BA	2171	A	N1-C6-N6	-9.61	112.83	118.60
57	BA	2572	A	N1-C6-N6	-9.61	112.83	118.60
57	BA	2810	A	N1-C6-N6	-9.61	112.83	118.60
57	BA	2376	A	N1-C6-N6	-9.61	112.83	118.60
22	AA	1396	A	N1-C6-N6	-9.61	112.84	118.60
57	BA	1147	A	N1-C6-N6	-9.61	112.84	118.60
22	AA	975	A	N1-C6-N6	-9.60	112.84	118.60
44	B2	7	ARG	NE-CZ-NH1	9.60	125.10	120.30
57	BA	1453	A	N1-C6-N6	-9.59	112.85	118.60
57	BA	1919	A	N1-C6-N6	-9.59	112.85	118.60
57	BA	2575	C	N1-C2-O2	9.58	124.65	118.90
34	BT	38	ARG	NE-CZ-NH2	9.58	125.09	120.30
57	BA	429	A	N1-C6-N6	-9.58	112.85	118.60
57	BA	2333	A	N1-C6-N6	-9.58	112.85	118.60
57	BA	1610	A	N1-C6-N6	-9.57	112.86	118.60
57	BA	909	A	N1-C6-N6	-9.57	112.86	118.60
57	BA	2126	A	N1-C6-N6	-9.57	112.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2346	A	N1-C6-N6	-9.57	112.86	118.60
22	AA	50	A	N1-C6-N6	-9.56	112.86	118.60
57	BA	1669	A	N1-C6-N6	-9.56	112.86	118.60
57	BA	793	A	N1-C6-N6	-9.56	112.86	118.60
57	BA	1014	A	N1-C6-N6	-9.56	112.86	118.60
57	BA	2813	A	N1-C6-N6	-9.56	112.86	118.60
30	BP	2	ARG	NE-CZ-NH1	9.56	125.08	120.30
22	AA	554	A	N1-C6-N6	-9.56	112.86	118.60
57	BA	668	A	N1-C6-N6	-9.56	112.86	118.60
57	BA	1586	A	N1-C6-N6	-9.56	112.86	118.60
57	BA	1900	A	N1-C6-N6	-9.56	112.86	118.60
57	BA	1901	A	N1-C6-N6	-9.55	112.87	118.60
57	BA	538	A	N1-C6-N6	-9.55	112.87	118.60
57	BA	2134	A	N1-C6-N6	-9.55	112.87	118.60
57	BA	1050	A	N1-C6-N6	-9.55	112.87	118.60
57	BA	371	A	N1-C6-N6	-9.54	112.88	118.60
57	BA	526	A	N1-C6-N6	-9.54	112.88	118.60
57	BA	1608	A	N1-C6-N6	-9.53	112.88	118.60
57	BA	689	A	N1-C6-N6	-9.53	112.88	118.60
57	BA	1434	A	N1-C6-N6	-9.53	112.88	118.60
7	AP	25	ARG	NE-CZ-NH1	9.52	125.06	120.30
22	AA	1493	A	N1-C6-N6	-9.52	112.89	118.60
22	AA	1502	A	N1-C6-N6	-9.52	112.89	118.60
57	BA	347	A	N1-C6-N6	-9.52	112.89	118.60
57	BA	2453	A	N1-C6-N6	-9.52	112.89	118.60
57	BA	165	A	N1-C6-N6	-9.52	112.89	118.60
22	AA	1180	A	N1-C6-N6	-9.52	112.89	118.60
57	BA	804	A	N1-C6-N6	-9.52	112.89	118.60
57	BA	1937	A	N1-C6-N6	-9.52	112.89	118.60
57	BA	849	A	N1-C6-N6	-9.51	112.89	118.60
23	A2	16	A	N1-C6-N6	-9.51	112.89	118.60
57	BA	1354	A	N1-C6-N6	-9.51	112.89	118.60
57	BA	2740	A	N1-C6-N6	-9.50	112.90	118.60
57	BA	608	A	N1-C6-N6	-9.50	112.90	118.60
22	AA	412	A	N1-C6-N6	-9.49	112.91	118.60
22	AA	1257	A	N1-C6-N6	-9.48	112.91	118.60
35	BD	216	ARG	NE-CZ-NH1	9.48	125.04	120.30
57	BA	1981	A	N1-C6-N6	-9.48	112.91	118.60
57	BA	2273	A	N1-C6-N6	-9.48	112.91	118.60
5	AN	89	ARG	NE-CZ-NH1	9.47	125.04	120.30
57	BA	227	A	N1-C6-N6	-9.47	112.92	118.60
57	BA	504	A	N1-C6-N6	-9.47	112.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2614	A	N1-C6-N6	-9.47	112.92	118.60
22	AA	177	G	O4'-C1'-N9	9.47	115.78	108.20
22	AA	676	A	N1-C6-N6	-9.47	112.92	118.60
57	BA	1503	A	N1-C6-N6	-9.47	112.92	118.60
22	AA	1339	A	N1-C6-N6	-9.47	112.92	118.60
22	AA	1239	A	N1-C6-N6	-9.46	112.92	118.60
22	AA	167	A	N1-C6-N6	-9.46	112.92	118.60
57	BA	2778	A	N1-C6-N6	-9.46	112.92	118.60
23	A2	41	A	N1-C6-N6	-9.45	112.93	118.60
38	BW	95	ARG	NE-CZ-NH2	9.45	125.03	120.30
22	AA	262	A	C5-C6-N1	9.45	122.42	117.70
22	AA	777	A	N1-C6-N6	-9.45	112.93	118.60
22	AA	1280	A	N1-C6-N6	-9.45	112.93	118.60
57	BA	1304	A	N1-C6-N6	-9.45	112.93	118.60
57	BA	2792	A	N1-C6-N6	-9.45	112.93	118.60
22	AA	712	A	N1-C6-N6	-9.44	112.94	118.60
57	BA	262	A	N1-C6-N6	-9.44	112.94	118.60
57	BA	752	A	N1-C6-N6	-9.44	112.94	118.60
57	BA	1077	A	N1-C6-N6	-9.44	112.94	118.60
57	BA	1505	A	N1-C6-N6	-9.44	112.94	118.60
22	AA	533	A	N1-C6-N6	-9.44	112.94	118.60
57	BA	181	A	N1-C6-N6	-9.44	112.94	118.60
57	BA	502	A	N1-C6-N6	-9.43	112.94	118.60
57	BA	1274	A	N1-C6-N6	-9.43	112.94	118.60
57	BA	1085	A	N1-C6-N6	-9.43	112.94	118.60
22	AA	913	A	N1-C6-N6	-9.42	112.95	118.60
22	AA	1447	A	N1-C6-N6	-9.42	112.95	118.60
30	BP	126	ARG	NE-CZ-NH1	9.42	125.01	120.30
14	AC	53	ARG	NE-CZ-NH1	9.42	125.01	120.30
22	AA	1	A	N1-C6-N6	-9.41	112.95	118.60
57	BA	1711	A	N1-C6-N6	-9.41	112.95	118.60
58	Ba	34	A	N1-C6-N6	-9.41	112.96	118.60
15	AD	62	ARG	NE-CZ-NH1	9.40	125.00	120.30
57	BA	2163	A	N1-C6-N6	-9.40	112.96	118.60
22	AA	1377	A	N1-C6-N6	-9.40	112.96	118.60
57	BA	1403	A	N1-C6-N6	-9.40	112.96	118.60
30	BP	60	ARG	NE-CZ-NH1	9.39	125.00	120.30
57	BA	1226	A	N1-C6-N6	-9.38	112.97	118.60
22	AA	889	A	N1-C6-N6	-9.38	112.97	118.60
57	BA	979	A	N1-C6-N6	-9.38	112.97	118.60
22	AA	819	A	N1-C6-N6	-9.38	112.97	118.60
37	BV	84	ARG	NE-CZ-NH2	9.38	124.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	300	A	N1-C6-N6	-9.38	112.97	118.60
57	BA	1532	A	N1-C6-N6	-9.37	112.98	118.60
22	AA	935	A	N1-C6-N6	-9.37	112.98	118.60
57	BA	10	A	N1-C6-N6	-9.37	112.98	118.60
57	BA	2666	C	N3-C2-O2	-9.37	115.34	121.90
22	AA	1179	A	N1-C6-N6	-9.36	112.98	118.60
22	AA	1216	A	N1-C6-N6	-9.36	112.98	118.60
57	BA	1876	A	N1-C6-N6	-9.36	112.98	118.60
23	A2	59	A	N1-C6-N6	-9.36	112.98	118.60
57	BA	654	A	N1-C6-N6	-9.36	112.99	118.60
57	BA	1477	A	N1-C6-N6	-9.36	112.99	118.60
22	AA	422	C	N3-C2-O2	-9.35	115.35	121.90
57	BA	73	A	N1-C6-N6	-9.35	112.99	118.60
57	BA	324	A	N1-C6-N6	-9.35	112.99	118.60
57	BA	348	A	N1-C6-N6	-9.35	112.99	118.60
57	BA	2392	A	N1-C6-N6	-9.35	112.99	118.60
57	BA	1679	A	N1-C6-N6	-9.34	113.00	118.60
57	BA	2679	A	N1-C6-N6	-9.34	113.00	118.60
57	BA	2736	A	N1-C6-N6	-9.34	113.00	118.60
57	BA	878	A	N1-C6-N6	-9.33	113.00	118.60
22	AA	466	A	N1-C6-N6	-9.33	113.00	118.60
24	A3	74	A	N1-C6-N6	-9.33	113.00	118.60
57	BA	2566	A	N1-C6-N6	-9.33	113.00	118.60
22	AA	520	A	N1-C6-N6	-9.32	113.00	118.60
22	AA	1492	A	N1-C6-N6	-9.32	113.01	118.60
57	BA	527	C	O4'-C1'-N1	9.32	115.66	108.20
57	BA	1762	A	N1-C6-N6	-9.32	113.01	118.60
22	AA	344	A	N1-C6-N6	-9.32	113.01	118.60
57	BA	1308	A	N1-C6-N6	-9.32	113.01	118.60
22	AA	1151	A	N1-C6-N6	-9.31	113.01	118.60
57	BA	750	A	N1-C6-N6	-9.31	113.01	118.60
57	BA	2211	A	N1-C6-N6	-9.31	113.01	118.60
57	BA	503	A	N1-C6-N6	-9.31	113.01	118.60
57	BA	368	A	N1-C6-N6	-9.31	113.01	118.60
22	AA	181	A	N1-C6-N6	-9.31	113.02	118.60
22	AA	702	A	N1-C6-N6	-9.31	113.02	118.60
58	Ba	50	A	N1-C6-N6	-9.31	113.02	118.60
57	BA	866	A	C5-C6-N1	9.31	122.35	117.70
57	BA	125	A	N1-C6-N6	-9.30	113.02	118.60
22	AA	3	A	N1-C6-N6	-9.30	113.02	118.60
22	AA	1446	A	N1-C6-N6	-9.30	113.02	118.60
57	BA	1020	A	N1-C6-N6	-9.30	113.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2602	A	N1-C6-N6	-9.30	113.02	118.60
57	BA	2766	A	C5-C6-N1	9.30	122.35	117.70
22	AA	1176	A	N1-C6-N6	-9.29	113.02	118.60
22	AA	493	A	O4'-C1'-N9	9.29	115.64	108.20
22	AA	509	A	N1-C6-N6	-9.29	113.03	118.60
57	BA	2225	A	C5-C6-N1	9.29	122.34	117.70
22	AA	715	A	N1-C6-N6	-9.29	113.03	118.60
57	BA	83	A	N1-C6-N6	-9.29	113.03	118.60
57	BA	320	A	N1-C6-N6	-9.28	113.03	118.60
22	AA	1019	A	N1-C6-N6	-9.28	113.03	118.60
57	BA	927	A	N1-C6-N6	-9.28	113.03	118.60
58	Ba	58	A	N1-C6-N6	-9.28	113.03	118.60
22	AA	1246	A	N1-C6-N6	-9.28	113.03	118.60
57	BA	980	A	N1-C6-N6	-9.28	113.03	118.60
57	BA	439	A	N1-C6-N6	-9.28	113.03	118.60
22	AA	1022	A	N1-C6-N6	-9.27	113.03	118.60
57	BA	2199	A	N1-C6-N6	-9.27	113.04	118.60
57	BA	432	A	N1-C6-N6	-9.27	113.04	118.60
57	BA	111	A	N1-C6-N6	-9.26	113.04	118.60
57	BA	1276	A	N1-C6-N6	-9.26	113.04	118.60
22	AA	456	A	N1-C6-N6	-9.26	113.04	118.60
22	AA	461	A	N1-C6-N6	-9.26	113.04	118.60
57	BA	614	A	N1-C6-N6	-9.26	113.04	118.60
57	BA	685	A	C5-C6-N1	9.26	122.33	117.70
57	BA	692	C	N3-C2-O2	-9.26	115.42	121.90
57	BA	1420	A	N1-C6-N6	-9.26	113.04	118.60
57	BA	2873	A	N1-C6-N6	-9.26	113.05	118.60
22	AA	51	A	N1-C6-N6	-9.25	113.05	118.60
57	BA	1253	A	N1-C6-N6	-9.25	113.05	118.60
57	BA	1847	A	N1-C6-N6	-9.25	113.05	118.60
22	AA	1480	A	N1-C6-N6	-9.25	113.05	118.60
57	BA	1469	A	N1-C6-N6	-9.25	113.05	118.60
57	BA	1616	A	N1-C6-N6	-9.25	113.05	118.60
22	AA	119	A	N1-C6-N6	-9.24	113.06	118.60
57	BA	988	A	N1-C6-N6	-9.24	113.05	118.60
57	BA	1960	A	N1-C6-N6	-9.24	113.06	118.60
22	AA	845	A	N1-C6-N6	-9.24	113.06	118.60
22	AA	1093	A	N1-C6-N6	-9.24	113.06	118.60
57	BA	322	A	N1-C6-N6	-9.24	113.06	118.60
57	BA	2856	A	N1-C6-N6	-9.24	113.06	118.60
57	BA	2169	A	N1-C6-N6	-9.23	113.06	118.60
57	BA	2020	A	N1-C6-N6	-9.23	113.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1359	A	C5-C6-N1	9.23	122.31	117.70
57	BA	1890	A	N1-C6-N6	-9.23	113.06	118.60
22	AA	374	A	C5-C6-N1	9.23	122.31	117.70
22	AA	397	A	C5-C6-N1	9.23	122.31	117.70
57	BA	2887	A	N1-C6-N6	-9.23	113.06	118.60
57	BA	1927	A	N1-C6-N6	-9.23	113.06	118.60
22	AA	969	A	N1-C6-N6	-9.22	113.06	118.60
57	BA	2267	A	N1-C6-N6	-9.22	113.07	118.60
22	AA	197	A	N1-C6-N6	-9.22	113.07	118.60
57	BA	127	A	N1-C6-N6	-9.22	113.07	118.60
57	BA	344	A	N1-C6-N6	-9.22	113.07	118.60
57	BA	984	A	N1-C6-N6	-9.22	113.07	118.60
57	BA	1603	A	N1-C6-N6	-9.22	113.07	118.60
57	BA	2005	A	N1-C6-N6	-9.22	113.07	118.60
57	BA	2461	A	N1-C6-N6	-9.22	113.07	118.60
57	BA	2534	A	N1-C6-N6	-9.22	113.07	118.60
57	BA	204	A	N1-C6-N6	-9.22	113.07	118.60
22	AA	996	A	N1-C6-N6	-9.22	113.07	118.60
57	BA	914	G	O4'-C1'-N9	9.21	115.57	108.20
57	BA	101	A	N1-C6-N6	-9.21	113.08	118.60
57	BA	1095	A	O4'-C1'-N9	9.21	115.56	108.20
57	BA	1609	A	N1-C6-N6	-9.20	113.08	118.60
22	AA	26	A	N1-C6-N6	-9.20	113.08	118.60
57	BA	613	A	N1-C6-N6	-9.20	113.08	118.60
22	AA	1155	A	N1-C6-N6	-9.20	113.08	118.60
57	BA	14	A	N1-C6-N6	-9.19	113.08	118.60
57	BA	547	A	N1-C6-N6	-9.19	113.09	118.60
57	BA	443	A	N1-C6-N6	-9.19	113.09	118.60
57	BA	1241	A	N1-C6-N6	-9.19	113.09	118.60
57	BA	1815	A	N1-C6-N6	-9.18	113.09	118.60
57	BA	1446	C	N3-C2-O2	-9.18	115.48	121.90
57	BA	1080	A	N1-C6-N6	-9.17	113.10	118.60
57	BA	1134	A	N1-C6-N6	-9.17	113.10	118.60
57	BA	2670	A	N1-C6-N6	-9.17	113.10	118.60
57	BA	1244	A	N1-C6-N6	-9.17	113.10	118.60
57	BA	1365	A	N1-C6-N6	-9.17	113.10	118.60
22	AA	665	A	C5-C6-N1	9.17	122.28	117.70
32	BR	86	ARG	NE-CZ-NH1	9.16	124.88	120.30
22	AA	782	A	N1-C6-N6	-9.16	113.10	118.60
23	A2	13	A	N1-C6-N6	-9.16	113.10	118.60
57	BA	1598	A	N1-C6-N6	-9.15	113.11	118.60
57	BA	1821	A	N1-C6-N6	-9.15	113.11	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2176	A	N1-C6-N6	-9.15	113.11	118.60
57	BA	2424	C	O4'-C1'-N1	9.15	115.52	108.20
22	AA	936	C	N3-C2-O2	-9.15	115.50	121.90
57	BA	866	A	N1-C6-N6	-9.15	113.11	118.60
57	BA	2426	A	N1-C6-N6	-9.15	113.11	118.60
57	BA	2825	G	O4'-C1'-N9	9.15	115.52	108.20
57	BA	2513	A	N1-C6-N6	-9.14	113.11	118.60
57	BA	2829	A	N1-C6-N6	-9.14	113.11	118.60
57	BA	602	A	N1-C6-N6	-9.14	113.11	118.60
57	BA	384	A	N1-C6-N6	-9.14	113.12	118.60
57	BA	858	G	O4'-C1'-N9	9.14	115.51	108.20
57	BA	2800	A	N1-C6-N6	-9.13	113.12	118.60
57	BA	2435	A	N1-C6-N6	-9.13	113.12	118.60
22	AA	7	A	N1-C6-N6	-9.13	113.12	118.60
22	AA	162	A	N1-C6-N6	-9.13	113.12	118.60
57	BA	1384	A	N1-C6-N6	-9.12	113.13	118.60
22	AA	8	A	N1-C6-N6	-9.12	113.13	118.60
22	AA	353	A	O4'-C1'-N9	9.12	115.50	108.20
22	AA	767	A	N1-C6-N6	-9.12	113.13	118.60
57	BA	453	A	N1-C6-N6	-9.12	113.13	118.60
22	AA	1542	A	N1-C6-N6	-9.12	113.13	118.60
57	BA	2589	A	N1-C6-N6	-9.12	113.13	118.60
57	BA	1787	A	N1-C6-N6	-9.12	113.13	118.60
22	AA	1410	A	N1-C6-N6	-9.11	113.13	118.60
57	BA	1046	A	N1-C6-N6	-9.11	113.13	118.60
57	BA	2734	A	N1-C6-N6	-9.11	113.13	118.60
57	BA	2634	A	N1-C6-N6	-9.11	113.13	118.60
22	AA	270	A	N1-C6-N6	-9.11	113.14	118.60
22	AA	1188	A	N1-C6-N6	-9.11	113.14	118.60
57	BA	2314	A	N1-C6-N6	-9.11	113.13	118.60
57	BA	2660	A	N1-C6-N6	-9.11	113.13	118.60
57	BA	2886	A	O4'-C1'-N9	9.11	115.49	108.20
57	BA	1535	A	N1-C6-N6	-9.10	113.14	118.60
22	AA	831	A	N1-C6-N6	-9.10	113.14	118.60
22	AA	968	A	N1-C6-N6	-9.10	113.14	118.60
57	BA	142	A	N1-C6-N6	-9.09	113.14	118.60
57	BA	1641	A	N1-C6-N6	-9.09	113.14	118.60
22	AA	2	A	N1-C6-N6	-9.09	113.15	118.60
22	AA	649	A	N1-C6-N6	-9.09	113.15	118.60
57	BA	2114	A	N1-C6-N6	-9.09	113.15	118.60
57	BA	2058	A	N1-C6-N6	-9.08	113.15	118.60
22	AA	415	A	C5-C6-N1	9.08	122.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Ba	29	A	N1-C6-N6	-9.08	113.15	118.60
57	BA	675	A	N1-C6-N6	-9.07	113.16	118.60
22	AA	1360	A	C5-C6-N1	9.07	122.24	117.70
57	BA	2765	A	N1-C6-N6	-9.07	113.16	118.60
22	AA	422	C	N1-C2-O2	9.07	124.34	118.90
57	BA	715	A	N1-C6-N6	-9.07	113.16	118.60
18	AG	3	ARG	NE-CZ-NH1	9.07	124.83	120.30
22	AA	411	A	C5-C6-N1	9.07	122.23	117.70
22	AA	1431	A	N1-C6-N6	-9.07	113.16	118.60
22	AA	1430	A	N1-C6-N6	-9.07	113.16	118.60
57	BA	918	A	N1-C6-N6	-9.06	113.16	118.60
57	BA	2748	A	N1-C6-N6	-9.06	113.16	118.60
22	AA	411	A	N1-C6-N6	-9.06	113.17	118.60
57	BA	802	A	N1-C6-N6	-9.06	113.17	118.60
22	AA	609	A	N1-C6-N6	-9.05	113.17	118.60
23	A2	55	A	N1-C6-N6	-9.05	113.17	118.60
57	BA	2814	A	N1-C6-N6	-9.05	113.17	118.60
22	AA	600	A	N1-C6-N6	-9.05	113.17	118.60
57	BA	2441	U	O4'-C1'-N1	9.05	115.44	108.20
57	BA	1717	A	C5-C6-N1	9.05	122.22	117.70
22	AA	621	A	N1-C6-N6	-9.04	113.17	118.60
57	BA	2835	A	N1-C6-N6	-9.04	113.17	118.60
57	BA	401	A	N1-C6-N6	-9.04	113.17	118.60
57	BA	1785	A	N1-C6-N6	-9.04	113.17	118.60
57	BA	886	A	N1-C6-N6	-9.04	113.18	118.60
57	BA	1427	A	C5-C6-N1	9.04	122.22	117.70
57	BA	1508	A	N1-C6-N6	-9.04	113.18	118.60
22	AA	363	A	N1-C6-N6	-9.03	113.18	118.60
22	AA	1000	A	N1-C6-N6	-9.04	113.18	118.60
57	BA	1744	A	N1-C6-N6	-9.03	113.18	118.60
22	AA	1398	A	N1-C6-N6	-9.03	113.18	118.60
57	BA	2055	C	O4'-C1'-N1	9.03	115.43	108.20
57	BA	2406	A	N1-C6-N6	-9.03	113.18	118.60
57	BA	1502	A	N1-C6-N6	-9.03	113.18	118.60
57	BA	2590	A	N1-C6-N6	-9.03	113.18	118.60
22	AA	1130	A	C5-C6-N1	9.03	122.21	117.70
57	BA	1545	A	N1-C6-N6	-9.03	113.18	118.60
29	BO	30	ARG	NE-CZ-NH1	9.02	124.81	120.30
57	BA	1275	A	C5-C6-N1	9.02	122.21	117.70
22	AA	860	A	N1-C6-N6	-9.02	113.19	118.60
24	A3	60	A	N1-C6-N6	-9.02	113.19	118.60
33	BS	9	ARG	NE-CZ-NH1	9.02	124.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Ba	52	A	N1-C6-N6	-9.02	113.19	118.60
58	Ba	78	A	C5-C6-N1	9.02	122.21	117.70
35	BD	211	ARG	NE-CZ-NH1	9.02	124.81	120.30
57	BA	2407	A	N1-C6-N6	-9.01	113.19	118.60
22	AA	1256	A	N1-C6-N6	-9.01	113.19	118.60
57	BA	1889	A	N1-C6-N6	-9.01	113.19	118.60
57	BA	2003	A	N1-C6-N6	-9.01	113.20	118.60
57	BA	892	A	N1-C6-N6	-9.00	113.20	118.60
22	AA	1434	A	N1-C6-N6	-9.00	113.20	118.60
57	BA	789	A	C5-C6-N1	9.00	122.20	117.70
57	BA	2657	A	N1-C6-N6	-9.00	113.20	118.60
22	AA	85	U	O4'-C1'-N1	8.99	115.39	108.20
34	BT	52	ARG	NE-CZ-NH1	8.99	124.80	120.30
57	BA	1089	A	N1-C6-N6	-8.99	113.20	118.60
57	BA	1393	A	N1-C6-N6	-8.99	113.20	118.60
57	BA	2468	A	N1-C6-N6	-8.99	113.20	118.60
57	BA	1928	A	N1-C6-N6	-8.99	113.21	118.60
22	AA	382	A	N1-C6-N6	-8.99	113.21	118.60
57	BA	514	A	N1-C6-N6	-8.98	113.21	118.60
57	BA	1213	A	N1-C6-N6	-8.98	113.21	118.60
57	BA	2117	A	N1-C6-N6	-8.98	113.21	118.60
57	BA	2749	A	N1-C6-N6	-8.98	113.21	118.60
57	BA	472	A	N1-C6-N6	-8.98	113.21	118.60
57	BA	2761	A	N1-C6-N6	-8.98	113.21	118.60
22	AA	130	A	C5-C6-N1	8.98	122.19	117.70
22	AA	374	A	N1-C6-N6	-8.98	113.21	118.60
57	BA	2598	A	N1-C6-N6	-8.98	113.21	118.60
57	BA	278	A	C5-C6-N1	8.97	122.19	117.70
57	BA	2090	A	N1-C6-N6	-8.97	113.22	118.60
22	AA	899	C	N1-C2-O2	8.97	124.28	118.90
57	BA	345	A	N1-C6-N6	-8.97	113.22	118.60
57	BA	782	A	N1-C6-N6	-8.97	113.22	118.60
57	BA	2727	A	N1-C6-N6	-8.97	113.22	118.60
22	AA	279	A	N1-C6-N6	-8.97	113.22	118.60
32	BR	63	ARG	NE-CZ-NH1	8.96	124.78	120.30
57	BA	1393	A	C5-C6-N1	8.96	122.18	117.70
57	BA	2173	A	N1-C6-N6	-8.96	113.22	118.60
57	BA	89	A	N1-C6-N6	-8.96	113.22	118.60
57	BA	244	A	N1-C6-N6	-8.96	113.23	118.60
22	AA	131	A	N1-C6-N6	-8.96	113.23	118.60
57	BA	497	A	N1-C6-N6	-8.95	113.23	118.60
22	AA	179	A	N1-C6-N6	-8.95	113.23	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	602	A	N1-C6-N6	-8.95	113.23	118.60
57	BA	332	A	N1-C6-N6	-8.95	113.23	118.60
57	BA	1392	A	N1-C6-N6	-8.95	113.23	118.60
35	BD	269	ARG	NE-CZ-NH1	8.94	124.77	120.30
57	BA	2635	A	N1-C6-N6	-8.95	113.23	118.60
57	BA	362	A	N1-C6-N6	-8.94	113.23	118.60
57	BA	1342	A	N1-C6-N6	-8.94	113.23	118.60
22	AA	243	A	N1-C6-N6	-8.94	113.23	118.60
57	BA	1668	A	N1-C6-N6	-8.94	113.23	118.60
22	AA	964	A	N1-C6-N6	-8.94	113.24	118.60
57	BA	1953	A	N1-C6-N6	-8.94	113.24	118.60
23	A2	27	A	N1-C6-N6	-8.93	113.24	118.60
57	BA	1759	A	N1-C6-N6	-8.93	113.24	118.60
57	BA	972	A	N1-C6-N6	-8.93	113.24	118.60
57	BA	2135	A	N1-C6-N6	-8.93	113.24	118.60
18	AG	91	ARG	NE-CZ-NH1	8.93	124.77	120.30
22	AA	964	A	C5-C6-N1	8.93	122.16	117.70
24	A3	16	C	N3-C2-O2	-8.93	115.65	121.90
57	BA	1854	A	N1-C6-N6	-8.93	113.24	118.60
22	AA	1152	A	N1-C6-N6	-8.93	113.24	118.60
57	BA	821	A	N1-C6-N6	-8.93	113.25	118.60
22	AA	974	A	N1-C6-N6	-8.92	113.25	118.60
57	BA	1757	A	N1-C6-N6	-8.92	113.25	118.60
22	AA	1163	A	N1-C6-N6	-8.92	113.25	118.60
22	AA	983	A	C5-C6-N1	8.92	122.16	117.70
57	BA	310	A	N1-C6-N6	-8.92	113.25	118.60
57	BA	2059	A	C5-C6-N1	8.92	122.16	117.70
46	B3	44	ARG	NE-CZ-NH2	8.91	124.76	120.30
57	BA	470	A	N1-C6-N6	-8.91	113.25	118.60
22	AA	704	A	C5-C6-N1	8.91	122.16	117.70
57	BA	1008	A	N1-C6-N6	-8.91	113.25	118.60
57	BA	2868	A	N1-C6-N6	-8.91	113.26	118.60
57	BA	1287	A	N1-C6-N6	-8.90	113.26	118.60
57	BA	2317	A	N1-C6-N6	-8.90	113.26	118.60
57	BA	481	G	O4'-C1'-N9	8.90	115.32	108.20
22	AA	468	A	N1-C6-N6	-8.90	113.26	118.60
58	Ba	109	A	N1-C6-N6	-8.90	113.26	118.60
22	AA	313	A	N1-C6-N6	-8.90	113.26	118.60
57	BA	1454	C	O4'-C1'-N1	8.90	115.32	108.20
22	AA	120	A	N1-C6-N6	-8.90	113.26	118.60
57	BA	1086	A	N1-C6-N6	-8.90	113.26	118.60
45	BE	83	ARG	NE-CZ-NH2	8.89	124.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	172	A	N1-C6-N6	-8.89	113.27	118.60
22	AA	495	A	N1-C6-N6	-8.89	113.27	118.60
22	AA	397	A	N1-C6-N6	-8.88	113.27	118.60
57	BA	2097	A	N1-C6-N6	-8.88	113.27	118.60
57	BA	2850	A	N1-C6-N6	-8.89	113.27	118.60
58	Ba	99	A	N1-C6-N6	-8.88	113.27	118.60
22	AA	673	A	N1-C6-N6	-8.88	113.27	118.60
57	BA	323	C	N3-C2-O2	-8.88	115.68	121.90
57	BA	626	A	N1-C6-N6	-8.88	113.27	118.60
57	BA	676	A	N1-C6-N6	-8.88	113.27	118.60
57	BA	1366	A	N1-C6-N6	-8.88	113.27	118.60
57	BA	1966	A	N1-C6-N6	-8.88	113.27	118.60
23	A2	59	A	O4'-C1'-N9	8.88	115.30	108.20
24	A3	73	A	N1-C6-N6	-8.88	113.27	118.60
57	BA	2147	A	O4'-C1'-N9	8.88	115.30	108.20
22	AA	1055	A	N1-C6-N6	-8.88	113.28	118.60
4	AM	78	ARG	NE-CZ-NH1	8.87	124.74	120.30
22	AA	648	A	N1-C6-N6	-8.87	113.28	118.60
22	AA	59	A	N1-C6-N6	-8.87	113.28	118.60
57	BA	104	A	N1-C6-N6	-8.86	113.28	118.60
22	AA	1171	A	N1-C6-N6	-8.86	113.28	118.60
54	BG	149	ARG	NE-CZ-NH1	8.86	124.73	120.30
22	AA	560	A	N1-C6-N6	-8.86	113.28	118.60
57	BA	739	A	N1-C6-N6	-8.86	113.28	118.60
57	BA	1912	A	N1-C6-N6	-8.86	113.28	118.60
57	BA	2336	A	N1-C6-N6	-8.85	113.29	118.60
58	Ba	39	A	N1-C6-N6	-8.85	113.29	118.60
58	Ba	88	C	O4'-C1'-N1	8.85	115.28	108.20
22	AA	1250	A	N1-C6-N6	-8.85	113.29	118.60
57	BA	233	A	C5-C6-N1	8.85	122.12	117.70
58	Ba	45	A	N1-C6-N6	-8.85	113.29	118.60
22	AA	182	A	N1-C6-N6	-8.85	113.29	118.60
57	BA	527	C	N3-C2-O2	-8.85	115.71	121.90
57	BA	2019	A	N1-C6-N6	-8.85	113.29	118.60
22	AA	238	A	N1-C6-N6	-8.84	113.30	118.60
54	BG	166	ARG	NE-CZ-NH1	8.84	124.72	120.30
57	BA	2060	A	N1-C6-N6	-8.84	113.30	118.60
22	AA	263	A	N1-C6-N6	-8.83	113.30	118.60
22	AA	1080	A	N1-C6-N6	-8.83	113.30	118.60
22	AA	1158	C	N3-C2-O2	-8.83	115.72	121.90
57	BA	2322	A	N1-C6-N6	-8.83	113.30	118.60
57	BA	2706	A	N1-C6-N6	-8.83	113.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1165	A	N1-C6-N6	-8.83	113.30	118.60
57	BA	2313	C	N3-C2-O2	-8.83	115.72	121.90
50	B7	34	ARG	NE-CZ-NH1	8.83	124.71	120.30
57	BA	1626	A	N1-C6-N6	-8.83	113.31	118.60
22	AA	58	C	N3-C2-O2	-8.82	115.72	121.90
57	BA	447	A	N1-C6-N6	-8.82	113.31	118.60
57	BA	1253	A	C5-C6-N1	8.82	122.11	117.70
57	BA	1700	A	N1-C6-N6	-8.82	113.31	118.60
57	BA	2765	A	C5-C6-N1	8.82	122.11	117.70
22	AA	1322	C	N3-C2-O2	-8.81	115.73	121.90
23	A2	45	G	O4'-C1'-N9	8.81	115.25	108.20
33	BS	10	ARG	NE-CZ-NH1	8.81	124.71	120.30
35	BD	86	ARG	NE-CZ-NH1	8.81	124.70	120.30
57	BA	1230	A	N1-C6-N6	-8.81	113.31	118.60
57	BA	1773	A	N1-C6-N6	-8.81	113.31	118.60
22	AA	152	A	C5-C6-N1	8.81	122.10	117.70
22	AA	298	A	N1-C6-N6	-8.80	113.32	118.60
22	AA	1374	A	N1-C6-N6	-8.80	113.32	118.60
57	BA	1057	A	N1-C6-N6	-8.80	113.32	118.60
22	AA	250	A	N1-C6-N6	-8.80	113.32	118.60
57	BA	515	A	C5-C6-N1	8.80	122.10	117.70
57	BA	1084	A	C5-C6-N1	8.80	122.10	117.70
57	BA	2076	U	O4'-C1'-N1	8.80	115.24	108.20
57	BA	670	A	N1-C6-N6	-8.80	113.32	118.60
57	BA	1987	A	N1-C6-N6	-8.80	113.32	118.60
21	A1	463	ARG	NE-CZ-NH1	8.79	124.70	120.30
22	AA	81	A	N1-C6-N6	-8.79	113.33	118.60
22	AA	1279	G	O4'-C1'-N9	8.79	115.23	108.20
57	BA	146	A	N1-C6-N6	-8.79	113.33	118.60
57	BA	936	A	N1-C6-N6	-8.78	113.33	118.60
57	BA	2432	A	O4'-C1'-N9	8.78	115.22	108.20
22	AA	794	A	N1-C6-N6	-8.78	113.33	118.60
57	BA	2358	A	N1-C6-N6	-8.78	113.33	118.60
24	A3	58	A	N1-C6-N6	-8.78	113.33	118.60
57	BA	2183	A	N1-C6-N6	-8.78	113.33	118.60
22	AA	814	A	C5-C6-N1	8.77	122.09	117.70
57	BA	1246	A	N1-C6-N6	-8.77	113.34	118.60
57	BA	1548	A	N1-C6-N6	-8.77	113.34	118.60
22	AA	759	A	N1-C6-N6	-8.77	113.34	118.60
22	AA	366	A	N1-C6-N6	-8.77	113.34	118.60
57	BA	2741	A	N1-C6-N6	-8.76	113.34	118.60
23	A2	18	A	N1-C6-N6	-8.76	113.34	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	215	C	N3-C2-O2	-8.76	115.77	121.90
22	AA	693	G	O4'-C1'-N9	8.76	115.21	108.20
57	BA	1808	A	N1-C6-N6	-8.76	113.34	118.60
4	AM	69	ARG	NE-CZ-NH1	8.76	124.68	120.30
23	A2	29	G	O4'-C1'-N9	8.75	115.20	108.20
57	BA	1086	A	C5-C6-N1	8.74	122.07	117.70
57	BA	2518	A	N1-C6-N6	-8.74	113.36	118.60
22	AA	510	A	N1-C6-N6	-8.74	113.36	118.60
22	AA	1005	A	N1-C6-N6	-8.74	113.36	118.60
22	AA	1146	A	N1-C6-N6	-8.74	113.36	118.60
22	AA	574	A	N1-C6-N6	-8.73	113.36	118.60
57	BA	586	A	N1-C6-N6	-8.73	113.36	118.60
57	BA	1676	A	C5-C6-N1	8.73	122.06	117.70
22	AA	65	A	N1-C6-N6	-8.72	113.37	118.60
22	AA	1408	A	N1-C6-N6	-8.72	113.36	118.60
22	AA	1429	A	N1-C6-N6	-8.72	113.36	118.60
57	BA	1413	A	N1-C6-N6	-8.72	113.37	118.60
57	BA	582	A	C5-C6-N1	8.72	122.06	117.70
57	BA	1630	A	N1-C6-N6	-8.72	113.37	118.60
57	BA	1504	A	N1-C6-N6	-8.72	113.37	118.60
57	BA	1522	A	N1-C6-N6	-8.72	113.37	118.60
57	BA	2328	A	N1-C6-N6	-8.71	113.37	118.60
57	BA	2721	A	C5-C6-N1	8.71	122.06	117.70
57	BA	1936	A	N1-C6-N6	-8.71	113.37	118.60
57	BA	2700	A	N1-C6-N6	-8.71	113.37	118.60
57	BA	750	A	C5-C6-N1	8.71	122.06	117.70
57	BA	1525	A	N1-C6-N6	-8.71	113.38	118.60
45	BE	128	ARG	NE-CZ-NH1	8.70	124.65	120.30
57	BA	2170	A	N1-C6-N6	-8.70	113.38	118.60
17	AF	91	ARG	NE-CZ-NH1	8.70	124.65	120.30
22	AA	535	A	N1-C6-N6	-8.70	113.38	118.60
57	BA	981	A	C5-C6-N1	8.70	122.05	117.70
57	BA	1385	A	N1-C6-N6	-8.70	113.38	118.60
57	BA	1677	A	N1-C6-N6	-8.70	113.38	118.60
22	AA	78	A	N1-C6-N6	-8.70	113.38	118.60
57	BA	637	A	N1-C6-N6	-8.70	113.38	118.60
18	AG	110	ARG	NE-CZ-NH1	8.69	124.65	120.30
22	AA	1014	A	C5-C6-N1	8.69	122.05	117.70
57	BA	516	C	N3-C2-O2	-8.69	115.81	121.90
57	BA	621	A	N1-C6-N6	-8.69	113.39	118.60
57	BA	2014	A	N1-C6-N6	-8.69	113.39	118.60
22	AA	228	A	N1-C6-N6	-8.69	113.39	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1347	A	C5-C6-N1	8.69	122.04	117.70
22	AA	371	A	N1-C6-N6	-8.69	113.39	118.60
22	AA	432	A	N1-C6-N6	-8.68	113.39	118.60
57	BA	507	A	N1-C6-N6	-8.68	113.39	118.60
57	BA	1419	A	C5-C6-N1	8.68	122.04	117.70
22	AA	1363	A	C5-C6-N1	8.68	122.04	117.70
57	BA	52	A	N1-C6-N6	-8.68	113.39	118.60
57	BA	1070	A	N1-C6-N6	-8.68	113.39	118.60
57	BA	2288	A	N1-C6-N6	-8.68	113.39	118.60
57	BA	2450	A	C5-C6-N1	8.68	122.04	117.70
57	BA	2432	A	C5-C6-N1	8.68	122.04	117.70
57	BA	63	A	N1-C6-N6	-8.67	113.40	118.60
57	BA	2342	C	N3-C2-O2	-8.67	115.83	121.90
22	AA	223	A	N1-C6-N6	-8.67	113.40	118.60
22	AA	246	A	N1-C6-N6	-8.67	113.40	118.60
22	AA	1238	A	C5-C6-N1	8.67	122.03	117.70
24	A3	36	A	N1-C6-N6	-8.67	113.40	118.60
57	BA	1583	A	N1-C6-N6	-8.67	113.40	118.60
20	AI	123	ARG	NE-CZ-NH1	8.67	124.63	120.30
24	A3	59	A	N1-C6-N6	-8.67	113.40	118.60
57	BA	53	A	N1-C6-N6	-8.67	113.40	118.60
57	BA	2070	A	N1-C6-N6	-8.67	113.40	118.60
57	BA	1012	U	O4'-C1'-N1	8.66	115.13	108.20
57	BA	899	A	N1-C6-N6	-8.66	113.40	118.60
57	BA	911	A	C5-C6-N1	8.66	122.03	117.70
57	BA	1275	A	O4'-C1'-N9	8.66	115.13	108.20
57	BA	2101	A	N1-C6-N6	-8.66	113.40	118.60
22	AA	934	C	N3-C2-O2	-8.66	115.84	121.90
57	BA	574	A	N1-C6-N6	-8.66	113.41	118.60
57	BA	2632	A	N1-C6-N6	-8.65	113.41	118.60
57	BA	2835	A	C5-C6-N1	8.65	122.03	117.70
57	BA	352	A	N1-C6-N6	-8.65	113.41	118.60
15	AD	183	ARG	NE-CZ-NH1	8.65	124.62	120.30
57	BA	2095	A	N1-C6-N6	-8.65	113.41	118.60
57	BA	160	A	N1-C6-N6	-8.64	113.41	118.60
22	AA	349	A	N1-C6-N6	-8.64	113.41	118.60
22	AA	1157	A	C5-C6-N1	8.64	122.02	117.70
57	BA	980	A	C5-C6-N1	8.64	122.02	117.70
22	AA	461	A	C5-C6-N1	8.63	122.02	117.70
22	AA	1275	A	N1-C6-N6	-8.63	113.42	118.60
57	BA	38	A	C5-C6-N1	8.63	122.02	117.70
22	AA	1252	A	N1-C6-N6	-8.63	113.42	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	182	A	N1-C6-N6	-8.62	113.42	118.60
57	BA	2614	A	C5-C6-N1	8.63	122.01	117.70
22	AA	872	A	C5-C6-N1	8.62	122.01	117.70
57	BA	1871	A	N1-C6-N6	-8.62	113.43	118.60
57	BA	2797	U	O4'-C1'-N1	8.62	115.10	108.20
14	AC	231	ARG	NE-CZ-NH2	8.62	124.61	120.30
57	BA	1268	A	N1-C6-N6	-8.62	113.43	118.60
57	BA	1322	A	N1-C6-N6	-8.62	113.43	118.60
22	AA	189	A	N1-C6-N6	-8.62	113.43	118.60
57	BA	222	A	N1-C6-N6	-8.62	113.43	118.60
57	BA	635	C	N3-C2-O2	-8.62	115.87	121.90
57	BA	1805	A	N1-C6-N6	-8.62	113.43	118.60
57	BA	2008	C	N3-C2-O2	-8.61	115.87	121.90
57	BA	2247	A	N1-C6-N6	-8.61	113.43	118.60
22	AA	1287	A	N1-C6-N6	-8.61	113.43	118.60
57	BA	1678	A	N1-C6-N6	-8.61	113.43	118.60
57	BA	1938	A	N1-C6-N6	-8.61	113.43	118.60
24	A3	14	A	N1-C6-N6	-8.61	113.44	118.60
48	B5	49	ARG	NE-CZ-NH1	8.61	124.60	120.30
57	BA	226	A	N1-C6-N6	-8.61	113.44	118.60
22	AA	1046	A	N1-C6-N6	-8.61	113.44	118.60
22	AA	1167	A	N1-C6-N6	-8.61	113.44	118.60
57	BA	1932	A	C5-C6-N1	8.61	122.00	117.70
57	BA	1009	A	N1-C6-N6	-8.60	113.44	118.60
57	BA	1912	A	C5-C6-N1	8.60	122.00	117.70
57	BA	2732	G	O4'-C1'-N9	8.60	115.08	108.20
22	AA	315	A	C5-C6-N1	8.60	122.00	117.70
30	BP	78	ARG	NE-CZ-NH1	8.60	124.60	120.30
57	BA	765	C	N3-C2-O2	-8.60	115.88	121.90
57	BA	838	C	N3-C2-O2	-8.60	115.88	121.90
22	AA	499	A	C5-C6-N1	8.60	122.00	117.70
57	BA	1040	A	N1-C6-N6	-8.60	113.44	118.60
57	BA	2560	A	N1-C6-N6	-8.60	113.44	118.60
57	BA	943	A	N1-C6-N6	-8.60	113.44	118.60
57	BA	794	A	N1-C6-N6	-8.59	113.44	118.60
57	BA	1268	A	C5-C6-N1	8.59	122.00	117.70
22	AA	579	A	N1-C6-N6	-8.59	113.44	118.60
22	AA	1004	A	N1-C6-N6	-8.59	113.45	118.60
57	BA	947	A	C5-C6-N1	8.59	122.00	117.70
57	BA	2758	A	N1-C6-N6	-8.59	113.45	118.60
3	AL	85	ARG	NE-CZ-NH1	8.59	124.59	120.30
22	AA	1092	A	N1-C6-N6	-8.59	113.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1786	A	C5-C6-N1	8.59	121.99	117.70
57	BA	103	A	N1-C6-N6	-8.58	113.45	118.60
57	BA	1204	A	C5-C6-N1	8.58	121.99	117.70
22	AA	77	A	N1-C6-N6	-8.58	113.45	118.60
57	BA	572	A	C5-C6-N1	8.57	121.99	117.70
57	BA	13	A	C5-C6-N1	8.57	121.99	117.70
22	AA	696	A	N1-C6-N6	-8.57	113.46	118.60
22	AA	1394	A	N1-C6-N6	-8.57	113.46	118.60
8	AQ	10	ARG	NE-CZ-NH1	8.57	124.58	120.30
22	AA	530	G	O4'-C1'-N9	8.57	115.05	108.20
57	BA	1496	A	N1-C6-N6	-8.56	113.46	118.60
22	AA	327	A	N1-C6-N6	-8.56	113.46	118.60
22	AA	1433	A	C5-C6-N1	8.56	121.98	117.70
57	BA	1302	A	C5-C6-N1	8.56	121.98	117.70
43	B1	73	ARG	NE-CZ-NH2	8.56	124.58	120.30
57	BA	73	A	C5-C6-N1	8.56	121.98	117.70
57	BA	155	A	N1-C6-N6	-8.56	113.46	118.60
57	BA	265	A	N1-C6-N6	-8.56	113.46	118.60
22	AA	781	A	C5-C6-N1	8.56	121.98	117.70
57	BA	199	A	N1-C6-N6	-8.56	113.46	118.60
57	BA	2071	A	C5-C6-N1	8.56	121.98	117.70
57	BA	1544	A	N1-C6-N6	-8.55	113.47	118.60
57	BA	960	A	N1-C6-N6	-8.55	113.47	118.60
57	BA	1383	A	N1-C6-N6	-8.55	113.47	118.60
57	BA	1454	C	N3-C2-O2	-8.55	115.91	121.90
42	B0	38	ARG	NE-CZ-NH1	8.55	124.58	120.30
57	BA	844	A	N1-C6-N6	-8.55	113.47	118.60
57	BA	514	A	C5-C6-N1	8.55	121.97	117.70
57	BA	751	A	N1-C6-N6	-8.55	113.47	118.60
57	BA	2882	A	C5-C6-N1	8.55	121.97	117.70
57	BA	294	A	C5-C6-N1	8.55	121.97	117.70
22	AA	630	A	N1-C6-N6	-8.54	113.47	118.60
22	AA	729	A	N1-C6-N6	-8.54	113.47	118.60
57	BA	2184	A	N1-C6-N6	-8.54	113.47	118.60
57	BA	2278	A	C5-C6-N1	8.54	121.97	117.70
57	BA	2534	A	C5-C6-N1	8.54	121.97	117.70
57	BA	2883	A	N1-C6-N6	-8.54	113.47	118.60
20	AI	32	ARG	NE-CZ-NH1	8.54	124.57	120.30
57	BA	269	C	O4'-C1'-N1	8.54	115.03	108.20
4	AM	91	ARG	NE-CZ-NH1	8.54	124.57	120.30
10	AS	36	ARG	NE-CZ-NH1	8.54	124.57	120.30
22	AA	282	A	N1-C6-N6	-8.54	113.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1597	A	N1-C6-N6	-8.54	113.48	118.60
57	BA	2781	A	C5-C6-N1	8.53	121.97	117.70
22	AA	1042	A	N1-C6-N6	-8.53	113.48	118.60
22	AA	583	A	N1-C6-N6	-8.53	113.48	118.60
57	BA	1665	A	C5-C6-N1	8.53	121.96	117.70
57	BA	2639	A	N1-C6-N6	-8.53	113.48	118.60
22	AA	681	A	N1-C6-N6	-8.53	113.48	118.60
22	AA	747	A	N1-C6-N6	-8.52	113.49	118.60
57	BA	661	A	C5-C6-N1	8.52	121.96	117.70
57	BA	1652	A	N1-C6-N6	-8.52	113.49	118.60
22	AA	695	A	C5-C6-N1	8.52	121.96	117.70
57	BA	2266	A	C5-C6-N1	8.52	121.96	117.70
57	BA	176	A	N1-C6-N6	-8.52	113.49	118.60
57	BA	1275	A	N1-C6-N6	-8.52	113.49	118.60
57	BA	1286	A	N1-C6-N6	-8.51	113.49	118.60
22	AA	211	G	O4'-C1'-N9	8.51	115.01	108.20
22	AA	1299	A	N1-C6-N6	-8.51	113.50	118.60
57	BA	478	A	N1-C6-N6	-8.51	113.49	118.60
57	BA	1084	A	N1-C6-N6	-8.51	113.50	118.60
57	BA	2154	A	N1-C6-N6	-8.51	113.50	118.60
57	BA	2119	A	N1-C6-N6	-8.51	113.50	118.60
22	AA	1093	A	C5-C6-N1	8.50	121.95	117.70
22	AA	28	A	N1-C6-N6	-8.50	113.50	118.60
57	BA	1434	A	O4'-C1'-N9	8.50	115.00	108.20
22	AA	621	A	C5-C6-N1	8.50	121.95	117.70
57	BA	1528	A	N1-C6-N6	-8.50	113.50	118.60
57	BA	1899	A	N1-C6-N6	-8.50	113.50	118.60
57	BA	2275	C	O4'-C1'-N1	8.49	115.00	108.20
22	AA	1169	A	N1-C6-N6	-8.49	113.50	118.60
22	AA	1368	A	N1-C6-N6	-8.49	113.50	118.60
48	B5	39	ARG	NE-CZ-NH1	8.49	124.55	120.30
57	BA	423	A	C5-C6-N1	8.49	121.95	117.70
18	AG	2	ARG	NE-CZ-NH1	8.49	124.54	120.30
57	BA	119	A	C5-C6-N1	8.49	121.94	117.70
22	AA	787	A	N1-C6-N6	-8.49	113.51	118.60
22	AA	572	A	C5-C6-N1	8.48	121.94	117.70
57	BA	94	A	N1-C6-N6	-8.48	113.51	118.60
22	AA	109	A	C5-C6-N1	8.48	121.94	117.70
57	BA	301	G	O4'-C1'-N9	8.48	114.98	108.20
57	BA	1069	A	N1-C6-N6	-8.48	113.51	118.60
57	BA	131	A	N1-C6-N6	-8.48	113.51	118.60
57	BA	2738	A	N1-C6-N6	-8.48	113.51	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2893	A	N1-C6-N6	-8.48	113.51	118.60
57	BA	655	A	C5-C6-N1	8.47	121.94	117.70
22	AA	1456	A	N1-C6-N6	-8.47	113.52	118.60
57	BA	2810	A	C5-C6-N1	8.47	121.94	117.70
22	AA	393	A	N1-C6-N6	-8.47	113.52	118.60
57	BA	906	U	O4'-C1'-N1	8.47	114.98	108.20
22	AA	106	C	N3-C2-O2	-8.47	115.97	121.90
24	A3	77	A	N1-C6-N6	-8.47	113.52	118.60
57	BA	221	A	N1-C6-N6	-8.47	113.52	118.60
57	BA	845	A	N1-C6-N6	-8.47	113.52	118.60
57	BA	1111	A	N1-C6-N6	-8.47	113.52	118.60
57	BA	2705	A	N1-C6-N6	-8.47	113.52	118.60
22	AA	1155	A	C5-C6-N1	8.47	121.93	117.70
22	AA	914	A	N1-C6-N6	-8.46	113.52	118.60
22	AA	408	A	N1-C6-N6	-8.46	113.52	118.60
57	BA	1990	C	N3-C2-O2	-8.46	115.98	121.90
57	BA	2662	A	C5-C6-N1	8.46	121.93	117.70
22	AA	687	A	N1-C6-N6	-8.46	113.53	118.60
53	BF	102	ARG	NE-CZ-NH2	8.46	124.53	120.30
22	AA	303	A	N1-C6-N6	-8.46	113.53	118.60
57	BA	131	A	C5-C6-N1	8.45	121.93	117.70
57	BA	2202	U	O4'-C1'-N1	8.46	114.96	108.20
22	AA	501	C	N3-C2-O2	-8.45	115.98	121.90
22	AA	1014	A	N1-C6-N6	-8.45	113.53	118.60
57	BA	718	A	C5-C6-N1	8.45	121.93	117.70
22	AA	873	A	N1-C6-N6	-8.45	113.53	118.60
22	AA	1441	A	C5-C6-N1	8.45	121.92	117.70
22	AA	1167	A	C5-C6-N1	8.44	121.92	117.70
57	BA	1367	A	N1-C6-N6	-8.44	113.53	118.60
57	BA	2542	A	N1-C6-N6	-8.44	113.53	118.60
57	BA	981	A	N1-C6-N6	-8.44	113.54	118.60
57	BA	1433	A	C5-C6-N1	8.44	121.92	117.70
47	B4	49	ARG	NE-CZ-NH1	8.44	124.52	120.30
22	AA	728	A	C5-C6-N1	8.44	121.92	117.70
22	AA	1150	A	N1-C6-N6	-8.44	113.54	118.60
57	BA	668	A	C5-C6-N1	8.44	121.92	117.70
22	AA	1499	A	C5-C6-N1	8.44	121.92	117.70
22	AA	814	A	N1-C6-N6	-8.43	113.54	118.60
22	AA	1197	A	C5-C6-N1	8.43	121.92	117.70
57	BA	1783	A	C5-C6-N1	8.43	121.92	117.70
57	BA	756	A	N1-C6-N6	-8.43	113.54	118.60
57	BA	2860	A	N1-C6-N6	-8.43	113.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	71	A	C5-C6-N1	8.43	121.91	117.70
57	BA	152	A	N1-C6-N6	-8.43	113.54	118.60
57	BA	2281	A	N1-C6-N6	-8.42	113.55	118.60
57	BA	631	A	C5-C6-N1	8.42	121.91	117.70
57	BA	490	C	N3-C2-O2	-8.42	116.01	121.90
57	BA	1635	A	C5-C6-N1	8.42	121.91	117.70
4	AM	112	ARG	NE-CZ-NH1	8.41	124.51	120.30
22	AA	553	A	N1-C6-N6	-8.41	113.55	118.60
22	AA	1050	G	O4'-C1'-N9	8.41	114.93	108.20
57	BA	322	A	C5-C6-N1	8.41	121.91	117.70
22	AA	328	C	N3-C2-O2	-8.41	116.01	121.90
22	AA	1333	A	N1-C6-N6	-8.41	113.56	118.60
22	AA	1035	A	N1-C6-N6	-8.41	113.56	118.60
57	BA	1551	A	C5-C6-N1	8.40	121.90	117.70
57	BA	1800	C	N3-C2-O2	-8.40	116.02	121.90
57	BA	2054	A	C4-C5-C6	-8.40	112.80	117.00
24	A3	38	A	C5-C6-N1	8.40	121.90	117.70
57	BA	2297	A	N1-C6-N6	-8.40	113.56	118.60
57	BA	1070	A	C5-C6-N1	8.40	121.90	117.70
57	BA	1213	A	C5-C6-N1	8.40	121.90	117.70
22	AA	1201	A	N1-C6-N6	-8.40	113.56	118.60
57	BA	2381	A	N1-C6-N6	-8.40	113.56	118.60
58	Ba	108	A	C5-C6-N1	8.40	121.90	117.70
57	BA	480	A	N1-C6-N6	-8.39	113.56	118.60
22	AA	532	A	C5-C6-N1	8.39	121.90	117.70
22	AA	622	A	C5-C6-N1	8.39	121.90	117.70
23	A2	18	A	C5-C6-N1	8.39	121.89	117.70
57	BA	279	A	N1-C6-N6	-8.39	113.56	118.60
57	BA	1847	A	O4'-C1'-N9	8.39	114.91	108.20
57	BA	2412	A	N1-C6-N6	-8.39	113.56	118.60
22	AA	949	A	N1-C6-N6	-8.39	113.57	118.60
22	AA	234	C	N3-C2-O2	-8.38	116.03	121.90
57	BA	249	C	N3-C2-O2	-8.39	116.03	121.90
57	BA	743	A	N1-C6-N6	-8.38	113.57	118.60
57	BA	1129	A	C5-C6-N1	8.38	121.89	117.70
57	BA	1689	A	N1-C6-N6	-8.38	113.57	118.60
57	BA	2158	A	N1-C6-N6	-8.38	113.57	118.60
22	AA	10	A	N1-C6-N6	-8.38	113.57	118.60
22	AA	327	A	C5-C6-N1	8.38	121.89	117.70
57	BA	192	C	O4'-C1'-N1	8.38	114.90	108.20
57	BA	222	A	C5-C6-N1	8.38	121.89	117.70
57	BA	1439	A	N1-C6-N6	-8.38	113.57	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2861	U	O4'-C1'-N1	8.38	114.90	108.20
22	AA	1274	A	N1-C6-N6	-8.38	113.57	118.60
57	BA	457	A	N1-C6-N6	-8.38	113.58	118.60
57	BA	1156	A	N1-C6-N6	-8.38	113.58	118.60
57	BA	1515	A	C5-C6-N1	8.37	121.89	117.70
22	AA	1196	A	N1-C6-N6	-8.37	113.58	118.60
57	BA	126	A	C5-C6-N1	8.37	121.88	117.70
57	BA	1359	A	N1-C6-N6	-8.37	113.58	118.60
57	BA	1952	A	C5-C6-N1	8.37	121.88	117.70
57	BA	2411	A	C5-C6-N1	8.37	121.88	117.70
58	Ba	53	A	C5-C6-N1	8.37	121.89	117.70
57	BA	330	A	C5-C6-N1	8.37	121.88	117.70
57	BA	752	A	O4'-C1'-N9	8.37	114.89	108.20
57	BA	2284	A	C5-C6-N1	8.37	121.88	117.70
57	BA	2497	A	N1-C6-N6	-8.37	113.58	118.60
57	BA	2531	A	C5-C6-N1	8.37	121.88	117.70
57	BA	21	A	N1-C6-N6	-8.36	113.58	118.60
57	BA	1260	A	N1-C6-N6	-8.36	113.58	118.60
57	BA	1676	A	N1-C6-N6	-8.36	113.58	118.60
57	BA	101	A	C5-C6-N1	8.36	121.88	117.70
57	BA	925	A	C5-C6-N1	8.36	121.88	117.70
57	BA	753	A	N1-C6-N6	-8.36	113.59	118.60
57	BA	1189	A	N1-C6-N6	-8.36	113.59	118.60
57	BA	1713	A	N1-C6-N6	-8.36	113.59	118.60
57	BA	1997	C	O4'-C1'-N1	8.36	114.88	108.20
22	AA	1257	A	O4'-C1'-N9	8.35	114.88	108.20
57	BA	342	A	N1-C6-N6	-8.35	113.59	118.60
22	AA	1339	A	C5-C6-N1	8.35	121.88	117.70
22	AA	1396	A	C5-C6-N1	8.35	121.88	117.70
57	BA	730	A	C5-C6-N1	8.35	121.87	117.70
57	BA	1205	A	C5-C6-N1	8.35	121.87	117.70
57	BA	2434	A	C5-C6-N1	8.35	121.87	117.70
57	BA	1916	A	N1-C6-N6	-8.34	113.59	118.60
22	AA	499	A	C4-C5-C6	-8.34	112.83	117.00
22	AA	493	A	C5-C6-N1	8.34	121.87	117.70
57	BA	1580	A	C5-C6-N1	8.34	121.87	117.70
22	AA	640	A	C5-C6-N1	8.34	121.87	117.70
22	AA	1200	C	N3-C2-O2	-8.34	116.06	121.90
57	BA	727	A	N1-C6-N6	-8.34	113.60	118.60
57	BA	920	A	N1-C6-N6	-8.34	113.60	118.60
57	BA	1791	A	C5-C6-N1	8.34	121.87	117.70
57	BA	975	A	C5-C6-N1	8.34	121.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AD	80	ARG	NE-CZ-NH1	8.33	124.47	120.30
57	BA	1978	A	N1-C6-N6	-8.33	113.60	118.60
22	AA	1096	C	N3-C2-O2	-8.33	116.07	121.90
46	B3	10	ARG	NE-CZ-NH2	8.33	124.47	120.30
57	BA	556	A	N1-C6-N6	-8.33	113.60	118.60
58	Ba	119	A	N1-C6-N6	-8.33	113.60	118.60
57	BA	71	A	C5-C6-N1	8.33	121.86	117.70
57	BA	730	A	N1-C6-N6	-8.33	113.60	118.60
17	AF	112	ARG	NE-CZ-NH1	8.32	124.46	120.30
22	AA	161	A	C5-C6-N1	8.32	121.86	117.70
24	A3	47	A	N1-C6-N6	-8.32	113.61	118.60
39	BX	73	ARG	NE-CZ-NH1	8.32	124.46	120.30
57	BA	466	A	N1-C6-N6	-8.32	113.61	118.60
22	AA	977	A	C5-C6-N1	8.32	121.86	117.70
57	BA	677	A	N1-C6-N6	-8.32	113.61	118.60
57	BA	792	A	N1-C6-N6	-8.32	113.61	118.60
57	BA	2766	A	N1-C6-N6	-8.32	113.61	118.60
57	BA	2872	A	C5-C6-N1	8.31	121.86	117.70
57	BA	223	A	C5-C6-N1	8.31	121.86	117.70
57	BA	231	A	N1-C6-N6	-8.31	113.61	118.60
57	BA	1893	C	N3-C2-O2	-8.31	116.08	121.90
22	AA	53	A	N1-C6-N6	-8.31	113.61	118.60
37	BV	80	ARG	NE-CZ-NH1	8.31	124.45	120.30
57	BA	354	A	N1-C6-N6	-8.31	113.61	118.60
57	BA	2191	A	N1-C6-N6	-8.31	113.61	118.60
22	AA	825	A	N1-C6-N6	-8.31	113.62	118.60
22	AA	1306	A	C5-C6-N1	8.31	121.85	117.70
57	BA	167	A	N1-C6-N6	-8.31	113.62	118.60
57	BA	2369	A	N1-C6-N6	-8.31	113.62	118.60
22	AA	1368	A	C5-C6-N1	8.31	121.85	117.70
57	BA	941	A	C5-C6-N1	8.31	121.85	117.70
53	BF	49	ARG	NE-CZ-NH2	8.30	124.45	120.30
57	BA	244	A	C5-C6-N1	8.30	121.85	117.70
57	BA	920	A	C5-C6-N1	8.30	121.85	117.70
57	BA	1085	A	C5-C6-N1	8.30	121.85	117.70
22	AA	892	A	N1-C6-N6	-8.30	113.62	118.60
22	AA	236	A	N1-C6-N6	-8.30	113.62	118.60
57	BA	1336	A	N1-C6-N6	-8.30	113.62	118.60
22	AA	400	C	N3-C2-O2	-8.30	116.09	121.90
57	BA	340	A	N1-C6-N6	-8.30	113.62	118.60
57	BA	449	A	C5-C6-N1	8.30	121.85	117.70
57	BA	1048	A	C5-C6-N1	8.30	121.85	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BQ	6	ARG	NE-CZ-NH1	8.30	124.45	120.30
57	BA	644	A	N1-C6-N6	-8.29	113.62	118.60
57	BA	800	A	N1-C6-N6	-8.29	113.62	118.60
57	BA	1590	A	N1-C6-N6	-8.29	113.62	118.60
22	AA	798	U	O4'-C1'-N1	8.29	114.83	108.20
57	BA	5	A	C5-C6-N1	8.29	121.85	117.70
57	BA	699	A	N1-C6-N6	-8.29	113.62	118.60
57	BA	505	A	C5-C6-N1	8.29	121.84	117.70
57	BA	933	A	N1-C6-N6	-8.29	113.63	118.60
57	BA	2809	A	C5-C6-N1	8.29	121.84	117.70
57	BA	2883	A	C5-C6-N1	8.29	121.84	117.70
42	B0	76	ARG	NE-CZ-NH1	8.29	124.44	120.30
57	BA	1065	U	O4'-C1'-N1	8.28	114.83	108.20
57	BA	2126	A	C5-C6-N1	8.28	121.84	117.70
57	BA	1133	A	C5-C6-N1	8.28	121.84	117.70
5	AN	12	ARG	NE-CZ-NH1	8.28	124.44	120.30
57	BA	1427	A	C4-C5-C6	-8.28	112.86	117.00
57	BA	1654	A	C5-C6-N1	8.28	121.84	117.70
22	AA	199	A	C5-C6-N1	8.28	121.84	117.70
22	AA	1254	A	N1-C6-N6	-8.28	113.63	118.60
57	BA	1395	A	C5-C6-N1	8.28	121.84	117.70
57	BA	1829	A	C5-C6-N1	8.28	121.84	117.70
57	BA	305	C	N3-C2-O2	-8.28	116.11	121.90
57	BA	1919	A	C5-C6-N1	8.28	121.84	117.70
57	BA	2435	A	C5-C6-N1	8.28	121.84	117.70
22	AA	55	A	N1-C6-N6	-8.27	113.64	118.60
22	AA	1111	A	C5-C6-N1	8.27	121.84	117.70
22	AA	160	A	C5-C6-N1	8.27	121.83	117.70
22	AA	938	A	C5-C6-N1	8.27	121.83	117.70
22	AA	1468	A	N1-C6-N6	-8.27	113.64	118.60
57	BA	928	A	N1-C6-N6	-8.27	113.64	118.60
57	BA	2297	A	C5-C6-N1	8.27	121.84	117.70
57	BA	1032	A	C5-C6-N1	8.27	121.83	117.70
57	BA	1611	C	N3-C2-O2	-8.27	116.11	121.90
58	Ba	15	A	C5-C6-N1	8.27	121.83	117.70
57	BA	237	C	N3-C2-O2	-8.27	116.11	121.90
57	BA	1143	A	C5-C6-N1	8.27	121.83	117.70
22	AA	972	C	N3-C2-O2	-8.26	116.11	121.90
22	AA	749	A	N1-C6-N6	-8.26	113.64	118.60
22	AA	174	A	N1-C6-N6	-8.26	113.64	118.60
22	AA	1219	A	C5-C6-N1	8.26	121.83	117.70
57	BA	1669	A	C5-C6-N1	8.26	121.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1377	A	C5-C6-N1	8.26	121.83	117.70
3	AL	113	ARG	NE-CZ-NH1	8.26	124.43	120.30
33	BS	102	ARG	NE-CZ-NH1	8.26	124.43	120.30
22	AA	1180	A	C5-C6-N1	8.25	121.83	117.70
57	BA	886	A	C5-C6-N1	8.25	121.83	117.70
57	BA	1434	A	C5-C6-N1	8.25	121.83	117.70
22	AA	1340	A	N1-C6-N6	-8.25	113.65	118.60
22	AA	1531	A	N1-C6-N6	-8.25	113.65	118.60
57	BA	340	A	C5-C6-N1	8.25	121.83	117.70
57	BA	2655	G	O4'-C1'-N9	8.25	114.80	108.20
22	AA	983	A	C4-C5-C6	-8.25	112.88	117.00
22	AA	629	A	N1-C6-N6	-8.25	113.65	118.60
22	AA	906	A	N1-C6-N6	-8.25	113.65	118.60
57	BA	2660	A	C5-C6-N1	8.25	121.82	117.70
57	BA	964	C	N3-C2-O2	-8.25	116.13	121.90
57	BA	83	A	C5-C6-N1	8.24	121.82	117.70
57	BA	2376	A	C5-C6-N1	8.24	121.82	117.70
57	BA	1598	A	O4'-C1'-N9	8.24	114.79	108.20
57	BA	1940	U	O4'-C1'-N1	8.24	114.79	108.20
57	BA	2587	A	C5-C6-N1	8.24	121.82	117.70
22	AA	743	A	N1-C6-N6	-8.24	113.66	118.60
57	BA	197	A	C5-C6-N1	8.24	121.82	117.70
57	BA	49	A	C5-C6-N1	8.23	121.82	117.70
57	BA	323	C	O4'-C1'-N1	8.23	114.79	108.20
57	BA	391	A	C5-C6-N1	8.23	121.82	117.70
1	AJ	45	ARG	NE-CZ-NH1	8.23	124.42	120.30
57	BA	945	A	C5-C6-N1	8.23	121.81	117.70
22	AA	98	A	N1-C6-N6	-8.23	113.66	118.60
22	AA	121	U	O4'-C1'-N1	8.23	114.78	108.20
57	BA	2211	A	C5-C6-N1	8.23	121.81	117.70
57	BA	2565	A	N1-C6-N6	-8.23	113.66	118.60
57	BA	2886	A	C5-C6-N1	8.23	121.81	117.70
22	AA	50	A	C5-C6-N1	8.22	121.81	117.70
22	AA	777	A	C5-C6-N1	8.22	121.81	117.70
57	BA	783	A	O4'-C1'-N9	8.22	114.78	108.20
21	A1	560	ARG	NE-CZ-NH1	8.22	124.41	120.30
12	AT	73	ARG	NE-CZ-NH1	8.22	124.41	120.30
22	AA	1349	A	C5-C6-N1	8.22	121.81	117.70
57	BA	1269	A	N1-C6-N6	-8.22	113.67	118.60
22	AA	1213	A	C4-C5-C6	-8.21	112.89	117.00
57	BA	2646	C	N3-C2-O2	-8.21	116.15	121.90
57	BA	2868	A	C5-C6-N1	8.21	121.81	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	143	A	C5-C6-N1	8.21	121.81	117.70
22	AA	502	A	C5-C6-N1	8.21	121.81	117.70
57	BA	1956	U	O4'-C1'-N1	8.21	114.77	108.20
58	Ba	94	A	N1-C6-N6	-8.21	113.67	118.60
57	BA	528	A	N1-C6-N6	-8.21	113.67	118.60
57	BA	650	C	N3-C2-O2	-8.21	116.15	121.90
22	AA	26	A	C5-C6-N1	8.21	121.80	117.70
33	BS	16	ARG	NE-CZ-NH1	8.21	124.40	120.30
22	AA	101	A	C5-C6-N1	8.21	121.80	117.70
22	AA	878	A	C5-C6-N1	8.21	121.80	117.70
22	AA	915	A	C5-C6-N1	8.20	121.80	117.70
57	BA	49	A	N1-C6-N6	-8.20	113.68	118.60
22	AA	1399	C	N3-C2-O2	-8.20	116.16	121.90
57	BA	28	A	C5-C6-N1	8.20	121.80	117.70
57	BA	1301	A	C5-C6-N1	8.20	121.80	117.70
57	BA	1788	C	N3-C2-O2	-8.20	116.16	121.90
22	AA	648	A	C5-C6-N1	8.20	121.80	117.70
57	BA	1028	A	C5-C6-N1	8.20	121.80	117.70
57	BA	2374	C	N3-C2-O2	-8.20	116.16	121.90
22	AA	1251	A	C5-C6-N1	8.19	121.80	117.70
22	AA	539	A	N1-C6-N6	-8.19	113.68	118.60
57	BA	2518	A	C5-C6-N1	8.19	121.80	117.70
10	AS	2	ARG	NE-CZ-NH1	8.19	124.39	120.30
22	AA	129	A	C5-C6-N1	8.19	121.79	117.70
22	AA	1236	A	C5-C6-N1	8.19	121.80	117.70
48	B5	51	ARG	NE-CZ-NH2	8.19	124.39	120.30
57	BA	677	A	C5-C6-N1	8.19	121.79	117.70
22	AA	574	A	C5-C6-N1	8.19	121.79	117.70
57	BA	1143	A	N1-C6-N6	-8.19	113.69	118.60
57	BA	426	C	N3-C2-O2	-8.18	116.17	121.90
57	BA	2750	A	C5-C6-N1	8.18	121.79	117.70
22	AA	300	A	N1-C6-N6	-8.18	113.69	118.60
22	AA	116	A	C5-C6-N1	8.18	121.79	117.70
22	AA	149	A	N1-C6-N6	-8.18	113.69	118.60
22	AA	1016	A	N1-C6-N6	-8.18	113.69	118.60
57	BA	56	A	C5-C6-N1	8.18	121.79	117.70
57	BA	1616	A	C5-C6-N1	8.18	121.79	117.70
57	BA	1526	C	N3-C2-O2	-8.18	116.18	121.90
22	AA	2	A	C5-C6-N1	8.17	121.79	117.70
57	BA	544	C	N3-C2-O2	-8.17	116.18	121.90
29	BO	108	ARG	NE-CZ-NH1	8.17	124.39	120.30
57	BA	1103	A	C5-C6-N1	8.17	121.78	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1537	G	O4'-C1'-N9	8.17	114.73	108.20
4	AM	100	ARG	NE-CZ-NH1	8.17	124.38	120.30
21	A1	207	ARG	NE-CZ-NH1	8.17	124.38	120.30
57	BA	787	C	N3-C2-O2	-8.17	116.18	121.90
57	BA	2433	A	C5-C6-N1	8.17	121.78	117.70
22	AA	726	C	N3-C2-O2	-8.17	116.18	121.90
57	BA	2378	A	N1-C6-N6	-8.16	113.70	118.60
57	BA	2380	C	N3-C2-O2	-8.16	116.18	121.90
22	AA	336	A	N1-C6-N6	-8.16	113.70	118.60
57	BA	2288	A	C5-C6-N1	8.16	121.78	117.70
13	AU	65	ARG	NE-CZ-NH1	8.16	124.38	120.30
57	BA	1579	A	C5-C6-N1	8.16	121.78	117.70
22	AA	356	A	C5-C6-N1	8.16	121.78	117.70
57	BA	1001	A	N1-C6-N6	-8.15	113.71	118.60
22	AA	468	A	C5-C6-N1	8.15	121.78	117.70
24	A3	57	C	N3-C2-O2	-8.15	116.19	121.90
57	BA	933	A	C5-C6-N1	8.15	121.78	117.70
22	AA	197	A	C5-C6-N1	8.15	121.77	117.70
22	AA	1332	A	C5-C6-N1	8.15	121.78	117.70
50	B7	34	ARG	NE-CZ-NH2	-8.15	116.23	120.30
57	BA	268	C	N3-C2-O2	-8.15	116.20	121.90
57	BA	2879	A	C5-C6-N1	8.15	121.77	117.70
57	BA	1021	A	N1-C6-N6	-8.15	113.71	118.60
57	BA	1664	A	C5-C6-N1	8.15	121.77	117.70
58	Ba	99	A	C5-C6-N1	8.15	121.78	117.70
57	BA	1705	A	N1-C6-N6	-8.15	113.71	118.60
57	BA	1067	A	C5-C6-N1	8.14	121.77	117.70
57	BA	2483	C	N3-C2-O2	-8.14	116.20	121.90
57	BA	1327	A	C5-C6-N1	8.14	121.77	117.70
22	AA	1465	A	N1-C6-N6	-8.14	113.72	118.60
57	BA	1745	A	N1-C6-N6	-8.14	113.72	118.60
58	Ba	53	A	N1-C6-N6	-8.13	113.72	118.60
57	BA	420	C	N3-C2-O2	-8.13	116.21	121.90
57	BA	783	A	N1-C6-N6	-8.13	113.72	118.60
57	BA	1717	A	C4-C5-C6	-8.13	112.93	117.00
58	Ba	104	A	C5-C6-N1	8.13	121.77	117.70
57	BA	2710	C	N3-C2-O2	-8.13	116.21	121.90
57	BA	1307	A	C5-C6-N1	8.13	121.76	117.70
57	BA	1370	C	N3-C2-O2	-8.13	116.21	121.90
57	BA	2019	A	C5-C6-N1	8.13	121.76	117.70
22	AA	205	A	N1-C6-N6	-8.12	113.72	118.60
57	BA	753	A	C5-C6-N1	8.12	121.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	496	A	N1-C6-N6	-8.12	113.73	118.60
57	BA	1998	A	N1-C6-N6	-8.12	113.73	118.60
22	AA	635	A	N1-C6-N6	-8.12	113.73	118.60
22	AA	151	A	C5-C6-N1	8.12	121.76	117.70
22	AA	205	A	C5-C6-N1	8.12	121.76	117.70
57	BA	1879	C	N3-C2-O2	-8.12	116.22	121.90
22	AA	560	A	C5-C6-N1	8.12	121.76	117.70
57	BA	2826	A	N1-C6-N6	-8.12	113.73	118.60
57	BA	849	A	C5-C6-N1	8.11	121.76	117.70
22	AA	385	C	N3-C2-O2	-8.11	116.22	121.90
22	AA	509	A	C5-C6-N1	8.11	121.76	117.70
57	BA	1095	A	C5-C6-N1	8.11	121.76	117.70
57	BA	624	C	N3-C2-O2	-8.11	116.22	121.90
22	AA	3	A	C5-C6-N1	8.11	121.75	117.70
22	AA	59	A	C5-C6-N1	8.11	121.75	117.70
22	AA	321	A	C5-C6-N1	8.11	121.75	117.70
22	AA	1188	A	C5-C6-N1	8.11	121.75	117.70
57	BA	1027	A	C5-C6-N1	8.11	121.75	117.70
57	BA	581	C	N3-C2-O2	-8.11	116.22	121.90
57	BA	1366	A	C5-C6-N1	8.11	121.75	117.70
22	AA	403	C	N3-C2-O2	-8.11	116.22	121.90
22	AA	768	A	N1-C6-N6	-8.11	113.74	118.60
17	AF	2	ARG	NE-CZ-NH1	8.11	124.35	120.30
57	BA	457	A	C5-C6-N1	8.11	121.75	117.70
57	BA	1090	A	C5-C6-N1	8.11	121.75	117.70
57	BA	2062	A	C5-C6-N1	8.11	121.75	117.70
20	AI	94	ARG	NE-CZ-NH1	8.10	124.35	120.30
57	BA	764	A	N1-C6-N6	-8.10	113.74	118.60
57	BA	1503	A	C5-C6-N1	8.10	121.75	117.70
22	AA	356	A	N1-C6-N6	-8.10	113.74	118.60
22	AA	718	A	C5-C6-N1	8.10	121.75	117.70
57	BA	1958	C	N3-C2-O2	-8.10	116.23	121.90
22	AA	1256	A	O4'-C1'-N9	8.10	114.68	108.20
23	A2	19	A	C5-C6-N1	8.10	121.75	117.70
35	BD	237	ARG	NE-CZ-NH2	-8.10	116.25	120.30
57	BA	116	C	N3-C2-O2	-8.10	116.23	121.90
57	BA	423	A	C4-C5-C6	-8.10	112.95	117.00
57	BA	601	C	N3-C2-O2	-8.10	116.23	121.90
57	BA	1151	A	C5-C6-N1	8.10	121.75	117.70
57	BA	1384	A	C5-C6-N1	8.10	121.75	117.70
57	BA	239	C	N3-C2-O2	-8.09	116.23	121.90
57	BA	633	A	N1-C6-N6	-8.09	113.74	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	482	A	N1-C6-N6	-8.09	113.75	118.60
41	BZ	79	ARG	NE-CZ-NH1	8.09	124.34	120.30
57	BA	1759	A	C5-C6-N1	8.09	121.75	117.70
57	BA	1982	U	O4'-C1'-N1	8.09	114.67	108.20
57	BA	2658	C	C4'-C3'-C2'	-8.09	94.51	102.60
57	BA	2850	A	C5-C6-N1	8.09	121.75	117.70
57	BA	118	A	N1-C6-N6	-8.09	113.75	118.60
57	BA	2753	A	N1-C6-N6	-8.09	113.75	118.60
22	AA	325	A	C5-C6-N1	8.08	121.74	117.70
22	AA	919	A	N1-C6-N6	-8.08	113.75	118.60
22	AA	1158	C	N1-C2-O2	8.08	123.75	118.90
57	BA	1490	A	C5-C6-N1	8.08	121.74	117.70
57	BA	2847	U	O4'-C1'-N1	8.08	114.67	108.20
57	BA	1378	A	C5-C6-N1	8.08	121.74	117.70
22	AA	689	C	N3-C2-O2	-8.08	116.24	121.90
22	AA	889	A	C5-C6-N1	8.08	121.74	117.70
57	BA	1705	A	C5-C6-N1	8.08	121.74	117.70
22	AA	1044	A	N1-C6-N6	-8.08	113.75	118.60
57	BA	191	A	N1-C6-N6	-8.08	113.75	118.60
57	BA	1142	A	C5-C6-N1	8.08	121.74	117.70
57	BA	2094	A	N1-C6-N6	-8.08	113.75	118.60
22	AA	1476	A	N1-C6-N6	-8.07	113.75	118.60
57	BA	433	C	N3-C2-O2	-8.07	116.25	121.90
22	AA	161	A	O4'-C1'-N9	8.07	114.66	108.20
22	AA	1434	A	C5-C6-N1	8.07	121.73	117.70
57	BA	216	A	C5-C6-N1	8.07	121.74	117.70
57	BA	1848	A	C5-C6-N1	8.07	121.73	117.70
57	BA	2634	A	C5-C6-N1	8.07	121.73	117.70
22	AA	665	A	C4-C5-C6	-8.07	112.97	117.00
22	AA	1384	C	N3-C2-O2	-8.07	116.25	121.90
57	BA	2660	A	O4'-C1'-N9	8.07	114.65	108.20
22	AA	1101	A	C5-C6-N1	8.06	121.73	117.70
57	BA	854	C	N3-C2-O2	-8.06	116.25	121.90
57	BA	1713	A	C5-C6-N1	8.06	121.73	117.70
57	BA	2478	A	C5-C6-N1	8.06	121.73	117.70
22	AA	288	A	C5-C6-N1	8.06	121.73	117.70
57	BA	795	C	N3-C2-O2	-8.06	116.26	121.90
57	BA	918	A	C5-C6-N1	8.06	121.73	117.70
57	BA	1069	A	C5-C6-N1	8.06	121.73	117.70
57	BA	1803	A	C5-C6-N1	8.06	121.73	117.70
57	BA	1847	A	C5-C6-N1	8.06	121.73	117.70
57	BA	2564	A	C5-C6-N1	8.06	121.73	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2900	A	N1-C6-N6	-8.06	113.77	118.60
22	AA	1413	A	N1-C6-N6	-8.06	113.77	118.60
57	BA	2734	A	C5-C6-N1	8.06	121.73	117.70
57	BA	13	A	C4-C5-C6	-8.05	112.97	117.00
57	BA	802	A	C5-C6-N1	8.05	121.73	117.70
57	BA	819	A	N1-C6-N6	-8.05	113.77	118.60
57	BA	1167	C	N3-C2-O2	-8.05	116.26	121.90
57	BA	2273	A	C5-C6-N1	8.05	121.73	117.70
22	AA	1124	G	O4'-C1'-N9	8.05	114.64	108.20
57	BA	1054	A	C5-C6-N1	8.05	121.73	117.70
57	BA	1937	A	C5-C6-N1	8.05	121.73	117.70
22	AA	1534	A	N1-C6-N6	-8.05	113.77	118.60
57	BA	1570	A	C5-C6-N1	8.05	121.73	117.70
57	BA	2882	A	C4-C5-C6	-8.05	112.97	117.00
57	BA	2778	A	C5-C6-N1	8.05	121.72	117.70
22	AA	547	A	C5-C6-N1	8.05	121.72	117.70
57	BA	91	A	C5-C6-N1	8.05	121.72	117.70
22	AA	909	A	N1-C6-N6	-8.05	113.77	118.60
43	B1	44	ARG	NE-CZ-NH1	8.05	124.32	120.30
57	BA	1241	A	O4'-C1'-N9	8.05	114.64	108.20
57	BA	2327	A	C5-C6-N1	8.05	121.72	117.70
22	AA	179	A	C5-C6-N1	8.05	121.72	117.70
22	AA	614	C	N3-C2-O2	-8.05	116.27	121.90
57	BA	1155	A	C5-C6-N1	8.05	121.72	117.70
57	BA	1637	A	N1-C6-N6	-8.05	113.77	118.60
57	BA	2358	A	C5-C6-N1	8.05	121.72	117.70
49	B6	43	ARG	NE-CZ-NH1	8.04	124.32	120.30
22	AA	132	C	N3-C2-O2	-8.04	116.27	121.90
57	BA	127	A	C5-C6-N1	8.04	121.72	117.70
57	BA	896	A	C5-C6-N1	8.04	121.72	117.70
57	BA	1262	A	C5-C6-N1	8.04	121.72	117.70
22	AA	65	A	C5-C6-N1	8.04	121.72	117.70
22	AA	790	A	N1-C6-N6	-8.04	113.78	118.60
23	A2	27	A	C5-C6-N1	8.04	121.72	117.70
57	BA	309	A	C5-C6-N1	8.04	121.72	117.70
57	BA	199	A	C5-C6-N1	8.04	121.72	117.70
57	BA	378	C	N3-C2-O2	-8.04	116.27	121.90
57	BA	735	A	N1-C6-N6	-8.04	113.78	118.60
57	BA	1073	A	C5-C6-N1	8.04	121.72	117.70
57	BA	1095	A	N1-C6-N6	-8.03	113.78	118.60
57	BA	2042	A	N1-C6-N6	-8.04	113.78	118.60
57	BA	2800	A	C5-C6-N1	8.04	121.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	363	A	C5-C6-N1	8.03	121.72	117.70
57	BA	1819	A	N1-C6-N6	-8.03	113.78	118.60
22	AA	435	A	N1-C6-N6	-8.03	113.78	118.60
22	AA	1428	A	C5-C6-N1	8.03	121.72	117.70
57	BA	1265	A	N1-C6-N6	-8.03	113.78	118.60
22	AA	712	A	C5-C6-N1	8.03	121.71	117.70
53	BF	102	ARG	NE-CZ-NH1	-8.03	116.29	120.30
57	BA	788	A	C5-C6-N1	8.03	121.71	117.70
57	BA	2078	C	N3-C2-O2	-8.03	116.28	121.90
22	AA	1012	A	N1-C6-N6	-8.03	113.78	118.60
22	AA	1225	A	C5-C6-N1	8.03	121.71	117.70
57	BA	727	A	C5-C6-N1	8.03	121.71	117.70
58	Ba	66	A	C5-C6-N1	8.03	121.71	117.70
57	BA	183	C	N3-C2-O2	-8.02	116.28	121.90
57	BA	1987	A	C5-C6-N1	8.02	121.71	117.70
22	AA	974	A	C5-C6-N1	8.02	121.71	117.70
22	AA	1324	A	N1-C6-N6	-8.02	113.79	118.60
57	BA	749	A	N1-C6-N6	-8.02	113.79	118.60
22	AA	1346	A	C5-C6-N1	8.02	121.71	117.70
57	BA	1997	C	N3-C2-O2	-8.02	116.29	121.90
4	AM	2	ARG	NE-CZ-NH1	8.02	124.31	120.30
8	AQ	64	ARG	NE-CZ-NH1	8.02	124.31	120.30
22	AA	1447	A	C5-C6-N1	8.02	121.71	117.70
35	BD	237	ARG	NE-CZ-NH1	8.02	124.31	120.30
57	BA	905	A	C5-C6-N1	8.02	121.71	117.70
16	AE	111	ARG	NH1-CZ-NH2	-8.02	110.58	119.40
22	AA	19	A	N1-C6-N6	-8.02	113.79	118.60
57	BA	603	A	C5-C6-N1	8.02	121.71	117.70
22	AA	1227	A	C5-C6-N1	8.02	121.71	117.70
57	BA	1098	A	N1-C6-N6	-8.02	113.79	118.60
57	BA	2764	A	C5-C6-N1	8.02	121.71	117.70
22	AA	80	A	N1-C6-N6	-8.01	113.79	118.60
57	BA	1247	A	C5-C6-N1	8.01	121.71	117.70
57	BA	1398	C	N3-C2-O2	-8.01	116.29	121.90
57	BA	1039	A	C5-C6-N1	8.01	121.71	117.70
57	BA	1722	A	N1-C6-N6	-8.01	113.79	118.60
57	BA	2333	A	C5-C6-N1	8.01	121.71	117.70
22	AA	1303	C	N3-C2-O2	-8.01	116.29	121.90
57	BA	172	A	N1-C6-N6	-8.01	113.79	118.60
57	BA	204	A	C5-C6-N1	8.01	121.70	117.70
57	BA	2870	C	N3-C2-O2	-8.01	116.30	121.90
22	AA	1513	A	C5-C6-N1	8.01	121.70	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1403	A	C5-C6-N1	8.01	121.70	117.70
57	BA	2516	A	N1-C6-N6	-8.01	113.80	118.60
22	AA	60	A	N1-C6-N6	-8.00	113.80	118.60
22	AA	311	C	N3-C2-O2	-8.00	116.30	121.90
22	AA	624	C	N3-C2-O2	-8.00	116.30	121.90
57	BA	1153	C	N3-C2-O2	-8.00	116.30	121.90
57	BA	95	A	C5-C6-N1	8.00	121.70	117.70
24	A3	11	A	N1-C6-N6	-8.00	113.80	118.60
57	BA	2258	C	N3-C2-O2	-8.00	116.30	121.90
57	BA	156	A	N1-C6-N6	-8.00	113.80	118.60
57	BA	1010	A	C5-C6-N1	8.00	121.70	117.70
57	BA	705	A	C5-C6-N1	8.00	121.70	117.70
57	BA	1342	A	C5-C6-N1	8.00	121.70	117.70
57	BA	2134	A	C5-C6-N1	8.00	121.70	117.70
57	BA	2459	A	C5-C6-N1	8.00	121.70	117.70
57	BA	2851	A	C5-C6-N1	8.00	121.70	117.70
22	AA	1325	C	N3-C2-O2	-7.99	116.31	121.90
22	AA	1428	A	N1-C6-N6	-7.99	113.80	118.60
22	AA	430	A	C5-C6-N1	7.99	121.70	117.70
57	BA	1598	A	C5-C6-N1	7.99	121.70	117.70
22	AA	608	A	C5-C6-N1	7.99	121.69	117.70
22	AA	767	A	C5-C6-N1	7.99	121.69	117.70
57	BA	2679	A	C5-C6-N1	7.99	121.69	117.70
57	BA	1593	A	N1-C6-N6	-7.99	113.81	118.60
57	BA	257	C	O4'-C1'-N1	7.99	114.59	108.20
57	BA	1549	A	N1-C6-N6	-7.99	113.81	118.60
57	BA	2541	A	C5-C6-N1	7.99	121.69	117.70
57	BA	2573	C	O4'-C1'-N1	7.99	114.59	108.20
22	AA	430	A	N1-C6-N6	-7.99	113.81	118.60
22	AA	1502	A	C5-C6-N1	7.99	121.69	117.70
56	BL	123	ARG	NE-CZ-NH1	7.99	124.29	120.30
57	BA	960	A	C5-C6-N1	7.99	121.69	117.70
57	BA	2287	A	C5-C6-N1	7.99	121.69	117.70
57	BA	282	A	N1-C6-N6	-7.98	113.81	118.60
57	BA	2283	C	N3-C2-O2	-7.98	116.31	121.90
57	BA	2309	A	C5-C6-N1	7.98	121.69	117.70
57	BA	2450	A	C4-C5-C6	-7.98	113.01	117.00
22	AA	353	A	C5-C6-N1	7.98	121.69	117.70
57	BA	783	A	C5-C6-N1	7.98	121.69	117.70
57	BA	903	C	N3-C2-O2	-7.98	116.31	121.90
57	BA	2579	C	O4'-C1'-N1	7.98	114.58	108.20
57	BA	272	A	C5-C6-N1	7.98	121.69	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	441	A	N1-C6-N6	-7.98	113.81	118.60
22	AA	732	C	N3-C2-O2	-7.98	116.31	121.90
42	B0	10	ARG	NE-CZ-NH1	7.98	124.29	120.30
57	BA	896	A	O4'-C1'-N9	7.98	114.58	108.20
43	B1	49	ARG	NE-CZ-NH2	7.98	124.29	120.30
57	BA	2212	A	C5-C6-N1	7.98	121.69	117.70
22	AA	1542	A	O4'-C1'-N9	7.97	114.58	108.20
24	A3	41	C	N3-C2-O2	-7.97	116.32	121.90
57	BA	173	A	N1-C6-N6	-7.97	113.81	118.60
57	BA	531	C	N3-C2-O2	-7.97	116.32	121.90
57	BA	2101	A	C5-C6-N1	7.97	121.69	117.70
22	AA	1261	A	C5-C6-N1	7.97	121.69	117.70
57	BA	761	A	N1-C6-N6	-7.97	113.82	118.60
57	BA	2225	A	C4-C5-C6	-7.97	113.01	117.00
57	BA	1238	G	O4'-C1'-N9	7.97	114.58	108.20
57	BA	1640	A	C5-C6-N1	7.97	121.69	117.70
57	BA	1969	A	N1-C6-N6	-7.97	113.82	118.60
58	Ba	115	A	N1-C6-N6	-7.97	113.82	118.60
57	BA	1009	A	C5-C6-N1	7.97	121.68	117.70
22	AA	130	A	N1-C6-N6	-7.97	113.82	118.60
22	AA	495	A	C5-C6-N1	7.97	121.68	117.70
57	BA	812	C	O4'-C1'-N1	7.97	114.57	108.20
57	BA	2417	C	N3-C2-O2	-7.97	116.32	121.90
57	BA	1872	A	N1-C6-N6	-7.96	113.82	118.60
57	BA	2542	A	C5-C6-N1	7.96	121.68	117.70
22	AA	320	A	N1-C6-N6	-7.96	113.82	118.60
22	AA	233	C	N3-C2-O2	-7.96	116.33	121.90
23	A2	26	U	O4'-C1'-N1	7.96	114.57	108.20
57	BA	5	A	N1-C6-N6	-7.96	113.82	118.60
22	AA	1513	A	C4-C5-C6	-7.96	113.02	117.00
57	BA	2322	A	C5-C6-N1	7.96	121.68	117.70
57	BA	1507	C	N3-C2-O2	-7.96	116.33	121.90
22	AA	878	A	N1-C6-N6	-7.96	113.83	118.60
22	AA	1110	A	N1-C6-N6	-7.96	113.83	118.60
57	BA	2051	A	N1-C6-N6	-7.96	113.83	118.60
57	BA	2088	A	C5-C6-N1	7.96	121.68	117.70
22	AA	53	A	C5-C6-N1	7.95	121.68	117.70
22	AA	320	A	C5-C6-N1	7.95	121.68	117.70
22	AA	826	C	N3-C2-O2	-7.95	116.33	121.90
57	BA	752	A	C5-C6-N1	7.95	121.68	117.70
22	AA	1542	A	C5-C6-N1	7.95	121.67	117.70
57	BA	213	A	C5-C6-N1	7.95	121.67	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	515	A	N1-C6-N6	-7.95	113.83	118.60
57	BA	1000	A	C5-C6-N1	7.95	121.67	117.70
57	BA	1328	A	C5-C6-N1	7.95	121.68	117.70
57	BA	2088	A	N1-C6-N6	-7.95	113.83	118.60
57	BA	2497	A	C5-C6-N1	7.95	121.67	117.70
22	AA	119	A	C5-C6-N1	7.95	121.67	117.70
22	AA	475	C	N3-C2-O2	-7.95	116.34	121.90
22	AA	906	A	C5-C6-N1	7.95	121.67	117.70
57	BA	382	A	C5-C6-N1	7.95	121.67	117.70
57	BA	1900	A	C5-C6-N1	7.95	121.67	117.70
57	BA	722	A	N1-C6-N6	-7.95	113.83	118.60
57	BA	1970	A	N1-C6-N6	-7.95	113.83	118.60
57	BA	1966	A	C5-C6-N1	7.94	121.67	117.70
57	BA	2378	A	C5-C6-N1	7.94	121.67	117.70
22	AA	1081	A	N1-C6-N6	-7.94	113.83	118.60
57	BA	130	C	N3-C2-O2	-7.94	116.34	121.90
57	BA	342	A	C5-C6-N1	7.94	121.67	117.70
57	BA	602	A	C5-C6-N1	7.94	121.67	117.70
57	BA	1610	A	C5-C6-N1	7.94	121.67	117.70
9	AR	5	ARG	NE-CZ-NH1	7.94	124.27	120.30
22	AA	996	A	C5-C6-N1	7.94	121.67	117.70
57	BA	2412	A	C5-C6-N1	7.94	121.67	117.70
57	BA	2564	A	N1-C6-N6	-7.94	113.84	118.60
22	AA	1507	A	C5-C6-N1	7.94	121.67	117.70
22	AA	1004	A	C5-C6-N1	7.94	121.67	117.70
22	AA	1499	A	N1-C6-N6	-7.94	113.84	118.60
57	BA	1439	A	C5-C6-N1	7.94	121.67	117.70
58	Ba	29	A	C5-C6-N1	7.94	121.67	117.70
57	BA	2468	A	C5-C6-N1	7.94	121.67	117.70
57	BA	2507	C	N3-C2-O2	-7.94	116.34	121.90
57	BA	2602	A	C5-C6-N1	7.94	121.67	117.70
57	BA	2814	A	C5-C6-N1	7.94	121.67	117.70
22	AA	195	A	C5-C6-N1	7.93	121.67	117.70
22	AA	663	A	N1-C6-N6	-7.93	113.84	118.60
22	AA	253	A	C5-C6-N1	7.93	121.67	117.70
57	BA	251	A	N1-C6-N6	-7.93	113.84	118.60
57	BA	371	A	C5-C6-N1	7.93	121.67	117.70
57	BA	415	A	N1-C6-N6	-7.93	113.84	118.60
57	BA	821	A	C5-C6-N1	7.93	121.67	117.70
57	BA	972	A	C5-C6-N1	7.93	121.67	117.70
57	BA	1287	A	C5-C6-N1	7.93	121.67	117.70
57	BA	541	A	N1-C6-N6	-7.93	113.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1050	A	C5-C6-N1	7.93	121.67	117.70
57	BA	1827	U	O4'-C1'-N1	7.93	114.55	108.20
57	BA	1833	C	N3-C2-O2	-7.93	116.35	121.90
22	AA	968	A	C5-C6-N1	7.93	121.67	117.70
22	AA	1282	C	N3-C2-O2	-7.93	116.35	121.90
57	BA	191	A	C5-C6-N1	7.93	121.67	117.70
57	BA	2758	A	C5-C6-N1	7.93	121.67	117.70
22	AA	1492	A	C5-C6-N1	7.93	121.66	117.70
57	BA	1986	C	N3-C2-O2	-7.93	116.35	121.90
57	BA	654	A	C5-C6-N1	7.93	121.66	117.70
57	BA	1981	A	C5-C6-N1	7.93	121.66	117.70
57	BA	2214	C	N3-C2-O2	-7.93	116.35	121.90
4	AM	97	ARG	NE-CZ-NH1	7.92	124.26	120.30
21	A1	632	ARG	NE-CZ-NH1	7.92	124.26	120.30
22	AA	596	A	C5-C6-N1	7.92	121.66	117.70
22	AA	1261	A	N1-C6-N6	-7.92	113.85	118.60
57	BA	1755	A	C5-C6-N1	7.92	121.66	117.70
57	BA	2388	A	C5-C6-N1	7.92	121.66	117.70
22	AA	28	A	C5-C6-N1	7.92	121.66	117.70
57	BA	44	A	N1-C6-N6	-7.92	113.85	118.60
22	AA	175	C	N3-C2-O2	-7.92	116.36	121.90
22	AA	622	A	C4-C5-C6	-7.92	113.04	117.00
22	AA	743	A	C5-C6-N1	7.92	121.66	117.70
57	BA	207	A	C5-C6-N1	7.92	121.66	117.70
57	BA	2031	A	C5-C6-N1	7.92	121.66	117.70
22	AA	1069	C	N3-C2-O2	-7.92	116.36	121.90
57	BA	1264	A	C5-C6-N1	7.92	121.66	117.70
22	AA	749	A	C5-C6-N1	7.92	121.66	117.70
22	AA	857	C	N3-C2-O2	-7.92	116.36	121.90
22	AA	907	A	N1-C6-N6	-7.92	113.85	118.60
57	BA	1089	A	C5-C6-N1	7.92	121.66	117.70
22	AA	267	C	N3-C2-O2	-7.92	116.36	121.90
57	BA	1079	C	N3-C2-O2	-7.92	116.36	121.90
57	BA	1175	A	C5-C6-N1	7.92	121.66	117.70
57	BA	2823	A	C5-C6-N1	7.92	121.66	117.70
22	AA	815	A	C5-C6-N1	7.92	121.66	117.70
57	BA	526	A	C5-C6-N1	7.92	121.66	117.70
57	BA	2723	C	N3-C2-O2	-7.92	116.36	121.90
22	AA	358	U	O4'-C1'-N1	7.91	114.53	108.20
57	BA	988	A	C5-C6-N1	7.91	121.66	117.70
57	BA	2169	A	C5-C6-N1	7.91	121.66	117.70
22	AA	312	C	N3-C2-O2	-7.91	116.36	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	72	A	C5-C6-N1	7.91	121.66	117.70
22	AA	95	C	N3-C2-O2	-7.91	116.36	121.90
23	A2	27	A	O4'-C1'-N9	7.91	114.53	108.20
57	BA	430	A	C5-C6-N1	7.91	121.66	117.70
57	BA	699	A	C5-C6-N1	7.91	121.66	117.70
57	BA	1040	A	C5-C6-N1	7.91	121.66	117.70
22	AA	306	A	N1-C6-N6	-7.91	113.86	118.60
22	AA	398	U	O4'-C1'-N1	7.91	114.53	108.20
22	AA	610	U	N3-C2-O2	-7.91	116.66	122.20
22	AA	1146	A	C5-C6-N1	7.91	121.65	117.70
57	BA	1226	A	C5-C6-N1	7.91	121.65	117.70
57	BA	1614	A	C5-C6-N1	7.91	121.65	117.70
57	BA	1678	A	C5-C6-N1	7.91	121.65	117.70
57	BA	2590	A	C4-C5-C6	-7.91	113.05	117.00
22	AA	1503	A	N1-C6-N6	-7.91	113.86	118.60
22	AA	190	A	N1-C6-N6	-7.91	113.86	118.60
57	BA	1749	A	N1-C6-N6	-7.91	113.86	118.60
57	BA	2510	C	N3-C2-O2	-7.91	116.37	121.90
22	AA	559	A	C5-C6-N1	7.90	121.65	117.70
57	BA	368	A	C5-C6-N1	7.90	121.65	117.70
57	BA	1021	A	C5-C6-N1	7.90	121.65	117.70
57	BA	2052	A	N1-C6-N6	-7.90	113.86	118.60
57	BA	2711	A	C5-C6-N1	7.90	121.65	117.70
22	AA	1346	A	C4-C5-C6	-7.90	113.05	117.00
37	BV	90	ARG	NE-CZ-NH1	7.90	124.25	120.30
57	BA	1583	A	C5-C6-N1	7.90	121.65	117.70
57	BA	2005	A	C5-C6-N1	7.90	121.65	117.70
56	BL	97	ARG	NE-CZ-NH1	7.90	124.25	120.30
22	AA	176	C	N3-C2-O2	-7.90	116.37	121.90
22	AA	243	A	C5-C6-N1	7.90	121.65	117.70
57	BA	693	A	C5-C6-N1	7.90	121.65	117.70
57	BA	1134	A	C5-C6-N1	7.90	121.65	117.70
58	Ba	4	C	N3-C2-O2	-7.90	116.37	121.90
57	BA	1794	A	C5-C6-N1	7.90	121.65	117.70
22	AA	120	A	C5-C6-N1	7.89	121.65	117.70
22	AA	1289	A	C5-C6-N1	7.89	121.65	117.70
57	BA	1499	C	N3-C2-O2	-7.89	116.37	121.90
57	BA	323	C	N1-C2-O2	7.89	123.64	118.90
57	BA	503	A	C5-C6-N1	7.89	121.65	117.70
57	BA	825	A	C5-C6-N1	7.89	121.65	117.70
57	BA	863	A	C5-C6-N1	7.89	121.65	117.70
57	BA	2033	A	C5-C6-N1	7.89	121.65	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2094	A	C5-C6-N1	7.89	121.65	117.70
21	A1	228	ARG	NE-CZ-NH1	7.89	124.25	120.30
22	AA	792	A	C5-C6-N1	7.89	121.65	117.70
57	BA	1977	A	N1-C6-N6	-7.89	113.87	118.60
22	AA	373	A	C5-C6-N1	7.89	121.64	117.70
57	BA	718	A	O4'-C1'-N9	7.89	114.51	108.20
57	BA	1961	C	N3-C2-O2	-7.89	116.38	121.90
57	BA	2366	A	C5-C6-N1	7.89	121.64	117.70
22	AA	1503	A	C5-C6-N1	7.89	121.64	117.70
57	BA	144	A	N1-C6-N6	-7.89	113.87	118.60
57	BA	1387	A	C5-C6-N1	7.89	121.64	117.70
57	BA	829	A	C5-C6-N1	7.88	121.64	117.70
57	BA	1544	A	C5-C6-N1	7.88	121.64	117.70
57	BA	2170	A	C5-C6-N1	7.88	121.64	117.70
57	BA	2521	C	N3-C2-O2	-7.88	116.38	121.90
58	Ba	59	A	N1-C6-N6	-7.88	113.87	118.60
57	BA	671	C	N3-C2-O2	-7.88	116.38	121.90
57	BA	1169	A	N1-C6-N6	-7.88	113.87	118.60
57	BA	1639	C	O4'-C1'-N1	7.88	114.50	108.20
57	BA	1677	A	C5-C6-N1	7.88	121.64	117.70
57	BA	2439	A	C5-C6-N1	7.88	121.64	117.70
22	AA	546	A	N1-C6-N6	-7.88	113.87	118.60
22	AA	595	A	N1-C6-N6	-7.88	113.87	118.60
57	BA	1274	A	C5-C6-N1	7.88	121.64	117.70
57	BA	1328	A	N1-C6-N6	-7.88	113.87	118.60
57	BA	1575	C	N3-C2-O2	-7.88	116.38	121.90
57	BA	2579	C	N3-C2-O2	-7.88	116.38	121.90
57	BA	2771	C	N3-C2-O2	-7.88	116.38	121.90
22	AA	962	C	N3-C2-O2	-7.88	116.39	121.90
22	AA	1480	A	C5-C6-N1	7.88	121.64	117.70
57	BA	538	A	C5-C6-N1	7.88	121.64	117.70
57	BA	2001	C	N3-C2-O2	-7.88	116.39	121.90
57	BA	2347	C	N3-C2-O2	-7.88	116.39	121.90
57	BA	2611	C	N3-C2-O2	-7.88	116.39	121.90
23	A2	16	A	C5-C6-N1	7.88	121.64	117.70
57	BA	1244	A	C5-C6-N1	7.88	121.64	117.70
58	Ba	88	C	N3-C2-O2	-7.88	116.39	121.90
22	AA	73	C	N3-C2-O2	-7.88	116.39	121.90
57	BA	225	C	N3-C2-O2	-7.88	116.39	121.90
57	BA	1237	A	C5-C6-N1	7.88	121.64	117.70
22	AA	131	A	O4'-C1'-N9	7.87	114.50	108.20
22	AA	600	A	C5-C6-N1	7.87	121.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A1	590	ARG	NE-CZ-NH1	7.87	124.23	120.30
22	AA	178	C	N3-C2-O2	-7.87	116.39	121.90
57	BA	394	C	N3-C2-O2	-7.87	116.39	121.90
57	BA	1528	A	C5-C6-N1	7.87	121.64	117.70
57	BA	2427	C	N3-C2-O2	-7.87	116.39	121.90
58	Ba	39	A	C5-C6-N1	7.87	121.63	117.70
57	BA	2813	A	C5-C6-N1	7.87	121.63	117.70
57	BA	2266	A	C4-C5-C6	-7.87	113.07	117.00
43	B1	26	ARG	NE-CZ-NH1	7.86	124.23	120.30
55	BH	94	ARG	NE-CZ-NH1	7.86	124.23	120.30
57	BA	269	C	N3-C2-O2	-7.86	116.39	121.90
22	AA	412	A	C5-C6-N1	7.86	121.63	117.70
54	BG	101	ARG	NE-CZ-NH2	7.86	124.23	120.30
57	BA	689	A	C5-C6-N1	7.86	121.63	117.70
57	BA	990	A	C5-C6-N1	7.86	121.63	117.70
22	AA	630	A	C5-C6-N1	7.86	121.63	117.70
57	BA	227	A	C4-C5-C6	-7.86	113.07	117.00
57	BA	1090	A	N1-C6-N6	-7.86	113.89	118.60
22	AA	395	C	N3-C2-O2	-7.86	116.40	121.90
22	AA	1299	A	C5-C6-N1	7.86	121.63	117.70
22	AA	1508	A	C5-C6-N1	7.86	121.63	117.70
57	BA	53	A	C5-C6-N1	7.86	121.63	117.70
58	Ba	25	U	O4'-C1'-N1	7.86	114.49	108.20
2	AK	126	ARG	NE-CZ-NH2	-7.86	116.37	120.30
22	AA	174	A	C5-C6-N1	7.86	121.63	117.70
22	AA	865	A	N1-C6-N6	-7.86	113.89	118.60
22	AA	1169	A	C5-C6-N1	7.86	121.63	117.70
57	BA	63	A	C5-C6-N1	7.85	121.63	117.70
22	AA	536	C	N3-C2-O2	-7.85	116.40	121.90
26	BJ	45	ARG	NE-CZ-NH1	7.85	124.23	120.30
57	BA	998	C	N3-C2-O2	-7.85	116.40	121.90
57	BA	1308	A	C5-C6-N1	7.85	121.63	117.70
57	BA	2717	C	N3-C2-O2	-7.85	116.40	121.90
57	BA	412	A	C5-C6-N1	7.85	121.63	117.70
57	BA	1591	A	N1-C6-N6	-7.85	113.89	118.60
57	BA	2215	C	N3-C2-O2	-7.85	116.40	121.90
22	AA	1005	A	C5-C6-N1	7.85	121.62	117.70
23	A2	16	A	O4'-C1'-N9	7.85	114.48	108.20
23	A2	59	A	C5-C6-N1	7.85	121.62	117.70
54	BG	109	ARG	NE-CZ-NH2	7.85	124.22	120.30
57	BA	1772	A	C5-C6-N1	7.85	121.62	117.70
22	AA	1114	C	N3-C2-O2	-7.85	116.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1286	A	C5-C6-N1	7.85	121.62	117.70
58	Ba	78	A	C4-C5-C6	-7.85	113.08	117.00
57	BA	1453	A	C5-C6-N1	7.85	121.62	117.70
18	AG	94	ARG	NE-CZ-NH1	7.84	124.22	120.30
57	BA	2147	A	N1-C6-N6	-7.84	113.89	118.60
24	A3	16	C	N1-C2-O2	7.84	123.61	118.90
57	BA	1564	C	N3-C2-O2	-7.84	116.41	121.90
22	AA	607	A	C5-C6-N1	7.84	121.62	117.70
22	AA	1118	U	C5'-C4'-C3'	-7.84	103.45	116.00
57	BA	1634	A	N1-C6-N6	-7.84	113.89	118.60
57	BA	487	C	N3-C2-O2	-7.84	116.41	121.90
57	BA	2620	C	N3-C2-O2	-7.84	116.41	121.90
18	AG	69	ARG	NE-CZ-NH1	7.84	124.22	120.30
22	AA	872	A	O4'-C1'-N9	7.84	114.47	108.20
57	BA	900	A	C5-C6-N1	7.84	121.62	117.70
22	AA	308	C	N3-C2-O2	-7.83	116.42	121.90
57	BA	141	G	O4'-C1'-N9	7.83	114.47	108.20
22	AA	274	A	C5-C6-N1	7.83	121.62	117.70
57	BA	94	A	C5-C6-N1	7.83	121.62	117.70
57	BA	522	A	N1-C6-N6	-7.83	113.90	118.60
57	BA	706	A	N1-C6-N6	-7.83	113.90	118.60
22	AA	1035	A	C5-C6-N1	7.83	121.62	117.70
43	B1	36	ARG	NE-CZ-NH2	7.83	124.22	120.30
57	BA	300	A	C5-C6-N1	7.83	121.62	117.70
22	AA	382	A	C5-C6-N1	7.83	121.61	117.70
57	BA	483	A	N1-C6-N6	-7.83	113.90	118.60
57	BA	2899	A	C5-C6-N1	7.83	121.61	117.70
15	AD	153	ARG	NE-CZ-NH1	7.83	124.21	120.30
22	AA	864	A	C5-C6-N1	7.83	121.61	117.70
22	AA	149	A	C5-C6-N1	7.83	121.61	117.70
22	AA	583	A	C5-C6-N1	7.83	121.61	117.70
22	AA	1163	A	C5-C6-N1	7.83	121.61	117.70
57	BA	574	A	C5-C6-N1	7.83	121.61	117.70
57	BA	987	C	N3-C2-O2	-7.83	116.42	121.90
57	BA	2448	A	C5-C6-N1	7.83	121.61	117.70
22	AA	1141	C	N3-C2-O2	-7.82	116.42	121.90
57	BA	2632	A	C5-C6-N1	7.82	121.61	117.70
23	A2	17	U	O4'-C1'-N1	7.82	114.46	108.20
57	BA	944	C	O4'-C1'-N1	7.82	114.46	108.20
57	BA	2122	U	O4'-C1'-N1	7.82	114.46	108.20
22	AA	840	C	N3-C2-O2	-7.82	116.43	121.90
22	AA	1394	A	C5-C6-N1	7.82	121.61	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	181	A	C5-C6-N1	7.82	121.61	117.70
57	BA	1801	A	C5-C6-N1	7.82	121.61	117.70
57	BA	1336	A	C5-C6-N1	7.82	121.61	117.70
57	BA	2060	A	C5-C6-N1	7.82	121.61	117.70
57	BA	2443	C	N3-C2-O2	-7.82	116.43	121.90
22	AA	284	C	N3-C2-O2	-7.82	116.43	121.90
57	BA	203	A	N1-C6-N6	-7.82	113.91	118.60
57	BA	2547	A	N1-C6-N6	-7.82	113.91	118.60
22	AA	706	A	C5-C6-N1	7.81	121.61	117.70
57	BA	873	C	N3-C2-O2	-7.81	116.43	121.90
57	BA	2009	A	N1-C6-N6	-7.81	113.91	118.60
22	AA	546	A	C5-C6-N1	7.81	121.61	117.70
58	Ba	90	C	N3-C2-O2	-7.81	116.43	121.90
57	BA	1382	G	O4'-C1'-N9	7.81	114.45	108.20
22	AA	66	A	C5-C6-N1	7.81	121.61	117.70
22	AA	1322	C	N1-C2-O2	7.81	123.58	118.90
57	BA	210	C	N3-C2-O2	-7.81	116.43	121.90
57	BA	1273	U	O4'-C1'-N1	7.81	114.45	108.20
57	BA	1569	A	C4-C5-C6	-7.81	113.09	117.00
2	AK	55	ARG	NE-CZ-NH1	7.81	124.20	120.30
22	AA	704	A	C4-C5-C6	-7.81	113.10	117.00
57	BA	1732	C	N3-C2-O2	-7.81	116.44	121.90
22	AA	1446	A	C5-C6-N1	7.81	121.60	117.70
57	BA	497	A	C5-C6-N1	7.81	121.60	117.70
57	BA	104	A	C5-C6-N1	7.80	121.60	117.70
57	BA	2773	C	N3-C2-O2	-7.80	116.44	121.90
22	AA	236	A	C5-C6-N1	7.80	121.60	117.70
29	BO	98	ARG	NE-CZ-NH1	7.80	124.20	120.30
22	AA	1296	C	N3-C2-O2	-7.80	116.44	121.90
57	BA	1365	A	C5-C6-N1	7.80	121.60	117.70
22	AA	1501	C	N3-C2-O2	-7.80	116.44	121.90
58	Ba	93	C	N3-C2-O2	-7.80	116.44	121.90
22	AA	675	A	C5-C6-N1	7.80	121.60	117.70
22	AA	998	C	N3-C2-O2	-7.80	116.44	121.90
57	BA	2366	A	N1-C6-N6	-7.80	113.92	118.60
22	AA	1251	A	N1-C6-N6	-7.80	113.92	118.60
57	BA	161	A	C5-C6-N1	7.80	121.60	117.70
57	BA	627	A	N1-C6-N6	-7.80	113.92	118.60
57	BA	740	C	N3-C2-O2	-7.79	116.44	121.90
57	BA	742	A	N1-C6-N6	-7.79	113.92	118.60
57	BA	814	C	N3-C2-O2	-7.79	116.44	121.90
57	BA	1029	A	N1-C6-N6	-7.79	113.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	511	C	N3-C2-O2	-7.79	116.45	121.90
57	BA	270	A	C5-C6-N1	7.79	121.60	117.70
57	BA	482	A	N1-C6-N6	-7.79	113.92	118.60
23	A2	13	A	C5-C6-N1	7.79	121.59	117.70
57	BA	1305	C	O4'-C1'-N1	7.79	114.43	108.20
57	BA	14	A	C5-C6-N1	7.79	121.59	117.70
57	BA	1552	A	C5-C6-N1	7.79	121.59	117.70
57	BA	1605	C	N3-C2-O2	-7.79	116.45	121.90
57	BA	1638	C	N3-C2-O2	-7.79	116.45	121.90
22	AA	1042	A	C5-C6-N1	7.79	121.59	117.70
22	AA	1520	C	N3-C2-O2	-7.79	116.45	121.90
22	AA	1524	C	N3-C2-O2	-7.79	116.45	121.90
22	AA	329	A	N1-C6-N6	-7.79	113.93	118.60
57	BA	1890	A	C5-C6-N1	7.79	121.59	117.70
57	BA	2416	C	N3-C2-O2	-7.79	116.45	121.90
22	AA	152	A	C4-C5-C6	-7.78	113.11	117.00
22	AA	448	A	C5-C6-N1	7.78	121.59	117.70
24	A3	75	C	N3-C2-O2	-7.78	116.45	121.90
57	BA	262	A	C5-C6-N1	7.78	121.59	117.70
57	BA	623	C	N3-C2-O2	-7.78	116.45	121.90
57	BA	761	A	C5-C6-N1	7.78	121.59	117.70
57	BA	1596	A	C5-C6-N1	7.78	121.59	117.70
58	Ba	50	A	C5-C6-N1	7.78	121.59	117.70
22	AA	432	A	C5-C6-N1	7.78	121.59	117.70
22	AA	845	A	C5-C6-N1	7.78	121.59	117.70
22	AA	969	A	C5-C6-N1	7.78	121.59	117.70
22	AA	1036	A	C5-C6-N1	7.78	121.59	117.70
57	BA	1938	A	C5-C6-N1	7.78	121.59	117.70
22	AA	143	A	N1-C6-N6	-7.78	113.93	118.60
22	AA	163	C	N3-C2-O2	-7.78	116.46	121.90
57	BA	614	A	C5-C6-N1	7.78	121.59	117.70
57	BA	2565	A	C5-C6-N1	7.78	121.59	117.70
57	BA	2761	A	C5-C6-N1	7.78	121.59	117.70
21	A1	622	ARG	NE-CZ-NH1	7.78	124.19	120.30
57	BA	666	A	C5-C6-N1	7.78	121.59	117.70
57	BA	1054	A	N1-C6-N6	-7.78	113.94	118.60
58	Ba	66	A	N1-C6-N6	-7.78	113.93	118.60
22	AA	466	A	C5-C6-N1	7.77	121.59	117.70
22	AA	913	A	C5-C6-N1	7.77	121.59	117.70
22	AA	1418	A	N1-C6-N6	-7.77	113.94	118.60
22	AA	1443	C	N3-C2-O2	-7.77	116.46	121.90
57	BA	1151	A	N1-C6-N6	-7.77	113.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1578	U	O4'-C1'-N1	7.77	114.42	108.20
57	BA	2207	C	N3-C2-O2	-7.77	116.46	121.90
22	AA	873	A	C5-C6-N1	7.77	121.58	117.70
57	BA	2095	A	C5-C6-N1	7.77	121.59	117.70
22	AA	510	A	C5-C6-N1	7.77	121.58	117.70
24	A3	73	A	C5-C6-N1	7.77	121.58	117.70
57	BA	986	C	N3-C2-O2	-7.77	116.46	121.90
57	BA	1794	A	N1-C6-N6	-7.77	113.94	118.60
57	BA	1808	A	C5-C6-N1	7.77	121.58	117.70
22	AA	994	A	N1-C6-N6	-7.77	113.94	118.60
57	BA	1745	A	C5-C6-N1	7.77	121.58	117.70
22	AA	1496	C	N3-C2-O2	-7.76	116.46	121.90
26	BJ	152	ARG	NE-CZ-NH1	7.76	124.18	120.30
57	BA	428	A	C5-C6-N1	7.76	121.58	117.70
57	BA	575	A	C4-C5-C6	-7.76	113.12	117.00
57	BA	846	U	O4'-C1'-N1	7.76	114.41	108.20
57	BA	1502	A	C5-C6-N1	7.76	121.58	117.70
22	AA	492	C	N3-C2-O2	-7.76	116.47	121.90
57	BA	1254	A	C5-C6-N1	7.76	121.58	117.70
57	BA	1354	A	C5-C6-N1	7.76	121.58	117.70
57	BA	1970	A	C5-C6-N1	7.76	121.58	117.70
57	BA	2475	C	N3-C2-O2	-7.76	116.47	121.90
22	AA	44	A	N1-C6-N6	-7.76	113.94	118.60
22	AA	279	A	C5-C6-N1	7.76	121.58	117.70
57	BA	1321	A	C5-C6-N1	7.76	121.58	117.70
57	BA	1632	A	C5-C6-N1	7.76	121.58	117.70
58	Ba	46	A	C5-C6-N1	7.76	121.58	117.70
57	BA	676	A	C5-C6-N1	7.76	121.58	117.70
57	BA	1032	A	N1-C6-N6	-7.76	113.94	118.60
57	BA	1967	C	N3-C2-O2	-7.76	116.47	121.90
57	BA	2346	A	C5-C6-N1	7.76	121.58	117.70
57	BA	2665	A	N1-C6-N6	-7.76	113.94	118.60
57	BA	739	A	C5-C6-N1	7.76	121.58	117.70
57	BA	2008	C	O4'-C1'-N1	7.76	114.41	108.20
22	AA	139	A	C5-C6-N1	7.76	121.58	117.70
22	AA	643	C	N3-C2-O2	-7.76	116.47	121.90
57	BA	227	A	C5-C6-N1	7.76	121.58	117.70
57	BA	995	C	N3-C2-O2	-7.76	116.47	121.90
57	BA	2307	G	O4'-C1'-N9	7.76	114.41	108.20
57	BA	1885	A	N1-C6-N6	-7.75	113.95	118.60
22	AA	1219	A	N1-C6-N6	-7.75	113.95	118.60
57	BA	190	A	C5-C6-N1	7.75	121.58	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2725	A	N1-C6-N6	-7.75	113.95	118.60
25	BC	12	ARG	NE-CZ-NH1	7.75	124.17	120.30
57	BA	1876	A	C5-C6-N1	7.75	121.58	117.70
22	AA	1252	A	C5-C6-N1	7.75	121.58	117.70
23	A2	41	A	C5-C6-N1	7.75	121.58	117.70
57	BA	1092	C	N3-C2-O2	-7.75	116.47	121.90
57	BA	1508	A	C5-C6-N1	7.75	121.58	117.70
57	BA	1553	A	C5-C6-N1	7.75	121.58	117.70
57	BA	1773	A	C5-C6-N1	7.75	121.58	117.70
24	A3	59	A	C5-C6-N1	7.75	121.58	117.70
57	BA	608	A	C5-C6-N1	7.75	121.57	117.70
57	BA	947	A	N1-C6-N6	-7.75	113.95	118.60
57	BA	1509	A	C5-C6-N1	7.75	121.57	117.70
19	AH	76	ARG	NE-CZ-NH1	7.75	124.17	120.30
57	BA	144	A	C5-C6-N1	7.75	121.57	117.70
22	AA	123	U	O4'-C1'-N1	7.75	114.40	108.20
57	BA	2222	C	N3-C2-O2	-7.75	116.48	121.90
24	A3	70	C	N3-C2-O2	-7.74	116.48	121.90
50	B7	19	ARG	NE-CZ-NH2	7.74	124.17	120.30
57	BA	724	U	O4'-C1'-N1	7.74	114.40	108.20
57	BA	2014	A	C5-C6-N1	7.74	121.57	117.70
22	AA	167	A	C5-C6-N1	7.74	121.57	117.70
57	BA	299	A	C5-C6-N1	7.74	121.57	117.70
57	BA	195	A	C5-C6-N1	7.74	121.57	117.70
57	BA	1936	A	C5-C6-N1	7.74	121.57	117.70
57	BA	2661	G	O4'-C1'-N9	7.74	114.39	108.20
57	BA	2873	A	O4'-C1'-N9	7.74	114.39	108.20
57	BA	2873	A	C5-C6-N1	7.74	121.57	117.70
22	AA	1059	C	N3-C2-O2	-7.74	116.48	121.90
22	AA	802	A	C5-C6-N1	7.74	121.57	117.70
22	AA	1229	A	C5-C6-N1	7.74	121.57	117.70
24	A3	13	C	N3-C2-O2	-7.74	116.48	121.90
57	BA	2856	A	C5-C6-N1	7.74	121.57	117.70
22	AA	901	A	C5-C6-N1	7.74	121.57	117.70
22	AA	1132	C	N3-C2-O2	-7.74	116.48	121.90
22	AA	1201	A	C5-C6-N1	7.74	121.57	117.70
22	AA	1493	A	C5-C6-N1	7.74	121.57	117.70
24	A3	60	A	C5-C6-N1	7.74	121.57	117.70
24	A3	72	C	N3-C2-O2	-7.74	116.48	121.90
57	BA	179	C	N3-C2-O2	-7.74	116.48	121.90
57	BA	482	A	C5-C6-N1	7.74	121.57	117.70
57	BA	996	A	N1-C6-N6	-7.74	113.96	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1118	C	N3-C2-O2	-7.74	116.48	121.90
57	BA	1133	A	C4-C5-C6	-7.74	113.13	117.00
57	BA	2406	A	C5-C6-N1	7.74	121.57	117.70
57	BA	2736	A	C5-C6-N1	7.74	121.57	117.70
24	A3	45	A	C5-C6-N1	7.73	121.57	117.70
57	BA	820	A	C5-C6-N1	7.73	121.57	117.70
22	AA	841	C	N3-C2-O2	-7.73	116.49	121.90
22	AA	1408	A	C5-C6-N1	7.73	121.57	117.70
57	BA	422	A	C5-C6-N1	7.73	121.57	117.70
57	BA	693	A	N1-C6-N6	-7.73	113.96	118.60
57	BA	921	C	N3-C2-O2	-7.73	116.49	121.90
57	BA	1156	A	C5-C6-N1	7.73	121.57	117.70
57	BA	1264	A	N1-C6-N6	-7.73	113.96	118.60
57	BA	6	A	N1-C6-N6	-7.73	113.96	118.60
22	AA	819	A	C5-C6-N1	7.73	121.56	117.70
57	BA	817	C	N3-C2-O2	-7.73	116.49	121.90
24	A3	39	A	C5-C6-N1	7.73	121.56	117.70
57	BA	362	A	C5-C6-N1	7.73	121.56	117.70
57	BA	453	A	C5-C6-N1	7.73	121.56	117.70
22	AA	52	C	N3-C2-O2	-7.73	116.49	121.90
22	AA	1465	A	C5-C6-N1	7.73	121.56	117.70
22	AA	514	C	N3-C2-O2	-7.72	116.49	121.90
57	BA	219	A	C5-C6-N1	7.72	121.56	117.70
22	AA	655	A	N1-C6-N6	-7.72	113.97	118.60
30	BP	59	ARG	NE-CZ-NH1	7.72	124.16	120.30
22	AA	1082	A	N1-C6-N6	-7.72	113.97	118.60
24	A3	47	A	C5-C6-N1	7.72	121.56	117.70
57	BA	84	A	C5-C6-N1	7.72	121.56	117.70
22	AA	7	A	C5-C6-N1	7.72	121.56	117.70
22	AA	223	A	C5-C6-N1	7.72	121.56	117.70
22	AA	418	C	N3-C2-O2	-7.72	116.50	121.90
22	AA	477	C	N3-C2-O2	-7.72	116.50	121.90
22	AA	286	C	N3-C2-O2	-7.71	116.50	121.90
22	AA	419	C	N3-C2-O2	-7.71	116.50	121.90
22	AA	1314	C	N3-C2-O2	-7.71	116.50	121.90
24	A3	1	C	O4'-C1'-N1	7.71	114.37	108.20
24	A3	44	A	C5-C6-N1	7.71	121.56	117.70
57	BA	848	C	N3-C2-O2	-7.71	116.50	121.90
22	AA	1479	C	N3-C2-O2	-7.71	116.50	121.90
57	BA	316	C	N3-C2-O2	-7.71	116.50	121.90
57	BA	2160	C	N3-C2-O2	-7.71	116.50	121.90
57	BA	1241	A	C5-C6-N1	7.71	121.56	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1323	C	O4'-C1'-N1	7.71	114.37	108.20
57	BA	2740	A	C5-C6-N1	7.71	121.56	117.70
24	A3	58	A	C5-C6-N1	7.71	121.56	117.70
22	AA	78	A	C5-C6-N1	7.71	121.55	117.70
22	AA	1218	C	N3-C2-O2	-7.71	116.50	121.90
22	AA	1389	C	N3-C2-O2	-7.71	116.50	121.90
57	BA	255	A	N1-C6-N6	-7.71	113.97	118.60
57	BA	790	U	N3-C2-O2	-7.71	116.80	122.20
22	AA	478	A	N1-C6-N6	-7.71	113.98	118.60
22	AA	595	A	C5-C6-N1	7.71	121.55	117.70
22	AA	1105	A	C5-C6-N1	7.71	121.55	117.70
22	AA	1362	A	C5-C6-N1	7.71	121.55	117.70
57	BA	479	A	C5-C6-N1	7.71	121.55	117.70
57	BA	816	C	N3-C2-O2	-7.71	116.51	121.90
57	BA	532	A	C5-C6-N1	7.71	121.55	117.70
57	BA	2707	U	O4'-C1'-N1	7.71	114.36	108.20
57	BA	118	A	C5-C6-N1	7.70	121.55	117.70
57	BA	1535	A	C5-C6-N1	7.70	121.55	117.70
57	BA	2176	A	C5-C6-N1	7.70	121.55	117.70
57	BA	2547	A	C5-C6-N1	7.70	121.55	117.70
22	AA	919	A	C5-C6-N1	7.70	121.55	117.70
22	AA	1038	C	N3-C2-O2	-7.70	116.51	121.90
22	AA	1256	A	C5-C6-N1	7.70	121.55	117.70
44	B2	52	ARG	NE-CZ-NH2	7.70	124.15	120.30
57	BA	443	A	C5-C6-N1	7.70	121.55	117.70
57	BA	547	A	C5-C6-N1	7.70	121.55	117.70
57	BA	1013	C	N3-C2-O2	-7.70	116.51	121.90
57	BA	1454	C	N1-C2-O2	7.70	123.52	118.90
57	BA	1746	A	C5-C6-N1	7.70	121.55	117.70
57	BA	2772	C	N3-C2-O2	-7.70	116.51	121.90
22	AA	414	A	C5-C6-N1	7.70	121.55	117.70
22	AA	441	A	C5-C6-N1	7.70	121.55	117.70
23	A2	55	A	C5-C6-N1	7.70	121.55	117.70
57	BA	1420	A	C5-C6-N1	7.70	121.55	117.70
57	BA	1270	C	N3-C2-O2	-7.70	116.51	121.90
22	AA	1148	U	O4'-C1'-N1	7.70	114.36	108.20
57	BA	2496	C	N3-C2-O2	-7.70	116.51	121.90
11	AB	20	ARG	NE-CZ-NH1	7.69	124.15	120.30
22	AA	907	A	C5-C6-N1	7.69	121.55	117.70
57	BA	2820	A	N1-C6-N6	-7.69	113.98	118.60
22	AA	574	A	C4-C5-C6	-7.69	113.16	117.00
57	BA	156	A	C5-C6-N1	7.69	121.54	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	927	A	C5-C6-N1	7.69	121.54	117.70
57	BA	1221	C	N3-C2-O2	-7.69	116.52	121.90
57	BA	1630	A	C5-C6-N1	7.69	121.54	117.70
57	BA	2675	A	C5-C6-N1	7.69	121.54	117.70
1	AJ	9	ARG	NE-CZ-NH1	7.69	124.14	120.30
22	AA	522	C	N3-C2-O2	-7.69	116.52	121.90
57	BA	2364	C	N3-C2-O2	-7.69	116.52	121.90
58	Ba	31	C	N3-C2-O2	-7.69	116.52	121.90
22	AA	503	C	N3-C2-O2	-7.68	116.52	121.90
22	AA	535	A	C5-C6-N1	7.68	121.54	117.70
22	AA	1067	A	C4-C5-C6	-7.68	113.16	117.00
22	AA	1170	A	C5-C6-N1	7.68	121.54	117.70
22	AA	816	A	C5-C6-N1	7.68	121.54	117.70
57	BA	1127	A	C5-C6-N1	7.68	121.54	117.70
57	BA	1155	A	C4-C5-C6	-7.68	113.16	117.00
57	BA	246	C	N3-C2-O2	-7.68	116.52	121.90
22	AA	790	A	C5-C6-N1	7.68	121.54	117.70
57	BA	348	A	C5-C6-N1	7.68	121.54	117.70
57	BA	1541	C	N3-C2-O2	-7.68	116.53	121.90
57	BA	2037	A	N1-C6-N6	-7.68	113.99	118.60
57	BA	2301	C	N3-C2-O2	-7.68	116.53	121.90
22	AA	8	A	C5-C6-N1	7.68	121.54	117.70
57	BA	1561	C	N3-C2-O2	-7.68	116.53	121.90
57	BA	2066	C	N3-C2-O2	-7.68	116.53	121.90
57	BA	2278	A	C4-C5-C6	-7.68	113.16	117.00
22	AA	706	A	N1-C6-N6	-7.68	113.99	118.60
57	BA	1864	U	O4'-C1'-N1	7.68	114.34	108.20
57	BA	2456	C	N3-C2-O2	-7.68	116.53	121.90
57	BA	2591	C	N3-C2-O2	-7.68	116.53	121.90
57	BA	2598	A	C5-C6-N1	7.68	121.54	117.70
22	AA	923	A	C5-C6-N1	7.67	121.54	117.70
22	AA	1500	A	C5-C6-N1	7.67	121.54	117.70
24	A3	45	A	N1-C6-N6	-7.67	114.00	118.60
57	BA	404	A	C5-C6-N1	7.67	121.54	117.70
57	BA	716	A	C5-C6-N1	7.67	121.54	117.70
57	BA	2163	A	C5-C6-N1	7.67	121.54	117.70
57	BA	2540	C	N3-C2-O2	-7.67	116.53	121.90
58	Ba	11	C	O4'-C1'-N1	7.67	114.34	108.20
58	Ba	60	C	N3-C2-O2	-7.67	116.53	121.90
57	BA	877	A	C5-C6-N1	7.67	121.54	117.70
57	BA	2298	A	N1-C6-N6	-7.67	114.00	118.60
22	AA	556	C	N3-C2-O2	-7.67	116.53	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	528	A	C5-C6-N1	7.67	121.54	117.70
57	BA	2458	G	O4'-C1'-N9	7.67	114.34	108.20
58	Ba	94	A	C5-C6-N1	7.67	121.54	117.70
22	AA	190	A	C5-C6-N1	7.67	121.53	117.70
22	AA	1328	C	N3-C2-O2	-7.67	116.53	121.90
10	AS	35	ARG	NE-CZ-NH1	7.67	124.13	120.30
22	AA	1019	A	C5-C6-N1	7.67	121.53	117.70
22	AA	1466	C	N3-C2-O2	-7.67	116.53	121.90
57	BA	781	A	C5-C6-N1	7.67	121.53	117.70
57	BA	2114	A	C5-C6-N1	7.67	121.53	117.70
22	AA	523	A	C4-C5-C6	-7.67	113.17	117.00
22	AA	1199	U	O4'-C1'-N1	7.67	114.33	108.20
22	AA	1237	C	O4'-C1'-N1	7.67	114.33	108.20
57	BA	432	A	C5-C6-N1	7.67	121.53	117.70
57	BA	928	A	C5-C6-N1	7.67	121.53	117.70
57	BA	2403	C	N3-C2-O2	-7.67	116.53	121.90
57	BA	2572	A	C5-C6-N1	7.67	121.53	117.70
57	BA	1462	C	N3-C2-O2	-7.67	116.53	121.90
58	Ba	52	A	C5-C6-N1	7.67	121.53	117.70
21	A1	110	ARG	NE-CZ-NH1	7.66	124.13	120.30
22	AA	452	A	C5-C6-N1	7.66	121.53	117.70
57	BA	749	A	C5-C6-N1	7.66	121.53	117.70
57	BA	2741	A	C5-C6-N1	7.66	121.53	117.70
22	AA	451	A	C5-C6-N1	7.66	121.53	117.70
22	AA	1369	C	N3-C2-O2	-7.66	116.54	121.90
32	BR	90	ARG	NE-CZ-NH1	7.66	124.13	120.30
43	B1	27	ARG	NE-CZ-NH1	7.66	124.13	120.30
22	AA	25	C	N3-C2-O2	-7.66	116.54	121.90
22	AA	554	A	C5-C6-N1	7.66	121.53	117.70
22	AA	580	C	N3-C2-O2	-7.66	116.54	121.90
55	BH	2	ARG	NE-CZ-NH2	7.66	124.13	120.30
57	BA	1126	A	C5-C6-N1	7.66	121.53	117.70
57	BA	2045	C	N3-C2-O2	-7.66	116.54	121.90
57	BA	2267	A	C5-C6-N1	7.66	121.53	117.70
22	AA	344	A	C5-C6-N1	7.66	121.53	117.70
57	BA	1877	A	C5-C6-N1	7.66	121.53	117.70
22	AA	1317	C	N3-C4-C5	7.65	124.96	121.90
57	BA	563	A	C5-C6-N1	7.65	121.53	117.70
57	BA	2749	A	C5-C6-N1	7.65	121.53	117.70
22	AA	1398	A	C5-C6-N1	7.65	121.53	117.70
24	A3	22	A	C5-C6-N1	7.65	121.53	117.70
57	BA	1417	C	N3-C2-O2	-7.65	116.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	897	C	N3-C2-O2	-7.65	116.55	121.90
57	BA	504	A	C5-C6-N1	7.65	121.53	117.70
57	BA	1943	U	N3-C2-O2	-7.65	116.84	122.20
57	BA	155	A	C5-C6-N1	7.65	121.52	117.70
57	BA	878	A	C5-C6-N1	7.65	121.52	117.70
57	BA	1853	A	C4-C5-C6	-7.65	113.17	117.00
57	BA	756	A	C5-C6-N1	7.65	121.52	117.70
57	BA	984	A	C5-C6-N1	7.65	121.52	117.70
22	AA	274	A	C4-C5-C6	-7.65	113.18	117.00
57	BA	1741	C	N3-C2-O2	-7.65	116.55	121.90
22	AA	779	C	N3-C2-O2	-7.64	116.55	121.90
57	BA	1383	A	C5-C6-N1	7.64	121.52	117.70
57	BA	1772	A	N1-C6-N6	-7.64	114.01	118.60
57	BA	2147	A	C5-C6-N1	7.64	121.52	117.70
22	AA	228	A	C5-C6-N1	7.64	121.52	117.70
22	AA	456	A	C5-C6-N1	7.64	121.52	117.70
22	AA	918	A	C5-C6-N1	7.64	121.52	117.70
43	B1	17	ARG	NE-CZ-NH2	7.64	124.12	120.30
57	BA	160	A	C5-C6-N1	7.64	121.52	117.70
57	BA	2020	A	C5-C6-N1	7.64	121.52	117.70
22	AA	937	A	C5-C6-N1	7.64	121.52	117.70
57	BA	1686	C	N3-C2-O2	-7.64	116.55	121.90
22	AA	136	C	N3-C2-O2	-7.64	116.55	121.90
22	AA	794	A	C5-C6-N1	7.64	121.52	117.70
57	BA	1077	A	C5-C6-N1	7.64	121.52	117.70
57	BA	1140	C	N3-C2-O2	-7.64	116.55	121.90
57	BA	2191	A	C5-C6-N1	7.64	121.52	117.70
57	BA	2860	A	C5-C6-N1	7.64	121.52	117.70
22	AA	181	A	C5-C6-N1	7.64	121.52	117.70
22	AA	1055	A	C5-C6-N1	7.64	121.52	117.70
22	AA	1234	C	N3-C2-O2	-7.64	116.55	121.90
57	BA	346	A	N1-C6-N6	-7.64	114.02	118.60
57	BA	672	C	N3-C2-O2	-7.64	116.55	121.90
57	BA	1272	A	N1-C6-N6	-7.64	114.02	118.60
57	BA	1489	C	N3-C2-O2	-7.64	116.55	121.90
57	BA	19	A	N1-C6-N6	-7.63	114.02	118.60
57	BA	680	C	N3-C2-O2	-7.63	116.56	121.90
57	BA	833	A	N1-C6-N6	-7.63	114.02	118.60
57	BA	2560	A	C5-C6-N1	7.63	121.52	117.70
22	AA	1274	A	C5-C6-N1	7.63	121.52	117.70
22	AA	1484	C	N3-C2-O2	-7.63	116.56	121.90
35	BD	216	ARG	NE-CZ-NH2	-7.63	116.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	734	A	N1-C6-N6	-7.63	114.02	118.60
57	BA	1144	A	N1-C6-N6	-7.63	114.02	118.60
57	BA	1170	C	N3-C2-O2	-7.63	116.56	121.90
57	BA	157	C	N3-C2-O2	-7.63	116.56	121.90
57	BA	320	A	C5-C6-N1	7.63	121.51	117.70
57	BA	1386	C	N3-C2-O2	-7.63	116.56	121.90
57	BA	1771	C	N3-C2-O2	-7.63	116.56	121.90
24	A3	77	A	C5-C6-N1	7.63	121.51	117.70
57	BA	75	G	O4'-C1'-N9	7.63	114.30	108.20
57	BA	1008	A	C5-C6-N1	7.63	121.51	117.70
35	BD	13	ARG	NE-CZ-NH1	7.62	124.11	120.30
57	BA	766	U	O4'-C1'-N1	7.62	114.30	108.20
57	BA	1123	C	N3-C2-O2	-7.62	116.56	121.90
57	BA	1387	A	N1-C6-N6	-7.62	114.03	118.60
57	BA	351	C	N3-C2-O2	-7.62	116.56	121.90
57	BA	1102	C	N3-C2-O2	-7.62	116.56	121.90
57	BA	1793	C	N3-C2-O2	-7.62	116.56	121.90
57	BA	2776	A	C5-C6-N1	7.62	121.51	117.70
57	BA	2853	C	N3-C2-O2	-7.62	116.56	121.90
22	AA	948	C	N3-C2-O2	-7.62	116.56	121.90
22	AA	1203	C	N3-C2-O2	-7.62	116.56	121.90
22	AA	1271	A	C5-C6-N1	7.62	121.51	117.70
57	BA	404	A	C4-C5-C6	-7.62	113.19	117.00
22	AA	1152	A	C5-C6-N1	7.62	121.51	117.70
57	BA	959	A	C5-C6-N1	7.62	121.51	117.70
57	BA	1314	C	N3-C2-O2	-7.62	116.57	121.90
57	BA	1419	A	C4-C5-C6	-7.62	113.19	117.00
22	AA	386	C	N3-C2-O2	-7.62	116.57	121.90
22	AA	935	A	C5-C6-N1	7.62	121.51	117.70
57	BA	196	A	C5-C6-N1	7.62	121.51	117.70
57	BA	2613	U	O4'-C1'-N1	7.62	114.30	108.20
22	AA	526	C	N3-C2-O2	-7.62	116.57	121.90
57	BA	505	A	N1-C6-N6	-7.62	114.03	118.60
22	AA	77	A	C5-C6-N1	7.62	121.51	117.70
57	BA	983	A	C5-C6-N1	7.62	121.51	117.70
57	BA	1214	A	N1-C6-N6	-7.62	114.03	118.60
57	BA	1899	A	C5-C6-N1	7.62	121.51	117.70
22	AA	221	C	N3-C2-O2	-7.61	116.57	121.90
22	AA	787	A	C5-C6-N1	7.61	121.51	117.70
22	AA	890	G	O4'-C1'-N9	7.61	114.29	108.20
22	AA	1229	A	N1-C6-N6	-7.61	114.03	118.60
57	BA	61	C	N3-C2-O2	-7.61	116.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	321	A	N1-C6-N6	-7.61	114.03	118.60
22	AA	1191	A	C5-C6-N1	7.61	121.51	117.70
22	AA	1248	A	C5-C6-N1	7.61	121.51	117.70
22	AA	298	A	C5-C6-N1	7.61	121.50	117.70
22	AA	1456	A	C5-C6-N1	7.61	121.50	117.70
22	AA	1102	A	N1-C6-N6	-7.61	114.03	118.60
57	BA	2336	A	C5-C6-N1	7.61	121.50	117.70
58	Ba	30	C	N3-C2-O2	-7.61	116.58	121.90
58	Ba	115	A	C5-C6-N1	7.61	121.50	117.70
57	BA	10	A	C5-C6-N1	7.61	121.50	117.70
57	BA	595	C	N3-C2-O2	-7.61	116.58	121.90
57	BA	1978	A	C5-C6-N1	7.61	121.50	117.70
57	BA	2698	U	O4'-C1'-N1	7.61	114.28	108.20
58	Ba	73	A	N1-C6-N6	-7.61	114.04	118.60
57	BA	999	U	O4'-C1'-N1	7.60	114.28	108.20
57	BA	2426	A	C5-C6-N1	7.60	121.50	117.70
22	AA	946	A	N1-C6-N6	-7.60	114.04	118.60
22	AA	978	A	N1-C6-N6	-7.60	114.04	118.60
57	BA	324	A	C5-C6-N1	7.60	121.50	117.70
57	BA	1748	C	N3-C2-O2	-7.60	116.58	121.90
57	BA	1832	C	N3-C2-O2	-7.60	116.58	121.90
57	BA	2480	C	O4'-C1'-N1	7.60	114.28	108.20
19	AH	116	ARG	NE-CZ-NH1	7.60	124.10	120.30
22	AA	802	A	N1-C6-N6	-7.60	114.04	118.60
22	AA	1257	A	C5-C6-N1	7.60	121.50	117.70
57	BA	1595	C	N3-C2-O2	-7.60	116.58	121.90
22	AA	238	A	C5-C6-N1	7.60	121.50	117.70
22	AA	1449	C	N3-C2-O2	-7.60	116.58	121.90
57	BA	97	C	N3-C2-O2	-7.60	116.58	121.90
57	BA	2129	C	N3-C2-O2	-7.60	116.58	121.90
22	AA	116	A	N1-C6-N6	-7.60	114.04	118.60
57	BA	415	A	C5-C6-N1	7.60	121.50	117.70
57	BA	1233	C	N3-C2-O2	-7.60	116.58	121.90
57	BA	1701	A	N1-C6-N6	-7.60	114.04	118.60
57	BA	217	A	C5-C6-N1	7.59	121.50	117.70
57	BA	1064	C	N3-C2-O2	-7.59	116.58	121.90
57	BA	1494	A	C5-C6-N1	7.59	121.50	117.70
57	BA	1572	A	N1-C6-N6	-7.59	114.04	118.60
13	AU	32	ARG	NE-CZ-NH1	7.59	124.10	120.30
22	AA	1531	A	C5-C6-N1	7.59	121.50	117.70
57	BA	2142	A	C5-C6-N1	7.59	121.50	117.70
20	AI	118	ARG	NE-CZ-NH1	7.59	124.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	498	A	C5-C6-N1	7.59	121.50	117.70
22	AA	768	A	C5-C6-N1	7.59	121.50	117.70
22	AA	1418	A	C5-C6-N1	7.59	121.50	117.70
36	BU	52	ARG	NE-CZ-NH1	7.59	124.10	120.30
57	BA	56	A	N1-C6-N6	-7.59	114.05	118.60
57	BA	853	C	N3-C2-O2	-7.59	116.59	121.90
57	BA	1447	C	N3-C2-O2	-7.59	116.59	121.90
57	BA	2051	A	C5-C6-N1	7.59	121.50	117.70
57	BA	2829	A	C5-C6-N1	7.59	121.50	117.70
22	AA	155	A	C5-C6-N1	7.59	121.49	117.70
22	AA	272	C	N3-C2-O2	-7.59	116.59	121.90
22	AA	1150	A	C5-C6-N1	7.59	121.49	117.70
57	BA	1609	A	C5-C6-N1	7.59	121.50	117.70
57	BA	1658	C	N3-C2-O2	-7.59	116.59	121.90
57	BA	2715	C	N3-C2-O2	-7.59	116.59	121.90
57	BA	2720	U	O4'-C1'-N1	7.59	114.27	108.20
22	AA	1204	A	C4-C5-C6	-7.59	113.21	117.00
57	BA	2058	A	C5-C6-N1	7.59	121.49	117.70
58	Ba	28	C	N3-C2-O2	-7.59	116.59	121.90
46	B3	29	ARG	NE-CZ-NH2	7.59	124.09	120.30
57	BA	1082	U	O4'-C1'-N1	7.59	114.27	108.20
57	BA	1194	A	C5-C6-N1	7.59	121.49	117.70
22	AA	300	A	C5-C6-N1	7.58	121.49	117.70
42	B0	13	ARG	NE-CZ-NH1	7.58	124.09	120.30
57	BA	786	C	N3-C2-O2	-7.58	116.59	121.90
22	AA	32	A	C5-C6-N1	7.58	121.49	117.70
57	BA	332	A	C5-C6-N1	7.58	121.49	117.70
22	AA	1140	C	N3-C2-O2	-7.58	116.59	121.90
57	BA	460	A	N1-C6-N6	-7.58	114.05	118.60
57	BA	621	A	C5-C6-N1	7.58	121.49	117.70
17	AF	38	ARG	NE-CZ-NH1	7.58	124.09	120.30
22	AA	680	C	N3-C2-O2	-7.58	116.60	121.90
32	BR	22	ARG	NE-CZ-NH1	7.58	124.09	120.30
57	BA	6	A	C5-C6-N1	7.58	121.49	117.70
57	BA	1749	A	C5-C6-N1	7.58	121.49	117.70
57	BA	1768	C	N3-C2-O2	-7.58	116.59	121.90
57	BA	2208	C	N3-C2-O2	-7.58	116.59	121.90
57	BA	2654	A	C5-C6-N1	7.58	121.49	117.70
22	AA	1250	A	C5-C6-N1	7.58	121.49	117.70
57	BA	149	A	C5-C6-N1	7.58	121.49	117.70
57	BA	480	A	C5-C6-N1	7.58	121.49	117.70
57	BA	1142	A	C4-C5-C6	-7.58	113.21	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	979	C	N3-C2-O2	-7.57	116.60	121.90
22	AA	1311	A	C5-C6-N1	7.57	121.49	117.70
57	BA	337	C	N3-C2-O2	-7.57	116.60	121.90
57	BA	1305	C	N3-C2-O2	-7.57	116.60	121.90
57	BA	1787	A	C5-C6-N1	7.57	121.49	117.70
22	AA	1243	C	N3-C2-O2	-7.57	116.60	121.90
22	AA	1397	C	N3-C2-O2	-7.57	116.60	121.90
57	BA	613	A	C5-C6-N1	7.57	121.48	117.70
22	AA	1367	C	N3-C2-O2	-7.57	116.60	121.90
57	BA	996	A	C5-C6-N1	7.57	121.48	117.70
57	BA	2265	U	O4'-C1'-N1	7.57	114.25	108.20
57	BA	2647	U	O4'-C1'-N1	7.57	114.25	108.20
22	AA	596	A	N1-C6-N6	-7.57	114.06	118.60
22	AA	1427	C	N3-C2-O2	-7.57	116.61	121.90
57	BA	951	C	N3-C2-O2	-7.57	116.61	121.90
57	BA	1795	C	O4'-C1'-N1	7.57	114.25	108.20
57	BA	2678	C	N3-C2-O2	-7.57	116.60	121.90
22	AA	1045	C	N3-C2-O2	-7.56	116.61	121.90
22	AA	1437	A	N1-C6-N6	-7.56	114.06	118.60
22	AA	1228	C	N3-C2-O2	-7.56	116.61	121.90
57	BA	744	U	O4'-C1'-N1	7.56	114.25	108.20
57	BA	1706	C	N3-C2-O2	-7.56	116.61	121.90
22	AA	1397	C	O4'-C1'-N1	7.56	114.25	108.20
57	BA	1246	A	C5-C6-N1	7.56	121.48	117.70
57	BA	2899	A	N1-C6-N6	-7.56	114.06	118.60
21	A1	517	ARG	NE-CZ-NH1	7.56	124.08	120.30
22	AA	217	C	N3-C2-O2	-7.56	116.61	121.90
22	AA	231	U	O4'-C1'-N1	7.56	114.25	108.20
57	BA	145	C	N3-C2-O2	-7.56	116.61	121.90
57	BA	1315	C	N3-C2-O2	-7.56	116.61	121.90
57	BA	2084	C	N3-C2-O2	-7.56	116.61	121.90
13	AU	54	ARG	NE-CZ-NH1	7.56	124.08	120.30
22	AA	478	A	C5-C6-N1	7.56	121.48	117.70
33	BS	94	ARG	NE-CZ-NH1	7.56	124.08	120.30
57	BA	422	A	N1-C6-N6	-7.56	114.07	118.60
57	BA	2635	A	C5-C6-N1	7.56	121.48	117.70
57	BA	529	A	C5-C6-N1	7.56	121.48	117.70
57	BA	1650	A	C5-C6-N1	7.56	121.48	117.70
58	Ba	119	A	C5-C6-N1	7.56	121.48	117.70
22	AA	655	A	C5-C6-N1	7.55	121.48	117.70
33	BS	25	ARG	NE-CZ-NH1	7.55	124.08	120.30
57	BA	540	C	N3-C2-O2	-7.55	116.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	985	C	N3-C2-O2	-7.55	116.61	121.90
57	BA	2077	A	C5-C6-N1	7.55	121.48	117.70
57	BA	2752	C	O4'-C1'-N1	7.55	114.24	108.20
22	AA	1021	A	C5-C6-N1	7.55	121.48	117.70
57	BA	626	A	C5-C6-N1	7.55	121.48	117.70
57	BA	1784	A	C5-C6-N1	7.55	121.48	117.70
22	AA	151	A	C4-C5-C6	-7.55	113.22	117.00
22	AA	932	C	N3-C2-O2	-7.55	116.61	121.90
53	BF	162	ARG	NE-CZ-NH2	7.55	124.08	120.30
57	BA	318	C	N3-C2-O2	-7.55	116.61	121.90
57	BA	633	A	C5-C6-N1	7.55	121.47	117.70
57	BA	804	A	C5-C6-N1	7.55	121.48	117.70
57	BA	915	C	N3-C2-O2	-7.55	116.61	121.90
57	BA	1027	A	N1-C6-N6	-7.55	114.07	118.60
57	BA	1378	A	C4-C5-C6	-7.55	113.22	117.00
57	BA	2089	C	N3-C2-O2	-7.55	116.61	121.90
57	BA	2199	A	C5-C6-N1	7.55	121.47	117.70
57	BA	2275	C	N3-C2-O2	-7.55	116.61	121.90
57	BA	2815	C	N3-C2-O2	-7.55	116.61	121.90
57	BA	362	A	O4'-C1'-N9	7.55	114.24	108.20
57	BA	943	A	C5-C6-N1	7.55	121.47	117.70
57	BA	2551	C	N3-C2-O2	-7.55	116.62	121.90
22	AA	452	A	C4-C5-C6	-7.55	113.23	117.00
57	BA	861	A	C5-C6-N1	7.55	121.47	117.70
57	BA	1323	C	N3-C2-O2	-7.55	116.62	121.90
57	BA	1569	A	C5-C6-N1	7.55	121.47	117.70
22	AA	250	A	C5-C6-N1	7.55	121.47	117.70
22	AA	1217	C	N3-C2-O2	-7.55	116.62	121.90
57	BA	2037	A	C5-C6-N1	7.55	121.47	117.70
57	BA	2367	G	O4'-C1'-N9	7.55	114.24	108.20
22	AA	1430	A	C5-C6-N1	7.54	121.47	117.70
57	BA	440	C	N3-C2-O2	-7.54	116.62	121.90
57	BA	1928	A	C5-C6-N1	7.54	121.47	117.70
22	AA	796	C	N3-C2-O2	-7.54	116.62	121.90
22	AA	815	A	C4-C5-C6	-7.54	113.23	117.00
57	BA	345	A	C5-C6-N1	7.54	121.47	117.70
57	BA	835	C	N3-C2-O2	-7.54	116.62	121.90
57	BA	1918	A	C5-C6-N1	7.54	121.47	117.70
22	AA	1081	A	C5-C6-N1	7.54	121.47	117.70
57	BA	2328	A	C5-C6-N1	7.54	121.47	117.70
57	BA	2270	A	C5-C6-N1	7.54	121.47	117.70
22	AA	1324	A	C5-C6-N1	7.54	121.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1353	A	C5-C6-N1	7.54	121.47	117.70
57	BA	1577	C	N3-C2-O2	-7.54	116.62	121.90
57	BA	1872	A	C5-C6-N1	7.54	121.47	117.70
22	AA	1350	A	C5-C6-N1	7.54	121.47	117.70
22	AA	87	C	N3-C2-O2	-7.54	116.63	121.90
57	BA	310	A	C5-C6-N1	7.54	121.47	117.70
57	BA	509	C	N3-C2-O2	-7.54	116.62	121.90
22	AA	766	A	C5-C6-N1	7.53	121.47	117.70
22	AA	539	A	C5-C6-N1	7.53	121.47	117.70
57	BA	1556	C	N3-C2-O2	-7.53	116.63	121.90
22	AA	573	A	C4-C5-C6	-7.53	113.23	117.00
57	BA	522	A	C5-C6-N1	7.53	121.47	117.70
22	AA	1082	A	C5-C6-N1	7.53	121.47	117.70
57	BA	1126	A	N1-C6-N6	-7.53	114.08	118.60
57	BA	1755	A	C4-C5-C6	-7.53	113.24	117.00
57	BA	2705	A	C5-C6-N1	7.53	121.47	117.70
15	AD	25	ARG	NE-CZ-NH1	7.53	124.06	120.30
57	BA	917	A	N1-C6-N6	-7.53	114.08	118.60
57	BA	1052	C	N3-C2-O2	-7.53	116.63	121.90
57	BA	2311	A	C5-C6-N1	7.53	121.46	117.70
15	AD	145	ARG	NE-CZ-NH1	7.53	124.06	120.30
22	AA	1080	A	C5-C6-N1	7.53	121.46	117.70
24	A3	74	A	C5-C6-N1	7.53	121.46	117.70
57	BA	384	A	C5-C6-N1	7.53	121.46	117.70
57	BA	973	A	C5-C6-N1	7.53	121.46	117.70
57	BA	1272	A	C5-C6-N1	7.53	121.46	117.70
57	BA	1376	C	N3-C2-O2	-7.53	116.63	121.90
57	BA	1913	A	C5-C6-N1	7.53	121.46	117.70
57	BA	466	A	C5-C6-N1	7.52	121.46	117.70
22	AA	1046	A	C4-C5-C6	-7.52	113.24	117.00
50	B7	41	ARG	NE-CZ-NH2	7.52	124.06	120.30
57	BA	2482	A	N1-C6-N6	-7.52	114.09	118.60
57	BA	2727	A	C5-C6-N1	7.52	121.46	117.70
57	BA	1512	C	N3-C2-O2	-7.52	116.64	121.90
22	AA	408	A	C5-C6-N1	7.52	121.46	117.70
22	AA	702	A	C5-C6-N1	7.52	121.46	117.70
57	BA	1549	A	C5-C6-N1	7.52	121.46	117.70
57	BA	1593	A	C5-C6-N1	7.52	121.46	117.70
57	BA	2516	A	C5-C6-N1	7.52	121.46	117.70
22	AA	459	A	C4-C5-C6	-7.51	113.24	117.00
22	AA	914	A	C5-C6-N1	7.51	121.46	117.70
57	BA	2750	A	C4-C5-C6	-7.51	113.24	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	156	C	N3-C2-O2	-7.51	116.64	121.90
22	AA	371	A	C5-C6-N1	7.51	121.46	117.70
22	AA	1510	C	N3-C2-O2	-7.51	116.64	121.90
58	Ba	109	A	C5-C6-N1	7.51	121.45	117.70
11	AB	224	ARG	NE-CZ-NH1	7.51	124.06	120.30
57	BA	403	U	O4'-C1'-N1	7.51	114.21	108.20
57	BA	1080	A	C5-C6-N1	7.51	121.45	117.70
22	AA	609	A	C5-C6-N1	7.51	121.45	117.70
22	AA	910	C	N3-C2-O2	-7.51	116.64	121.90
22	AA	1246	A	C5-C6-N1	7.51	121.45	117.70
57	BA	2232	C	N3-C2-O2	-7.51	116.64	121.90
57	BA	2841	C	N3-C2-O2	-7.51	116.64	121.90
22	AA	1067	A	C5-C6-N1	7.51	121.45	117.70
57	BA	105	C	N3-C2-O2	-7.51	116.65	121.90
57	BA	542	C	N3-C2-O2	-7.51	116.65	121.90
57	BA	603	A	C4-C5-C6	-7.51	113.25	117.00
57	BA	611	C	N3-C2-O2	-7.51	116.65	121.90
57	BA	772	C	N3-C2-O2	-7.51	116.64	121.90
22	AA	366	A	C5-C6-N1	7.50	121.45	117.70
57	BA	1104	C	N3-C2-O2	-7.50	116.65	121.90
58	Ba	62	C	N3-C2-O2	-7.50	116.65	121.90
57	BA	968	C	N3-C2-O2	-7.50	116.65	121.90
57	BA	1194	A	C4-C5-C6	-7.50	113.25	117.00
57	BA	2792	A	C5-C6-N1	7.50	121.45	117.70
17	AF	44	ARG	NE-CZ-NH1	7.50	124.05	120.30
22	AA	1441	A	C4-C5-C6	-7.50	113.25	117.00
57	BA	510	C	N3-C2-O2	-7.50	116.65	121.90
57	BA	2139	U	O4'-C1'-N1	7.50	114.20	108.20
57	BA	2471	A	C5-C6-N1	7.50	121.45	117.70
57	BA	42	A	C5-C6-N1	7.50	121.45	117.70
57	BA	253	C	N3-C2-O2	-7.50	116.65	121.90
22	AA	1063	C	N3-C2-O2	-7.50	116.65	121.90
22	AA	1375	A	C5-C6-N1	7.50	121.45	117.70
57	BA	1367	A	C5-C6-N1	7.50	121.45	117.70
57	BA	1819	A	C5-C6-N1	7.50	121.45	117.70
57	BA	57	C	O4'-C1'-N1	7.50	114.20	108.20
57	BA	1189	A	C5-C6-N1	7.50	121.45	117.70
22	AA	883	C	N3-C2-O2	-7.50	116.65	121.90
57	BA	226	A	C5-C6-N1	7.50	121.45	117.70
22	AA	784	A	C5-C6-N1	7.49	121.45	117.70
24	A3	52	C	N3-C2-O2	-7.49	116.65	121.90
57	BA	45	G	O4'-C1'-N9	7.49	114.19	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	213	A	N1-C6-N6	-7.49	114.10	118.60
57	BA	1789	A	N1-C6-N6	-7.49	114.10	118.60
24	A3	1	C	N3-C2-O2	-7.49	116.66	121.90
57	BA	2317	A	C5-C6-N1	7.49	121.45	117.70
57	BA	2896	C	N3-C2-O2	-7.49	116.66	121.90
22	AA	411	A	C4-C5-C6	-7.49	113.25	117.00
22	AA	1117	A	C5-C6-N1	7.49	121.44	117.70
57	BA	806	C	N3-C2-O2	-7.49	116.66	121.90
57	BA	1214	A	C5-C6-N1	7.49	121.44	117.70
57	BA	1652	A	C5-C6-N1	7.49	121.44	117.70
22	AA	839	C	O4'-C1'-N1	7.49	114.19	108.20
57	BA	173	A	C5-C6-N1	7.49	121.44	117.70
22	AA	131	A	C5-C6-N1	7.49	121.44	117.70
22	AA	1176	A	C5-C6-N1	7.49	121.44	117.70
57	BA	125	A	C5-C6-N1	7.49	121.44	117.70
57	BA	294	A	C4-C5-C6	-7.49	113.26	117.00
57	BA	2392	A	C5-C6-N1	7.49	121.44	117.70
57	BA	2425	A	C5-C6-N1	7.49	121.44	117.70
57	BA	1121	C	N3-C2-O2	-7.48	116.66	121.90
57	BA	1881	C	N3-C2-O2	-7.48	116.66	121.90
22	AA	586	C	N3-C2-O2	-7.48	116.66	121.90
22	AA	716	A	C5-C6-N1	7.48	121.44	117.70
22	AA	879	C	N3-C2-O2	-7.48	116.66	121.90
22	AA	1255	G	O4'-C1'-N9	7.48	114.19	108.20
57	BA	590	A	C5-C6-N1	7.48	121.44	117.70
57	BA	691	C	N3-C2-O2	-7.48	116.66	121.90
57	BA	1306	C	N3-C2-O2	-7.48	116.66	121.90
57	BA	2117	A	C5-C6-N1	7.48	121.44	117.70
57	BA	302	C	N3-C2-O2	-7.48	116.66	121.90
57	BA	2733	A	C4-C5-C6	-7.48	113.26	117.00
58	Ba	45	A	C5-C6-N1	7.48	121.44	117.70
22	AA	199	A	N1-C6-N6	-7.48	114.11	118.60
22	AA	263	A	C5-C6-N1	7.48	121.44	117.70
22	AA	958	A	C5-C6-N1	7.48	121.44	117.70
57	BA	1386	C	O4'-C1'-N1	7.48	114.18	108.20
57	BA	2430	A	C5-C6-N1	7.48	121.44	117.70
57	BA	1496	A	C5-C6-N1	7.48	121.44	117.70
57	BA	1810	A	C5-C6-N1	7.48	121.44	117.70
57	BA	2420	C	N3-C2-O2	-7.48	116.67	121.90
57	BA	2721	A	C4-C5-C6	-7.48	113.26	117.00
24	A3	26	C	N3-C2-O2	-7.48	116.67	121.90
57	BA	1708	C	N3-C2-O2	-7.48	116.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1789	A	C5-C6-N1	7.48	121.44	117.70
57	BA	2855	C	N3-C2-O2	-7.48	116.67	121.90
58	Ba	90	C	N1-C2-O2	7.48	123.39	118.90
22	AA	753	A	N1-C6-N6	-7.47	114.12	118.60
22	AA	1284	C	N3-C2-O2	-7.47	116.67	121.90
57	BA	22	C	N3-C2-O2	-7.47	116.67	121.90
57	BA	1147	A	C5-C6-N1	7.47	121.44	117.70
57	BA	1357	C	N3-C2-O2	-7.47	116.67	121.90
57	BA	1586	A	C5-C6-N1	7.47	121.44	117.70
57	BA	2295	C	N3-C2-O2	-7.47	116.67	121.90
22	AA	435	A	C4-C5-C6	-7.47	113.26	117.00
22	AA	637	C	N3-C2-O2	-7.47	116.67	121.90
24	A3	42	C	N3-C2-O2	-7.47	116.67	121.90
57	BA	344	A	C5-C6-N1	7.47	121.44	117.70
57	BA	2764	A	C4-C5-C6	-7.47	113.26	117.00
22	AA	36	C	N3-C2-O2	-7.47	116.67	121.90
57	BA	1117	C	N3-C2-O2	-7.47	116.67	121.90
57	BA	1146	C	N3-C2-O2	-7.47	116.67	121.90
57	BA	2274	A	C5-C6-N1	7.47	121.44	117.70
57	BA	1866	A	N1-C6-N6	-7.47	114.12	118.60
22	AA	1196	A	C5-C6-N1	7.47	121.43	117.70
57	BA	723	C	N3-C2-O2	-7.47	116.67	121.90
57	BA	2733	A	C5-C6-N1	7.47	121.43	117.70
57	BA	374	A	N1-C6-N6	-7.47	114.12	118.60
57	BA	737	C	N3-C2-O2	-7.47	116.67	121.90
57	BA	1596	A	N1-C6-N6	-7.47	114.12	118.60
22	AA	735	C	N3-C2-O2	-7.46	116.67	121.90
22	AA	1374	A	C5-C6-N1	7.46	121.43	117.70
23	A2	24	A	C5-C6-N1	7.46	121.43	117.70
57	BA	563	A	N1-C6-N6	-7.46	114.12	118.60
57	BA	2015	A	C5-C6-N1	7.46	121.43	117.70
22	AA	269	C	N3-C2-O2	-7.46	116.68	121.90
22	AA	341	C	N3-C2-O2	-7.46	116.68	121.90
57	BA	508	A	C5-C6-N1	7.46	121.43	117.70
57	BA	2015	A	N1-C6-N6	-7.46	114.12	118.60
57	BA	2260	C	O4'-C1'-N1	7.46	114.17	108.20
57	BA	2395	C	N3-C2-O2	-7.46	116.68	121.90
22	AA	716	A	C4-C5-C6	-7.46	113.27	117.00
57	BA	401	A	C4-C5-C6	-7.46	113.27	117.00
57	BA	1057	A	C4-C5-C6	-7.46	113.27	117.00
57	BA	2150	C	N3-C2-O2	-7.46	116.68	121.90
57	BA	2241	A	C5-C6-N1	7.46	121.43	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2805	C	N3-C2-O2	-7.46	116.68	121.90
22	AA	443	C	N3-C2-O2	-7.46	116.68	121.90
57	BA	357	C	N3-C2-O2	-7.46	116.68	121.90
57	BA	643	A	N1-C6-N6	-7.46	114.12	118.60
22	AA	160	A	C4-C5-C6	-7.46	113.27	117.00
22	AA	1210	C	N3-C2-O2	-7.46	116.68	121.90
57	BA	279	A	C5-C6-N1	7.46	121.43	117.70
57	BA	640	C	N3-C2-O2	-7.46	116.68	121.90
57	BA	1927	A	C5-C6-N1	7.46	121.43	117.70
22	AA	1103	C	N3-C2-O2	-7.46	116.68	121.90
30	BP	132	ARG	NE-CZ-NH1	7.46	124.03	120.30
57	BA	152	A	C5-C6-N1	7.46	121.43	117.70
57	BA	2171	A	C4-C5-C6	-7.46	113.27	117.00
57	BA	2676	C	N3-C2-O2	-7.46	116.68	121.90
58	Ba	101	A	C5-C6-N1	7.46	121.43	117.70
22	AA	754	C	N3-C2-O2	-7.46	116.68	121.90
57	BA	1974	C	N3-C2-O2	-7.46	116.68	121.90
57	BA	2097	A	C5-C6-N1	7.46	121.43	117.70
57	BA	2227	A	C5-C6-N1	7.46	121.43	117.70
57	BA	2606	C	N3-C2-O2	-7.46	116.68	121.90
57	BA	1711	A	C5-C6-N1	7.45	121.43	117.70
57	BA	893	C	N3-C2-O2	-7.45	116.68	121.90
22	AA	60	A	C5-C6-N1	7.45	121.42	117.70
22	AA	862	C	N3-C2-O2	-7.45	116.69	121.90
22	AA	969	A	O4'-C1'-N9	7.45	114.16	108.20
57	BA	462	C	N3-C2-O2	-7.45	116.69	121.90
57	BA	632	A	N1-C6-N6	-7.45	114.13	118.60
57	BA	1853	A	C5-C6-N1	7.45	121.42	117.70
57	BA	2044	C	N3-C2-O2	-7.45	116.68	121.90
57	BA	2418	A	C5-C6-N1	7.45	121.42	117.70
22	AA	489	C	N3-C2-O2	-7.45	116.69	121.90
22	AA	663	A	C5-C6-N1	7.45	121.42	117.70
22	AA	839	C	N3-C2-O2	-7.45	116.69	121.90
22	AA	1129	C	N3-C2-O2	-7.45	116.69	121.90
57	BA	501	A	C5-C6-N1	7.45	121.42	117.70
57	BA	564	C	N3-C2-O2	-7.45	116.69	121.90
57	BA	128	C	N3-C2-O2	-7.45	116.69	121.90
57	BA	517	C	N3-C2-O2	-7.45	116.69	121.90
20	AI	98	ARG	NE-CZ-NH1	7.45	124.02	120.30
22	AA	649	A	C5-C6-N1	7.45	121.42	117.70
22	AA	1521	C	N3-C2-O2	-7.45	116.69	121.90
57	BA	515	A	C4-C5-C6	-7.45	113.28	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1169	A	C5-C6-N1	7.45	121.42	117.70
15	AD	69	ARG	NE-CZ-NH1	7.44	124.02	120.30
57	BA	1350	C	N3-C2-O2	-7.44	116.69	121.90
57	BA	1698	A	C5-C6-N1	7.44	121.42	117.70
57	BA	2291	U	O4'-C1'-N1	7.44	114.16	108.20
22	AA	1153	G	O4'-C1'-N9	7.44	114.15	108.20
57	BA	1328	A	C4-C5-C6	-7.44	113.28	117.00
57	BA	2376	A	C4-C5-C6	-7.44	113.28	117.00
22	AA	313	A	C5-C6-N1	7.44	121.42	117.70
22	AA	1410	A	C5-C6-N1	7.44	121.42	117.70
57	BA	147	C	N3-C2-O2	-7.44	116.69	121.90
57	BA	1284	A	C5-C6-N1	7.44	121.42	117.70
57	BA	418	C	N3-C2-O2	-7.44	116.69	121.90
22	AA	1269	A	C5-C6-N1	7.44	121.42	117.70
57	BA	278	A	C4-C5-C6	-7.44	113.28	117.00
57	BA	1996	C	N3-C2-O2	-7.44	116.69	121.90
57	BA	2200	C	N3-C2-O2	-7.44	116.69	121.90
22	AA	1071	C	N3-C2-O2	-7.44	116.69	121.90
57	BA	1901	A	C5-C6-N1	7.44	121.42	117.70
57	BA	2575	C	C2-N3-C4	7.44	123.62	119.90
57	BA	205	G	O4'-C1'-N9	7.43	114.15	108.20
57	BA	1276	A	C5-C6-N1	7.43	121.42	117.70
57	BA	1780	A	N1-C6-N6	-7.43	114.14	118.60
57	BA	1844	C	N3-C2-O2	-7.43	116.70	121.90
57	BA	2340	A	C5-C6-N1	7.43	121.42	117.70
22	AA	759	A	C5-C6-N1	7.43	121.42	117.70
22	AA	880	C	N3-C2-O2	-7.43	116.70	121.90
22	AA	1012	A	C5-C6-N1	7.43	121.42	117.70
57	BA	2704	C	N3-C2-O2	-7.43	116.70	121.90
22	AA	342	C	N3-C2-O2	-7.43	116.70	121.90
22	AA	1506	U	O4'-C1'-N1	7.43	114.14	108.20
57	BA	231	A	C5-C6-N1	7.43	121.42	117.70
57	BA	751	A	C5-C6-N1	7.43	121.42	117.70
57	BA	1566	A	C5-C6-N1	7.43	121.42	117.70
57	BA	2135	A	C5-C6-N1	7.43	121.42	117.70
22	AA	192	A	C5-C6-N1	7.43	121.42	117.70
22	AA	483	C	O4'-C1'-N1	7.43	114.14	108.20
57	BA	470	A	C5-C6-N1	7.43	121.41	117.70
57	BA	732	C	N3-C2-O2	-7.43	116.70	121.90
57	BA	936	A	C5-C6-N1	7.43	121.42	117.70
57	BA	1404	C	N3-C2-O2	-7.43	116.70	121.90
57	BA	1550	C	N3-C2-O2	-7.43	116.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2184	A	C5-C6-N1	7.43	121.42	117.70
22	AA	26	A	C4-C5-C6	-7.43	113.29	117.00
57	BA	2070	A	C5-C6-N1	7.43	121.41	117.70
22	AA	285	C	N3-C2-O2	-7.43	116.70	121.90
57	BA	1205	A	C4-C5-C6	-7.43	113.29	117.00
3	AL	109	ARG	NE-CZ-NH1	7.42	124.01	120.30
21	A1	584	ARG	NE-CZ-NH1	7.42	124.01	120.30
22	AA	290	C	N3-C2-O2	-7.42	116.70	121.90
22	AA	853	C	N3-C2-O2	-7.42	116.70	121.90
22	AA	1113	C	N3-C2-O2	-7.42	116.70	121.90
57	BA	734	A	C5-C6-N1	7.42	121.41	117.70
57	BA	1100	C	N3-C2-O2	-7.42	116.70	121.90
22	AA	750	C	N3-C2-O2	-7.42	116.70	121.90
22	AA	1239	A	C5-C6-N1	7.42	121.41	117.70
22	AA	1285	A	C5-C6-N1	7.42	121.41	117.70
57	BA	2527	C	N3-C2-O2	-7.42	116.70	121.90
57	BA	2757	A	C5-C6-N1	7.42	121.41	117.70
57	BA	2827	C	N3-C2-O2	-7.42	116.70	121.90
42	B0	38	ARG	NE-CZ-NH2	-7.42	116.59	120.30
22	AA	856	C	N3-C2-O2	-7.42	116.71	121.90
22	AA	1044	A	C5-C6-N1	7.42	121.41	117.70
57	BA	610	C	N3-C2-O2	-7.42	116.71	121.90
57	BA	2767	C	N3-C2-O2	-7.42	116.71	121.90
22	AA	207	C	N3-C2-O2	-7.42	116.71	121.90
57	BA	503	A	C4-C5-C6	-7.42	113.29	117.00
57	BA	937	C	N3-C2-O2	-7.42	116.71	121.90
57	BA	1204	A	C4-C5-C6	-7.42	113.29	117.00
57	BA	1505	A	C4-C5-C6	-7.42	113.29	117.00
57	BA	2534	A	C4-C5-C6	-7.42	113.29	117.00
57	BA	2787	C	N3-C2-O2	-7.42	116.71	121.90
57	BA	2880	C	N3-C2-O2	-7.42	116.71	121.90
57	BA	678	C	N3-C2-O2	-7.42	116.71	121.90
57	BA	2264	C	N3-C2-O2	-7.42	116.71	121.90
34	BT	108	ARG	NE-CZ-NH2	7.41	124.01	120.30
57	BA	2653	U	O4'-C1'-N1	7.41	114.13	108.20
57	BA	2762	C	N3-C2-O2	-7.41	116.71	121.90
22	AA	578	C	N3-C2-O2	-7.41	116.71	121.90
57	BA	944	C	N3-C2-O2	-7.41	116.71	121.90
57	BA	1739	A	C5-C6-N1	7.41	121.41	117.70
58	Ba	57	A	N1-C6-N6	-7.41	114.15	118.60
22	AA	80	A	C5-C6-N1	7.41	121.41	117.70
22	AA	1151	A	C4-C5-C6	-7.41	113.30	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2711	A	C4-C5-C6	-7.41	113.30	117.00
57	BA	1545	A	C5-C6-N1	7.41	121.40	117.70
57	BA	1809	A	C5-C6-N1	7.41	121.40	117.70
57	BA	2821	A	N1-C6-N6	-7.41	114.15	118.60
57	BA	103	A	C5-C6-N1	7.41	121.40	117.70
57	BA	1046	A	C5-C6-N1	7.41	121.40	117.70
57	BA	1806	C	N3-C2-O2	-7.41	116.72	121.90
22	AA	756	C	N3-C2-O2	-7.41	116.72	121.90
22	AA	1254	A	C5-C6-N1	7.41	121.40	117.70
57	BA	973	A	N1-C6-N6	-7.41	114.16	118.60
57	BA	1437	C	N3-C2-O2	-7.41	116.72	121.90
57	BA	1679	A	C5-C6-N1	7.41	121.40	117.70
22	AA	1411	C	N3-C2-O2	-7.40	116.72	121.90
57	BA	486	C	N3-C2-O2	-7.40	116.72	121.90
22	AA	1412	C	N3-C2-O2	-7.40	116.72	121.90
57	BA	513	A	C5-C6-N1	7.40	121.40	117.70
57	BA	2407	A	C5-C6-N1	7.40	121.40	117.70
58	Ba	68	C	N3-C2-O2	-7.40	116.72	121.90
22	AA	182	A	C5-C6-N1	7.40	121.40	117.70
22	AA	295	C	N3-C2-O2	-7.40	116.72	121.90
22	AA	1119	C	N3-C2-O2	-7.40	116.72	121.90
30	BP	21	ARG	NE-CZ-NH1	7.40	124.00	120.30
51	B8	7	ARG	NE-CZ-NH1	7.40	124.00	120.30
57	BA	1103	A	C4-C5-C6	-7.40	113.30	117.00
57	BA	2433	A	C4-C5-C6	-7.40	113.30	117.00
57	BA	73	A	C4-C5-C6	-7.40	113.30	117.00
57	BA	2354	C	N3-C2-O2	-7.40	116.72	121.90
57	BA	151	C	N3-C2-O2	-7.40	116.72	121.90
57	BA	314	C	N3-C2-O2	-7.40	116.72	121.90
57	BA	1672	A	C5-C6-N1	7.40	121.40	117.70
22	AA	1016	A	C5-C6-N1	7.40	121.40	117.70
22	AA	1172	C	N3-C2-O2	-7.40	116.72	121.90
57	BA	1960	A	C5-C6-N1	7.40	121.40	117.70
22	AA	99	C	N3-C2-O2	-7.39	116.72	121.90
57	BA	52	A	C5-C6-N1	7.39	121.40	117.70
22	AA	186	C	N3-C2-O2	-7.39	116.73	121.90
22	AA	860	A	C5-C6-N1	7.39	121.40	117.70
48	B5	15	ARG	NE-CZ-NH2	7.39	124.00	120.30
57	BA	31	C	N3-C2-O2	-7.39	116.72	121.90
57	BA	742	A	C5-C6-N1	7.39	121.40	117.70
57	BA	844	A	C5-C6-N1	7.39	121.40	117.70
57	BA	1164	C	N3-C2-O2	-7.39	116.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1909	C	N3-C2-O2	-7.39	116.72	121.90
57	BA	1319	C	N3-C2-O2	-7.39	116.73	121.90
22	AA	47	C	N3-C2-O2	-7.39	116.73	121.90
36	BU	32	ARG	NE-CZ-NH2	7.39	124.00	120.30
57	BA	1639	C	N3-C2-O2	-7.39	116.73	121.90
57	BA	2377	A	N1-C6-N6	-7.39	114.17	118.60
57	BA	2652	C	N3-C2-O2	-7.39	116.73	121.90
57	BA	76	C	N3-C2-O2	-7.39	116.73	121.90
24	A3	63	C	N3-C2-O2	-7.39	116.73	121.90
57	BA	225	C	O4'-C1'-N1	7.39	114.11	108.20
22	AA	958	A	C4-C5-C6	-7.38	113.31	117.00
35	BD	181	ARG	NE-CZ-NH1	7.38	123.99	120.30
57	BA	815	C	N3-C2-O2	-7.38	116.73	121.90
57	BA	979	A	C5-C6-N1	7.38	121.39	117.70
57	BA	1007	C	N3-C2-O2	-7.38	116.73	121.90
57	BA	1345	C	N3-C2-O2	-7.38	116.73	121.90
57	BA	1488	C	N3-C2-O2	-7.38	116.73	121.90
57	BA	2042	A	C5-C6-N1	7.38	121.39	117.70
57	BA	2559	C	N3-C2-O2	-7.38	116.73	121.90
22	AA	196	A	C5-C6-N1	7.38	121.39	117.70
22	AA	270	A	C5-C6-N1	7.38	121.39	117.70
57	BA	592	A	C5-C6-N1	7.38	121.39	117.70
57	BA	1757	A	C5-C6-N1	7.38	121.39	117.70
22	AA	1203	C	O4'-C1'-N1	7.38	114.11	108.20
57	BA	2726	A	C4-C5-C6	-7.38	113.31	117.00
57	BA	2730	C	N3-C2-O2	-7.38	116.73	121.90
57	BA	2837	A	C5-C6-N1	7.38	121.39	117.70
57	BA	2856	A	C4-C5-C6	-7.38	113.31	117.00
10	AS	54	ARG	NE-CZ-NH1	7.38	123.99	120.30
24	A3	14	A	C5-C6-N1	7.38	121.39	117.70
57	BA	715	A	C5-C6-N1	7.38	121.39	117.70
57	BA	991	C	N3-C2-O2	-7.38	116.73	121.90
57	BA	1144	A	C5-C6-N1	7.38	121.39	117.70
57	BA	2806	C	N3-C2-O2	-7.38	116.74	121.90
22	AA	282	A	C5-C6-N1	7.38	121.39	117.70
22	AA	676	A	C5-C6-N1	7.38	121.39	117.70
22	AA	994	A	C5-C6-N1	7.38	121.39	117.70
22	AA	1180	A	C4-C5-C6	-7.38	113.31	117.00
57	BA	21	A	C5-C6-N1	7.38	121.39	117.70
57	BA	2153	C	N3-C2-O2	-7.38	116.74	121.90
22	AA	549	C	N3-C2-O2	-7.38	116.74	121.90
57	BA	922	C	O4'-C1'-N1	7.38	114.10	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	343	C	N3-C2-O2	-7.37	116.74	121.90
57	BA	382	A	C4-C5-C6	-7.37	113.31	117.00
57	BA	1597	A	C5-C6-N1	7.37	121.39	117.70
57	BA	1796	U	O4'-C1'-N1	7.37	114.10	108.20
22	AA	189	A	C5-C6-N1	7.37	121.39	117.70
22	AA	1011	C	N3-C2-O2	-7.37	116.74	121.90
22	AA	1448	C	N3-C2-O2	-7.37	116.74	121.90
57	BA	910	A	C5-C6-N1	7.37	121.39	117.70
57	BA	1302	A	N1-C6-N6	-7.37	114.18	118.60
57	BA	1347	A	N1-C6-N6	-7.37	114.18	118.60
57	BA	1668	A	C5-C6-N1	7.37	121.39	117.70
22	AA	23	C	N3-C2-O2	-7.37	116.74	121.90
22	AA	673	A	C5-C6-N1	7.37	121.39	117.70
22	AA	553	A	C5-C6-N1	7.37	121.38	117.70
57	BA	2263	C	N3-C2-O2	-7.37	116.74	121.90
57	BA	2469	A	C5-C6-N1	7.37	121.39	117.70
22	AA	1409	C	N3-C2-O2	-7.37	116.74	121.90
22	AA	908	A	N1-C6-N6	-7.37	114.18	118.60
57	BA	523	C	N3-C2-O2	-7.37	116.74	121.90
57	BA	792	A	C5-C6-N1	7.37	121.38	117.70
57	BA	1752	C	N3-C2-O2	-7.37	116.74	121.90
57	BA	2154	A	C5-C6-N1	7.37	121.38	117.70
57	BA	2774	C	N3-C2-O2	-7.37	116.75	121.90
3	AL	30	ARG	NE-CZ-NH1	7.36	123.98	120.30
57	BA	364	C	N3-C2-O2	-7.36	116.75	121.90
57	BA	2340	A	N1-C6-N6	-7.36	114.18	118.60
22	AA	381	C	N3-C2-O2	-7.36	116.75	121.90
57	BA	1268	A	C4-C5-C6	-7.36	113.32	117.00
22	AA	71	A	N1-C6-N6	-7.36	114.18	118.60
22	AA	1245	C	N3-C2-O2	-7.36	116.75	121.90
57	BA	281	C	N3-C2-O2	-7.36	116.75	121.90
57	BA	1637	A	C5-C6-N1	7.36	121.38	117.70
57	BA	1985	C	N3-C2-O2	-7.36	116.75	121.90
22	AA	513	C	N3-C2-O2	-7.36	116.75	121.90
57	BA	885	C	N3-C2-O2	-7.36	116.75	121.90
57	BA	1547	C	N3-C2-O2	-7.36	116.75	121.90
57	BA	781	A	C4-C5-C6	-7.36	113.32	117.00
45	BE	83	ARG	NE-CZ-NH1	-7.36	116.62	120.30
54	BG	91	ARG	NE-CZ-NH2	7.36	123.98	120.30
57	BA	1918	A	C4-C5-C6	-7.36	113.32	117.00
57	BA	2440	C	N3-C2-O2	-7.36	116.75	121.90
57	BA	2670	A	C5-C6-N1	7.36	121.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	882	C	N3-C2-O2	-7.35	116.75	121.90
22	AA	889	A	C4-C5-C6	-7.35	113.32	117.00
22	AA	379	C	N3-C2-O2	-7.35	116.75	121.90
57	BA	224	U	O4'-C1'-N1	7.35	114.08	108.20
57	BA	1335	C	N3-C2-O2	-7.35	116.75	121.90
57	BA	1548	A	C5-C6-N1	7.35	121.38	117.70
57	BA	1744	A	C5-C6-N1	7.35	121.38	117.70
57	BA	2036	C	N3-C2-O2	-7.35	116.75	121.90
22	AA	651	C	N3-C2-O2	-7.35	116.75	121.90
22	AA	806	C	N3-C2-O2	-7.35	116.75	121.90
22	AA	975	A	C5-C6-N1	7.35	121.38	117.70
57	BA	1505	A	C5-C6-N1	7.35	121.38	117.70
22	AA	44	A	C5-C6-N1	7.35	121.37	117.70
22	AA	694	A	C5-C6-N1	7.35	121.37	117.70
22	AA	793	U	N3-C2-O2	-7.35	117.06	122.20
57	BA	66	C	N3-C2-O2	-7.35	116.76	121.90
57	BA	204	A	C4-C5-C6	-7.35	113.33	117.00
57	BA	541	A	C5-C6-N1	7.35	121.37	117.70
57	BA	1518	C	N3-C2-O2	-7.35	116.76	121.90
57	BA	2442	C	N3-C2-O2	-7.35	116.76	121.90
57	BA	2639	A	C5-C6-N1	7.35	121.37	117.70
22	AA	315	A	C4-C5-C6	-7.35	113.33	117.00
22	AA	1216	A	C5-C6-N1	7.35	121.37	117.70
22	AA	431	A	C5-C6-N1	7.34	121.37	117.70
22	AA	931	C	N3-C2-O2	-7.34	116.76	121.90
50	B7	12	ARG	NE-CZ-NH2	7.34	123.97	120.30
57	BA	119	A	C4-C5-C6	-7.34	113.33	117.00
57	BA	1327	A	C4-C5-C6	-7.34	113.33	117.00
57	BA	1414	C	N3-C2-O2	-7.34	116.76	121.90
57	BA	706	A	C5-C6-N1	7.34	121.37	117.70
57	BA	2281	A	C4-C5-C6	-7.34	113.33	117.00
22	AA	1130	A	N1-C6-N6	-7.34	114.19	118.60
57	BA	670	A	C5-C6-N1	7.34	121.37	117.70
57	BA	2177	C	N3-C2-O2	-7.34	116.76	121.90
57	BA	2691	C	N3-C2-O2	-7.34	116.76	121.90
22	AA	373	A	N1-C6-N6	-7.34	114.20	118.60
22	AA	487	A	N1-C6-N6	-7.34	114.20	118.60
57	BA	1815	A	C5-C6-N1	7.34	121.37	117.70
57	BA	2753	A	C5-C6-N1	7.34	121.37	117.70
22	AA	1223	C	N3-C2-O2	-7.34	116.76	121.90
24	A3	35	C	N3-C2-O2	-7.34	116.76	121.90
57	BA	1359	A	C4-C5-C6	-7.34	113.33	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1179	A	C4-C5-C6	-7.34	113.33	117.00
57	BA	1254	A	N1-C6-N6	-7.34	114.20	118.60
57	BA	2482	A	C5-C6-N1	7.34	121.37	117.70
57	BA	2558	C	N3-C2-O2	-7.34	116.76	121.90
57	BA	2820	A	C5-C6-N1	7.34	121.37	117.70
22	AA	383	A	N1-C6-N6	-7.33	114.20	118.60
22	AA	396	C	N3-C2-O2	-7.33	116.77	121.90
57	BA	143	C	N3-C2-O2	-7.33	116.77	121.90
31	BQ	44	ARG	NE-CZ-NH2	7.33	123.97	120.30
57	BA	794	A	C5-C6-N1	7.33	121.37	117.70
57	BA	1625	C	N3-C2-O2	-7.33	116.77	121.90
22	AA	1275	A	C5-C6-N1	7.33	121.36	117.70
57	BA	354	A	C5-C6-N1	7.33	121.37	117.70
22	AA	738	C	N3-C2-O2	-7.33	116.77	121.90
57	BA	161	A	C4-C5-C6	-7.33	113.33	117.00
57	BA	731	C	N3-C2-O2	-7.33	116.77	121.90
57	BA	2039	U	O4'-C1'-N1	7.33	114.06	108.20
22	AA	808	C	N3-C2-O2	-7.33	116.77	121.90
22	AA	1380	U	O4'-C1'-N1	7.33	114.06	108.20
57	BA	2082	A	C5-C6-N1	7.33	121.36	117.70
57	BA	2267	A	C4-C5-C6	-7.33	113.34	117.00
22	AA	448	A	C4-C5-C6	-7.33	113.34	117.00
57	BA	1230	A	C5-C6-N1	7.33	121.36	117.70
57	BA	2467	C	N3-C2-O2	-7.33	116.77	121.90
22	AA	1037	C	N3-C2-O2	-7.33	116.77	121.90
57	BA	37	C	N3-C2-O2	-7.33	116.77	121.90
57	BA	675	A	C5-C6-N1	7.33	121.36	117.70
22	AA	328	C	N1-C2-O2	7.32	123.29	118.90
22	AA	1293	C	N3-C2-O2	-7.32	116.77	121.90
22	AA	1318	A	N1-C6-N6	-7.32	114.21	118.60
57	BA	255	A	C5-C6-N1	7.32	121.36	117.70
57	BA	1999	C	N3-C2-O2	-7.32	116.77	121.90
57	BA	2893	A	C5-C6-N1	7.32	121.36	117.70
57	BA	1096	A	C5-C6-N1	7.32	121.36	117.70
21	A1	358	ARG	NE-CZ-NH1	7.32	123.96	120.30
22	AA	325	A	C4-C5-C6	-7.32	113.34	117.00
22	AA	681	A	C5-C6-N1	7.32	121.36	117.70
57	BA	1165	A	C5-C6-N1	7.32	121.36	117.70
57	BA	2451	A	C4-C5-C6	-7.32	113.34	117.00
57	BA	311	A	C5-C6-N1	7.32	121.36	117.70
57	BA	1152	C	N3-C2-O2	-7.32	116.78	121.90
57	BA	1480	C	N3-C2-O2	-7.32	116.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	917	A	C5-C6-N1	7.32	121.36	117.70
57	BA	1020	A	C5-C6-N1	7.32	121.36	117.70
22	AA	1179	A	C5-C6-N1	7.32	121.36	117.70
57	BA	1854	A	C5-C6-N1	7.32	121.36	117.70
57	BA	2023	C	N3-C2-O2	-7.32	116.78	121.90
57	BA	899	A	C5-C6-N1	7.31	121.36	117.70
22	AA	780	A	C5-C6-N1	7.31	121.36	117.70
57	BA	102	U	O4'-C1'-N1	7.31	114.05	108.20
57	BA	111	A	C5-C6-N1	7.31	121.36	117.70
57	BA	346	A	C5-C6-N1	7.31	121.36	117.70
57	BA	592	A	C4-C5-C6	-7.31	113.34	117.00
22	AA	55	A	C5-C6-N1	7.31	121.36	117.70
22	AA	1497	G	N1-C6-O6	-7.31	115.51	119.90
24	A3	38	A	C4-C5-C6	-7.31	113.35	117.00
57	BA	660	C	N3-C2-O2	-7.31	116.78	121.90
57	BA	2368	C	N3-C2-O2	-7.31	116.78	121.90
57	BA	2515	C	N3-C2-O2	-7.31	116.78	121.90
22	AA	1171	A	C5-C6-N1	7.31	121.35	117.70
57	BA	20	C	N3-C2-O2	-7.31	116.78	121.90
57	BA	336	C	N3-C2-O2	-7.31	116.78	121.90
57	BA	1001	A	C5-C6-N1	7.31	121.35	117.70
57	BA	2006	C	N3-C2-O2	-7.31	116.78	121.90
57	BA	2785	C	N3-C2-O2	-7.31	116.78	121.90
22	AA	807	A	C5-C6-N1	7.31	121.35	117.70
57	BA	2649	C	N3-C2-O2	-7.31	116.78	121.90
22	AA	1092	A	C5-C6-N1	7.30	121.35	117.70
22	AA	1311	A	C4-C5-C6	-7.30	113.35	117.00
57	BA	485	C	N3-C2-O2	-7.30	116.79	121.90
57	BA	1150	C	N3-C2-O2	-7.30	116.79	121.90
57	BA	2799	A	C5-C6-N1	7.30	121.35	117.70
22	AA	370	C	N3-C2-O2	-7.30	116.79	121.90
57	BA	479	A	C4-C5-C6	-7.30	113.35	117.00
57	BA	1504	A	C4-C5-C6	-7.30	113.35	117.00
57	BA	1893	C	O4'-C1'-N1	7.30	114.04	108.20
57	BA	2248	C	N3-C2-O2	-7.30	116.79	121.90
22	AA	401	C	N3-C2-O2	-7.30	116.79	121.90
54	BG	177	ARG	NE-CZ-NH1	7.30	123.95	120.30
24	A3	24	C	N3-C2-O2	-7.30	116.79	121.90
57	BA	176	A	C5-C6-N1	7.30	121.35	117.70
57	BA	668	A	C4-C5-C6	-7.30	113.35	117.00
58	Ba	110	C	N3-C2-O2	-7.30	116.79	121.90
22	AA	1349	A	C4-C5-C6	-7.30	113.35	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1735	A	C5-C6-N1	7.30	121.35	117.70
22	AA	1028	C	N3-C2-O2	-7.29	116.79	121.90
57	BA	1114	C	N3-C2-O2	-7.29	116.79	121.90
57	BA	2636	C	O4'-C1'-N1	7.29	114.04	108.20
22	AA	98	A	C5-C6-N1	7.29	121.35	117.70
22	AA	1413	A	C5-C6-N1	7.29	121.35	117.70
24	A3	69	C	N3-C2-O2	-7.29	116.80	121.90
57	BA	172	A	C5-C6-N1	7.29	121.35	117.70
57	BA	1399	C	N3-C2-O2	-7.29	116.80	121.90
57	BA	1732	C	O4'-C1'-N1	7.29	114.03	108.20
22	AA	81	A	C5-C6-N1	7.29	121.34	117.70
57	BA	833	A	C5-C6-N1	7.29	121.34	117.70
57	BA	1291	C	N3-C2-O2	-7.29	116.80	121.90
57	BA	2091	C	N3-C2-O2	-7.29	116.80	121.90
22	AA	338	A	C5-C6-N1	7.29	121.34	117.70
22	AA	1109	C	N3-C2-O2	-7.29	116.80	121.90
57	BA	1977	A	C5-C6-N1	7.29	121.34	117.70
57	BA	2326	C	N3-C2-O2	-7.29	116.80	121.90
57	BA	1532	A	C4-C5-C6	-7.29	113.36	117.00
57	BA	2486	C	N3-C2-O2	-7.29	116.80	121.90
22	AA	451	A	C4-C5-C6	-7.28	113.36	117.00
22	AA	460	A	C4-C5-C6	-7.28	113.36	117.00
22	AA	915	A	C4-C5-C6	-7.28	113.36	117.00
46	B3	15	ARG	NE-CZ-NH2	7.28	123.94	120.30
57	BA	1522	A	C5-C6-N1	7.28	121.34	117.70
58	Ba	3	C	N3-C2-O2	-7.28	116.80	121.90
57	BA	800	A	C5-C6-N1	7.28	121.34	117.70
57	BA	1533	C	N3-C2-O2	-7.28	116.80	121.90
22	AA	33	A	C5-C6-N1	7.28	121.34	117.70
22	AA	634	C	N3-C2-O2	-7.28	116.80	121.90
57	BA	366	C	N3-C2-O2	-7.28	116.80	121.90
57	BA	743	A	C5-C6-N1	7.28	121.34	117.70
57	BA	1158	C	N3-C2-O2	-7.28	116.80	121.90
57	BA	1363	C	N3-C2-O2	-7.28	116.80	121.90
57	BA	1431	A	C5-C6-N1	7.28	121.34	117.70
57	BA	1727	C	N3-C2-O2	-7.28	116.80	121.90
22	AA	171	A	C5-C6-N1	7.28	121.34	117.70
58	Ba	101	A	N1-C6-N6	-7.28	114.23	118.60
22	AA	662	U	O4'-C1'-N1	7.28	114.02	108.20
57	BA	1469	A	C5-C6-N1	7.28	121.34	117.70
57	BA	2418	A	C4-C5-C6	-7.28	113.36	117.00
22	AA	523	A	C5-C6-N1	7.28	121.34	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	256	A	C5-C6-N1	7.28	121.34	117.70
57	BA	1196	C	N3-C2-O2	-7.28	116.81	121.90
22	AA	658	C	N3-C2-O2	-7.27	116.81	121.90
13	AU	16	ARG	NE-CZ-NH1	7.27	123.94	120.30
22	AA	747	A	C5-C6-N1	7.27	121.34	117.70
57	BA	644	A	C5-C6-N1	7.27	121.34	117.70
57	BA	1265	A	C5-C6-N1	7.27	121.34	117.70
57	BA	1868	C	N3-C2-O2	-7.27	116.81	121.90
22	AA	784	A	N1-C6-N6	-7.27	114.24	118.60
27	BK	133	ARG	NE-CZ-NH1	7.27	123.94	120.30
22	AA	848	C	N3-C2-O2	-7.27	116.81	121.90
22	AA	1429	A	C5-C6-N1	7.27	121.33	117.70
22	AA	1431	A	C5-C6-N1	7.27	121.33	117.70
57	BA	2776	A	N1-C6-N6	-7.27	114.24	118.60
57	BA	2469	A	N1-C6-N6	-7.27	114.24	118.60
22	AA	1	A	C5-C6-N1	7.27	121.33	117.70
57	BA	2451	A	C5-C6-N1	7.26	121.33	117.70
58	Ba	63	C	N3-C2-O2	-7.26	116.81	121.90
22	AA	1280	A	C5-C6-N1	7.26	121.33	117.70
57	BA	1711	A	C4-C5-C6	-7.26	113.37	117.00
57	BA	2043	C	N3-C2-O2	-7.26	116.82	121.90
57	BA	1269	A	C5-C6-N1	7.26	121.33	117.70
57	BA	2682	A	C5-C6-N1	7.26	121.33	117.70
58	Ba	58	A	C4-C5-C6	-7.26	113.37	117.00
22	AA	225	C	N3-C2-O2	-7.26	116.82	121.90
22	AA	912	C	N3-C2-O2	-7.26	116.82	121.90
23	A2	58	C	N3-C2-O2	-7.26	116.82	121.90
24	A3	22	A	C4-C5-C6	-7.26	113.37	117.00
45	BE	59	ARG	NE-CZ-NH2	7.26	123.93	120.30
57	BA	609	A	N1-C6-N6	-7.26	114.24	118.60
57	BA	1384	A	C4-C5-C6	-7.26	113.37	117.00
57	BA	1685	C	N3-C2-O2	-7.26	116.82	121.90
58	Ba	71	C	N3-C2-O2	-7.26	116.82	121.90
57	BA	922	C	N3-C2-O2	-7.26	116.82	121.90
57	BA	2739	U	O4'-C1'-N1	7.26	114.01	108.20
58	Ba	46	A	C4-C5-C6	-7.26	113.37	117.00
22	AA	303	A	C5-C6-N1	7.26	121.33	117.70
57	BA	1161	C	N3-C2-O2	-7.26	116.82	121.90
57	BA	1472	C	N3-C2-O2	-7.26	116.82	121.90
57	BA	1571	A	N1-C6-N6	-7.26	114.25	118.60
22	AA	573	A	C5-C6-N1	7.25	121.33	117.70
57	BA	2317	A	C4-C5-C6	-7.25	113.37	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1388	C	N3-C2-O2	-7.25	116.82	121.90
24	A3	15	G	O4'-C1'-N9	7.25	114.00	108.20
22	AA	1329	A	C5-C6-N1	7.25	121.33	117.70
57	BA	472	A	C5-C6-N1	7.25	121.33	117.70
57	BA	1991	U	O4'-C1'-N1	7.25	114.00	108.20
22	AA	465	A	N1-C6-N6	-7.25	114.25	118.60
57	BA	1969	A	C5-C6-N1	7.25	121.33	117.70
22	AA	490	C	N3-C2-O2	-7.25	116.83	121.90
57	BA	1902	C	N3-C2-O2	-7.25	116.83	121.90
22	AA	40	C	N3-C2-O2	-7.25	116.83	121.90
32	BR	118	ARG	NE-CZ-NH1	7.25	123.92	120.30
22	AA	74	A	C5-C6-N1	7.25	121.32	117.70
57	BA	393	C	N3-C2-O2	-7.25	116.83	121.90
57	BA	599	A	C5-C6-N1	7.25	121.32	117.70
57	BA	1947	C	N3-C2-O2	-7.25	116.83	121.90
58	Ba	49	C	N3-C2-O2	-7.25	116.83	121.90
22	AA	329	A	C5-C6-N1	7.24	121.32	117.70
22	AA	334	C	N3-C2-O2	-7.24	116.83	121.90
22	AA	602	A	C4-C5-C6	-7.24	113.38	117.00
22	AA	946	A	C5-C6-N1	7.24	121.32	117.70
22	AA	1046	A	C5-C6-N1	7.24	121.32	117.70
50	B7	39	ARG	NE-CZ-NH1	7.24	123.92	120.30
57	BA	455	C	N3-C2-O2	-7.24	116.83	121.90
57	BA	1261	C	N3-C2-O2	-7.24	116.83	121.90
57	BA	1701	A	C5-C6-N1	7.24	121.32	117.70
57	BA	2175	C	N3-C2-O2	-7.24	116.83	121.90
57	BA	2888	C	N3-C2-O2	-7.24	116.83	121.90
22	AA	1318	A	C5-C6-N1	7.24	121.32	117.70
57	BA	1580	A	C4-C5-C6	-7.24	113.38	117.00
57	BA	1722	A	C5-C6-N1	7.24	121.32	117.70
57	BA	265	A	C5-C6-N1	7.24	121.32	117.70
57	BA	1247	A	C4-C5-C6	-7.24	113.38	117.00
57	BA	1330	C	N3-C2-O2	-7.24	116.83	121.90
57	BA	1804	C	N3-C2-O2	-7.24	116.83	121.90
57	BA	2863	C	N3-C2-O2	-7.24	116.83	121.90
22	AA	316	C	N3-C2-O2	-7.24	116.83	121.90
57	BA	1848	A	C4-C5-C6	-7.24	113.38	117.00
57	BA	2521	C	N1-C2-O2	7.24	123.24	118.90
57	BA	428	A	C4-C5-C6	-7.24	113.38	117.00
57	BA	2369	A	C5-C6-N1	7.24	121.32	117.70
22	AA	415	A	N1-C6-N6	-7.23	114.26	118.60
22	AA	1476	A	C5-C6-N1	7.23	121.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	696	A	C5-C6-N1	7.23	121.32	117.70
57	BA	115	C	N3-C2-O2	-7.23	116.84	121.90
57	BA	238	C	N3-C2-O2	-7.23	116.84	121.90
57	BA	253	C	O4'-C1'-N1	7.23	113.99	108.20
57	BA	1392	A	C5-C6-N1	7.23	121.32	117.70
57	BA	2003	A	C5-C6-N1	7.23	121.32	117.70
58	Ba	113	C	N3-C2-O2	-7.23	116.84	121.90
22	AA	805	C	N3-C2-O2	-7.23	116.84	121.90
24	A3	66	C	N3-C2-O2	-7.23	116.84	121.90
57	BA	2486	C	O4'-C1'-N1	7.23	113.98	108.20
57	BA	1243	C	N3-C2-O2	-7.23	116.84	121.90
57	BA	1494	A	C4-C5-C6	-7.23	113.39	117.00
57	BA	1551	A	N1-C6-N6	-7.23	114.26	118.60
22	AA	321	A	C4-C5-C6	-7.23	113.39	117.00
22	AA	1434	A	C4-C5-C6	-7.23	113.39	117.00
24	A3	40	C	N3-C2-O2	-7.23	116.84	121.90
57	BA	2600	A	C5-C6-N1	7.23	121.31	117.70
58	Ba	118	C	N3-C2-O2	-7.23	116.84	121.90
57	BA	2439	A	O4'-C1'-N9	7.23	113.98	108.20
22	AA	349	A	C5-C6-N1	7.22	121.31	117.70
57	BA	340	A	C4-C5-C6	-7.22	113.39	117.00
57	BA	1503	A	C4-C5-C6	-7.22	113.39	117.00
57	BA	2129	C	O4'-C1'-N1	7.22	113.98	108.20
22	AA	896	C	N3-C2-O2	-7.22	116.84	121.90
22	AA	1032	G	O4'-C1'-N9	7.22	113.98	108.20
57	BA	1495	A	C5-C6-N1	7.22	121.31	117.70
57	BA	1821	A	C4-C5-C6	-7.22	113.39	117.00
22	AA	1280	A	C4-C5-C6	-7.22	113.39	117.00
57	BA	516	C	O4'-C1'-N1	7.22	113.98	108.20
57	BA	929	U	O4'-C1'-N1	7.22	113.98	108.20
57	BA	2566	A	C5-C6-N1	7.22	121.31	117.70
57	BA	723	C	O4'-C1'-N1	7.22	113.97	108.20
57	BA	784	G	O4'-C1'-N9	7.22	113.97	108.20
57	BA	1229	C	N3-C2-O2	-7.22	116.85	121.90
57	BA	1600	C	N3-C2-O2	-7.22	116.85	121.90
57	BA	2657	A	C5-C6-N1	7.22	121.31	117.70
22	AA	1437	A	C5-C6-N1	7.21	121.31	117.70
24	A3	68	C	N3-C2-O2	-7.21	116.85	121.90
57	BA	244	A	C4-C5-C6	-7.21	113.39	117.00
57	BA	449	A	N1-C6-N6	-7.21	114.27	118.60
57	BA	1403	A	C4-C5-C6	-7.21	113.39	117.00
57	BA	1874	C	N3-C2-O2	-7.21	116.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Ba	59	A	C5-C6-N1	7.21	121.31	117.70
9	AR	2	ARG	NE-CZ-NH1	7.21	123.91	120.30
22	AA	90	C	N3-C2-O2	-7.21	116.85	121.90
57	BA	2196	C	N3-C2-O2	-7.21	116.85	121.90
22	AA	389	A	C5-C6-N1	7.21	121.31	117.70
22	AA	1306	A	N1-C6-N6	-7.21	114.27	118.60
24	A3	36	A	C5-C6-N1	7.21	121.31	117.70
57	BA	92	U	O4'-C1'-N1	7.21	113.97	108.20
57	BA	492	A	C5-C6-N1	7.21	121.31	117.70
57	BA	990	A	C4-C5-C6	-7.21	113.39	117.00
57	BA	1532	A	C5-C6-N1	7.21	121.31	117.70
57	BA	677	A	C4-C5-C6	-7.21	113.39	117.00
57	BA	840	C	N3-C2-O2	-7.21	116.85	121.90
22	AA	486	U	O4'-C1'-N1	7.21	113.97	108.20
22	AA	1197	A	N1-C6-N6	-7.21	114.28	118.60
57	BA	572	A	N1-C6-N6	-7.21	114.28	118.60
57	BA	1531	C	N3-C2-O2	-7.21	116.85	121.90
58	Ba	19	C	N3-C2-O2	-7.21	116.85	121.90
22	AA	488	C	N3-C2-O2	-7.21	116.86	121.90
22	AA	572	A	C4-C5-C6	-7.21	113.40	117.00
57	BA	1290	C	N3-C2-O2	-7.21	116.86	121.90
22	AA	74	A	C4-C5-C6	-7.20	113.40	117.00
22	AA	392	C	N3-C2-O2	-7.20	116.86	121.90
22	AA	892	A	C5-C6-N1	7.20	121.30	117.70
22	AA	1344	C	N3-C2-O2	-7.20	116.86	121.90
57	BA	209	C	N3-C2-O2	-7.20	116.86	121.90
57	BA	2119	A	C5-C6-N1	7.20	121.30	117.70
57	BA	201	C	N3-C2-O2	-7.20	116.86	121.90
57	BA	2751	G	O4'-C1'-N9	7.20	113.96	108.20
22	AA	699	C	N3-C2-O2	-7.20	116.86	121.90
22	AA	739	C	N3-C2-O2	-7.20	116.86	121.90
22	AA	1462	C	N3-C2-O2	-7.20	116.86	121.90
57	BA	385	C	N3-C2-O2	-7.20	116.86	121.90
57	BA	1916	A	C5-C6-N1	7.20	121.30	117.70
57	BA	2206	C	N3-C2-O2	-7.20	116.86	121.90
9	AR	47	ARG	NE-CZ-NH1	7.20	123.90	120.30
57	BA	959	A	N1-C6-N6	-7.20	114.28	118.60
57	BA	1612	C	N3-C2-O2	-7.20	116.86	121.90
58	Ba	0	U	O4'-C1'-N1	7.20	113.96	108.20
22	AA	364	A	C5-C6-N1	7.20	121.30	117.70
57	BA	1728	C	N3-C2-O2	-7.20	116.86	121.90
57	BA	2381	A	C4-C5-C6	-7.20	113.40	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	67	C	N3-C2-O2	-7.20	116.86	121.90
22	AA	153	C	N3-C2-O2	-7.20	116.86	121.90
22	AA	1001	C	N3-C2-O2	-7.20	116.86	121.90
57	BA	634	C	N3-C2-O2	-7.20	116.86	121.90
57	BA	870	U	O4'-C1'-N1	7.19	113.96	108.20
22	AA	1236	A	N1-C6-N6	-7.19	114.28	118.60
57	BA	290	U	O4'-C1'-N1	7.19	113.95	108.20
57	BA	436	C	N3-C2-O2	-7.19	116.86	121.90
57	BA	1726	C	N3-C2-O2	-7.19	116.86	121.90
57	BA	2716	C	N3-C2-O2	-7.19	116.86	121.90
22	AA	34	C	N3-C2-O2	-7.19	116.87	121.90
57	BA	221	A	C5-C6-N1	7.19	121.30	117.70
57	BA	2003	A	C4-C5-C6	-7.19	113.41	117.00
58	Ba	17	C	N3-C2-O2	-7.19	116.87	121.90
58	Ba	114	C	N3-C2-O2	-7.19	116.87	121.90
22	AA	393	A	C4-C5-C6	-7.19	113.41	117.00
22	AA	1329	A	C4-C5-C6	-7.19	113.41	117.00
57	BA	945	A	C4-C5-C6	-7.19	113.41	117.00
57	BA	1704	C	N3-C2-O2	-7.19	116.87	121.90
57	BA	1608	A	C5-C6-N1	7.19	121.29	117.70
22	AA	1302	C	N3-C2-O2	-7.19	116.87	121.90
24	A3	62	C	N3-C2-O2	-7.18	116.87	121.90
57	BA	32	C	N3-C2-O2	-7.18	116.87	121.90
57	BA	1014	A	C5-C6-N1	7.18	121.29	117.70
22	AA	374	A	C4-C5-C6	-7.18	113.41	117.00
22	AA	1195	C	N3-C2-O2	-7.18	116.87	121.90
57	BA	414	C	N3-C2-O2	-7.18	116.87	121.90
57	BA	793	A	C5-C6-N1	7.18	121.29	117.70
57	BA	2513	A	C5-C6-N1	7.18	121.29	117.70
21	A1	50	ARG	NE-CZ-NH1	7.18	123.89	120.30
57	BA	2463	C	N3-C2-O2	-7.18	116.87	121.90
13	AU	68	ARG	NE-CZ-NH1	7.18	123.89	120.30
22	AA	1273	C	N3-C2-O2	-7.18	116.87	121.90
57	BA	505	A	C4-C5-C6	-7.18	113.41	117.00
57	BA	758	C	N3-C2-O2	-7.18	116.88	121.90
57	BA	2063	C	N3-C2-O2	-7.18	116.88	121.90
57	BA	2902	C	N3-C2-O2	-7.18	116.88	121.90
22	AA	277	C	N3-C2-O2	-7.18	116.88	121.90
22	AA	1136	C	N3-C2-O2	-7.18	116.88	121.90
57	BA	203	A	C5-C6-N1	7.18	121.29	117.70
57	BA	211	C	N3-C2-O2	-7.18	116.88	121.90
57	BA	1001	A	C4-C5-C6	-7.18	113.41	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1572	A	C5-C6-N1	7.18	121.29	117.70
57	BA	1591	A	C5-C6-N1	7.18	121.29	117.70
57	BA	2636	C	N3-C2-O2	-7.18	116.88	121.90
22	AA	900	A	C5-C6-N1	7.17	121.29	117.70
57	BA	1172	C	N3-C2-O2	-7.17	116.88	121.90
43	B1	10	ARG	NE-CZ-NH2	7.17	123.89	120.30
57	BA	1237	A	C4-C5-C6	-7.17	113.41	117.00
57	BA	2112	G	O4'-C1'-N9	7.17	113.94	108.20
57	BA	1998	A	C5-C6-N1	7.17	121.29	117.70
57	BA	2103	C	N3-C2-O2	-7.17	116.88	121.90
58	Ba	26	C	N3-C2-O2	-7.17	116.88	121.90
57	BA	331	C	N3-C2-O2	-7.17	116.88	121.90
57	BA	2795	C	N3-C2-O2	-7.17	116.88	121.90
22	AA	63	C	N3-C2-O2	-7.17	116.88	121.90
22	AA	339	C	N3-C2-O2	-7.17	116.88	121.90
22	AA	930	C	N3-C2-O2	-7.17	116.88	121.90
22	AA	206	C	N3-C2-O2	-7.17	116.88	121.90
22	AA	1357	A	C5-C6-N1	7.17	121.28	117.70
22	AA	1366	C	N3-C2-O2	-7.17	116.88	121.90
57	BA	1005	C	N3-C2-O2	-7.17	116.88	121.90
57	BA	2826	A	C5-C6-N1	7.17	121.28	117.70
57	BA	679	C	N3-C2-O2	-7.16	116.89	121.90
57	BA	958	U	O4'-C1'-N1	7.16	113.93	108.20
57	BA	1920	C	N3-C2-O2	-7.16	116.89	121.90
57	BA	2837	A	N1-C6-N6	-7.16	114.30	118.60
22	AA	1340	A	C4-C5-C6	-7.16	113.42	117.00
22	AA	282	A	C4-C5-C6	-7.16	113.42	117.00
22	AA	1396	A	C4-C5-C6	-7.16	113.42	117.00
57	BA	445	C	N3-C2-O2	-7.16	116.89	121.90
57	BA	1848	A	N1-C6-N6	-7.16	114.31	118.60
57	BA	2080	A	C5-C6-N1	7.16	121.28	117.70
57	BA	2520	C	N3-C2-O2	-7.16	116.89	121.90
57	BA	2830	C	N3-C2-O2	-7.16	116.89	121.90
7	AP	31	ARG	NE-CZ-NH1	7.16	123.88	120.30
57	BA	2198	A	C5-C6-N1	7.16	121.28	117.70
57	BA	2338	C	N3-C2-O2	-7.16	116.89	121.90
3	AL	98	ARG	NE-CZ-NH1	7.16	123.88	120.30
57	BA	1298	C	N3-C2-O2	-7.16	116.89	121.90
57	BA	2670	A	C4-C5-C6	-7.16	113.42	117.00
22	AA	1045	C	O4'-C1'-N1	7.15	113.92	108.20
57	BA	877	A	C4-C5-C6	-7.15	113.42	117.00
18	AG	154	ARG	NE-CZ-NH1	7.15	123.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	B1	73	ARG	NE-CZ-NH1	-7.15	116.72	120.30
57	BA	2108	A	C5-C6-N1	7.15	121.28	117.70
57	BA	2171	A	C5-C6-N1	7.15	121.28	117.70
57	BA	341	C	N3-C2-O2	-7.15	116.89	121.90
57	BA	1366	A	C4-C5-C6	-7.15	113.42	117.00
57	BA	2874	C	N3-C2-O2	-7.15	116.90	121.90
22	AA	66	A	N1-C6-N6	-7.15	114.31	118.60
22	AA	83	C	N3-C2-O2	-7.15	116.90	121.90
35	BD	202	ARG	NE-CZ-NH1	7.15	123.87	120.30
57	BA	1278	C	N3-C2-O2	-7.15	116.90	121.90
57	BA	13	A	C1'-O4'-C4'	-7.15	104.18	109.90
57	BA	2335	A	C5-C6-N1	7.15	121.27	117.70
22	AA	520	A	O4'-C1'-N9	7.14	113.92	108.20
22	AA	1163	A	C4-C5-C6	-7.14	113.43	117.00
24	A3	11	A	C5-C6-N1	7.14	121.27	117.70
36	BU	54	ARG	NE-CZ-NH1	7.14	123.87	120.30
57	BA	616	A	C5-C6-N1	7.14	121.27	117.70
57	BA	1552	A	C1'-O4'-C4'	-7.14	104.18	109.90
57	BA	2270	A	C4-C5-C6	-7.14	113.43	117.00
57	BA	2419	U	O4'-C1'-N1	7.14	113.92	108.20
22	AA	271	C	N3-C2-O2	-7.14	116.90	121.90
57	BA	1351	C	N3-C2-O2	-7.14	116.90	121.90
57	BA	2872	A	C4-C5-C6	-7.14	113.43	117.00
22	AA	909	A	C5-C6-N1	7.14	121.27	117.70
22	AA	1342	C	N3-C2-O2	-7.14	116.90	121.90
22	AA	1404	C	N3-C2-O2	-7.14	116.90	121.90
57	BA	1284	A	C4-C5-C6	-7.14	113.43	117.00
57	BA	1545	A	C4-C5-C6	-7.14	113.43	117.00
57	BA	2471	A	C4-C5-C6	-7.14	113.43	117.00
20	AI	108	ARG	NE-CZ-NH1	7.14	123.87	120.30
31	BQ	10	ARG	NE-CZ-NH2	7.14	123.87	120.30
57	BA	8	C	N3-C2-O2	-7.14	116.90	121.90
57	BA	84	A	C4-C5-C6	-7.14	113.43	117.00
57	BA	2033	A	C4-C5-C6	-7.14	113.43	117.00
57	BA	2632	A	C4-C5-C6	-7.14	113.43	117.00
57	BA	2738	A	C5-C6-N1	7.14	121.27	117.70
22	AA	600	A	C4-C5-C6	-7.14	113.43	117.00
40	BY	6	ARG	NE-CZ-NH1	7.14	123.87	120.30
57	BA	2703	C	N3-C2-O2	-7.14	116.90	121.90
22	AA	19	A	C5-C6-N1	7.14	121.27	117.70
22	AA	309	A	C4-C5-C6	-7.14	113.43	117.00
57	BA	719	C	N3-C2-O2	-7.14	116.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	912	C	N3-C2-O2	-7.14	116.91	121.90
57	BA	1178	C	N3-C2-O2	-7.14	116.90	121.90
57	BA	2300	C	N3-C2-O2	-7.14	116.90	121.90
57	BA	2783	U	O4'-C1'-N1	7.14	113.91	108.20
22	AA	681	A	C4-C5-C6	-7.13	113.43	117.00
22	AA	1022	A	C4-C5-C6	-7.13	113.43	117.00
22	AA	1339	A	C4-C5-C6	-7.13	113.43	117.00
22	AA	712	A	C4-C5-C6	-7.13	113.43	117.00
22	AA	1000	A	C5-C6-N1	7.13	121.27	117.70
57	BA	19	A	C5-C6-N1	7.13	121.27	117.70
57	BA	1072	C	N3-C2-O2	-7.13	116.91	121.90
57	BA	2666	C	N1-C2-O2	7.13	123.18	118.90
22	AA	607	A	C4-C5-C6	-7.13	113.43	117.00
22	AA	1360	A	N1-C6-N6	-7.13	114.32	118.60
57	BA	129	C	N3-C2-O2	-7.13	116.91	121.90
57	BA	2072	C	N3-C2-O2	-7.13	116.91	121.90
57	BA	2594	C	N3-C2-O2	-7.13	116.91	121.90
22	AA	51	A	C5-C6-N1	7.13	121.27	117.70
22	AA	746	A	C5-C6-N1	7.13	121.27	117.70
38	BW	11	ARG	NE-CZ-NH1	7.13	123.86	120.30
57	BA	1129	A	C4-C5-C6	-7.13	113.44	117.00
22	AA	16	A	C5-C6-N1	7.13	121.26	117.70
57	BA	429	A	C4-C5-C6	-7.13	113.44	117.00
57	BA	1784	A	N1-C6-N6	-7.13	114.32	118.60
57	BA	1908	C	N3-C2-O2	-7.13	116.91	121.90
57	BA	2035	G	O4'-C1'-N9	7.13	113.90	108.20
57	BA	2339	C	N3-C2-O2	-7.13	116.91	121.90
57	BA	2466	C	N3-C2-O2	-7.13	116.91	121.90
57	BA	2700	A	C4-C5-C6	-7.13	113.44	117.00
58	Ba	51	G	N1-C6-O6	-7.13	115.62	119.90
22	AA	1200	C	N1-C2-O2	7.13	123.18	118.90
53	BF	88	ARG	NE-CZ-NH2	7.13	123.86	120.30
57	BA	892	A	C5-C6-N1	7.13	121.26	117.70
57	BA	908	C	N3-C2-O2	-7.13	116.91	121.90
22	AA	642	A	C5-C6-N1	7.12	121.26	117.70
22	AA	1230	C	N3-C2-O2	-7.12	116.91	121.90
52	B9	4	ARG	NE-CZ-NH1	7.12	123.86	120.30
57	BA	64	A	C5-C6-N1	7.12	121.26	117.70
57	BA	353	C	N3-C2-O2	-7.12	116.91	121.90
57	BA	2017	U	N3-C2-O2	-7.12	117.21	122.20
18	AG	118	ARG	NE-CZ-NH1	7.12	123.86	120.30
57	BA	1244	A	C4-C5-C6	-7.12	113.44	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2009	A	C4-C5-C6	-7.12	113.44	117.00
57	BA	2794	C	N3-C2-O2	-7.12	116.91	121.90
57	BA	2900	A	C5-C6-N1	7.12	121.26	117.70
22	AA	101	A	C4-C5-C6	-7.12	113.44	117.00
57	BA	2096	C	N3-C2-O2	-7.12	116.92	121.90
57	BA	2146	C	N3-C2-O2	-7.12	116.92	121.90
12	AT	23	ARG	NE-CZ-NH1	7.12	123.86	120.30
22	AA	243	A	C4-C5-C6	-7.12	113.44	117.00
22	AA	708	C	N3-C2-O2	-7.12	116.92	121.90
57	BA	1278	C	O4'-C1'-N1	7.12	113.89	108.20
57	BA	2362	C	N3-C2-O2	-7.12	116.92	121.90
57	BA	2654	A	C4-C5-C6	-7.12	113.44	117.00
22	AA	635	A	C5-C6-N1	7.12	121.26	117.70
22	AA	990	C	N3-C2-O2	-7.12	116.92	121.90
57	BA	1836	C	N3-C2-O2	-7.12	116.92	121.90
24	A3	76	C	N3-C2-O2	-7.12	116.92	121.90
37	BV	78	ARG	NE-CZ-NH2	7.12	123.86	120.30
45	BE	169	ARG	NE-CZ-NH2	7.12	123.86	120.30
57	BA	44	A	C4-C5-C6	-7.12	113.44	117.00
57	BA	1044	C	N3-C2-O2	-7.12	116.92	121.90
57	BA	1304	A	C4-C5-C6	-7.12	113.44	117.00
57	BA	2377	A	O4'-C1'-N9	7.12	113.89	108.20
22	AA	728	A	C4-C5-C6	-7.11	113.44	117.00
57	BA	1463	C	N3-C2-O2	-7.11	116.92	121.90
57	BA	2050	C	N3-C2-O2	-7.11	116.92	121.90
22	AA	715	A	C4-C5-C6	-7.11	113.44	117.00
22	AA	940	C	N3-C2-O2	-7.11	116.92	121.90
22	AA	1204	A	C5-C6-N1	7.11	121.25	117.70
22	AA	1460	C	N3-C2-O2	-7.11	116.92	121.90
23	A2	22	G	O4'-C1'-N9	7.11	113.89	108.20
23	A2	33	A	N1-C6-N6	-7.11	114.33	118.60
57	BA	655	A	C4-C5-C6	-7.11	113.44	117.00
57	BA	2821	A	C5-C6-N1	7.11	121.25	117.70
22	AA	309	A	C5-C6-N1	7.11	121.25	117.70
32	BR	2	ARG	NE-CZ-NH1	7.11	123.86	120.30
57	BA	282	A	C5-C6-N1	7.11	121.25	117.70
57	BA	2158	A	C5-C6-N1	7.11	121.25	117.70
22	AA	356	A	C4-C5-C6	-7.11	113.45	117.00
22	AA	1378	C	N3-C2-O2	-7.11	116.92	121.90
57	BA	41	C	N3-C2-O2	-7.11	116.92	121.90
57	BA	1805	A	C5-C6-N1	7.11	121.25	117.70
57	BA	1039	A	N1-C6-N6	-7.11	114.34	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1145	C	N3-C2-O2	-7.11	116.93	121.90
57	BA	1653	G	O4'-C1'-N9	7.11	113.88	108.20
57	BA	2501	C	N3-C2-O2	-7.11	116.93	121.90
22	AA	579	A	C4-C5-C6	-7.10	113.45	117.00
22	AA	629	A	C5-C6-N1	7.10	121.25	117.70
22	AA	1093	A	C4-C5-C6	-7.10	113.45	117.00
22	AA	1128	C	N3-C2-O2	-7.10	116.93	121.90
22	AA	336	A	C4-C5-C6	-7.10	113.45	117.00
22	AA	1022	A	C5-C6-N1	7.10	121.25	117.70
57	BA	492	A	C4-C5-C6	-7.10	113.45	117.00
57	BA	1148	U	O4'-C1'-N1	7.10	113.88	108.20
57	BA	1516	G	O4'-C1'-N9	7.10	113.88	108.20
57	BA	1889	A	C5-C6-N1	7.10	121.25	117.70
22	AA	368	U	N3-C2-O2	-7.10	117.23	122.20
57	BA	1184	U	O4'-C1'-N1	7.10	113.88	108.20
57	BA	142	A	C5-C6-N1	7.10	121.25	117.70
57	BA	702	U	O4'-C1'-N1	7.10	113.88	108.20
57	BA	2025	C	N3-C2-O2	-7.10	116.93	121.90
57	BA	2377	A	C5-C6-N1	7.10	121.25	117.70
57	BA	2626	C	N3-C2-O2	-7.10	116.93	121.90
22	AA	842	U	N3-C2-O2	-7.10	117.23	122.20
58	Ba	34	A	C5-C6-N1	7.10	121.25	117.70
22	AA	83	C	O4'-C1'-N1	7.09	113.88	108.20
22	AA	129	A	C4-C5-C6	-7.09	113.45	117.00
22	AA	355	C	N3-C2-O2	-7.09	116.93	121.90
22	AA	868	C	N3-C2-O2	-7.09	116.93	121.90
28	BN	120	ARG	NE-CZ-NH2	7.09	123.85	120.30
57	BA	1030	C	N3-C2-O2	-7.09	116.93	121.90
57	BA	1592	C	N3-C2-O2	-7.09	116.93	121.90
57	BA	2220	U	O4'-C1'-N1	7.09	113.87	108.20
57	BA	89	A	C4-C5-C6	-7.09	113.45	117.00
57	BA	942	G	C8-N9-C4	-7.09	103.56	106.40
22	AA	383	A	C5-C6-N1	7.09	121.25	117.70
22	AA	729	A	C5-C6-N1	7.09	121.25	117.70
22	AA	1287	A	C5-C6-N1	7.09	121.25	117.70
22	AA	1483	A	N1-C6-N6	-7.09	114.35	118.60
57	BA	1955	U	O4'-C1'-N1	7.09	113.87	108.20
57	BA	2424	C	C3'-C2'-C1'	7.09	107.17	101.50
22	AA	1263	C	N3-C2-O2	-7.09	116.94	121.90
57	BA	236	C	N3-C2-O2	-7.09	116.94	121.90
57	BA	1251	C	N3-C2-O2	-7.09	116.94	121.90
22	AA	280	C	N3-C2-O2	-7.09	116.94	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	602	A	C5-C6-N1	7.09	121.24	117.70
57	BA	1957	C	N3-C2-O2	-7.09	116.94	121.90
57	BA	2065	C	N3-C2-O2	-7.09	116.94	121.90
22	AA	810	C	N3-C2-O2	-7.08	116.94	121.90
22	AA	923	A	N1-C6-N6	-7.08	114.35	118.60
22	AA	414	A	C4-C5-C6	-7.08	113.46	117.00
57	BA	1174	U	O4'-C1'-N1	7.08	113.87	108.20
22	AA	908	A	C5-C6-N1	7.08	121.24	117.70
57	BA	1934	C	N3-C2-O2	-7.08	116.94	121.90
57	BA	2614	A	C4-C5-C6	-7.08	113.46	117.00
57	BA	2752	C	N3-C4-C5	7.08	124.73	121.90
22	AA	1368	A	C4-C5-C6	-7.08	113.46	117.00
22	AA	10	A	C5-C6-N1	7.08	121.24	117.70
22	AA	412	A	O4'-C1'-N9	7.08	113.86	108.20
22	AA	694	A	N1-C6-N6	-7.08	114.35	118.60
22	AA	1317	C	N3-C2-O2	-7.08	116.94	121.90
57	BA	146	A	C5-C6-N1	7.08	121.24	117.70
57	BA	372	G	O4'-C1'-N9	7.08	113.86	108.20
57	BA	1843	C	N3-C2-O2	-7.08	116.94	121.90
57	BA	2662	A	C3'-C2'-C1'	7.08	107.16	101.50
57	BA	1413	A	C5-C6-N1	7.08	121.24	117.70
22	AA	783	C	N3-C2-O2	-7.08	116.95	121.90
24	A3	44	A	N1-C6-N6	-7.08	114.36	118.60
57	BA	126	A	C4-C5-C6	-7.08	113.46	117.00
57	BA	216	A	C4-C5-C6	-7.08	113.46	117.00
57	BA	1200	C	N3-C2-O2	-7.08	116.95	121.90
57	BA	1895	C	N3-C2-O2	-7.08	116.95	121.90
2	AK	36	ARG	NE-CZ-NH1	7.07	123.84	120.30
22	AA	1111	A	C4-C5-C6	-7.07	113.46	117.00
57	BA	96	C	N3-C2-O2	-7.07	116.95	121.90
57	BA	241	A	C5-C6-N1	7.07	121.24	117.70
57	BA	1924	C	N3-C2-O2	-7.07	116.95	121.90
57	BA	2796	U	O4'-C1'-N1	7.07	113.86	108.20
57	BA	2840	C	N3-C2-O2	-7.07	116.95	121.90
57	BA	898	C	N3-C2-O2	-7.07	116.95	121.90
57	BA	1057	A	C5-C6-N1	7.07	121.24	117.70
57	BA	1053	C	N3-C2-O2	-7.07	116.95	121.90
57	BA	1871	A	C5-C6-N1	7.07	121.23	117.70
57	BA	2448	A	C4-C5-C6	-7.07	113.47	117.00
57	BA	632	A	C5-C6-N1	7.07	121.23	117.70
57	BA	1260	A	C5-C6-N1	7.07	121.23	117.70
22	AA	2	A	C4-C5-C6	-7.07	113.47	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1265	C	N3-C2-O2	-7.07	116.95	121.90
57	BA	374	A	C5-C6-N1	7.07	121.23	117.70
21	A1	269	ARG	NE-CZ-NH1	7.07	123.83	120.30
57	BA	95	A	C4-C5-C6	-7.07	113.47	117.00
57	BA	1821	A	C5-C6-N1	7.07	121.23	117.70
57	BA	2901	C	N3-C2-O2	-7.07	116.95	121.90
22	AA	183	C	N3-C2-O2	-7.06	116.95	121.90
22	AA	792	A	C4-C5-C6	-7.06	113.47	117.00
22	AA	1433	A	C4-C5-C6	-7.06	113.47	117.00
57	BA	106	C	N3-C2-O2	-7.06	116.96	121.90
57	BA	2020	A	C4-C5-C6	-7.06	113.47	117.00
57	BA	2461	A	C5-C6-N1	7.06	121.23	117.70
58	Ba	104	A	C4-C5-C6	-7.06	113.47	117.00
57	BA	274	C	N3-C2-O2	-7.06	116.96	121.90
57	BA	1088	A	C5-C6-N1	7.06	121.23	117.70
57	BA	2793	C	N3-C2-O2	-7.06	116.96	121.90
58	Ba	8	C	N3-C2-O2	-7.06	116.96	121.90
22	AA	124	C	N3-C2-O2	-7.06	116.96	121.90
22	AA	248	C	N3-C2-O2	-7.06	116.96	121.90
22	AA	1167	A	C4-C5-C6	-7.06	113.47	117.00
57	BA	756	A	C4-C5-C6	-7.06	113.47	117.00
57	BA	2061	G	P-O3'-C3'	7.06	128.17	119.70
57	BA	2350	C	N3-C2-O2	-7.06	116.96	121.90
58	Ba	58	A	C5-C6-N1	7.06	121.23	117.70
22	AA	1027	C	N3-C2-O2	-7.06	116.96	121.90
22	AA	1214	C	N3-C2-O2	-7.06	116.96	121.90
38	BW	88	ARG	NE-CZ-NH2	7.06	123.83	120.30
57	BA	1307	A	C4-C5-C6	-7.06	113.47	117.00
57	BA	1731	G	O4'-C1'-N9	7.06	113.85	108.20
57	BA	2064	C	N3-C2-O2	-7.06	116.96	121.90
22	AA	918	A	C4-C5-C6	-7.06	113.47	117.00
57	BA	845	A	C4-C5-C6	-7.06	113.47	117.00
57	BA	1357	C	O4'-C1'-N1	7.06	113.84	108.20
57	BA	1712	U	O4'-C1'-N1	7.06	113.84	108.20
57	BA	2465	C	N3-C2-O2	-7.06	116.96	121.90
22	AA	528	C	N3-C2-O2	-7.05	116.96	121.90
57	BA	965	C	N3-C2-O2	-7.05	116.96	121.90
57	BA	2241	A	C4-C5-C6	-7.05	113.47	117.00
57	BA	1048	A	C4-C5-C6	-7.05	113.47	117.00
22	AA	172	A	C5-C6-N1	7.05	121.22	117.70
22	AA	545	C	N3-C2-O2	-7.05	116.96	121.90
22	AA	167	A	C4-C5-C6	-7.05	113.47	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	825	A	C5-C6-N1	7.05	121.22	117.70
22	AA	1161	C	N3-C2-O2	-7.05	116.97	121.90
24	A3	3	C	N3-C2-O2	-7.05	116.97	121.90
57	BA	1579	A	C4-C5-C6	-7.05	113.47	117.00
57	BA	1838	C	N3-C2-O2	-7.05	116.97	121.90
57	BA	2792	A	C4-C5-C6	-7.05	113.48	117.00
22	AA	941	G	O4'-C1'-N9	7.05	113.84	108.20
57	BA	167	A	C5-C6-N1	7.05	121.22	117.70
57	BA	417	C	O4'-C1'-N1	7.05	113.84	108.20
57	BA	591	U	O4'-C1'-N1	7.05	113.84	108.20
57	BA	1322	A	C5-C6-N1	7.05	121.22	117.70
57	BA	2875	C	N3-C2-O2	-7.05	116.97	121.90
22	AA	612	C	N3-C2-O2	-7.04	116.97	121.90
29	BO	17	ARG	NE-CZ-NH1	7.04	123.82	120.30
57	BA	2512	C	N3-C2-O2	-7.04	116.97	121.90
22	AA	807	A	C4-C5-C6	-7.04	113.48	117.00
24	A3	36	A	C4-C5-C6	-7.04	113.48	117.00
22	AA	579	A	C5-C6-N1	7.04	121.22	117.70
22	AA	1237	C	N3-C2-O2	-7.04	116.97	121.90
57	BA	422	A	C4-C5-C6	-7.04	113.48	117.00
57	BA	800	A	C4-C5-C6	-7.04	113.48	117.00
57	BA	2327	A	C4-C5-C6	-7.04	113.48	117.00
57	BA	2450	A	O4'-C1'-N9	7.04	113.83	108.20
22	AA	1289	A	C4-C5-C6	-7.04	113.48	117.00
30	BP	41	ARG	NE-CZ-NH1	7.04	123.82	120.30
57	BA	2480	C	N3-C2-O2	-7.04	116.97	121.90
22	AA	974	A	C4-C5-C6	-7.04	113.48	117.00
22	AA	1055	A	C4-C5-C6	-7.04	113.48	117.00
22	AA	1080	A	C4-C5-C6	-7.04	113.48	117.00
22	AA	1120	C	N3-C2-O2	-7.04	116.97	121.90
57	BA	460	A	C5-C6-N1	7.04	121.22	117.70
57	BA	782	A	C5-C6-N1	7.04	121.22	117.70
57	BA	1539	U	O4'-C1'-N1	7.04	113.83	108.20
57	BA	1590	A	C5-C6-N1	7.04	121.22	117.70
22	AA	78	A	C4-C5-C6	-7.03	113.48	117.00
22	AA	502	A	N1-C6-N6	-7.03	114.38	118.60
22	AA	865	A	C5-C6-N1	7.03	121.22	117.70
22	AA	937	A	C4-C5-C6	-7.03	113.48	117.00
22	AA	1239	A	C4-C5-C6	-7.03	113.48	117.00
57	BA	796	C	N3-C2-O2	-7.03	116.98	121.90
57	BA	981	A	C4-C5-C6	-7.03	113.48	117.00
57	BA	1700	A	C5-C6-N1	7.03	121.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2284	A	N1-C6-N6	-7.03	114.38	118.60
22	AA	959	A	N1-C6-N6	-7.03	114.38	118.60
57	BA	544	C	N1-C2-O2	7.03	123.12	118.90
57	BA	2381	A	C5-C6-N1	7.03	121.22	117.70
57	BA	2699	C	N3-C2-O2	-7.03	116.98	121.90
57	BA	352	A	C5-C6-N1	7.03	121.21	117.70
57	BA	2311	A	C4-C5-C6	-7.03	113.49	117.00
22	AA	461	A	C4-C5-C6	-7.03	113.49	117.00
57	BA	554	U	O4'-C1'-N1	7.03	113.82	108.20
57	BA	1014	A	C4-C5-C6	-7.03	113.49	117.00
22	AA	174	A	C4-C5-C6	-7.02	113.49	117.00
57	BA	1780	A	C5-C6-N1	7.02	121.21	117.70
22	AA	736	C	N3-C2-O2	-7.02	116.98	121.90
24	A3	49	C	N3-C2-O2	-7.02	116.98	121.90
24	A3	67	C	N3-C2-O2	-7.02	116.98	121.90
57	BA	1477	A	C5-C6-N1	7.02	121.21	117.70
57	BA	1902	C	O4'-C1'-N1	7.02	113.82	108.20
57	BA	2260	C	N3-C2-O2	-7.02	116.99	121.90
22	AA	647	C	N3-C2-O2	-7.02	116.99	121.90
22	AA	436	C	N3-C2-O2	-7.02	116.99	121.90
22	AA	1395	C	N3-C2-O2	-7.02	116.99	121.90
22	AA	1102	A	C5-C6-N1	7.01	121.21	117.70
57	BA	231	A	C4-C5-C6	-7.01	113.49	117.00
57	BA	2143	C	N3-C2-O2	-7.01	116.99	121.90
57	BA	42	A	C4-C5-C6	-7.01	113.49	117.00
57	BA	398	C	N3-C2-O2	-7.01	116.99	121.90
57	BA	918	A	C4-C5-C6	-7.01	113.49	117.00
57	BA	1794	A	C4-C5-C6	-7.01	113.49	117.00
22	AA	938	A	C4-C5-C6	-7.01	113.49	117.00
22	AA	989	U	O4'-C1'-N1	7.01	113.81	108.20
22	AA	1107	C	N3-C2-O2	-7.01	116.99	121.90
57	BA	179	C	O4'-C1'-N1	7.01	113.81	108.20
57	BA	242	G	C1'-O4'-C4'	-7.01	104.29	109.90
57	BA	1091	G	O4'-C1'-N9	7.01	113.81	108.20
57	BA	1941	C	O4'-C1'-N1	7.01	113.81	108.20
57	BA	2297	A	C4-C5-C6	-7.01	113.50	117.00
57	BA	584	C	N3-C2-O2	-7.01	116.99	121.90
22	AA	456	A	C4-C5-C6	-7.01	113.50	117.00
23	A2	57	C	N3-C2-O2	-7.01	117.00	121.90
57	BA	1181	U	O4'-C1'-N1	7.01	113.81	108.20
57	BA	1764	C	N3-C2-O2	-7.01	117.00	121.90
57	BA	2404	U	O4'-C1'-N1	7.01	113.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2476	A	C4-C5-C6	-7.01	113.50	117.00
57	BA	909	A	C5-C6-N1	7.00	121.20	117.70
57	BA	2755	C	N3-C2-O2	-7.00	117.00	121.90
58	Ba	27	C	N3-C2-O2	-7.00	117.00	121.90
22	AA	623	C	N3-C2-O2	-7.00	117.00	121.90
57	BA	109	C	N3-C2-O2	-7.00	117.00	121.90
22	AA	901	A	N1-C6-N6	-7.00	114.40	118.60
22	AA	1327	C	N3-C2-O2	-7.00	117.00	121.90
57	BA	1574	C	N3-C2-O2	-7.00	117.00	121.90
15	AD	46	ARG	NE-CZ-NH1	7.00	123.80	120.30
22	AA	1146	A	C4-C5-C6	-7.00	113.50	117.00
22	AA	1354	U	O4'-C1'-N1	7.00	113.80	108.20
57	BA	64	A	C4-C5-C6	-7.00	113.50	117.00
19	AH	113	ARG	NE-CZ-NH1	7.00	123.80	120.30
24	A3	13	C	O4'-C1'-N1	7.00	113.80	108.20
57	BA	2080	A	C4-C5-C6	-7.00	113.50	117.00
20	AI	121	ARG	NE-CZ-NH1	7.00	123.80	120.30
22	AA	831	A	C5-C6-N1	7.00	121.20	117.70
57	BA	1509	A	C4-C5-C6	-7.00	113.50	117.00
57	BA	2804	U	O4'-C1'-N1	7.00	113.80	108.20
57	BA	16	C	N3-C2-O2	-6.99	117.00	121.90
57	BA	1289	C	N3-C2-O2	-6.99	117.00	121.90
57	BA	490	C	N1-C2-O2	6.99	123.09	118.90
58	Ba	52	A	C4-C5-C6	-6.99	113.50	117.00
22	AA	96	U	O4'-C1'-N1	6.99	113.79	108.20
22	AA	782	A	C5-C6-N1	6.99	121.20	117.70
57	BA	861	A	N1-C6-N6	-6.99	114.41	118.60
57	BA	1147	A	C4-C5-C6	-6.99	113.50	117.00
57	BA	2052	A	C5-C6-N1	6.99	121.20	117.70
57	BA	2738	A	C4-C5-C6	-6.99	113.50	117.00
2	AK	12	ARG	NE-CZ-NH1	6.99	123.80	120.30
57	BA	735	A	C5-C6-N1	6.99	121.19	117.70
57	BA	2314	A	C5-C6-N1	6.99	121.19	117.70
57	BA	2519	U	O4'-C1'-N1	6.99	113.79	108.20
22	AA	1500	A	N1-C6-N6	-6.99	114.41	118.60
22	AA	1216	A	C4-C5-C6	-6.98	113.51	117.00
22	AA	1333	A	C5-C6-N1	6.98	121.19	117.70
22	AA	737	C	N3-C2-O2	-6.98	117.01	121.90
57	BA	1029	A	C5-C6-N1	6.98	121.19	117.70
57	BA	2090	A	C4-C5-C6	-6.98	113.51	117.00
22	AA	1138	G	N3-C4-C5	-6.98	125.11	128.60
22	AA	1312	G	N1-C6-O6	-6.98	115.71	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	649	A	C4-C5-C6	-6.98	113.51	117.00
22	AA	950	U	O4'-C1'-N1	6.98	113.78	108.20
26	BJ	93	ARG	NE-CZ-NH1	6.98	123.79	120.30
57	BA	692	C	N1-C2-O2	6.98	123.08	118.90
57	BA	1775	U	O4'-C1'-N1	6.98	113.78	108.20
57	BA	1785	A	C5-C6-N1	6.98	121.19	117.70
22	AA	221	C	O4'-C1'-N1	6.97	113.78	108.20
29	BO	31	ARG	NE-CZ-NH1	6.97	123.79	120.30
57	BA	2013	A	C5-C6-N1	6.97	121.19	117.70
57	BA	722	A	C5-C6-N1	6.97	121.19	117.70
57	BA	983	A	N1-C6-N6	-6.97	114.42	118.60
22	AA	797	C	N3-C2-O2	-6.97	117.02	121.90
57	BA	2332	C	N3-C2-O2	-6.97	117.02	121.90
22	AA	1288	A	C4-C5-C6	-6.97	113.52	117.00
57	BA	218	A	N1-C6-N6	-6.97	114.42	118.60
57	BA	391	A	N1-C6-N6	-6.97	114.42	118.60
22	AA	924	C	N3-C2-O2	-6.96	117.02	121.90
57	BA	249	C	O4'-C1'-N1	6.96	113.77	108.20
57	BA	1077	A	C4-C5-C6	-6.96	113.52	117.00
57	BA	1385	A	C5-C6-N1	6.96	121.18	117.70
58	Ba	88	C	N1-C2-O2	6.96	123.08	118.90
22	AA	984	C	N3-C2-O2	-6.96	117.03	121.90
57	BA	1207	C	N3-C2-O2	-6.96	117.03	121.90
57	BA	1498	C	N3-C2-O2	-6.96	117.03	121.90
57	BA	1772	A	C4-C5-C6	-6.96	113.52	117.00
22	AA	238	A	C4-C5-C6	-6.96	113.52	117.00
57	BA	2199	A	C4-C5-C6	-6.96	113.52	117.00
22	AA	389	A	C4-C5-C6	-6.96	113.52	117.00
22	AA	1098	C	N3-C2-O2	-6.96	117.03	121.90
57	BA	1477	A	C4-C5-C6	-6.96	113.52	117.00
57	BA	2434	A	C4-C5-C6	-6.96	113.52	117.00
22	AA	1308	U	O4'-C1'-N1	6.96	113.77	108.20
57	BA	739	A	C4-C5-C6	-6.96	113.52	117.00
57	BA	2725	A	C5-C6-N1	6.96	121.18	117.70
57	BA	2745	C	N3-C2-O2	-6.96	117.03	121.90
58	Ba	73	A	C5-C6-N1	6.96	121.18	117.70
2	AK	52	ARG	NE-CZ-NH1	6.96	123.78	120.30
41	BZ	9	ARG	NE-CZ-NH1	6.96	123.78	120.30
57	BA	2430	A	O4'-C1'-N9	6.96	113.76	108.20
22	AA	81	A	C4-C5-C6	-6.95	113.52	117.00
22	AA	1246	A	C4-C5-C6	-6.95	113.52	117.00
57	BA	47	C	N3-C2-O2	-6.95	117.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	439	A	C5-C6-N1	6.95	121.18	117.70
57	BA	1304	A	C5-C6-N1	6.95	121.18	117.70
57	BA	2728	U	O4'-C1'-N1	6.95	113.76	108.20
57	BA	979	A	C4-C5-C6	-6.95	113.52	117.00
24	A3	39	A	C4-C5-C6	-6.95	113.52	117.00
57	BA	447	A	C5-C6-N1	6.95	121.17	117.70
22	AA	47	C	O4'-C1'-N1	6.95	113.76	108.20
22	AA	525	C	N3-C2-O2	-6.95	117.03	121.90
57	BA	631	A	C4-C5-C6	-6.95	113.53	117.00
57	BA	946	C	N3-C2-O2	-6.95	117.04	121.90
57	BA	1634	A	C5-C6-N1	6.95	121.17	117.70
57	BA	2198	A	C4-C5-C6	-6.95	113.53	117.00
22	AA	58	C	N1-C2-O2	6.95	123.07	118.90
22	AA	913	A	C4-C5-C6	-6.95	113.53	117.00
32	BR	4	ARG	NE-CZ-NH2	-6.95	116.83	120.30
22	AA	757	U	O4'-C1'-N1	6.95	113.76	108.20
22	AA	1410	A	C4-C5-C6	-6.95	113.53	117.00
57	BA	2108	A	C4-C5-C6	-6.95	113.53	117.00
57	BA	970	U	O4'-C1'-N1	6.94	113.75	108.20
57	BA	1876	A	C4-C5-C6	-6.94	113.53	117.00
57	BA	1049	C	N3-C2-O2	-6.94	117.04	121.90
57	BA	1786	A	C4-C5-C6	-6.94	113.53	117.00
57	BA	1885	A	C5-C6-N1	6.94	121.17	117.70
57	BA	2560	A	C4-C5-C6	-6.94	113.53	117.00
22	AA	162	A	C5-C6-N1	6.94	121.17	117.70
57	BA	442	G	O4'-C1'-N9	6.94	113.75	108.20
57	BA	1557	C	N3-C2-O2	-6.94	117.04	121.90
57	BA	2285	C	N3-C2-O2	-6.94	117.04	121.90
57	BA	851	C	N3-C2-O2	-6.94	117.04	121.90
57	BA	2000	C	N3-C2-O2	-6.94	117.04	121.90
22	AA	262	A	C4-C5-C6	-6.93	113.53	117.00
22	AA	872	A	C4-C5-C6	-6.93	113.53	117.00
57	BA	1405	U	O4'-C1'-N1	6.93	113.75	108.20
57	BA	1745	A	C4-C5-C6	-6.93	113.53	117.00
57	BA	1928	A	C4-C5-C6	-6.93	113.53	117.00
3	AL	55	ARG	NE-CZ-NH1	6.93	123.77	120.30
22	AA	16	A	C4-C5-C6	-6.93	113.53	117.00
57	BA	53	A	C4-C5-C6	-6.93	113.53	117.00
57	BA	309	A	C4-C5-C6	-6.93	113.53	117.00
57	BA	560	C	N3-C2-O2	-6.93	117.05	121.90
57	BA	637	A	C4-C5-C6	-6.93	113.53	117.00
57	BA	721	A	C5-C6-N1	6.93	121.17	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	941	A	C4-C5-C6	-6.93	113.53	117.00
57	BA	165	A	C5-C6-N1	6.93	121.17	117.70
57	BA	439	A	C4-C5-C6	-6.93	113.53	117.00
22	AA	229	U	O4'-C1'-N1	6.93	113.74	108.20
22	AA	780	A	N1-C6-N6	-6.93	114.44	118.60
22	AA	1021	A	C4-C5-C6	-6.93	113.54	117.00
57	BA	33	C	N3-C2-O2	-6.93	117.05	121.90
57	BA	1858	A	C5-C6-N1	6.93	121.17	117.70
22	AA	1536	C	N3-C2-O2	-6.93	117.05	121.90
32	BR	103	ARG	NE-CZ-NH1	6.93	123.76	120.30
57	BA	89	A	C5-C6-N1	6.93	121.16	117.70
57	BA	2021	C	N3-C2-O2	-6.93	117.05	121.90
57	BA	2889	C	N3-C2-O2	-6.93	117.05	121.90
22	AA	121	U	N3-C2-O2	-6.93	117.35	122.20
22	AA	1419	G	O4'-C1'-N9	6.93	113.74	108.20
24	A3	29	C	N3-C2-O2	-6.93	117.05	121.90
57	BA	817	C	O4'-C1'-N1	6.93	113.74	108.20
57	BA	2274	A	C4-C5-C6	-6.93	113.54	117.00
57	BA	2884	U	N3-C2-O2	-6.93	117.35	122.20
22	AA	143	A	C4-C5-C6	-6.92	113.54	117.00
57	BA	83	A	C4-C5-C6	-6.92	113.54	117.00
57	BA	352	A	C4-C5-C6	-6.92	113.54	117.00
57	BA	743	A	C4-C5-C6	-6.92	113.54	117.00
57	BA	2824	C	N3-C2-O2	-6.92	117.05	121.90
22	AA	996	A	C4-C5-C6	-6.92	113.54	117.00
9	AR	62	ARG	NE-CZ-NH1	6.92	123.76	120.30
57	BA	330	A	N1-C6-N6	-6.92	114.45	118.60
57	BA	480	A	C4-C5-C6	-6.92	113.54	117.00
57	BA	980	A	C4-C5-C6	-6.92	113.54	117.00
57	BA	1040	A	C4-C5-C6	-6.92	113.54	117.00
57	BA	1433	A	N1-C6-N6	-6.92	114.45	118.60
57	BA	2681	C	N3-C2-O2	-6.92	117.06	121.90
58	Ba	92	C	N3-C2-O2	-6.92	117.06	121.90
22	AA	128	G	O4'-C1'-N9	6.92	113.74	108.20
22	AA	246	A	C5-C6-N1	6.92	121.16	117.70
57	BA	935	C	N3-C2-O2	-6.92	117.06	121.90
57	BA	609	A	C5-C6-N1	6.92	121.16	117.70
57	BA	634	C	O4'-C1'-N1	6.92	113.73	108.20
57	BA	833	A	C4-C5-C6	-6.92	113.54	117.00
57	BA	1102	C	O4'-C1'-N1	6.92	113.73	108.20
57	BA	2298	A	C5-C6-N1	6.92	121.16	117.70
57	BA	2530	A	C5-C6-N1	6.92	121.16	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2577	A	C5-C6-N1	6.92	121.16	117.70
22	AA	1227	A	C4-C5-C6	-6.92	113.54	117.00
57	BA	2095	A	C4-C5-C6	-6.92	113.54	117.00
22	AA	607	A	N1-C6-N6	-6.92	114.45	118.60
22	AA	1097	C	N3-C2-O2	-6.92	117.06	121.90
57	BA	1054	A	C4-C5-C6	-6.92	113.54	117.00
57	BA	2090	A	C5-C6-N1	6.92	121.16	117.70
57	BA	2205	A	N1-C6-N6	-6.92	114.45	118.60
22	AA	841	C	N1-C2-O2	6.91	123.05	118.90
22	AA	1408	A	C4-C5-C6	-6.91	113.54	117.00
57	BA	1635	A	C4-C5-C6	-6.91	113.54	117.00
57	BA	1691	C	N3-C2-O2	-6.91	117.06	121.90
57	BA	2589	A	C4-C5-C6	-6.91	113.54	117.00
58	Ba	35	C	N3-C2-O2	-6.91	117.06	121.90
39	BX	12	ARG	NE-CZ-NH1	6.91	123.76	120.30
22	AA	496	A	C5-C6-N1	6.91	121.16	117.70
57	BA	234	U	O4'-C1'-N1	6.91	113.73	108.20
57	BA	1665	A	C4-C5-C6	-6.91	113.55	117.00
58	Ba	38	C	N3-C2-O2	-6.91	117.06	121.90
57	BA	104	A	C4-C5-C6	-6.91	113.55	117.00
57	BA	218	A	C5-C6-N1	6.91	121.15	117.70
57	BA	643	A	C5-C6-N1	6.91	121.15	117.70
57	BA	1914	C	N3-C2-O2	-6.91	117.06	121.90
57	BA	2369	A	C4-C5-C6	-6.91	113.55	117.00
57	BA	57	C	N3-C2-O2	-6.91	117.06	121.90
22	AA	197	A	C4-C5-C6	-6.91	113.55	117.00
22	AA	565	U	O4'-C1'-N1	6.91	113.72	108.20
22	AA	1149	C	N3-C2-O2	-6.90	117.07	121.90
22	AA	510	A	C4-C5-C6	-6.90	113.55	117.00
22	AA	1447	A	C4-C5-C6	-6.90	113.55	117.00
22	AA	1105	A	C4-C5-C6	-6.90	113.55	117.00
57	BA	69	C	N3-C2-O2	-6.90	117.07	121.90
57	BA	267	C	N3-C2-O2	-6.90	117.07	121.90
22	AA	504	C	N3-C2-O2	-6.90	117.07	121.90
57	BA	666	A	C4-C5-C6	-6.90	113.55	117.00
57	BA	986	C	N1-C2-O2	6.90	123.04	118.90
57	BA	1373	A	N1-C6-N6	-6.90	114.46	118.60
57	BA	1385	A	C4-C5-C6	-6.90	113.55	117.00
57	BA	1960	A	C4-C5-C6	-6.90	113.55	117.00
22	AA	352	C	N3-C2-O2	-6.90	117.07	121.90
22	AA	1208	C	N3-C2-O2	-6.90	117.07	121.90
22	AA	790	A	C4-C5-C6	-6.90	113.55	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2679	A	C4-C5-C6	-6.90	113.55	117.00
22	AA	235	C	N3-C2-O2	-6.89	117.07	121.90
22	AA	482	A	C5-C6-N1	6.89	121.15	117.70
23	A2	51	C	N3-C2-O2	-6.89	117.07	121.90
57	BA	198	C	N3-C2-O2	-6.89	117.07	121.90
58	Ba	105	G	O4'-C1'-N9	6.89	113.72	108.20
22	AA	432	A	C4-C5-C6	-6.89	113.55	117.00
22	AA	733	G	N1-C6-O6	-6.89	115.77	119.90
57	BA	1570	A	N1-C6-N6	-6.89	114.46	118.60
57	BA	1759	A	C4-C5-C6	-6.89	113.55	117.00
22	AA	460	A	C5-C6-N1	6.89	121.15	117.70
57	BA	1306	C	O4'-C1'-N1	6.89	113.71	108.20
22	AA	1319	A	C5-C6-N1	6.89	121.14	117.70
43	B1	56	ARG	NE-CZ-NH2	6.89	123.74	120.30
57	BA	565	C	N3-C2-O2	-6.89	117.08	121.90
22	AA	1533	C	N3-C2-O2	-6.89	117.08	121.90
57	BA	413	C	N3-C2-O2	-6.89	117.08	121.90
57	BA	819	A	C5-C6-N1	6.89	121.14	117.70
57	BA	948	C	N3-C2-O2	-6.89	117.08	121.90
22	AA	393	A	C5-C6-N1	6.89	121.14	117.70
57	BA	927	A	C4-C5-C6	-6.89	113.56	117.00
57	BA	2554	U	O4'-C1'-N1	6.89	113.71	108.20
57	BA	417	C	N3-C2-O2	-6.88	117.08	121.90
57	BA	866	A	C4-C5-C6	-6.88	113.56	117.00
57	BA	1615	C	N3-C2-O2	-6.88	117.08	121.90
57	BA	1883	U	O4'-C1'-N1	6.88	113.71	108.20
57	BA	2589	A	C5-C6-N1	6.88	121.14	117.70
22	AA	139	A	C4-C5-C6	-6.88	113.56	117.00
57	BA	1127	A	C4-C5-C6	-6.88	113.56	117.00
57	BA	1320	C	N3-C2-O2	-6.88	117.08	121.90
57	BA	1672	A	C4-C5-C6	-6.88	113.56	117.00
57	BA	2073	C	N3-C2-O2	-6.88	117.08	121.90
57	BA	272	A	N1-C6-N6	-6.88	114.47	118.60
57	BA	698	C	N3-C2-O2	-6.88	117.08	121.90
57	BA	2411	A	C4-C5-C6	-6.88	113.56	117.00
22	AA	32	A	N1-C6-N6	-6.88	114.47	118.60
22	AA	547	A	C4-C5-C6	-6.88	113.56	117.00
57	BA	2023	C	O4'-C1'-N1	6.88	113.70	108.20
57	BA	2814	A	C4-C5-C6	-6.88	113.56	117.00
56	BL	68	ARG	NE-CZ-NH1	6.88	123.74	120.30
57	BA	1208	C	N3-C2-O2	-6.88	117.09	121.90
57	BA	1230	A	C4-C5-C6	-6.88	113.56	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2058	A	C4-C5-C6	-6.88	113.56	117.00
22	AA	1509	C	N3-C2-O2	-6.88	117.09	121.90
50	B7	3	ARG	NE-CZ-NH2	6.88	123.74	120.30
57	BA	226	A	C4-C5-C6	-6.87	113.56	117.00
22	AA	375	U	O4'-C1'-N1	6.87	113.70	108.20
57	BA	311	A	N1-C6-N6	-6.87	114.48	118.60
57	BA	757	G	O4'-C1'-N9	6.87	113.70	108.20
57	BA	1616	A	C4-C5-C6	-6.87	113.56	117.00
57	BA	2287	A	C4-C5-C6	-6.87	113.56	117.00
58	Ba	97	C	N3-C2-O2	-6.87	117.09	121.90
17	AF	109	ARG	NE-CZ-NH1	6.87	123.73	120.30
19	AH	79	ARG	NE-CZ-NH1	6.87	123.73	120.30
57	BA	28	A	N1-C6-N6	-6.87	114.48	118.60
22	AA	193	C	N3-C2-O2	-6.87	117.09	121.90
57	BA	582	A	C4-C5-C6	-6.87	113.57	117.00
57	BA	1076	C	N3-C2-O2	-6.87	117.09	121.90
57	BA	1746	A	C4-C5-C6	-6.87	113.57	117.00
58	Ba	50	A	C4-C5-C6	-6.87	113.57	117.00
22	AA	1151	A	C5-C6-N1	6.87	121.13	117.70
57	BA	823	C	N3-C2-O2	-6.87	117.09	121.90
57	BA	1953	A	C4-C5-C6	-6.87	113.57	117.00
22	AA	222	C	N3-C2-O2	-6.87	117.09	121.90
22	AA	336	A	C5-C6-N1	6.87	121.13	117.70
22	AA	1000	A	C4-C5-C6	-6.87	113.57	117.00
22	AA	1248	A	C4-C5-C6	-6.87	113.57	117.00
57	BA	401	A	C5-C6-N1	6.87	121.13	117.70
57	BA	1175	A	C4-C5-C6	-6.87	113.57	117.00
57	BA	1414	C	O4'-C1'-N1	6.87	113.69	108.20
57	BA	703	U	O4'-C1'-N1	6.86	113.69	108.20
57	BA	750	A	C4-C5-C6	-6.86	113.57	117.00
57	BA	1998	A	C4-C5-C6	-6.86	113.57	117.00
57	BA	2170	A	O4'-C1'-N9	6.86	113.69	108.20
57	BA	1151	A	C4-C5-C6	-6.86	113.57	117.00
57	BA	1656	C	N3-C2-O2	-6.86	117.10	121.90
57	BA	2441	U	N3-C2-O2	-6.86	117.40	122.20
12	AT	9	ARG	NE-CZ-NH1	6.86	123.73	120.30
22	AA	744	C	N3-C2-O2	-6.86	117.10	121.90
57	BA	637	A	C5-C6-N1	6.86	121.13	117.70
57	BA	2394	C	N3-C2-O2	-6.86	117.10	121.90
57	BA	2590	A	C5-C6-N1	6.86	121.13	117.70
57	BA	1349	C	N3-C2-O2	-6.86	117.10	121.90
22	AA	719	C	N3-C2-O2	-6.86	117.10	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	79	C	N3-C2-O2	-6.86	117.10	121.90
57	BA	421	C	N3-C2-O2	-6.86	117.10	121.90
22	AA	440	C	N3-C2-O2	-6.86	117.10	121.90
22	AA	764	C	N3-C2-O2	-6.86	117.10	121.90
57	BA	550	C	N3-C2-O2	-6.86	117.10	121.90
57	BA	1437	C	O4'-C1'-N1	6.86	113.68	108.20
57	BA	1362	C	N3-C2-O2	-6.85	117.10	121.90
22	AA	1229	A	C4-C5-C6	-6.85	113.57	117.00
57	BA	1664	A	C4-C5-C6	-6.85	113.57	117.00
21	A1	206	ARG	NE-CZ-NH1	6.85	123.72	120.30
22	AA	311	C	N1-C2-O2	6.85	123.01	118.90
22	AA	363	A	C4-C5-C6	-6.85	113.58	117.00
57	BA	1043	C	N3-C2-O2	-6.85	117.11	121.90
57	BA	1626	A	C5-C6-N1	6.85	121.12	117.70
22	AA	1352	C	N3-C2-O2	-6.85	117.11	121.90
44	B2	48	ARG	NE-CZ-NH1	6.85	123.72	120.30
57	BA	44	A	C5-C6-N1	6.85	121.12	117.70
57	BA	1264	A	C4-C5-C6	-6.85	113.58	117.00
57	BA	2778	A	C4-C5-C6	-6.85	113.58	117.00
57	BA	502	A	C4-C5-C6	-6.85	113.58	117.00
22	AA	279	A	C4-C5-C6	-6.84	113.58	117.00
22	AA	1259	C	N3-C2-O2	-6.84	117.11	121.90
57	BA	2616	C	N3-C2-O2	-6.84	117.11	121.90
22	AA	635	A	C4-C5-C6	-6.84	113.58	117.00
22	AA	934	C	N1-C2-O2	6.84	123.01	118.90
57	BA	1816	C	N3-C2-O2	-6.84	117.11	121.90
57	BA	2194	U	O4'-C1'-N1	6.84	113.67	108.20
22	AA	1225	A	N1-C6-N6	-6.84	114.50	118.60
57	BA	1795	C	N3-C2-O2	-6.84	117.11	121.90
22	AA	994	A	C4-C5-C6	-6.84	113.58	117.00
36	BU	29	ARG	NE-CZ-NH1	6.84	123.72	120.30
57	BA	125	A	C4-C5-C6	-6.84	113.58	117.00
57	BA	1272	A	C4-C5-C6	-6.84	113.58	117.00
57	BA	1526	C	O4'-C1'-N1	6.84	113.67	108.20
57	BA	1582	C	N3-C2-O2	-6.84	117.11	121.90
57	BA	2163	A	C4-C5-C6	-6.84	113.58	117.00
57	BA	2651	C	N3-C2-O2	-6.84	117.11	121.90
28	BN	35	ARG	NE-CZ-NH1	6.84	123.72	120.30
57	BA	155	A	C4-C5-C6	-6.84	113.58	117.00
57	BA	586	A	C5-C6-N1	6.84	121.12	117.70
57	BA	715	A	C4-C5-C6	-6.84	113.58	117.00
57	BA	114	U	O4'-C1'-N1	6.83	113.67	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1604	C	N3-C2-O2	-6.83	117.12	121.90
22	AA	487	A	C5-C6-N1	6.83	121.12	117.70
34	BT	71	ARG	NE-CZ-NH1	6.83	123.72	120.30
57	BA	111	A	C4-C5-C6	-6.83	113.58	117.00
57	BA	295	G	O4'-C1'-N9	6.83	113.67	108.20
57	BA	1373	A	C5-C6-N1	6.83	121.12	117.70
22	AA	679	C	N3-C2-O2	-6.83	117.12	121.90
57	BA	1932	A	C4-C5-C6	-6.83	113.58	117.00
22	AA	126	G	O4'-C1'-N9	6.83	113.66	108.20
57	BA	222	A	C4-C5-C6	-6.83	113.59	117.00
57	BA	614	A	C4-C5-C6	-6.83	113.59	117.00
57	BA	764	A	C5-C6-N1	6.83	121.11	117.70
57	BA	2788	C	N3-C2-O2	-6.83	117.12	121.90
22	AA	770	C	N3-C2-O2	-6.83	117.12	121.90
22	AA	936	C	O4'-C1'-N1	6.83	113.66	108.20
22	AA	1081	A	C4-C5-C6	-6.83	113.59	117.00
56	BL	116	ARG	NE-CZ-NH1	6.83	123.71	120.30
57	BA	483	A	C5-C6-N1	6.83	121.11	117.70
57	BA	911	A	C4-C5-C6	-6.83	113.59	117.00
57	BA	1344	U	O4'-C1'-N1	6.83	113.66	108.20
57	BA	2183	A	C5-C6-N1	6.83	121.11	117.70
57	BA	788	A	C4-C5-C6	-6.82	113.59	117.00
57	BA	1428	C	N3-C2-O2	-6.82	117.12	121.90
57	BA	2423	U	O4'-C1'-N1	6.82	113.66	108.20
57	BA	837	C	N3-C2-O2	-6.82	117.12	121.90
57	BA	2440	C	C6-N1-C2	-6.82	117.57	120.30
22	AA	13	U	O4'-C1'-N1	6.82	113.66	108.20
57	BA	2468	A	C4-C5-C6	-6.82	113.59	117.00
57	BA	378	C	N1-C2-O2	6.82	122.99	118.90
57	BA	1285	A	C4-C5-C6	-6.82	113.59	117.00
57	BA	1977	A	C4-C5-C6	-6.82	113.59	117.00
22	AA	559	A	O4'-C1'-N9	6.82	113.65	108.20
22	AA	1073	U	O4'-C1'-N1	6.82	113.65	108.20
57	BA	548	G	O4'-C1'-N9	6.82	113.65	108.20
22	AA	18	C	N3-C2-O2	-6.81	117.13	121.90
57	BA	599	A	C4-C5-C6	-6.81	113.59	117.00
22	AA	291	U	O4'-C1'-N1	6.81	113.65	108.20
57	BA	2600	A	C4-C5-C6	-6.81	113.59	117.00
22	AA	50	A	C4-C5-C6	-6.81	113.59	117.00
22	AA	1069	C	O4'-C1'-N1	6.81	113.65	108.20
22	AA	1394	A	C4-C5-C6	-6.81	113.59	117.00
57	BA	1470	A	C5-C6-N1	6.81	121.11	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	430	A	C4-C5-C6	-6.81	113.59	117.00
57	BA	909	A	C4-C5-C6	-6.81	113.60	117.00
57	BA	933	A	O4'-C1'-N9	6.81	113.65	108.20
58	Ba	12	C	N3-C2-O2	-6.81	117.13	121.90
22	AA	435	A	C5-C6-N1	6.81	121.10	117.70
22	AA	1070	U	O4'-C1'-N1	6.81	113.64	108.20
57	BA	2358	A	C4-C5-C6	-6.81	113.60	117.00
57	BA	2757	A	N1-C6-N6	-6.81	114.52	118.60
22	AA	781	A	C4-C5-C6	-6.80	113.60	117.00
57	BA	2411	A	N1-C6-N6	-6.80	114.52	118.60
22	AA	80	A	C4-C5-C6	-6.80	113.60	117.00
22	AA	576	C	N3-C2-O2	-6.80	117.14	121.90
40	BY	93	ARG	NE-CZ-NH1	6.80	123.70	120.30
46	B3	15	ARG	NE-CZ-NH1	6.80	123.70	120.30
57	BA	793	A	C4-C5-C6	-6.80	113.60	117.00
57	BA	1590	A	C4-C5-C6	-6.80	113.60	117.00
22	AA	371	A	C4-C5-C6	-6.80	113.60	117.00
22	AA	866	C	N3-C2-O2	-6.80	117.14	121.90
57	BA	412	A	C4-C5-C6	-6.80	113.60	117.00
57	BA	2314	A	C4-C5-C6	-6.80	113.60	117.00
22	AA	753	A	C5-C6-N1	6.80	121.10	117.70
57	BA	911	A	N1-C6-N6	-6.80	114.52	118.60
22	AA	10	A	C4-C5-C6	-6.80	113.60	117.00
22	AA	1016	A	C4-C5-C6	-6.80	113.60	117.00
57	BA	550	C	O4'-C1'-N1	6.80	113.64	108.20
58	Ba	91	C	N3-C2-O2	-6.80	117.14	121.90
57	BA	2070	A	C4-C5-C6	-6.79	113.60	117.00
22	AA	1340	A	C5-C6-N1	6.79	121.10	117.70
24	A3	11	A	C4-C5-C6	-6.79	113.60	117.00
22	AA	660	C	N3-C2-O2	-6.79	117.15	121.90
22	AA	306	A	C5-C6-N1	6.79	121.09	117.70
22	AA	1465	A	C4-C5-C6	-6.79	113.61	117.00
57	BA	1762	A	C5-C6-N1	6.79	121.09	117.70
57	BA	1952	A	C4-C5-C6	-6.79	113.61	117.00
31	BQ	50	ARG	NE-CZ-NH2	6.79	123.69	120.30
57	BA	208	C	N3-C2-O2	-6.79	117.15	121.90
57	BA	1302	A	C4-C5-C6	-6.79	113.61	117.00
57	BA	2675	A	C4-C5-C6	-6.79	113.61	117.00
57	BA	556	A	C5-C6-N1	6.79	121.09	117.70
57	BA	1046	A	C4-C5-C6	-6.79	113.61	117.00
57	BA	1803	A	N1-C6-N6	-6.79	114.53	118.60
22	AA	554	A	C4-C5-C6	-6.78	113.61	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	475	C	N3-C2-O2	-6.78	117.15	121.90
57	BA	838	C	N1-C2-O2	6.78	122.97	118.90
57	BA	2683	C	N3-C2-O2	-6.78	117.15	121.90
22	AA	995	C	O4'-C1'-N1	6.78	113.63	108.20
57	BA	1119	U	O4'-C1'-N1	6.78	113.62	108.20
22	AA	303	A	C4-C5-C6	-6.78	113.61	117.00
22	AA	1035	A	C4-C5-C6	-6.78	113.61	117.00
22	AA	1155	A	C4-C5-C6	-6.78	113.61	117.00
22	AA	1453	G	O4'-C1'-N9	6.78	113.62	108.20
57	BA	902	C	N3-C2-O2	-6.78	117.15	121.90
57	BA	1080	A	C4-C5-C6	-6.78	113.61	117.00
57	BA	2851	A	C4-C5-C6	-6.78	113.61	117.00
14	AC	171	ARG	NE-CZ-NH1	6.78	123.69	120.30
22	AA	236	A	C4-C5-C6	-6.78	113.61	117.00
57	BA	184	C	N3-C2-O2	-6.78	117.16	121.90
57	BA	1901	A	C4-C5-C6	-6.78	113.61	117.00
57	BA	2665	A	C5-C6-N1	6.78	121.09	117.70
54	BG	147	ARG	NE-CZ-NH1	6.78	123.69	120.30
57	BA	538	A	C4-C5-C6	-6.78	113.61	117.00
57	BA	994	C	N3-C2-O2	-6.78	117.16	121.90
57	BA	1525	A	C4-C5-C6	-6.78	113.61	117.00
57	BA	1801	A	C4-C5-C6	-6.77	113.61	117.00
22	AA	1152	A	C4-C5-C6	-6.77	113.61	117.00
23	A2	47	C	N3-C2-O2	-6.77	117.16	121.90
57	BA	661	A	N1-C6-N6	-6.77	114.54	118.60
57	BA	1073	A	C4-C5-C6	-6.77	113.61	117.00
57	BA	2001	C	O4'-C1'-N1	6.77	113.62	108.20
57	BA	2170	A	C4-C5-C6	-6.77	113.61	117.00
57	BA	2425	A	C4-C5-C6	-6.77	113.61	117.00
22	AA	355	C	N3-C4-C5	6.77	124.61	121.90
22	AA	1493	A	O4'-C1'-N9	6.77	113.62	108.20
57	BA	2887	A	C5-C6-N1	6.77	121.08	117.70
24	A3	43	G	O4'-C1'-N9	6.77	113.61	108.20
57	BA	627	A	C4-C5-C6	-6.77	113.62	117.00
57	BA	627	A	C5-C6-N1	6.77	121.08	117.70
57	BA	942	G	N7-C8-N9	6.77	116.48	113.10
57	BA	2094	A	C4-C5-C6	-6.77	113.62	117.00
57	BA	2346	A	C4-C5-C6	-6.77	113.62	117.00
57	BA	2823	A	N1-C6-N6	-6.77	114.54	118.60
19	AH	12	ARG	NE-CZ-NH1	6.76	123.68	120.30
22	AA	1209	C	N3-C2-O2	-6.76	117.17	121.90
42	B0	13	ARG	NE-CZ-NH2	6.76	123.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	37	U	O4'-C1'-N1	6.76	113.61	108.20
57	BA	2810	A	C4-C5-C6	-6.76	113.62	117.00
57	BA	2878	U	O4'-C1'-N1	6.76	113.61	108.20
22	AA	1145	A	N1-C6-N6	-6.76	114.54	118.60
58	Ba	34	A	C4-C5-C6	-6.76	113.62	117.00
22	AA	1397	C	N1-C2-O2	6.76	122.96	118.90
57	BA	984	A	C4-C5-C6	-6.76	113.62	117.00
57	BA	1111	A	C5-C6-N1	6.76	121.08	117.70
57	BA	1969	A	C4-C5-C6	-6.76	113.62	117.00
57	BA	482	A	C4-C5-C6	-6.76	113.62	117.00
22	AA	1130	A	C4-C5-C6	-6.76	113.62	117.00
22	AA	1484	C	O4'-C1'-N1	6.76	113.61	108.20
36	BU	63	ARG	NE-CZ-NH1	6.76	123.68	120.30
57	BA	502	A	C5-C6-N1	6.76	121.08	117.70
57	BA	305	C	N1-C2-O2	6.75	122.95	118.90
57	BA	2748	A	C5-C6-N1	6.75	121.08	117.70
22	AA	507	C	N3-C2-O2	-6.75	117.17	121.90
22	AA	1157	A	N1-C6-N6	-6.75	114.55	118.60
22	AA	1430	A	C4-C5-C6	-6.75	113.62	117.00
57	BA	5	A	C4-C5-C6	-6.75	113.62	117.00
22	AA	831	A	C4-C5-C6	-6.75	113.62	117.00
22	AA	412	A	C1'-O4'-C4'	-6.75	104.50	109.90
29	BO	18	ARG	NE-CZ-NH1	6.75	123.67	120.30
33	BS	33	ARG	NE-CZ-NH1	6.75	123.67	120.30
57	BA	165	A	C4-C5-C6	-6.75	113.63	117.00
57	BA	765	C	N1-C2-O2	6.75	122.95	118.90
22	AA	253	A	N1-C6-N6	-6.75	114.55	118.60
22	AA	609	A	C4-C5-C6	-6.75	113.63	117.00
37	BV	13	ARG	NE-CZ-NH1	6.75	123.67	120.30
57	BA	21	A	C4-C5-C6	-6.75	113.63	117.00
57	BA	1183	U	O4'-C1'-N1	6.75	113.60	108.20
57	BA	1641	A	C5-C6-N1	6.75	121.07	117.70
57	BA	1765	U	O4'-C1'-N1	6.75	113.60	108.20
57	BA	2883	A	C4-C5-C6	-6.75	113.63	117.00
31	BQ	16	ARG	NE-CZ-NH1	6.75	123.67	120.30
57	BA	541	A	C4-C5-C6	-6.75	113.63	117.00
57	BA	1953	A	C5-C6-N1	6.75	121.07	117.70
57	BA	103	A	C4-C5-C6	-6.74	113.63	117.00
57	BA	146	A	C4-C5-C6	-6.74	113.63	117.00
22	AA	1350	A	N1-C6-N6	-6.74	114.56	118.60
22	AA	1377	A	C4-C5-C6	-6.74	113.63	117.00
22	AA	1406	U	O4'-C1'-N1	6.74	113.59	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	557	C	N3-C2-O2	-6.74	117.18	121.90
57	BA	2019	A	C4-C5-C6	-6.74	113.63	117.00
22	AA	212	G	O4'-C1'-N9	6.74	113.59	108.20
4	AM	108	ARG	NE-CZ-NH1	6.74	123.67	120.30
57	BA	1650	A	C4-C5-C6	-6.74	113.63	117.00
22	AA	1066	C	N3-C2-O2	-6.73	117.19	121.90
57	BA	1774	C	N3-C2-O2	-6.73	117.19	121.90
58	Ba	39	A	C4-C5-C6	-6.73	113.63	117.00
57	BA	3	U	O4'-C1'-N1	6.73	113.58	108.20
57	BA	1502	A	C4-C5-C6	-6.73	113.64	117.00
26	BJ	124	ARG	NE-CZ-NH1	6.73	123.67	120.30
57	BA	2173	A	C5-C6-N1	6.73	121.06	117.70
22	AA	181	A	C4-C5-C6	-6.73	113.64	117.00
22	AA	1133	G	O4'-C1'-N9	6.73	113.58	108.20
35	BD	257	ARG	NE-CZ-NH1	6.73	123.66	120.30
51	B8	12	ARG	NE-CZ-NH2	6.73	123.66	120.30
57	BA	1630	A	C4-C5-C6	-6.73	113.64	117.00
57	BA	1802	A	N1-C6-N6	-6.73	114.56	118.60
57	BA	1085	A	C4-C5-C6	-6.73	113.64	117.00
57	BA	1035	U	O4'-C1'-N1	6.72	113.58	108.20
57	BA	1576	U	O4'-C1'-N1	6.72	113.58	108.20
22	AA	382	A	C4-C5-C6	-6.72	113.64	117.00
22	AA	1188	A	C4-C5-C6	-6.72	113.64	117.00
22	AA	1479	C	O4'-C1'-N1	6.72	113.58	108.20
57	BA	384	A	C4-C5-C6	-6.72	113.64	117.00
57	BA	749	A	C4-C5-C6	-6.72	113.64	117.00
57	BA	1805	A	C4-C5-C6	-6.72	113.64	117.00
22	AA	747	A	C4-C5-C6	-6.72	113.64	117.00
57	BA	408	G	N1-C6-O6	-6.72	115.87	119.90
57	BA	1088	A	N1-C6-N6	-6.72	114.57	118.60
57	BA	1213	A	C4-C5-C6	-6.72	113.64	117.00
57	BA	574	A	C4-C5-C6	-6.72	113.64	117.00
57	BA	1313	U	N3-C2-O2	-6.72	117.50	122.20
57	BA	507	A	C5-C6-N1	6.72	121.06	117.70
57	BA	1566	A	C4-C5-C6	-6.72	113.64	117.00
57	BA	2541	A	C4-C5-C6	-6.72	113.64	117.00
15	AD	43	ARG	NE-CZ-NH1	6.72	123.66	120.30
57	BA	2009	A	C5-C6-N1	6.72	121.06	117.70
57	BA	2179	C	N3-C2-O2	-6.72	117.20	121.90
57	BA	2736	A	C4-C5-C6	-6.72	113.64	117.00
3	AL	49	ARG	NE-CZ-NH1	6.71	123.66	120.30
22	AA	779	C	O4'-C1'-N1	6.71	113.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	239	C	O4'-C1'-N1	6.71	113.57	108.20
57	BA	453	A	C4-C5-C6	-6.71	113.64	117.00
57	BA	1000	A	C4-C5-C6	-6.71	113.64	117.00
22	AA	288	A	N1-C6-N6	-6.71	114.57	118.60
22	AA	131	A	C4-C5-C6	-6.71	113.64	117.00
35	BD	12	ARG	NE-CZ-NH1	6.71	123.66	120.30
57	BA	2077	A	N1-C6-N6	-6.71	114.57	118.60
46	B3	30	ARG	NE-CZ-NH1	6.71	123.65	120.30
57	BA	1058	U	O4'-C1'-N1	6.71	113.57	108.20
57	BA	1306	C	N3-C4-N4	-6.71	113.30	118.00
57	BA	1353	A	C4-C5-C6	-6.71	113.65	117.00
57	BA	2461	A	C4-C5-C6	-6.71	113.65	117.00
22	AA	483	C	N3-C2-O2	-6.71	117.21	121.90
23	A2	33	A	C5-C6-N1	6.71	121.05	117.70
57	BA	2118	U	O4'-C1'-N1	6.71	113.56	108.20
17	AF	79	ARG	NE-CZ-NH1	6.70	123.65	120.30
57	BA	335	C	N3-C2-O2	-6.70	117.21	121.90
57	BA	1413	A	C4-C5-C6	-6.70	113.65	117.00
57	BA	1889	A	C4-C5-C6	-6.70	113.65	117.00
16	AE	92	ARG	NE-CZ-NH1	6.70	123.65	120.30
22	AA	1419	G	N1-C6-O6	-6.70	115.88	119.90
57	BA	94	A	C4-C5-C6	-6.70	113.65	117.00
57	BA	1706	C	O4'-C1'-N1	6.70	113.56	108.20
57	BA	2565	A	C4-C5-C6	-6.70	113.65	117.00
57	BA	1075	C	N3-C2-O2	-6.70	117.21	121.90
57	BA	1905	C	N3-C2-O2	-6.70	117.21	121.90
57	BA	2200	C	O4'-C1'-N1	6.70	113.56	108.20
7	AP	5	ARG	NE-CZ-NH1	6.70	123.65	120.30
57	BA	454	A	C4-C5-C6	-6.70	113.65	117.00
57	BA	1109	C	N3-C2-O2	-6.70	117.21	121.90
57	BA	1341	G	O4'-C1'-N9	6.70	113.56	108.20
57	BA	1548	A	C4-C5-C6	-6.70	113.65	117.00
57	BA	2281	A	C5-C6-N1	6.70	121.05	117.70
57	BA	334	C	N3-C2-O2	-6.70	117.21	121.90
57	BA	654	A	O4'-C1'-N9	6.70	113.56	108.20
22	AA	728	A	O4'-C1'-N9	6.70	113.56	108.20
57	BA	11	C	N3-C2-O2	-6.70	117.21	121.90
57	BA	477	A	C5-C6-N1	6.70	121.05	117.70
57	BA	1515	A	C4-C5-C6	-6.70	113.65	117.00
57	BA	1877	A	C4-C5-C6	-6.70	113.65	117.00
22	AA	1446	A	C4-C5-C6	-6.69	113.65	117.00
22	AA	214	C	N3-C2-O2	-6.69	117.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1496	A	C4-C5-C6	-6.69	113.65	117.00
57	BA	2071	A	N1-C6-N6	-6.69	114.58	118.60
57	BA	2223	G	O4'-C1'-N9	6.69	113.55	108.20
22	AA	1507	A	N1-C6-N6	-6.69	114.59	118.60
57	BA	197	A	C4-C5-C6	-6.69	113.66	117.00
57	BA	158	U	O4'-C1'-N1	6.69	113.55	108.20
57	BA	770	G	O4'-C1'-N9	6.69	113.55	108.20
22	AA	155	A	C4-C5-C6	-6.69	113.66	117.00
22	AA	959	A	C5-C6-N1	6.69	121.04	117.70
57	BA	441	U	O4'-C1'-N1	6.69	113.55	108.20
57	BA	504	A	C4-C5-C6	-6.69	113.66	117.00
57	BA	1490	A	C4-C5-C6	-6.69	113.66	117.00
57	BA	1586	A	C4-C5-C6	-6.69	113.66	117.00
57	BA	2726	A	C5-C6-N1	6.69	121.04	117.70
22	AA	767	A	C4-C5-C6	-6.69	113.66	117.00
22	AA	179	A	C4-C5-C6	-6.68	113.66	117.00
22	AA	1534	A	C5-C6-N1	6.68	121.04	117.70
57	BA	19	A	C4-C5-C6	-6.68	113.66	117.00
57	BA	219	A	C4-C5-C6	-6.68	113.66	117.00
57	BA	1729	U	O4'-C1'-N1	6.68	113.55	108.20
57	BA	2129	C	N1-C2-O2	6.68	122.91	118.90
58	Ba	60	C	N1-C2-O2	6.68	122.91	118.90
22	AA	583	A	C4-C5-C6	-6.68	113.66	117.00
57	BA	1822	C	N3-C2-O2	-6.68	117.22	121.90
57	BA	2078	C	N1-C2-O2	6.68	122.91	118.90
57	BA	2309	A	C4-C5-C6	-6.68	113.66	117.00
57	BA	2227	A	N1-C6-N6	-6.68	114.59	118.60
22	AA	192	A	N1-C6-N6	-6.68	114.59	118.60
22	AA	322	C	N3-C2-O2	-6.68	117.22	121.90
57	BA	962	G	N1-C6-O6	-6.68	115.89	119.90
57	BA	2761	A	C4-C5-C6	-6.68	113.66	117.00
57	BA	347	A	C4-C5-C6	-6.68	113.66	117.00
57	BA	2247	A	O4'-C1'-N9	6.68	113.54	108.20
57	BA	2619	C	N3-C2-O2	-6.68	117.23	121.90
57	BA	2085	U	O4'-C1'-N1	6.68	113.54	108.20
57	BA	2573	C	N3-C2-O2	-6.68	117.23	121.90
57	BA	1815	A	C4-C5-C6	-6.67	113.66	117.00
57	BA	2195	U	O4'-C1'-N1	6.67	113.54	108.20
57	BA	2199	A	C5'-C4'-C3'	-6.67	105.32	116.00
57	BA	2205	A	C5-C6-N1	6.67	121.04	117.70
57	BA	1786	A	O4'-C1'-N9	6.67	113.54	108.20
22	AA	741	G	O4'-C1'-N9	6.67	113.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2211	A	O4'-C1'-N9	6.67	113.54	108.20
22	AA	1110	A	C5-C6-N1	6.67	121.03	117.70
57	BA	207	A	N1-C6-N6	-6.67	114.60	118.60
57	BA	2900	A	C4-C5-C6	-6.67	113.67	117.00
57	BA	1713	A	C4-C5-C6	-6.67	113.67	117.00
22	AA	640	A	C4-C5-C6	-6.67	113.67	117.00
57	BA	1354	A	C4-C5-C6	-6.67	113.67	117.00
58	Ba	70	C	N3-C2-O2	-6.67	117.23	121.90
22	AA	814	A	C4-C5-C6	-6.66	113.67	117.00
22	AA	1147	C	O4'-C1'-N1	6.66	113.53	108.20
22	AA	1162	C	N3-C2-O2	-6.66	117.23	121.90
22	AA	1288	A	C5-C6-N1	6.66	121.03	117.70
57	BA	1937	A	C4-C5-C6	-6.66	113.67	117.00
22	AA	1100	C	N3-C2-O2	-6.66	117.24	121.90
57	BA	1287	A	C4-C5-C6	-6.66	113.67	117.00
7	AP	35	ARG	NE-CZ-NH1	6.66	123.63	120.30
22	AA	313	A	C4-C5-C6	-6.66	113.67	117.00
22	AA	1017	U	O4'-C1'-N1	6.66	113.53	108.20
57	BA	2476	A	C5-C6-N1	6.66	121.03	117.70
57	BA	2887	A	C4-C5-C6	-6.66	113.67	117.00
9	AR	72	ARG	NE-CZ-NH1	6.66	123.63	120.30
22	AA	1501	C	O4'-C1'-N1	6.66	113.53	108.20
57	BA	1504	A	C5-C6-N1	6.66	121.03	117.70
57	BA	1612	C	O4'-C1'-N1	6.66	113.53	108.20
57	BA	1790	C	O4'-C1'-N1	6.66	113.53	108.20
57	BA	2805	C	O4'-C1'-N1	6.66	113.53	108.20
57	BA	63	A	C4-C5-C6	-6.66	113.67	117.00
57	BA	1640	A	C4-C5-C6	-6.66	113.67	117.00
57	BA	2288	A	C4-C5-C6	-6.66	113.67	117.00
57	BA	2378	A	C4-C5-C6	-6.66	113.67	117.00
22	AA	1429	A	C4-C5-C6	-6.65	113.67	117.00
22	AA	48	C	N3-C2-O2	-6.65	117.24	121.90
22	AA	1103	C	O4'-C1'-N1	6.65	113.52	108.20
55	BH	148	ARG	NE-CZ-NH1	6.65	123.63	120.30
57	BA	972	A	C4-C5-C6	-6.65	113.67	117.00
57	BA	1790	C	N3-C2-O2	-6.65	117.24	121.90
22	AA	642	A	N1-C6-N6	-6.65	114.61	118.60
57	BA	888	C	N3-C2-O2	-6.65	117.25	121.90
57	BA	1010	A	C4-C5-C6	-6.65	113.67	117.00
57	BA	2386	A	C5-C6-N1	6.65	121.03	117.70
57	BA	2145	C	N3-C2-O2	-6.65	117.25	121.90
20	AI	84	ARG	NE-CZ-NH1	6.65	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	849	A	C4-C5-C6	-6.65	113.68	117.00
57	BA	1084	A	C4-C5-C6	-6.65	113.68	117.00
22	AA	1051	C	N3-C2-O2	-6.65	117.25	121.90
57	BA	182	A	C5-C6-N1	6.65	121.02	117.70
57	BA	1453	A	C4-C5-C6	-6.65	113.68	117.00
57	BA	2497	A	C4-C5-C6	-6.65	113.68	117.00
22	AA	58	C	O4'-C1'-N1	6.64	113.52	108.20
57	BA	1690	A	C5-C6-N1	6.64	121.02	117.70
57	BA	1837	C	N3-C2-O2	-6.64	117.25	121.90
57	BA	2451	A	O4'-C1'-N9	6.64	113.52	108.20
22	AA	120	A	C4-C5-C6	-6.64	113.68	117.00
22	AA	545	C	O4'-C1'-N1	6.64	113.51	108.20
22	AA	1019	A	C4-C5-C6	-6.64	113.68	117.00
57	BA	223	A	C4-C5-C6	-6.64	113.68	117.00
57	BA	454	A	C5-C6-N1	6.64	121.02	117.70
57	BA	1393	A	C4-C5-C6	-6.64	113.68	117.00
57	BA	2407	A	C4-C5-C6	-6.64	113.68	117.00
57	BA	2426	A	C4-C5-C6	-6.64	113.68	117.00
57	BA	804	A	C4-C5-C6	-6.64	113.68	117.00
57	BA	905	A	C4-C5-C6	-6.64	113.68	117.00
22	AA	228	A	C4-C5-C6	-6.64	113.68	117.00
57	BA	2453	A	C5-C6-N1	6.64	121.02	117.70
57	BA	2813	A	C4-C5-C6	-6.64	113.68	117.00
24	A3	74	A	C4-C5-C6	-6.64	113.68	117.00
57	BA	1423	G	O4'-C1'-N9	6.64	113.51	108.20
57	BA	1689	A	C5-C6-N1	6.64	121.02	117.70
57	BA	91	A	C4-C5-C6	-6.64	113.68	117.00
57	BA	501	A	N1-C6-N6	-6.64	114.62	118.60
57	BA	602	A	C4-C5-C6	-6.64	113.68	117.00
57	BA	1735	A	C4-C5-C6	-6.64	113.68	117.00
22	AA	496	A	O4'-C1'-N9	6.63	113.51	108.20
22	AA	1375	A	N1-C6-N6	-6.63	114.62	118.60
57	BA	1564	C	N1-C2-O2	6.63	122.88	118.90
57	BA	1757	A	C4-C5-C6	-6.63	113.68	117.00
57	BA	1830	C	N3-C2-O2	-6.63	117.26	121.90
57	BA	2730	C	O4'-C1'-N1	6.63	113.51	108.20
57	BA	1269	A	C4-C5-C6	-6.63	113.68	117.00
57	BA	402	A	C5-C6-N1	6.63	121.02	117.70
57	BA	825	A	C4-C5-C6	-6.63	113.69	117.00
57	BA	1809	A	N1-C6-N6	-6.63	114.62	118.60
22	AA	560	A	C4-C5-C6	-6.63	113.69	117.00
57	BA	14	A	C4-C5-C6	-6.63	113.69	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1263	U	O4'-C1'-N1	6.63	113.50	108.20
57	BA	1321	A	C4-C5-C6	-6.63	113.69	117.00
57	BA	1754	A	C4-C5-C6	-6.63	113.69	117.00
57	BA	1783	A	C4-C5-C6	-6.63	113.69	117.00
57	BA	2385	C	N3-C2-O2	-6.63	117.26	121.90
57	BA	2743	U	O4'-C1'-N1	6.63	113.50	108.20
22	AA	495	A	C4-C5-C6	-6.62	113.69	117.00
57	BA	177	G	O4'-C1'-N9	6.62	113.50	108.20
22	AA	107	G	N1-C6-O6	-6.62	115.92	119.90
46	B3	10	ARG	NE-CZ-NH1	-6.62	116.99	120.30
57	BA	892	A	C4-C5-C6	-6.62	113.69	117.00
57	BA	142	A	C4-C5-C6	-6.62	113.69	117.00
57	BA	2310	C	N3-C2-O2	-6.62	117.27	121.90
57	BA	2333	A	C4-C5-C6	-6.62	113.69	117.00
57	BA	478	A	C5-C6-N1	6.62	121.01	117.70
57	BA	210	C	O4'-C1'-N1	6.62	113.49	108.20
57	BA	928	A	C4-C5-C6	-6.62	113.69	117.00
57	BA	1568	G	N1-C6-O6	-6.62	115.93	119.90
19	AH	87	ARG	NE-CZ-NH1	6.61	123.61	120.30
57	BA	761	A	C4-C5-C6	-6.61	113.69	117.00
57	BA	1892	C	N3-C2-O2	-6.61	117.27	121.90
22	AA	564	C	O4'-C1'-N1	6.61	113.49	108.20
22	AA	718	A	C4-C5-C6	-6.61	113.69	117.00
57	BA	1938	A	C4-C5-C6	-6.61	113.69	117.00
22	AA	946	A	C4-C5-C6	-6.61	113.69	117.00
57	BA	2634	A	C4-C5-C6	-6.61	113.70	117.00
22	AA	1145	A	C5-C6-N1	6.61	121.00	117.70
36	BU	2	ARG	NE-CZ-NH2	6.61	123.60	120.30
57	BA	2340	A	C4-C5-C6	-6.61	113.70	117.00
22	AA	720	C	N3-C2-O2	-6.61	117.28	121.90
57	BA	59	U	O4'-C1'-N1	6.61	113.48	108.20
57	BA	1705	A	C4-C5-C6	-6.61	113.70	117.00
22	AA	121	U	C3'-C2'-C1'	6.60	106.78	101.50
32	BR	45	ARG	NE-CZ-NH1	6.60	123.60	120.30
57	BA	2347	C	N1-C2-O2	6.60	122.86	118.90
22	AA	801	U	O4'-C1'-N1	6.60	113.48	108.20
22	AA	1539	C	N3-C2-O2	-6.60	117.28	121.90
57	BA	1190	G	O4'-C1'-N9	6.60	113.48	108.20
57	BA	1941	C	N3-C2-O2	-6.60	117.28	121.90
57	BA	203	A	C4-C5-C6	-6.60	113.70	117.00
57	BA	213	A	C4-C5-C6	-6.60	113.70	117.00
57	BA	1591	A	C4-C5-C6	-6.60	113.70	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2101	A	C4-C5-C6	-6.60	113.70	117.00
22	AA	564	C	N3-C2-O2	-6.60	117.28	121.90
22	AA	1171	A	O4'-C1'-N9	6.60	113.48	108.20
57	BA	2781	A	C4-C5-C6	-6.60	113.70	117.00
57	BA	821	A	C4-C5-C6	-6.60	113.70	117.00
57	BA	2494	G	N1-C6-O6	-6.60	115.94	119.90
24	A3	40	C	N1-C2-O2	6.59	122.86	118.90
36	BU	52	ARG	NE-CZ-NH2	-6.59	117.00	120.30
57	BA	2055	C	N3-C2-O2	-6.59	117.28	121.90
57	BA	2198	A	O4'-C1'-N9	6.59	113.47	108.20
58	Ba	14	U	O4'-C1'-N1	6.59	113.48	108.20
22	AA	715	A	C5-C6-N1	6.59	121.00	117.70
57	BA	527	C	N1-C2-O2	6.59	122.86	118.90
57	BA	2866	U	O4'-C1'-N1	6.59	113.47	108.20
22	AA	1252	A	C4-C5-C6	-6.59	113.71	117.00
57	BA	1646	C	N3-C2-O2	-6.59	117.29	121.90
57	BA	2667	C	N3-C2-O2	-6.59	117.29	121.90
22	AA	1492	A	C4-C5-C6	-6.59	113.71	117.00
57	BA	1493	C	N3-C2-O2	-6.59	117.29	121.90
22	AA	1269	A	C4-C5-C6	-6.58	113.71	117.00
22	AA	1463	U	O4'-C1'-N1	6.58	113.47	108.20
57	BA	1143	A	C4-C5-C6	-6.58	113.71	117.00
57	BA	2273	A	C4-C5-C6	-6.58	113.71	117.00
57	BA	2602	A	O4'-C1'-N9	6.58	113.47	108.20
58	Ba	11	C	N3-C2-O2	-6.58	117.29	121.90
58	Ba	27	C	O4'-C1'-N1	6.58	113.47	108.20
22	AA	1236	A	C4-C5-C6	-6.58	113.71	117.00
57	BA	948	C	O4'-C1'-N1	6.58	113.47	108.20
57	BA	1167	C	N1-C2-O2	6.58	122.85	118.90
57	BA	2179	C	O4'-C1'-N1	6.58	113.47	108.20
57	BA	1301	A	C4-C5-C6	-6.58	113.71	117.00
11	AB	94	ARG	NE-CZ-NH1	6.58	123.59	120.30
57	BA	1987	A	C4-C5-C6	-6.58	113.71	117.00
22	AA	338	A	N1-C6-N6	-6.58	114.65	118.60
22	AA	468	A	C4-C5-C6	-6.58	113.71	117.00
57	BA	2435	A	C4-C5-C6	-6.58	113.71	117.00
57	BA	16	C	O4'-C1'-N1	6.58	113.46	108.20
57	BA	1352	U	O4'-C1'-N1	6.58	113.46	108.20
22	AA	1513	A	O4'-C1'-N9	6.57	113.46	108.20
35	BD	101	ARG	NE-CZ-NH1	6.57	123.59	120.30
57	BA	471	A	C5-C6-N1	6.57	120.99	117.70
22	AA	1170	A	C4-C5-C6	-6.57	113.71	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	925	A	C4-C5-C6	-6.57	113.72	117.00
57	BA	1069	A	C4-C5-C6	-6.57	113.72	117.00
57	BA	1654	A	N1-C6-N6	-6.57	114.66	118.60
22	AA	1226	C	N3-C2-O2	-6.57	117.30	121.90
22	AA	1342	C	O4'-C1'-N1	6.57	113.45	108.20
42	B0	13	ARG	NH1-CZ-NH2	-6.57	112.18	119.40
57	BA	447	A	C4-C5-C6	-6.57	113.72	117.00
57	BA	1165	A	C4-C5-C6	-6.57	113.72	117.00
57	BA	1276	A	C4-C5-C6	-6.57	113.72	117.00
57	BA	1438	U	O4'-C1'-N1	6.57	113.45	108.20
22	AA	848	C	O4'-C1'-N1	6.57	113.45	108.20
57	BA	354	A	C4-C5-C6	-6.57	113.72	117.00
57	BA	1323	C	N1-C2-O2	6.57	122.84	118.90
57	BA	1583	A	C4-C5-C6	-6.57	113.72	117.00
57	BA	2276	G	O4'-C1'-N9	6.57	113.45	108.20
57	BA	2366	A	C4-C5-C6	-6.57	113.72	117.00
22	AA	288	A	C4-C5-C6	-6.56	113.72	117.00
57	BA	508	A	C4-C5-C6	-6.56	113.72	117.00
57	BA	525	U	O4'-C1'-N1	6.56	113.45	108.20
57	BA	2875	C	O4'-C1'-N1	6.56	113.45	108.20
58	Ba	119	A	C4-C5-C6	-6.56	113.72	117.00
57	BA	722	A	C4-C5-C6	-6.56	113.72	117.00
57	BA	1440	U	O4'-C1'-N1	6.56	113.45	108.20
57	BA	166	U	O4'-C1'-N1	6.56	113.45	108.20
57	BA	575	A	C5-C6-N1	6.56	120.98	117.70
57	BA	1679	A	C4-C5-C6	-6.56	113.72	117.00
57	BA	2394	C	O4'-C1'-N1	6.56	113.45	108.20
57	BA	2478	A	C4-C5-C6	-6.56	113.72	117.00
22	AA	470	C	N3-C2-O2	-6.56	117.31	121.90
57	BA	599	A	N1-C6-N6	-6.56	114.67	118.60
57	BA	2837	A	C4-C5-C6	-6.56	113.72	117.00
38	BW	84	ARG	NE-CZ-NH2	6.56	123.58	120.30
22	AA	400	C	N1-C2-O2	6.55	122.83	118.90
22	AA	518	C	N3-C2-O2	-6.55	117.31	121.90
22	AA	630	A	C4-C5-C6	-6.55	113.72	117.00
57	BA	721	A	N1-C6-N6	-6.55	114.67	118.60
57	BA	1152	C	O4'-C1'-N1	6.55	113.44	108.20
22	AA	1520	C	O4'-C1'-N1	6.55	113.44	108.20
24	A3	25	U	O4'-C1'-N1	6.55	113.44	108.20
58	Ba	108	A	N1-C6-N6	-6.55	114.67	118.60
22	AA	19	A	C4-C5-C6	-6.55	113.72	117.00
22	AA	72	A	N1-C6-N6	-6.55	114.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	430	A	C4-C5-C6	-6.55	113.72	117.00
57	BA	233	A	N1-C6-N6	-6.55	114.67	118.60
57	BA	2097	A	C4-C5-C6	-6.55	113.72	117.00
57	BA	2176	A	C4-C5-C6	-6.55	113.72	117.00
57	BA	2577	A	C4-C5-C6	-6.55	113.72	117.00
22	AA	270	A	C4-C5-C6	-6.55	113.72	117.00
22	AA	1468	A	C5-C6-N1	6.55	120.97	117.70
57	BA	1070	A	O4'-C1'-N9	6.55	113.44	108.20
57	BA	992	C	N3-C2-O2	-6.55	117.32	121.90
57	BA	1754	A	N1-C6-N6	-6.55	114.67	118.60
22	AA	349	A	C4-C5-C6	-6.55	113.73	117.00
22	AA	535	A	C4-C5-C6	-6.55	113.73	117.00
22	AA	872	A	C1'-O4'-C4'	-6.55	104.66	109.90
22	AA	1005	A	C4-C5-C6	-6.55	113.73	117.00
22	AA	1171	A	C4-C5-C6	-6.55	113.73	117.00
57	BA	2284	A	C4-C5-C6	-6.55	113.73	117.00
57	BA	528	A	C4-C5-C6	-6.54	113.73	117.00
51	B8	41	ARG	NE-CZ-NH2	6.54	123.57	120.30
57	BA	86	G	O4'-C1'-N9	6.54	113.44	108.20
22	AA	43	C	N3-C2-O2	-6.54	117.32	121.90
22	AA	1036	A	C4-C5-C6	-6.54	113.73	117.00
22	AA	1261	A	C4-C5-C6	-6.54	113.73	117.00
22	AA	1437	A	C4-C5-C6	-6.54	113.73	117.00
57	BA	844	A	C4-C5-C6	-6.54	113.73	117.00
22	AA	969	A	C4-C5-C6	-6.54	113.73	117.00
57	BA	779	U	O4'-C1'-N1	6.54	113.43	108.20
57	BA	1887	C	N3-C2-O2	-6.54	117.32	121.90
22	AA	563	A	C5-C6-N1	6.54	120.97	117.70
57	BA	1297	C	N3-C2-O2	-6.54	117.32	121.90
22	AA	676	A	C4-C5-C6	-6.54	113.73	117.00
22	AA	702	A	C4-C5-C6	-6.54	113.73	117.00
57	BA	416	U	O4'-C1'-N1	6.54	113.43	108.20
57	BA	497	A	C4-C5-C6	-6.54	113.73	117.00
57	BA	1090	A	C4-C5-C6	-6.54	113.73	117.00
57	BA	2063	C	N3-C4-C5	6.54	124.51	121.90
14	AC	58	ARG	NE-CZ-NH1	6.53	123.57	120.30
57	BA	249	C	N1-C2-O2	6.53	122.82	118.90
57	BA	257	C	N3-C2-O2	-6.53	117.33	121.90
57	BA	890	C	N3-C2-O2	-6.53	117.33	121.90
57	BA	1866	A	C5-C6-N1	6.53	120.97	117.70
22	AA	1413	A	C4-C5-C6	-6.53	113.73	117.00
22	AA	906	A	C4-C5-C6	-6.53	113.73	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2247	A	C4-C5-C6	-6.53	113.73	117.00
57	BA	484	C	N3-C2-O2	-6.53	117.33	121.90
57	BA	829	A	C4-C5-C6	-6.53	113.74	117.00
22	AA	754	C	N1-C2-O2	6.53	122.82	118.90
22	AA	819	A	C4-C5-C6	-6.53	113.74	117.00
22	AA	1483	A	C5-C6-N1	6.53	120.96	117.70
57	BA	2183	A	C4-C5-C6	-6.53	113.74	117.00
14	AC	228	ARG	NE-CZ-NH1	6.53	123.56	120.30
22	AA	949	A	C5-C6-N1	6.53	120.96	117.70
22	AA	1042	A	C4-C5-C6	-6.53	113.74	117.00
57	BA	2059	A	C4-C5-C6	-6.53	113.74	117.00
22	AA	54	C	N3-C2-O2	-6.52	117.33	121.90
57	BA	1599	U	O4'-C1'-N1	6.52	113.42	108.20
57	BA	2432	A	C4-C5-C6	-6.52	113.74	117.00
57	BA	152	A	C4-C5-C6	-6.52	113.74	117.00
57	BA	987	C	O4'-C1'-N1	6.52	113.42	108.20
57	BA	1749	A	C4-C5-C6	-6.52	113.74	117.00
58	Ba	110	C	O4'-C1'-N1	6.52	113.42	108.20
13	AU	46	ARG	NE-CZ-NH1	6.52	123.56	120.30
22	AA	1185	G	N1-C6-O6	-6.52	115.99	119.90
22	AA	1497	G	O4'-C1'-N9	6.52	113.42	108.20
57	BA	655	A	N1-C6-N6	-6.52	114.69	118.60
57	BA	878	A	C4-C5-C6	-6.52	113.74	117.00
57	BA	1098	A	C5-C6-N1	6.52	120.96	117.70
57	BA	1257	C	N3-C2-O2	-6.52	117.34	121.90
57	BA	1431	A	N1-C6-N6	-6.52	114.69	118.60
58	Ba	70	C	O4'-C1'-N1	6.52	113.42	108.20
9	AR	52	ARG	NE-CZ-NH1	6.52	123.56	120.30
22	AA	65	A	C4-C5-C6	-6.52	113.74	117.00
22	AA	533	A	C4-C5-C6	-6.52	113.74	117.00
57	BA	522	A	C4-C5-C6	-6.52	113.74	117.00
57	BA	1512	C	O4'-C1'-N1	6.52	113.41	108.20
31	BQ	55	ARG	NE-CZ-NH2	6.52	123.56	120.30
57	BA	348	A	C4-C5-C6	-6.52	113.74	117.00
57	BA	71	A	C4-C5-C6	-6.51	113.74	117.00
57	BA	237	C	N1-C2-O2	6.51	122.81	118.90
57	BA	501	A	C4-C5-C6	-6.51	113.74	117.00
57	BA	2336	A	C4-C5-C6	-6.51	113.74	117.00
22	AA	1431	A	C4-C5-C6	-6.51	113.74	117.00
22	AA	675	A	C4-C5-C6	-6.51	113.74	117.00
22	AA	1238	A	C4-C5-C6	-6.51	113.74	117.00
22	AA	281	G	O4'-C1'-N9	6.51	113.41	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	17	C	N3-C2-O2	-6.51	117.34	121.90
57	BA	1535	A	C4-C5-C6	-6.51	113.75	117.00
57	BA	1124	G	O4'-C1'-N9	6.51	113.41	108.20
57	BA	2563	U	O4'-C1'-N1	6.51	113.41	108.20
22	AA	837	U	O4'-C1'-N1	6.51	113.41	108.20
57	BA	1609	A	C4-C5-C6	-6.51	113.75	117.00
57	BA	2076	U	N3-C2-O2	-6.51	117.65	122.20
22	AA	300	A	C4-C5-C6	-6.50	113.75	117.00
57	BA	74	A	C4-C5-C6	-6.50	113.75	117.00
57	BA	456	C	N3-C2-O2	-6.50	117.35	121.90
57	BA	1611	C	N1-C2-O2	6.50	122.80	118.90
57	BA	2239	G	N1-C6-O6	-6.50	116.00	119.90
57	BA	2797	U	N3-C2-O2	-6.50	117.65	122.20
22	AA	519	C	C5'-C4'-C3'	-6.50	105.60	116.00
22	AA	689	C	O4'-C1'-N1	6.50	113.40	108.20
22	AA	1145	A	C4-C5-C6	-6.50	113.75	117.00
57	BA	429	A	C5-C6-N1	6.50	120.95	117.70
57	BA	613	A	C4-C5-C6	-6.50	113.75	117.00
57	BA	672	C	N1-C2-O2	6.50	122.80	118.90
57	BA	1654	A	C4-C5-C6	-6.50	113.75	117.00
57	BA	2842	G	O4'-C1'-N9	6.50	113.40	108.20
22	AA	176	C	N1-C2-O2	6.50	122.80	118.90
22	AA	546	A	C4-C5-C6	-6.50	113.75	117.00
22	AA	796	C	O4'-C1'-N1	6.50	113.40	108.20
57	BA	299	A	C4-C5-C6	-6.50	113.75	117.00
22	AA	1213	A	C5-C6-N1	6.50	120.95	117.70
35	BD	268	ARG	NE-CZ-NH1	6.50	123.55	120.30
57	BA	881	G	N1-C6-O6	-6.50	116.00	119.90
57	BA	1204	A	O4'-C1'-N9	6.50	113.40	108.20
57	BA	2429	G	O4'-C1'-N9	6.50	113.40	108.20
22	AA	77	A	C4-C5-C6	-6.50	113.75	117.00
22	AA	335	C	N3-C2-O2	-6.50	117.35	121.90
22	AA	501	C	N1-C2-O2	6.50	122.80	118.90
22	AA	825	A	C4-C5-C6	-6.50	113.75	117.00
57	BA	344	A	C4-C5-C6	-6.50	113.75	117.00
57	BA	908	C	O4'-C1'-N1	6.50	113.40	108.20
57	BA	444	C	O4'-C1'-N1	6.50	113.40	108.20
22	AA	7	A	C4-C5-C6	-6.49	113.75	117.00
22	AA	48	C	O4'-C1'-N1	6.49	113.39	108.20
22	AA	964	A	C4-C5-C6	-6.49	113.75	117.00
24	A3	47	A	C4-C5-C6	-6.49	113.75	117.00
57	BA	262	A	C4-C5-C6	-6.49	113.75	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	732	C	O4'-C1'-N1	6.49	113.39	108.20
57	BA	1978	A	C4-C5-C6	-6.49	113.75	117.00
57	BA	2755	C	O4'-C1'-N1	6.49	113.39	108.20
22	AA	613	C	N3-C2-O2	-6.49	117.36	121.90
57	BA	2513	A	C4-C5-C6	-6.49	113.75	117.00
22	AA	1096	C	N1-C2-O2	6.49	122.79	118.90
22	AA	1117	A	C4-C5-C6	-6.49	113.75	117.00
57	BA	201	C	O4'-C1'-N1	6.49	113.39	108.20
57	BA	716	A	C4-C5-C6	-6.49	113.75	117.00
22	AA	312	C	N1-C2-O2	6.49	122.79	118.90
22	AA	673	A	C4-C5-C6	-6.49	113.76	117.00
22	AA	985	C	N3-C2-O2	-6.49	117.36	121.90
22	AA	1493	A	C4-C5-C6	-6.49	113.76	117.00
57	BA	131	A	C4-C5-C6	-6.49	113.76	117.00
57	BA	2598	A	C4-C5-C6	-6.49	113.75	117.00
24	A3	59	A	C4-C5-C6	-6.49	113.76	117.00
28	BN	116	ARG	NE-CZ-NH1	6.49	123.54	120.30
22	AA	381	C	N1-C2-O2	6.49	122.79	118.90
38	BW	88	ARG	NE-CZ-NH1	-6.49	117.06	120.30
57	BA	1603	A	C4-C5-C6	-6.49	113.76	117.00
37	BV	79	ARG	NE-CZ-NH2	6.48	123.54	120.30
57	BA	99	U	N3-C2-O2	-6.48	117.66	122.20
22	AA	520	A	C5-C6-N1	6.48	120.94	117.70
28	BN	96	ARG	NE-CZ-NH2	6.48	123.54	120.30
39	BX	69	ARG	NE-CZ-NH1	6.48	123.54	120.30
57	BA	391	A	C4-C5-C6	-6.48	113.76	117.00
22	AA	522	C	N1-C2-O2	6.48	122.79	118.90
22	AA	784	A	C4-C5-C6	-6.48	113.76	117.00
57	BA	415	A	C4-C5-C6	-6.48	113.76	117.00
57	BA	1189	A	C4-C5-C6	-6.48	113.76	117.00
57	BA	1802	A	C5-C6-N1	6.48	120.94	117.70
57	BA	2205	A	C4-C5-C6	-6.48	113.76	117.00
13	AU	34	ARG	NH1-CZ-NH2	-6.48	112.27	119.40
57	BA	1870	C	N3-C2-O2	-6.48	117.36	121.90
22	AA	223	A	C4-C5-C6	-6.48	113.76	117.00
22	AA	314	C	N3-C2-O2	-6.48	117.37	121.90
51	B8	29	ARG	NE-CZ-NH2	6.48	123.54	120.30
57	BA	426	C	N1-C2-O2	6.48	122.79	118.90
57	BA	1495	A	C4-C5-C6	-6.48	113.76	117.00
57	BA	1997	C	N1-C2-O2	6.48	122.79	118.90
57	BA	2499	C	N3-C2-O2	-6.48	117.37	121.90
53	BF	114	ARG	NE-CZ-NH1	6.48	123.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	38	A	C4-C5-C6	-6.48	113.76	117.00
57	BA	2666	C	O4'-C1'-N1	6.48	113.38	108.20
22	AA	234	C	O4'-C1'-N1	6.47	113.38	108.20
23	A2	46	C	N3-C2-O2	-6.47	117.37	121.90
57	BA	1677	A	C4-C5-C6	-6.47	113.76	117.00
57	BA	2261	C	N3-C2-O2	-6.47	117.37	121.90
57	BA	2672	U	O4'-C1'-N1	6.47	113.38	108.20
22	AA	296	U	O4'-C1'-N1	6.47	113.38	108.20
22	AA	862	C	N1-C2-O2	6.47	122.78	118.90
57	BA	37	C	O4'-C1'-N1	6.47	113.38	108.20
57	BA	975	A	C4-C5-C6	-6.47	113.76	117.00
22	AA	195	A	C4-C5-C6	-6.47	113.77	117.00
22	AA	53	A	C4-C5-C6	-6.47	113.77	117.00
22	AA	1196	A	C4-C5-C6	-6.47	113.77	117.00
57	BA	1219	U	O4'-C1'-N1	6.47	113.38	108.20
57	BA	2133	G	N3-C4-C5	-6.47	125.36	128.60
57	BA	118	A	C4-C5-C6	-6.47	113.77	117.00
57	BA	206	U	O4'-C1'-N1	6.47	113.37	108.20
57	BA	320	A	C4-C5-C6	-6.47	113.77	117.00
57	BA	56	A	C4-C5-C6	-6.47	113.77	117.00
57	BA	127	A	C4-C5-C6	-6.47	113.77	117.00
57	BA	657	U	O4'-C1'-N1	6.47	113.37	108.20
57	BA	1919	A	C4-C5-C6	-6.46	113.77	117.00
57	BA	2465	C	O4'-C1'-N1	6.46	113.37	108.20
22	AA	648	A	C4-C5-C6	-6.46	113.77	117.00
22	AA	340	U	O4'-C1'-N1	6.46	113.37	108.20
22	AA	1508	A	N1-C6-N6	-6.46	114.72	118.60
58	Ba	57	A	C5-C6-N1	6.46	120.93	117.70
22	AA	1004	A	C4-C5-C6	-6.46	113.77	117.00
57	BA	646	U	O4'-C1'-N1	6.46	113.37	108.20
57	BA	1571	A	C5-C6-N1	6.46	120.93	117.70
20	AI	122	ARG	NE-CZ-NH2	-6.46	117.07	120.30
22	AA	98	A	C4-C5-C6	-6.46	113.77	117.00
57	BA	639	U	O4'-C1'-N1	6.46	113.37	108.20
57	BA	1525	A	C5-C6-N1	6.46	120.93	117.70
22	AA	655	A	C4-C5-C6	-6.46	113.77	117.00
22	AA	1357	A	N1-C6-N6	-6.46	114.73	118.60
51	B8	1	PRO	CA-N-CD	-6.46	102.46	111.50
57	BA	82	U	O4'-C1'-N1	6.46	113.37	108.20
57	BA	2462	C	N3-C2-O2	-6.46	117.38	121.90
22	AA	496	A	C1'-O4'-C4'	-6.46	104.74	109.90
57	BA	2175	C	O4'-C1'-N1	6.45	113.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2459	A	N1-C6-N6	-6.45	114.73	118.60
57	BA	2487	G	O4'-C1'-N9	6.45	113.36	108.20
22	AA	959	A	C4-C5-C6	-6.45	113.78	117.00
22	AA	1074	G	N1-C6-O6	-6.45	116.03	119.90
57	BA	233	A	C4-C5-C6	-6.45	113.77	117.00
57	BA	1295	C	N3-C2-O2	-6.45	117.38	121.90
57	BA	1700	A	C4-C5-C6	-6.45	113.77	117.00
57	BA	2283	C	O4'-C1'-N1	6.45	113.36	108.20
57	BA	2359	C	N3-C2-O2	-6.45	117.39	121.90
22	AA	459	A	C5-C6-N1	6.45	120.92	117.70
22	AA	1262	C	N3-C2-O2	-6.45	117.39	121.90
22	AA	1500	A	C4-C5-C6	-6.45	113.78	117.00
57	BA	347	A	C5-C6-N1	6.45	120.92	117.70
57	BA	2104	C	N3-C2-O2	-6.45	117.39	121.90
35	BD	270	ARG	NE-CZ-NH1	6.45	123.52	120.30
57	BA	176	A	C4-C5-C6	-6.45	113.78	117.00
57	BA	2007	U	O4'-C1'-N1	6.45	113.36	108.20
57	BA	2386	A	C4-C5-C6	-6.45	113.78	117.00
57	BA	172	A	C4-C5-C6	-6.44	113.78	117.00
57	BA	920	A	C4-C5-C6	-6.44	113.78	117.00
57	BA	1009	A	C4-C5-C6	-6.44	113.78	117.00
57	BA	1433	A	C4-C5-C6	-6.44	113.78	117.00
57	BA	2196	C	N1-C2-O2	6.44	122.77	118.90
57	BA	2601	C	N3-C2-O2	-6.44	117.39	121.90
57	BA	116	C	O4'-C1'-N1	6.44	113.35	108.20
57	BA	1221	C	O4'-C1'-N1	6.44	113.35	108.20
57	BA	2031	A	C4-C5-C6	-6.44	113.78	117.00
22	AA	882	C	O4'-C1'-N1	6.44	113.35	108.20
57	BA	163	C	N3-C2-O2	-6.44	117.39	121.90
57	BA	240	C	N3-C2-O2	-6.44	117.39	121.90
57	BA	311	A	C4-C5-C6	-6.44	113.78	117.00
57	BA	889	C	N3-C2-O2	-6.44	117.39	121.90
57	BA	1558	C	N3-C2-O2	-6.44	117.39	121.90
57	BA	1890	A	C4-C5-C6	-6.44	113.78	117.00
57	BA	2773	C	O4'-C1'-N1	6.44	113.35	108.20
57	BA	754	U	O4'-C1'-N1	6.43	113.35	108.20
57	BA	1810	A	C4-C5-C6	-6.43	113.78	117.00
3	AL	11	ARG	NE-CZ-NH1	6.43	123.52	120.30
57	BA	444	C	N3-C2-O2	-6.43	117.40	121.90
57	BA	1275	A	C4-C5-C6	-6.43	113.78	117.00
57	BA	1803	A	C4-C5-C6	-6.43	113.78	117.00
57	BA	2047	C	N3-C2-O2	-6.43	117.40	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1342	A	C4-C5-C6	-6.43	113.78	117.00
22	AA	263	A	C4-C5-C6	-6.43	113.78	117.00
22	AA	703	G	O4'-C1'-N9	6.43	113.34	108.20
22	AA	893	C	N3-C2-O2	-6.43	117.40	121.90
22	AA	1542	A	C4-C5-C6	-6.43	113.78	117.00
57	BA	1375	U	O4'-C1'-N1	6.43	113.34	108.20
57	BA	2028	U	O4'-C1'-N1	6.43	113.34	108.20
45	BE	77	ARG	NE-CZ-NH2	6.43	123.51	120.30
57	BA	1597	A	C4-C5-C6	-6.43	113.79	117.00
57	BA	1772	A	C4'-C3'-C2'	-6.43	96.17	102.60
22	AA	344	A	C4-C5-C6	-6.43	113.79	117.00
22	AA	687	A	C5-C6-N1	6.43	120.91	117.70
22	AA	1101	A	N1-C6-N6	-6.43	114.74	118.60
22	AA	1480	A	C4-C5-C6	-6.43	113.79	117.00
22	AA	119	A	C4-C5-C6	-6.42	113.79	117.00
22	AA	1382	C	N3-C4-C5	6.42	124.47	121.90
22	AA	1451	U	O4'-C1'-N1	6.42	113.34	108.20
45	BE	128	ARG	NH1-CZ-NH2	-6.42	112.33	119.40
57	BA	1047	G	O4'-C1'-N9	6.42	113.34	108.20
57	BA	1632	A	C4-C5-C6	-6.42	113.79	117.00
57	BA	2342	C	N1-C2-O2	6.42	122.75	118.90
57	BA	832	U	O4'-C1'-N1	6.42	113.34	108.20
57	BA	2564	A	C4-C5-C6	-6.42	113.79	117.00
22	AA	110	C	N3-C2-O2	-6.42	117.41	121.90
57	BA	1308	A	C4-C5-C6	-6.42	113.79	117.00
57	BA	1028	A	C4-C5-C6	-6.42	113.79	117.00
57	BA	717	C	N3-C2-O2	-6.42	117.41	121.90
57	BA	1610	A	C4-C5-C6	-6.42	113.79	117.00
57	BA	1644	C	N3-C2-O2	-6.42	117.41	121.90
57	BA	2114	A	C4-C5-C6	-6.42	113.79	117.00
22	AA	787	A	C4-C5-C6	-6.42	113.79	117.00
22	AA	999	C	N3-C2-O2	-6.42	117.41	121.90
22	AA	1403	C	N3-C2-O2	-6.42	117.41	121.90
57	BA	590	A	C4-C5-C6	-6.42	113.79	117.00
57	BA	1565	C	N3-C2-O2	-6.42	117.41	121.90
22	AA	307	C	N3-C2-O2	-6.41	117.41	121.90
24	A3	58	A	C4-C5-C6	-6.41	113.79	117.00
57	BA	440	C	N1-C2-O2	6.41	122.75	118.90
57	BA	742	A	C4-C5-C6	-6.41	113.79	117.00
35	BD	62	ARG	NE-CZ-NH1	6.41	123.50	120.30
57	BA	300	A	C4-C5-C6	-6.41	113.79	117.00
57	BA	1760	C	N3-C2-O2	-6.41	117.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2119	A	C4-C5-C6	-6.41	113.80	117.00
57	BA	2424	C	C1'-O4'-C4'	-6.41	104.77	109.90
57	BA	2511	U	O4'-C1'-N1	6.41	113.33	108.20
13	AU	20	ARG	NE-CZ-NH1	6.41	123.50	120.30
22	AA	1219	A	C4-C5-C6	-6.41	113.80	117.00
24	A3	73	A	C4-C5-C6	-6.41	113.80	117.00
57	BA	608	A	C4-C5-C6	-6.41	113.80	117.00
57	BA	1638	C	N1-C2-O2	6.41	122.75	118.90
23	A2	41	A	C4-C5-C6	-6.41	113.80	117.00
57	BA	2658	C	N3-C2-O2	-6.41	117.42	121.90
22	AA	559	A	C4-C5-C6	-6.41	113.80	117.00
22	AA	1176	A	C4-C5-C6	-6.41	113.80	117.00
22	AA	1360	A	C4-C5-C6	-6.41	113.80	117.00
24	A3	1	C	N1-C2-O2	6.41	122.74	118.90
57	BA	1265	A	C4-C5-C6	-6.41	113.80	117.00
57	BA	1882	U	O4'-C1'-N1	6.40	113.32	108.20
23	A2	14	G	O4'-C1'-N9	6.40	113.32	108.20
46	B3	15	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
57	BA	432	A	C4-C5-C6	-6.40	113.80	117.00
57	BA	1742	U	O4'-C1'-N1	6.40	113.32	108.20
58	Ba	55	U	O4'-C1'-N1	6.40	113.32	108.20
22	AA	189	A	C4-C5-C6	-6.40	113.80	117.00
22	AA	749	A	C4-C5-C6	-6.40	113.80	117.00
22	AA	948	C	O4'-C1'-N1	6.40	113.32	108.20
57	BA	1261	C	O4'-C1'-N1	6.40	113.32	108.20
57	BA	1900	A	C4-C5-C6	-6.40	113.80	117.00
57	BA	2115	G	O4'-C1'-N9	6.40	113.32	108.20
57	BA	2188	U	O4'-C1'-N1	6.40	113.32	108.20
22	AA	599	C	N3-C2-O2	-6.40	117.42	121.90
57	BA	650	C	O4'-C1'-N1	6.40	113.32	108.20
57	BA	1020	A	C4-C5-C6	-6.40	113.80	117.00
21	A1	278	ARG	NE-CZ-NH1	6.40	123.50	120.30
22	AA	169	C	O4'-C1'-N1	6.40	113.32	108.20
22	AA	845	A	C4-C5-C6	-6.40	113.80	117.00
33	BS	13	ARG	NE-CZ-NH1	6.40	123.50	120.30
57	BA	563	A	C4-C5-C6	-6.40	113.80	117.00
57	BA	1685	C	O4'-C1'-N1	6.40	113.32	108.20
57	BA	1942	C	N3-C2-O2	-6.40	117.42	121.90
22	AA	320	A	C4-C5-C6	-6.40	113.80	117.00
22	AA	498	A	C4-C5-C6	-6.39	113.80	117.00
22	AA	614	C	N1-C2-O2	6.39	122.74	118.90
57	BA	264	C	N3-C2-O2	-6.39	117.42	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	899	A	C4-C5-C6	-6.39	113.80	117.00
22	AA	135	C	N3-C2-O2	-6.39	117.42	121.90
22	AA	234	C	N1-C2-O2	6.39	122.74	118.90
22	AA	1362	A	C4-C5-C6	-6.39	113.80	117.00
57	BA	1067	A	C4-C5-C6	-6.39	113.80	117.00
22	AA	1210	C	N1-C2-O2	6.39	122.73	118.90
57	BA	626	A	C4-C5-C6	-6.39	113.80	117.00
57	BA	1211	C	N3-C2-O2	-6.39	117.43	121.90
22	AA	978	A	C5-C6-N1	6.39	120.89	117.70
57	BA	1996	C	O4'-C1'-N1	6.39	113.31	108.20
58	Ba	59	A	C4-C5-C6	-6.39	113.81	117.00
22	AA	1169	A	C4-C5-C6	-6.39	113.81	117.00
22	AA	1534	A	C4-C5-C6	-6.39	113.81	117.00
57	BA	2142	A	N1-C6-N6	-6.39	114.77	118.60
57	BA	2479	U	O4'-C1'-N1	6.39	113.31	108.20
22	AA	290	C	N1-C2-O2	6.38	122.73	118.90
57	BA	2135	A	C4-C5-C6	-6.38	113.81	117.00
57	BA	2637	U	O4'-C1'-N1	6.38	113.31	108.20
58	Ba	43	C	N3-C2-O2	-6.38	117.43	121.90
22	AA	478	A	C4-C5-C6	-6.38	113.81	117.00
22	AA	479	U	O4'-C1'-N1	6.38	113.31	108.20
22	AA	553	A	C4-C5-C6	-6.38	113.81	117.00
57	BA	1002	G	O4'-C1'-N9	6.38	113.31	108.20
22	AA	768	A	C4-C5-C6	-6.38	113.81	117.00
57	BA	164	C	N3-C2-O2	-6.38	117.43	121.90
57	BA	598	U	O4'-C1'-N1	6.38	113.30	108.20
22	AA	207	C	O4'-C1'-N1	6.38	113.30	108.20
22	AA	493	A	C4-C5-C6	-6.38	113.81	117.00
57	BA	786	C	N1-C2-O2	6.38	122.73	118.90
57	BA	1312	U	O4'-C1'-N1	6.38	113.30	108.20
57	BA	2704	C	N1-C2-O2	6.38	122.73	118.90
22	AA	873	A	C4-C5-C6	-6.38	113.81	117.00
57	BA	867	C	O4'-C1'-N1	6.38	113.30	108.20
57	BA	1251	C	C1'-O4'-C4'	-6.38	104.80	109.90
57	BA	1257	C	O4'-C1'-N1	6.38	113.30	108.20
57	BA	1322	A	C4-C5-C6	-6.38	113.81	117.00
57	BA	1641	A	C4-C5-C6	-6.38	113.81	117.00
57	BA	2226	C	N3-C2-O2	-6.38	117.44	121.90
57	BA	2829	A	C4-C5-C6	-6.38	113.81	117.00
57	BA	2734	A	C4-C5-C6	-6.38	113.81	117.00
57	BA	478	A	C4-C5-C6	-6.37	113.81	117.00
57	BA	1446	C	N1-C2-O2	6.37	122.72	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1681	G	O4'-C1'-N9	6.37	113.30	108.20
57	BA	2305	U	O4'-C1'-N1	6.37	113.30	108.20
22	AA	923	A	C4-C5-C6	-6.37	113.81	117.00
57	BA	10	A	C4-C5-C6	-6.37	113.81	117.00
57	BA	1469	A	C4-C5-C6	-6.37	113.81	117.00
57	BA	2088	A	C4-C5-C6	-6.37	113.81	117.00
57	BA	2160	C	N1-C2-O2	6.37	122.72	118.90
57	BA	2207	C	N1-C2-O2	6.37	122.72	118.90
57	BA	816	C	N1-C2-O2	6.37	122.72	118.90
22	AA	732	C	N1-C2-O2	6.37	122.72	118.90
57	BA	459	U	O4'-C1'-N1	6.37	113.29	108.20
57	BA	633	A	C4-C5-C6	-6.37	113.82	117.00
57	BA	1246	A	C4-C5-C6	-6.37	113.82	117.00
57	BA	2037	A	C4-C5-C6	-6.37	113.82	117.00
58	Ba	95	U	O4'-C1'-N1	6.37	113.30	108.20
22	AA	597	G	N1-C6-O6	-6.37	116.08	119.90
50	B7	34	ARG	CD-NE-CZ	6.37	132.51	123.60
22	AA	215	C	O4'-C1'-N1	6.37	113.29	108.20
22	AA	342	C	N1-C2-O2	6.37	122.72	118.90
22	AA	812	G	O4'-C1'-N9	6.37	113.29	108.20
22	AA	1258	G	N1-C6-O6	-6.37	116.08	119.90
57	BA	466	A	C4-C5-C6	-6.37	113.82	117.00
57	BA	2473	U	O4'-C1'-N1	6.37	113.29	108.20
57	BA	2706	A	C4-C5-C6	-6.37	113.82	117.00
22	AA	1277	C	N3-C2-O2	-6.36	117.45	121.90
28	BN	95	ARG	NE-CZ-NH1	6.36	123.48	120.30
57	BA	2364	C	O4'-C1'-N1	6.36	113.29	108.20
57	BA	2516	A	C4-C5-C6	-6.36	113.82	117.00
57	BA	2612	C	N3-C2-O2	-6.36	117.45	121.90
22	AA	1054	C	N3-C2-O2	-6.36	117.45	121.90
57	BA	2406	A	C4-C5-C6	-6.36	113.82	117.00
57	BA	1379	U	O4'-C1'-N1	6.36	113.29	108.20
57	BA	1655	A	N1-C6-N6	-6.36	114.78	118.60
57	BA	2352	A	C5-C6-N1	6.36	120.88	117.70
29	BO	78	ARG	NE-CZ-NH1	6.36	123.48	120.30
57	BA	1894	C	N3-C2-O2	-6.36	117.45	121.90
57	BA	1417	C	O4'-C1'-N1	6.36	113.29	108.20
22	AA	1507	A	C4-C5-C6	-6.36	113.82	117.00
41	BZ	93	ARG	NE-CZ-NH1	6.36	123.48	120.30
57	BA	275	C	N3-C2-O2	-6.36	117.45	121.90
57	BA	2706	A	C5-C6-N1	6.36	120.88	117.70
22	AA	130	A	C4-C5-C6	-6.35	113.82	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	296	U	O4'-C1'-N1	6.35	113.28	108.20
57	BA	1544	A	C4-C5-C6	-6.35	113.82	117.00
24	A3	48	U	O4'-C1'-N1	6.35	113.28	108.20
24	A3	77	A	C4-C5-C6	-6.35	113.82	117.00
57	BA	2602	A	C4-C5-C6	-6.35	113.82	117.00
57	BA	457	A	C4-C5-C6	-6.35	113.82	117.00
57	BA	1286	A	C4-C5-C6	-6.35	113.82	117.00
22	AA	864	A	C4-C5-C6	-6.35	113.83	117.00
24	A3	46	G	O4'-C1'-N9	6.35	113.28	108.20
29	BO	64	ARG	NE-CZ-NH1	6.35	123.47	120.30
57	BA	157	C	O4'-C1'-N1	6.35	113.28	108.20
57	BA	547	A	C4-C5-C6	-6.35	113.83	117.00
57	BA	2823	A	C4-C5-C6	-6.35	113.83	117.00
22	AA	364	A	C4-C5-C6	-6.35	113.83	117.00
57	BA	1347	A	C4-C5-C6	-6.35	113.83	117.00
22	AA	1274	A	C4-C5-C6	-6.35	113.83	117.00
57	BA	195	A	N1-C6-N6	-6.35	114.79	118.60
18	AG	78	ARG	NE-CZ-NH1	6.34	123.47	120.30
22	AA	338	A	C4-C5-C6	-6.34	113.83	117.00
35	BD	51	ARG	NE-CZ-NH2	-6.34	117.13	120.30
57	BA	1474	U	O4'-C1'-N1	6.34	113.27	108.20
57	BA	2568	U	O4'-C1'-N1	6.34	113.27	108.20
22	AA	151	A	O4'-C1'-N9	6.34	113.27	108.20
57	BA	1791	A	C4-C5-C6	-6.34	113.83	117.00
57	BA	2542	A	C4-C5-C6	-6.34	113.83	117.00
57	BA	1596	A	C4-C5-C6	-6.34	113.83	117.00
57	BA	1676	A	C4-C5-C6	-6.34	113.83	117.00
22	AA	457	G	O4'-C1'-N9	6.34	113.27	108.20
57	BA	251	A	C5-C6-N1	6.34	120.87	117.70
22	AA	188	C	N3-C2-O2	-6.33	117.47	121.90
22	AA	306	A	C4-C5-C6	-6.33	113.83	117.00
22	AA	1012	A	C4-C5-C6	-6.33	113.83	117.00
57	BA	1172	C	N1-C2-O2	6.33	122.70	118.90
57	BA	1285	A	C5-C6-N1	6.33	120.87	117.70
24	A3	44	A	C4-C5-C6	-6.33	113.83	117.00
57	BA	1913	A	C4-C5-C6	-6.33	113.83	117.00
57	BA	845	A	C5-C6-N1	6.33	120.87	117.70
57	BA	1156	A	C4-C5-C6	-6.33	113.83	117.00
57	BA	1226	A	C4-C5-C6	-6.33	113.83	117.00
57	BA	2268	A	C5-C6-N1	6.33	120.87	117.70
57	BA	2412	A	C4-C5-C6	-6.33	113.83	117.00
22	AA	731	G	O4'-C1'-N9	6.33	113.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1593	A	C4-C5-C6	-6.33	113.83	117.00
22	AA	853	C	O4'-C1'-N1	6.33	113.26	108.20
22	AA	1267	C	N3-C2-O2	-6.33	117.47	121.90
57	BA	645	C	N3-C2-O2	-6.33	117.47	121.90
57	BA	1261	C	N1-C2-O2	6.33	122.70	118.90
57	BA	1614	A	C4-C5-C6	-6.33	113.84	117.00
6	AO	88	ARG	NE-CZ-NH1	6.33	123.46	120.30
22	AA	264	C	O4'-C1'-N1	6.33	113.26	108.20
57	BA	1096	A	C4-C5-C6	-6.33	113.84	117.00
57	BA	1395	A	C4-C5-C6	-6.33	113.84	117.00
57	BA	2184	A	C4-C5-C6	-6.33	113.84	117.00
22	AA	562	U	O4'-C1'-N1	6.32	113.26	108.20
57	BA	109	C	O4'-C1'-N1	6.32	113.26	108.20
57	BA	194	G	N1-C6-O6	-6.32	116.11	119.90
57	BA	379	G	N1-C6-O6	-6.32	116.11	119.90
57	BA	961	C	N3-C2-O2	-6.32	117.47	121.90
57	BA	1570	A	C4-C5-C6	-6.32	113.84	117.00
57	BA	2688	G	O4'-C1'-N9	6.32	113.26	108.20
57	BA	228	C	N3-C2-O2	-6.32	117.47	121.90
57	BA	820	A	C4-C5-C6	-6.32	113.84	117.00
22	AA	1194	U	O4'-C1'-N1	6.32	113.26	108.20
52	B9	24	ARG	NE-CZ-NH2	6.32	123.46	120.30
57	BA	1336	A	C4-C5-C6	-6.32	113.84	117.00
57	BA	1739	A	C4-C5-C6	-6.32	113.84	117.00
57	BA	2463	C	N1-C2-O2	6.32	122.69	118.90
57	BA	2388	A	C4-C5-C6	-6.32	113.84	117.00
57	BA	383	C	N3-C2-O2	-6.32	117.48	121.90
57	BA	324	A	C4-C5-C6	-6.31	113.84	117.00
57	BA	736	C	N3-C2-O2	-6.31	117.48	121.90
22	AA	403	C	N1-C2-O2	6.31	122.69	118.90
57	BA	710	U	O4'-C1'-N1	6.31	113.25	108.20
22	AA	365	U	N3-C2-O2	-6.31	117.78	122.20
57	BA	164	C	O4'-C1'-N1	6.31	113.25	108.20
57	BA	1159	U	O4'-C1'-N1	6.31	113.25	108.20
57	BA	2809	A	N1-C6-N6	-6.31	114.81	118.60
57	BA	342	A	C4-C5-C6	-6.31	113.84	117.00
57	BA	1111	A	C4-C5-C6	-6.31	113.84	117.00
57	BA	2799	A	C4-C5-C6	-6.31	113.85	117.00
57	BA	1241	A	C4-C5-C6	-6.31	113.85	117.00
57	BA	2150	C	O4'-C1'-N1	6.31	113.25	108.20
57	BA	1829	A	C4-C5-C6	-6.31	113.85	117.00
22	AA	620	C	O4'-C1'-N1	6.30	113.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1476	A	C4-C5-C6	-6.30	113.85	117.00
57	BA	624	C	N1-C2-O2	6.30	122.68	118.90
57	BA	1551	A	C4-C5-C6	-6.30	113.85	117.00
57	BA	1800	C	N1-C2-O2	6.30	122.68	118.90
57	BA	2106	U	O4'-C1'-N1	6.30	113.24	108.20
57	BA	2322	A	C4-C5-C6	-6.30	113.85	117.00
57	BA	2587	A	N1-C6-N6	-6.30	114.82	118.60
22	AA	975	A	C4-C5-C6	-6.30	113.85	117.00
58	Ba	42	C	N3-C2-O2	-6.30	117.49	121.90
22	AA	663	A	C4-C5-C6	-6.30	113.85	117.00
57	BA	566	U	O4'-C1'-N1	6.30	113.24	108.20
57	BA	1420	A	C4-C5-C6	-6.30	113.85	117.00
57	BA	2809	A	C4-C5-C6	-6.30	113.85	117.00
57	BA	217	A	C4-C5-C6	-6.30	113.85	117.00
57	BA	2155	U	O4'-C1'-N1	6.30	113.24	108.20
57	BA	2328	A	C4-C5-C6	-6.30	113.85	117.00
57	BA	2062	A	C4-C5-C6	-6.30	113.85	117.00
57	BA	635	C	N1-C2-O2	6.30	122.68	118.90
57	BA	640	C	N1-C2-O2	6.29	122.68	118.90
22	AA	509	A	C4-C5-C6	-6.29	113.85	117.00
57	BA	14	A	O4'-C1'-N9	6.29	113.23	108.20
57	BA	2885	G	O4'-C1'-N9	6.29	113.24	108.20
57	BA	277	G	O4'-C1'-N9	6.29	113.23	108.20
22	AA	412	A	C4-C5-C6	-6.29	113.86	117.00
22	AA	1510	C	C5'-C4'-O4'	6.29	116.65	109.10
57	BA	120	U	O4'-C1'-N1	6.29	113.23	108.20
57	BA	1013	C	O4'-C1'-N1	6.29	113.23	108.20
57	BA	1169	A	C4-C5-C6	-6.29	113.86	117.00
15	AD	55	ARG	NE-CZ-NH1	6.29	123.44	120.30
15	AD	110	ARG	NE-CZ-NH1	6.29	123.44	120.30
22	AA	545	C	N1-C2-O2	6.29	122.67	118.90
57	BA	362	A	C4-C5-C6	-6.29	113.86	117.00
57	BA	1092	C	O4'-C1'-N1	6.29	113.23	108.20
22	AA	106	C	N1-C2-O2	6.28	122.67	118.90
22	AA	1132	C	O4'-C1'-N1	6.28	113.23	108.20
22	AA	1150	A	C4-C5-C6	-6.28	113.86	117.00
57	BA	604	G	C5'-C4'-O4'	6.28	116.64	109.10
58	Ba	53	A	C4-C5-C6	-6.28	113.86	117.00
57	BA	2178	C	O4'-C1'-N1	6.28	113.23	108.20
57	BA	2227	A	C4-C5-C6	-6.28	113.86	117.00
18	AG	1	PRO	CA-N-CD	-6.28	102.71	111.50
22	AA	1271	A	C4-C5-C6	-6.28	113.86	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BH	169	ARG	NE-CZ-NH2	6.28	123.44	120.30
57	BA	1236	G	O4'-C1'-N9	6.28	113.22	108.20
57	BA	1777	U	N3-C2-O2	-6.28	117.80	122.20
57	BA	2452	C	N3-C2-O2	-6.28	117.50	121.90
57	BA	2539	C	N3-C2-O2	-6.28	117.50	121.90
22	AA	284	C	O4'-C1'-N1	6.28	113.22	108.20
22	AA	1504	G	O4'-C1'-N9	6.28	113.22	108.20
57	BA	451	U	O4'-C1'-N1	6.28	113.22	108.20
22	AA	624	C	O4'-C1'-N1	6.28	113.22	108.20
31	BQ	114	ARG	NE-CZ-NH2	6.28	123.44	120.30
57	BA	545	U	O4'-C1'-N1	6.28	113.22	108.20
57	BA	688	U	O4'-C1'-N1	6.28	113.22	108.20
57	BA	2374	C	N1-C2-O2	6.28	122.67	118.90
22	AA	802	A	C4-C5-C6	-6.28	113.86	117.00
22	AA	865	A	C4-C5-C6	-6.28	113.86	117.00
22	AA	1456	A	C4-C5-C6	-6.28	113.86	117.00
57	BA	2456	C	N1-C2-O2	6.28	122.67	118.90
57	BA	2774	C	O4'-C1'-N1	6.28	113.22	108.20
57	BA	1994	C	N3-C2-O2	-6.27	117.51	121.90
22	AA	182	A	C4-C5-C6	-6.27	113.86	117.00
22	AA	1472	U	O4'-C1'-N1	6.27	113.22	108.20
57	BA	1398	C	N1-C2-O2	6.27	122.66	118.90
22	AA	1201	A	C4-C5-C6	-6.27	113.86	117.00
57	BA	1675	C	N3-C2-O2	-6.27	117.51	121.90
57	BA	2422	C	N3-C2-O2	-6.27	117.51	121.90
22	AA	71	A	C4-C5-C6	-6.27	113.87	117.00
44	B2	7	ARG	NH1-CZ-NH2	-6.27	112.51	119.40
57	BA	675	A	C4-C5-C6	-6.27	113.87	117.00
57	BA	2061	G	C4'-C3'-C2'	-6.27	96.33	102.60
57	BA	1319	C	N1-C2-O2	6.26	122.66	118.90
57	BA	2247	A	C5-C6-N1	6.26	120.83	117.70
57	BA	2762	C	O4'-C1'-N1	6.26	113.21	108.20
22	AA	473	U	O4'-C1'-N1	6.26	113.21	108.20
23	A2	48	C	N3-C2-O2	-6.26	117.52	121.90
58	Ba	47	C	N3-C2-O2	-6.26	117.52	121.90
47	B4	63	ARG	NE-CZ-NH1	6.26	123.43	120.30
57	BA	910	A	C4-C5-C6	-6.26	113.87	117.00
57	BA	1462	C	O4'-C1'-N1	6.26	113.21	108.20
57	BA	1652	A	C4-C5-C6	-6.26	113.87	117.00
57	BA	1791	A	N1-C6-N6	-6.26	114.84	118.60
22	AA	721	G	O4'-C1'-N9	6.26	113.21	108.20
28	BN	37	ARG	NE-CZ-NH2	6.26	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	196	A	C4-C5-C6	-6.26	113.87	117.00
22	AA	8	A	C4-C5-C6	-6.26	113.87	117.00
22	AA	796	C	N1-C2-O2	6.26	122.66	118.90
24	A3	45	A	C4-C5-C6	-6.26	113.87	117.00
22	AA	1538	C	N3-C2-O2	-6.26	117.52	121.90
57	BA	31	C	O4'-C1'-N1	6.26	113.21	108.20
57	BA	1553	A	C4-C5-C6	-6.26	113.87	117.00
57	BA	2005	A	C4-C5-C6	-6.26	113.87	117.00
57	BA	2899	A	C4-C5-C6	-6.26	113.87	117.00
57	BA	29	U	O4'-C1'-N1	6.25	113.20	108.20
57	BA	752	A	C4-C5-C6	-6.25	113.87	117.00
22	AA	1092	A	C4-C5-C6	-6.25	113.87	117.00
24	A3	72	C	O4'-C1'-N1	6.25	113.20	108.20
57	BA	2708	G	O4'-C1'-N9	6.25	113.20	108.20
22	AA	1112	C	N3-C2-O2	-6.25	117.52	121.90
22	AA	1161	C	N1-C2-O2	6.25	122.65	118.90
22	AA	1287	A	C4-C5-C6	-6.25	113.87	117.00
57	BA	437	U	O4'-C1'-N1	6.25	113.20	108.20
57	BA	2417	C	O4'-C1'-N1	6.25	113.20	108.20
22	AA	333	U	O4'-C1'-N1	6.25	113.20	108.20
22	AA	480	U	O4'-C1'-N1	6.25	113.20	108.20
22	AA	1023	U	O4'-C1'-N1	6.25	113.20	108.20
22	AA	1254	A	C4-C5-C6	-6.25	113.88	117.00
46	B3	37	ARG	NE-CZ-NH1	6.25	123.42	120.30
57	BA	727	A	C4-C5-C6	-6.25	113.88	117.00
57	BA	2015	A	C4-C5-C6	-6.25	113.88	117.00
57	BA	2610	C	N3-C4-C5	6.25	124.40	121.90
57	BA	2758	A	C4-C5-C6	-6.25	113.88	117.00
57	BA	2766	A	C4-C5-C6	-6.25	113.88	117.00
58	Ba	28	C	N1-C2-O2	6.25	122.65	118.90
58	Ba	45	A	C4-C5-C6	-6.25	113.88	117.00
22	AA	419	C	N1-C2-O2	6.25	122.65	118.90
22	AA	953	G	N1-C6-O6	-6.25	116.15	119.90
22	AA	977	A	C4-C5-C6	-6.25	113.88	117.00
57	BA	823	C	N1-C2-O2	6.25	122.65	118.90
57	BA	2236	U	O4'-C1'-N1	6.25	113.20	108.20
57	BA	1549	A	C4-C5-C6	-6.25	113.88	117.00
32	BR	96	ARG	NE-CZ-NH1	6.24	123.42	120.30
57	BA	143	C	O4'-C1'-N1	6.24	113.19	108.20
57	BA	1839	G	O4'-C1'-N9	6.24	113.19	108.20
22	AA	73	C	O4'-C1'-N1	6.24	113.19	108.20
57	BA	2436	G	N1-C6-O6	-6.24	116.16	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	287	U	O4'-C1'-N1	6.24	113.19	108.20
22	AA	659	U	O4'-C1'-N1	6.24	113.19	108.20
22	AA	1428	A	C4-C5-C6	-6.24	113.88	117.00
57	BA	794	A	C4-C5-C6	-6.24	113.88	117.00
57	BA	1221	C	N1-C2-O2	6.24	122.64	118.90
57	BA	1754	A	C5-C6-N1	6.24	120.82	117.70
57	BA	1762	A	C4-C5-C6	-6.24	113.88	117.00
57	BA	418	C	N1-C2-O2	6.24	122.64	118.90
57	BA	569	U	O4'-C1'-N1	6.24	113.19	108.20
57	BA	740	C	O4'-C1'-N1	6.24	113.19	108.20
57	BA	1144	A	C4-C5-C6	-6.24	113.88	117.00
57	BA	1227	G	N1-C6-O6	-6.24	116.16	119.90
57	BA	2279	G	N1-C6-O6	-6.24	116.16	119.90
22	AA	741	G	N1-C6-O6	-6.24	116.16	119.90
57	BA	936	A	C4-C5-C6	-6.24	113.88	117.00
58	Ba	115	A	C4-C5-C6	-6.24	113.88	117.00
57	BA	1217	U	O4'-C1'-N1	6.23	113.19	108.20
57	BA	2635	A	C4-C5-C6	-6.23	113.88	117.00
57	BA	1270	C	O4'-C1'-N1	6.23	113.19	108.20
57	BA	2860	A	C4-C5-C6	-6.23	113.88	117.00
3	AL	53	ARG	NE-CZ-NH1	6.23	123.42	120.30
22	AA	689	C	N1-C2-O2	6.23	122.64	118.90
22	AA	876	C	N3-C2-O2	-6.23	117.54	121.90
23	A2	18	A	C4-C5-C6	-6.23	113.89	117.00
38	BW	110	ARG	NE-CZ-NH2	6.23	123.42	120.30
57	BA	330	A	O4'-C1'-N9	6.23	113.18	108.20
57	BA	982	C	N3-C2-O2	-6.23	117.54	121.90
57	BA	944	C	N3-C4-N4	-6.23	113.64	118.00
57	BA	2173	A	C4-C5-C6	-6.23	113.89	117.00
22	AA	108	G	N3-C4-C5	-6.23	125.49	128.60
22	AA	192	A	C4-C5-C6	-6.23	113.89	117.00
22	AA	1132	C	N1-C2-O2	6.23	122.64	118.90
22	AA	1425	U	O4'-C1'-N1	6.23	113.18	108.20
35	BD	42	ARG	NE-CZ-NH1	6.23	123.41	120.30
57	BA	383	C	O4'-C1'-N1	6.23	113.18	108.20
57	BA	1936	A	C4-C5-C6	-6.23	113.89	117.00
57	BA	1561	C	N1-C2-O2	6.23	122.64	118.90
16	AE	53	ARG	NE-CZ-NH1	6.22	123.41	120.30
55	BH	68	ARG	NE-CZ-NH1	6.22	123.41	120.30
8	AQ	61	ARG	NE-CZ-NH1	6.22	123.41	120.30
14	AC	126	ARG	NE-CZ-NH1	6.22	123.41	120.30
57	BA	282	A	C4-C5-C6	-6.22	113.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	998	C	N1-C2-O2	6.22	122.63	118.90
57	BA	2566	A	C4-C5-C6	-6.22	113.89	117.00
22	AA	376	G	N1-C6-O6	-6.22	116.17	119.90
57	BA	2169	A	C4-C5-C6	-6.22	113.89	117.00
5	AN	64	ARG	NE-CZ-NH1	6.22	123.41	120.30
22	AA	621	A	C4-C5-C6	-6.22	113.89	117.00
27	BK	126	ARG	NE-CZ-NH1	6.22	123.41	120.30
32	BR	30	ARG	NE-CZ-NH1	6.22	123.41	120.30
57	BA	1392	A	C4-C5-C6	-6.22	113.89	117.00
57	BA	2424	C	N3-C2-O2	-6.22	117.55	121.90
57	BA	1933	G	O4'-C1'-N9	6.22	113.17	108.20
22	AA	623	C	O4'-C1'-N1	6.22	113.17	108.20
22	AA	1358	U	N3-C2-O2	-6.22	117.85	122.20
57	BA	6	A	C4-C5-C6	-6.22	113.89	117.00
57	BA	116	C	N1-C2-O2	6.22	122.63	118.90
57	BA	1008	A	C4-C5-C6	-6.22	113.89	117.00
57	BA	1520	U	O4'-C1'-N1	6.22	113.17	108.20
57	BA	2332	C	O4'-C1'-N1	6.22	113.17	108.20
16	AE	44	ARG	NE-CZ-NH1	6.21	123.41	120.30
22	AA	385	C	N1-C2-O2	6.21	122.63	118.90
22	AA	779	C	N1-C2-O2	6.21	122.63	118.90
57	BA	1045	C	N3-C2-O2	-6.21	117.55	121.90
57	BA	2142	A	C4-C5-C6	-6.21	113.89	117.00
58	Ba	101	A	C4-C5-C6	-6.21	113.89	117.00
22	AA	33	A	N1-C6-N6	-6.21	114.87	118.60
22	AA	816	A	C4-C5-C6	-6.21	113.89	117.00
57	BA	1439	A	C4-C5-C6	-6.21	113.89	117.00
57	BA	2443	C	N1-C2-O2	6.21	122.63	118.90
13	AU	44	ARG	NE-CZ-NH1	6.21	123.41	120.30
22	AA	782	A	C4-C5-C6	-6.21	113.89	117.00
22	AA	998	C	N1-C2-O2	6.21	122.63	118.90
57	BA	1022	G	N1-C6-O6	-6.21	116.17	119.90
57	BA	1585	C	N3-C2-O2	-6.21	117.55	121.90
57	BA	689	A	C4-C5-C6	-6.21	113.89	117.00
57	BA	1698	A	N1-C6-N6	-6.21	114.88	118.60
57	BA	1761	C	N3-C2-O2	-6.21	117.55	121.90
57	BA	2815	C	O4'-C1'-N1	6.21	113.17	108.20
22	AA	441	A	C4-C5-C6	-6.21	113.90	117.00
22	AA	1314	C	N1-C2-O2	6.21	122.62	118.90
22	AA	28	A	C4-C5-C6	-6.20	113.90	117.00
22	AA	431	A	C4-C5-C6	-6.20	113.90	117.00
57	BA	357	C	O4'-C1'-N1	6.20	113.16	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1135	C	N3-C2-O2	-6.20	117.56	121.90
57	BA	2126	A	C4-C5-C6	-6.20	113.90	117.00
57	BA	2610	C	N3-C2-O2	-6.20	117.56	121.90
57	BA	2617	U	O4'-C1'-N1	6.20	113.16	108.20
57	BA	2700	A	C5-C6-N1	6.20	120.80	117.70
57	BA	2710	C	N1-C2-O2	6.20	122.62	118.90
22	AA	215	C	N1-C2-O2	6.20	122.62	118.90
57	BA	80	G	N1-C6-O6	-6.20	116.18	119.90
57	BA	2824	C	O4'-C1'-N1	6.20	113.16	108.20
22	AA	232	G	N3-C2-N2	-6.20	115.56	119.90
22	AA	919	A	C4-C5-C6	-6.20	113.90	117.00
57	BA	241	A	N1-C6-N6	-6.20	114.88	118.60
57	BA	683	U	O4'-C1'-N1	6.20	113.16	108.20
22	AA	490	C	O4'-C1'-N1	6.20	113.16	108.20
22	AA	569	C	N3-C2-O2	-6.20	117.56	121.90
57	BA	1173	U	O4'-C1'-N1	6.20	113.16	108.20
57	BA	1406	U	O4'-C1'-N1	6.20	113.16	108.20
57	BA	2759	G	N1-C6-O6	-6.20	116.18	119.90
22	AA	1467	C	N3-C2-O2	-6.20	117.56	121.90
57	BA	1253	A	C4-C5-C6	-6.20	113.90	117.00
57	BA	2850	A	C4-C5-C6	-6.20	113.90	117.00
57	BA	1655	A	C5-C6-N1	6.19	120.80	117.70
57	BA	2752	C	N3-C2-O2	-6.19	117.56	121.90
57	BA	734	A	C4-C5-C6	-6.19	113.90	117.00
57	BA	2178	C	N3-C2-O2	-6.19	117.57	121.90
22	AA	539	A	C4-C5-C6	-6.19	113.91	117.00
22	AA	25	C	N1-C2-O2	6.19	122.61	118.90
27	BK	102	ARG	NE-CZ-NH1	6.19	123.39	120.30
22	AA	298	A	C4-C5-C6	-6.19	113.91	117.00
22	AA	1359	C	N3-C2-O2	-6.19	117.57	121.90
57	BA	817	C	N1-C2-O2	6.19	122.61	118.90
57	BA	1064	C	C4'-C3'-C2'	-6.19	96.41	102.60
57	BA	1176	U	O4'-C1'-N1	6.19	113.15	108.20
57	BA	1326	U	O4'-C1'-N1	6.19	113.15	108.20
57	BA	1541	C	O4'-C1'-N1	6.19	113.15	108.20
57	BA	1758	U	N3-C2-O2	-6.19	117.87	122.20
57	BA	1925	C	N3-C2-O2	-6.19	117.57	121.90
57	BA	581	C	O4'-C1'-N1	6.19	113.15	108.20
57	BA	2649	C	O4'-C1'-N1	6.19	113.15	108.20
7	AP	28	ARG	NE-CZ-NH1	6.18	123.39	120.30
22	AA	582	C	N3-C2-O2	-6.18	117.57	121.90
57	BA	1178	C	N1-C2-O2	6.18	122.61	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1881	C	O4'-C1'-N1	6.18	113.15	108.20
22	AA	226	G	N1-C6-O6	-6.18	116.19	119.90
45	BE	124	ARG	NE-CZ-NH1	6.18	123.39	120.30
57	BA	2329	U	O4'-C1'-N1	6.18	113.15	108.20
22	AA	1117	A	O4'-C1'-N9	6.18	113.14	108.20
57	BA	737	C	O4'-C1'-N1	6.18	113.14	108.20
57	BA	2079	U	O4'-C1'-N1	6.18	113.14	108.20
57	BA	676	A	C4-C5-C6	-6.18	113.91	117.00
57	BA	919	U	O4'-C1'-N1	6.18	113.14	108.20
57	BA	1180	U	O4'-C1'-N1	6.18	113.14	108.20
57	BA	1306	C	N1-C2-O2	6.18	122.61	118.90
58	Ba	90	C	N3-C4-N4	-6.18	113.67	118.00
4	AM	106	ARG	NE-CZ-NH1	6.18	123.39	120.30
15	AD	13	ARG	NE-CZ-NH1	6.18	123.39	120.30
57	BA	129	C	O4'-C1'-N1	6.18	113.14	108.20
57	BA	182	A	C4-C5-C6	-6.18	113.91	117.00
9	AR	60	ARG	NE-CZ-NH1	6.18	123.39	120.30
22	AA	1121	U	O4'-C1'-N1	6.18	113.14	108.20
22	AA	1208	C	N1-C2-O2	6.18	122.61	118.90
57	BA	1080	A	O4'-C1'-N9	6.18	113.14	108.20
57	BA	1365	A	C4-C5-C6	-6.18	113.91	117.00
57	BA	1457	U	O4'-C1'-N1	6.18	113.14	108.20
57	BA	1528	A	C4-C5-C6	-6.18	113.91	117.00
57	BA	2055	C	C3'-C2'-C1'	-6.18	96.56	101.50
26	BJ	52	ARG	NE-CZ-NH1	6.17	123.39	120.30
57	BA	512	G	O4'-C1'-N9	6.17	113.14	108.20
57	BA	1006	C	N3-C2-O2	-6.17	117.58	121.90
13	AU	6	ARG	NE-CZ-NH1	6.17	123.39	120.30
22	AA	398	U	C1'-O4'-C4'	-6.17	104.96	109.90
22	AA	880	C	O4'-C1'-N1	6.17	113.14	108.20
22	AA	1140	C	N1-C2-O2	6.17	122.60	118.90
57	BA	310	A	C4-C5-C6	-6.17	113.92	117.00
19	AH	14	ARG	NE-CZ-NH1	6.17	123.39	120.30
57	BA	377	G	N1-C6-O6	-6.17	116.20	119.90
57	BA	2146	C	N1-C2-O2	6.17	122.60	118.90
22	AA	275	G	C5'-C4'-C3'	-6.17	106.13	116.00
22	AA	979	C	O4'-C1'-N1	6.17	113.14	108.20
22	AA	1531	A	C4-C5-C6	-6.17	113.92	117.00
57	BA	368	A	C4-C5-C6	-6.17	113.92	117.00
57	BA	1637	A	C4-C5-C6	-6.17	113.92	117.00
57	BA	239	C	N1-C2-O2	6.17	122.60	118.90
57	BA	693	A	C4-C5-C6	-6.17	113.92	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	867	C	N3-C2-O2	-6.17	117.58	121.90
57	BA	1666	G	N1-C6-O6	-6.17	116.20	119.90
57	BA	1924	C	N1-C2-O2	6.17	122.60	118.90
57	BA	2042	A	C4-C5-C6	-6.17	113.92	117.00
57	BA	2472	G	C4'-C3'-C2'	-6.17	96.43	102.60
57	BA	2657	A	C4-C5-C6	-6.17	113.92	117.00
22	AA	493	A	C3'-C2'-C1'	6.17	106.43	101.50
36	BU	50	ARG	NE-CZ-NH1	6.17	123.38	120.30
57	BA	101	A	C4-C5-C6	-6.16	113.92	117.00
57	BA	944	C	N1-C2-O2	6.16	122.60	118.90
57	BA	1731	G	N3-C4-C5	-6.16	125.52	128.60
22	AA	327	A	C4-C5-C6	-6.16	113.92	117.00
57	BA	181	A	C4-C5-C6	-6.16	113.92	117.00
57	BA	421	C	N1-C2-O2	6.16	122.60	118.90
22	AA	1157	A	C4-C5-C6	-6.16	113.92	117.00
57	BA	1785	A	C4-C5-C6	-6.16	113.92	117.00
57	BA	2723	C	N1-C2-O2	6.16	122.60	118.90
58	Ba	10	G	C5'-C4'-C3'	-6.16	106.14	116.00
11	AB	20	ARG	NE-CZ-NH2	-6.16	117.22	120.30
22	AA	1384	C	N1-C2-O2	6.16	122.59	118.90
57	BA	791	C	N3-C2-O2	-6.16	117.59	121.90
11	AB	138	ARG	NE-CZ-NH1	6.16	123.38	120.30
57	BA	670	A	C4-C5-C6	-6.16	113.92	117.00
57	BA	2800	A	C4-C5-C6	-6.16	113.92	117.00
31	BQ	16	ARG	NE-CZ-NH2	-6.16	117.22	120.30
57	BA	1854	A	C4-C5-C6	-6.16	113.92	117.00
22	AA	388	G	N3-C4-C5	-6.15	125.52	128.60
22	AA	1424	U	O4'-C1'-N1	6.15	113.12	108.20
55	BH	152	ARG	NE-CZ-NH2	6.15	123.38	120.30
57	BA	2190	G	O4'-C1'-N9	6.15	113.12	108.20
57	BA	385	C	N1-C2-O2	6.15	122.59	118.90
57	BA	1126	A	C4-C5-C6	-6.15	113.92	117.00
57	BA	2264	C	N3-C4-N4	-6.15	113.69	118.00
22	AA	878	A	C4-C5-C6	-6.15	113.92	117.00
22	AA	1282	C	N1-C2-O2	6.15	122.59	118.90
24	A3	49	C	N1-C2-O2	6.15	122.59	118.90
57	BA	1350	C	N1-C2-O2	6.15	122.59	118.90
57	BA	1362	C	O4'-C1'-N1	6.15	113.12	108.20
23	A2	45	G	C3'-C2'-C1'	6.15	106.42	101.50
45	BE	179	ARG	NE-CZ-NH1	6.15	123.37	120.30
22	AA	140	U	O4'-C1'-N1	6.15	113.12	108.20
22	AA	429	U	C5-C6-N1	-6.15	119.63	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1141	C	O4'-C1'-N1	6.15	113.12	108.20
22	AA	1191	A	C4-C5-C6	-6.15	113.93	117.00
22	AA	1503	A	C4-C5-C6	-6.15	113.93	117.00
57	BA	20	C	O4'-C1'-N1	6.15	113.12	108.20
57	BA	751	A	C4-C5-C6	-6.15	113.93	117.00
57	BA	2354	C	O4'-C1'-N1	6.15	113.12	108.20
22	AA	280	C	N1-C2-O2	6.14	122.59	118.90
54	BG	79	ARG	NE-CZ-NH2	6.14	123.37	120.30
57	BA	2294	G	O4'-C1'-N9	6.14	113.12	108.20
22	AA	736	C	O4'-C1'-N1	6.14	113.11	108.20
25	BC	9	ARG	NE-CZ-NH1	6.14	123.37	120.30
57	BA	1234	U	O4'-C1'-N1	6.14	113.11	108.20
57	BA	1958	C	N1-C2-O2	6.14	122.58	118.90
22	AA	1205	U	O4'-C1'-N1	6.14	113.11	108.20
22	AA	1499	A	C4-C5-C6	-6.14	113.93	117.00
57	BA	472	A	C4-C5-C6	-6.14	113.93	117.00
57	BA	552	U	O4'-C1'-N1	6.14	113.11	108.20
57	BA	2628	C	N3-C2-O2	-6.14	117.60	121.90
57	BA	1606	C	O4'-C1'-N1	6.14	113.11	108.20
22	AA	330	C	N3-C2-O2	-6.14	117.60	121.90
22	AA	502	A	C4-C5-C6	-6.14	113.93	117.00
57	BA	74	A	C2-N3-C4	6.14	113.67	110.60
57	BA	2740	A	C4-C5-C6	-6.13	113.93	117.00
57	BA	2154	A	C4-C5-C6	-6.13	113.93	117.00
57	BA	2537	U	O4'-C1'-N1	6.13	113.11	108.20
22	AA	18	C	O4'-C1'-N1	6.13	113.11	108.20
22	AA	416	G	N1-C6-O6	-6.13	116.22	119.90
57	BA	2510	C	N1-C2-O2	6.13	122.58	118.90
20	AI	79	ARG	NE-CZ-NH1	6.13	123.36	120.30
22	AA	44	A	C4-C5-C6	-6.13	113.94	117.00
43	B1	71	ARG	NE-CZ-NH1	6.13	123.36	120.30
57	BA	270	A	C4-C5-C6	-6.13	113.94	117.00
57	BA	957	C	N3-C2-O2	-6.13	117.61	121.90
57	BA	1367	A	C4-C5-C6	-6.13	113.94	117.00
57	BA	2071	A	C4-C5-C6	-6.13	113.94	117.00
15	AD	2	ARG	NE-CZ-NH1	6.13	123.36	120.30
57	BA	1499	C	O4'-C1'-N1	6.13	113.10	108.20
22	AA	127	G	O4'-C1'-N9	6.12	113.10	108.20
22	AA	824	G	O4'-C1'-N9	6.12	113.10	108.20
57	BA	659	G	N1-C6-O6	-6.12	116.23	119.90
57	BA	1348	C	N3-C2-O2	-6.12	117.61	121.90
57	BA	1736	U	O4'-C1'-N1	6.12	113.10	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2901	C	O4'-C1'-N1	6.12	113.10	108.20
57	BA	526	A	C4-C5-C6	-6.12	113.94	117.00
22	AA	1535	C	N3-C2-O2	-6.12	117.62	121.90
57	BA	1065	U	N3-C2-O2	-6.12	117.92	122.20
57	BA	2667	C	O4'-C1'-N1	6.12	113.09	108.20
22	AA	1082	A	C4-C5-C6	-6.12	113.94	117.00
57	BA	399	U	O4'-C1'-N1	6.12	113.09	108.20
57	BA	1730	C	N3-C2-O2	-6.12	117.62	121.90
22	AA	328	C	P-O3'-C3'	6.12	127.04	119.70
22	AA	1014	A	C4-C5-C6	-6.12	113.94	117.00
57	BA	968	C	N1-C2-O2	6.12	122.57	118.90
24	A3	52	C	N1-C2-O2	6.11	122.57	118.90
56	BL	50	ARG	NE-CZ-NH1	6.11	123.36	120.30
57	BA	987	C	N1-C2-O2	6.11	122.57	118.90
22	AA	366	A	C4-C5-C6	-6.11	113.94	117.00
22	AA	788	U	O4'-C1'-N1	6.11	113.09	108.20
57	BA	1607	C	N3-C2-O2	-6.11	117.62	121.90
22	AA	1324	A	C4-C5-C6	-6.11	113.94	117.00
57	BA	792	A	C4-C5-C6	-6.11	113.94	117.00
57	BA	954	G	N1-C6-O6	-6.11	116.23	119.90
22	AA	171	A	C4-C5-C6	-6.11	113.95	117.00
22	AA	285	C	O4'-C1'-N1	6.11	113.09	108.20
22	AA	618	C	N3-C2-O2	-6.11	117.62	121.90
22	AA	230	G	N1-C6-O6	-6.11	116.24	119.90
22	AA	860	A	C4-C5-C6	-6.11	113.95	117.00
57	BA	2873	A	C4-C5-C6	-6.11	113.95	117.00
21	A1	627	ARG	NE-CZ-NH1	6.11	123.35	120.30
22	AA	900	A	C4-C5-C6	-6.11	113.95	117.00
45	BE	13	ARG	NE-CZ-NH2	6.11	123.35	120.30
57	BA	229	C	N3-C2-O2	-6.11	117.63	121.90
57	BA	418	C	O4'-C1'-N1	6.11	113.08	108.20
57	BA	1450	G	N1-C6-O6	-6.11	116.24	119.90
22	AA	190	A	C4-C5-C6	-6.10	113.95	117.00
57	BA	195	A	C4-C5-C6	-6.10	113.95	117.00
57	BA	1049	C	N1-C2-O2	6.10	122.56	118.90
1	AJ	62	ARG	NE-CZ-NH1	6.10	123.35	120.30
22	AA	879	C	N1-C2-O2	6.10	122.56	118.90
22	AA	1390	U	O4'-C1'-N1	6.10	113.08	108.20
22	AA	1458	G	O4'-C1'-N9	6.10	113.08	108.20
57	BA	144	A	C4-C5-C6	-6.10	113.95	117.00
57	BA	1929	G	N3-C4-C5	-6.10	125.55	128.60
14	AC	64	ARG	NE-CZ-NH1	6.10	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	614	C	O4'-C1'-N1	6.10	113.08	108.20
38	BW	8	ARG	NE-CZ-NH1	6.10	123.35	120.30
22	AA	631	C	N3-C2-O2	-6.10	117.63	121.90
22	AA	1281	C	N3-C2-O2	-6.10	117.63	121.90
57	BA	435	C	N3-C2-O2	-6.10	117.63	121.90
57	BA	1867	G	O4'-C1'-N9	6.10	113.08	108.20
22	AA	1285	A	C4-C5-C6	-6.10	113.95	117.00
22	AA	1336	C	N3-C2-O2	-6.10	117.63	121.90
57	BA	607	U	O4'-C1'-N1	6.10	113.08	108.20
57	BA	1463	C	O4'-C1'-N1	6.10	113.08	108.20
57	BA	1771	C	N1-C2-O2	6.10	122.56	118.90
57	BA	2060	A	C4-C5-C6	-6.10	113.95	117.00
57	BA	2254	C	N3-C2-O2	-6.10	117.63	121.90
57	BA	2712	C	N3-C2-O2	-6.10	117.63	121.90
57	BA	1871	A	C4-C5-C6	-6.10	113.95	117.00
57	BA	2222	C	O4'-C1'-N1	6.10	113.08	108.20
22	AA	817	C	N3-C2-O2	-6.09	117.63	121.90
57	BA	40	U	O4'-C1'-N1	6.09	113.08	108.20
57	BA	606	U	O4'-C1'-N1	6.09	113.08	108.20
57	BA	983	A	C4-C5-C6	-6.09	113.95	117.00
57	BA	943	A	C4-C5-C6	-6.09	113.95	117.00
57	BA	1542	U	O4'-C1'-N1	6.09	113.07	108.20
57	BA	2313	C	N1-C2-O2	6.09	122.56	118.90
22	AA	308	C	O4'-C1'-N1	6.09	113.07	108.20
57	BA	1722	A	C4-C5-C6	-6.09	113.95	117.00
57	BA	1899	A	C4-C5-C6	-6.09	113.95	117.00
57	BA	2776	A	C4-C5-C6	-6.09	113.95	117.00
22	AA	823	C	N3-C2-O2	-6.09	117.64	121.90
57	BA	1981	A	C4-C5-C6	-6.09	113.96	117.00
57	BA	2660	A	C3'-C2'-C1'	6.09	106.37	101.50
57	BA	2786	U	O4'-C1'-N1	6.09	113.07	108.20
57	BA	2820	A	C4-C5-C6	-6.09	113.96	117.00
57	BA	2117	A	C4-C5-C6	-6.08	113.96	117.00
22	AA	408	A	C4-C5-C6	-6.08	113.96	117.00
22	AA	571	U	O4'-C1'-N1	6.08	113.07	108.20
22	AA	576	C	O4'-C1'-N1	6.08	113.07	108.20
57	BA	332	A	C4-C5-C6	-6.08	113.96	117.00
57	BA	1083	U	C1'-O4'-C4'	-6.08	105.03	109.90
57	BA	1859	U	O4'-C1'-N1	6.08	113.07	108.20
57	BA	2576	G	N3-C4-C5	-6.08	125.56	128.60
50	B7	28	ARG	NE-CZ-NH1	6.08	123.34	120.30
57	BA	318	C	O4'-C1'-N1	6.08	113.06	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	373	U	O4'-C1'-N1	6.08	113.06	108.20
57	BA	394	C	N1-C2-O2	6.08	122.55	118.90
22	AA	425	G	N1-C6-O6	-6.08	116.25	119.90
22	AA	1457	G	O4'-C1'-N9	6.08	113.06	108.20
57	BA	28	A	O4'-C1'-N9	6.08	113.06	108.20
57	BA	2013	A	N1-C6-N6	-6.08	114.95	118.60
57	BA	2015	A	O4'-C1'-N9	6.08	113.06	108.20
22	AA	59	A	C4-C5-C6	-6.08	113.96	117.00
22	AA	471	U	O4'-C1'-N1	6.08	113.06	108.20
22	AA	907	A	C4-C5-C6	-6.08	113.96	117.00
26	BJ	41	ARG	NE-CZ-NH1	6.08	123.34	120.30
57	BA	55	G	N1-C6-O6	-6.08	116.25	119.90
57	BA	2159	G	O4'-C1'-N9	6.08	113.06	108.20
21	A1	336	ARG	NE-CZ-NH1	6.07	123.34	120.30
22	AA	563	A	C4-C5-C6	-6.07	113.96	117.00
22	AA	870	U	O4'-C1'-N1	6.07	113.06	108.20
22	AA	1101	A	C4-C5-C6	-6.07	113.96	117.00
57	BA	156	A	C4-C5-C6	-6.07	113.96	117.00
57	BA	1507	C	N1-C2-O2	6.07	122.55	118.90
57	BA	1603	A	C5-C6-N1	6.07	120.74	117.70
9	AR	69	TYR	CB-CG-CD1	-6.07	117.36	121.00
12	AT	59	ARG	NE-CZ-NH1	6.07	123.33	120.30
22	AA	852	G	N1-C6-O6	-6.07	116.26	119.90
22	AA	955	U	O4'-C1'-N1	6.07	113.06	108.20
22	AA	969	A	C1'-O4'-C4'	-6.07	105.04	109.90
57	BA	130	C	N1-C2-O2	6.07	122.54	118.90
57	BA	2587	A	C4-C5-C6	-6.07	113.97	117.00
22	AA	1521	C	N1-C2-O2	6.07	122.54	118.90
57	BA	621	A	C4-C5-C6	-6.07	113.97	117.00
57	BA	661	A	C4-C5-C6	-6.07	113.97	117.00
57	BA	900	A	C4-C5-C6	-6.07	113.97	117.00
57	BA	998	C	O4'-C1'-N1	6.07	113.06	108.20
57	BA	2281	A	O4'-C1'-N9	6.07	113.06	108.20
22	AA	242	G	N1-C6-O6	-6.07	116.26	119.90
22	AA	1512	U	O4'-C1'-N1	6.07	113.05	108.20
57	BA	461	C	N3-C2-O2	-6.07	117.65	121.90
57	BA	673	C	N3-C2-O2	-6.07	117.65	121.90
57	BA	1083	U	O4'-C1'-N1	6.07	113.05	108.20
57	BA	66	C	N1-C2-O2	6.07	122.54	118.90
57	BA	2392	A	C4-C5-C6	-6.07	113.97	117.00
57	BA	2667	C	N3-C4-C5	6.07	124.33	121.90
57	BA	2189	U	O4'-C1'-N1	6.06	113.05	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	267	C	N1-C2-O2	6.06	122.54	118.90
57	BA	802	A	C4-C5-C6	-6.06	113.97	117.00
22	AA	832	G	N1-C6-O6	-6.06	116.27	119.90
57	BA	942	G	N3-C4-C5	-6.06	125.57	128.60
24	A3	7	G	O4'-C1'-N9	6.06	113.05	108.20
57	BA	1694	C	N3-C2-O2	-6.06	117.66	121.90
57	BA	2676	C	O4'-C1'-N1	6.06	113.05	108.20
22	AA	672	U	O4'-C1'-N1	6.05	113.04	108.20
22	AA	1414	U	O4'-C1'-N1	6.05	113.04	108.20
22	AA	1460	C	O4'-C1'-N1	6.05	113.04	108.20
57	BA	896	A	C4-C5-C6	-6.05	113.97	117.00
57	BA	1625	C	N1-C2-O2	6.05	122.53	118.90
57	BA	288	U	O4'-C1'-N1	6.05	113.04	108.20
18	AG	159	ARG	NE-CZ-NH1	6.05	123.33	120.30
22	AA	595	A	C4-C5-C6	-6.05	113.97	117.00
22	AA	687	A	C4-C5-C6	-6.05	113.97	117.00
22	AA	896	C	O4'-C1'-N1	6.05	113.04	108.20
22	AA	968	A	C4-C5-C6	-6.05	113.97	117.00
35	BD	220	ARG	NH1-CZ-NH2	-6.05	112.74	119.40
36	BU	91	ARG	NE-CZ-NH1	6.05	123.33	120.30
57	BA	664	G	N1-C6-O6	-6.05	116.27	119.90
57	BA	1773	A	C4-C5-C6	-6.05	113.97	117.00
57	BA	2603	G	N1-C6-O6	-6.05	116.27	119.90
58	Ba	109	A	C4-C5-C6	-6.05	113.97	117.00
22	AA	51	A	C1'-O4'-C4'	-6.05	105.06	109.90
22	AA	483	C	N1-C2-O2	6.05	122.53	118.90
33	BS	81	ARG	NE-CZ-NH1	6.05	123.33	120.30
57	BA	1758	U	O4'-C1'-N1	6.05	113.04	108.20
57	BA	2352	A	N1-C6-N6	-6.05	114.97	118.60
22	AA	52	C	N1-C2-O2	6.05	122.53	118.90
57	BA	940	G	N9-C1'-C2'	-6.05	105.35	112.00
22	AA	1195	C	N1-C2-O2	6.05	122.53	118.90
22	AA	1223	C	N3-C4-N4	-6.05	113.77	118.00
22	AA	1251	A	C4-C5-C6	-6.05	113.98	117.00
57	BA	1266	G	O4'-C1'-N9	6.05	113.04	108.20
57	BA	1443	U	O4'-C1'-N1	6.05	113.04	108.20
57	BA	1462	C	N1-C2-O2	6.05	122.53	118.90
57	BA	2882	A	C6-C5-N7	6.05	136.53	132.30
58	Ba	94	A	C4-C5-C6	-6.05	113.98	117.00
57	BA	2253	G	C1'-O4'-C4'	-6.04	105.06	109.90
22	AA	117	G	N1-C6-O6	-6.04	116.27	119.90
23	A2	13	A	C4-C5-C6	-6.04	113.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	218	A	C4-C5-C6	-6.04	113.98	117.00
57	BA	784	G	N3-C4-C5	-6.04	125.58	128.60
57	BA	791	C	N3-C4-C5	6.04	124.32	121.90
57	BA	1089	A	C4-C5-C6	-6.04	113.98	117.00
22	AA	1277	C	O4'-C1'-N1	6.04	113.03	108.20
57	BA	157	C	N1-C2-O2	6.04	122.53	118.90
57	BA	1320	C	N1-C2-O2	6.04	122.53	118.90
57	BA	2164	C	N3-C2-O2	-6.04	117.67	121.90
57	BA	2886	A	C4-C5-C6	-6.04	113.98	117.00
22	AA	482	A	C4-C5-C6	-6.04	113.98	117.00
22	AA	1471	U	O4'-C1'-N1	6.04	113.03	108.20
57	BA	336	C	O4'-C1'-N1	6.04	113.03	108.20
23	A2	24	A	C4-C5-C6	-6.04	113.98	117.00
29	BO	70	ARG	NE-CZ-NH1	6.04	123.32	120.30
22	AA	504	C	N1-C2-O2	6.04	122.52	118.90
22	AA	1478	U	O4'-C1'-N1	6.04	113.03	108.20
22	AA	1529	G	O4'-C1'-N9	6.04	113.03	108.20
57	BA	721	A	C4-C5-C6	-6.04	113.98	117.00
5	AN	62	ARG	NE-CZ-NH2	6.03	123.32	120.30
22	AA	151	A	C6-C5-N7	6.03	136.52	132.30
22	AA	1224	U	O4'-C1'-N1	6.03	113.03	108.20
22	AA	1228	C	N1-C2-O2	6.03	122.52	118.90
57	BA	1575	C	O4'-C1'-N1	6.03	113.03	108.20
57	BA	2368	C	O4'-C1'-N1	6.03	113.03	108.20
57	BA	366	C	O4'-C1'-N1	6.03	113.03	108.20
57	BA	601	C	N1-C2-O2	6.03	122.52	118.90
57	BA	1124	G	N1-C6-O6	-6.03	116.28	119.90
57	BA	1670	C	N3-C2-O2	-6.03	117.68	121.90
23	A2	23	C	N3-C2-O2	-6.03	117.68	121.90
22	AA	993	G	N3-C4-C5	-6.03	125.59	128.60
47	B4	25	ARG	NE-CZ-NH1	6.03	123.31	120.30
57	BA	207	A	C4-C5-C6	-6.03	113.99	117.00
57	BA	286	U	O4'-C1'-N1	6.03	113.02	108.20
57	BA	529	A	C4-C5-C6	-6.03	113.99	117.00
57	BA	789	A	N1-C6-N6	-6.03	114.98	118.60
57	BA	1039	A	C4-C5-C6	-6.03	113.99	117.00
57	BA	1489	C	O4'-C1'-N1	6.03	113.02	108.20
57	BA	1678	A	C4-C5-C6	-6.03	113.99	117.00
57	BA	2427	C	N1-C2-O2	6.03	122.52	118.90
57	BA	2717	C	N1-C2-O2	6.03	122.52	118.90
57	BA	2806	C	N1-C2-O2	6.03	122.52	118.90
57	BA	130	C	O4'-C1'-N1	6.03	113.02	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	865	C	N3-C2-O2	-6.03	117.68	121.90
22	AA	726	C	N1-C2-O2	6.02	122.52	118.90
57	BA	1990	C	O4'-C1'-N1	6.02	113.02	108.20
57	BA	2295	C	O4'-C1'-N1	6.02	113.02	108.20
57	BA	947	A	C4-C5-C6	-6.02	113.99	117.00
57	BA	1150	C	O4'-C1'-N1	6.02	113.02	108.20
57	BA	2868	A	C4-C5-C6	-6.02	113.99	117.00
22	AA	1044	A	C4-C5-C6	-6.02	113.99	117.00
57	BA	901	C	N3-C2-O2	-6.02	117.69	121.90
22	AA	3	A	C4-C5-C6	-6.02	113.99	117.00
22	AA	1389	C	O4'-C1'-N1	6.02	113.02	108.20
57	BA	753	A	C4-C5-C6	-6.02	113.99	117.00
57	BA	2044	C	N1-C2-O2	6.02	122.51	118.90
22	AA	1056	U	O4'-C1'-N1	6.02	113.01	108.20
22	AA	1332	A	N1-C6-N6	-6.02	114.99	118.60
24	A3	57	C	N1-C2-O2	6.02	122.51	118.90
57	BA	1019	U	O4'-C1'-N1	6.02	113.01	108.20
57	BA	1856	U	O4'-C1'-N1	6.02	113.01	108.20
58	Ba	120	U	N3-C2-O2	-6.02	117.99	122.20
57	BA	2469	A	C4-C5-C6	-6.02	113.99	117.00
22	AA	436	C	O4'-C1'-N1	6.01	113.01	108.20
57	BA	1872	A	C4-C5-C6	-6.01	113.99	117.00
57	BA	1892	C	O4'-C1'-N1	6.01	113.01	108.20
57	BA	2811	G	O4'-C1'-N9	6.01	113.01	108.20
22	AA	895	G	N1-C6-O6	-6.01	116.29	119.90
22	AA	1477	U	O4'-C1'-N1	6.01	113.01	108.20
57	BA	392	U	O4'-C1'-N1	6.01	113.01	108.20
57	BA	1573	G	O4'-C1'-N9	6.01	113.01	108.20
57	BA	1789	A	C4-C5-C6	-6.01	113.99	117.00
57	BA	253	C	N1-C2-O2	6.01	122.51	118.90
57	BA	1481	U	O4'-C1'-N1	6.01	113.01	108.20
57	BA	2841	C	N1-C2-O2	6.01	122.51	118.90
10	AS	77	ARG	NH1-CZ-NH2	-6.01	112.79	119.40
57	BA	2611	C	N1-C2-O2	6.01	122.50	118.90
57	BA	1595	C	N1-C2-O2	6.01	122.50	118.90
57	BA	1642	G	O4'-C1'-N9	6.01	113.00	108.20
57	BA	1904	G	O4'-C1'-N9	6.01	113.01	108.20
57	BA	2661	G	N1-C6-O6	-6.01	116.30	119.90
57	BA	2793	C	O4'-C1'-N1	6.01	113.00	108.20
58	Ba	71	C	O4'-C1'-N1	6.01	113.00	108.20
22	AA	521	G	N1-C6-O6	-6.00	116.30	119.90
22	AA	1427	C	N1-C2-O2	6.00	122.50	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2196	C	N3-C4-N4	-6.00	113.80	118.00
22	AA	205	A	C4-C5-C6	-6.00	114.00	117.00
24	A3	66	C	N1-C2-O2	6.00	122.50	118.90
57	BA	443	A	C4-C5-C6	-6.00	114.00	117.00
57	BA	730	A	C4-C5-C6	-6.00	114.00	117.00
57	BA	962	G	C5'-C4'-O4'	6.00	116.31	109.10
57	BA	1254	A	C4-C5-C6	-6.00	114.00	117.00
17	AF	38	ARG	NE-CZ-NH2	-6.00	117.30	120.30
22	AA	350	G	N1-C6-O6	-6.00	116.30	119.90
22	AA	948	C	N1-C2-O2	6.00	122.50	118.90
22	AA	1104	G	N1-C6-O6	-6.00	116.30	119.90
22	AA	1319	A	N1-C6-N6	-6.00	115.00	118.60
22	AA	130	A	O4'-C1'-N9	6.00	113.00	108.20
22	AA	1383	C	O4'-C1'-N1	6.00	113.00	108.20
22	AA	1462	C	O4'-C1'-N1	6.00	113.00	108.20
35	BD	47	ARG	NE-CZ-NH1	6.00	123.30	120.30
57	BA	1416	G	O4'-C1'-N9	6.00	113.00	108.20
57	BA	2258	C	N1-C2-O2	6.00	122.50	118.90
57	BA	2356	U	O4'-C1'-N1	6.00	113.00	108.20
57	BA	2662	A	C4-C5-C6	-6.00	114.00	117.00
22	AA	1400	C	N3-C2-O2	-6.00	117.70	121.90
57	BA	2001	C	N1-C2-O2	6.00	122.50	118.90
22	AA	528	C	O4'-C1'-N1	6.00	113.00	108.20
22	AA	1281	C	N3-C4-C5	6.00	124.30	121.90
57	BA	2282	G	N1-C6-O6	-6.00	116.30	119.90
57	BA	1179	G	N1-C6-O6	-6.00	116.30	119.90
34	BT	100	ARG	NE-CZ-NH2	5.99	123.30	120.30
57	BA	4	U	O4'-C1'-N1	5.99	113.00	108.20
57	BA	440	C	O4'-C1'-N1	5.99	113.00	108.20
22	AA	611	C	N3-C2-O2	-5.99	117.70	121.90
22	AA	765	G	C1'-O4'-C4'	-5.99	105.11	109.90
57	BA	1245	G	N1-C6-O6	-5.99	116.31	119.90
22	AA	578	C	O4'-C1'-N1	5.99	112.99	108.20
22	AA	638	U	O4'-C1'-N1	5.99	112.99	108.20
22	AA	983	A	C6-C5-N7	5.99	136.49	132.30
22	AA	1484	C	N1-C2-O2	5.99	122.50	118.90
57	BA	301	G	N3-C4-C5	-5.99	125.61	128.60
22	AA	520	A	C4-C5-C6	-5.99	114.01	117.00
57	BA	1164	C	O4'-C1'-N1	5.99	112.99	108.20
22	AA	578	C	N1-C2-O2	5.99	122.49	118.90
22	AA	777	A	C4-C5-C6	-5.99	114.01	117.00
22	AA	475	C	N1-C2-O2	5.99	122.49	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1103	C	N1-C2-O2	5.99	122.49	118.90
22	AA	1524	C	N3-C4-C5	5.99	124.30	121.90
57	BA	171	U	O4'-C1'-N1	5.99	112.99	108.20
57	BA	712	G	O4'-C1'-N9	5.99	112.99	108.20
57	BA	1262	A	C4-C5-C6	-5.99	114.01	117.00
57	BA	2191	A	C4-C5-C6	-5.99	114.01	117.00
58	Ba	29	A	C4-C5-C6	-5.99	114.01	117.00
57	BA	1370	C	N1-C2-O2	5.98	122.49	118.90
57	BA	1670	C	O4'-C1'-N1	5.98	112.99	108.20
20	AI	48	ARG	NE-CZ-NH1	5.98	123.29	120.30
22	AA	72	A	C4-C5-C6	-5.98	114.01	117.00
57	BA	140	C	N3-C2-O2	-5.98	117.71	121.90
57	BA	1927	A	C4-C5-C6	-5.98	114.01	117.00
4	AM	97	ARG	NE-CZ-NH2	-5.98	117.31	120.30
18	AG	2	ARG	NH1-CZ-NH2	-5.98	112.82	119.40
22	AA	1275	A	C4-C5-C6	-5.98	114.01	117.00
22	AA	1344	C	O4'-C1'-N1	5.98	112.98	108.20
57	BA	173	A	C4-C5-C6	-5.98	114.01	117.00
57	BA	1072	C	N1-C2-O2	5.98	122.49	118.90
57	BA	1166	G	O4'-C1'-N9	5.98	112.98	108.20
57	BA	1966	A	C4-C5-C6	-5.98	114.01	117.00
22	AA	45	G	O4'-C1'-N9	5.98	112.98	108.20
22	AA	753	A	C4-C5-C6	-5.98	114.01	117.00
57	BA	402	A	N1-C6-N6	-5.98	115.01	118.60
57	BA	2551	C	N1-C2-O2	5.98	122.49	118.90
58	Ba	120	U	O4'-C1'-N1	5.98	112.98	108.20
24	A3	42	C	N1-C2-O2	5.98	122.49	118.90
57	BA	618	G	N1-C6-O6	-5.98	116.31	119.90
22	AA	17	U	O4'-C1'-N1	5.98	112.98	108.20
22	AA	556	C	N1-C2-O2	5.98	122.48	118.90
22	AA	60	A	C4-C5-C6	-5.97	114.01	117.00
22	AA	348	G	O4'-C1'-N9	5.97	112.98	108.20
22	AA	403	C	O4'-C1'-N1	5.97	112.98	108.20
22	AA	797	C	O4'-C1'-N1	5.97	112.98	108.20
22	AA	824	G	N1-C6-O6	-5.97	116.31	119.90
57	BA	160	A	C4-C5-C6	-5.97	114.01	117.00
57	BA	935	C	O4'-C1'-N1	5.97	112.98	108.20
57	BA	1626	A	C4-C5-C6	-5.97	114.01	117.00
57	BA	1737	G	N3-C2-N2	-5.97	115.72	119.90
57	BA	1912	A	C4-C5-C6	-5.97	114.01	117.00
24	A3	51	U	O4'-C1'-N1	5.97	112.98	108.20
57	BA	507	A	C4-C5-C6	-5.97	114.01	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1920	C	N1-C2-O2	5.97	122.48	118.90
57	BA	2214	C	N1-C2-O2	5.97	122.48	118.90
57	BA	2575	C	N3-C4-C5	-5.97	119.51	121.90
57	BA	2380	C	N1-C2-O2	5.97	122.48	118.90
8	AQ	5	ARG	NE-CZ-NH1	5.97	123.28	120.30
22	AA	612	C	N1-C2-O2	5.97	122.48	118.90
22	AA	1328	C	N1-C2-O2	5.97	122.48	118.90
57	BA	265	A	C4-C5-C6	-5.97	114.02	117.00
57	BA	2635	A	O4'-C1'-N9	5.97	112.98	108.20
22	AA	1235	U	O4'-C1'-N1	5.97	112.97	108.20
57	BA	1686	C	O4'-C1'-N1	5.97	112.97	108.20
57	BA	2083	G	N1-C6-O6	-5.97	116.32	119.90
22	AA	196	A	C4-C5-C6	-5.97	114.02	117.00
22	AA	706	A	C4-C5-C6	-5.97	114.02	117.00
22	AA	1443	C	O4'-C1'-N1	5.97	112.97	108.20
57	BA	873	C	N1-C2-O2	5.97	122.48	118.90
57	BA	1847	A	C4-C5-C6	-5.97	114.02	117.00
57	BA	2283	C	N1-C2-O2	5.97	122.48	118.90
22	AA	1510	C	N1-C2-O2	5.96	122.48	118.90
57	BA	272	A	C4-C5-C6	-5.96	114.02	117.00
57	BA	1086	A	C4-C5-C6	-5.96	114.02	117.00
57	BA	28	A	C4-C5-C6	-5.96	114.02	117.00
58	Ba	15	A	C4-C5-C6	-5.96	114.02	117.00
22	AA	1226	C	N1-C2-O2	5.96	122.48	118.90
57	BA	221	A	C4-C5-C6	-5.96	114.02	117.00
57	BA	705	A	C4-C5-C6	-5.96	114.02	117.00
57	BA	728	G	O4'-C1'-N9	5.96	112.97	108.20
57	BA	1313	U	C3'-C2'-C1'	5.96	106.27	101.50
57	BA	1404	C	N1-C2-O2	5.96	122.48	118.90
57	BA	2169	A	O4'-C1'-N9	5.96	112.97	108.20
57	BA	2177	C	N1-C2-O2	5.96	122.48	118.90
22	AA	246	A	C4-C5-C6	-5.96	114.02	117.00
22	AA	810	C	N1-C2-O2	5.96	122.48	118.90
22	AA	507	C	O4'-C1'-N1	5.96	112.97	108.20
22	AA	839	C	N1-C2-O2	5.96	122.47	118.90
57	BA	652	U	O4'-C1'-N1	5.96	112.97	108.20
57	BA	1070	A	C4-C5-C6	-5.96	114.02	117.00
57	BA	1651	G	N1-C6-O6	-5.96	116.33	119.90
22	AA	387	U	O4'-C1'-N1	5.96	112.97	108.20
57	BA	1552	A	N1-C6-N6	-5.96	115.03	118.60
16	AE	19	ARG	NE-CZ-NH1	5.96	123.28	120.30
22	AA	217	C	N1-C2-O2	5.96	122.47	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1643	G	O4'-C1'-N9	5.96	112.96	108.20
32	BR	8	ARG	NE-CZ-NH1	5.95	123.28	120.30
57	BA	2832	U	O4'-C1'-N1	5.95	112.96	108.20
57	BA	1617	C	N3-C2-O2	-5.95	117.73	121.90
22	AA	163	C	N1-C2-O2	5.95	122.47	118.90
22	AA	433	G	N1-C6-O6	-5.95	116.33	119.90
22	AA	1137	C	N3-C2-O2	-5.95	117.73	121.90
28	BN	69	ARG	NE-CZ-NH1	5.95	123.28	120.30
57	BA	1200	C	O4'-C1'-N1	5.95	112.96	108.20
57	BA	1862	G	N1-C6-O6	-5.95	116.33	119.90
57	BA	1934	C	N1-C2-O2	5.95	122.47	118.90
57	BA	2066	C	N1-C2-O2	5.95	122.47	118.90
57	BA	2727	A	C4-C5-C6	-5.95	114.02	117.00
24	A3	28	U	O4'-C1'-N1	5.95	112.96	108.20
57	BA	2547	A	C4-C5-C6	-5.95	114.03	117.00
22	AA	1444	U	O4'-C1'-N1	5.95	112.96	108.20
22	AA	397	A	C4-C5-C6	-5.95	114.03	117.00
22	AA	759	A	C4-C5-C6	-5.95	114.03	117.00
23	A2	45	G	N3-C4-C5	-5.95	125.63	128.60
57	BA	1293	C	N3-C2-O2	-5.95	117.74	121.90
57	BA	2505	G	O4'-C1'-N9	5.95	112.96	108.20
22	AA	111	G	N3-C2-N2	-5.94	115.74	119.90
44	B2	23	ARG	NE-CZ-NH1	5.94	123.27	120.30
57	BA	1007	C	N1-C2-O2	5.94	122.47	118.90
22	AA	695	A	C4-C5-C6	-5.94	114.03	117.00
22	AA	1508	A	C4-C5-C6	-5.94	114.03	117.00
57	BA	349	U	O4'-C1'-N1	5.94	112.95	108.20
18	AG	9	ARG	NE-CZ-NH1	5.94	123.27	120.30
22	AA	603	U	O4'-C1'-N1	5.94	112.95	108.20
22	AA	1255	G	N1-C6-O6	-5.94	116.33	119.90
22	AA	1458	G	N1-C6-O6	-5.94	116.34	119.90
57	BA	723	C	N1-C2-O2	5.94	122.47	118.90
57	BA	985	C	N1-C2-O2	5.94	122.46	118.90
57	BA	1879	C	N1-C2-O2	5.94	122.46	118.90
57	BA	1986	C	N1-C2-O2	5.94	122.46	118.90
22	AA	1334	G	N1-C6-O6	-5.94	116.34	119.90
57	BA	886	A	C4-C5-C6	-5.94	114.03	117.00
22	AA	69	G	N1-C6-O6	-5.94	116.34	119.90
22	AA	1259	C	N1-C2-O2	5.94	122.46	118.90
22	AA	1502	A	C4-C5-C6	-5.94	114.03	117.00
57	BA	345	A	C4-C5-C6	-5.94	114.03	117.00
57	BA	836	G	N1-C6-O6	-5.94	116.34	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2530	A	C4-C5-C6	-5.94	114.03	117.00
4	AM	92	ARG	NE-CZ-NH1	5.94	123.27	120.30
22	AA	489	C	O4'-C1'-N1	5.94	112.95	108.20
57	BA	1490	A	O4'-C1'-N9	5.94	112.95	108.20
57	BA	1747	U	O4'-C1'-N1	5.94	112.95	108.20
10	AS	2	ARG	NH1-CZ-NH2	-5.93	112.87	119.40
22	AA	35	G	N1-C6-O6	-5.93	116.34	119.90
22	AA	309	A	O4'-C1'-N9	5.93	112.95	108.20
22	AA	840	C	N1-C2-O2	5.93	122.46	118.90
22	AA	1204	A	C6-C5-N7	5.93	136.45	132.30
22	AA	1208	C	O4'-C1'-N1	5.93	112.95	108.20
22	AA	1230	C	O4'-C1'-N1	5.93	112.94	108.20
22	AA	1234	C	O4'-C1'-N1	5.93	112.95	108.20
22	AA	1256	A	C1'-O4'-C4'	-5.93	105.15	109.90
57	BA	474	G	N1-C6-O6	-5.93	116.34	119.90
57	BA	2401	U	O4'-C1'-N1	5.93	112.95	108.20
57	BA	2687	U	O4'-C1'-N1	5.93	112.95	108.20
57	BA	1121	C	N1-C2-O2	5.93	122.46	118.90
57	BA	2714	G	N3-C4-C5	-5.93	125.64	128.60
22	AA	194	C	N3-C2-O2	-5.93	117.75	121.90
57	BA	1033	U	N3-C2-O2	-5.93	118.05	122.20
57	BA	1201	U	O4'-C1'-N1	5.93	112.94	108.20
57	BA	2104	C	O4'-C1'-N1	5.93	112.94	108.20
57	BA	2301	C	O4'-C1'-N1	5.93	112.94	108.20
57	BA	2864	G	N1-C6-O6	-5.93	116.34	119.90
22	AA	856	C	O4'-C1'-N1	5.93	112.94	108.20
22	AA	1382	C	N3-C2-O2	-5.93	117.75	121.90
23	A2	27	A	C4-C5-C6	-5.93	114.04	117.00
57	BA	2397	G	N1-C6-O6	-5.93	116.34	119.90
13	AU	1	PRO	CA-N-CD	-5.93	103.20	111.50
42	B0	19	ARG	NE-CZ-NH1	5.93	123.26	120.30
57	BA	739	A	O4'-C1'-N9	5.93	112.94	108.20
57	BA	1214	A	C4-C5-C6	-5.93	114.04	117.00
22	AA	751	U	O4'-C1'-N1	5.92	112.94	108.20
57	BA	104	A	O4'-C1'-N9	5.92	112.94	108.20
57	BA	1387	A	C4-C5-C6	-5.92	114.04	117.00
57	BA	1832	C	O4'-C1'-N1	5.92	112.94	108.20
57	BA	2052	A	C4-C5-C6	-5.92	114.04	117.00
57	BA	2065	C	O4'-C1'-N1	5.92	112.94	108.20
22	AA	466	A	C4-C5-C6	-5.92	114.04	117.00
22	AA	866	C	O4'-C1'-N1	5.92	112.94	108.20
22	AA	892	A	C4-C5-C6	-5.92	114.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1008	U	O4'-C1'-N1	5.92	112.94	108.20
22	AA	1330	U	O4'-C1'-N1	5.92	112.94	108.20
33	BS	102	ARG	NE-CZ-NH2	-5.92	117.34	120.30
57	BA	595	C	N1-C2-O2	5.92	122.45	118.90
57	BA	387	U	O4'-C1'-N1	5.92	112.94	108.20
57	BA	1833	C	N1-C2-O2	5.92	122.45	118.90
57	BA	2715	C	N1-C2-O2	5.92	122.45	118.90
57	BA	2818	U	O4'-C1'-N1	5.92	112.94	108.20
58	Ba	108	A	C4-C5-C6	-5.92	114.04	117.00
22	AA	251	G	N3-C4-C5	-5.92	125.64	128.60
57	BA	2089	C	N1-C2-O2	5.92	122.45	118.90
57	BA	2765	A	C4-C5-C6	-5.92	114.04	117.00
22	AA	169	C	N3-C2-O2	-5.92	117.76	121.90
22	AA	811	C	N3-C2-O2	-5.92	117.76	121.90
22	AA	901	A	C4-C5-C6	-5.92	114.04	117.00
57	BA	610	C	O4'-C1'-N1	5.92	112.93	108.20
57	BA	2359	C	O4'-C1'-N1	5.92	112.93	108.20
57	BA	2402	U	O4'-C1'-N1	5.92	112.93	108.20
57	BA	304	U	O4'-C1'-N1	5.92	112.93	108.20
57	BA	876	C	N3-C2-O2	-5.92	117.76	121.90
22	AA	485	U	O4'-C1'-N1	5.91	112.93	108.20
22	AA	843	U	N3-C2-O2	-5.91	118.06	122.20
57	BA	506	G	N1-C6-O6	-5.91	116.35	119.90
57	BA	1227	G	O4'-C1'-N9	5.91	112.93	108.20
57	BA	1242	U	O4'-C1'-N1	5.91	112.93	108.20
57	BA	1451	C	N3-C4-C5	5.91	124.27	121.90
22	AA	1037	C	O4'-C1'-N1	5.91	112.93	108.20
57	BA	196	A	O4'-C1'-N9	5.91	112.93	108.20
57	BA	211	C	O4'-C1'-N1	5.91	112.93	108.20
57	BA	1386	C	N1-C2-O2	5.91	122.45	118.90
22	AA	826	C	N1-C2-O2	5.91	122.45	118.90
22	AA	1396	A	O4'-C1'-N9	5.91	112.93	108.20
23	A2	17	U	N3-C2-O2	-5.91	118.06	122.20
57	BA	359	G	N1-C6-O6	-5.91	116.35	119.90
57	BA	1908	C	N1-C2-O2	5.91	122.45	118.90
57	BA	2403	C	O4'-C1'-N1	5.91	112.93	108.20
22	AA	137	U	O4'-C1'-N1	5.91	112.93	108.20
22	AA	857	C	O4'-C1'-N1	5.91	112.93	108.20
57	BA	96	C	N1-C2-O2	5.91	122.44	118.90
57	BA	699	A	C4-C5-C6	-5.91	114.05	117.00
57	BA	718	A	C4-C5-C6	-5.91	114.05	117.00
57	BA	854	C	N1-C2-O2	5.91	122.44	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1382	G	N3-C4-C5	-5.91	125.65	128.60
57	BA	2705	A	C4-C5-C6	-5.91	114.05	117.00
57	BA	2741	A	C4-C5-C6	-5.91	114.05	117.00
58	Ba	106	G	N1-C6-O6	-5.91	116.36	119.90
34	BT	92	ARG	NE-CZ-NH1	5.91	123.25	120.30
22	AA	210	C	N3-C2-O2	-5.91	117.77	121.90
22	AA	746	A	C4-C5-C6	-5.91	114.05	117.00
57	BA	2606	C	N1-C2-O2	5.91	122.44	118.90
57	BA	1068	G	O4'-C1'-N9	5.90	112.92	108.20
57	BA	1451	C	N3-C2-O2	-5.90	117.77	121.90
57	BA	1550	C	N1-C2-O2	5.90	122.44	118.90
22	AA	1232	U	O4'-C1'-N1	5.90	112.92	108.20
57	BA	2621	G	N1-C6-O6	-5.90	116.36	119.90
22	AA	596	A	C4-C5-C6	-5.90	114.05	117.00
22	AA	1485	U	O4'-C1'-N1	5.90	112.92	108.20
57	BA	2801	G	O4'-C1'-N9	5.90	112.92	108.20
22	AA	615	G	N1-C6-O6	-5.90	116.36	119.90
57	BA	1258	U	O4'-C1'-N1	5.90	112.92	108.20
57	BA	2364	C	N1-C2-O2	5.90	122.44	118.90
11	AB	221	ARG	NE-CZ-NH1	5.90	123.25	120.30
24	A3	60	A	C4-C5-C6	-5.90	114.05	117.00
57	BA	933	A	C4-C5-C6	-5.90	114.05	117.00
57	BA	2144	G	O4'-C1'-N9	5.90	112.92	108.20
57	BA	2791	G	O4'-C1'-N9	5.90	112.92	108.20
57	BA	2335	A	C4-C5-C6	-5.90	114.05	117.00
57	BA	2789	C	N3-C2-O2	-5.90	117.77	121.90
22	AA	36	C	N1-C2-O2	5.89	122.44	118.90
22	AA	95	C	N1-C2-O2	5.89	122.44	118.90
22	AA	629	A	C4-C5-C6	-5.89	114.05	117.00
22	AA	909	A	C4-C5-C6	-5.89	114.05	117.00
57	BA	457	A	O4'-C1'-N9	5.89	112.92	108.20
57	BA	1050	A	C4-C5-C6	-5.89	114.05	117.00
57	BA	1170	C	N1-C2-O2	5.89	122.44	118.90
57	BA	2608	G	O4'-C1'-N9	5.89	112.92	108.20
22	AA	477	C	N1-C2-O2	5.89	122.44	118.90
22	AA	1481	U	O4'-C1'-N1	5.89	112.91	108.20
57	BA	643	A	C4-C5-C6	-5.89	114.05	117.00
57	BA	1397	U	O4'-C1'-N1	5.89	112.91	108.20
57	BA	1434	A	C4-C5-C6	-5.89	114.05	117.00
22	AA	149	A	C4-C5-C6	-5.89	114.06	117.00
22	AA	272	C	N1-C2-O2	5.89	122.43	118.90
22	AA	795	C	N3-C2-O2	-5.89	117.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1032	G	N3-C4-C5	-5.89	125.66	128.60
23	A2	33	A	C4-C5-C6	-5.89	114.06	117.00
57	BA	869	G	N1-C6-O6	-5.89	116.37	119.90
57	BA	2626	C	O4'-C1'-N1	5.89	112.91	108.20
58	Ba	36	C	N3-C2-O2	-5.89	117.78	121.90
23	A2	16	A	C4-C5-C6	-5.89	114.06	117.00
57	BA	2572	A	O4'-C1'-N9	5.89	112.91	108.20
22	AA	180	U	O4'-C1'-N1	5.88	112.91	108.20
57	BA	2013	A	C4-C5-C6	-5.88	114.06	117.00
57	BA	2682	A	C4-C5-C6	-5.88	114.06	117.00
57	BA	2826	A	C4-C5-C6	-5.88	114.06	117.00
22	AA	1186	G	N1-C6-O6	-5.88	116.37	119.90
57	BA	2197	U	O4'-C1'-N1	5.88	112.91	108.20
22	AA	114	U	O4'-C1'-N1	5.88	112.91	108.20
22	AA	865	A	O4'-C1'-N9	5.88	112.91	108.20
57	BA	687	C	N3-C2-O2	-5.88	117.78	121.90
57	BA	706	A	O4'-C1'-N9	5.88	112.91	108.20
57	BA	1508	A	C4-C5-C6	-5.88	114.06	117.00
57	BA	2570	G	N1-C6-O6	-5.88	116.37	119.90
22	AA	436	C	N1-C2-O2	5.88	122.43	118.90
57	BA	1018	U	O4'-C1'-N1	5.88	112.90	108.20
30	BP	2	ARG	NH1-CZ-NH2	-5.88	112.93	119.40
57	BA	1752	C	N1-C2-O2	5.88	122.43	118.90
57	BA	2151	U	O4'-C1'-N1	5.88	112.90	108.20
57	BA	2805	C	N1-C2-O2	5.88	122.43	118.90
57	BA	471	A	N1-C6-N6	-5.88	115.07	118.60
57	BA	1305	C	N3-C4-N4	-5.88	113.89	118.00
22	AA	1223	C	N3-C4-C5	5.88	124.25	121.90
57	BA	653	U	P-O3'-C3'	5.88	126.75	119.70
57	BA	1842	G	N1-C6-O6	-5.88	116.38	119.90
57	BA	2496	C	N1-C2-O2	5.88	122.42	118.90
57	BA	2556	C	N3-C2-O2	-5.88	117.79	121.90
22	AA	1045	C	N1-C2-O2	5.87	122.42	118.90
22	AA	1398	A	C4-C5-C6	-5.87	114.06	117.00
57	BA	241	A	C4-C5-C6	-5.87	114.06	117.00
57	BA	679	C	N1-C2-O2	5.87	122.42	118.90
57	BA	2518	A	C4-C5-C6	-5.87	114.06	117.00
22	AA	519	C	N3-C2-O2	-5.87	117.79	121.90
57	BA	915	C	N1-C2-O2	5.87	122.42	118.90
22	AA	341	C	N1-C2-O2	5.87	122.42	118.90
36	BU	12	ARG	NE-CZ-NH2	5.87	123.23	120.30
57	BA	331	C	O4'-C1'-N1	5.87	112.90	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AF	2	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
22	AA	930	C	O4'-C1'-N1	5.87	112.89	108.20
57	BA	1788	C	N1-C2-O2	5.87	122.42	118.90
57	BA	1809	A	C4-C5-C6	-5.87	114.07	117.00
57	BA	281	C	O4'-C1'-N1	5.87	112.89	108.20
57	BA	1166	G	N3-C2-N2	-5.87	115.79	119.90
22	AA	88	U	O4'-C1'-N1	5.87	112.89	108.20
57	BA	190	A	C4-C5-C6	-5.87	114.07	117.00
57	BA	609	A	C4-C5-C6	-5.87	114.07	117.00
58	Ba	44	G	N1-C6-O6	-5.87	116.38	119.90
58	Ba	113	C	N1-C2-O2	5.87	122.42	118.90
22	AA	446	G	O4'-C1'-N9	5.86	112.89	108.20
22	AA	646	G	N1-C6-O6	-5.86	116.38	119.90
57	BA	764	A	C4-C5-C6	-5.86	114.07	117.00
57	BA	1153	C	N1-C2-O2	5.86	122.42	118.90
57	BA	1666	G	O4'-C1'-N9	5.86	112.89	108.20
57	BA	1874	C	O4'-C1'-N1	5.86	112.89	108.20
57	BA	2051	A	C4-C5-C6	-5.86	114.07	117.00
57	BA	2153	C	N1-C2-O2	5.86	122.42	118.90
57	BA	2221	G	N1-C6-O6	-5.86	116.38	119.90
22	AA	705	G	N3-C2-N2	-5.86	115.80	119.90
57	BA	616	A	N1-C6-N6	-5.86	115.08	118.60
57	BA	2715	C	O4'-C1'-N1	5.86	112.89	108.20
22	AA	593	U	O4'-C1'-N1	5.86	112.89	108.20
22	AA	995	C	N3-C2-O2	-5.86	117.80	121.90
22	AA	1350	A	C4-C5-C6	-5.86	114.07	117.00
57	BA	322	A	C4-C5-C6	-5.86	114.07	117.00
57	BA	811	U	O4'-C1'-N1	5.86	112.89	108.20
57	BA	1488	C	O4'-C1'-N1	5.86	112.89	108.20
57	BA	1691	C	O4'-C1'-N1	5.86	112.89	108.20
57	BA	2377	A	C4-C5-C6	-5.86	114.07	117.00
22	AA	897	C	N1-C2-O2	5.86	122.42	118.90
57	BA	2768	U	O4'-C1'-N1	5.86	112.89	108.20
57	BA	2771	C	N1-C2-O2	5.86	122.42	118.90
22	AA	1257	A	C4-C5-C6	-5.86	114.07	117.00
22	AA	1372	U	O4'-C1'-N1	5.86	112.89	108.20
57	BA	934	U	O4'-C1'-N1	5.86	112.89	108.20
57	BA	957	C	N3-C4-C5	5.86	124.24	121.90
57	BA	1415	U	O4'-C1'-N1	5.86	112.89	108.20
57	BA	1442	U	O4'-C1'-N1	5.86	112.89	108.20
57	BA	1986	C	O4'-C1'-N1	5.86	112.89	108.20
24	A3	26	C	N1-C2-O2	5.86	122.41	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1278	C	N1-C2-O2	5.86	122.41	118.90
57	BA	1408	G	N1-C6-O6	-5.86	116.39	119.90
57	BA	1470	A	N1-C6-N6	-5.86	115.09	118.60
57	BA	2170	A	C3'-C2'-C1'	5.86	106.19	101.50
58	Ba	4	C	N1-C2-O2	5.86	122.41	118.90
57	BA	170	U	O4'-C1'-N1	5.85	112.88	108.20
22	AA	356	A	C4'-C3'-C2'	-5.85	96.75	102.60
22	AA	696	A	C4-C5-C6	-5.85	114.07	117.00
22	AA	960	U	N3-C2-O2	-5.85	118.10	122.20
57	BA	1536	C	N3-C2-O2	-5.85	117.80	121.90
57	BA	1961	C	N1-C2-O2	5.85	122.41	118.90
57	BA	1383	A	O4'-C1'-N9	5.85	112.88	108.20
57	BA	1572	A	C4-C5-C6	-5.85	114.08	117.00
57	BA	2549	G	N1-C6-O6	-5.85	116.39	119.90
22	AA	357	G	N1-C6-O6	-5.85	116.39	119.90
22	AA	1303	C	N1-C2-O2	5.85	122.41	118.90
57	BA	331	C	N1-C2-O2	5.85	122.41	118.90
57	BA	1662	U	O4'-C1'-N1	5.85	112.88	108.20
57	BA	540	C	N1-C2-O2	5.85	122.41	118.90
14	AC	171	ARG	NE-CZ-NH2	-5.85	117.38	120.30
57	BA	2748	A	C4-C5-C6	-5.85	114.08	117.00
22	AA	1197	A	C4-C5-C6	-5.84	114.08	117.00
57	BA	251	A	C4-C5-C6	-5.84	114.08	117.00
57	BA	2221	G	O4'-C1'-N9	5.84	112.88	108.20
57	BA	2893	A	C4-C5-C6	-5.84	114.08	117.00
22	AA	388	G	O4'-C1'-N9	5.84	112.87	108.20
22	AA	5	U	N3-C2-O2	-5.84	118.11	122.20
22	AA	492	C	N1-C2-O2	5.84	122.41	118.90
22	AA	742	G	N1-C6-O6	-5.84	116.39	119.90
22	AA	1250	A	C4-C5-C6	-5.84	114.08	117.00
57	BA	771	G	C5'-C4'-C3'	-5.84	106.65	116.00
57	BA	2147	A	C4-C5-C6	-5.84	114.08	117.00
6	AO	57	ARG	NE-CZ-NH1	5.84	123.22	120.30
22	AA	116	A	C4-C5-C6	-5.84	114.08	117.00
57	BA	1965	C	N3-C2-O2	-5.84	117.81	121.90
57	BA	2852	G	N1-C6-O6	-5.84	116.40	119.90
57	BA	97	C	O4'-C1'-N1	5.84	112.87	108.20
57	BA	112	U	O4'-C1'-N1	5.84	112.87	108.20
57	BA	1331	G	C5'-C4'-O4'	5.84	116.11	109.10
57	BA	1819	A	C4-C5-C6	-5.84	114.08	117.00
22	AA	770	C	O4'-C1'-N1	5.84	112.87	108.20
22	AA	968	A	O4'-C1'-N9	5.84	112.87	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1147	C	N3-C2-O2	-5.84	117.81	121.90
57	BA	53	A	O4'-C1'-N9	5.84	112.87	108.20
57	BA	1193	G	N1-C6-O6	-5.84	116.40	119.90
57	BA	2066	C	O4'-C1'-N1	5.84	112.87	108.20
57	BA	2453	A	C4-C5-C6	-5.84	114.08	117.00
57	BA	2806	C	O4'-C1'-N1	5.84	112.87	108.20
22	AA	963	G	N1-C6-O6	-5.83	116.40	119.90
57	BA	1813	G	O4'-C1'-N9	5.83	112.87	108.20
22	AA	1438	G	N1-C6-O6	-5.83	116.40	119.90
57	BA	587	C	N3-C2-O2	-5.83	117.82	121.90
57	BA	835	C	N1-C2-O2	5.83	122.40	118.90
57	BA	1526	C	N1-C2-O2	5.83	122.40	118.90
57	BA	1999	C	N1-C2-O2	5.83	122.40	118.90
57	BA	2320	U	O4'-C1'-N1	5.83	112.87	108.20
58	Ba	26	C	C5'-C4'-C3'	-5.83	106.67	116.00
57	BA	1134	A	O4'-C1'-N9	5.83	112.86	108.20
57	BA	1634	A	C4-C5-C6	-5.83	114.08	117.00
57	BA	1880	U	O4'-C1'-N1	5.83	112.86	108.20
57	BA	863	A	N1-C6-N6	-5.83	115.10	118.60
22	AA	286	C	N1-C2-O2	5.83	122.40	118.90
22	AA	794	A	C4-C5-C6	-5.83	114.09	117.00
22	AA	1242	G	N1-C6-O6	-5.83	116.40	119.90
57	BA	914	G	C4'-C3'-C2'	-5.83	96.77	102.60
57	BA	1027	A	C4-C5-C6	-5.83	114.09	117.00
22	AA	1110	A	C4-C5-C6	-5.83	114.09	117.00
57	BA	41	C	O4'-C1'-N1	5.83	112.86	108.20
57	BA	235	U	O4'-C1'-N1	5.83	112.86	108.20
57	BA	583	G	O4'-C1'-N9	5.83	112.86	108.20
57	BA	1787	A	C4-C5-C6	-5.83	114.09	117.00
22	AA	277	C	O4'-C1'-N1	5.82	112.86	108.20
22	AA	384	G	O4'-C1'-N9	5.82	112.86	108.20
23	A2	55	A	C4-C5-C6	-5.82	114.09	117.00
57	BA	177	G	N3-C4-C5	-5.82	125.69	128.60
57	BA	2032	G	N1-C6-O6	-5.82	116.41	119.90
22	AA	85	U	N3-C2-O2	-5.82	118.12	122.20
22	AA	156	C	O4'-C1'-N1	5.82	112.86	108.20
22	AA	201	G	N1-C6-O6	-5.82	116.41	119.90
57	BA	434	U	O4'-C1'-N1	5.82	112.86	108.20
57	BA	694	U	O4'-C1'-N1	5.82	112.86	108.20
58	Ba	111	U	O4'-C1'-N1	5.82	112.86	108.20
22	AA	1318	A	C4-C5-C6	-5.82	114.09	117.00
48	B5	12	ARG	NE-CZ-NH2	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	316	C	O4'-C1'-N1	5.82	112.86	108.20
57	BA	2368	C	N3-C4-C5	5.82	124.23	121.90
57	BA	2660	A	C4-C5-C6	-5.82	114.09	117.00
22	AA	124	C	O4'-C1'-N1	5.82	112.85	108.20
22	AA	1107	C	O4'-C1'-N1	5.82	112.86	108.20
22	AA	1299	A	C4-C5-C6	-5.82	114.09	117.00
57	BA	327	G	N3-C2-N2	-5.82	115.83	119.90
57	BA	1073	A	C5-C6-N6	5.82	128.35	123.70
57	BA	2788	C	N1-C2-O2	5.82	122.39	118.90
22	AA	1411	C	N1-C2-O2	5.82	122.39	118.90
31	BQ	51	ARG	NE-CZ-NH2	5.82	123.21	120.30
57	BA	2182	U	O4'-C1'-N1	5.82	112.85	108.20
57	BA	2749	A	C4-C5-C6	-5.82	114.09	117.00
57	BA	821	A	O4'-C1'-N9	5.81	112.85	108.20
57	BA	2152	G	N1-C6-O6	-5.81	116.41	119.90
22	AA	373	A	C4-C5-C6	-5.81	114.09	117.00
57	BA	387	U	N3-C2-O2	-5.81	118.13	122.20
57	BA	2175	C	N1-C2-O2	5.81	122.39	118.90
57	BA	2181	U	O4'-C1'-N1	5.81	112.85	108.20
22	AA	156	C	N1-C2-O2	5.81	122.39	118.90
22	AA	760	G	O4'-C1'-N9	5.81	112.85	108.20
22	AA	372	C	N3-C2-O2	-5.81	117.83	121.90
22	AA	1038	C	N1-C2-O2	5.81	122.39	118.90
22	AA	1509	C	O4'-C1'-N1	5.81	112.85	108.20
57	BA	828	U	N3-C2-O2	-5.81	118.13	122.20
57	BA	355	U	O4'-C1'-N1	5.81	112.84	108.20
57	BA	1424	G	N1-C6-O6	-5.81	116.42	119.90
24	A3	54	G	N1-C6-O6	-5.81	116.42	119.90
55	BH	151	ARG	NE-CZ-NH1	5.81	123.20	120.30
57	BA	506	G	O4'-C1'-N9	5.81	112.84	108.20
57	BA	2450	A	C6-C5-N7	5.81	136.36	132.30
22	AA	177	G	N3-C4-C5	-5.80	125.70	128.60
57	BA	594	U	O4'-C1'-N1	5.80	112.84	108.20
57	BA	680	C	N1-C2-O2	5.80	122.38	118.90
57	BA	2219	U	O4'-C1'-N1	5.80	112.84	108.20
57	BA	2527	C	N1-C2-O2	5.80	122.38	118.90
57	BA	1052	C	N1-C2-O2	5.80	122.38	118.90
57	BA	1079	C	O4'-C1'-N1	5.80	112.84	108.20
57	BA	1513	U	O4'-C1'-N1	5.80	112.84	108.20
57	BA	1695	G	O4'-C1'-N9	5.80	112.84	108.20
57	BA	2277	G	N1-C6-O6	-5.80	116.42	119.90
22	AA	427	U	N3-C2-O2	-5.80	118.14	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	835	U	O4'-C1'-N1	5.80	112.84	108.20
22	AA	1033	G	O4'-C1'-N9	5.80	112.84	108.20
22	AA	1303	C	O4'-C1'-N1	5.80	112.84	108.20
57	BA	47	C	O4'-C1'-N1	5.80	112.84	108.20
57	BA	2753	A	C4-C5-C6	-5.80	114.10	117.00
57	BA	960	A	C4-C5-C6	-5.80	114.10	117.00
57	BA	1658	C	N1-C2-O2	5.80	122.38	118.90
22	AA	773	G	O4'-C1'-N9	5.80	112.84	108.20
33	BS	16	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
57	BA	842	U	O4'-C1'-N1	5.80	112.84	108.20
57	BA	988	A	C4-C5-C6	-5.80	114.10	117.00
57	BA	2014	A	C4-C5-C6	-5.80	114.10	117.00
57	BA	2338	C	O4'-C1'-N1	5.80	112.84	108.20
57	BA	2896	C	N1-C2-O2	5.80	122.38	118.90
58	Ba	13	G	N1-C6-O6	-5.80	116.42	119.90
22	AA	927	G	N1-C6-O6	-5.79	116.42	119.90
22	AA	52	C	O4'-C1'-N1	5.79	112.83	108.20
22	AA	109	A	C4-C5-C6	-5.79	114.10	117.00
57	BA	1192	G	N1-C6-O6	-5.79	116.42	119.90
57	BA	1471	G	N1-C6-O6	-5.79	116.42	119.90
22	AA	166	U	O4'-C1'-N1	5.79	112.83	108.20
22	AA	1105	A	O4'-C1'-N9	5.79	112.83	108.20
22	AA	1504	G	N1-C6-O6	-5.79	116.42	119.90
57	BA	1970	A	C4-C5-C6	-5.79	114.10	117.00
58	Ba	16	G	O4'-C1'-N9	5.79	112.83	108.20
30	BP	59	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
57	BA	1780	A	C4-C5-C6	-5.79	114.11	117.00
22	AA	162	A	C4-C5-C6	-5.79	114.11	117.00
22	AA	988	G	O4'-C1'-N9	5.79	112.83	108.20
22	AA	1031	C	N3-C2-O2	-5.79	117.85	121.90
22	AA	1050	G	C4'-C3'-C2'	-5.79	96.81	102.60
24	A3	53	G	O4'-C1'-N9	5.79	112.83	108.20
57	BA	1487	U	O4'-C1'-N1	5.79	112.83	108.20
57	BA	2531	A	C4-C5-C6	-5.79	114.11	117.00
22	AA	172	A	C4-C5-C6	-5.79	114.11	117.00
22	AA	395	C	N1-C2-O2	5.79	122.37	118.90
57	BA	789	A	C4-C5-C6	-5.79	114.11	117.00
57	BA	1644	C	O4'-C1'-N1	5.79	112.83	108.20
57	BA	2008	C	N1-C2-O2	5.79	122.37	118.90
22	AA	136	C	N1-C2-O2	5.79	122.37	118.90
22	AA	200	G	O4'-C1'-N9	5.79	112.83	108.20
22	AA	253	A	C4-C5-C6	-5.79	114.11	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	210	C	N1-C2-O2	5.79	122.37	118.90
57	BA	1074	G	N1-C6-O6	-5.78	116.43	119.90
57	BA	2646	C	C5'-C4'-O4'	5.78	116.04	109.10
22	AA	651	C	N1-C2-O2	5.78	122.37	118.90
22	AA	935	A	C4-C5-C6	-5.78	114.11	117.00
57	BA	558	U	O4'-C1'-N1	5.78	112.82	108.20
57	BA	1600	C	O4'-C1'-N1	5.78	112.82	108.20
57	BA	1748	C	N1-C2-O2	5.78	122.37	118.90
57	BA	1988	G	N1-C6-O6	-5.78	116.43	119.90
57	BA	2361	G	O4'-C1'-N9	5.78	112.83	108.20
57	BA	2460	U	O4'-C1'-N1	5.78	112.83	108.20
57	BA	1678	A	O4'-C1'-N9	5.78	112.82	108.20
21	A1	142	ARG	NE-CZ-NH1	5.78	123.19	120.30
22	AA	623	C	N1-C2-O2	5.78	122.37	118.90
22	AA	912	C	N1-C2-O2	5.78	122.37	118.90
22	AA	1503	A	O4'-C1'-N9	5.78	112.82	108.20
53	BF	21	ARG	NE-CZ-NH2	5.78	123.19	120.30
57	BA	557	C	O4'-C1'-N1	5.78	112.82	108.20
57	BA	671	C	N1-C2-O2	5.78	122.37	118.90
57	BA	991	C	N1-C2-O2	5.78	122.37	118.90
57	BA	1266	G	C3'-C2'-C1'	-5.78	96.88	101.50
57	BA	2017	U	N1-C2-N3	5.78	118.37	114.90
22	AA	13	U	C1'-O4'-C4'	-5.78	105.28	109.90
22	AA	745	G	N1-C6-O6	-5.78	116.43	119.90
35	BD	166	ARG	NE-CZ-NH1	5.78	123.19	120.30
57	BA	1431	A	C4-C5-C6	-5.78	114.11	117.00
57	BA	1993	U	O4'-C1'-N1	5.78	112.82	108.20
57	BA	2639	A	C4-C5-C6	-5.78	114.11	117.00
22	AA	437	U	O4'-C1'-N1	5.77	112.82	108.20
22	AA	463	U	O4'-C4'-C3'	5.77	110.72	106.10
22	AA	717	U	O4'-C1'-N1	5.77	112.82	108.20
57	BA	611	C	N1-C2-O2	5.77	122.36	118.90
57	BA	1832	C	N1-C2-O2	5.77	122.36	118.90
22	AA	308	C	N1-C2-O2	5.77	122.36	118.90
22	AA	738	C	N1-C2-O2	5.77	122.36	118.90
22	AA	1306	A	C4-C5-C6	-5.77	114.11	117.00
57	BA	8	C	O4'-C1'-N1	5.77	112.82	108.20
57	BA	464	U	O4'-C1'-N1	5.77	112.82	108.20
57	BA	509	C	N1-C2-O2	5.77	122.36	118.90
57	BA	812	C	N3-C2-O2	-5.77	117.86	121.90
22	AA	259	G	N1-C6-O6	-5.77	116.44	119.90
22	AA	735	C	N1-C2-O2	5.77	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	654	A	C4-C5-C6	-5.77	114.11	117.00
22	AA	513	C	N1-C2-O2	5.77	122.36	118.90
57	BA	988	A	O4'-C1'-N9	5.77	112.82	108.20
57	BA	1022	G	O4'-C1'-N9	5.77	112.82	108.20
57	BA	1541	C	N1-C2-O2	5.77	122.36	118.90
57	BA	2561	U	O4'-C1'-N1	5.77	112.82	108.20
22	AA	402	G	N1-C6-O6	-5.77	116.44	119.90
57	BA	193	U	O4'-C1'-N1	5.77	112.81	108.20
57	BA	879	G	O4'-C1'-N9	5.77	112.81	108.20
22	AA	1069	C	N1-C2-O2	5.77	122.36	118.90
22	AA	1114	C	N1-C2-O2	5.76	122.36	118.90
57	BA	1452	G	C5-C6-N1	5.76	114.38	111.50
57	BA	1768	C	N1-C2-O2	5.76	122.36	118.90
57	BA	2204	G	C5'-C4'-C3'	-5.76	106.78	116.00
57	BA	2423	U	N3-C2-O2	-5.76	118.16	122.20
57	BA	2556	C	O4'-C1'-N1	5.76	112.81	108.20
57	BA	2589	A	O4'-C1'-N9	5.76	112.81	108.20
3	AL	120	ARG	NE-CZ-NH1	5.76	123.18	120.30
22	AA	1090	U	O4'-C1'-N1	5.76	112.81	108.20
57	BA	279	A	C4-C5-C6	-5.76	114.12	117.00
57	BA	2050	C	N1-C2-O2	5.76	122.36	118.90
22	AA	62	U	O4'-C1'-N1	5.76	112.81	108.20
22	AA	438	U	O4'-C1'-N1	5.76	112.81	108.20
22	AA	857	C	N1-C2-O2	5.76	122.36	118.90
22	AA	561	U	O4'-C1'-N1	5.76	112.81	108.20
22	AA	683	G	N1-C6-O6	-5.76	116.44	119.90
22	AA	1374	A	C4-C5-C6	-5.76	114.12	117.00
57	BA	105	C	N1-C2-O2	5.76	122.36	118.90
57	BA	149	A	C4-C5-C6	-5.76	114.12	117.00
57	BA	1036	G	N1-C6-O6	-5.76	116.44	119.90
57	BA	2092	U	N3-C2-O2	-5.76	118.17	122.20
57	BA	371	A	C4-C5-C6	-5.76	114.12	117.00
57	BA	1461	C	N3-C2-O2	-5.76	117.87	121.90
22	AA	658	C	O4'-C1'-N1	5.75	112.80	108.20
57	BA	135	U	O4'-C1'-N1	5.75	112.80	108.20
57	BA	535	G	N1-C6-O6	-5.75	116.45	119.90
57	BA	872	U	O4'-C1'-N1	5.75	112.80	108.20
57	BA	1310	G	O4'-C1'-N9	5.75	112.80	108.20
57	BA	2643	G	N1-C6-O6	-5.75	116.45	119.90
58	Ba	99	A	C4-C5-C6	-5.75	114.12	117.00
22	AA	943	U	O4'-C1'-N1	5.75	112.80	108.20
22	AA	965	U	N3-C2-O2	-5.75	118.17	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	36	G	N3-C2-N2	-5.75	115.87	119.90
57	BA	421	C	O4'-C1'-N1	5.75	112.80	108.20
57	BA	1274	A	C4-C5-C6	-5.75	114.12	117.00
57	BA	1959	G	N1-C6-O6	-5.75	116.45	119.90
57	BA	2512	C	O4'-C1'-N1	5.75	112.80	108.20
22	AA	370	C	O4'-C1'-N1	5.75	112.80	108.20
22	AA	469	C	N3-C2-O2	-5.75	117.88	121.90
1	AJ	7	ARG	NE-CZ-NH1	5.75	123.17	120.30
57	BA	1215	G	N1-C6-O6	-5.75	116.45	119.90
57	BA	1216	G	N1-C6-O6	-5.75	116.45	119.90
57	BA	1288	G	N3-C4-C5	-5.75	125.72	128.60
57	BA	2192	U	O4'-C1'-N1	5.75	112.80	108.20
22	AA	1153	G	N1-C6-O6	-5.75	116.45	119.90
22	AA	1389	C	N1-C2-O2	5.75	122.35	118.90
57	BA	863	A	C4-C5-C6	-5.75	114.13	117.00
57	BA	1329	U	N3-C2-O2	-5.75	118.18	122.20
22	AA	199	A	C4-C5-C6	-5.75	114.13	117.00
24	A3	70	C	O4'-C1'-N1	5.75	112.80	108.20
22	AA	608	A	C4-C5-C6	-5.74	114.13	117.00
57	BA	267	C	O4'-C1'-N1	5.74	112.80	108.20
57	BA	1292	G	N1-C6-O6	-5.74	116.45	119.90
23	A2	36	U	O4'-C1'-N1	5.74	112.79	108.20
57	BA	952	G	N1-C6-O6	-5.74	116.45	119.90
22	AA	1504	G	C1'-O4'-C4'	-5.74	105.31	109.90
57	BA	838	C	O4'-C1'-N1	5.74	112.79	108.20
57	BA	885	C	N1-C2-O2	5.74	122.34	118.90
57	BA	1624	U	O4'-C1'-N1	5.74	112.79	108.20
22	AA	843	U	C3'-C2'-C1'	5.74	106.09	101.50
57	BA	87	U	N3-C2-O2	-5.74	118.18	122.20
57	BA	2493	U	O4'-C1'-N1	5.74	112.79	108.20
22	AA	67	C	O4'-C1'-N1	5.74	112.79	108.20
22	AA	1284	C	N1-C2-O2	5.74	122.34	118.90
57	BA	199	A	C4-C5-C6	-5.74	114.13	117.00
57	BA	506	G	N3-C4-C5	-5.74	125.73	128.60
57	BA	576	U	O4'-C1'-N1	5.74	112.79	108.20
57	BA	1231	U	O4'-C1'-N1	5.74	112.79	108.20
57	BA	1719	G	N1-C6-O6	-5.74	116.46	119.90
57	BA	2614	A	O4'-C1'-N9	5.74	112.79	108.20
22	AA	250	A	C4-C5-C6	-5.73	114.13	117.00
22	AA	1466	C	N1-C2-O2	5.73	122.34	118.90
22	AA	1449	C	N1-C2-O2	5.73	122.34	118.90
35	BD	174	ARG	NE-CZ-NH1	5.73	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	514	A	C4-C5-C6	-5.73	114.13	117.00
57	BA	1422	G	N1-C6-O6	-5.73	116.46	119.90
57	BA	2041	U	O4'-C1'-N1	5.73	112.79	108.20
57	BA	2737	G	N1-C6-O6	-5.73	116.46	119.90
57	BA	2821	A	C4-C5-C6	-5.73	114.13	117.00
22	AA	1452	C	N3-C2-O2	-5.73	117.89	121.90
57	BA	364	C	N1-C2-O2	5.73	122.34	118.90
58	Ba	62	C	N1-C2-O2	5.73	122.34	118.90
22	AA	204	G	N1-C6-O6	-5.73	116.46	119.90
22	AA	1217	C	N1-C2-O2	5.73	122.34	118.90
30	BP	69	ARG	NE-CZ-NH1	5.73	123.16	120.30
57	BA	353	C	O4'-C1'-N1	5.73	112.78	108.20
57	BA	2646	C	N1-C2-O2	5.73	122.34	118.90
57	BA	42	A	O4'-C1'-N9	5.73	112.78	108.20
57	BA	1024	G	O4'-C1'-N9	5.73	112.78	108.20
57	BA	1409	U	O4'-C1'-N1	5.73	112.78	108.20
22	AA	189	A	O4'-C1'-N9	5.72	112.78	108.20
22	AA	405	U	O4'-C1'-N1	5.72	112.78	108.20
22	AA	1520	C	N1-C2-O2	5.72	122.33	118.90
57	BA	650	C	N1-C2-O2	5.72	122.33	118.90
57	BA	1489	C	N1-C2-O2	5.72	122.33	118.90
57	BA	2301	C	N1-C2-O2	5.72	122.33	118.90
57	BA	2735	G	N1-C6-O6	-5.72	116.47	119.90
22	AA	426	U	O4'-C1'-N1	5.72	112.78	108.20
22	AA	914	A	C5'-C4'-O4'	5.72	115.97	109.10
57	BA	2730	C	N1-C2-O2	5.72	122.33	118.90
22	AA	888	G	O4'-C1'-N9	5.72	112.78	108.20
57	BA	576	U	C3'-C2'-C1'	5.72	106.08	101.50
57	BA	1094	U	O4'-C1'-N1	5.72	112.78	108.20
57	BA	1100	C	O4'-C1'-N1	5.72	112.78	108.20
57	BA	2438	U	C5-C6-N1	-5.72	119.84	122.70
21	A1	263	ARG	NE-CZ-NH1	5.72	123.16	120.30
22	AA	295	C	N1-C2-O2	5.72	122.33	118.90
22	AA	339	C	N1-C2-O2	5.72	122.33	118.90
22	AA	404	G	C5-C6-N1	5.72	114.36	111.50
22	AA	795	C	O4'-C1'-N1	5.72	112.78	108.20
57	BA	783	A	C4-C5-C6	-5.72	114.14	117.00
57	BA	1317	G	N1-C6-O6	-5.72	116.47	119.90
57	BA	2016	U	O4'-C1'-N1	5.72	112.78	108.20
57	BA	2215	C	N1-C2-O2	5.72	122.33	118.90
57	BA	635	C	O4'-C1'-N1	5.72	112.77	108.20
57	BA	1118	C	N1-C2-O2	5.72	122.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2023	C	N1-C2-O2	5.72	122.33	118.90
22	AA	1075	U	O4'-C1'-N1	5.72	112.77	108.20
22	AA	1483	A	C4-C5-C6	-5.72	114.14	117.00
57	BA	2187	U	O4'-C1'-N1	5.72	112.77	108.20
22	AA	1037	C	N1-C2-O2	5.71	122.33	118.90
22	AA	1366	C	N1-C2-O2	5.71	122.33	118.90
57	BA	1755	A	C6-C5-N7	5.71	136.30	132.30
57	BA	2416	C	N1-C2-O2	5.71	122.33	118.90
22	AA	894	G	N1-C6-O6	-5.71	116.47	119.90
22	AA	1011	C	N1-C2-O2	5.71	122.33	118.90
22	AA	164	G	N1-C6-O6	-5.71	116.47	119.90
22	AA	552	U	N3-C2-O2	-5.71	118.20	122.20
57	BA	2076	U	P-O3'-C3'	5.71	126.55	119.70
22	AA	91	U	O4'-C1'-N1	5.71	112.77	108.20
22	AA	677	U	O4'-C1'-N1	5.71	112.77	108.20
22	AA	1270	G	N1-C6-O6	-5.71	116.47	119.90
57	BA	2295	C	N1-C2-O2	5.71	122.33	118.90
57	BA	764	A	O4'-C1'-N9	5.71	112.77	108.20
57	BA	1095	A	C4-C5-C6	-5.71	114.15	117.00
22	AA	419	C	O4'-C1'-N1	5.71	112.77	108.20
57	BA	2572	A	C4-C5-C6	-5.71	114.15	117.00
22	AA	1046	A	O4'-C1'-N9	5.71	112.76	108.20
57	BA	893	C	N1-C2-O2	5.71	122.32	118.90
23	A2	24	A	O3'-P-O5'	-5.70	93.16	104.00
57	BA	836	G	C5-C6-N1	5.70	114.35	111.50
58	Ba	26	C	N1-C2-O2	5.70	122.32	118.90
57	BA	691	C	N1-C2-O2	5.70	122.32	118.90
11	AB	136	ARG	NE-CZ-NH1	5.70	123.15	120.30
22	AA	1302	C	N1-C2-O2	5.70	122.32	118.90
57	BA	133	U	O4'-C1'-N1	5.70	112.76	108.20
57	BA	496	G	N1-C6-O6	-5.70	116.48	119.90
57	BA	1120	G	N1-C6-O6	-5.70	116.48	119.90
57	BA	1498	C	N1-C2-O2	5.70	122.32	118.90
57	BA	1686	C	N1-C2-O2	5.70	122.32	118.90
58	Ba	9	G	N1-C6-O6	-5.70	116.48	119.90
22	AA	877	G	N1-C6-O6	-5.70	116.48	119.90
22	AA	1294	G	N1-C6-O6	-5.70	116.48	119.90
57	BA	1653	G	P-O3'-C3'	5.70	126.54	119.70
57	BA	2240	U	O4'-C1'-N1	5.70	112.76	108.20
22	AA	580	C	N1-C2-O2	5.70	122.32	118.90
22	AA	1143	G	N1-C6-O6	-5.70	116.48	119.90
57	BA	951	C	N1-C2-O2	5.70	122.32	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1602	U	N3-C2-O2	-5.70	118.21	122.20
57	BA	1617	C	O4'-C1'-N1	5.70	112.76	108.20
57	BA	1663	G	N3-C4-C5	-5.70	125.75	128.60
57	BA	1777	U	O4'-C1'-N1	5.70	112.76	108.20
58	Ba	93	C	N1-C2-O2	5.70	122.32	118.90
23	A2	59	A	C4-C5-C6	-5.69	114.15	117.00
57	BA	2429	G	C3'-C2'-C1'	5.69	106.06	101.50
22	AA	1276	G	N1-C6-O6	-5.69	116.48	119.90
57	BA	36	G	N1-C6-O6	-5.69	116.48	119.90
57	BA	2158	A	C4-C5-C6	-5.69	114.15	117.00
57	BA	2285	C	N1-C2-O2	5.69	122.31	118.90
57	BA	2842	G	N1-C6-O6	-5.69	116.48	119.90
57	BA	2853	C	O4'-C1'-N1	5.69	112.75	108.20
24	A3	26	C	O4'-C1'-N1	5.69	112.75	108.20
29	BO	105	ARG	NE-CZ-NH1	5.69	123.15	120.30
31	BQ	38	ARG	NE-CZ-NH1	5.69	123.14	120.30
57	BA	2601	C	O4'-C1'-N1	5.69	112.75	108.20
22	AA	86	G	O4'-C1'-N9	5.69	112.75	108.20
22	AA	514	C	N1-C2-O2	5.69	122.31	118.90
22	AA	739	C	N1-C2-O2	5.69	122.31	118.90
57	BA	1594	U	O4'-C1'-N1	5.69	112.75	108.20
22	AA	709	U	O4'-C1'-N1	5.69	112.75	108.20
57	BA	1330	C	N1-C2-O2	5.69	122.31	118.90
57	BA	2508	G	C4'-C3'-C2'	-5.69	96.91	102.60
57	BA	2652	C	O4'-C1'-N1	5.69	112.75	108.20
57	BA	2902	C	N1-C2-O2	5.69	122.31	118.90
22	AA	496	A	C4-C5-C6	-5.69	114.16	117.00
22	AA	871	U	O4'-C1'-N1	5.69	112.75	108.20
57	BA	803	U	O4'-C1'-N1	5.69	112.75	108.20
57	BA	1128	G	N1-C6-O6	-5.69	116.49	119.90
57	BA	1480	C	O4'-C1'-N1	5.69	112.75	108.20
22	AA	162	A	O4'-C1'-N9	5.68	112.75	108.20
22	AA	1383	C	N3-C2-O2	-5.68	117.92	121.90
57	BA	29	U	N1-C2-N3	5.68	118.31	114.90
57	BA	343	C	N1-C2-O2	5.68	122.31	118.90
14	AC	130	ARG	NE-CZ-NH1	5.68	123.14	120.30
22	AA	936	C	C4'-C3'-C2'	-5.68	96.92	102.60
22	AA	1059	C	N1-C2-O2	5.68	122.31	118.90
24	A3	24	C	N1-C2-O2	5.68	122.31	118.90
57	BA	487	C	N1-C2-O2	5.68	122.31	118.90
57	BA	990	A	C3'-C2'-C1'	5.68	106.05	101.50
57	BA	1334	G	N1-C6-O6	-5.68	116.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AD	164	ARG	NE-CZ-NH1	5.68	123.14	120.30
57	BA	2430	A	C1'-O4'-C4'	-5.68	105.36	109.90
22	AA	908	A	C4-C5-C6	-5.68	114.16	117.00
57	BA	41	C	N1-C2-O2	5.68	122.31	118.90
57	BA	597	G	N1-C6-O6	-5.68	116.49	119.90
57	BA	793	A	O4'-C1'-N9	5.68	112.74	108.20
57	BA	1229	C	O4'-C1'-N1	5.68	112.74	108.20
57	BA	1967	C	O4'-C1'-N1	5.68	112.74	108.20
57	BA	2232	C	O4'-C1'-N1	5.68	112.74	108.20
57	BA	2699	C	O4'-C1'-N1	5.68	112.74	108.20
22	AA	65	A	O4'-C1'-N9	5.68	112.74	108.20
22	AA	624	C	N1-C2-O2	5.68	122.31	118.90
57	BA	644	A	C4-C5-C6	-5.68	114.16	117.00
57	BA	2548	U	O4'-C1'-N1	5.68	112.74	108.20
22	AA	883	C	N1-C2-O2	5.68	122.31	118.90
57	BA	143	C	N1-C2-O2	5.68	122.31	118.90
57	BA	517	C	O4'-C1'-N1	5.68	112.74	108.20
57	BA	2110	G	O4'-C1'-N9	5.68	112.74	108.20
22	AA	1114	C	O4'-C1'-N1	5.67	112.74	108.20
22	AA	1314	C	N3-C4-C5	5.67	124.17	121.90
57	BA	1013	C	N1-C2-O2	5.67	122.31	118.90
57	BA	1185	G	C3'-C2'-C1'	5.67	106.04	101.50
57	BA	1238	G	N1-C6-O6	-5.67	116.50	119.90
57	BA	2438	U	O4'-C1'-N1	5.67	112.74	108.20
22	AA	165	G	N1-C6-O6	-5.67	116.50	119.90
22	AA	1187	G	N1-C6-O6	-5.67	116.50	119.90
57	BA	1314	C	N1-C2-O2	5.67	122.30	118.90
57	BA	2584	U	O4'-C1'-N1	5.67	112.74	108.20
58	Ba	66	A	C4-C5-C6	-5.67	114.16	117.00
22	AA	1192	C	N3-C2-O2	-5.67	117.93	121.90
57	BA	623	C	N1-C2-O2	5.67	122.30	118.90
57	BA	1140	C	N1-C2-O2	5.67	122.30	118.90
57	BA	1346	G	N1-C6-O6	-5.67	116.50	119.90
7	AP	14	ARG	NE-CZ-NH1	5.67	123.13	120.30
22	AA	87	C	N1-C2-O2	5.67	122.30	118.90
22	AA	216	U	O4'-C1'-N1	5.67	112.73	108.20
57	BA	719	C	N1-C2-O2	5.67	122.30	118.90
57	BA	1228	G	O4'-C1'-N9	5.67	112.73	108.20
57	BA	2222	C	N1-C2-O2	5.67	122.30	118.90
22	AA	1341	U	O4'-C1'-N1	5.67	112.73	108.20
57	BA	142	A	O4'-C1'-N9	5.67	112.73	108.20
57	BA	1203	U	O4'-C1'-N1	5.67	112.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1728	C	O4'-C1'-N1	5.67	112.73	108.20
57	BA	2699	C	N1-C2-O2	5.67	122.30	118.90
22	AA	766	A	C4-C5-C6	-5.66	114.17	117.00
57	BA	291	G	N1-C6-O6	-5.66	116.50	119.90
57	BA	2306	C	N3-C2-O2	-5.66	117.94	121.90
57	BA	2855	C	N1-C2-O2	5.66	122.30	118.90
57	BA	486	C	N1-C2-O2	5.66	122.30	118.90
57	BA	903	C	N1-C2-O2	5.66	122.30	118.90
57	BA	1402	U	O4'-C1'-N1	5.66	112.73	108.20
22	AA	392	C	O4'-C1'-N1	5.66	112.73	108.20
29	BO	49	ARG	NE-CZ-NH1	5.66	123.13	120.30
57	BA	283	G	N1-C6-O6	-5.66	116.50	119.90
57	BA	914	G	C3'-C2'-C1'	-5.66	96.97	101.50
57	BA	1575	C	N1-C2-O2	5.66	122.30	118.90
4	AM	89	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
22	AA	1213	A	P-O3'-C3'	5.66	126.49	119.70
57	BA	831	G	N1-C6-O6	-5.66	116.50	119.90
57	BA	1270	C	N1-C2-O2	5.66	122.29	118.90
57	BA	1974	C	N1-C2-O2	5.66	122.29	118.90
22	AA	32	A	C4-C5-C6	-5.66	114.17	117.00
57	BA	1138	G	O4'-C1'-N9	5.66	112.72	108.20
57	BA	2676	C	N1-C2-O2	5.66	122.29	118.90
22	AA	1342	C	N1-C2-O2	5.65	122.29	118.90
57	BA	2579	C	N1-C2-O2	5.65	122.29	118.90
22	AA	758	C	N3-C2-O2	-5.65	117.94	121.90
35	BD	61	TYR	CB-CG-CD1	-5.65	117.61	121.00
38	BW	11	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
57	BA	996	A	C4-C5-C6	-5.65	114.17	117.00
57	BA	1646	C	C3'-C2'-C1'	5.65	106.02	101.50
57	BA	2773	C	N1-C2-O2	5.65	122.29	118.90
57	BA	2858	C	N3-C2-O2	-5.65	117.94	121.90
22	AA	1072	G	N1-C6-O6	-5.65	116.51	119.90
22	AA	1234	C	N1-C2-O2	5.65	122.29	118.90
7	AP	8	ARG	NE-CZ-NH1	5.65	123.12	120.30
57	BA	297	G	O4'-C1'-N9	5.65	112.72	108.20
57	BA	1383	A	C4-C5-C6	-5.65	114.17	117.00
57	BA	1585	C	O4'-C1'-N1	5.65	112.72	108.20
57	BA	1727	C	N1-C2-O2	5.65	122.29	118.90
57	BA	2507	C	N1-C2-O2	5.65	122.29	118.90
22	AA	153	C	N1-C2-O2	5.65	122.29	118.90
22	AA	194	C	O4'-C1'-N1	5.65	112.72	108.20
22	AA	952	U	O4'-C1'-N1	5.65	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	326	G	N1-C6-O6	-5.65	116.51	119.90
57	BA	531	C	N1-C2-O2	5.65	122.29	118.90
58	Ba	68	C	O4'-C1'-N1	5.65	112.72	108.20
22	AA	761	G	N1-C6-O6	-5.65	116.51	119.90
57	BA	2211	A	C4-C5-C6	-5.65	114.18	117.00
22	AA	258	G	N1-C6-O6	-5.64	116.51	119.90
57	BA	2006	C	O4'-C1'-N1	5.64	112.72	108.20
57	BA	2174	C	N3-C2-O2	-5.64	117.95	121.90
12	AT	59	ARG	NE-CZ-NH2	5.64	123.12	120.30
57	BA	268	C	N1-C2-O2	5.64	122.28	118.90
57	BA	738	G	N1-C6-O6	-5.64	116.52	119.90
57	BA	814	C	N1-C2-O2	5.64	122.28	118.90
57	BA	903	C	O4'-C1'-N1	5.64	112.71	108.20
57	BA	1522	A	C4-C5-C6	-5.64	114.18	117.00
57	BA	2300	C	O4'-C1'-N1	5.64	112.71	108.20
57	BA	2447	G	N3-C4-C5	-5.64	125.78	128.60
57	BA	2889	C	O4'-C1'-N1	5.64	112.71	108.20
22	AA	68	G	N3-C2-N2	-5.64	115.95	119.90
57	BA	1160	G	N1-C6-O6	-5.64	116.52	119.90
57	BA	2103	C	O4'-C1'-N1	5.64	112.71	108.20
22	AA	90	C	O4'-C1'-N1	5.64	112.71	108.20
22	AA	1218	C	N1-C2-O2	5.64	122.28	118.90
22	AA	1399	C	O4'-C1'-N1	5.64	112.71	108.20
57	BA	76	C	N1-C2-O2	5.64	122.28	118.90
57	BA	1073	A	C6-C5-N7	5.64	136.25	132.30
57	BA	2555	U	O4'-C1'-N1	5.64	112.71	108.20
52	B9	12	ARG	NE-CZ-NH1	5.64	123.12	120.30
57	BA	36	G	N9-C4-C5	5.64	107.66	105.40
57	BA	1706	C	N1-C2-O2	5.64	122.28	118.90
57	BA	1849	G	N1-C6-O6	-5.64	116.52	119.90
24	A3	68	C	O4'-C1'-N1	5.64	112.71	108.20
57	BA	604	G	C5'-C4'-C3'	-5.64	106.98	116.00
57	BA	740	C	N1-C2-O2	5.64	122.28	118.90
57	BA	970	U	N3-C2-O2	-5.64	118.25	122.20
57	BA	1260	A	C4-C5-C6	-5.64	114.18	117.00
57	BA	2300	C	N1-C2-O2	5.64	122.28	118.90
22	AA	33	A	C4-C5-C6	-5.63	114.18	117.00
22	AA	590	U	O4'-C1'-N1	5.63	112.71	108.20
22	AA	1272	G	N1-C6-O6	-5.63	116.52	119.90
57	BA	969	G	O4'-C1'-N9	5.63	112.71	108.20
57	BA	2208	C	N1-C2-O2	5.63	122.28	118.90
57	BA	2326	C	N1-C2-O2	5.63	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2439	A	C4-C5-C6	-5.63	114.18	117.00
57	BA	2665	A	C4-C5-C6	-5.63	114.18	117.00
22	AA	956	U	O4'-C1'-N1	5.63	112.70	108.20
57	BA	13	A	C6-C5-N7	5.63	136.24	132.30
57	BA	1123	C	O4'-C1'-N1	5.63	112.70	108.20
57	BA	1311	G	O4'-C1'-N9	5.63	112.70	108.20
57	BA	2483	C	N1-C2-O2	5.63	122.28	118.90
57	BA	2835	A	C4-C5-C6	-5.63	114.19	117.00
22	AA	386	C	O4'-C1'-N1	5.63	112.70	108.20
57	BA	22	C	N1-C2-O2	5.63	122.28	118.90
57	BA	959	A	C4-C5-C6	-5.63	114.19	117.00
22	AA	886	G	N1-C6-O6	-5.63	116.52	119.90
57	BA	1843	C	N1-C2-O2	5.63	122.28	118.90
57	BA	2212	A	C4-C5-C6	-5.63	114.19	117.00
57	BA	2223	G	N1-C6-O6	-5.63	116.52	119.90
57	BA	2785	C	N1-C2-O2	5.63	122.28	118.90
22	AA	1320	C	N3-C2-O2	-5.62	117.96	121.90
57	BA	1233	C	N1-C2-O2	5.62	122.28	118.90
57	BA	2631	G	N1-C6-O6	-5.62	116.53	119.90
2	AK	105	ARG	NE-CZ-NH1	5.62	123.11	120.30
22	AA	183	C	C1'-O4'-C4'	-5.62	105.40	109.90
22	AA	1113	C	N1-C2-O2	5.62	122.27	118.90
57	BA	912	C	N1-C2-O2	5.62	122.27	118.90
57	BA	1744	A	C4-C5-C6	-5.62	114.19	117.00
22	AA	932	C	N1-C2-O2	5.62	122.27	118.90
57	BA	705	A	N1-C6-N6	-5.62	115.23	118.60
57	BA	2190	G	N1-C6-O6	-5.62	116.53	119.90
57	BA	2542	A	O4'-C1'-N9	5.62	112.70	108.20
6	AO	71	ARG	NE-CZ-NH1	5.62	123.11	120.30
22	AA	225	C	N1-C2-O2	5.62	122.27	118.90
22	AA	230	G	O4'-C1'-N9	5.62	112.70	108.20
57	BA	678	C	N1-C2-O2	5.62	122.27	118.90
58	Ba	3	C	N1-C2-O2	5.62	122.27	118.90
22	AA	580	C	O4'-C1'-N1	5.62	112.69	108.20
57	BA	1263	U	N3-C2-O2	-5.62	118.27	122.20
57	BA	1352	U	C5-C6-N1	-5.62	119.89	122.70
57	BA	2545	G	N1-C6-O6	-5.62	116.53	119.90
22	AA	1348	U	N3-C2-O2	-5.62	118.27	122.20
57	BA	2533	U	O4'-C1'-N1	5.62	112.69	108.20
57	BA	2562	U	O4'-C1'-N1	5.62	112.69	108.20
22	AA	1094	G	N1-C6-O6	-5.62	116.53	119.90
57	BA	238	C	N1-C2-O2	5.62	122.27	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1185	G	N1-C6-O6	-5.62	116.53	119.90
57	BA	1577	C	N1-C2-O2	5.62	122.27	118.90
57	BA	2063	C	N3-C4-N4	-5.62	114.07	118.00
22	AA	225	C	O4'-C1'-N1	5.61	112.69	108.20
22	AA	316	C	N1-C2-O2	5.61	122.27	118.90
22	AA	409	U	O4'-C1'-N1	5.61	112.69	108.20
22	AA	457	G	N1-C6-O6	-5.61	116.53	119.90
22	AA	634	C	N1-C2-O2	5.61	122.27	118.90
22	AA	1130	A	O4'-C1'-N9	5.61	112.69	108.20
22	AA	1443	C	N1-C2-O2	5.61	122.27	118.90
57	BA	105	C	O4'-C1'-N1	5.61	112.69	108.20
57	BA	1451	C	O4'-C1'-N1	5.61	112.69	108.20
57	BA	2063	C	N1-C2-O2	5.61	122.27	118.90
22	AA	990	C	N1-C2-O2	5.61	122.27	118.90
57	BA	285	G	N1-C6-O6	-5.61	116.53	119.90
57	BA	787	C	N1-C2-O2	5.61	122.27	118.90
23	A2	49	U	O4'-C1'-N1	5.61	112.69	108.20
57	BA	301	G	N1-C6-O6	-5.61	116.53	119.90
57	BA	584	C	O4'-C1'-N1	5.61	112.69	108.20
57	BA	1185	G	O4'-C1'-N9	5.61	112.69	108.20
57	BA	1316	U	O4'-C1'-N1	5.61	112.69	108.20
57	BA	1448	G	N1-C6-O6	-5.61	116.53	119.90
57	BA	1956	U	N3-C2-O2	-5.61	118.27	122.20
57	BA	1996	C	N1-C2-O2	5.61	122.27	118.90
57	BA	2361	G	N1-C6-O6	-5.61	116.53	119.90
22	AA	275	G	N1-C6-O6	-5.61	116.54	119.90
22	AA	1296	C	N1-C2-O2	5.61	122.27	118.90
57	BA	256	A	C4-C5-C6	-5.61	114.20	117.00
57	BA	1045	C	C3'-C2'-C1'	5.61	105.99	101.50
22	AA	1448	C	N1-C2-O2	5.61	122.26	118.90
57	BA	2870	C	N1-C2-O2	5.61	122.26	118.90
22	AA	351	G	O4'-C1'-N9	5.60	112.68	108.20
57	BA	134	G	N1-C6-O6	-5.60	116.54	119.90
57	BA	521	U	O4'-C1'-N1	5.60	112.68	108.20
57	BA	565	C	N3-C4-C5	5.60	124.14	121.90
57	BA	1996	C	N3-C4-C5	5.60	124.14	121.90
57	BA	2831	G	N1-C6-O6	-5.60	116.54	119.90
57	BA	711	G	N1-C6-O6	-5.60	116.54	119.90
57	BA	1134	A	C4-C5-C6	-5.60	114.20	117.00
22	AA	772	U	O4'-C1'-N1	5.60	112.68	108.20
22	AA	1198	G	N1-C6-O6	-5.60	116.54	119.90
22	AA	202	G	N3-C4-C5	-5.60	125.80	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	BF	117	ARG	NE-CZ-NH1	5.60	123.10	120.30
57	BA	468	G	O4'-C1'-N9	5.60	112.68	108.20
57	BA	551	G	O4'-C1'-N9	5.60	112.68	108.20
57	BA	2098	U	O4'-C1'-N1	5.60	112.68	108.20
57	BA	2779	U	O4'-C1'-N1	5.60	112.68	108.20
22	AA	1218	C	O4'-C1'-N1	5.59	112.68	108.20
22	AA	1243	C	N1-C2-O2	5.59	122.26	118.90
57	BA	580	U	N3-C2-O2	-5.59	118.28	122.20
57	BA	2398	U	O4'-C1'-N1	5.59	112.68	108.20
22	AA	420	U	C5'-C4'-O4'	5.59	115.81	109.10
57	BA	509	C	N3-C4-C5	5.59	124.14	121.90
57	BA	1340	U	N3-C2-O2	-5.59	118.28	122.20
57	BA	2784	U	O4'-C1'-N1	5.59	112.67	108.20
22	AA	243	A	O4'-C1'-N9	5.59	112.67	108.20
22	AA	931	C	N1-C2-O2	5.59	122.25	118.90
22	AA	1469	C	N3-C2-O2	-5.59	117.99	121.90
31	BQ	18	ARG	NE-CZ-NH2	5.59	123.10	120.30
57	BA	211	C	N1-C2-O2	5.59	122.25	118.90
57	BA	252	G	O4'-C1'-N9	5.59	112.67	108.20
57	BA	2446	G	N1-C6-O6	-5.59	116.55	119.90
57	BA	2795	C	N1-C2-O2	5.59	122.25	118.90
57	BA	565	C	O4'-C1'-N1	5.59	112.67	108.20
22	AA	283	U	O4'-C1'-N1	5.59	112.67	108.20
22	AA	1019	A	O4'-C1'-N9	5.59	112.67	108.20
22	AA	1369	C	N1-C2-O2	5.59	122.25	118.90
22	AA	1509	C	N1-C2-O2	5.59	122.25	118.90
57	BA	467	G	O4'-C1'-N9	5.59	112.67	108.20
57	BA	1844	C	N1-C2-O2	5.59	122.25	118.90
20	AI	44	ARG	NE-CZ-NH1	5.59	123.09	120.30
22	AA	532	A	C2-N3-C4	5.59	113.39	110.60
22	AA	849	G	N1-C6-O6	-5.59	116.55	119.90
22	AA	932	C	O4'-C1'-N1	5.59	112.67	108.20
57	BA	1868	C	N1-C2-O2	5.59	122.25	118.90
58	Ba	20	G	N1-C6-O6	-5.59	116.55	119.90
58	Ba	57	A	C4-C5-C6	-5.59	114.21	117.00
57	BA	302	C	O4'-C1'-N1	5.58	112.67	108.20
57	BA	1191	G	O4'-C1'-N9	5.58	112.67	108.20
57	BA	2084	C	O4'-C1'-N1	5.58	112.67	108.20
22	AA	41	G	N1-C6-O6	-5.58	116.55	119.90
22	AA	202	G	N1-C6-O6	-5.58	116.55	119.90
57	BA	581	C	N1-C2-O2	5.58	122.25	118.90
57	BA	1114	C	N1-C2-O2	5.58	122.25	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Ba	27	C	N1-C2-O2	5.58	122.25	118.90
22	AA	868	C	N1-C2-O2	5.58	122.25	118.90
22	AA	1165	U	O4'-C1'-N1	5.58	112.67	108.20
22	AA	1256	A	C4-C5-C6	-5.58	114.21	117.00
57	BA	74	A	C5'-C4'-C3'	-5.58	107.07	116.00
57	BA	556	A	C4-C5-C6	-5.58	114.21	117.00
57	BA	1022	G	C5-C6-N1	5.58	114.29	111.50
57	BA	1993	U	N3-C2-O2	-5.58	118.29	122.20
57	BA	2061	G	C2'-C3'-O3'	5.58	122.63	113.70
57	BA	2102	G	N1-C6-O6	-5.58	116.55	119.90
22	AA	284	C	N1-C2-O2	5.58	122.25	118.90
22	AA	637	C	N1-C2-O2	5.58	122.25	118.90
22	AA	828	U	O4'-C1'-N1	5.58	112.66	108.20
57	BA	1860	G	N1-C6-O6	-5.58	116.55	119.90
22	AA	132	C	N1-C2-O2	5.58	122.25	118.90
22	AA	221	C	N1-C2-O2	5.58	122.25	118.90
22	AA	334	C	N1-C2-O2	5.58	122.25	118.90
22	AA	1282	C	N3-C4-C5	5.58	124.13	121.90
24	A3	14	A	C4-C5-C6	-5.58	114.21	117.00
57	BA	908	C	N1-C2-O2	5.58	122.25	118.90
57	BA	2307	G	N1-C6-O6	-5.58	116.55	119.90
57	BA	2769	U	O4'-C1'-N1	5.58	112.66	108.20
57	BA	2061	G	O4'-C1'-N9	5.58	112.66	108.20
57	BA	2470	G	N1-C6-O6	-5.58	116.55	119.90
22	AA	54	C	O4'-C1'-N1	5.58	112.66	108.20
22	AA	111	G	N1-C6-O6	-5.58	116.56	119.90
57	BA	149	A	N1-C6-N6	-5.58	115.25	118.60
57	BA	183	C	N1-C2-O2	5.58	122.25	118.90
57	BA	523	C	N1-C2-O2	5.58	122.25	118.90
57	BA	2235	G	N1-C6-O6	-5.58	116.55	119.90
57	BA	2416	C	O4'-C1'-N1	5.58	112.66	108.20
58	Ba	88	C	C1'-O4'-C4'	-5.58	105.44	109.90
22	AA	1470	U	O4'-C1'-N1	5.57	112.66	108.20
57	BA	1153	C	O4'-C1'-N1	5.57	112.66	108.20
57	BA	1841	U	O4'-C1'-N1	5.57	112.66	108.20
57	BA	1846	G	N1-C6-O6	-5.57	116.56	119.90
57	BA	1985	C	O4'-C1'-N1	5.57	112.66	108.20
24	A3	75	C	N1-C2-O2	5.57	122.24	118.90
57	BA	1916	A	C4-C5-C6	-5.57	114.21	117.00
57	BA	2248	C	N1-C2-O2	5.57	122.24	118.90
57	BA	795	C	N1-C2-O2	5.57	122.24	118.90
57	BA	848	C	N1-C2-O2	5.57	122.24	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2793	C	N1-C2-O2	5.57	122.24	118.90
22	AA	1231	G	N1-C6-O6	-5.57	116.56	119.90
35	BD	176	ARG	NE-CZ-NH1	5.57	123.08	120.30
57	BA	1772	A	O4'-C1'-N9	5.57	112.65	108.20
57	BA	2350	C	O4'-C1'-N1	5.57	112.65	108.20
57	BA	2517	C	N3-C2-O2	-5.57	118.00	121.90
22	AA	736	C	N1-C2-O2	5.57	122.24	118.90
57	BA	445	C	N3-C4-C5	5.57	124.13	121.90
57	BA	1064	C	N1-C2-O2	5.57	122.24	118.90
57	BA	1330	C	O4'-C1'-N1	5.57	112.65	108.20
57	BA	1701	A	C4-C5-C6	-5.57	114.22	117.00
57	BA	1881	C	N1-C2-O2	5.57	122.24	118.90
57	BA	2854	G	N1-C6-O6	-5.57	116.56	119.90
57	BA	2901	C	N1-C2-O2	5.57	122.24	118.90
22	AA	346	G	N3-C4-C5	-5.56	125.82	128.60
57	BA	1764	C	O4'-C1'-N1	5.56	112.65	108.20
57	BA	1905	C	N1-C2-O2	5.56	122.24	118.90
57	BA	2615	U	O4'-C1'-N1	5.56	112.65	108.20
58	Ba	3	C	O4'-C1'-N1	5.56	112.65	108.20
22	AA	3	A	C3'-C2'-C1'	5.56	105.95	101.50
22	AA	23	C	N1-C2-O2	5.56	122.24	118.90
22	AA	232	G	O4'-C1'-N9	5.56	112.65	108.20
22	AA	717	U	P-O3'-C3'	5.56	126.38	119.70
22	AA	785	G	N1-C6-O6	-5.56	116.56	119.90
22	AA	1423	G	N1-C6-O6	-5.56	116.56	119.90
57	BA	97	C	N1-C2-O2	5.56	122.24	118.90
57	BA	1465	G	N1-C6-O6	-5.56	116.56	119.90
57	BA	1750	G	N1-C6-O6	-5.56	116.56	119.90
57	BA	2141	G	O4'-C1'-N9	5.56	112.65	108.20
57	BA	706	A	C4-C5-C6	-5.56	114.22	117.00
57	BA	1519	G	N1-C6-O6	-5.56	116.56	119.90
22	AA	1147	C	N3-C4-C5	5.56	124.12	121.90
22	AA	1540	U	O4'-C1'-N1	5.56	112.65	108.20
57	BA	414	C	C4'-C3'-C2'	-5.56	97.04	102.60
57	BA	685	A	C4-C5-C6	-5.56	114.22	117.00
57	BA	1990	C	N1-C2-O2	5.56	122.24	118.90
57	BA	2129	C	C1'-O4'-C4'	-5.56	105.45	109.90
57	BA	2593	U	O4'-C1'-N1	5.56	112.65	108.20
22	AA	108	G	N1-C6-O6	-5.56	116.56	119.90
57	BA	43	G	N1-C6-O6	-5.56	116.57	119.90
57	BA	928	A	O4'-C1'-N9	5.56	112.65	108.20
57	BA	1130	U	O4'-C1'-N1	5.56	112.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	99	C	O4'-C1'-N1	5.56	112.64	108.20
57	BA	60	G	O3'-P-O5'	-5.56	93.44	104.00
24	A3	67	C	N1-C2-O2	5.55	122.23	118.90
57	BA	806	C	N1-C2-O2	5.55	122.23	118.90
57	BA	840	C	O4'-C1'-N1	5.55	112.64	108.20
57	BA	1414	C	N1-C2-O2	5.55	122.23	118.90
57	BA	1690	A	N1-C6-N6	-5.55	115.27	118.60
57	BA	2017	U	O4'-C1'-N1	5.55	112.64	108.20
58	Ba	110	C	N1-C2-O2	5.55	122.23	118.90
57	BA	816	C	O4'-C1'-N1	5.55	112.64	108.20
57	BA	2843	G	O4'-C1'-N9	5.55	112.64	108.20
15	AD	187	ARG	NE-CZ-NH1	5.55	123.08	120.30
22	AA	245	U	N3-C2-O2	-5.55	118.31	122.20
22	AA	470	C	O4'-C1'-N1	5.55	112.64	108.20
43	B1	26	ARG	NH1-CZ-NH2	-5.55	113.29	119.40
57	BA	58	G	O4'-C1'-N9	5.55	112.64	108.20
57	BA	2355	G	N1-C6-O6	-5.55	116.57	119.90
22	AA	135	C	O4'-C1'-N1	5.55	112.64	108.20
57	BA	367	G	O4'-C1'-N9	5.55	112.64	108.20
57	BA	496	G	O4'-C1'-N9	5.55	112.64	108.20
57	BA	861	A	C4-C5-C6	-5.55	114.22	117.00
57	BA	2354	C	N1-C2-O2	5.55	122.23	118.90
22	AA	855	U	O4'-C1'-N1	5.55	112.64	108.20
54	BG	70	ARG	NE-CZ-NH2	5.55	123.07	120.30
57	BA	141	G	N3-C4-C5	-5.55	125.83	128.60
22	AA	386	C	N1-C2-O2	5.55	122.23	118.90
22	AA	1020	G	N1-C6-O6	-5.55	116.57	119.90
22	AA	1302	C	N3-C4-C5	5.55	124.12	121.90
57	BA	575	A	C1'-O4'-C4'	-5.55	105.46	109.90
57	BA	1121	C	O4'-C1'-N1	5.55	112.64	108.20
57	BA	1888	G	O4'-C1'-N9	5.55	112.64	108.20
57	BA	2816	G	N1-C6-O6	-5.55	116.57	119.90
27	BK	64	ARG	NE-CZ-NH1	5.54	123.07	120.30
57	BA	153	U	O4'-C1'-N1	5.54	112.64	108.20
57	BA	2045	C	N1-C2-O2	5.54	122.23	118.90
57	BA	2839	G	N1-C6-O6	-5.54	116.57	119.90
21	A1	623	ARG	NE-CZ-NH1	5.54	123.07	120.30
22	AA	443	C	N1-C2-O2	5.54	122.23	118.90
22	AA	708	C	N1-C2-O2	5.54	122.23	118.90
22	AA	845	A	C1'-O4'-C4'	-5.54	105.47	109.90
22	AA	1071	C	O4'-C1'-N1	5.54	112.64	108.20
22	AA	1332	A	C4-C5-C6	-5.54	114.23	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A2	29	G	N3-C4-C5	-5.54	125.83	128.60
57	BA	475	C	O4'-C1'-N1	5.54	112.63	108.20
57	BA	1480	C	N1-C2-O2	5.54	122.23	118.90
58	Ba	112	G	N1-C6-O6	-5.54	116.57	119.90
22	AA	66	A	C4-C5-C6	-5.54	114.23	117.00
22	AA	444	G	N1-C6-O6	-5.54	116.58	119.90
22	AA	980	C	N3-C2-O2	-5.54	118.02	121.90
22	AA	1384	C	O4'-C1'-N1	5.54	112.63	108.20
57	BA	188	G	N1-C6-O6	-5.54	116.58	119.90
57	BA	351	C	N1-C2-O2	5.54	122.22	118.90
57	BA	1129	A	C5'-C4'-O4'	5.54	115.75	109.10
57	BA	1332	G	P-O3'-C3'	5.54	126.35	119.70
57	BA	2064	C	N1-C2-O2	5.54	122.22	118.90
58	Ba	31	C	N1-C2-O2	5.54	122.22	118.90
22	AA	756	C	N1-C2-O2	5.54	122.22	118.90
57	BA	268	C	O4'-C1'-N1	5.54	112.63	108.20
57	BA	462	C	N1-C2-O2	5.54	122.22	118.90
57	BA	882	G	N1-C6-O6	-5.54	116.58	119.90
57	BA	2535	G	N3-C2-N2	-5.54	116.02	119.90
57	BA	2616	C	O4'-C1'-N1	5.54	112.63	108.20
58	Ba	37	C	N3-C2-O2	-5.54	118.02	121.90
22	AA	87	C	O4'-C1'-N1	5.54	112.63	108.20
57	BA	1621	U	O4'-C1'-N1	5.54	112.63	108.20
12	AT	24	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
22	AA	815	A	C6-C5-N7	5.54	136.17	132.30
22	AA	1039	G	N1-C6-O6	-5.54	116.58	119.90
24	A3	72	C	N1-C2-O2	5.54	122.22	118.90
57	BA	246	C	O4'-C1'-N1	5.54	112.63	108.20
57	BA	714	U	O4'-C1'-N1	5.54	112.63	108.20
57	BA	924	G	N1-C6-O6	-5.54	116.58	119.90
57	BA	2739	U	C5-C6-N1	-5.54	119.93	122.70
57	BA	2843	G	N1-C6-O6	-5.54	116.58	119.90
24	A3	43	G	N1-C6-O6	-5.53	116.58	119.90
57	BA	1908	C	O4'-C1'-N1	5.53	112.63	108.20
57	BA	2403	C	N1-C2-O2	5.53	122.22	118.90
57	BA	2646	C	O4'-C1'-N1	5.53	112.63	108.20
22	AA	714	G	O4'-C1'-N9	5.53	112.63	108.20
57	BA	1607	C	O4'-C1'-N1	5.53	112.63	108.20
57	BA	2653	U	N3-C2-O2	-5.53	118.33	122.20
57	BA	2000	C	O4'-C1'-N1	5.53	112.62	108.20
22	AA	841	C	O4'-C1'-N1	5.53	112.62	108.20
22	AA	1047	G	N3-C4-C5	-5.53	125.83	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1526	G	N1-C6-O6	-5.53	116.58	119.90
57	BA	1533	C	N1-C2-O2	5.53	122.22	118.90
22	AA	74	A	C6-C5-N7	5.53	136.17	132.30
22	AA	764	C	O4'-C1'-N1	5.53	112.62	108.20
22	AA	973	G	N1-C6-O6	-5.53	116.58	119.90
22	AA	1364	U	O4'-C1'-N1	5.53	112.62	108.20
57	BA	393	C	N1-C2-O2	5.53	122.22	118.90
57	BA	636	G	N1-C6-O6	-5.53	116.58	119.90
57	BA	832	U	N3-C2-O2	-5.53	118.33	122.20
57	BA	1585	C	N3-C4-C5	5.53	124.11	121.90
57	BA	1768	C	O4'-C1'-N1	5.53	112.62	108.20
22	AA	573	A	C6-C5-N7	5.53	136.17	132.30
22	AA	1253	G	C5'-C4'-C3'	-5.53	107.16	116.00
57	BA	1926	U	N3-C2-O2	-5.53	118.33	122.20
57	BA	2143	C	O4'-C1'-N1	5.53	112.62	108.20
57	BA	2458	G	N3-C4-C5	-5.53	125.84	128.60
57	BA	1388	G	O4'-C1'-N9	5.52	112.62	108.20
22	AA	558	G	O4'-C1'-N9	5.52	112.62	108.20
22	AA	1040	U	O4'-C1'-N1	5.52	112.62	108.20
22	AA	1501	C	N1-C2-O2	5.52	122.21	118.90
57	BA	1718	G	N1-C6-O6	-5.52	116.59	119.90
22	AA	161	A	C8-N9-C4	-5.52	103.59	105.80
22	AA	218	U	O4'-C1'-N1	5.52	112.62	108.20
22	AA	1292	G	N1-C6-O6	-5.52	116.59	119.90
22	AA	1307	U	O4'-C1'-N1	5.52	112.62	108.20
57	BA	665	U	O4'-C1'-N1	5.52	112.62	108.20
57	BA	1076	C	N1-C2-O2	5.52	122.21	118.90
57	BA	1569	A	C6-C5-N7	5.52	136.16	132.30
57	BA	2082	A	N1-C6-N6	-5.52	115.29	118.60
57	BA	2422	C	C1'-O4'-C4'	-5.52	105.48	109.90
57	BA	2476	A	C6-C5-N7	5.52	136.16	132.30
57	BA	2771	C	O4'-C1'-N1	5.52	112.61	108.20
58	Ba	93	C	O4'-C1'-N1	5.52	112.61	108.20
57	BA	580	U	O4'-C1'-N1	5.52	112.61	108.20
57	BA	1793	C	N1-C2-O2	5.52	122.21	118.90
57	BA	2161	C	N3-C2-O2	-5.52	118.04	121.90
22	AA	536	C	N1-C2-O2	5.51	122.21	118.90
57	BA	100	U	N3-C2-O2	-5.51	118.34	122.20
57	BA	256	A	N1-C6-N6	-5.51	115.29	118.60
57	BA	315	G	N1-C6-O6	-5.51	116.59	119.90
57	BA	1615	C	C2-N3-C4	-5.51	117.14	119.90
20	AI	129	ARG	NH1-CZ-NH2	-5.51	113.34	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1496	C	N1-C2-O2	5.51	122.21	118.90
57	BA	542	C	O4'-C1'-N1	5.51	112.61	108.20
20	AI	48	ARG	NE-CZ-NH2	-5.51	117.55	120.30
22	AA	203	G	N1-C6-O6	-5.51	116.59	119.90
24	A3	9	G	N3-C4-C5	-5.51	125.84	128.60
57	BA	49	A	C4-C5-C6	-5.51	114.24	117.00
57	BA	1499	C	N1-C2-O2	5.51	122.21	118.90
57	BA	2691	C	N1-C2-O2	5.51	122.21	118.90
57	BA	2785	C	O4'-C1'-N1	5.51	112.61	108.20
22	AA	129	A	C6-C5-N7	5.51	136.16	132.30
22	AA	1144	G	N1-C6-O6	-5.51	116.59	119.90
57	BA	645	C	O4'-C1'-N1	5.51	112.61	108.20
57	BA	709	U	O4'-C1'-N1	5.51	112.61	108.20
22	AA	383	A	C4-C5-C6	-5.51	114.25	117.00
57	BA	560	C	N1-C2-O2	5.51	122.20	118.90
57	BA	1021	A	C4-C5-C6	-5.51	114.25	117.00
57	BA	2099	U	O4'-C1'-N1	5.51	112.61	108.20
57	BA	2206	C	N1-C2-O2	5.51	122.20	118.90
57	BA	2558	C	N1-C2-O2	5.51	122.20	118.90
22	AA	1109	C	O4'-C1'-N1	5.51	112.61	108.20
22	AA	1228	C	O4'-C1'-N1	5.51	112.61	108.20
22	AA	1474	U	O4'-C1'-N1	5.51	112.61	108.20
49	B6	5	ARG	NE-CZ-NH1	5.51	123.05	120.30
53	BF	79	ARG	NE-CZ-NH1	5.51	123.05	120.30
57	BA	647	G	N1-C6-O6	-5.51	116.60	119.90
57	BA	1091	G	N1-C6-O6	-5.51	116.60	119.90
57	BA	1162	G	N1-C6-O6	-5.51	116.60	119.90
57	BA	2368	C	N1-C2-O2	5.51	122.20	118.90
57	BA	2815	C	N1-C2-O2	5.51	122.20	118.90
57	BA	2840	C	N1-C2-O2	5.51	122.20	118.90
40	BY	81	ARG	NE-CZ-NH1	5.50	123.05	120.30
57	BA	1130	U	C3'-C2'-C1'	-5.50	97.10	101.50
57	BA	1931	U	N3-C2-O2	-5.50	118.35	122.20
57	BA	2671	G	N1-C6-O6	-5.50	116.60	119.90
57	BA	2704	C	N3-C4-C5	5.50	124.10	121.90
51	B8	39	ARG	NE-CZ-NH2	5.50	123.05	120.30
57	BA	984	A	O4'-C1'-N9	5.50	112.60	108.20
58	Ba	1	U	O4'-C1'-N1	5.50	112.60	108.20
22	AA	665	A	C6-C5-N7	5.50	136.15	132.30
22	AA	793	U	C4'-C3'-C2'	-5.50	97.10	102.60
57	BA	782	A	C4-C5-C6	-5.50	114.25	117.00
57	BA	2036	C	N1-C2-O2	5.50	122.20	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2141	G	N1-C6-O6	-5.50	116.60	119.90
12	AT	9	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
57	BA	2622	U	O4'-C1'-N1	5.50	112.60	108.20
22	AA	914	A	C4-C5-C6	-5.50	114.25	117.00
57	BA	2532	G	N3-C2-N2	-5.50	116.05	119.90
22	AA	1203	C	N1-C2-O2	5.50	122.20	118.90
57	BA	516	C	N1-C2-O2	5.50	122.20	118.90
57	BA	551	G	N1-C6-O6	-5.50	116.60	119.90
57	BA	1131	G	N1-C6-O6	-5.50	116.60	119.90
57	BA	2107	G	N1-C6-O6	-5.50	116.60	119.90
57	BA	2772	C	N1-C2-O2	5.50	122.20	118.90
58	Ba	71	C	N1-C2-O2	5.50	122.20	118.90
22	AA	264	C	N3-C2-O2	-5.50	118.05	121.90
22	AA	639	G	N1-C6-O6	-5.50	116.60	119.90
22	AA	999	C	O4'-C1'-N1	5.50	112.60	108.20
57	BA	1101	U	O4'-C1'-N1	5.50	112.60	108.20
57	BA	1204	A	C2-N3-C4	5.50	113.35	110.60
57	BA	2339	C	N1-C2-O2	5.50	122.20	118.90
22	AA	993	G	O4'-C1'-N9	5.49	112.59	108.20
40	BY	85	ARG	NE-CZ-NH1	5.49	123.05	120.30
57	BA	314	C	N1-C2-O2	5.49	122.20	118.90
57	BA	1137	G	O4'-C1'-N9	5.49	112.59	108.20
57	BA	1363	C	O4'-C1'-N1	5.49	112.59	108.20
57	BA	1830	C	N3-C4-N4	-5.49	114.16	118.00
57	BA	2678	C	N1-C2-O2	5.49	122.20	118.90
57	BA	2789	C	O4'-C1'-N1	5.49	112.59	108.20
57	BA	620	G	N1-C6-O6	-5.49	116.61	119.90
57	BA	1941	C	N3-C4-C5	5.49	124.10	121.90
57	BA	2180	U	O4'-C1'-N1	5.49	112.59	108.20
22	AA	329	A	C4-C5-C6	-5.49	114.25	117.00
22	AA	971	G	O4'-C1'-N9	5.49	112.59	108.20
23	A2	19	A	C4-C5-C6	-5.49	114.25	117.00
23	A2	23	C	N3-C4-C5	5.49	124.10	121.90
57	BA	255	A	C4-C5-C6	-5.49	114.25	117.00
57	BA	772	C	N1-C2-O2	5.49	122.19	118.90
57	BA	2442	C	N1-C2-O2	5.49	122.19	118.90
22	AA	193	C	N1-C2-O2	5.49	122.19	118.90
22	AA	307	C	O4'-C1'-N1	5.49	112.59	108.20
22	AA	1521	C	O4'-C1'-N1	5.49	112.59	108.20
57	BA	897	C	N3-C2-O2	-5.49	118.06	121.90
57	BA	1059	G	N1-C6-O6	-5.49	116.61	119.90
57	BA	1135	C	O4'-C1'-N1	5.49	112.59	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2200	C	C2-N3-C4	-5.49	117.16	119.90
57	BA	2540	C	N1-C2-O2	5.49	122.19	118.90
22	AA	620	C	N3-C2-O2	-5.49	118.06	121.90
22	AA	1214	C	N3-C4-C5	5.49	124.09	121.90
57	BA	1257	C	N1-C2-O2	5.49	122.19	118.90
57	BA	2238	G	N3-C4-C5	-5.49	125.86	128.60
57	BA	519	U	O4'-C1'-N1	5.48	112.59	108.20
57	BA	2757	A	C5'-C4'-O4'	5.48	115.68	109.10
22	AA	622	A	C6-C5-N7	5.48	136.14	132.30
57	BA	353	C	N1-C2-O2	5.48	122.19	118.90
57	BA	699	A	O4'-C1'-N9	5.48	112.59	108.20
57	BA	1310	G	N1-C6-O6	-5.48	116.61	119.90
57	BA	2033	A	C6-C5-N7	5.48	136.14	132.30
57	BA	2760	C	N3-C2-O2	-5.48	118.06	121.90
22	AA	304	U	O4'-C1'-N1	5.48	112.58	108.20
22	AA	429	U	C3'-C2'-C1'	-5.48	97.12	101.50
22	AA	542	G	N1-C6-O6	-5.48	116.61	119.90
22	AA	856	C	N1-C2-O2	5.48	122.19	118.90
22	AA	1109	C	N1-C2-O2	5.48	122.19	118.90
57	BA	398	C	N1-C2-O2	5.48	122.19	118.90
57	BA	1668	A	C4-C5-C6	-5.48	114.26	117.00
57	BA	2103	C	N1-C2-O2	5.48	122.19	118.90
22	AA	592	G	N1-C6-O6	-5.48	116.61	119.90
57	BA	209	C	O4'-C1'-N1	5.48	112.58	108.20
57	BA	921	C	N1-C2-O2	5.48	122.19	118.90
22	AA	434	U	O4'-C1'-N1	5.48	112.58	108.20
22	AA	517	G	O4'-C1'-N9	5.48	112.58	108.20
57	BA	1725	U	O4'-C1'-N1	5.48	112.58	108.20
22	AA	1183	U	N3-C2-O2	-5.47	118.37	122.20
22	AA	1367	C	N1-C2-O2	5.47	122.19	118.90
57	BA	1015	U	O4'-C1'-N1	5.47	112.58	108.20
57	BA	2636	C	N1-C2-O2	5.47	122.19	118.90
58	Ba	89	U	O4'-C1'-N1	5.47	112.58	108.20
22	AA	743	A	C4-C5-C6	-5.47	114.26	117.00
57	BA	1258	U	N3-C2-O2	-5.47	118.37	122.20
57	BA	1531	C	N1-C2-O2	5.47	122.18	118.90
57	BA	2313	C	N3-C4-N4	-5.47	114.17	118.00
57	BA	2393	U	O4'-C1'-N1	5.47	112.58	108.20
57	BA	2629	U	N3-C2-O2	-5.47	118.37	122.20
57	BA	2825	G	N3-C4-C5	-5.47	125.86	128.60
22	AA	942	G	N1-C6-O6	-5.47	116.62	119.90
28	BN	27	ARG	NE-CZ-NH1	5.47	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	914	G	N1-C6-O6	-5.47	116.62	119.90
57	BA	1963	U	N3-C2-O2	-5.47	118.37	122.20
22	AA	586	C	N1-C2-O2	5.47	122.18	118.90
22	AA	868	C	O4'-C1'-N1	5.47	112.58	108.20
57	BA	1615	C	N3-C4-C5	5.47	124.09	121.90
57	BA	2459	A	C4-C5-C6	-5.47	114.27	117.00
22	AA	128	G	N1-C6-O6	-5.47	116.62	119.90
23	A2	24	A	C5'-C4'-C3'	-5.47	107.25	116.00
57	BA	532	A	C4-C5-C6	-5.47	114.27	117.00
57	BA	1769	U	O4'-C1'-N1	5.47	112.57	108.20
22	AA	215	C	N3-C4-N4	-5.47	114.17	118.00
22	AA	986	U	O4'-C1'-N1	5.47	112.57	108.20
22	AA	1225	A	C4-C5-C6	-5.47	114.27	117.00
57	BA	191	A	C4-C5-C6	-5.47	114.27	117.00
57	BA	877	A	C6-C5-N7	5.47	136.13	132.30
57	BA	971	G	O4'-C1'-N9	5.47	112.57	108.20
57	BA	2752	C	C2-N3-C4	-5.47	117.17	119.90
22	AA	1281	C	O4'-C1'-N1	5.46	112.57	108.20
22	AA	1388	C	N1-C2-O2	5.46	122.18	118.90
34	BT	52	ARG	NE-CZ-NH2	-5.46	117.57	120.30
36	BU	69	ARG	NE-CZ-NH2	5.46	123.03	120.30
57	BA	147	C	N1-C2-O2	5.46	122.18	118.90
57	BA	735	A	C4-C5-C6	-5.46	114.27	117.00
57	BA	809	G	N1-C6-O6	-5.46	116.62	119.90
57	BA	1667	G	O4'-C1'-N9	5.46	112.57	108.20
22	AA	512	U	O4'-C1'-N1	5.46	112.57	108.20
57	BA	1378	A	C6-C5-N7	5.46	136.12	132.30
57	BA	1512	C	N1-C2-O2	5.46	122.18	118.90
57	BA	1592	C	O4'-C1'-N1	5.46	112.57	108.20
57	BA	2430	A	N1-C6-N6	-5.46	115.32	118.60
58	Ba	48	U	O4'-C1'-N1	5.46	112.57	108.20
22	AA	1491	G	N1-C6-O6	-5.46	116.62	119.90
57	BA	1472	C	N1-C2-O2	5.46	122.18	118.90
57	BA	2096	C	O4'-C1'-N1	5.46	112.57	108.20
57	BA	1110	G	O4'-C1'-N9	5.46	112.57	108.20
22	AA	526	C	N1-C2-O2	5.46	122.18	118.90
22	AA	971	G	N1-C6-O6	-5.46	116.62	119.90
57	BA	1092	C	N1-C2-O2	5.46	122.17	118.90
57	BA	1812	U	O4'-C1'-N1	5.46	112.57	108.20
58	Ba	40	U	O4'-C1'-N1	5.46	112.57	108.20
22	AA	39	G	N3-C4-C5	-5.46	125.87	128.60
22	AA	750	C	N1-C2-O2	5.46	122.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1129	C	N1-C2-O2	5.46	122.17	118.90
57	BA	2879	A	C4-C5-C6	-5.46	114.27	117.00
15	AD	61	ARG	NE-CZ-NH1	5.46	123.03	120.30
57	BA	1909	C	N1-C2-O2	5.46	122.17	118.90
57	BA	2620	C	N1-C2-O2	5.46	122.17	118.90
23	A2	58	C	N1-C2-O2	5.45	122.17	118.90
57	BA	2238	G	N1-C6-O6	-5.45	116.63	119.90
22	AA	47	C	N3-C4-N4	-5.45	114.18	118.00
57	BA	1037	G	N1-C6-O6	-5.45	116.63	119.90
58	Ba	26	C	C5'-C4'-O4'	5.45	115.64	109.10
22	AA	1369	C	O4'-C1'-N1	5.45	112.56	108.20
57	BA	215	G	N1-C6-O6	-5.45	116.63	119.90
57	BA	937	C	N1-C2-O2	5.45	122.17	118.90
22	AA	465	A	C4-C5-C6	-5.45	114.28	117.00
22	AA	526	C	O4'-C1'-N1	5.45	112.56	108.20
22	AA	900	A	O4'-C1'-N9	5.45	112.56	108.20
57	BA	808	G	O4'-C1'-N9	5.45	112.56	108.20
57	BA	872	U	N3-C2-O2	-5.45	118.39	122.20
57	BA	2254	C	O4'-C1'-N1	5.45	112.56	108.20
22	AA	833	G	N1-C6-O6	-5.45	116.63	119.90
57	BA	1760	C	O4'-C1'-N1	5.45	112.56	108.20
22	AA	209	U	O4'-C1'-N1	5.45	112.56	108.20
57	BA	1115	G	O4'-C1'-N9	5.45	112.56	108.20
57	BA	1243	C	O4'-C1'-N1	5.45	112.56	108.20
57	BA	1547	C	O4'-C1'-N1	5.45	112.56	108.20
22	AA	1344	C	N1-C2-O2	5.44	122.17	118.90
57	BA	1117	C	N1-C2-O2	5.44	122.17	118.90
57	BA	2641	G	N1-C6-O6	-5.44	116.63	119.90
22	AA	931	C	O4'-C1'-N1	5.44	112.55	108.20
57	BA	765	C	O4'-C1'-N1	5.44	112.55	108.20
57	BA	965	C	O4'-C1'-N1	5.44	112.55	108.20
57	BA	1207	C	N1-C2-O2	5.44	122.17	118.90
57	BA	1795	C	N1-C2-O2	5.44	122.17	118.90
57	BA	2650	U	O4'-C1'-N1	5.44	112.55	108.20
22	AA	1258	G	N9-C4-C5	5.44	107.58	105.40
57	BA	2621	G	O4'-C1'-N9	5.44	112.55	108.20
22	AA	331	G	N1-C6-O6	-5.44	116.64	119.90
24	A3	53	G	N1-C6-O6	-5.44	116.64	119.90
12	AT	28	ARG	NE-CZ-NH1	5.44	123.02	120.30
22	AA	13	U	N3-C2-O2	-5.44	118.39	122.20
22	AA	522	C	N3-C4-N4	-5.44	114.19	118.00
57	BA	277	G	N1-C6-O6	-5.44	116.64	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	874	G	N1-C6-O6	-5.44	116.64	119.90
57	BA	999	U	C5-C6-N1	-5.44	119.98	122.70
57	BA	1281	G	N1-C6-O6	-5.44	116.64	119.90
58	Ba	17	C	O4'-C1'-N1	5.44	112.55	108.20
22	AA	591	U	O4'-C1'-N1	5.44	112.55	108.20
22	AA	1164	G	N1-C6-O6	-5.44	116.64	119.90
22	AA	1453	G	N3-C4-C5	-5.44	125.88	128.60
58	Ba	19	C	N1-C2-O2	5.44	122.16	118.90
57	BA	225	C	N3-C4-N4	-5.43	114.19	118.00
57	BA	1844	C	O4'-C1'-N1	5.43	112.55	108.20
57	BA	2892	G	C5'-C4'-C3'	-5.43	107.30	116.00
22	AA	1089	G	N1-C6-O6	-5.43	116.64	119.90
23	A2	28	U	O4'-C1'-N1	5.43	112.55	108.20
24	A3	5	G	O4'-C1'-N9	5.43	112.55	108.20
24	A3	52	C	O4'-C1'-N1	5.43	112.55	108.20
57	BA	29	U	N3-C2-O2	-5.43	118.40	122.20
57	BA	225	C	N1-C2-O2	5.43	122.16	118.90
57	BA	246	C	N1-C2-O2	5.43	122.16	118.90
57	BA	310	A	O4'-C1'-N9	5.43	112.55	108.20
57	BA	904	G	N1-C6-O6	-5.43	116.64	119.90
57	BA	1188	U	O4'-C1'-N1	5.43	112.55	108.20
57	BA	2710	C	O4'-C1'-N1	5.43	112.55	108.20
58	Ba	81	G	N1-C6-O6	-5.43	116.64	119.90
22	AA	507	C	N1-C2-O2	5.43	122.16	118.90
57	BA	470	A	C4-C5-C6	-5.43	114.28	117.00
57	BA	2026	U	O4'-C1'-N1	5.43	112.55	108.20
57	BA	2655	G	N3-C4-C5	-5.43	125.88	128.60
22	AA	423	G	N3-C4-C5	-5.43	125.89	128.60
22	AA	1047	G	C5-C6-N1	5.43	114.22	111.50
22	AA	1286	U	C1'-O4'-C4'	-5.43	105.56	109.90
57	BA	453	A	O4'-C1'-N9	5.43	112.54	108.20
57	BA	575	A	O4'-C1'-N9	5.43	112.54	108.20
57	BA	1537	G	N3-C4-C5	-5.43	125.89	128.60
57	BA	1684	G	N1-C6-O6	-5.43	116.64	119.90
57	BA	2807	U	O4'-C1'-N1	5.43	112.54	108.20
22	AA	1475	G	N1-C6-O6	-5.43	116.64	119.90
57	BA	1005	C	N1-C2-O2	5.43	122.16	118.90
22	AA	43	C	O4'-C1'-N1	5.43	112.54	108.20
22	AA	124	C	N1-C2-O2	5.43	122.16	118.90
22	AA	1194	U	N3-C2-O2	-5.43	118.40	122.20
22	AA	1409	C	N1-C2-O2	5.43	122.16	118.90
57	BA	573	U	C5'-C4'-C3'	-5.43	107.32	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2136	G	N1-C6-O6	-5.43	116.64	119.90
57	BA	2413	G	N1-C6-O6	-5.43	116.64	119.90
57	BA	2588	G	O4'-C1'-N9	5.43	112.54	108.20
57	BA	2796	U	N3-C2-O2	-5.43	118.40	122.20
22	AA	722	G	N1-C6-O6	-5.42	116.64	119.90
57	BA	1351	C	N1-C2-O2	5.42	122.16	118.90
57	BA	2904	U	O4'-C1'-N1	5.42	112.54	108.20
32	BR	46	ARG	NE-CZ-NH1	5.42	123.01	120.30
57	BA	441	U	N3-C2-O2	-5.42	118.40	122.20
57	BA	2450	A	C1'-O4'-C4'	-5.42	105.56	109.90
22	AA	513	C	O4'-C1'-N1	5.42	112.54	108.20
22	AA	799	G	N1-C6-O6	-5.42	116.65	119.90
24	A3	70	C	N1-C2-O2	5.42	122.15	118.90
57	BA	210	C	N3-C4-N4	-5.42	114.20	118.00
57	BA	871	U	N3-C2-O2	-5.42	118.41	122.20
57	BA	901	C	O4'-C1'-N1	5.42	112.54	108.20
58	Ba	33	G	N1-C6-O6	-5.42	116.65	119.90
57	BA	1680	U	O4'-C1'-N1	5.42	112.54	108.20
57	BA	1726	C	N1-C2-O2	5.42	122.15	118.90
57	BA	2299	U	O4'-C1'-N1	5.42	112.54	108.20
22	AA	267	C	O4'-C1'-N1	5.42	112.53	108.20
57	BA	2484	G	N1-C6-O6	-5.42	116.65	119.90
58	Ba	96	G	N1-C6-O6	-5.42	116.65	119.90
22	AA	339	C	O4'-C1'-N1	5.42	112.53	108.20
57	BA	269	C	N1-C2-O2	5.42	122.15	118.90
57	BA	737	C	N1-C2-O2	5.42	122.15	118.90
57	BA	1427	A	C6-C5-N7	5.42	136.09	132.30
22	AA	949	A	C4-C5-C6	-5.42	114.29	117.00
57	BA	1808	A	O4'-C1'-N9	5.42	112.53	108.20
57	BA	2121	G	N1-C6-O6	-5.42	116.65	119.90
57	BA	2417	C	N1-C2-O2	5.42	122.15	118.90
57	BA	2877	G	O4'-C1'-N9	5.42	112.53	108.20
58	Ba	27	C	N3-C4-C5	5.42	124.07	121.90
3	AL	13	ARG	NE-CZ-NH1	5.41	123.01	120.30
22	AA	268	U	C5-C6-N1	-5.41	119.99	122.70
22	AA	1190	G	N3-C2-N2	-5.41	116.11	119.90
57	BA	61	C	N1-C2-O2	5.41	122.15	118.90
57	BA	404	A	O4'-C1'-N9	5.41	112.53	108.20
57	BA	1399	C	N3-C4-N4	-5.41	114.21	118.00
57	BA	1689	A	C4-C5-C6	-5.41	114.29	117.00
45	BE	128	ARG	NE-CZ-NH2	5.41	123.01	120.30
57	BA	528	A	O4'-C1'-N9	5.41	112.53	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1724	G	N1-C6-O6	-5.41	116.65	119.90
22	AA	106	C	O4'-C1'-N1	5.41	112.53	108.20
22	AA	887	G	N1-C6-O6	-5.41	116.65	119.90
22	AA	1487	G	O4'-C1'-N9	5.41	112.53	108.20
37	BV	68	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
43	B1	36	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
57	BA	1357	C	N1-C2-O2	5.41	122.15	118.90
57	BA	2666	C	N3-C4-C5	5.41	124.06	121.90
22	AA	808	C	N1-C2-O2	5.41	122.14	118.90
22	AA	1524	C	N1-C2-O2	5.41	122.14	118.90
57	BA	573	U	O4'-C1'-N1	5.41	112.53	108.20
57	BA	1017	G	N1-C6-O6	-5.41	116.65	119.90
57	BA	1370	C	O4'-C1'-N1	5.41	112.53	108.20
57	BA	1533	C	O4'-C1'-N1	5.41	112.53	108.20
57	BA	1914	C	N1-C2-O2	5.41	122.14	118.90
58	Ba	11	C	N1-C2-O2	5.41	122.14	118.90
22	AA	1120	C	O4'-C1'-N1	5.41	112.53	108.20
57	BA	114	U	N3-C2-O2	-5.41	118.42	122.20
57	BA	731	C	O4'-C1'-N1	5.41	112.53	108.20
22	AA	691	G	N3-C2-N2	-5.41	116.12	119.90
22	AA	699	C	N1-C2-O2	5.41	122.14	118.90
22	AA	1523	G	N3-C2-N2	-5.41	116.12	119.90
24	A3	75	C	O4'-C1'-N1	5.41	112.52	108.20
57	BA	280	U	O4'-C1'-N1	5.41	112.53	108.20
57	BA	413	C	O4'-C1'-N1	5.41	112.52	108.20
57	BA	1146	C	N1-C2-O2	5.41	122.14	118.90
57	BA	1298	C	N1-C2-O2	5.41	122.14	118.90
57	BA	1931	U	O4'-C1'-N1	5.41	112.53	108.20
57	BA	2673	G	N1-C6-O6	-5.41	116.66	119.90
11	AB	136	ARG	NE-CZ-NH2	-5.40	117.60	120.30
11	AB	207	ARG	NE-CZ-NH1	5.40	123.00	120.30
22	AA	1388	C	O4'-C1'-N1	5.40	112.52	108.20
57	BA	15	G	O4'-C1'-N9	5.40	112.52	108.20
22	AA	472	U	O4'-C1'-N1	5.40	112.52	108.20
57	BA	510	C	N1-C2-O2	5.40	122.14	118.90
57	BA	1518	C	N1-C2-O2	5.40	122.14	118.90
58	Ba	18	G	N1-C6-O6	-5.40	116.66	119.90
58	Ba	77	U	O4'-C1'-N1	5.40	112.52	108.20
22	AA	737	C	N1-C2-O2	5.40	122.14	118.90
22	AA	1313	U	O4'-C1'-N1	5.40	112.52	108.20
24	A3	40	C	C6-N1-C2	-5.40	118.14	120.30
57	BA	116	C	N3-C4-N4	-5.40	114.22	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	273	G	N1-C6-O6	-5.40	116.66	119.90
57	BA	660	C	N1-C2-O2	5.40	122.14	118.90
57	BA	1161	C	N1-C2-O2	5.40	122.14	118.90
58	Ba	58	A	C6-C5-N7	5.40	136.08	132.30
22	AA	160	A	O4'-C1'-N9	5.40	112.52	108.20
22	AA	345	C	N3-C2-O2	-5.40	118.12	121.90
38	BW	99	ARG	NE-CZ-NH1	5.40	123.00	120.30
57	BA	902	C	N1-C2-O2	5.40	122.14	118.90
57	BA	1291	C	N1-C2-O2	5.40	122.14	118.90
22	AA	126	G	N1-C6-O6	-5.40	116.66	119.90
22	AA	1106	G	N1-C6-O6	-5.40	116.66	119.90
24	A3	69	C	N1-C2-O2	5.40	122.14	118.90
57	BA	1985	C	N1-C2-O2	5.40	122.14	118.90
57	BA	2658	C	N3-C4-C5	5.40	124.06	121.90
22	AA	1	A	C4-C5-C6	-5.39	114.30	117.00
22	AA	601	G	N1-C6-O6	-5.39	116.66	119.90
22	AA	1119	C	O4'-C1'-N1	5.39	112.52	108.20
57	BA	200	U	O4'-C1'-N1	5.39	112.52	108.20
57	BA	303	G	N1-C6-O6	-5.39	116.66	119.90
57	BA	351	C	O4'-C1'-N1	5.39	112.52	108.20
57	BA	445	C	N1-C2-O2	5.39	122.14	118.90
57	BA	1663	G	C5-C6-N1	5.39	114.20	111.50
57	BA	2774	C	N1-C2-O2	5.39	122.14	118.90
57	BA	2865	U	N3-C2-O2	-5.39	118.42	122.20
58	Ba	54	G	N1-C6-O6	-5.39	116.66	119.90
22	AA	1399	C	N1-C2-O2	5.39	122.14	118.90
31	BQ	66	ARG	NE-CZ-NH1	5.39	123.00	120.30
57	BA	823	C	N3-C4-C5	5.39	124.06	121.90
57	BA	1332	G	N3-C4-C5	-5.39	125.90	128.60
57	BA	2193	G	N1-C6-O6	-5.39	116.67	119.90
22	AA	341	C	O4'-C1'-N1	5.39	112.51	108.20
26	BJ	55	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
57	BA	840	C	N1-C2-O2	5.39	122.14	118.90
57	BA	1720	U	O4'-C1'-N1	5.39	112.51	108.20
14	AC	178	ARG	NE-CZ-NH1	5.39	122.99	120.30
22	AA	63	C	N1-C2-O2	5.39	122.13	118.90
22	AA	474	G	N1-C6-O6	-5.39	116.67	119.90
22	AA	817	C	N3-C4-C5	5.39	124.06	121.90
22	AA	930	C	N1-C2-O2	5.39	122.13	118.90
57	BA	151	C	N1-C2-O2	5.39	122.13	118.90
57	BA	433	C	O4'-C1'-N1	5.39	112.51	108.20
22	AA	139	A	C6-C5-N7	5.39	136.07	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1038	G	N1-C6-O6	-5.39	116.67	119.90
57	BA	2817	U	N3-C2-O2	-5.39	118.43	122.20
45	BE	46	ARG	NE-CZ-NH1	5.39	122.99	120.30
57	BA	289	G	N1-C6-O6	-5.39	116.67	119.90
57	BA	820	A	N1-C6-N6	-5.39	115.37	118.60
57	BA	1376	C	N1-C2-O2	5.39	122.13	118.90
57	BA	2064	C	N3-C4-N4	-5.39	114.23	118.00
22	AA	183	C	N1-C2-O2	5.38	122.13	118.90
22	AA	245	U	N1-C2-N3	5.38	118.13	114.90
22	AA	719	C	C3'-C2'-C1'	5.38	105.81	101.50
57	BA	248	G	N1-C6-O6	-5.38	116.67	119.90
57	BA	788	A	O4'-C1'-N9	5.38	112.51	108.20
57	BA	2510	C	O4'-C1'-N1	5.38	112.51	108.20
57	BA	2692	G	C4'-C3'-C2'	-5.38	97.22	102.60
22	AA	780	A	C4-C5-C6	-5.38	114.31	117.00
22	AA	1054	C	O4'-C1'-N1	5.38	112.51	108.20
57	BA	851	C	N1-C2-O2	5.38	122.13	118.90
22	AA	848	C	N1-C2-O2	5.38	122.13	118.90
22	AA	1105	A	C6-C5-N7	5.38	136.07	132.30
24	A3	57	C	O4'-C1'-N1	5.38	112.50	108.20
57	BA	370	G	N1-C6-O6	-5.38	116.67	119.90
57	BA	1300	G	O4'-C1'-N9	5.38	112.50	108.20
57	BA	2043	C	N1-C2-O2	5.38	122.13	118.90
57	BA	2458	G	N1-C6-O6	-5.38	116.67	119.90
57	BA	2606	C	N3-C4-C5	5.38	124.05	121.90
57	BA	1660	G	N1-C6-O6	-5.38	116.67	119.90
57	BA	1898	U	O4'-C1'-N1	5.38	112.50	108.20
57	BA	2812	G	N1-C6-O6	-5.38	116.67	119.90
24	A3	68	C	N1-C2-O2	5.38	122.13	118.90
57	BA	31	C	N1-C2-O2	5.38	122.13	118.90
57	BA	42	A	C6-C5-N7	5.38	136.06	132.30
57	BA	196	A	C1'-O4'-C4'	-5.38	105.60	109.90
57	BA	1335	C	N1-C2-O2	5.38	122.13	118.90
57	BA	1565	C	O4'-C1'-N1	5.38	112.50	108.20
57	BA	1601	G	N1-C6-O6	-5.38	116.67	119.90
57	BA	2515	C	N1-C2-O2	5.38	122.13	118.90
22	AA	458	U	O4'-C1'-N1	5.38	112.50	108.20
22	AA	1086	U	N3-C2-O2	-5.38	118.44	122.20
57	BA	1356	G	N1-C6-O6	-5.38	116.67	119.90
58	Ba	12	C	N1-C2-O2	5.38	122.13	118.90
22	AA	396	C	N1-C2-O2	5.38	122.12	118.90
22	AA	774	G	N1-C6-O6	-5.38	116.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	778	G	N1-C6-O6	-5.38	116.67	119.90
22	AA	896	C	N1-C2-O2	5.38	122.12	118.90
22	AA	1479	C	N1-C2-O2	5.38	122.12	118.90
24	A3	20	G	N1-C6-O6	-5.38	116.67	119.90
57	BA	209	C	N1-C2-O2	5.38	122.12	118.90
57	BA	252	G	N1-C6-O6	-5.38	116.67	119.90
57	BA	2794	C	N1-C2-O2	5.38	122.12	118.90
22	AA	70	U	N3-C2-O2	-5.37	118.44	122.20
22	AA	763	G	N7-C8-N9	5.37	115.79	113.10
22	AA	818	G	O4'-C1'-N9	5.37	112.50	108.20
22	AA	1081	A	C5'-C4'-O4'	5.37	115.55	109.10
22	AA	1264	U	O4'-C1'-N1	5.37	112.50	108.20
34	BT	20	ARG	NE-CZ-NH2	5.37	122.99	120.30
57	BA	145	C	N1-C2-O2	5.37	122.12	118.90
57	BA	1741	C	N1-C2-O2	5.37	122.12	118.90
57	BA	2057	G	N1-C6-O6	-5.37	116.68	119.90
57	BA	2347	C	O4'-C1'-N1	5.37	112.50	108.20
57	BA	2571	U	N3-C2-O2	-5.37	118.44	122.20
22	AA	487	A	C4-C5-C6	-5.37	114.31	117.00
22	AA	1412	C	N1-C2-O2	5.37	122.12	118.90
22	AA	353	A	C4-C5-C6	-5.37	114.31	117.00
22	AA	1355	G	N1-C6-O6	-5.37	116.68	119.90
57	BA	2056	G	O4'-C1'-N9	5.37	112.50	108.20
22	AA	773	G	N1-C6-O6	-5.37	116.68	119.90
57	BA	963	U	O4'-C1'-N1	5.37	112.50	108.20
22	AA	1279	G	N1-C6-O6	-5.37	116.68	119.90
6	AO	83	ARG	NE-CZ-NH1	5.37	122.98	120.30
22	AA	8	A	O4'-C1'-N9	5.37	112.49	108.20
22	AA	1064	G	O4'-C1'-N9	5.37	112.49	108.20
57	BA	284	U	O4'-C1'-N1	5.37	112.49	108.20
57	BA	596	U	O4'-C1'-N1	5.37	112.49	108.20
57	BA	796	C	N1-C2-O2	5.37	122.12	118.90
57	BA	1417	C	N1-C2-O2	5.37	122.12	118.90
57	BA	1702	G	N1-C6-O6	-5.37	116.68	119.90
57	BA	1808	A	C4-C5-C6	-5.37	114.32	117.00
57	BA	1885	A	C4-C5-C6	-5.37	114.32	117.00
57	BA	2331	G	N1-C6-O6	-5.37	116.68	119.90
57	BA	2895	G	N1-C6-O6	-5.37	116.68	119.90
22	AA	1273	C	N1-C2-O2	5.36	122.12	118.90
57	BA	1140	C	O4'-C1'-N1	5.36	112.49	108.20
57	BA	1612	C	N1-C2-O2	5.36	122.12	118.90
57	BA	2150	C	N1-C2-O2	5.36	122.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2243	U	N3-C2-O2	-5.36	118.44	122.20
57	BA	2889	C	N1-C2-O2	5.36	122.12	118.90
58	Ba	92	C	O4'-C1'-N1	5.36	112.49	108.20
22	AA	489	C	N1-C2-O2	5.36	122.12	118.90
22	AA	1490	U	O4'-C1'-N1	5.36	112.49	108.20
57	BA	524	G	N1-C6-O6	-5.36	116.68	119.90
57	BA	592	A	C6-C5-N7	5.36	136.05	132.30
57	BA	871	U	O4'-C1'-N1	5.36	112.49	108.20
57	BA	1830	C	N1-C2-O2	5.36	122.12	118.90
58	Ba	13	G	C3'-C2'-C1'	5.36	105.79	101.50
22	AA	1	A	O4'-C1'-N9	5.36	112.49	108.20
22	AA	1420	U	O4'-C1'-N1	5.36	112.49	108.20
41	BZ	19	ARG	NH1-CZ-NH2	-5.36	113.50	119.40
57	BA	1267	U	N3-C2-O2	-5.36	118.45	122.20
57	BA	1447	C	N1-C2-O2	5.36	122.12	118.90
57	BA	1798	U	O4'-C1'-N1	5.36	112.49	108.20
57	BA	1858	A	N1-C6-N6	-5.36	115.38	118.60
57	BA	2145	C	O4'-C1'-N1	5.36	112.49	108.20
57	BA	2311	A	O4'-C1'-N9	5.36	112.49	108.20
58	Ba	4	C	O4'-C1'-N1	5.36	112.49	108.20
22	AA	285	C	N1-C2-O2	5.36	122.11	118.90
22	AA	729	A	C4'-C3'-C2'	-5.36	97.24	102.60
22	AA	1223	C	N1-C2-O2	5.36	122.11	118.90
22	AA	1337	G	N1-C6-O6	-5.36	116.69	119.90
57	BA	2131	U	N3-C2-O2	-5.36	118.45	122.20
57	BA	2657	A	O4'-C1'-N9	5.36	112.49	108.20
22	AA	854	U	O4'-C1'-N1	5.36	112.49	108.20
57	BA	1598	A	C4-C5-C6	-5.36	114.32	117.00
57	BA	1961	C	O4'-C1'-N1	5.36	112.49	108.20
22	AA	428	G	C5-C6-N1	5.36	114.18	111.50
22	AA	732	C	O4'-C1'-N1	5.36	112.48	108.20
57	BA	455	C	N1-C2-O2	5.36	122.11	118.90
57	BA	1164	C	N1-C2-O2	5.36	122.11	118.90
57	BA	1277	G	N1-C6-O6	-5.36	116.69	119.90
57	BA	1488	C	N1-C2-O2	5.36	122.11	118.90
57	BA	2081	U	O4'-C1'-N1	5.36	112.48	108.20
57	BA	2538	C	N3-C2-O2	-5.36	118.15	121.90
22	AA	564	C	N3-C4-C5	5.35	124.04	121.90
57	BA	2780	G	O4'-C1'-N9	5.35	112.48	108.20
57	BA	268	C	N3-C4-N4	-5.35	114.25	118.00
57	BA	1199	U	O4'-C1'-N1	5.35	112.48	108.20
57	BA	1290	C	O4'-C1'-N1	5.35	112.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2742	G	N1-C6-O6	-5.35	116.69	119.90
23	A2	19	A	C2-N3-C4	5.35	113.28	110.60
2	AK	6	ARG	NE-CZ-NH1	5.35	122.97	120.30
22	AA	693	G	C3'-C2'-C1'	5.35	105.78	101.50
57	BA	1944	U	N3-C2-O2	-5.35	118.45	122.20
22	AA	695	A	N1-C6-N6	-5.35	115.39	118.60
22	AA	726	C	O4'-C1'-N1	5.35	112.48	108.20
57	BA	561	G	P-O3'-C3'	5.35	126.12	119.70
57	BA	1044	C	N1-C2-O2	5.35	122.11	118.90
57	BA	1303	G	N3-C4-C5	-5.35	125.93	128.60
57	BA	2362	C	O4'-C1'-N1	5.35	112.48	108.20
22	AA	6	G	N1-C6-O6	-5.35	116.69	119.90
57	BA	2828	G	N1-C6-O6	-5.35	116.69	119.90
58	Ba	75	G	N1-C6-O6	-5.35	116.69	119.90
22	AA	157	U	O4'-C1'-N1	5.34	112.48	108.20
22	AA	1409	C	O4'-C1'-N1	5.34	112.48	108.20
50	B7	14	ARG	NE-CZ-NH2	5.34	122.97	120.30
57	BA	819	A	C4-C5-C6	-5.34	114.33	117.00
57	BA	922	C	N1-C2-O2	5.34	122.11	118.90
57	BA	1368	G	O4'-C1'-N9	5.34	112.47	108.20
57	BA	2303	G	N1-C6-O6	-5.34	116.69	119.90
57	BA	1662	U	N3-C2-O2	-5.34	118.46	122.20
57	BA	2232	C	N1-C2-O2	5.34	122.11	118.90
22	AA	1115	U	N1-C2-N3	5.34	118.10	114.90
22	AA	1262	C	O4'-C1'-N1	5.34	112.47	108.20
57	BA	785	G	N1-C6-O6	-5.34	116.69	119.90
57	BA	878	A	O4'-C1'-N9	5.34	112.47	108.20
57	BA	1866	A	C4-C5-C6	-5.34	114.33	117.00
57	BA	1918	A	C6-C5-N7	5.34	136.04	132.30
57	BA	2595	G	N1-C6-O6	-5.34	116.69	119.90
57	BA	2788	C	N3-C4-C5	5.34	124.04	121.90
22	AA	355	C	N1-C2-O2	5.34	122.10	118.90
22	AA	369	G	N1-C6-O6	-5.34	116.70	119.90
24	A3	66	C	O4'-C1'-N1	5.34	112.47	108.20
38	BW	95	ARG	NH1-CZ-NH2	-5.34	113.53	119.40
57	BA	366	C	N1-C2-O2	5.34	122.10	118.90
57	BA	2134	A	C4-C5-C6	-5.34	114.33	117.00
12	AT	59	ARG	NH1-CZ-NH2	-5.34	113.53	119.40
22	AA	644	U	O4'-C1'-N1	5.34	112.47	108.20
22	AA	1086	U	O4'-C1'-N1	5.34	112.47	108.20
22	AA	1154	G	N1-C6-O6	-5.34	116.70	119.90
22	AA	1539	C	N1-C2-O2	5.34	122.10	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	813	U	O4'-C1'-N1	5.34	112.47	108.20
57	BA	2077	A	C4-C5-C6	-5.34	114.33	117.00
57	BA	312	G	N3-C4-C5	-5.34	125.93	128.60
57	BA	776	G	O4'-C1'-N9	5.34	112.47	108.20
57	BA	1106	G	N1-C6-O6	-5.34	116.70	119.90
57	BA	2206	C	O4'-C1'-N1	5.34	112.47	108.20
57	BA	2554	U	N3-C2-O2	-5.34	118.47	122.20
57	BA	2629	U	C3'-C2'-C1'	5.34	105.77	101.50
6	AO	76	ARG	NE-CZ-NH1	5.33	122.97	120.30
57	BA	164	C	N3-C4-C5	5.33	124.03	121.90
57	BA	1123	C	N1-C2-O2	5.33	122.10	118.90
22	AA	142	G	N1-C6-O6	-5.33	116.70	119.90
22	AA	1028	C	N1-C2-O2	5.33	122.10	118.90
57	BA	295	G	N1-C6-O6	-5.33	116.70	119.90
57	BA	868	U	O4'-C1'-N1	5.33	112.47	108.20
57	BA	1290	C	N1-C2-O2	5.33	122.10	118.90
57	BA	2149	U	O4'-C1'-N1	5.33	112.47	108.20
14	AC	231	ARG	NH1-CZ-NH2	-5.33	113.53	119.40
22	AA	175	C	N1-C2-O2	5.33	122.10	118.90
22	AA	203	G	N3-C2-N2	-5.33	116.17	119.90
22	AA	680	C	N1-C2-O2	5.33	122.10	118.90
22	AA	1136	C	N1-C2-O2	5.33	122.10	118.90
22	AA	1260	G	N1-C6-O6	-5.33	116.70	119.90
22	AA	1488	G	N1-C6-O6	-5.33	116.70	119.90
57	BA	95	A	O4'-C1'-N9	5.33	112.47	108.20
57	BA	593	U	O4'-C1'-N1	5.33	112.47	108.20
57	BA	1399	C	N1-C2-O2	5.33	122.10	118.90
57	BA	1823	G	N1-C6-O6	-5.33	116.70	119.90
57	BA	1838	C	N3-C4-C5	5.33	124.03	121.90
57	BA	2263	C	N1-C2-O2	5.33	122.10	118.90
22	AA	269	C	N1-C2-O2	5.33	122.10	118.90
22	AA	1174	G	N1-C6-O6	-5.33	116.70	119.90
22	AA	1249	C	N3-C2-O2	-5.33	118.17	121.90
22	AA	18	C	N1-C2-O2	5.33	122.10	118.90
22	AA	488	C	O4'-C1'-N1	5.33	112.46	108.20
22	AA	884	U	N3-C2-O2	-5.33	118.47	122.20
57	BA	2084	C	N1-C2-O2	5.33	122.10	118.90
22	AA	713	G	O4'-C1'-N9	5.33	112.46	108.20
57	BA	1703	G	N1-C6-O6	-5.33	116.70	119.90
57	BA	2863	C	O4'-C1'-N1	5.33	112.46	108.20
22	AA	697	U	O4'-C1'-N1	5.33	112.46	108.20
22	AA	1009	U	O4'-C1'-N1	5.33	112.46	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	84	A	O4'-C1'-N9	5.33	112.46	108.20
57	BA	707	G	N1-C6-O6	-5.33	116.70	119.90
57	BA	1029	A	C4-C5-C6	-5.33	114.34	117.00
57	BA	1051	G	N1-C6-O6	-5.33	116.70	119.90
57	BA	1802	A	C4-C5-C6	-5.33	114.34	117.00
57	BA	2207	C	O4'-C1'-N1	5.33	112.46	108.20
57	BA	2888	C	N1-C2-O2	5.33	122.10	118.90
23	A2	57	C	N1-C2-O2	5.32	122.09	118.90
57	BA	264	C	O4'-C1'-N1	5.32	112.46	108.20
57	BA	856	G	N1-C6-O6	-5.32	116.70	119.90
57	BA	969	G	N3-C2-N2	-5.32	116.17	119.90
57	BA	1122	G	N1-C6-O6	-5.32	116.71	119.90
57	BA	1694	C	N1-C2-O2	5.32	122.09	118.90
57	BA	1704	C	N1-C2-O2	5.32	122.09	118.90
57	BA	2305	U	N3-C2-O2	-5.32	118.47	122.20
35	BD	68	ARG	NE-CZ-NH1	5.32	122.96	120.30
57	BA	451	U	C1'-O4'-C4'	-5.32	105.64	109.90
57	BA	570	G	N3-C4-C5	-5.32	125.94	128.60
57	BA	718	A	C2-N3-C4	5.32	113.26	110.60
57	BA	1988	G	O4'-C1'-N9	5.32	112.46	108.20
22	AA	534	U	O4'-C1'-N1	5.32	112.45	108.20
22	AA	711	G	N1-C6-O6	-5.32	116.71	119.90
57	BA	423	A	C6-C5-N7	5.32	136.02	132.30
22	AA	1172	C	N1-C2-O2	5.32	122.09	118.90
57	BA	1195	G	N1-C6-O6	-5.32	116.71	119.90
57	BA	1222	U	O4'-C1'-N1	5.32	112.45	108.20
57	BA	2658	C	C1'-O4'-C4'	-5.32	105.65	109.90
22	AA	625	U	O4'-C1'-N1	5.32	112.45	108.20
23	A2	29	G	N1-C6-O6	-5.32	116.71	119.90
57	BA	529	A	O4'-C1'-N9	5.32	112.45	108.20
57	BA	1194	A	O4'-C1'-N9	5.32	112.45	108.20
57	BA	1568	G	N3-C2-N2	-5.32	116.18	119.90
57	BA	433	C	N1-C2-O2	5.31	122.09	118.90
57	BA	1266	G	N1-C6-O6	-5.31	116.71	119.90
57	BA	1374	G	N1-C6-O6	-5.31	116.71	119.90
57	BA	2006	C	N1-C2-O2	5.31	122.09	118.90
57	BA	2280	G	N1-C6-O6	-5.31	116.71	119.90
57	BA	2425	A	O4'-C1'-N9	5.31	112.45	108.20
22	AA	1133	G	N1-C6-O6	-5.31	116.71	119.90
22	AA	1286	U	N3-C2-O2	-5.31	118.48	122.20
57	BA	413	C	N1-C2-O2	5.31	122.09	118.90
57	BA	1838	C	N1-C2-O2	5.31	122.09	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2502	G	C3'-C2'-C1'	5.31	105.75	101.50
57	BA	2661	G	C2'-C3'-O3'	5.31	122.20	113.70
22	AA	74	A	O4'-C1'-N9	5.31	112.45	108.20
57	BA	337	C	N1-C2-O2	5.31	122.09	118.90
57	BA	625	G	C5'-C4'-O4'	5.31	115.47	109.10
57	BA	873	C	O4'-C1'-N1	5.31	112.45	108.20
57	BA	2827	C	N1-C2-O2	5.31	122.09	118.90
22	AA	995	C	N3-C4-C5	5.31	124.02	121.90
22	AA	1421	G	N1-C6-O6	-5.31	116.72	119.90
57	BA	732	C	N3-C4-N4	-5.31	114.28	118.00
57	BA	1427	A	C3'-C2'-C1'	-5.31	97.25	101.50
57	BA	1653	G	N1-C6-O6	-5.31	116.72	119.90
57	BA	2065	C	N1-C2-O2	5.31	122.08	118.90
57	BA	2161	C	O4'-C1'-N1	5.31	112.45	108.20
57	BA	2891	U	O4'-C1'-N1	5.31	112.45	108.20
22	AA	661	G	N1-C6-O6	-5.31	116.72	119.90
22	AA	1317	C	C2-N3-C4	-5.31	117.25	119.90
57	BA	357	C	N1-C2-O2	5.31	122.08	118.90
58	Ba	38	C	N1-C2-O2	5.31	122.08	118.90
58	Ba	118	C	N1-C2-O2	5.31	122.08	118.90
2	AK	97	ARG	NE-CZ-NH1	5.30	122.95	120.30
22	AA	1449	C	O4'-C1'-N1	5.30	112.44	108.20
57	BA	23	G	N1-C6-O6	-5.30	116.72	119.90
57	BA	75	G	C1'-O4'-C4'	-5.30	105.66	109.90
57	BA	493	G	O4'-C1'-N9	5.30	112.44	108.20
57	BA	2080	A	C6-C5-N7	5.30	136.01	132.30
57	BA	2160	C	O4'-C1'-N1	5.30	112.44	108.20
57	BA	2072	C	N1-C2-O2	5.30	122.08	118.90
57	BA	2312	U	C3'-C2'-C1'	5.30	105.74	101.50
35	BD	100	ARG	NE-CZ-NH1	5.30	122.95	120.30
57	BA	395	U	N3-C2-O2	-5.30	118.49	122.20
57	BA	1587	G	N1-C6-O6	-5.30	116.72	119.90
57	BA	1629	U	N3-C2-O2	-5.30	118.49	122.20
57	BA	2452	C	O4'-C1'-N1	5.30	112.44	108.20
22	AA	534	U	N3-C2-O2	-5.30	118.49	122.20
22	AA	853	C	N1-C2-O2	5.30	122.08	118.90
22	AA	1525	G	N1-C6-O6	-5.30	116.72	119.90
57	BA	2599	G	N1-C6-O6	-5.30	116.72	119.90
57	BA	150	U	O4'-C1'-N1	5.30	112.44	108.20
57	BA	330	A	C4-C5-C6	-5.30	114.35	117.00
22	AA	575	G	N1-C6-O6	-5.30	116.72	119.90
22	AA	737	C	O4'-C1'-N1	5.30	112.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1732	C	N1-C2-O2	5.30	122.08	118.90
57	BA	2573	C	N3-C4-C5	5.30	124.02	121.90
57	BA	2845	U	O4'-C1'-N1	5.30	112.44	108.20
22	AA	972	C	N1-C2-O2	5.29	122.08	118.90
30	BP	132	ARG	NE-CZ-NH2	-5.29	117.65	120.30
57	BA	2038	G	N1-C6-O6	-5.29	116.72	119.90
57	BA	2666	C	C2-N3-C4	-5.29	117.25	119.90
57	BA	459	U	N3-C2-O2	-5.29	118.49	122.20
57	BA	462	C	O4'-C1'-N1	5.29	112.44	108.20
57	BA	1351	C	O4'-C1'-N1	5.29	112.43	108.20
57	BA	1693	U	N3-C2-O2	-5.29	118.50	122.20
57	BA	2367	G	N1-C6-O6	-5.29	116.72	119.90
22	AA	255	G	N1-C6-O6	-5.29	116.72	119.90
22	AA	832	G	O4'-C1'-N9	5.29	112.43	108.20
22	AA	936	C	N3-C4-N4	-5.29	114.30	118.00
57	BA	228	C	N1-C2-O2	5.29	122.08	118.90
57	BA	2023	C	C5'-C4'-C3'	-5.29	107.53	116.00
57	BA	2096	C	N1-C2-O2	5.29	122.08	118.90
57	BA	2145	C	N1-C2-O2	5.29	122.08	118.90
57	BA	2225	A	O4'-C1'-N9	5.29	112.43	108.20
57	BA	239	C	N3-C4-N4	-5.29	114.30	118.00
57	BA	2512	C	N1-C2-O2	5.29	122.07	118.90
22	AA	47	C	N1-C2-O2	5.29	122.07	118.90
22	AA	1115	U	O4'-C1'-N1	5.29	112.43	108.20
57	BA	1571	A	C4-C5-C6	-5.29	114.36	117.00
57	BA	1995	U	N3-C2-O2	-5.29	118.50	122.20
58	Ba	17	C	N1-C2-O2	5.29	122.07	118.90
57	BA	837	C	O4'-C1'-N1	5.29	112.43	108.20
22	AA	616	G	N1-C6-O6	-5.29	116.73	119.90
22	AA	882	C	N1-C2-O2	5.29	122.07	118.90
57	BA	20	C	N1-C2-O2	5.29	122.07	118.90
57	BA	2678	C	O4'-C1'-N1	5.29	112.43	108.20
22	AA	198	G	N1-C6-O6	-5.28	116.73	119.90
22	AA	485	U	N3-C2-O2	-5.28	118.50	122.20
22	AA	1184	G	N3-C2-N2	-5.28	116.20	119.90
22	AA	1513	A	C6-C5-N7	5.28	136.00	132.30
57	BA	917	A	C5'-C4'-C3'	-5.28	107.55	116.00
57	BA	1363	C	N1-C2-O2	5.28	122.07	118.90
57	BA	1897	G	N1-C6-O6	-5.28	116.73	119.90
57	BA	2443	C	N3-C4-C5	5.28	124.01	121.90
58	Ba	89	U	N3-C2-O2	-5.28	118.50	122.20
22	AA	20	U	O4'-C1'-N1	5.28	112.42	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	970	C	O4'-C1'-N1	5.28	112.43	108.20
13	AU	66	ARG	NE-CZ-NH1	5.28	122.94	120.30
57	BA	994	C	O4'-C1'-N1	5.28	112.42	108.20
57	BA	2652	C	N1-C2-O2	5.28	122.07	118.90
35	BD	211	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
57	BA	658	U	O4'-C1'-N1	5.28	112.42	108.20
57	BA	2601	C	N1-C2-O2	5.28	122.07	118.90
22	AA	962	C	N1-C2-O2	5.28	122.07	118.90
22	AA	1375	A	C4-C5-C6	-5.28	114.36	117.00
22	AA	1504	G	N3-C2-N2	-5.28	116.21	119.90
24	A3	77	A	C1'-O4'-C4'	-5.28	105.68	109.90
57	BA	622	G	N1-C6-O6	-5.28	116.73	119.90
57	BA	1032	A	C4-C5-C6	-5.28	114.36	117.00
57	BA	1202	G	N1-C6-O6	-5.28	116.73	119.90
57	BA	1576	U	C5-C6-N1	-5.28	120.06	122.70
57	BA	2506	U	N3-C2-O2	-5.28	118.50	122.20
22	AA	1194	U	N1-C2-N3	5.28	118.06	114.90
22	AA	1279	G	C1'-O4'-C4'	-5.28	105.68	109.90
57	BA	838	C	N3-C4-C5	5.28	124.01	121.90
57	BA	1098	A	C5'-C4'-O4'	5.28	115.43	109.10
57	BA	1423	G	N1-C6-O6	-5.28	116.73	119.90
22	AA	433	G	O4'-C1'-N9	5.27	112.42	108.20
22	AA	499	A	C1'-O4'-C4'	-5.27	105.68	109.90
57	BA	1895	C	N1-C2-O2	5.27	122.06	118.90
22	AA	866	C	N1-C2-O2	5.27	122.06	118.90
22	AA	1464	U	O4'-C1'-N1	5.27	112.42	108.20
57	BA	700	G	O4'-C1'-N9	5.27	112.42	108.20
57	BA	1043	C	N1-C2-O2	5.27	122.06	118.90
57	BA	1608	A	C4-C5-C6	-5.27	114.36	117.00
57	BA	187	G	N1-C6-O6	-5.27	116.74	119.90
57	BA	1969	A	O4'-C1'-N9	5.27	112.42	108.20
22	AA	314	C	N3-C4-C5	5.27	124.01	121.90
22	AA	315	A	C6-C5-N7	5.27	135.99	132.30
57	BA	37	C	C4'-C3'-C2'	-5.27	97.33	102.60
57	BA	1081	U	O4'-C1'-N1	5.27	112.42	108.20
57	BA	1168	G	N1-C6-O6	-5.27	116.74	119.90
57	BA	1275	A	C5'-C4'-O4'	5.27	115.42	109.10
57	BA	2209	G	N1-C6-O6	-5.27	116.74	119.90
57	BA	2279	G	O4'-C1'-N9	5.27	112.42	108.20
58	Ba	26	C	N3-C4-C5	5.27	124.01	121.90
5	AN	52	ARG	NH1-CZ-NH2	-5.27	113.61	119.40
22	AA	167	A	C6-C5-N7	5.27	135.99	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A2	15	G	N3-C4-C5	-5.27	125.97	128.60
57	BA	906	U	N1-C2-N3	5.27	118.06	114.90
57	BA	2133	G	N1-C6-O6	-5.27	116.74	119.90
57	BA	2165	C	N3-C2-O2	-5.27	118.21	121.90
57	BA	2594	C	N1-C2-O2	5.27	122.06	118.90
58	Ba	83	G	N1-C6-O6	-5.27	116.74	119.90
22	AA	518	C	N3-C4-C5	5.27	124.01	121.90
22	AA	822	U	N3-C2-O2	-5.27	118.51	122.20
53	BF	67	ARG	NE-CZ-NH1	5.27	122.93	120.30
6	AO	16	ARG	NE-CZ-NH1	5.26	122.93	120.30
22	AA	904	U	O4'-C1'-N1	5.26	112.41	108.20
22	AA	1186	G	O4'-C1'-N9	5.26	112.41	108.20
22	AA	1280	A	C6-C5-N7	5.26	135.99	132.30
57	BA	680	C	O4'-C1'-N1	5.26	112.41	108.20
57	BA	2045	C	O4'-C1'-N1	5.26	112.41	108.20
57	BA	2395	C	O4'-C1'-N1	5.26	112.41	108.20
58	Ba	97	C	O4'-C1'-N1	5.26	112.41	108.20
57	BA	973	A	C4-C5-C6	-5.26	114.37	117.00
5	AN	8	ARG	NE-CZ-NH1	5.26	122.93	120.30
22	AA	177	G	N3-C2-N2	-5.26	116.22	119.90
22	AA	597	G	O4'-C1'-N9	5.26	112.41	108.20
22	AA	846	G	N1-C6-O6	-5.26	116.74	119.90
57	BA	205	G	N1-C6-O6	-5.26	116.74	119.90
57	BA	567	U	O4'-C1'-N1	5.26	112.41	108.20
57	BA	1019	U	N3-C2-O2	-5.26	118.52	122.20
57	BA	1194	A	C6-C5-N7	5.26	135.98	132.30
57	BA	1475	G	O4'-C1'-N9	5.26	112.41	108.20
57	BA	2409	G	N1-C6-O6	-5.26	116.74	119.90
58	Ba	91	C	N1-C2-O2	5.26	122.06	118.90
22	AA	985	C	O4'-C1'-N1	5.26	112.41	108.20
22	AA	1241	G	N1-C6-O6	-5.26	116.74	119.90
57	BA	758	C	O4'-C1'-N1	5.26	112.41	108.20
57	BA	1109	C	N1-C2-O2	5.26	122.06	118.90
57	BA	2577	A	C3'-C2'-C1'	5.26	105.71	101.50
57	BA	2661	G	C5'-C4'-O4'	5.26	115.41	109.10
22	AA	227	G	N1-C6-O6	-5.26	116.75	119.90
22	AA	544	G	O4'-C1'-N9	5.26	112.41	108.20
22	AA	642	A	C4-C5-C6	-5.26	114.37	117.00
22	AA	1395	C	N1-C2-O2	5.26	122.06	118.90
32	BR	4	ARG	CD-NE-CZ	5.26	130.96	123.60
57	BA	112	U	C4'-C3'-C2'	-5.26	97.34	102.60
57	BA	2138	G	N1-C6-O6	-5.26	116.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2768	U	N3-C2-O2	-5.26	118.52	122.20
22	AA	206	C	N1-C2-O2	5.26	122.05	118.90
22	AA	385	C	O4'-C1'-N1	5.26	112.41	108.20
22	AA	444	G	O4'-C1'-N9	5.26	112.41	108.20
22	AA	1352	C	O4'-C1'-N1	5.26	112.41	108.20
57	BA	712	G	C4'-C3'-C2'	-5.26	97.34	102.60
57	BA	990	A	O4'-C1'-N9	5.26	112.41	108.20
57	BA	1104	C	N1-C2-O2	5.26	122.05	118.90
57	BA	2640	G	N1-C6-O6	-5.26	116.75	119.90
22	AA	1007	U	O4'-C1'-N1	5.25	112.40	108.20
57	BA	784	G	C5-C6-N1	5.25	114.13	111.50
57	BA	907	G	N1-C6-O6	-5.25	116.75	119.90
57	BA	1337	G	N1-C6-O6	-5.25	116.75	119.90
22	AA	34	C	N1-C2-O2	5.25	122.05	118.90
22	AA	37	U	C5-C6-N1	-5.25	120.07	122.70
22	AA	756	C	O4'-C1'-N1	5.25	112.40	108.20
22	AA	1001	C	N1-C2-O2	5.25	122.05	118.90
57	BA	536	G	N1-C6-O6	-5.25	116.75	119.90
57	BA	588	U	O4'-C1'-N1	5.25	112.40	108.20
57	BA	2855	C	O4'-C1'-N1	5.25	112.40	108.20
22	AA	94	G	C5-C6-N1	5.25	114.13	111.50
22	AA	271	C	N1-C2-O2	5.25	122.05	118.90
57	BA	79	C	N1-C2-O2	5.25	122.05	118.90
57	BA	401	A	C6-C5-N7	5.25	135.98	132.30
57	BA	1476	U	O4'-C1'-N1	5.25	112.40	108.20
57	BA	1478	G	N1-C6-O6	-5.25	116.75	119.90
57	BA	2421	G	N1-C6-O6	-5.25	116.75	119.90
58	Ba	92	C	N1-C2-O2	5.25	122.05	118.90
2	AK	121	ARG	NE-CZ-NH2	-5.25	117.67	120.30
22	AA	1457	G	N1-C6-O6	-5.25	116.75	119.90
26	BJ	60	ARG	NE-CZ-NH1	5.25	122.92	120.30
57	BA	1972	G	N1-C6-O6	-5.25	116.75	119.90
8	AQ	10	ARG	NH1-CZ-NH2	-5.25	113.63	119.40
22	AA	483	C	N3-C4-N4	-5.25	114.33	118.00
22	AA	1119	C	N1-C2-O2	5.25	122.05	118.90
22	AA	1491	G	O4'-C1'-N9	5.25	112.40	108.20
57	BA	1325	U	N3-C2-O2	-5.25	118.53	122.20
57	BA	1867	G	N1-C6-O6	-5.25	116.75	119.90
57	BA	2757	A	C4-C5-C6	-5.25	114.38	117.00
9	AR	11	ARG	NE-CZ-NH1	-5.25	117.68	120.30
22	AA	207	C	N1-C2-O2	5.25	122.05	118.90
22	AA	1063	C	N1-C2-O2	5.25	122.05	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BU	49	ARG	NE-CZ-NH1	5.25	122.92	120.30
51	B8	7	ARG	NH1-CZ-NH2	-5.25	113.63	119.40
57	BA	872	U	N1-C2-N3	5.25	118.05	114.90
57	BA	917	A	C4-C5-C6	-5.25	114.38	117.00
57	BA	2329	U	N3-C2-O2	-5.25	118.53	122.20
57	BA	2540	C	N3-C4-C5	5.25	124.00	121.90
22	AA	40	C	N1-C2-O2	5.25	122.05	118.90
22	AA	112	G	N1-C6-O6	-5.25	116.75	119.90
22	AA	197	A	C1'-O4'-C4'	-5.25	105.70	109.90
22	AA	662	U	C5-C6-N1	-5.24	120.08	122.70
22	AA	1011	C	O4'-C1'-N1	5.24	112.39	108.20
57	BA	167	A	C4-C5-C6	-5.24	114.38	117.00
57	BA	227	A	O4'-C1'-N9	5.24	112.39	108.20
57	BA	673	C	O4'-C1'-N1	5.24	112.39	108.20
57	BA	673	C	N3-C4-C5	5.24	124.00	121.90
58	Ba	37	C	O4'-C1'-N1	5.24	112.39	108.20
57	BA	54	G	O4'-C1'-N9	5.24	112.39	108.20
57	BA	1145	C	O4'-C1'-N1	5.24	112.39	108.20
57	BA	2482	A	C4-C5-C6	-5.24	114.38	117.00
22	AA	810	C	N3-C4-C5	5.24	124.00	121.90
57	BA	499	U	N3-C2-O2	-5.24	118.53	122.20
57	BA	666	A	C6-C5-N7	5.24	135.97	132.30
57	BA	1284	A	C6-C5-N7	5.24	135.97	132.30
57	BA	1790	C	N3-C4-C5	5.24	124.00	121.90
58	Ba	8	C	N1-C2-O2	5.24	122.04	118.90
22	AA	997	U	O4'-C1'-N1	5.24	112.39	108.20
57	BA	409	G	O4'-C1'-N9	5.24	112.39	108.20
57	BA	1965	C	N1-C2-O2	5.24	122.04	118.90
57	BA	2081	U	C5-C6-N1	-5.24	120.08	122.70
57	BA	2374	C	C5'-C4'-O4'	5.24	115.39	109.10
57	BA	2414	G	N1-C6-O6	-5.24	116.76	119.90
20	AI	10	ARG	NE-CZ-NH1	5.24	122.92	120.30
57	BA	1218	G	N1-C6-O6	-5.24	116.76	119.90
22	AA	293	G	N1-C6-O6	-5.24	116.76	119.90
22	AA	922	G	N1-C6-O6	-5.24	116.76	119.90
22	AA	979	C	N1-C2-O2	5.24	122.04	118.90
23	A2	51	C	N1-C2-O2	5.24	122.04	118.90
24	A3	31	G	N1-C6-O6	-5.24	116.76	119.90
57	BA	96	C	O4'-C1'-N1	5.24	112.39	108.20
57	BA	382	A	O4'-C1'-N9	5.24	112.39	108.20
57	BA	2055	C	N1-C2-O2	5.24	122.04	118.90
57	BA	514	A	C5'-C4'-O4'	5.23	115.38	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1486	U	O4'-C1'-N1	5.23	112.39	108.20
57	BA	2801	G	N1-C6-O6	-5.23	116.76	119.90
16	AE	67	ARG	NE-CZ-NH1	5.23	122.92	120.30
53	BF	102	ARG	CD-NE-CZ	5.23	130.93	123.60
57	BA	360	U	N3-C2-O2	-5.23	118.54	122.20
57	BA	524	G	O4'-C1'-N9	5.23	112.39	108.20
57	BA	1397	U	C5-C6-N1	-5.23	120.08	122.70
57	BA	1465	G	N3-C4-C5	-5.23	125.98	128.60
57	BA	1529	G	N1-C6-O6	-5.23	116.76	119.90
57	BA	1698	A	C4-C5-C6	-5.23	114.38	117.00
14	AC	163	ARG	NE-CZ-NH1	5.23	122.92	120.30
22	AA	585	G	N1-C6-O6	-5.23	116.76	119.90
22	AA	1290	G	N1-C6-O6	-5.23	116.76	119.90
22	AA	1416	G	N1-C6-O6	-5.23	116.76	119.90
23	A2	47	C	N1-C2-O2	5.23	122.04	118.90
57	BA	1329	U	C5-C6-N1	-5.23	120.08	122.70
57	BA	1858	A	C4-C5-C6	-5.23	114.39	117.00
18	AG	77	ARG	NE-CZ-NH1	5.23	122.92	120.30
22	AA	90	C	N1-C2-O2	5.23	122.04	118.90
22	AA	322	C	N1-C2-O2	5.23	122.04	118.90
22	AA	893	C	N3-C4-C5	5.23	123.99	121.90
22	AA	1460	C	N1-C2-O2	5.23	122.04	118.90
57	BA	219	A	C6-C5-N7	5.23	135.96	132.30
57	BA	570	G	C3'-C2'-C1'	5.23	105.68	101.50
57	BA	2332	C	N1-C2-O2	5.23	122.04	118.90
22	AA	70	U	O4'-C1'-N1	5.23	112.38	108.20
22	AA	936	C	N1-C2-O2	5.23	122.04	118.90
53	BF	44	ARG	NE-CZ-NH2	5.23	122.91	120.30
57	BA	645	C	N1-C2-O2	5.23	122.04	118.90
57	BA	2214	C	N3-C4-C5	5.23	123.99	121.90
12	AT	9	ARG	NE-CZ-NH2	5.23	122.91	120.30
14	AC	155	ARG	NE-CZ-NH1	5.23	122.91	120.30
57	BA	632	A	C4-C5-C6	-5.23	114.39	117.00
57	BA	2710	C	C3'-C2'-C1'	5.23	105.68	101.50
22	AA	213	G	O4'-C1'-N9	5.22	112.38	108.20
22	AA	1378	C	N1-C2-O2	5.22	122.03	118.90
57	BA	468	G	N3-C2-N2	-5.22	116.24	119.90
57	BA	2020	A	C1'-O4'-C4'	-5.22	105.72	109.90
57	BA	2228	G	N1-C6-O6	-5.22	116.77	119.90
57	BA	2502	G	O4'-C4'-C3'	5.22	110.28	106.10
57	BA	2728	U	C5-C6-N1	-5.22	120.09	122.70
22	AA	505	G	N1-C6-O6	-5.22	116.77	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	710	G	N1-C6-O6	-5.22	116.77	119.90
22	AA	1376	U	O4'-C1'-N1	5.22	112.38	108.20
22	AA	1487	G	N1-C6-O6	-5.22	116.77	119.90
57	BA	382	A	C6-C5-N7	5.22	135.96	132.30
57	BA	638	G	C5'-C4'-O4'	5.22	115.37	109.10
57	BA	281	C	N1-C2-O2	5.22	122.03	118.90
57	BA	1233	C	O4'-C1'-N1	5.22	112.38	108.20
57	BA	1778	U	O4'-C1'-N1	5.22	112.38	108.20
57	BA	2100	G	N1-C6-O6	-5.22	116.77	119.90
12	AT	73	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
13	AU	17	ARG	NE-CZ-NH1	5.22	122.91	120.30
22	AA	73	C	N3-C4-N4	-5.22	114.35	118.00
22	AA	178	C	O4'-C1'-N1	5.22	112.38	108.20
22	AA	219	U	O4'-C1'-N1	5.22	112.38	108.20
22	AA	1060	U	N3-C2-O2	-5.22	118.55	122.20
57	BA	69	C	O4'-C1'-N1	5.22	112.38	108.20
57	BA	214	G	N1-C6-O6	-5.22	116.77	119.90
57	BA	1016	G	N1-C6-O6	-5.22	116.77	119.90
57	BA	1374	G	O4'-C1'-N9	5.22	112.38	108.20
57	BA	1547	C	N1-C2-O2	5.22	122.03	118.90
57	BA	1902	C	N3-C4-N4	-5.22	114.35	118.00
57	BA	2395	C	N1-C2-O2	5.22	122.03	118.90
57	BA	2754	U	N3-C2-O2	-5.22	118.55	122.20
22	AA	456	A	C6-C5-N7	5.22	135.95	132.30
22	AA	694	A	C4-C5-C6	-5.22	114.39	117.00
22	AA	829	G	N1-C6-O6	-5.22	116.77	119.90
22	AA	934	C	N3-C4-N4	-5.22	114.35	118.00
57	BA	1441	G	N1-C6-O6	-5.22	116.77	119.90
57	BA	1804	C	O4'-C1'-N1	5.22	112.37	108.20
57	BA	2241	A	C6-C5-N7	5.22	135.95	132.30
57	BA	2558	C	O4'-C1'-N1	5.22	112.37	108.20
57	BA	2563	U	C5-C6-N1	-5.22	120.09	122.70
57	BA	2642	G	N1-C6-O6	-5.22	116.77	119.90
22	AA	235	C	N1-C2-O2	5.21	122.03	118.90
22	AA	523	A	C6-C5-N7	5.21	135.95	132.30
25	BC	134	ARG	NE-CZ-NH1	5.21	122.91	120.30
51	B8	29	ARG	NH1-CZ-NH2	-5.21	113.66	119.40
57	BA	294	A	C1'-O4'-C4'	-5.21	105.73	109.90
58	Ba	14	U	N3-C2-O2	-5.21	118.55	122.20
22	AA	1124	G	N1-C6-O6	-5.21	116.77	119.90
57	BA	962	G	C1'-O4'-C4'	-5.21	105.73	109.90
22	AA	920	U	O4'-C1'-N1	5.21	112.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	493	G	N1-C6-O6	-5.21	116.77	119.90
57	BA	1182	G	N1-C6-O6	-5.21	116.77	119.90
57	BA	2261	C	C5'-C4'-C3'	-5.21	107.66	116.00
24	A3	67	C	O4'-C1'-N1	5.21	112.37	108.20
57	BA	1116	G	O4'-C1'-N9	5.21	112.37	108.20
57	BA	1310	G	N3-C2-N2	-5.21	116.25	119.90
57	BA	1784	A	C5'-C4'-O4'	5.21	115.35	109.10
57	BA	2298	A	C4-C5-C6	-5.21	114.39	117.00
22	AA	353	A	C3'-C2'-C1'	5.21	105.67	101.50
22	AA	448	A	C6-C5-N7	5.21	135.94	132.30
22	AA	961	U	O4'-C1'-N1	5.21	112.37	108.20
57	BA	26	G	N3-C2-N2	-5.21	116.25	119.90
57	BA	1203	U	C5-C6-N1	-5.21	120.10	122.70
57	BA	1254	A	O4'-C4'-C3'	5.21	110.27	106.10
57	BA	1437	C	N1-C2-O2	5.21	122.03	118.90
57	BA	1659	G	N1-C6-O6	-5.21	116.78	119.90
57	BA	2215	C	O4'-C1'-N1	5.21	112.37	108.20
22	AA	43	C	N1-C2-O2	5.21	122.02	118.90
22	AA	645	G	N1-C6-O6	-5.21	116.78	119.90
22	AA	729	A	C4-C5-C6	-5.21	114.40	117.00
22	AA	771	G	N1-C6-O6	-5.21	116.78	119.90
22	AA	903	G	N1-C6-O6	-5.21	116.78	119.90
22	AA	989	U	C5-C6-N1	-5.21	120.10	122.70
22	AA	1027	C	N1-C2-O2	5.21	122.02	118.90
57	BA	175	G	N1-C6-O6	-5.21	116.78	119.90
57	BA	2462	C	O4'-C1'-N1	5.21	112.37	108.20
57	BA	2712	C	N3-C4-C5	5.21	123.98	121.90
58	Ba	20	G	O4'-C1'-N9	5.21	112.37	108.20
33	BS	13	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
57	BA	2311	A	C1'-O4'-C4'	-5.21	105.74	109.90
22	AA	239	U	O4'-C1'-N1	5.20	112.36	108.20
22	AA	464	U	C5'-C4'-O4'	5.20	115.34	109.10
22	AA	897	C	N3-C4-C5	5.20	123.98	121.90
28	BN	13	ARG	NE-CZ-NH2	5.20	122.90	120.30
57	BA	1997	C	N3-C4-C5	5.20	123.98	121.90
57	BA	2010	G	N1-C6-O6	-5.20	116.78	119.90
57	BA	2027	G	N1-C6-O6	-5.20	116.78	119.90
57	BA	2846	G	N1-C6-O6	-5.20	116.78	119.90
24	A3	3	C	O4'-C1'-N1	5.20	112.36	108.20
57	BA	395	U	O4'-C1'-N1	5.20	112.36	108.20
57	BA	590	A	O4'-C1'-N9	5.20	112.36	108.20
7	AP	25	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AC	135	ARG	NE-CZ-NH1	5.20	122.90	120.30
22	AA	113	G	N1-C6-O6	-5.20	116.78	119.90
22	AA	953	G	C5-C6-N1	5.20	114.10	111.50
22	AA	1221	G	N1-C6-O6	-5.20	116.78	119.90
22	AA	1321	U	N3-C2-O2	-5.20	118.56	122.20
28	BN	99	ARG	NE-CZ-NH1	5.20	122.90	120.30
57	BA	23	G	O4'-C1'-N9	5.20	112.36	108.20
57	BA	132	G	N1-C6-O6	-5.20	116.78	119.90
57	BA	257	C	N3-C4-C5	5.20	123.98	121.90
57	BA	2053	G	N1-C6-O6	-5.20	116.78	119.90
22	AA	1230	C	N1-C2-O2	5.20	122.02	118.90
23	A2	29	G	C5-C6-N1	5.20	114.10	111.50
57	BA	769	U	N3-C2-O2	-5.20	118.56	122.20
57	BA	1624	U	C5'-C4'-C3'	-5.20	107.68	116.00
57	BA	2139	U	N1-C2-N3	5.20	118.02	114.90
22	AA	1508	A	O4'-C1'-N9	5.20	112.36	108.20
57	BA	57	C	N1-C2-O2	5.20	122.02	118.90
57	BA	427	U	O4'-C1'-N1	5.20	112.36	108.20
57	BA	1716	U	N3-C2-O2	-5.20	118.56	122.20
57	BA	2225	A	C6-C5-N7	5.20	135.94	132.30
57	BA	2243	U	N1-C2-N3	5.20	118.02	114.90
57	BA	2465	C	N1-C2-O2	5.20	122.02	118.90
57	BA	2848	G	O4'-C1'-N9	5.20	112.36	108.20
22	AA	633	G	O4'-C1'-N9	5.20	112.36	108.20
22	AA	925	G	N1-C6-O6	-5.20	116.78	119.90
22	AA	1273	C	N3-C4-C5	5.20	123.98	121.90
36	BU	27	ARG	NE-CZ-NH1	5.20	122.90	120.30
53	BF	49	ARG	NH1-CZ-NH2	-5.20	113.69	119.40
57	BA	460	A	C4-C5-C6	-5.20	114.40	117.00
57	BA	2615	U	N3-C2-O2	-5.20	118.56	122.20
22	AA	73	C	N1-C2-O2	5.19	122.02	118.90
57	BA	1663	G	N1-C6-O6	-5.19	116.78	119.90
57	BA	1863	G	N1-C6-O6	-5.19	116.78	119.90
58	Ba	65	U	O4'-C1'-N1	5.19	112.36	108.20
21	A1	42	ARG	NE-CZ-NH1	5.19	122.90	120.30
22	AA	392	C	N1-C2-O2	5.19	122.02	118.90
24	A3	17	C	N1-C2-O2	5.19	122.02	118.90
57	BA	51	G	O4'-C1'-N9	5.19	112.35	108.20
57	BA	123	G	N1-C6-O6	-5.19	116.78	119.90
57	BA	2011	U	O4'-C1'-N1	5.19	112.35	108.20
57	BA	2171	A	C6-C5-N7	5.19	135.93	132.30
57	BA	2499	C	N1-C2-O2	5.19	122.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1220	G	C4'-C3'-C2'	-5.19	97.41	102.60
57	BA	151	C	O4'-C1'-N1	5.19	112.35	108.20
57	BA	1068	G	N1-C6-O6	-5.19	116.79	119.90
57	BA	1393	A	C5'-C4'-O4'	5.19	115.33	109.10
57	BA	2703	C	N1-C2-O2	5.19	122.02	118.90
57	BA	2802	G	N1-C6-O6	-5.19	116.79	119.90
22	AA	378	G	N1-C6-O6	-5.19	116.79	119.90
22	AA	712	A	C6-C5-N7	5.19	135.93	132.30
1	AJ	89	ARG	NE-CZ-NH1	5.19	122.89	120.30
22	AA	497	G	P-O3'-C3'	5.19	125.92	119.70
22	AA	716	A	C6-C5-N7	5.19	135.93	132.30
22	AA	879	C	N3-C4-C5	5.19	123.97	121.90
22	AA	1138	G	C8-N9-C4	-5.19	104.33	106.40
22	AA	1317	C	N1-C2-O2	5.19	122.01	118.90
38	BW	11	ARG	NE-CZ-NH2	5.19	122.89	120.30
57	BA	814	C	O4'-C1'-N1	5.19	112.35	108.20
57	BA	1458	U	O4'-C1'-N1	5.19	112.35	108.20
57	BA	1770	G	N1-C6-O6	-5.19	116.79	119.90
57	BA	1837	C	N1-C2-O2	5.19	122.01	118.90
57	BA	2349	G	C5-C6-N1	5.19	114.09	111.50
22	AA	40	C	O4'-C1'-N1	5.19	112.35	108.20
22	AA	740	U	O4'-C1'-N1	5.19	112.35	108.20
24	A3	13	C	N1-C2-O2	5.19	122.01	118.90
24	A3	15	G	N3-C2-N2	-5.19	116.27	119.90
57	BA	446	G	O4'-C1'-N9	5.19	112.35	108.20
57	BA	1133	A	O4'-C1'-N9	5.19	112.35	108.20
57	BA	1293	C	O4'-C1'-N1	5.19	112.35	108.20
57	BA	2290	G	N3-C4-C5	-5.19	126.01	128.60
22	AA	67	C	N1-C2-O2	5.18	122.01	118.90
22	AA	627	G	N1-C6-O6	-5.18	116.79	119.90
22	AA	1333	A	C4-C5-C6	-5.18	114.41	117.00
57	BA	423	A	C5-C6-N6	5.18	127.85	123.70
57	BA	436	C	O4'-C1'-N1	5.18	112.35	108.20
57	BA	956	G	N1-C6-O6	-5.18	116.79	119.90
57	BA	1493	C	N1-C2-O2	5.18	122.01	118.90
57	BA	1556	C	N1-C2-O2	5.18	122.01	118.90
57	BA	2384	U	O4'-C1'-N1	5.18	112.35	108.20
57	BA	2585	U	N3-C2-O2	-5.18	118.57	122.20
57	BA	2600	A	C6-C5-N7	5.18	135.93	132.30
57	BA	2663	G	C5'-C4'-O4'	5.18	115.32	109.10
57	BA	2669	G	N1-C6-O6	-5.18	116.79	119.90
57	BA	2674	G	N1-C6-O6	-5.18	116.79	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	191	G	O4'-C1'-N9	5.18	112.35	108.20
57	BA	2277	G	C5'-C4'-O4'	5.18	115.32	109.10
22	AA	629	A	O4'-C1'-N9	5.18	112.34	108.20
22	AA	939	G	N1-C6-O6	-5.18	116.79	119.90
57	BA	1726	C	O4'-C1'-N1	5.18	112.34	108.20
57	BA	2576	G	N9-C1'-C2'	-5.18	106.30	112.00
57	BA	2811	G	N1-C6-O6	-5.18	116.79	119.90
22	AA	92	U	O4'-C1'-N1	5.18	112.34	108.20
22	AA	563	A	C1'-O4'-C4'	-5.18	105.76	109.90
57	BA	426	C	O4'-C1'-N1	5.18	112.34	108.20
57	BA	1003	G	N1-C6-O6	-5.18	116.79	119.90
57	BA	1166	G	C8-N9-C4	-5.18	104.33	106.40
57	BA	1843	C	O4'-C1'-N1	5.18	112.34	108.20
57	BA	2880	C	N1-C2-O2	5.18	122.01	118.90
58	Ba	76	G	O4'-C1'-N9	5.18	112.34	108.20
22	AA	305	G	O4'-C4'-C3'	5.18	110.24	106.10
57	BA	485	C	N1-C2-O2	5.18	122.01	118.90
22	AA	5	U	N1-C2-N3	5.18	118.01	114.90
22	AA	974	A	C6-C5-N7	5.18	135.92	132.30
22	AA	987	G	N1-C6-O6	-5.18	116.79	119.90
57	BA	302	C	N1-C2-O2	5.18	122.01	118.90
57	BA	898	C	N1-C2-O2	5.18	122.01	118.90
57	BA	2140	G	N1-C6-O6	-5.18	116.79	119.90
57	BA	2474	U	O4'-C1'-N1	5.18	112.34	108.20
22	AA	958	A	C6-C5-N7	5.17	135.92	132.30
57	BA	274	C	N1-C2-O2	5.17	122.00	118.90
57	BA	560	C	O4'-C1'-N1	5.17	112.34	108.20
57	BA	579	G	N3-C4-C5	-5.17	126.01	128.60
57	BA	582	A	O4'-C1'-N9	5.17	112.34	108.20
57	BA	1203	U	N3-C2-O2	-5.17	118.58	122.20
57	BA	1259	G	N1-C6-O6	-5.17	116.80	119.90
57	BA	2693	G	N1-C6-O6	-5.17	116.80	119.90
13	AU	20	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
22	AA	417	G	N1-C6-O6	-5.17	116.80	119.90
22	AA	830	G	N1-C6-O6	-5.17	116.80	119.90
22	AA	1351	U	O4'-C1'-N1	5.17	112.34	108.20
57	BA	1369	G	N1-C6-O6	-5.17	116.80	119.90
57	BA	2078	C	N3-C4-C5	5.17	123.97	121.90
57	BA	2582	G	N3-C4-C5	-5.17	126.02	128.60
57	BA	2782	G	N1-C6-O6	-5.17	116.80	119.90
22	AA	398	U	C5'-C4'-O4'	5.17	115.30	109.10
22	AA	722	G	N3-C4-C5	-5.17	126.02	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1131	G	N1-C6-O6	-5.17	116.80	119.90
57	BA	33	C	N3-C4-C5	5.17	123.97	121.90
57	BA	154	U	O4'-C1'-N1	5.17	112.33	108.20
57	BA	179	C	N1-C2-O2	5.17	122.00	118.90
57	BA	963	U	N1-C2-N3	5.17	118.00	114.90
57	BA	971	G	N1-C6-O6	-5.17	116.80	119.90
57	BA	1606	C	C4'-C3'-C2'	-5.17	97.43	102.60
57	BA	1879	C	O4'-C1'-N1	5.17	112.33	108.20
58	Ba	25	U	N3-C2-O2	-5.17	118.58	122.20
16	AE	68	ARG	NE-CZ-NH1	5.17	122.88	120.30
22	AA	469	C	N3-C4-C5	5.17	123.97	121.90
22	AA	1128	C	N1-C2-O2	5.17	122.00	118.90
22	AA	1380	U	N3-C2-O2	-5.17	118.58	122.20
23	A2	26	U	N3-C2-O2	-5.17	118.58	122.20
57	BA	334	C	O4'-C1'-N1	5.17	112.33	108.20
57	BA	728	G	N1-C6-O6	-5.17	116.80	119.90
57	BA	1145	C	N1-C2-O2	5.17	122.00	118.90
57	BA	1305	C	N1-C2-O2	5.17	122.00	118.90
57	BA	1448	G	O4'-C1'-N9	5.17	112.33	108.20
57	BA	1649	G	N1-C6-O6	-5.17	116.80	119.90
57	BA	1894	C	O4'-C1'-N1	5.17	112.33	108.20
22	AA	289	G	N3-C4-C5	-5.17	126.02	128.60
22	AA	748	G	N1-C6-O6	-5.17	116.80	119.90
57	BA	2486	C	N1-C2-O2	5.17	122.00	118.90
57	BA	2881	U	O4'-C1'-N1	5.17	112.33	108.20
22	AA	16	A	C6-C5-N7	5.16	135.91	132.30
22	AA	511	C	N1-C2-O2	5.16	122.00	118.90
57	BA	1007	C	N3-C4-C5	5.16	123.97	121.90
57	BA	1401	G	N1-C6-O6	-5.16	116.80	119.90
57	BA	1494	A	C6-C5-N7	5.16	135.91	132.30
57	BA	1993	U	N1-C2-N3	5.16	118.00	114.90
22	AA	152	A	C6-C5-N7	5.16	135.91	132.30
57	BA	854	C	O4'-C1'-N1	5.16	112.33	108.20
57	BA	894	U	C5-C6-N1	-5.16	120.12	122.70
57	BA	1753	G	N3-C2-N2	-5.16	116.29	119.90
7	AP	56	ARG	NE-CZ-NH1	5.16	122.88	120.30
22	AA	384	G	N1-C6-O6	-5.16	116.80	119.90
22	AA	464	U	O4'-C1'-N1	5.16	112.33	108.20
24	A3	17	C	O4'-C1'-N1	5.16	112.33	108.20
57	BA	407	G	N1-C6-O6	-5.16	116.80	119.90
57	BA	1484	U	O4'-C1'-N1	5.16	112.33	108.20
57	BA	2102	G	O4'-C1'-N9	5.16	112.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2420	C	O4'-C1'-N1	5.16	112.33	108.20
57	BA	2620	C	O4'-C1'-N1	5.16	112.33	108.20
22	AA	459	A	C6-C5-N7	5.16	135.91	132.30
22	AA	792	A	O4'-C1'-N9	5.16	112.33	108.20
22	AA	1293	C	N1-C2-O2	5.16	122.00	118.90
22	AA	1511	G	C5-C6-N1	5.16	114.08	111.50
57	BA	1192	G	O4'-C1'-N9	5.16	112.33	108.20
57	BA	1896	G	N1-C6-O6	-5.16	116.81	119.90
22	AA	12	U	O4'-C1'-N1	5.16	112.33	108.20
22	AA	483	C	C3'-C2'-C1'	5.16	105.62	101.50
22	AA	1244	G	N1-C6-O6	-5.16	116.81	119.90
35	BD	188	ARG	NE-CZ-NH1	5.16	122.88	120.30
57	BA	966	G	N1-C6-O6	-5.16	116.81	119.90
57	BA	2488	G	N1-C6-O6	-5.16	116.81	119.90
22	AA	134	G	N1-C6-O6	-5.16	116.81	119.90
22	AA	427	U	O4'-C1'-N1	5.16	112.32	108.20
57	BA	1063	G	N1-C6-O6	-5.16	116.81	119.90
22	AA	664	G	N3-C4-C5	-5.15	126.02	128.60
57	BA	629	G	N1-C6-O6	-5.15	116.81	119.90
57	BA	738	G	O4'-C1'-N9	5.15	112.32	108.20
57	BA	2902	C	O4'-C1'-N1	5.15	112.32	108.20
58	Ba	30	C	N1-C2-O2	5.15	121.99	118.90
7	AP	14	ARG	NE-CZ-NH2	5.15	122.88	120.30
22	AA	637	C	O4'-C1'-N1	5.15	112.32	108.20
22	AA	717	U	N3-C2-O2	-5.15	118.59	122.20
22	AA	787	A	O4'-C1'-N9	5.15	112.32	108.20
57	BA	449	A	C4-C5-C6	-5.15	114.42	117.00
57	BA	456	C	N1-C2-O2	5.15	121.99	118.90
57	BA	702	U	N3-C2-O2	-5.15	118.59	122.20
57	BA	2467	C	O4'-C1'-N1	5.15	112.32	108.20
57	BA	2475	C	N1-C2-O2	5.15	121.99	118.90
57	BA	2836	U	C5-C6-N1	-5.15	120.12	122.70
22	AA	1055	A	O4'-C1'-N9	5.15	112.32	108.20
22	AA	1291	U	O4'-C1'-N1	5.15	112.32	108.20
22	AA	1524	C	C2-N3-C4	-5.15	117.33	119.90
23	A2	46	C	N1-C2-O2	5.15	121.99	118.90
57	BA	236	C	O4'-C1'-N1	5.15	112.32	108.20
57	BA	923	G	N1-C6-O6	-5.15	116.81	119.90
57	BA	1202	G	O4'-C1'-N9	5.15	112.32	108.20
57	BA	2585	U	O4'-C1'-N1	5.15	112.32	108.20
57	BA	2762	C	N1-C2-O2	5.15	121.99	118.90
58	Ba	23	G	N1-C6-O6	-5.15	116.81	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	44	A	O4'-C1'-N9	5.15	112.32	108.20
57	BA	383	C	N3-C4-N4	-5.15	114.39	118.00
4	AM	91	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
22	AA	314	C	N1-C2-O2	5.15	121.99	118.90
22	AA	1439	G	N1-C6-O6	-5.15	116.81	119.90
57	BA	108	G	O4'-C1'-N9	5.15	112.32	108.20
57	BA	254	G	C5'-C4'-O4'	5.15	115.28	109.10
57	BA	356	G	N1-C6-O6	-5.15	116.81	119.90
57	BA	674	G	N1-C6-O6	-5.15	116.81	119.90
57	BA	841	G	N1-C6-O6	-5.15	116.81	119.90
57	BA	853	C	N1-C2-O2	5.15	121.99	118.90
57	BA	1153	C	N3-C4-C5	5.15	123.96	121.90
57	BA	1853	A	C6-C5-N7	5.15	135.90	132.30
57	BA	77	G	N1-C6-O6	-5.15	116.81	119.90
57	BA	744	U	N3-C2-O2	-5.15	118.60	122.20
57	BA	1100	C	N1-C2-O2	5.15	121.99	118.90
57	BA	2677	G	N1-C6-O6	-5.15	116.81	119.90
57	BA	2822	G	N1-C6-O6	-5.15	116.81	119.90
22	AA	48	C	N1-C2-O2	5.14	121.99	118.90
22	AA	243	A	C1'-O4'-C4'	-5.14	105.78	109.90
22	AA	799	G	O4'-C1'-N9	5.14	112.32	108.20
57	BA	188	G	O4'-C1'-N9	5.14	112.31	108.20
57	BA	600	G	N1-C6-O6	-5.14	116.81	119.90
57	BA	1198	U	N3-C2-O2	-5.14	118.60	122.20
57	BA	1361	G	N1-C6-O6	-5.14	116.81	119.90
57	BA	2755	C	N1-C2-O2	5.14	121.99	118.90
22	AA	274	A	C6-C5-N7	5.14	135.90	132.30
57	BA	1206	G	N1-C6-O6	-5.14	116.81	119.90
57	BA	1335	C	O4'-C1'-N1	5.14	112.31	108.20
57	BA	1782	U	O4'-C1'-N1	5.14	112.31	108.20
57	BA	2176	A	C6-C5-N7	5.14	135.90	132.30
57	BA	2431	U	O4'-C1'-N1	5.14	112.31	108.20
22	AA	921	U	O4'-C1'-N1	5.14	112.31	108.20
24	A3	29	C	O4'-C1'-N1	5.14	112.31	108.20
57	BA	1847	A	C2-N3-C4	5.14	113.17	110.60
57	BA	2858	C	N3-C4-C5	5.14	123.96	121.90
58	Ba	82	U	O4'-C1'-N1	5.14	112.31	108.20
6	AO	79	ARG	NE-CZ-NH1	5.14	122.87	120.30
22	AA	269	C	O4'-C1'-N1	5.14	112.31	108.20
57	BA	81	G	N1-C6-O6	-5.14	116.82	119.90
57	BA	901	C	N3-C4-C5	5.14	123.95	121.90
57	BA	1309	G	N1-C6-O6	-5.14	116.82	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1352	U	N1-C2-N3	5.14	117.98	114.90
57	BA	1597	A	O4'-C1'-N9	5.14	112.31	108.20
58	Ba	73	A	C4-C5-C6	-5.14	114.43	117.00
22	AA	811	C	N3-C4-C5	5.14	123.95	121.90
22	AA	1245	C	N1-C2-O2	5.14	121.98	118.90
45	BE	124	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
45	BE	184	ARG	NE-CZ-NH2	5.14	122.87	120.30
57	BA	1314	C	C5'-C4'-O4'	5.14	115.26	109.10
57	BA	1349	C	O4'-C1'-N1	5.14	112.31	108.20
57	BA	2517	C	C1'-O4'-C4'	-5.14	105.79	109.90
57	BA	2853	C	N1-C2-O2	5.14	121.98	118.90
22	AA	37	U	O4'-C1'-N1	5.13	112.31	108.20
22	AA	286	C	O4'-C1'-N1	5.13	112.31	108.20
22	AA	1278	G	N1-C6-O6	-5.13	116.82	119.90
22	AA	1293	C	O4'-C1'-N1	5.13	112.31	108.20
22	AA	1370	G	N1-C6-O6	-5.13	116.82	119.90
57	BA	208	C	N1-C2-O2	5.13	121.98	118.90
57	BA	337	C	O4'-C1'-N1	5.13	112.31	108.20
57	BA	374	A	C4-C5-C6	-5.13	114.43	117.00
57	BA	1146	C	O4'-C1'-N1	5.13	112.31	108.20
57	BA	1957	C	N1-C2-O2	5.13	121.98	118.90
57	BA	905	A	C6-C5-N7	5.13	135.89	132.30
9	AR	11	ARG	NE-CZ-NH2	5.13	122.87	120.30
16	AE	137	ARG	NE-CZ-NH1	5.13	122.87	120.30
22	AA	155	A	C6-C5-N7	5.13	135.89	132.30
22	AA	266	G	N3-C4-C5	-5.13	126.03	128.60
48	B5	9	ARG	NH1-CZ-NH2	-5.13	113.76	119.40
57	BA	236	C	N1-C2-O2	5.13	121.98	118.90
57	BA	2342	C	C6-N1-C2	-5.13	118.25	120.30
57	BA	2049	G	N1-C6-O6	-5.13	116.82	119.90
20	AI	17	ARG	NH1-CZ-NH2	-5.13	113.76	119.40
22	AA	834	U	O4'-C1'-N1	5.13	112.30	108.20
22	AA	846	G	O4'-C1'-N9	5.13	112.30	108.20
57	BA	381	G	N1-C6-O6	-5.13	116.82	119.90
57	BA	641	U	N3-C2-O2	-5.13	118.61	122.20
57	BA	2526	G	N1-C6-O6	-5.13	116.82	119.90
57	BA	2711	A	C6-C5-N7	5.13	135.89	132.30
22	AA	488	C	N1-C2-O2	5.13	121.98	118.90
22	AA	678	U	O4'-C1'-N1	5.13	112.30	108.20
22	AA	816	A	C5'-C4'-O4'	5.13	115.25	109.10
22	AA	991	U	N3-C2-O2	-5.13	118.61	122.20
22	AA	1279	G	C5-C6-N1	5.13	114.06	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	B2	47	ARG	NE-CZ-NH2	5.13	122.86	120.30
57	BA	208	C	O4'-C1'-N1	5.13	112.30	108.20
57	BA	378	C	N3-C4-C5	5.13	123.95	121.90
57	BA	475	C	N1-C2-O2	5.13	121.98	118.90
57	BA	523	C	C4'-C3'-C2'	-5.13	97.47	102.60
57	BA	546	U	O4'-C1'-N1	5.13	112.30	108.20
57	BA	843	G	N1-C6-O6	-5.13	116.82	119.90
57	BA	1028	A	O4'-C1'-N9	5.13	112.30	108.20
57	BA	1865	U	O4'-C1'-N1	5.13	112.30	108.20
38	BW	92	ARG	NE-CZ-NH1	5.12	122.86	120.30
57	BA	313	G	N1-C6-O6	-5.12	116.83	119.90
22	AA	371	A	C5'-C4'-O4'	5.12	115.25	109.10
22	AA	671	G	O4'-C1'-N9	5.12	112.30	108.20
57	BA	1312	U	C5-C6-N1	-5.12	120.14	122.70
57	BA	1410	G	N1-C6-O6	-5.12	116.83	119.90
57	BA	1800	C	N3-C4-C5	5.12	123.95	121.90
57	BA	1904	G	N1-C6-O6	-5.12	116.83	119.90
22	AA	647	C	N1-C2-O2	5.12	121.97	118.90
22	AA	1018	G	N1-C6-O6	-5.12	116.83	119.90
57	BA	1028	A	N1-C6-N6	-5.12	115.53	118.60
22	AA	1021	A	C6-C5-N7	5.12	135.88	132.30
57	BA	2808	G	N3-C2-N2	-5.12	116.32	119.90
14	AC	10	ARG	NE-CZ-NH1	5.12	122.86	120.30
17	AF	24	ARG	NE-CZ-NH1	5.12	122.86	120.30
22	AA	335	C	N1-C2-O2	5.12	121.97	118.90
22	AA	442	G	N1-C6-O6	-5.12	116.83	119.90
22	AA	514	C	O4'-C1'-N1	5.12	112.30	108.20
22	AA	1329	A	C6-C5-N7	5.12	135.88	132.30
23	A2	22	G	N3-C4-C5	-5.12	126.04	128.60
57	BA	1529	G	O4'-C1'-N9	5.12	112.29	108.20
57	BA	2245	U	N1-C2-N3	5.12	117.97	114.90
22	AA	724	G	C5-C6-N1	5.12	114.06	111.50
23	A2	45	G	N1-C6-O6	-5.12	116.83	119.90
22	AA	163	C	O4'-C1'-N1	5.12	112.29	108.20
22	AA	319	G	N1-C6-O6	-5.12	116.83	119.90
22	AA	1006	G	N1-C6-O6	-5.12	116.83	119.90
45	BE	124	ARG	NE-CZ-NH2	5.12	122.86	120.30
48	B5	16	ARG	NE-CZ-NH1	5.12	122.86	120.30
57	BA	698	C	N1-C2-O2	5.12	121.97	118.90
57	BA	731	C	N1-C2-O2	5.12	121.97	118.90
57	BA	1141	U	N3-C2-O2	-5.12	118.62	122.20
57	BA	2714	G	C5'-C4'-O4'	5.12	115.24	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1025	U	O4'-C1'-N1	5.11	112.29	108.20
48	B5	12	ARG	NE-CZ-NH1	5.11	122.86	120.30
57	BA	568	U	N3-C2-O2	-5.11	118.62	122.20
22	AA	245	U	O4'-C1'-N1	5.11	112.29	108.20
57	BA	882	G	N3-C4-C5	-5.11	126.04	128.60
57	BA	964	C	N3-C4-N4	-5.11	114.42	118.00
22	AA	1327	C	N1-C2-O2	5.11	121.97	118.90
22	AA	1328	C	O4'-C1'-N1	5.11	112.29	108.20
57	BA	327	G	N1-C6-O6	-5.11	116.83	119.90
57	BA	815	C	N1-C2-O2	5.11	121.97	118.90
57	BA	1379	U	N3-C2-O2	-5.11	118.62	122.20
57	BA	2649	C	N1-C2-O2	5.11	121.97	118.90
57	BA	2695	U	O4'-C1'-N1	5.11	112.29	108.20
57	BA	2897	U	O4'-C1'-N1	5.11	112.29	108.20
22	AA	144	G	N1-C6-O6	-5.11	116.83	119.90
22	AA	1346	A	C6-C5-N7	5.11	135.88	132.30
47	B4	59	ARG	NE-CZ-NH1	5.11	122.85	120.30
57	BA	1119	U	C5-C6-N1	-5.11	120.15	122.70
21	A1	87	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
22	AA	969	A	C5'-C4'-O4'	5.11	115.23	109.10
22	AA	1206	G	C5-C6-N1	5.11	114.05	111.50
22	AA	1221	G	C4'-C3'-C2'	-5.11	97.49	102.60
22	AA	1326	U	O4'-C1'-N1	5.11	112.29	108.20
57	BA	129	C	N1-C2-O2	5.11	121.96	118.90
57	BA	847	U	C3'-C2'-C1'	5.11	105.59	101.50
57	BA	1098	A	C4-C5-C6	-5.11	114.45	117.00
57	BA	1295	C	O4'-C1'-N1	5.11	112.29	108.20
57	BA	1639	C	N1-C2-O2	5.11	121.96	118.90
57	BA	2517	C	N3-C4-C5	5.11	123.94	121.90
58	Ba	49	C	N1-C2-O2	5.11	121.96	118.90
22	AA	498	A	C6-C5-N7	5.11	135.87	132.30
22	AA	782	A	O4'-C1'-N9	5.11	112.28	108.20
22	AA	895	G	O4'-C1'-N9	5.11	112.28	108.20
22	AA	1210	C	N3-C4-C5	5.11	123.94	121.90
22	AA	1248	A	C6-C5-N7	5.11	135.87	132.30
22	AA	1263	C	N1-C2-O2	5.11	121.96	118.90
22	AA	1405	G	O4'-C1'-N9	5.11	112.28	108.20
57	BA	7	G	N1-C6-O6	-5.11	116.84	119.90
57	BA	16	C	N1-C2-O2	5.11	121.96	118.90
57	BA	121	G	N3-C4-C5	-5.11	126.05	128.60
57	BA	234	U	N3-C2-O2	-5.11	118.62	122.20
57	BA	1513	U	N3-C2-O2	-5.11	118.63	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1568	G	N9-C4-C5	5.11	107.44	105.40
57	BA	1830	C	N3-C4-C5	5.11	123.94	121.90
57	BA	1887	C	N1-C2-O2	5.11	121.96	118.90
57	BA	249	C	N3-C4-C5	5.10	123.94	121.90
57	BA	448	U	N3-C2-O2	-5.10	118.63	122.20
57	BA	2312	U	O4'-C4'-C3'	5.10	110.18	106.10
57	BA	2651	C	O4'-C1'-N1	5.10	112.28	108.20
22	AA	1265	C	N1-C2-O2	5.10	121.96	118.90
57	BA	1388	G	N1-C6-O6	-5.10	116.84	119.90
57	BA	1403	A	C6-C5-N7	5.10	135.87	132.30
57	BA	1888	G	N3-C4-C5	-5.10	126.05	128.60
57	BA	2400	G	N1-C6-O6	-5.10	116.84	119.90
57	BA	2452	C	N1-C2-O2	5.10	121.96	118.90
22	AA	1098	C	N1-C2-O2	5.10	121.96	118.90
47	B4	56	ARG	NE-CZ-NH1	5.10	122.85	120.30
57	BA	389	G	N1-C6-O6	-5.10	116.84	119.90
57	BA	2294	G	N1-C6-O6	-5.10	116.84	119.90
58	Ba	21	G	O4'-C1'-N9	5.10	112.28	108.20
22	AA	105	G	N1-C6-O6	-5.10	116.84	119.90
22	AA	1090	U	N3-C2-O2	-5.10	118.63	122.20
22	AA	1535	C	N1-C2-O2	5.10	121.96	118.90
22	AA	1538	C	N1-C2-O2	5.10	121.96	118.90
57	BA	825	A	C6-C5-N7	5.10	135.87	132.30
57	BA	1107	G	O4'-C1'-N9	5.10	112.28	108.20
57	BA	1552	A	C4-C5-C6	-5.10	114.45	117.00
57	BA	2706	A	O4'-C1'-N9	5.10	112.28	108.20
58	Ba	114	C	N1-C2-O2	5.10	121.96	118.90
22	AA	211	G	N3-C4-C5	-5.10	126.05	128.60
22	AA	1118	U	N1-C2-N3	5.10	117.96	114.90
24	A3	6	G	N1-C6-O6	-5.10	116.84	119.90
57	BA	407	G	O4'-C1'-N9	5.10	112.28	108.20
57	BA	2117	A	O4'-C1'-N9	5.10	112.28	108.20
57	BA	2186	G	N1-C6-O6	-5.10	116.84	119.90
57	BA	2874	C	N1-C2-O2	5.10	121.96	118.90
58	Ba	35	C	N1-C2-O2	5.10	121.96	118.90
5	AN	60	ARG	NE-CZ-NH1	5.10	122.85	120.30
10	AS	54	ARG	NH1-CZ-NH2	-5.10	113.80	119.40
22	AA	936	C	C2-N3-C4	-5.10	117.35	119.90
57	BA	1779	U	N3-C2-O2	-5.10	118.63	122.20
57	BA	2245	U	N3-C2-O2	-5.10	118.63	122.20
57	BA	2310	C	N1-C2-O2	5.10	121.96	118.90
22	AA	370	C	N1-C2-O2	5.09	121.96	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	576	C	N1-C2-O2	5.09	121.96	118.90
22	AA	862	C	N3-C4-C5	5.09	123.94	121.90
22	AA	1385	G	N1-C6-O6	-5.09	116.84	119.90
57	BA	703	U	N3-C2-O2	-5.09	118.63	122.20
57	BA	962	G	O4'-C1'-N9	5.09	112.28	108.20
57	BA	1115	G	N1-C6-O6	-5.09	116.84	119.90
57	BA	1188	U	N3-C2-O2	-5.09	118.63	122.20
57	BA	2271	G	O4'-C1'-N9	5.09	112.28	108.20
57	BA	2581	G	N3-C4-C5	-5.09	126.05	128.60
57	BA	536	G	O4'-C1'-N9	5.09	112.27	108.20
57	BA	1075	C	O4'-C1'-N1	5.09	112.28	108.20
57	BA	1271	G	N1-C6-O6	-5.09	116.84	119.90
57	BA	2584	U	N3-C2-O2	-5.09	118.64	122.20
58	Ba	19	C	O4'-C1'-N1	5.09	112.27	108.20
58	Ba	105	G	N1-C6-O6	-5.09	116.84	119.90
4	AM	112	ARG	NE-CZ-NH2	-5.09	117.75	120.30
22	AA	325	A	C6-C5-N7	5.09	135.86	132.30
57	BA	334	C	N1-C2-O2	5.09	121.95	118.90
57	BA	1105	U	O4'-C1'-N1	5.09	112.27	108.20
57	BA	1176	U	N3-C2-O2	-5.09	118.64	122.20
57	BA	1271	G	N3-C4-C5	-5.09	126.05	128.60
57	BA	1275	A	C2-N3-C4	5.09	113.14	110.60
57	BA	1958	C	O4'-C1'-N1	5.09	112.27	108.20
57	BA	2108	A	C6-C5-N7	5.09	135.86	132.30
22	AA	13	U	N1-C2-N3	5.09	117.95	114.90
22	AA	501	C	C5'-C4'-O4'	5.09	115.21	109.10
22	AA	976	G	N1-C6-O6	-5.09	116.85	119.90
22	AA	1507	A	O4'-C1'-N9	5.09	112.27	108.20
22	AA	1522	U	N3-C2-O2	-5.09	118.64	122.20
57	BA	623	C	O4'-C1'-N1	5.09	112.27	108.20
57	BA	1023	U	C5-C6-N1	-5.09	120.16	122.70
57	BA	1920	C	O4'-C1'-N1	5.09	112.27	108.20
57	BA	2234	G	N7-C8-N9	5.09	115.64	113.10
57	BA	2308	G	N1-C6-O6	-5.09	116.85	119.90
57	BA	2323	G	N1-C6-O6	-5.09	116.85	119.90
57	BA	2349	G	N1-C6-O6	-5.09	116.85	119.90
57	BA	2637	U	N3-C2-O2	-5.09	118.64	122.20
58	Ba	46	A	C6-C5-N7	5.09	135.86	132.30
20	AI	122	ARG	NE-CZ-NH1	5.09	122.84	120.30
22	AA	378	G	C5'-C4'-O4'	5.09	115.21	109.10
57	BA	897	C	N3-C4-N4	-5.09	114.44	118.00
57	BA	1655	A	C4-C5-C6	-5.09	114.46	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2591	C	N3-C4-C5	5.09	123.94	121.90
22	AA	783	C	O4'-C1'-N1	5.09	112.27	108.20
22	AA	807	A	C6-C5-N7	5.09	135.86	132.30
22	AA	1118	U	C5'-C4'-O4'	5.09	115.20	109.10
57	BA	59	U	N3-C2-O2	-5.09	118.64	122.20
57	BA	112	U	N3-C2-O2	-5.09	118.64	122.20
57	BA	306	U	O4'-C1'-N1	5.09	112.27	108.20
57	BA	1417	C	N3-C4-N4	-5.09	114.44	118.00
57	BA	1646	C	N1-C2-O2	5.09	121.95	118.90
57	BA	1886	U	O4'-C1'-N1	5.09	112.27	108.20
57	BA	1967	C	N1-C2-O2	5.09	121.95	118.90
57	BA	2591	C	O4'-C1'-N1	5.09	112.27	108.20
22	AA	318	G	N1-C6-O6	-5.08	116.85	119.90
57	BA	1199	U	C5-C6-N1	-5.08	120.16	122.70
57	BA	2201	G	N1-C6-O6	-5.08	116.85	119.90
57	BA	2875	C	N1-C2-O2	5.08	121.95	118.90
57	BA	199	A	O3'-P-O5'	-5.08	94.34	104.00
57	BA	1157	G	N3-C4-C5	-5.08	126.06	128.60
57	BA	1729	U	N3-C2-O2	-5.08	118.64	122.20
57	BA	2509	G	N1-C6-O6	-5.08	116.85	119.90
57	BA	58	G	N1-C6-O6	-5.08	116.85	119.90
57	BA	1005	C	C5'-C4'-O4'	5.08	115.20	109.10
58	Ba	56	G	N1-C6-O6	-5.08	116.85	119.90
23	A2	52	U	N3-C2-O2	-5.08	118.64	122.20
57	BA	445	C	N3-C4-N4	-5.08	114.44	118.00
57	BA	2143	C	N1-C2-O2	5.08	121.95	118.90
22	AA	276	G	N1-C6-O6	-5.08	116.85	119.90
24	A3	3	C	N1-C2-O2	5.08	121.95	118.90
33	BS	94	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
57	BA	1107	G	N1-C6-O6	-5.08	116.85	119.90
57	BA	1344	U	N3-C2-O2	-5.08	118.64	122.20
57	BA	1581	G	N1-C6-O6	-5.08	116.85	119.90
57	BA	1582	C	N1-C2-O2	5.08	121.95	118.90
57	BA	1648	U	C5'-C4'-C3'	-5.08	107.87	116.00
57	BA	2892	G	O4'-C1'-N9	5.08	112.26	108.20
57	BA	24	G	N1-C6-O6	-5.08	116.85	119.90
57	BA	109	C	N1-C2-O2	5.08	121.95	118.90
57	BA	317	G	N1-C6-O6	-5.08	116.85	119.90
57	BA	2880	C	C5'-C4'-O4'	5.08	115.19	109.10
2	AK	126	ARG	CD-NE-CZ	5.08	130.71	123.60
22	AA	564	C	N1-C2-O2	5.08	121.94	118.90
57	BA	122	G	N1-C6-O6	-5.08	116.85	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	505	A	O4'-C1'-N9	5.08	112.26	108.20
57	BA	1532	A	C6-C5-N7	5.08	135.85	132.30
57	BA	2001	C	N3-C4-C5	5.08	123.93	121.90
57	BA	2467	C	N3-C4-C5	5.08	123.93	121.90
15	AD	80	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
22	AA	150	U	O4'-C1'-N1	5.07	112.26	108.20
22	AA	805	C	C5'-C4'-O4'	5.07	115.19	109.10
22	AA	839	C	C3'-C2'-C1'	-5.07	97.44	101.50
57	BA	192	C	N3-C2-O2	-5.07	118.35	121.90
57	BA	1244	A	C6-C5-N7	5.07	135.85	132.30
57	BA	2000	C	N1-C2-O2	5.07	121.94	118.90
57	BA	2249	U	O4'-C4'-C3'	5.07	110.16	106.10
57	BA	2266	A	C6-C5-N7	5.07	135.85	132.30
58	Ba	43	C	N1-C2-O2	5.07	121.94	118.90
22	AA	521	G	O4'-C1'-N9	5.07	112.26	108.20
57	BA	2496	C	N3-C4-C5	5.07	123.93	121.90
58	Ba	16	G	N1-C6-O6	-5.07	116.86	119.90
22	AA	25	C	N3-C4-C5	5.07	123.93	121.90
22	AA	377	G	N1-C6-O6	-5.07	116.86	119.90
22	AA	474	G	O4'-C1'-N9	5.07	112.26	108.20
22	AA	764	C	N1-C2-O2	5.07	121.94	118.90
22	AA	1343	G	N1-C6-O6	-5.07	116.86	119.90
22	AA	1494	G	N1-C6-O6	-5.07	116.86	119.90
57	BA	999	U	N1-C2-N3	5.07	117.94	114.90
57	BA	1013	C	C5'-C4'-C3'	-5.07	107.89	116.00
57	BA	1304	A	C6-C5-N7	5.07	135.85	132.30
57	BA	1370	C	N3-C4-C5	5.07	123.93	121.90
57	BA	1779	U	O4'-C1'-N1	5.07	112.26	108.20
57	BA	2725	A	C4-C5-C6	-5.07	114.46	117.00
57	BA	2728	U	N3-C2-O2	-5.07	118.65	122.20
22	AA	194	C	N3-C4-C5	5.07	123.93	121.90
57	BA	100	U	O4'-C1'-N1	5.07	112.25	108.20
10	AS	31	ARG	NE-CZ-NH1	5.07	122.83	120.30
57	BA	2394	C	N1-C2-O2	5.07	121.94	118.90
57	BA	2731	G	N1-C6-O6	-5.07	116.86	119.90
21	A1	206	ARG	NE-CZ-NH2	-5.07	117.77	120.30
22	AA	662	U	N3-C2-O2	-5.07	118.65	122.20
22	AA	980	C	N3-C4-C5	5.07	123.93	121.90
56	BL	123	ARG	NE-CZ-NH2	-5.07	117.77	120.30
57	BA	261	G	N1-C6-O6	-5.07	116.86	119.90
57	BA	940	G	O4'-C1'-N9	5.07	112.25	108.20
57	BA	1058	U	N3-C2-O2	-5.07	118.65	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1752	C	O4'-C1'-N1	5.07	112.25	108.20
57	BA	2016	U	N3-C2-O2	-5.07	118.65	122.20
57	BA	2373	G	N1-C6-O6	-5.07	116.86	119.90
24	A3	41	C	O4'-C1'-N1	5.06	112.25	108.20
57	BA	1437	C	C3'-C2'-C1'	5.06	105.55	101.50
57	BA	1592	C	N1-C2-O2	5.06	121.94	118.90
57	BA	2613	U	N3-C2-O2	-5.06	118.66	122.20
22	AA	202	G	C5-C6-N1	5.06	114.03	111.50
22	AA	731	G	C4'-C3'-C2'	-5.06	97.54	102.60
22	AA	875	U	O4'-C1'-N1	5.06	112.25	108.20
57	BA	85	G	N1-C6-O6	-5.06	116.86	119.90
57	BA	325	G	N1-C6-O6	-5.06	116.86	119.90
57	BA	669	G	N1-C6-O6	-5.06	116.86	119.90
57	BA	2199	A	C5'-C4'-O4'	5.06	115.17	109.10
57	BA	2766	A	C2-N3-C4	5.06	113.13	110.60
22	AA	96	U	C5-C6-N1	-5.06	120.17	122.70
22	AA	722	G	C5-C6-N1	5.06	114.03	111.50
22	AA	1112	C	N1-C2-O2	5.06	121.94	118.90
57	BA	190	A	C4'-C3'-C2'	-5.06	97.54	102.60
57	BA	1133	A	C6-C5-N7	5.06	135.84	132.30
22	AA	56	U	O4'-C1'-N1	5.06	112.25	108.20
22	AA	409	U	N3-C2-O2	-5.06	118.66	122.20
22	AA	443	C	O4'-C1'-N1	5.06	112.25	108.20
22	AA	1086	U	N1-C2-N3	5.06	117.94	114.90
22	AA	1319	A	C4-C5-C6	-5.06	114.47	117.00
57	BA	87	U	O4'-C1'-N1	5.06	112.25	108.20
57	BA	565	C	N1-C2-O2	5.06	121.94	118.90
57	BA	827	U	O4'-C1'-N1	5.06	112.25	108.20
22	AA	401	C	N1-C2-O2	5.06	121.93	118.90
22	AA	911	U	O4'-C1'-N1	5.06	112.25	108.20
22	AA	1051	C	N1-C2-O2	5.06	121.93	118.90
22	AA	1434	A	O4'-C1'-N9	5.06	112.25	108.20
23	A2	27	A	C4'-C3'-C2'	-5.06	97.54	102.60
49	B6	27	ARG	NE-CZ-NH1	5.06	122.83	120.30
57	BA	206	U	N3-C2-O2	-5.06	118.66	122.20
57	BA	510	C	O4'-C1'-N1	5.06	112.25	108.20
57	BA	1209	U	N3-C2-O2	-5.06	118.66	122.20
57	BA	1315	C	N1-C2-O2	5.06	121.94	118.90
57	BA	1701	A	O4'-C1'-N9	5.06	112.25	108.20
57	BA	1822	C	N1-C2-O2	5.06	121.93	118.90
57	BA	2733	A	C6-C5-N7	5.06	135.84	132.30
57	BA	2792	A	O4'-C1'-N9	5.06	112.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AM	56	ARG	NE-CZ-NH1	5.06	122.83	120.30
22	AA	394	G	N3-C2-N2	-5.06	116.36	119.90
29	BO	71	ARG	NE-CZ-NH1	5.06	122.83	120.30
57	BA	993	G	N1-C6-O6	-5.06	116.87	119.90
57	BA	2489	U	C3'-C2'-C1'	5.06	105.55	101.50
22	AA	1533	C	N1-C2-O2	5.05	121.93	118.90
35	BD	12	ARG	NE-CZ-NH2	-5.05	117.77	120.30
56	BL	51	ARG	NE-CZ-NH1	5.05	122.83	120.30
57	BA	93	G	N1-C6-O6	-5.05	116.87	119.90
57	BA	229	C	N1-C2-O2	5.05	121.93	118.90
57	BA	318	C	N1-C2-O2	5.05	121.93	118.90
57	BA	451	U	N3-C2-O2	-5.05	118.66	122.20
57	BA	601	C	O4'-C1'-N1	5.05	112.24	108.20
57	BA	1489	C	N3-C4-C5	5.05	123.92	121.90
57	BA	1697	G	N9-C1'-C2'	-5.05	106.44	112.00
57	BA	1784	A	C4-C5-C6	-5.05	114.47	117.00
8	AQ	76	ARG	NE-CZ-NH1	5.05	122.83	120.30
22	AA	107	G	C5'-C4'-O4'	5.05	115.16	109.10
22	AA	1415	G	N1-C6-O6	-5.05	116.87	119.90
57	BA	678	C	O4'-C1'-N1	5.05	112.24	108.20
57	BA	1887	C	O4'-C1'-N1	5.05	112.24	108.20
22	AA	205	A	C3'-C2'-C1'	5.05	105.54	101.50
22	AA	445	G	N1-C6-O6	-5.05	116.87	119.90
22	AA	666	G	N3-C2-N2	-5.05	116.36	119.90
22	AA	1118	U	N3-C2-O2	-5.05	118.66	122.20
22	AA	1336	C	N1-C2-O2	5.05	121.93	118.90
24	A3	69	C	O4'-C1'-N1	5.05	112.24	108.20
57	BA	559	G	C5-C6-N1	5.05	114.03	111.50
57	BA	688	U	C5-C6-N1	-5.05	120.17	122.70
57	BA	2275	C	N1-C2-O2	5.05	121.93	118.90
57	BA	2603	G	N9-C4-C5	5.05	107.42	105.40
57	BA	2696	U	N3-C2-O2	-5.05	118.66	122.20
57	BA	2874	C	C3'-C2'-C1'	5.05	105.54	101.50
58	Ba	47	C	O4'-C1'-N1	5.05	112.24	108.20
22	AA	671	G	N1-C6-O6	-5.05	116.87	119.90
22	AA	941	G	N1-C6-O6	-5.05	116.87	119.90
22	AA	1028	C	O4'-C1'-N1	5.05	112.24	108.20
22	AA	1468	A	C4-C5-C6	-5.05	114.47	117.00
57	BA	87	U	C3'-C2'-C1'	5.05	105.54	101.50
57	BA	119	A	C6-C5-N7	5.05	135.83	132.30
57	BA	719	C	O4'-C1'-N1	5.05	112.24	108.20
57	BA	1087	G	N1-C6-O6	-5.05	116.87	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2089	C	N3-C4-C5	5.05	123.92	121.90
22	AA	445	G	O4'-C1'-N9	5.05	112.24	108.20
22	AA	924	C	N1-C2-O2	5.05	121.93	118.90
22	AA	940	C	O4'-C1'-N1	5.05	112.24	108.20
22	AA	1300	G	O4'-C1'-N9	5.05	112.24	108.20
57	BA	409	G	C4'-C3'-C2'	-5.05	97.55	102.60
57	BA	1691	C	N1-C2-O2	5.05	121.93	118.90
57	BA	2667	C	N1-C2-O2	5.05	121.93	118.90
22	AA	117	G	C5-C6-N1	5.05	114.02	111.50
22	AA	248	C	N1-C2-O2	5.05	121.93	118.90
22	AA	358	U	N3-C2-O2	-5.05	118.67	122.20
22	AA	670	G	N1-C6-O6	-5.05	116.87	119.90
22	AA	731	G	N1-C6-O6	-5.05	116.87	119.90
22	AA	952	U	C5'-C4'-O4'	5.05	115.16	109.10
22	AA	1447	A	O4'-C1'-N9	5.05	112.24	108.20
22	AA	1527	U	O4'-C1'-N1	5.05	112.24	108.20
37	BV	21	ARG	NE-CZ-NH2	5.05	122.82	120.30
57	BA	301	G	C4'-C3'-C2'	-5.05	97.55	102.60
57	BA	772	C	O4'-C1'-N1	5.05	112.24	108.20
57	BA	1728	C	N1-C2-O2	5.05	121.93	118.90
57	BA	1893	C	N1-C2-O2	5.05	121.93	118.90
57	BA	2283	C	N3-C4-N4	-5.05	114.47	118.00
57	BA	2375	G	N1-C6-O6	-5.05	116.87	119.90
22	AA	186	C	N1-C2-O2	5.04	121.93	118.90
22	AA	985	C	N1-C2-O2	5.04	121.93	118.90
57	BA	1099	G	N1-C6-O6	-5.04	116.87	119.90
57	BA	1102	C	N1-C2-O2	5.04	121.93	118.90
22	AA	186	C	O4'-C1'-N1	5.04	112.23	108.20
22	AA	277	C	N1-C2-O2	5.04	121.93	118.90
22	AA	1071	C	N1-C2-O2	5.04	121.93	118.90
22	AA	1330	U	N3-C2-O2	-5.04	118.67	122.20
57	BA	147	C	O4'-C1'-N1	5.04	112.23	108.20
57	BA	611	C	O4'-C1'-N1	5.04	112.23	108.20
57	BA	1841	U	N3-C2-O2	-5.04	118.67	122.20
57	BA	1851	U	N3-C2-O2	-5.04	118.67	122.20
57	BA	2750	A	C6-C5-N7	5.04	135.83	132.30
22	AA	15	G	N1-C6-O6	-5.04	116.88	119.90
22	AA	233	C	N1-C2-O2	5.04	121.92	118.90
57	BA	243	U	O4'-C1'-N1	5.04	112.23	108.20
57	BA	287	G	N1-C6-O6	-5.04	116.88	119.90
57	BA	347	A	O4'-C1'-N9	5.04	112.23	108.20
57	BA	1589	U	O4'-C1'-N1	5.04	112.23	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1965	C	N3-C4-C5	5.04	123.92	121.90
57	BA	2439	A	C2-N3-C4	5.04	113.12	110.60
57	BA	2703	C	O4'-C1'-N1	5.04	112.23	108.20
57	BA	1531	C	O4'-C1'-N1	5.04	112.23	108.20
57	BA	2491	U	O4'-C1'-N1	5.04	112.23	108.20
57	BA	2731	G	C5'-C4'-C3'	-5.04	107.94	116.00
58	Ba	10	G	O4'-C4'-C3'	5.04	110.13	106.10
58	Ba	31	C	O4'-C1'-N1	5.04	112.23	108.20
17	AF	110	ARG	NE-CZ-NH1	5.04	122.82	120.30
22	AA	271	C	O4'-C1'-N1	5.04	112.23	108.20
57	BA	339	U	O4'-C1'-N1	5.04	112.23	108.20
57	BA	816	C	C5'-C4'-C3'	-5.04	107.94	116.00
57	BA	2480	C	N3-C4-N4	-5.04	114.47	118.00
57	BA	2736	A	C6-C5-N7	5.04	135.83	132.30
58	Ba	28	C	O4'-C1'-N1	5.04	112.23	108.20
22	AA	768	A	O4'-C1'-N9	5.04	112.23	108.20
57	BA	2270	A	C6-C5-N7	5.04	135.83	132.30
57	BA	2675	A	C6-C5-N7	5.04	135.83	132.30
22	AA	406	G	N3-C4-C5	-5.04	126.08	128.60
22	AA	460	A	C6-C5-N7	5.04	135.83	132.30
22	AA	544	G	N1-C6-O6	-5.04	116.88	119.90
22	AA	550	G	N1-C6-O6	-5.04	116.88	119.90
22	AA	1273	C	O4'-C1'-N1	5.04	112.23	108.20
57	BA	241	A	O4'-C1'-N9	5.04	112.23	108.20
57	BA	997	G	N1-C6-O6	-5.04	116.88	119.90
57	BA	1195	G	O4'-C1'-N9	5.04	112.23	108.20
57	BA	2824	C	N3-C4-C5	5.04	123.91	121.90
58	Ba	64	G	N1-C6-O6	-5.04	116.88	119.90
22	AA	224	U	O4'-C1'-N1	5.03	112.23	108.20
22	AA	1067	A	C6-C5-N7	5.03	135.82	132.30
22	AA	1102	A	C4-C5-C6	-5.03	114.48	117.00
57	BA	588	U	N3-C2-O2	-5.03	118.68	122.20
57	BA	1277	G	O4'-C1'-N9	5.03	112.23	108.20
57	BA	1971	U	O4'-C1'-N1	5.03	112.23	108.20
22	AA	1038	C	O4'-C1'-N1	5.03	112.23	108.20
22	AA	1481	U	N1-C2-N3	5.03	117.92	114.90
57	BA	66	C	N3-C4-N4	-5.03	114.48	118.00
57	BA	767	U	O4'-C1'-N1	5.03	112.22	108.20
57	BA	1566	A	C6-C5-N7	5.03	135.82	132.30
57	BA	2007	U	N3-C2-O2	-5.03	118.68	122.20
57	BA	916	G	N7-C8-N9	5.03	115.61	113.10
57	BA	926	G	N1-C6-O6	-5.03	116.88	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1578	U	N1-C2-N3	5.03	117.92	114.90
57	BA	1818	U	C5-C6-N1	-5.03	120.19	122.70
57	BA	2717	C	N3-C4-C5	5.03	123.91	121.90
22	AA	290	C	O4'-C1'-N1	5.03	112.22	108.20
57	BA	1159	U	N3-C2-O2	-5.03	118.68	122.20
57	BA	1822	C	O4'-C1'-N1	5.03	112.22	108.20
57	BA	1974	C	O4'-C1'-N1	5.03	112.22	108.20
22	AA	496	A	C5'-C4'-O4'	5.03	115.13	109.10
25	BC	122	ARG	NE-CZ-NH1	5.03	122.81	120.30
56	BL	116	ARG	NE-CZ-NH2	-5.03	117.79	120.30
57	BA	310	A	C5'-C4'-C3'	-5.03	107.95	116.00
57	BA	376	G	N1-C6-O6	-5.03	116.88	119.90
57	BA	396	G	N3-C4-C5	-5.03	126.09	128.60
57	BA	897	C	N3-C4-C5	5.03	123.91	121.90
57	BA	1774	C	N1-C2-O2	5.03	121.92	118.90
22	AA	79	G	N1-C6-O6	-5.03	116.89	119.90
22	AA	518	C	N1-C2-O2	5.03	121.92	118.90
22	AA	1211	U	N3-C2-O2	-5.03	118.68	122.20
22	AA	1312	G	N9-C4-C5	5.03	107.41	105.40
57	BA	156	A	O4'-C1'-N9	5.03	112.22	108.20
57	BA	1473	G	N1-C6-O6	-5.03	116.88	119.90
57	BA	1645	G	O4'-C1'-N9	5.03	112.22	108.20
57	BA	1650	A	C6-C5-N7	5.03	135.82	132.30
57	BA	2856	A	C6-C5-N7	5.03	135.82	132.30
58	Ba	10	G	N1-C6-O6	-5.03	116.89	119.90
22	AA	359	G	N1-C6-O6	-5.02	116.89	119.90
22	AA	811	C	O4'-C1'-N1	5.02	112.22	108.20
22	AA	836	G	N1-C6-O6	-5.02	116.89	119.90
57	BA	1243	C	N1-C2-O2	5.02	121.92	118.90
57	BA	1313	U	O4'-C1'-N1	5.02	112.22	108.20
57	BA	1607	C	N1-C2-O2	5.02	121.92	118.90
22	AA	792	A	C1'-O4'-C4'	-5.02	105.88	109.90
22	AA	1053	G	O4'-C1'-N9	5.02	112.22	108.20
22	AA	1074	G	C5'-C4'-C3'	-5.02	107.97	116.00
29	BO	78	ARG	NE-CZ-NH2	-5.02	117.79	120.30
35	BD	132	ARG	NE-CZ-NH1	5.02	122.81	120.30
57	BA	52	A	C4-C5-C6	-5.02	114.49	117.00
57	BA	631	A	C6-C5-N7	5.02	135.81	132.30
57	BA	1244	A	O4'-C1'-N9	5.02	112.22	108.20
57	BA	1251	C	N1-C2-O2	5.02	121.91	118.90
57	BA	1508	A	C1'-O4'-C4'	-5.02	105.88	109.90
57	BA	2216	G	N1-C6-O6	-5.02	116.89	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2644	G	N1-C6-O6	-5.02	116.89	119.90
22	AA	1107	C	N1-C2-O2	5.02	121.91	118.90
57	BA	1669	A	C4-C5-C6	-5.02	114.49	117.00
57	BA	2233	U	N3-C2-O2	-5.02	118.69	122.20
22	AA	56	U	N1-C2-N3	5.02	117.91	114.90
22	AA	455	G	N1-C6-O6	-5.02	116.89	119.90
22	AA	945	G	C5-C6-N1	5.02	114.01	111.50
57	BA	480	A	C5'-C4'-O4'	5.02	115.12	109.10
57	BA	888	C	N1-C2-O2	5.02	121.91	118.90
57	BA	1901	A	C6-C5-N7	5.02	135.81	132.30
57	BA	2061	G	N3-C4-C5	-5.02	126.09	128.60
57	BA	2471	A	C6-C5-N7	5.02	135.81	132.30
57	BA	2681	C	N1-C2-O2	5.02	121.91	118.90
57	BA	2880	C	C6-N1-C2	-5.02	118.29	120.30
3	AL	11	ARG	NE-CZ-NH2	-5.02	117.79	120.30
22	AA	191	G	N1-C6-O6	-5.02	116.89	119.90
22	AA	1384	C	N3-C4-C5	5.02	123.91	121.90
57	BA	294	A	C6-C5-N7	5.02	135.81	132.30
57	BA	544	C	N3-C4-C5	5.02	123.91	121.90
57	BA	1021	A	C5'-C4'-C3'	-5.02	107.97	116.00
57	BA	1435	G	N1-C6-O6	-5.02	116.89	119.90
57	BA	1824	G	N1-C6-O6	-5.02	116.89	119.90
14	AC	142	ARG	NE-CZ-NH1	5.02	122.81	120.30
22	AA	257	G	N1-C6-O6	-5.02	116.89	119.90
22	AA	414	A	C6-C5-N7	5.02	135.81	132.30
57	BA	2562	U	N3-C2-O2	-5.02	118.69	122.20
4	AM	78	ARG	NH1-CZ-NH2	-5.01	113.88	119.40
22	AA	64	G	N1-C6-O6	-5.01	116.89	119.90
22	AA	641	U	O4'-C4'-C3'	5.01	110.11	106.10
28	BN	34	ARG	NE-CZ-NH1	5.01	122.81	120.30
57	BA	855	G	O4'-C1'-N9	5.01	112.21	108.20
57	BA	1055	G	N1-C6-O6	-5.01	116.89	119.90
57	BA	1078	U	O4'-C4'-C3'	5.01	110.11	106.10
57	BA	1363	C	N3-C4-C5	5.01	123.91	121.90
57	BA	1808	A	C3'-C2'-C1'	5.01	105.51	101.50
57	BA	1826	G	N1-C6-O6	-5.01	116.89	119.90
57	BA	1836	C	N1-C2-O2	5.01	121.91	118.90
57	BA	2025	C	O4'-C1'-N1	5.01	112.21	108.20
57	BA	2087	G	N1-C6-O6	-5.01	116.89	119.90
57	BA	2188	U	N3-C2-O2	-5.01	118.69	122.20
57	BA	2792	A	C6-C5-N7	5.01	135.81	132.30
22	AA	490	C	N1-C2-O2	5.01	121.91	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	812	G	N1-C6-O6	-5.01	116.89	119.90
30	BP	59	ARG	NE-CZ-NH2	5.01	122.81	120.30
57	BA	858	G	C1'-O4'-C4'	-5.01	105.89	109.90
57	BA	1567	G	N1-C6-O6	-5.01	116.89	119.90
22	AA	309	A	N9-C1'-C2'	-5.01	106.49	112.00
22	AA	311	C	N3-C4-C5	5.01	123.90	121.90
22	AA	805	C	N1-C2-O2	5.01	121.91	118.90
22	AA	1297	G	O4'-C1'-N9	5.01	112.21	108.20
22	AA	1459	G	N1-C6-O6	-5.01	116.89	119.90
24	A3	19	G	N1-C6-O6	-5.01	116.89	119.90
33	BS	13	ARG	NE-CZ-NH2	5.01	122.81	120.30
57	BA	38	A	O4'-C1'-N9	5.01	112.21	108.20
57	BA	1463	C	N1-C2-O2	5.01	121.91	118.90
57	BA	2264	C	O4'-C1'-N1	5.01	112.21	108.20
57	BA	2653	U	N1-C2-N3	5.01	117.91	114.90
57	BA	2761	A	O4'-C1'-N9	5.01	112.21	108.20
22	AA	102	G	N1-C6-O6	-5.01	116.89	119.90
22	AA	352	C	N3-C4-C5	5.01	123.90	121.90
57	BA	1711	A	C6-C5-N7	5.01	135.81	132.30
57	BA	2304	G	N1-C6-O6	-5.01	116.89	119.90
57	BA	2765	A	C1'-O4'-C4'	-5.01	105.89	109.90
22	AA	110	C	N3-C4-C5	5.01	123.90	121.90
22	AA	1441	A	C6-C5-N7	5.01	135.81	132.30
57	BA	754	U	C5'-C4'-O4'	5.01	115.11	109.10
57	BA	964	C	O4'-C1'-N1	5.01	112.20	108.20
57	BA	1411	U	O4'-C1'-N1	5.01	112.21	108.20
57	BA	1610	A	O4'-C1'-N9	5.01	112.21	108.20
57	BA	1685	C	N1-C2-O2	5.01	121.90	118.90
57	BA	1786	A	C1'-O4'-C4'	-5.01	105.89	109.90
57	BA	1811	G	N1-C6-O6	-5.01	116.90	119.90
4	AM	100	ARG	NH1-CZ-NH2	-5.00	113.89	119.40
22	AA	532	A	C4-C5-C6	-5.00	114.50	117.00
57	BA	2035	G	N1-C6-O6	-5.00	116.90	119.90
58	Ba	79	G	N1-C6-O6	-5.00	116.90	119.90
22	AA	1353	G	O4'-C1'-N9	5.00	112.20	108.20
57	BA	341	C	O4'-C1'-N1	5.00	112.20	108.20
57	BA	346	A	C1'-O4'-C4'	-5.00	105.90	109.90
57	BA	554	U	N3-C2-O2	-5.00	118.70	122.20
57	BA	605	G	C5'-C4'-O4'	5.00	115.10	109.10
57	BA	1118	C	O4'-C1'-N1	5.00	112.20	108.20
57	BA	1136	G	C5'-C4'-O4'	5.00	115.10	109.10
58	Ba	100	G	N1-C6-O6	-5.00	116.90	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	368	U	N1-C2-N3	5.00	117.90	114.90
22	AA	380	G	O4'-C1'-N9	5.00	112.20	108.20
22	AA	429	U	N3-C2-O2	-5.00	118.70	122.20
22	AA	500	G	C5'-C4'-O4'	5.00	115.10	109.10
22	AA	859	G	N1-C6-O6	-5.00	116.90	119.90
22	AA	1401	G	N3-C4-C5	-5.00	126.10	128.60
23	A2	40	G	N1-C6-O6	-5.00	116.90	119.90
57	BA	442	G	N1-C6-O6	-5.00	116.90	119.90
57	BA	1623	G	N1-C6-O6	-5.00	116.90	119.90
57	BA	2352	A	C4-C5-C6	-5.00	114.50	117.00
57	BA	2683	C	N3-C4-C5	5.00	123.90	121.90

There are no chirality outliers.

All (1070) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	A1	289	ILE	Peptide
21	A1	374	LEU	Peptide
23	A2	23	C	Sidechain
23	A2	34	U	Sidechain
23	A2	39	U	Sidechain
23	A2	44	U	Sidechain
23	A2	45	G	Sidechain
24	A3	1	C	Sidechain
24	A3	14	A	Sidechain
24	A3	15	G	Sidechain
24	A3	20	G	Sidechain
24	A3	23	G	Sidechain
24	A3	28	U	Sidechain
24	A3	30	G	Sidechain
24	A3	40	C	Sidechain
24	A3	46	G	Sidechain
24	A3	47	A	Sidechain
24	A3	60	A	Sidechain
24	A3	64	G	Sidechain
24	A3	65	G	Sidechain
24	A3	69	C	Sidechain
24	A3	7	G	Sidechain
22	AA	100	G	Sidechain
22	AA	1008	U	Sidechain
22	AA	1010	U	Sidechain
22	AA	1013	G	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	1016	A	Sidechain
22	AA	1026	G	Sidechain
22	AA	1027	C	Sidechain
22	AA	1028	C	Sidechain
22	AA	1030	U	Sidechain
22	AA	1032	G	Sidechain
22	AA	1051	C	Sidechain
22	AA	1054	C	Sidechain
22	AA	1067	A	Sidechain
22	AA	1071	C	Sidechain
22	AA	1072	G	Sidechain
22	AA	1077	G	Sidechain
22	AA	1080	A	Sidechain
22	AA	1082	A	Sidechain
22	AA	1084	G	Sidechain
22	AA	1087	G	Sidechain
22	AA	1093	A	Sidechain
22	AA	1094	G	Sidechain
22	AA	1095	U	Sidechain
22	AA	1099	G	Sidechain
22	AA	110	C	Sidechain
22	AA	1100	C	Sidechain
22	AA	1101	A	Sidechain
22	AA	1109	C	Sidechain
22	AA	1111	A	Sidechain
22	AA	1112	C	Sidechain
22	AA	1114	C	Sidechain
22	AA	1115	U	Sidechain
22	AA	1117	A	Sidechain
22	AA	1118	U	Sidechain
22	AA	1120	C	Sidechain
22	AA	1122	U	Sidechain
22	AA	1131	G	Sidechain
22	AA	1139	G	Sidechain
22	AA	1142	G	Sidechain
22	AA	1148	U	Sidechain
22	AA	1149	C	Sidechain
22	AA	1153	G	Sidechain
22	AA	1155	A	Sidechain
22	AA	1157	A	Sidechain
22	AA	1160	G	Sidechain
22	AA	1169	A	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	117	G	Sidechain
22	AA	1170	A	Sidechain
22	AA	1176	A	Sidechain
22	AA	1178	G	Sidechain
22	AA	1179	A	Sidechain
22	AA	119	A	Sidechain
22	AA	1191	A	Sidechain
22	AA	1195	C	Sidechain
22	AA	1209	C	Sidechain
22	AA	121	U	Sidechain
22	AA	1213	A	Sidechain
22	AA	1225	A	Sidechain
22	AA	1226	C	Sidechain
22	AA	1233	G	Sidechain
22	AA	1234	C	Sidechain
22	AA	1240	U	Sidechain
22	AA	1250	A	Sidechain
22	AA	1251	A	Sidechain
22	AA	1264	U	Sidechain
22	AA	1266	G	Sidechain
22	AA	1267	C	Sidechain
22	AA	1269	A	Sidechain
22	AA	1278	G	Sidechain
22	AA	128	G	Sidechain
22	AA	1282	C	Sidechain
22	AA	1287	A	Sidechain
22	AA	1289	A	Sidechain
22	AA	1296	C	Sidechain
22	AA	1297	G	Sidechain
22	AA	1298	U	Sidechain
22	AA	1299	A	Sidechain
22	AA	130	A	Sidechain
22	AA	1300	G	Sidechain
22	AA	1303	C	Sidechain
22	AA	1304	G	Sidechain
22	AA	1305	G	Sidechain
22	AA	1306	A	Sidechain
22	AA	1308	U	Sidechain
22	AA	1316	G	Sidechain
22	AA	1317	C	Sidechain
22	AA	1319	A	Sidechain
22	AA	1326	U	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	1330	U	Sidechain
22	AA	1343	G	Sidechain
22	AA	1345	U	Sidechain
22	AA	1349	A	Sidechain
22	AA	1357	A	Sidechain
22	AA	1358	U	Sidechain
22	AA	1360	A	Sidechain
22	AA	1361	G	Sidechain
22	AA	1362	A	Sidechain
22	AA	1363	A	Sidechain
22	AA	1366	C	Sidechain
22	AA	1373	G	Sidechain
22	AA	1374	A	Sidechain
22	AA	1380	U	Sidechain
22	AA	1382	C	Sidechain
22	AA	1392	G	Sidechain
22	AA	1394	A	Sidechain
22	AA	1396	A	Sidechain
22	AA	1400	C	Sidechain
22	AA	1401	G	Sidechain
22	AA	1411	C	Sidechain
22	AA	1419	G	Sidechain
22	AA	1426	G	Sidechain
22	AA	143	A	Sidechain
22	AA	1430	A	Sidechain
22	AA	1432	G	Sidechain
22	AA	1433	A	Sidechain
22	AA	1447	A	Sidechain
22	AA	1448	C	Sidechain
22	AA	1449	C	Sidechain
22	AA	1451	U	Sidechain
22	AA	1453	G	Sidechain
22	AA	1468	A	Sidechain
22	AA	1477	U	Sidechain
22	AA	1489	G	Sidechain
22	AA	149	A	Sidechain
22	AA	1490	U	Sidechain
22	AA	1502	A	Sidechain
22	AA	1503	A	Sidechain
22	AA	1506	U	Sidechain
22	AA	1512	U	Sidechain
22	AA	1513	A	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	1517	G	Sidechain
22	AA	1528	U	Sidechain
22	AA	153	C	Sidechain
22	AA	1535	C	Sidechain
22	AA	1537	U	Sidechain
22	AA	1542	A	Sidechain
22	AA	158	G	Sidechain
22	AA	159	G	Sidechain
22	AA	161	A	Sidechain
22	AA	173	U	Sidechain
22	AA	179	A	Sidechain
22	AA	182	A	Sidechain
22	AA	184	G	Sidechain
22	AA	187	G	Sidechain
22	AA	188	C	Sidechain
22	AA	2	A	Sidechain
22	AA	201	G	Sidechain
22	AA	202	G	Sidechain
22	AA	205	A	Sidechain
22	AA	209	U	Sidechain
22	AA	21	G	Sidechain
22	AA	212	G	Sidechain
22	AA	214	C	Sidechain
22	AA	215	C	Sidechain
22	AA	217	C	Sidechain
22	AA	222	C	Sidechain
22	AA	223	A	Sidechain
22	AA	234	C	Sidechain
22	AA	236	A	Sidechain
22	AA	244	U	Sidechain
22	AA	245	U	Sidechain
22	AA	246	A	Sidechain
22	AA	249	U	Sidechain
22	AA	252	U	Sidechain
22	AA	262	A	Sidechain
22	AA	264	C	Sidechain
22	AA	268	U	Sidechain
22	AA	269	C	Sidechain
22	AA	270	A	Sidechain
22	AA	272	C	Sidechain
22	AA	278	G	Sidechain
22	AA	279	A	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	281	G	Sidechain
22	AA	282	A	Sidechain
22	AA	285	C	Sidechain
22	AA	286	C	Sidechain
22	AA	293	G	Sidechain
22	AA	3	A	Sidechain
22	AA	304	U	Sidechain
22	AA	306	A	Sidechain
22	AA	308	C	Sidechain
22	AA	313	A	Sidechain
22	AA	314	C	Sidechain
22	AA	316	C	Sidechain
22	AA	324	G	Sidechain
22	AA	325	A	Sidechain
22	AA	33	A	Sidechain
22	AA	330	C	Sidechain
22	AA	332	G	Sidechain
22	AA	333	U	Sidechain
22	AA	336	A	Sidechain
22	AA	345	C	Sidechain
22	AA	346	G	Sidechain
22	AA	354	G	Sidechain
22	AA	36	C	Sidechain
22	AA	362	G	Sidechain
22	AA	368	U	Sidechain
22	AA	371	A	Sidechain
22	AA	376	G	Sidechain
22	AA	380	G	Sidechain
22	AA	383	A	Sidechain
22	AA	387	U	Sidechain
22	AA	390	U	Sidechain
22	AA	391	G	Sidechain
22	AA	392	C	Sidechain
22	AA	394	G	Sidechain
22	AA	395	C	Sidechain
22	AA	404	G	Sidechain
22	AA	410	G	Sidechain
22	AA	42	G	Sidechain
22	AA	423	G	Sidechain
22	AA	426	U	Sidechain
22	AA	428	G	Sidechain
22	AA	429	U	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	442	G	Sidechain
22	AA	448	A	Sidechain
22	AA	455	G	Sidechain
22	AA	457	G	Sidechain
22	AA	459	A	Sidechain
22	AA	46	G	Sidechain
22	AA	460	A	Sidechain
22	AA	463	U	Sidechain
22	AA	469	C	Sidechain
22	AA	472	U	Sidechain
22	AA	48	C	Sidechain
22	AA	481	G	Sidechain
22	AA	488	C	Sidechain
22	AA	490	C	Sidechain
22	AA	491	G	Sidechain
22	AA	493	A	Sidechain
22	AA	506	G	Sidechain
22	AA	51	A	Sidechain
22	AA	517	G	Sidechain
22	AA	518	C	Sidechain
22	AA	521	G	Sidechain
22	AA	522	C	Sidechain
22	AA	529	G	Sidechain
22	AA	530	G	Sidechain
22	AA	534	U	Sidechain
22	AA	535	A	Sidechain
22	AA	540	G	Sidechain
22	AA	551	U	Sidechain
22	AA	554	A	Sidechain
22	AA	558	G	Sidechain
22	AA	56	U	Sidechain
22	AA	560	A	Sidechain
22	AA	562	U	Sidechain
22	AA	563	A	Sidechain
22	AA	566	G	Sidechain
22	AA	568	G	Sidechain
22	AA	572	A	Sidechain
22	AA	590	U	Sidechain
22	AA	592	G	Sidechain
22	AA	594	U	Sidechain
22	AA	595	A	Sidechain
22	AA	597	G	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	60	A	Sidechain
22	AA	600	A	Sidechain
22	AA	608	A	Sidechain
22	AA	612	C	Sidechain
22	AA	618	C	Sidechain
22	AA	620	C	Sidechain
22	AA	623	C	Sidechain
22	AA	631	C	Sidechain
22	AA	639	G	Sidechain
22	AA	640	A	Sidechain
22	AA	641	U	Sidechain
22	AA	642	A	Sidechain
22	AA	654	G	Sidechain
22	AA	664	G	Sidechain
22	AA	665	A	Sidechain
22	AA	666	G	Sidechain
22	AA	67	C	Sidechain
22	AA	676	A	Sidechain
22	AA	679	C	Sidechain
22	AA	686	U	Sidechain
22	AA	690	G	Sidechain
22	AA	691	G	Sidechain
22	AA	692	U	Sidechain
22	AA	695	A	Sidechain
22	AA	697	U	Sidechain
22	AA	70	U	Sidechain
22	AA	703	G	Sidechain
22	AA	71	A	Sidechain
22	AA	722	G	Sidechain
22	AA	725	G	Sidechain
22	AA	728	A	Sidechain
22	AA	737	C	Sidechain
22	AA	745	G	Sidechain
22	AA	752	G	Sidechain
22	AA	754	C	Sidechain
22	AA	761	G	Sidechain
22	AA	771	G	Sidechain
22	AA	775	G	Sidechain
22	AA	778	G	Sidechain
22	AA	779	C	Sidechain
22	AA	781	A	Sidechain
22	AA	788	U	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	790	A	Sidechain
22	AA	791	G	Sidechain
22	AA	793	U	Sidechain
22	AA	795	C	Sidechain
22	AA	8	A	Sidechain
22	AA	80	A	Sidechain
22	AA	802	A	Sidechain
22	AA	805	C	Sidechain
22	AA	811	C	Sidechain
22	AA	816	A	Sidechain
22	AA	824	G	Sidechain
22	AA	826	C	Sidechain
22	AA	828	U	Sidechain
22	AA	838	G	Sidechain
22	AA	842	U	Sidechain
22	AA	843	U	Sidechain
22	AA	855	U	Sidechain
22	AA	859	G	Sidechain
22	AA	860	A	Sidechain
22	AA	863	U	Sidechain
22	AA	864	A	Sidechain
22	AA	87	C	Sidechain
22	AA	872	A	Sidechain
22	AA	874	G	Sidechain
22	AA	883	C	Sidechain
22	AA	892	A	Sidechain
22	AA	898	G	Sidechain
22	AA	900	A	Sidechain
22	AA	906	A	Sidechain
22	AA	91	U	Sidechain
22	AA	912	C	Sidechain
22	AA	914	A	Sidechain
22	AA	937	A	Sidechain
22	AA	938	A	Sidechain
22	AA	939	G	Sidechain
22	AA	94	G	Sidechain
22	AA	942	G	Sidechain
22	AA	946	A	Sidechain
22	AA	949	A	Sidechain
22	AA	95	C	Sidechain
22	AA	951	G	Sidechain
22	AA	958	A	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	960	U	Sidechain
22	AA	961	U	Sidechain
22	AA	962	C	Sidechain
22	AA	971	G	Sidechain
22	AA	972	C	Sidechain
22	AA	979	C	Sidechain
22	AA	985	C	Sidechain
22	AA	99	C	Sidechain
22	AA	991	U	Sidechain
22	AA	997	U	Sidechain
15	AD	61	ARG	Sidechain
18	AG	101	ARG	Sidechain
18	AG	118	ARG	Sidechain
3	AL	109	ARG	Sidechain
6	AO	88	ARG	Sidechain
7	AP	25	ARG	Sidechain
9	AR	2	ARG	Sidechain
10	AS	79	TYR	Sidechain
42	B0	54	ARG	Sidechain
51	B8	12	ARG	Sidechain
57	BA	100	U	Sidechain
57	BA	1004	U	Sidechain
57	BA	1012	U	Sidechain
57	BA	1013	C	Sidechain
57	BA	1014	A	Sidechain
57	BA	1017	G	Sidechain
57	BA	102	U	Sidechain
57	BA	1025	G	Sidechain
57	BA	1026	G	Sidechain
57	BA	1027	A	Sidechain
57	BA	1028	A	Sidechain
57	BA	103	A	Sidechain
57	BA	104	A	Sidechain
57	BA	1045	C	Sidechain
57	BA	1046	A	Sidechain
57	BA	1047	G	Sidechain
57	BA	1048	A	Sidechain
57	BA	1050	A	Sidechain
57	BA	1057	A	Sidechain
57	BA	106	C	Sidechain
57	BA	1063	G	Sidechain
57	BA	1066	U	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1069	A	Sidechain
57	BA	107	G	Sidechain
57	BA	1071	G	Sidechain
57	BA	1072	C	Sidechain
57	BA	1075	C	Sidechain
57	BA	1081	U	Sidechain
57	BA	1082	U	Sidechain
57	BA	1083	U	Sidechain
57	BA	1085	A	Sidechain
57	BA	1088	A	Sidechain
57	BA	109	C	Sidechain
57	BA	1095	A	Sidechain
57	BA	1097	U	Sidechain
57	BA	1099	G	Sidechain
57	BA	1104	C	Sidechain
57	BA	1108	U	Sidechain
57	BA	1111	A	Sidechain
57	BA	1119	U	Sidechain
57	BA	1130	U	Sidechain
57	BA	1132	U	Sidechain
57	BA	1133	A	Sidechain
57	BA	1134	A	Sidechain
57	BA	1135	C	Sidechain
57	BA	1138	G	Sidechain
57	BA	1142	A	Sidechain
57	BA	1148	U	Sidechain
57	BA	1158	C	Sidechain
57	BA	1165	A	Sidechain
57	BA	1167	C	Sidechain
57	BA	1168	G	Sidechain
57	BA	1169	A	Sidechain
57	BA	1171	G	Sidechain
57	BA	1174	U	Sidechain
57	BA	1177	G	Sidechain
57	BA	1178	C	Sidechain
57	BA	1179	G	Sidechain
57	BA	1182	G	Sidechain
57	BA	1187	G	Sidechain
57	BA	1188	U	Sidechain
57	BA	1189	A	Sidechain
57	BA	1198	U	Sidechain
57	BA	12	U	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1200	C	Sidechain
57	BA	1202	G	Sidechain
57	BA	1205	A	Sidechain
57	BA	1206	G	Sidechain
57	BA	1209	U	Sidechain
57	BA	1210	G	Sidechain
57	BA	1223	G	Sidechain
57	BA	1225	G	Sidechain
57	BA	1226	A	Sidechain
57	BA	1227	G	Sidechain
57	BA	1230	A	Sidechain
57	BA	1232	G	Sidechain
57	BA	1236	G	Sidechain
57	BA	1238	G	Sidechain
57	BA	124	G	Sidechain
57	BA	1245	G	Sidechain
57	BA	1251	C	Sidechain
57	BA	1252	G	Sidechain
57	BA	1254	A	Sidechain
57	BA	1255	U	Sidechain
57	BA	1263	U	Sidechain
57	BA	1267	U	Sidechain
57	BA	1268	A	Sidechain
57	BA	1271	G	Sidechain
57	BA	1273	U	Sidechain
57	BA	1281	G	Sidechain
57	BA	1283	G	Sidechain
57	BA	1288	G	Sidechain
57	BA	1291	C	Sidechain
57	BA	1299	G	Sidechain
57	BA	1302	A	Sidechain
57	BA	1310	G	Sidechain
57	BA	1311	G	Sidechain
57	BA	1315	C	Sidechain
57	BA	1324	G	Sidechain
57	BA	1329	U	Sidechain
57	BA	1343	G	Sidechain
57	BA	1353	A	Sidechain
57	BA	1356	G	Sidechain
57	BA	1364	G	Sidechain
57	BA	1370	C	Sidechain
57	BA	1376	C	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1377	G	Sidechain
57	BA	1378	A	Sidechain
57	BA	138	U	Sidechain
57	BA	1398	C	Sidechain
57	BA	1402	U	Sidechain
57	BA	1405	U	Sidechain
57	BA	1406	U	Sidechain
57	BA	1410	G	Sidechain
57	BA	1425	G	Sidechain
57	BA	1427	A	Sidechain
57	BA	1431	A	Sidechain
57	BA	144	A	Sidechain
57	BA	1450	G	Sidechain
57	BA	146	A	Sidechain
57	BA	1464	G	Sidechain
57	BA	1465	G	Sidechain
57	BA	1467	U	Sidechain
57	BA	1469	A	Sidechain
57	BA	1473	G	Sidechain
57	BA	1474	U	Sidechain
57	BA	1482	G	Sidechain
57	BA	1483	G	Sidechain
57	BA	1492	G	Sidechain
57	BA	1494	A	Sidechain
57	BA	1495	A	Sidechain
57	BA	1508	A	Sidechain
57	BA	1517	G	Sidechain
57	BA	152	A	Sidechain
57	BA	1532	A	Sidechain
57	BA	1535	A	Sidechain
57	BA	1537	G	Sidechain
57	BA	1544	A	Sidechain
57	BA	1546	G	Sidechain
57	BA	1548	A	Sidechain
57	BA	1549	A	Sidechain
57	BA	1551	A	Sidechain
57	BA	1554	U	Sidechain
57	BA	1555	G	Sidechain
57	BA	1560	G	Sidechain
57	BA	1561	C	Sidechain
57	BA	1564	C	Sidechain
57	BA	1569	A	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1570	A	Sidechain
57	BA	1573	G	Sidechain
57	BA	1575	C	Sidechain
57	BA	1583	A	Sidechain
57	BA	1596	A	Sidechain
57	BA	1599	U	Sidechain
57	BA	160	A	Sidechain
57	BA	1601	G	Sidechain
57	BA	1602	U	Sidechain
57	BA	1606	C	Sidechain
57	BA	1610	A	Sidechain
57	BA	1616	A	Sidechain
57	BA	1627	G	Sidechain
57	BA	1630	A	Sidechain
57	BA	1631	G	Sidechain
57	BA	1632	A	Sidechain
57	BA	1639	C	Sidechain
57	BA	1641	A	Sidechain
57	BA	1643	G	Sidechain
57	BA	1645	G	Sidechain
57	BA	1650	A	Sidechain
57	BA	1651	G	Sidechain
57	BA	1652	A	Sidechain
57	BA	1653	G	Sidechain
57	BA	1656	C	Sidechain
57	BA	1663	G	Sidechain
57	BA	1667	G	Sidechain
57	BA	1671	U	Sidechain
57	BA	1672	A	Sidechain
57	BA	1680	U	Sidechain
57	BA	1681	G	Sidechain
57	BA	1682	G	Sidechain
57	BA	1687	G	Sidechain
57	BA	169	G	Sidechain
57	BA	1695	G	Sidechain
57	BA	1698	A	Sidechain
57	BA	17	G	Sidechain
57	BA	1701	A	Sidechain
57	BA	1704	C	Sidechain
57	BA	1705	A	Sidechain
57	BA	1706	C	Sidechain
57	BA	1708	C	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1710	G	Sidechain
57	BA	1713	A	Sidechain
57	BA	1721	G	Sidechain
57	BA	1726	C	Sidechain
57	BA	1736	U	Sidechain
57	BA	1739	A	Sidechain
57	BA	1744	A	Sidechain
57	BA	1745	A	Sidechain
57	BA	1749	A	Sidechain
57	BA	1750	G	Sidechain
57	BA	1761	C	Sidechain
57	BA	1762	A	Sidechain
57	BA	177	G	Sidechain
57	BA	1773	A	Sidechain
57	BA	1786	A	Sidechain
57	BA	179	C	Sidechain
57	BA	1797	G	Sidechain
57	BA	1798	U	Sidechain
57	BA	1799	G	Sidechain
57	BA	1802	A	Sidechain
57	BA	1805	A	Sidechain
57	BA	1807	G	Sidechain
57	BA	181	A	Sidechain
57	BA	1818	U	Sidechain
57	BA	182	A	Sidechain
57	BA	1821	A	Sidechain
57	BA	1830	C	Sidechain
57	BA	1831	G	Sidechain
57	BA	1842	G	Sidechain
57	BA	1848	A	Sidechain
57	BA	1851	U	Sidechain
57	BA	1857	G	Sidechain
57	BA	1865	U	Sidechain
57	BA	1866	A	Sidechain
57	BA	1869	G	Sidechain
57	BA	1870	C	Sidechain
57	BA	1881	C	Sidechain
57	BA	1883	U	Sidechain
57	BA	1885	A	Sidechain
57	BA	1900	A	Sidechain
57	BA	191	A	Sidechain
57	BA	1918	A	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1922	G	Sidechain
57	BA	1926	U	Sidechain
57	BA	1927	A	Sidechain
57	BA	1938	A	Sidechain
57	BA	194	G	Sidechain
57	BA	1941	C	Sidechain
57	BA	1945	G	Sidechain
57	BA	1948	G	Sidechain
57	BA	1952	A	Sidechain
57	BA	1953	A	Sidechain
57	BA	1970	A	Sidechain
57	BA	1972	G	Sidechain
57	BA	1973	G	Sidechain
57	BA	1976	U	Sidechain
57	BA	1982	U	Sidechain
57	BA	199	A	Sidechain
57	BA	1996	C	Sidechain
57	BA	1997	C	Sidechain
57	BA	2	G	Sidechain
57	BA	2002	G	Sidechain
57	BA	2007	U	Sidechain
57	BA	2011	U	Sidechain
57	BA	2012	G	Sidechain
57	BA	2019	A	Sidechain
57	BA	203	A	Sidechain
57	BA	2033	A	Sidechain
57	BA	2035	G	Sidechain
57	BA	2050	C	Sidechain
57	BA	2051	A	Sidechain
57	BA	2053	G	Sidechain
57	BA	2057	G	Sidechain
57	BA	2059	A	Sidechain
57	BA	2063	C	Sidechain
57	BA	2065	C	Sidechain
57	BA	2068	U	Sidechain
57	BA	207	A	Sidechain
57	BA	2074	U	Sidechain
57	BA	2077	A	Sidechain
57	BA	208	C	Sidechain
57	BA	2080	A	Sidechain
57	BA	2090	A	Sidechain
57	BA	2091	C	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2097	A	Sidechain
57	BA	21	A	Sidechain
57	BA	2102	G	Sidechain
57	BA	2111	U	Sidechain
57	BA	2112	G	Sidechain
57	BA	2113	U	Sidechain
57	BA	2114	A	Sidechain
57	BA	2120	G	Sidechain
57	BA	2133	G	Sidechain
57	BA	2138	G	Sidechain
57	BA	2152	G	Sidechain
57	BA	2153	C	Sidechain
57	BA	2154	A	Sidechain
57	BA	2167	U	Sidechain
57	BA	2168	G	Sidechain
57	BA	217	A	Sidechain
57	BA	218	A	Sidechain
57	BA	2182	U	Sidechain
57	BA	2188	U	Sidechain
57	BA	219	A	Sidechain
57	BA	2197	U	Sidechain
57	BA	2204	G	Sidechain
57	BA	2205	A	Sidechain
57	BA	2206	C	Sidechain
57	BA	2210	U	Sidechain
57	BA	2226	C	Sidechain
57	BA	2227	A	Sidechain
57	BA	2228	G	Sidechain
57	BA	223	A	Sidechain
57	BA	2230	G	Sidechain
57	BA	2236	U	Sidechain
57	BA	2246	G	Sidechain
57	BA	2252	G	Sidechain
57	BA	2253	G	Sidechain
57	BA	2254	C	Sidechain
57	BA	2258	C	Sidechain
57	BA	226	A	Sidechain
57	BA	2266	A	Sidechain
57	BA	2268	A	Sidechain
57	BA	227	A	Sidechain
57	BA	2273	A	Sidechain
57	BA	2282	G	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2286	G	Sidechain
57	BA	229	C	Sidechain
57	BA	2295	C	Sidechain
57	BA	2300	C	Sidechain
57	BA	2301	C	Sidechain
57	BA	2304	G	Sidechain
57	BA	2305	U	Sidechain
57	BA	2307	G	Sidechain
57	BA	2308	G	Sidechain
57	BA	231	A	Sidechain
57	BA	2324	U	Sidechain
57	BA	2325	G	Sidechain
57	BA	2327	A	Sidechain
57	BA	2333	A	Sidechain
57	BA	2337	G	Sidechain
57	BA	2341	G	Sidechain
57	BA	2357	G	Sidechain
57	BA	2358	A	Sidechain
57	BA	2365	G	Sidechain
57	BA	2369	A	Sidechain
57	BA	2375	G	Sidechain
57	BA	2376	A	Sidechain
57	BA	2382	G	Sidechain
57	BA	2384	U	Sidechain
57	BA	2391	G	Sidechain
57	BA	2392	A	Sidechain
57	BA	2399	G	Sidechain
57	BA	2400	G	Sidechain
57	BA	2405	G	Sidechain
57	BA	2408	U	Sidechain
57	BA	2411	A	Sidechain
57	BA	2420	C	Sidechain
57	BA	2422	C	Sidechain
57	BA	2424	C	Sidechain
57	BA	243	U	Sidechain
57	BA	2431	U	Sidechain
57	BA	2433	A	Sidechain
57	BA	2437	G	Sidechain
57	BA	2438	U	Sidechain
57	BA	2441	U	Sidechain
57	BA	2442	C	Sidechain
57	BA	2447	G	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2451	A	Sidechain
57	BA	2453	A	Sidechain
57	BA	2458	G	Sidechain
57	BA	2461	A	Sidechain
57	BA	2468	A	Sidechain
57	BA	2471	A	Sidechain
57	BA	2472	G	Sidechain
57	BA	2475	C	Sidechain
57	BA	2476	A	Sidechain
57	BA	248	G	Sidechain
57	BA	2488	G	Sidechain
57	BA	249	C	Sidechain
57	BA	25	U	Sidechain
57	BA	250	G	Sidechain
57	BA	2507	C	Sidechain
57	BA	2508	G	Sidechain
57	BA	2516	A	Sidechain
57	BA	2517	C	Sidechain
57	BA	2518	A	Sidechain
57	BA	2520	C	Sidechain
57	BA	2521	C	Sidechain
57	BA	2522	U	Sidechain
57	BA	2530	A	Sidechain
57	BA	2531	A	Sidechain
57	BA	2532	G	Sidechain
57	BA	2536	G	Sidechain
57	BA	2542	A	Sidechain
57	BA	2550	G	Sidechain
57	BA	2555	U	Sidechain
57	BA	2557	G	Sidechain
57	BA	2560	A	Sidechain
57	BA	2562	U	Sidechain
57	BA	2565	A	Sidechain
57	BA	2566	A	Sidechain
57	BA	2573	C	Sidechain
57	BA	2575	C	Sidechain
57	BA	2576	G	Sidechain
57	BA	2583	G	Sidechain
57	BA	2588	G	Sidechain
57	BA	2591	C	Sidechain
57	BA	2601	C	Sidechain
57	BA	2608	G	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2611	C	Sidechain
57	BA	2613	U	Sidechain
57	BA	2624	G	Sidechain
57	BA	2625	G	Sidechain
57	BA	263	G	Sidechain
57	BA	2637	U	Sidechain
57	BA	2638	G	Sidechain
57	BA	264	C	Sidechain
57	BA	2645	G	Sidechain
57	BA	265	A	Sidechain
57	BA	2650	U	Sidechain
57	BA	2659	G	Sidechain
57	BA	2663	G	Sidechain
57	BA	2664	G	Sidechain
57	BA	2679	A	Sidechain
57	BA	2680	U	Sidechain
57	BA	2682	A	Sidechain
57	BA	2700	A	Sidechain
57	BA	2708	G	Sidechain
57	BA	2718	G	Sidechain
57	BA	272	A	Sidechain
57	BA	2721	A	Sidechain
57	BA	2723	C	Sidechain
57	BA	2726	A	Sidechain
57	BA	2727	A	Sidechain
57	BA	2732	G	Sidechain
57	BA	2734	A	Sidechain
57	BA	2737	G	Sidechain
57	BA	2739	U	Sidechain
57	BA	2740	A	Sidechain
57	BA	275	C	Sidechain
57	BA	2751	G	Sidechain
57	BA	2753	A	Sidechain
57	BA	2756	U	Sidechain
57	BA	276	U	Sidechain
57	BA	2768	U	Sidechain
57	BA	277	G	Sidechain
57	BA	2772	C	Sidechain
57	BA	2776	A	Sidechain
57	BA	278	A	Sidechain
57	BA	2780	G	Sidechain
57	BA	2786	U	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2787	C	Sidechain
57	BA	279	A	Sidechain
57	BA	2796	U	Sidechain
57	BA	2797	U	Sidechain
57	BA	28	A	Sidechain
57	BA	2807	U	Sidechain
57	BA	2809	A	Sidechain
57	BA	2810	A	Sidechain
57	BA	2816	G	Sidechain
57	BA	2824	C	Sidechain
57	BA	2831	G	Sidechain
57	BA	2832	U	Sidechain
57	BA	2836	U	Sidechain
57	BA	2839	G	Sidechain
57	BA	2840	C	Sidechain
57	BA	2848	G	Sidechain
57	BA	2851	A	Sidechain
57	BA	2856	A	Sidechain
57	BA	2857	G	Sidechain
57	BA	2866	U	Sidechain
57	BA	2868	A	Sidechain
57	BA	2869	G	Sidechain
57	BA	2874	C	Sidechain
57	BA	2879	A	Sidechain
57	BA	2881	U	Sidechain
57	BA	2885	G	Sidechain
57	BA	2888	C	Sidechain
57	BA	2889	C	Sidechain
57	BA	2892	G	Sidechain
57	BA	2895	G	Sidechain
57	BA	2899	A	Sidechain
57	BA	293	U	Sidechain
57	BA	297	G	Sidechain
57	BA	301	G	Sidechain
57	BA	303	G	Sidechain
57	BA	307	G	Sidechain
57	BA	308	G	Sidechain
57	BA	313	G	Sidechain
57	BA	33	C	Sidechain
57	BA	333	G	Sidechain
57	BA	343	C	Sidechain
57	BA	346	A	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	347	A	Sidechain
57	BA	352	A	Sidechain
57	BA	354	A	Sidechain
57	BA	361	G	Sidechain
57	BA	363	G	Sidechain
57	BA	367	G	Sidechain
57	BA	374	A	Sidechain
57	BA	377	G	Sidechain
57	BA	380	G	Sidechain
57	BA	385	C	Sidechain
57	BA	39	G	Sidechain
57	BA	390	U	Sidechain
57	BA	392	U	Sidechain
57	BA	394	C	Sidechain
57	BA	395	U	Sidechain
57	BA	403	U	Sidechain
57	BA	415	A	Sidechain
57	BA	416	U	Sidechain
57	BA	418	C	Sidechain
57	BA	420	C	Sidechain
57	BA	422	A	Sidechain
57	BA	43	G	Sidechain
57	BA	442	G	Sidechain
57	BA	446	G	Sidechain
57	BA	447	A	Sidechain
57	BA	449	A	Sidechain
57	BA	45	G	Sidechain
57	BA	450	G	Sidechain
57	BA	455	C	Sidechain
57	BA	457	A	Sidechain
57	BA	459	U	Sidechain
57	BA	460	A	Sidechain
57	BA	461	C	Sidechain
57	BA	463	G	Sidechain
57	BA	464	U	Sidechain
57	BA	474	G	Sidechain
57	BA	477	A	Sidechain
57	BA	478	A	Sidechain
57	BA	48	G	Sidechain
57	BA	480	A	Sidechain
57	BA	481	G	Sidechain
57	BA	486	C	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	492	A	Sidechain
57	BA	493	G	Sidechain
57	BA	498	G	Sidechain
57	BA	500	G	Sidechain
57	BA	501	A	Sidechain
57	BA	507	A	Sidechain
57	BA	510	C	Sidechain
57	BA	52	A	Sidechain
57	BA	528	A	Sidechain
57	BA	53	A	Sidechain
57	BA	544	C	Sidechain
57	BA	568	U	Sidechain
57	BA	573	U	Sidechain
57	BA	575	A	Sidechain
57	BA	576	U	Sidechain
57	BA	577	G	Sidechain
57	BA	58	G	Sidechain
57	BA	581	C	Sidechain
57	BA	583	G	Sidechain
57	BA	587	C	Sidechain
57	BA	59	U	Sidechain
57	BA	592	A	Sidechain
57	BA	594	U	Sidechain
57	BA	60	G	Sidechain
57	BA	603	A	Sidechain
57	BA	607	U	Sidechain
57	BA	608	A	Sidechain
57	BA	611	C	Sidechain
57	BA	617	G	Sidechain
57	BA	622	G	Sidechain
57	BA	623	C	Sidechain
57	BA	626	A	Sidechain
57	BA	63	A	Sidechain
57	BA	630	G	Sidechain
57	BA	632	A	Sidechain
57	BA	636	G	Sidechain
57	BA	637	A	Sidechain
57	BA	642	U	Sidechain
57	BA	666	A	Sidechain
57	BA	671	C	Sidechain
57	BA	672	C	Sidechain
57	BA	676	A	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	685	A	Sidechain
57	BA	687	C	Sidechain
57	BA	688	U	Sidechain
57	BA	692	C	Sidechain
57	BA	693	A	Sidechain
57	BA	697	G	Sidechain
57	BA	700	G	Sidechain
57	BA	708	G	Sidechain
57	BA	71	A	Sidechain
57	BA	715	A	Sidechain
57	BA	717	C	Sidechain
57	BA	718	A	Sidechain
57	BA	72	U	Sidechain
57	BA	721	A	Sidechain
57	BA	726	G	Sidechain
57	BA	728	G	Sidechain
57	BA	729	G	Sidechain
57	BA	73	A	Sidechain
57	BA	735	A	Sidechain
57	BA	736	C	Sidechain
57	BA	738	G	Sidechain
57	BA	74	A	Sidechain
57	BA	75	G	Sidechain
57	BA	751	A	Sidechain
57	BA	757	G	Sidechain
57	BA	764	A	Sidechain
57	BA	772	C	Sidechain
57	BA	776	G	Sidechain
57	BA	78	U	Sidechain
57	BA	782	A	Sidechain
57	BA	783	A	Sidechain
57	BA	786	C	Sidechain
57	BA	789	A	Sidechain
57	BA	791	C	Sidechain
57	BA	794	A	Sidechain
57	BA	795	C	Sidechain
57	BA	800	A	Sidechain
57	BA	801	G	Sidechain
57	BA	802	A	Sidechain
57	BA	804	A	Sidechain
57	BA	810	U	Sidechain
57	BA	813	U	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	819	A	Sidechain
57	BA	820	A	Sidechain
57	BA	828	U	Sidechain
57	BA	834	G	Sidechain
57	BA	837	C	Sidechain
57	BA	838	C	Sidechain
57	BA	841	G	Sidechain
57	BA	845	A	Sidechain
57	BA	858	G	Sidechain
57	BA	86	G	Sidechain
57	BA	861	A	Sidechain
57	BA	867	C	Sidechain
57	BA	87	U	Sidechain
57	BA	871	U	Sidechain
57	BA	876	C	Sidechain
57	BA	881	G	Sidechain
57	BA	883	G	Sidechain
57	BA	89	A	Sidechain
57	BA	894	U	Sidechain
57	BA	902	C	Sidechain
57	BA	905	A	Sidechain
57	BA	909	A	Sidechain
57	BA	910	A	Sidechain
57	BA	912	C	Sidechain
57	BA	914	G	Sidechain
57	BA	915	C	Sidechain
57	BA	916	G	Sidechain
57	BA	923	G	Sidechain
57	BA	927	A	Sidechain
57	BA	931	U	Sidechain
57	BA	934	U	Sidechain
57	BA	936	A	Sidechain
57	BA	940	G	Sidechain
57	BA	945	A	Sidechain
57	BA	950	G	Sidechain
57	BA	956	G	Sidechain
57	BA	957	C	Sidechain
57	BA	959	A	Sidechain
57	BA	962	G	Sidechain
57	BA	963	U	Sidechain
57	BA	966	G	Sidechain
57	BA	968	C	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	969	G	Sidechain
57	BA	970	U	Sidechain
57	BA	971	G	Sidechain
57	BA	983	A	Sidechain
57	BA	984	A	Sidechain
57	BA	989	G	Sidechain
57	BA	99	U	Sidechain
57	BA	990	A	Sidechain
35	BD	155	ARG	Sidechain
55	BH	175	LYS	Peptide
55	BH	57	TYR	Sidechain
26	BJ	137	ARG	Sidechain
28	BN	116	ARG	Sidechain
28	BN	52	ASP	Peptide
29	BO	31	ARG	Sidechain
32	BR	8	ARG	Sidechain
34	BT	71	ARG	Sidechain
36	BU	50	ARG	Sidechain
36	BU	54	ARG	Sidechain
38	BW	25	ARG	Sidechain
40	BY	6	ARG	Sidechain
58	Ba	105	G	Sidechain
58	Ba	11	C	Sidechain
58	Ba	117	G	Sidechain
58	Ba	15	A	Sidechain
58	Ba	21	G	Sidechain
58	Ba	35	C	Sidechain
58	Ba	40	U	Sidechain
58	Ba	41	G	Sidechain
58	Ba	50	A	Sidechain
58	Ba	51	G	Sidechain
58	Ba	57	A	Sidechain
58	Ba	64	G	Sidechain
58	Ba	73	A	Sidechain
58	Ba	90	C	Sidechain
58	Ba	92	C	Sidechain

## 5.2 Too-close contacts ⓘ

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



the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AJ	794	0	803	0	0
2	AK	923	0	912	0	0
3	AL	923	0	954	0	0
4	AM	876	0	910	0	0
5	AN	771	0	777	0	0
6	AO	690	0	691	0	0
7	AP	620	0	611	0	0
8	AQ	657	0	687	0	0
9	AR	603	0	602	0	0
10	AS	708	0	732	0	0
11	AB	1805	0	1750	0	0
12	AT	636	0	652	0	0
13	AU	564	0	579	0	0
14	AC	1761	0	1793	0	0
15	AD	1587	0	1596	0	0
16	AE	1182	0	1185	0	0
17	AF	1061	0	971	0	0
18	AG	1347	0	1347	0	0
19	AH	948	0	975	0	0
20	AI	1000	0	1011	0	0
21	A1	4989	0	4915	0	0
22	AA	33089	0	16668	0	0
23	A2	993	0	501	0	0
24	A3	1640	0	845	0	0
25	BC	1733	0	1824	0	0
26	BJ	1233	0	1283	0	0
27	BK	1032	0	1088	0	0
28	BN	1129	0	1162	0	0
29	BO	947	0	1023	0	0
30	BP	1053	0	1129	0	0
31	BQ	1074	0	1157	0	0
32	BR	1008	0	1045	0	0
33	BS	900	0	935	0	0
34	BT	917	0	965	0	0
35	BD	2092	0	2170	0	0
36	BU	947	0	1022	0	0
37	BV	816	0	839	0	0
38	BW	857	0	922	0	0
39	BX	787	0	846	0	0
40	BY	789	0	847	0	0
41	BZ	753	0	780	0	0
42	B0	634	0	656	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	B1	625	0	655	0	0
44	B2	509	0	543	0	0
45	BE	1565	0	1616	0	0
46	B3	449	0	491	0	0
47	B4	549	0	552	0	0
48	B5	444	0	461	0	0
49	B6	441	0	485	0	0
50	B7	377	0	418	0	0
51	B8	504	0	574	0	0
52	B9	302	0	343	0	0
53	BF	1552	0	1619	0	0
54	BG	1420	0	1460	0	0
55	BH	1323	0	1374	0	0
56	BL	1111	0	1148	0	0
57	BA	62351	0	31378	0	0
58	Ba	2566	0	1302	0	0
All	All	154956	0	106579	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	AJ	44/103 (43%)	40 (91%)	1 (2%)	3 (7%)	1	23
2	AK	57/128 (44%)	52 (91%)	5 (9%)	0	100	100
3	AL	64/123 (52%)	54 (84%)	8 (12%)	2 (3%)	5	42
4	AM	56/117 (48%)	51 (91%)	4 (7%)	1 (2%)	11	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AN	41/100 (41%)	37 (90%)	3 (7%)	1 (2%)	7	47
6	AO	44/88 (50%)	43 (98%)	1 (2%)	0	100	100
7	AP	34/82 (42%)	31 (91%)	3 (9%)	0	100	100
8	AQ	52/83 (63%)	48 (92%)	4 (8%)	0	100	100
9	AR	36/74 (49%)	34 (94%)	2 (6%)	0	100	100
10	AS	54/91 (59%)	53 (98%)	1 (2%)	0	100	100
11	AB	123/240 (51%)	114 (93%)	7 (6%)	2 (2%)	12	56
12	AT	32/86 (37%)	30 (94%)	2 (6%)	0	100	100
13	AU	24/70 (34%)	18 (75%)	3 (12%)	3 (12%)	0	8
14	AC	126/232 (54%)	122 (97%)	4 (3%)	0	100	100
15	AD	107/205 (52%)	102 (95%)	5 (5%)	0	100	100
16	AE	89/166 (54%)	84 (94%)	4 (4%)	1 (1%)	17	63
17	AF	65/135 (48%)	61 (94%)	4 (6%)	0	100	100
18	AG	84/178 (47%)	79 (94%)	5 (6%)	0	100	100
19	AH	77/129 (60%)	70 (91%)	7 (9%)	0	100	100
20	AI	69/129 (54%)	63 (91%)	6 (9%)	0	100	100
21	A1	434/639 (68%)	390 (90%)	38 (9%)	6 (1%)	14	58
25	BC	232/234 (99%)	213 (92%)	18 (8%)	1 (0%)	39	80
26	BJ	162/164 (99%)	158 (98%)	3 (2%)	1 (1%)	30	74
27	BK	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
28	BN	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
29	BO	121/123 (98%)	107 (88%)	11 (9%)	3 (2%)	7	46
30	BP	142/144 (99%)	127 (89%)	13 (9%)	2 (1%)	14	58
31	BQ	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	13	57
32	BR	125/127 (98%)	112 (90%)	11 (9%)	2 (2%)	12	56
33	BS	115/117 (98%)	115 (100%)	0	0	100	100
34	BT	112/114 (98%)	107 (96%)	3 (3%)	2 (2%)	11	53
35	BD	270/272 (99%)	252 (93%)	15 (6%)	3 (1%)	17	63
36	BU	115/117 (98%)	108 (94%)	5 (4%)	2 (2%)	11	55
37	BV	101/103 (98%)	94 (93%)	4 (4%)	3 (3%)	5	42
38	BW	108/110 (98%)	103 (95%)	4 (4%)	1 (1%)	21	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	BX	98/100 (98%)	83 (85%)	12 (12%)	3 (3%)	5	42
40	BY	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
41	BZ	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
42	B0	82/84 (98%)	72 (88%)	6 (7%)	4 (5%)	3	31
43	B1	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	15	60
44	B2	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
45	BE	207/209 (99%)	181 (87%)	20 (10%)	6 (3%)	6	43
46	B3	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
47	B4	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
48	B5	54/56 (96%)	50 (93%)	3 (6%)	1 (2%)	10	52
49	B6	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
50	B7	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	B8	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
52	B9	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	2	28
53	BF	199/201 (99%)	186 (94%)	7 (4%)	6 (3%)	5	42
54	BG	176/178 (99%)	155 (88%)	15 (8%)	6 (3%)	5	40
55	BH	174/176 (99%)	157 (90%)	14 (8%)	3 (2%)	11	55
56	BL	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	26	71
All	All	5512/7062 (78%)	5089 (92%)	349 (6%)	74 (1%)	20	60

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	A1	242	THR
21	A1	493	LYS
32	BR	13	ASN
35	BD	140	VAL
42	B0	40	ARG
45	BE	122	VAL
56	BL	35	LYS
1	AJ	57	VAL
13	AU	3	ILE
13	AU	19	LYS
21	A1	174	GLN
30	BP	53	GLY
34	BT	5	LYS

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Mol	Chain	Res	Type
35	BD	77	VAL
42	B0	36	ILE
43	B1	27	ARG
45	BE	37	VAL
53	BF	62	GLN
53	BF	79	ARG
53	BF	96	VAL
54	BG	132	ARG
55	BH	29	ASN
55	BH	46	ASP
4	AM	22	TYR
11	AB	18	GLN
16	AE	23	THR
21	A1	249	LEU
21	A1	284	SER
21	A1	566	VAL
30	BP	36	LYS
31	BQ	43	ALA
36	BU	5	ARG
38	BW	28	LYS
39	BX	51	PHE
53	BF	6	LYS
53	BF	46	GLN
54	BG	80	GLN
3	AL	75	GLU
31	BQ	58	LYS
35	BD	162	GLN
36	BU	102	LYS
37	BV	91	GLN
39	BX	69	ARG
42	B0	23	LYS
52	B9	16	ILE
1	AJ	42	LEU
3	AL	43	LYS
11	AB	17	HIS
25	BC	166	ASP
26	BJ	70	CYS
37	BV	53	PHE
42	B0	68	PHE
45	BE	119	ALA
45	BE	167	ASN
54	BG	81	GLY

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Mol	Chain	Res	Type
54	BG	88	VAL
54	BG	103	ILE
55	BH	94	ARG
29	BO	5	GLN
32	BR	80	PHE
37	BV	101	ILE
39	BX	74	ILE
45	BE	113	SER
48	B5	54	ILE
53	BF	183	PHE
54	BG	35	LEU
1	AJ	74	VAL
34	BT	32	VAL
45	BE	117	GLY
52	B9	7	VAL
29	BO	93	GLN
29	BO	122	VAL
5	AN	71	GLY
13	AU	2	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	AJ	90/90 (100%)	88 (98%)	2 (2%)	60	83
2	AK	98/98 (100%)	97 (99%)	1 (1%)	82	92
3	AL	103/103 (100%)	102 (99%)	1 (1%)	82	92
4	AM	95/95 (100%)	95 (100%)	0	100	100
5	AN	83/83 (100%)	82 (99%)	1 (1%)	78	90
6	AO	76/76 (100%)	74 (97%)	2 (3%)	54	80
7	AP	65/65 (100%)	64 (98%)	1 (2%)	72	88
8	AQ	77/77 (100%)	75 (97%)	2 (3%)	54	80
9	AR	64/64 (100%)	62 (97%)	2 (3%)	47	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AS	78/78 (100%)	74 (95%)	4 (5%)	29	66
11	AB	198/198 (100%)	196 (99%)	2 (1%)	82	92
12	AT	65/65 (100%)	65 (100%)	0	100	100
13	AU	60/60 (100%)	58 (97%)	2 (3%)	45	76
14	AC	189/189 (100%)	181 (96%)	8 (4%)	36	70
15	AD	172/172 (100%)	168 (98%)	4 (2%)	58	83
16	AE	125/125 (100%)	119 (95%)	6 (5%)	31	67
17	AF	116/116 (100%)	111 (96%)	5 (4%)	35	70
18	AG	146/146 (100%)	143 (98%)	3 (2%)	61	84
19	AH	104/104 (100%)	101 (97%)	3 (3%)	50	78
20	AI	106/106 (100%)	102 (96%)	4 (4%)	40	73
21	A1	568/568 (100%)	559 (98%)	9 (2%)	70	88
25	BC	181/181 (100%)	174 (96%)	7 (4%)	39	72
26	BJ	122/122 (100%)	120 (98%)	2 (2%)	70	88
27	BK	109/109 (100%)	106 (97%)	3 (3%)	51	78
28	BN	116/116 (100%)	110 (95%)	6 (5%)	29	65
29	BO	104/104 (100%)	95 (91%)	9 (9%)	13	45
30	BP	103/103 (100%)	96 (93%)	7 (7%)	20	57
31	BQ	109/109 (100%)	105 (96%)	4 (4%)	41	73
32	BR	103/103 (100%)	100 (97%)	3 (3%)	50	78
33	BS	87/87 (100%)	86 (99%)	1 (1%)	80	91
34	BT	99/99 (100%)	97 (98%)	2 (2%)	63	85
35	BD	217/217 (100%)	212 (98%)	5 (2%)	58	83
36	BU	89/89 (100%)	86 (97%)	3 (3%)	44	75
37	BV	84/84 (100%)	83 (99%)	1 (1%)	78	90
38	BW	93/93 (100%)	90 (97%)	3 (3%)	46	76
39	BX	84/84 (100%)	83 (99%)	1 (1%)	78	90
40	BY	84/84 (100%)	82 (98%)	2 (2%)	57	82
41	BZ	78/78 (100%)	77 (99%)	1 (1%)	76	89
42	B0	62/62 (100%)	56 (90%)	6 (10%)	10	40
43	B1	67/67 (100%)	66 (98%)	1 (2%)	72	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	B2	55/55 (100%)	54 (98%)	1 (2%)	66	87
45	BE	164/164 (100%)	163 (99%)	1 (1%)	90	95
46	B3	48/48 (100%)	48 (100%)	0	100	100
47	B4	62/62 (100%)	61 (98%)	1 (2%)	70	88
48	B5	47/47 (100%)	45 (96%)	2 (4%)	35	70
49	B6	48/48 (100%)	48 (100%)	0	100	100
50	B7	38/38 (100%)	37 (97%)	1 (3%)	54	80
51	B8	51/51 (100%)	51 (100%)	0	100	100
52	B9	34/34 (100%)	34 (100%)	0	100	100
53	BF	165/165 (100%)	161 (98%)	4 (2%)	57	82
54	BG	149/149 (100%)	141 (95%)	8 (5%)	27	64
55	BH	137/137 (100%)	132 (96%)	5 (4%)	42	74
56	BL	114/114 (100%)	114 (100%)	0	100	100
All	All	5781/5781 (100%)	5629 (97%)	152 (3%)	57	80

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AJ	37	ARG
1	AJ	58	ASN
2	AK	55	ARG
3	AL	49	ARG
5	AN	95	LEU
6	AO	57	ARG
6	AO	88	ARG
7	AP	47	GLU
8	AQ	64	ARG
8	AQ	68	LYS
9	AR	15	GLU
9	AR	65	SER
10	AS	6	LYS
10	AS	82	HIS
10	AS	86	LYS
10	AS	91	LYS
11	AB	14	HIS
11	AB	183	PHE
13	AU	19	LYS

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Mol	Chain	Res	Type
13	AU	68	ARG
14	AC	3	LYS
14	AC	28	PHE
14	AC	35	ASP
14	AC	48	LYS
14	AC	57	GLU
14	AC	187	GLU
14	AC	227	GLN
14	AC	231	ARG
15	AD	71	PHE
15	AD	72	ARG
15	AD	131	ILE
15	AD	187	ARG
16	AE	12	GLU
16	AE	22	LYS
16	AE	49	TYR
16	AE	92	ARG
16	AE	121	ASN
16	AE	122	VAL
17	AF	6	ILE
17	AF	69	GLU
17	AF	98	GLU
17	AF	112	ARG
17	AF	118	ASN
18	AG	143	MET
18	AG	150	PHE
18	AG	153	TYR
19	AH	26	MET
19	AH	65	PHE
19	AH	76	ARG
20	AI	26	LYS
20	AI	79	ARG
20	AI	80	HIS
20	AI	122	ARG
21	A1	228	ARG
21	A1	256	ILE
21	A1	322	GLN
21	A1	370	ASP
21	A1	421	MET
21	A1	468	TYR
21	A1	490	TYR
21	A1	526	GLN

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Mol	Chain	Res	Type
21	A1	561	TYR
25	BC	39	VAL
25	BC	105	LYS
25	BC	162	ARG
25	BC	172	HIS
25	BC	186	LYS
25	BC	208	TYR
25	BC	234	ASN
26	BJ	55	ARG
26	BJ	94	LEU
27	BK	4	VAL
27	BK	45	THR
27	BK	87	SER
28	BN	2	LYS
28	BN	44	TYR
28	BN	47	HIS
28	BN	49	ASP
28	BN	61	LYS
28	BN	98	GLU
29	BO	23	LYS
29	BO	31	ARG
29	BO	47	ILE
29	BO	64	ARG
29	BO	70	ARG
29	BO	80	ASP
29	BO	107	LEU
29	BO	113	MET
29	BO	122	VAL
30	BP	4	ASN
30	BP	21	ARG
30	BP	33	ARG
30	BP	39	LYS
30	BP	47	ARG
30	BP	111	ILE
30	BP	126	ARG
31	BQ	12	MET
31	BQ	63	ILE
31	BQ	93	VAL
31	BQ	97	GLN
32	BR	1	MET
32	BR	16	HIS
32	BR	99	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	BS	18	LEU
34	BT	50	ARG
34	BT	109	ILE
35	BD	200	MET
35	BD	211	ARG
35	BD	212	TRP
35	BD	217	PRO
35	BD	269	ARG
36	BU	4	LYS
36	BU	88	GLU
36	BU	96	ASP
37	BV	86	GLN
38	BW	60	HIS
38	BW	95	ARG
38	BW	110	ARG
39	BX	76	ARG
40	BY	46	LYS
40	BY	65	GLN
41	BZ	42	LEU
42	B0	19	ARG
42	B0	22	VAL
42	B0	23	LYS
42	B0	35	ILE
42	B0	40	ARG
42	B0	49	ASN
43	B1	26	ARG
44	B2	47	ARG
45	BE	128	ARG
47	B4	63	ARG
48	B5	6	LYS
48	B5	32	THR
50	B7	1	MET
53	BF	60	TRP
53	BF	67	ARG
53	BF	88	ARG
53	BF	152	GLU
54	BG	34	THR
54	BG	65	LEU
54	BG	91	ARG
54	BG	94	ARG
54	BG	103	ILE
54	BG	111	ARG

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Mol	Chain	Res	Type
54	BG	119	LYS
54	BG	134	GLN
55	BH	2	ARG
55	BH	68	ARG
55	BH	104	LEU
55	BH	154	GLU
55	BH	166	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AA	1538/1542 (99%)	194 (12%)	57 (3%)
23	A2	46/47 (97%)	13 (28%)	1 (2%)
24	A3	75/77 (97%)	12 (16%)	2 (2%)
57	BA	2899/2904 (99%)	404 (13%)	115 (3%)
58	Ba	119/120 (99%)	11 (9%)	0
All	All	4677/4690 (99%)	634 (13%)	175 (3%)

All (634) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	AA	2	A
22	AA	3	A
22	AA	5	U
22	AA	6	G
22	AA	7	A
22	AA	8	A
22	AA	9	G
22	AA	32	A
22	AA	39	G
22	AA	48	C
22	AA	49	U
22	AA	50	A
22	AA	52	C
22	AA	55	A
22	AA	56	U
22	AA	60	A
22	AA	84	U

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Mol	Chain	Res	Type
22	AA	108	G
22	AA	109	A
22	AA	120	A
22	AA	131	A
22	AA	144	G
22	AA	149	A
22	AA	153	C
22	AA	163	C
22	AA	184	G
22	AA	204	G
22	AA	214	C
22	AA	243	A
22	AA	244	U
22	AA	247	G
22	AA	250	A
22	AA	251	G
22	AA	262	A
22	AA	263	A
22	AA	266	G
22	AA	267	C
22	AA	280	C
22	AA	289	G
22	AA	298	A
22	AA	328	C
22	AA	329	A
22	AA	330	C
22	AA	332	G
22	AA	347	G
22	AA	352	C
22	AA	353	A
22	AA	354	G
22	AA	367	U
22	AA	368	U
22	AA	372	C
22	AA	373	A
22	AA	381	C
22	AA	390	U
22	AA	398	U
22	AA	406	G
22	AA	412	A
22	AA	413	G
22	AA	422	C

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Mol	Chain	Res	Type
22	AA	429	U
22	AA	451	A
22	AA	464	U
22	AA	465	A
22	AA	466	A
22	AA	468	A
22	AA	481	G
22	AA	482	A
22	AA	484	G
22	AA	486	U
22	AA	487	A
22	AA	494	G
22	AA	496	A
22	AA	498	A
22	AA	505	G
22	AA	508	U
22	AA	511	C
22	AA	512	U
22	AA	518	C
22	AA	519	C
22	AA	520	A
22	AA	524	G
22	AA	527	7MG
22	AA	531	U
22	AA	532	A
22	AA	547	A
22	AA	559	A
22	AA	564	C
22	AA	566	G
22	AA	572	A
22	AA	573	A
22	AA	576	C
22	AA	631	C
22	AA	633	G
22	AA	665	A
22	AA	688	G
22	AA	695	A
22	AA	718	A
22	AA	719	C
22	AA	720	C
22	AA	721	G
22	AA	723	U

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Mol	Chain	Res	Type
22	AA	755	G
22	AA	766	A
22	AA	812	G
22	AA	817	C
22	AA	821	G
22	AA	828	U
22	AA	840	C
22	AA	841	C
22	AA	843	U
22	AA	846	G
22	AA	874	G
22	AA	885	G
22	AA	889	A
22	AA	890	G
22	AA	914	A
22	AA	927	G
22	AA	934	C
22	AA	935	A
22	AA	938	A
22	AA	960	U
22	AA	962	C
22	AA	966	2MG
22	AA	968	A
22	AA	969	A
22	AA	975	A
22	AA	977	A
22	AA	981	U
22	AA	993	G
22	AA	1004	A
22	AA	1026	G
22	AA	1044	A
22	AA	1050	G
22	AA	1051	C
22	AA	1064	G
22	AA	1065	U
22	AA	1094	G
22	AA	1101	A
22	AA	1102	A
22	AA	1110	A
22	AA	1136	C
22	AA	1138	G
22	AA	1139	G

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Mol	Chain	Res	Type
22	AA	1140	C
22	AA	1152	A
22	AA	1159	U
22	AA	1168	U
22	AA	1169	A
22	AA	1183	U
22	AA	1184	G
22	AA	1191	A
22	AA	1196	A
22	AA	1212	U
22	AA	1214	C
22	AA	1215	G
22	AA	1228	C
22	AA	1238	A
22	AA	1241	G
22	AA	1256	A
22	AA	1257	A
22	AA	1258	G
22	AA	1279	G
22	AA	1280	A
22	AA	1281	C
22	AA	1285	A
22	AA	1297	G
22	AA	1302	C
22	AA	1303	C
22	AA	1305	G
22	AA	1306	A
22	AA	1319	A
22	AA	1320	C
22	AA	1322	C
22	AA	1340	A
22	AA	1346	A
22	AA	1359	C
22	AA	1360	A
22	AA	1398	A
22	AA	1401	G
22	AA	1447	A
22	AA	1491	G
22	AA	1492	A
22	AA	1493	A
22	AA	1502	A
22	AA	1503	A

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Mol	Chain	Res	Type
22	AA	1506	U
22	AA	1507	A
22	AA	1529	G
22	AA	1530	G
22	AA	1535	C
22	AA	1537	U
22	AA	1539	C
22	AA	1540	U
22	AA	1542	A
23	A2	14	G
23	A2	16	A
23	A2	19	A
23	A2	21	U
23	A2	25	U
23	A2	26	U
23	A2	27	A
23	A2	29	G
23	A2	30	U
23	A2	34	U
23	A2	46	C
23	A2	47	C
23	A2	56	G
24	A3	2	G
24	A3	9	G
24	A3	10	G
24	A3	16	C
24	A3	17	C
24	A3	21	H2U
24	A3	39	A
24	A3	49	C
24	A3	74	A
24	A3	75	C
24	A3	76	C
24	A3	77	A
57	BA	13	A
57	BA	35	G
57	BA	61	C
57	BA	62	U
57	BA	71	A
57	BA	74	A
57	BA	75	G
57	BA	91	A

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Mol	Chain	Res	Type
57	BA	98	G
57	BA	100	U
57	BA	119	A
57	BA	120	U
57	BA	139	U
57	BA	140	C
57	BA	149	A
57	BA	163	C
57	BA	180	G
57	BA	196	A
57	BA	197	A
57	BA	199	A
57	BA	204	A
57	BA	205	G
57	BA	216	A
57	BA	222	A
57	BA	230	G
57	BA	242	G
57	BA	243	U
57	BA	248	G
57	BA	250	G
57	BA	265	A
57	BA	266	G
57	BA	271	G
57	BA	272	A
57	BA	277	G
57	BA	299	A
57	BA	311	A
57	BA	324	A
57	BA	330	A
57	BA	332	A
57	BA	333	G
57	BA	338	G
57	BA	360	U
57	BA	361	G
57	BA	368	A
57	BA	372	G
57	BA	386	G
57	BA	387	U
57	BA	388	G
57	BA	394	C
57	BA	395	U

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Mol	Chain	Res	Type
57	BA	396	G
57	BA	406	G
57	BA	411	G
57	BA	424	G
57	BA	435	C
57	BA	451	U
57	BA	454	A
57	BA	458	G
57	BA	480	A
57	BA	481	G
57	BA	482	A
57	BA	489	G
57	BA	490	C
57	BA	491	G
57	BA	504	A
57	BA	505	A
57	BA	531	C
57	BA	532	A
57	BA	533	G
57	BA	544	C
57	BA	545	U
57	BA	546	U
57	BA	550	C
57	BA	562	U
57	BA	573	U
57	BA	575	A
57	BA	588	U
57	BA	603	A
57	BA	604	G
57	BA	613	A
57	BA	615	U
57	BA	637	A
57	BA	638	G
57	BA	652	U
57	BA	654	A
57	BA	671	C
57	BA	686	U
57	BA	718	A
57	BA	719	C
57	BA	730	A
57	BA	747	5MU
57	BA	752	A

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Mol	Chain	Res	Type
57	BA	764	A
57	BA	776	G
57	BA	781	A
57	BA	782	A
57	BA	783	A
57	BA	784	G
57	BA	789	A
57	BA	790	U
57	BA	791	C
57	BA	792	A
57	BA	805	G
57	BA	812	C
57	BA	846	U
57	BA	850	U
57	BA	851	C
57	BA	859	G
57	BA	866	A
57	BA	887	U
57	BA	890	C
57	BA	896	A
57	BA	901	C
57	BA	910	A
57	BA	914	G
57	BA	915	C
57	BA	920	A
57	BA	945	A
57	BA	946	C
57	BA	961	C
57	BA	974	G
57	BA	995	C
57	BA	996	A
57	BA	1009	A
57	BA	1012	U
57	BA	1019	U
57	BA	1020	A
57	BA	1022	G
57	BA	1025	G
57	BA	1033	U
57	BA	1046	A
57	BA	1047	G
57	BA	1048	A
57	BA	1057	A

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Mol	Chain	Res	Type
57	BA	1062	G
57	BA	1065	U
57	BA	1066	U
57	BA	1068	G
57	BA	1069	A
57	BA	1070	A
57	BA	1071	G
57	BA	1073	A
57	BA	1078	U
57	BA	1079	C
57	BA	1087	G
57	BA	1088	A
57	BA	1095	A
57	BA	1096	A
57	BA	1098	A
57	BA	1112	G
57	BA	1128	G
57	BA	1129	A
57	BA	1130	U
57	BA	1132	U
57	BA	1133	A
57	BA	1135	C
57	BA	1143	A
57	BA	1155	A
57	BA	1175	A
57	BA	1176	U
57	BA	1177	G
57	BA	1212	G
57	BA	1225	G
57	BA	1238	G
57	BA	1241	A
57	BA	1248	G
57	BA	1254	A
57	BA	1255	U
57	BA	1256	G
57	BA	1257	C
57	BA	1266	G
57	BA	1271	G
57	BA	1272	A
57	BA	1273	U
57	BA	1287	A
57	BA	1300	G

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Mol	Chain	Res	Type
57	BA	1301	A
57	BA	1302	A
57	BA	1303	G
57	BA	1314	C
57	BA	1324	G
57	BA	1329	U
57	BA	1332	G
57	BA	1333	G
57	BA	1341	G
57	BA	1348	C
57	BA	1349	C
57	BA	1350	C
57	BA	1365	A
57	BA	1366	A
57	BA	1379	U
57	BA	1383	A
57	BA	1384	A
57	BA	1386	C
57	BA	1394	U
57	BA	1396	U
57	BA	1416	G
57	BA	1417	C
57	BA	1451	C
57	BA	1452	G
57	BA	1455	G
57	BA	1458	U
57	BA	1459	G
57	BA	1475	G
57	BA	1482	G
57	BA	1493	C
57	BA	1508	A
57	BA	1509	A
57	BA	1524	G
57	BA	1552	A
57	BA	1568	G
57	BA	1569	A
57	BA	1598	A
57	BA	1607	C
57	BA	1608	A
57	BA	1610	A
57	BA	1611	C
57	BA	1619	G

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Mol	Chain	Res	Type
57	BA	1646	C
57	BA	1647	U
57	BA	1648	U
57	BA	1654	A
57	BA	1669	A
57	BA	1674	G
57	BA	1700	A
57	BA	1713	A
57	BA	1729	U
57	BA	1730	C
57	BA	1732	C
57	BA	1733	G
57	BA	1758	U
57	BA	1762	A
57	BA	1764	C
57	BA	1773	A
57	BA	1791	A
57	BA	1800	C
57	BA	1816	C
57	BA	1839	G
57	BA	1900	A
57	BA	1901	A
57	BA	1906	G
57	BA	1912	A
57	BA	1914	C
57	BA	1916	A
57	BA	1919	A
57	BA	1928	A
57	BA	1930	G
57	BA	1937	A
57	BA	1941	C
57	BA	1942	C
57	BA	1955	U
57	BA	1964	G
57	BA	1965	C
57	BA	1966	A
57	BA	1970	A
57	BA	1971	U
57	BA	1972	G
57	BA	1982	U
57	BA	1992	G
57	BA	1993	U

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Mol	Chain	Res	Type
57	BA	1998	A
57	BA	2023	C
57	BA	2031	A
57	BA	2032	G
57	BA	2056	G
57	BA	2061	G
57	BA	2062	A
57	BA	2068	U
57	BA	2069	7MG
57	BA	2076	U
57	BA	2077	A
57	BA	2092	U
57	BA	2111	U
57	BA	2112	G
57	BA	2113	U
57	BA	2116	G
57	BA	2117	A
57	BA	2118	U
57	BA	2119	A
57	BA	2126	A
57	BA	2127	G
57	BA	2130	U
57	BA	2131	U
57	BA	2132	U
57	BA	2133	G
57	BA	2134	A
57	BA	2146	C
57	BA	2147	A
57	BA	2148	G
57	BA	2154	A
57	BA	2158	A
57	BA	2164	C
57	BA	2165	C
57	BA	2170	A
57	BA	2198	A
57	BA	2203	U
57	BA	2212	A
57	BA	2213	U
57	BA	2239	G
57	BA	2249	U
57	BA	2250	G
57	BA	2251	OMG

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Mol	Chain	Res	Type
57	BA	2253	G
57	BA	2254	C
57	BA	2266	A
57	BA	2276	G
57	BA	2282	G
57	BA	2283	C
57	BA	2287	A
57	BA	2288	A
57	BA	2289	G
57	BA	2306	C
57	BA	2307	G
57	BA	2308	G
57	BA	2309	A
57	BA	2312	U
57	BA	2321	U
57	BA	2325	G
57	BA	2327	A
57	BA	2333	A
57	BA	2334	U
57	BA	2335	A
57	BA	2336	A
57	BA	2337	G
57	BA	2345	G
57	BA	2346	A
57	BA	2347	C
57	BA	2382	G
57	BA	2383	G
57	BA	2385	C
57	BA	2390	U
57	BA	2402	U
57	BA	2403	C
57	BA	2423	U
57	BA	2424	C
57	BA	2425	A
57	BA	2426	A
57	BA	2428	G
57	BA	2429	G
57	BA	2431	U
57	BA	2433	A
57	BA	2435	A
57	BA	2439	A
57	BA	2441	U

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Mol	Chain	Res	Type
57	BA	2447	G
57	BA	2448	A
57	BA	2449	H2U
57	BA	2452	C
57	BA	2472	G
57	BA	2476	A
57	BA	2478	A
57	BA	2489	U
57	BA	2490	G
57	BA	2491	U
57	BA	2492	U
57	BA	2493	U
57	BA	2501	C
57	BA	2502	G
57	BA	2504	PSU
57	BA	2505	G
57	BA	2507	C
57	BA	2513	A
57	BA	2518	A
57	BA	2519	U
57	BA	2529	G
57	BA	2534	A
57	BA	2555	U
57	BA	2565	A
57	BA	2566	A
57	BA	2572	A
57	BA	2573	C
57	BA	2574	G
57	BA	2577	A
57	BA	2585	U
57	BA	2599	G
57	BA	2602	A
57	BA	2613	U
57	BA	2629	U
57	BA	2654	A
57	BA	2658	C
57	BA	2659	G
57	BA	2661	G
57	BA	2663	G
57	BA	2685	G
57	BA	2689	U
57	BA	2690	U

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Mol	Chain	Res	Type
57	BA	2714	G
57	BA	2733	A
57	BA	2757	A
57	BA	2778	A
57	BA	2791	G
57	BA	2792	A
57	BA	2797	U
57	BA	2799	A
57	BA	2800	A
57	BA	2820	A
57	BA	2823	A
57	BA	2834	G
57	BA	2850	A
57	BA	2886	A
57	BA	2894	G
57	BA	2895	G
57	BA	2903	U
57	BA	2904	U
58	Ba	12	C
58	Ba	13	G
58	Ba	14	U
58	Ba	15	A
58	Ba	25	U
58	Ba	41	G
58	Ba	42	C
58	Ba	90	C
58	Ba	99	A
58	Ba	109	A
58	Ba	120	U

All (175) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	AA	2	A
22	AA	3	A
22	AA	5	U
22	AA	6	G
22	AA	13	U
22	AA	48	C
22	AA	49	U
22	AA	51	A
22	AA	71	A

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Mol	Chain	Res	Type
22	AA	121	U
22	AA	161	A
22	AA	197	A
22	AA	205	A
22	AA	243	A
22	AA	262	A
22	AA	279	A
22	AA	297	G
22	AA	305	G
22	AA	328	C
22	AA	329	A
22	AA	331	G
22	AA	367	U
22	AA	372	C
22	AA	412	A
22	AA	451	A
22	AA	464	U
22	AA	465	A
22	AA	497	G
22	AA	531	U
22	AA	575	G
22	AA	619	U
22	AA	700	G
22	AA	717	U
22	AA	719	C
22	AA	765	G
22	AA	812	G
22	AA	840	C
22	AA	845	A
22	AA	934	C
22	AA	974	A
22	AA	1101	A
22	AA	1183	U
22	AA	1213	A
22	AA	1214	C
22	AA	1225	A
22	AA	1238	A
22	AA	1256	A
22	AA	1281	C
22	AA	1302	C
22	AA	1305	G
22	AA	1319	A

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Mol	Chain	Res	Type
22	AA	1380	U
22	AA	1397	C
22	AA	1491	G
22	AA	1529	G
22	AA	1537	U
22	AA	1539	C
23	A2	33	A
24	A3	9	G
24	A3	10	G
57	BA	13	A
57	BA	48	G
57	BA	61	C
57	BA	119	A
57	BA	121	G
57	BA	140	C
57	BA	190	A
57	BA	196	A
57	BA	242	G
57	BA	249	C
57	BA	301	G
57	BA	311	A
57	BA	332	A
57	BA	387	U
57	BA	394	C
57	BA	395	U
57	BA	479	A
57	BA	489	G
57	BA	529	A
57	BA	544	C
57	BA	545	U
57	BA	561	G
57	BA	587	C
57	BA	603	A
57	BA	620	G
57	BA	637	A
57	BA	651	G
57	BA	653	U
57	BA	718	A
57	BA	752	A
57	BA	782	A
57	BA	804	A
57	BA	850	U

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Mol	Chain	Res	Type
57	BA	859	G
57	BA	866	A
57	BA	896	A
57	BA	920	A
57	BA	958	U
57	BA	960	A
57	BA	995	C
57	BA	1019	U
57	BA	1033	U
57	BA	1061	U
57	BA	1078	U
57	BA	1088	A
57	BA	1095	A
57	BA	1128	G
57	BA	1133	A
57	BA	1142	A
57	BA	1254	A
57	BA	1256	G
57	BA	1286	A
57	BA	1301	A
57	BA	1313	U
57	BA	1324	G
57	BA	1325	U
57	BA	1332	G
57	BA	1349	C
57	BA	1365	A
57	BA	1393	A
57	BA	1451	C
57	BA	1458	U
57	BA	1474	U
57	BA	1508	A
57	BA	1568	G
57	BA	1607	C
57	BA	1610	A
57	BA	1614	A
57	BA	1646	C
57	BA	1647	U
57	BA	1653	G
57	BA	1668	A
57	BA	1674	G
57	BA	1729	U
57	BA	1758	U

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Mol	Chain	Res	Type
57	BA	1786	A
57	BA	1929	G
57	BA	1937	A
57	BA	1939	5MU
57	BA	1941	C
57	BA	2042	A
57	BA	2060	A
57	BA	2061	G
57	BA	2062	A
57	BA	2068	U
57	BA	2076	U
57	BA	2092	U
57	BA	2117	A
57	BA	2131	U
57	BA	2133	G
57	BA	2248	C
57	BA	2251	OMG
57	BA	2253	G
57	BA	2308	G
57	BA	2336	A
57	BA	2345	G
57	BA	2402	U
57	BA	2422	C
57	BA	2423	U
57	BA	2430	A
57	BA	2440	C
57	BA	2447	G
57	BA	2489	U
57	BA	2529	G
57	BA	2564	A
57	BA	2571	U
57	BA	2615	U
57	BA	2629	U
57	BA	2655	G
57	BA	2660	A
57	BA	2755	C
57	BA	2756	U
57	BA	2790	U
57	BA	2885	G
57	BA	2894	G

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

39 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
24	H2U	A3	21	24	17,21,22	1.08	2 (11%)	23,30,33	1.09	2 (8%)
24	OMC	A3	33	24	15,22,23	1.04	1 (6%)	20,31,34	0.79	0
24	5MU	A3	55	24	13,22,23	0.99	1 (7%)	16,32,35	4.63	2 (12%)
24	PSU	A3	56	24	15,21,22	1.10	2 (13%)	16,30,33	3.45	4 (25%)
24	4SU	A3	8	24	12,21,22	1.04	1 (8%)	15,30,33	1.64	1 (6%)
22	2MG	AA	1207	22	18,26,27	1.07	1 (5%)	21,38,41	2.60	5 (23%)
22	4OC	AA	1402	22	15,23,24	0.94	1 (6%)	21,32,35	1.56	4 (19%)
22	5MC	AA	1407	22	14,22,23	1.11	1 (7%)	17,32,35	1.17	1 (5%)
22	UR3	AA	1498	22	13,22,23	0.82	0	18,32,35	1.12	1 (5%)
22	2MG	AA	1516	22	18,26,27	1.05	1 (5%)	21,38,41	2.75	7 (33%)
22	MA6	AA	1518	22	18,26,27	0.82	1 (5%)	15,38,41	1.36	1 (6%)
22	MA6	AA	1519	22	18,26,27	0.83	1 (5%)	15,38,41	1.35	1 (6%)
22	PSU	AA	516	22	15,21,22	1.08	2 (13%)	16,30,33	3.48	4 (25%)
22	7MG	AA	527	22	20,26,27	2.14	4 (20%)	23,39,42	2.11	2 (8%)
22	2MG	AA	966	22	18,26,27	1.11	1 (5%)	21,38,41	2.53	4 (19%)
22	5MC	AA	967	22	14,22,23	1.04	1 (7%)	17,32,35	1.25	2 (11%)
57	6MZ	BA	1618	57	17,25,26	0.86	0	15,36,39	1.46	2 (13%)
57	2MG	BA	1835	57	18,26,27	1.08	1 (5%)	21,38,41	2.48	5 (23%)
57	PSU	BA	1911	57	15,21,22	1.09	2 (13%)	16,30,33	3.65	3 (18%)
57	3TD	BA	1915	57	15,22,23	0.99	0	17,32,35	1.70	3 (17%)
57	PSU	BA	1917	57	15,21,22	1.07	2 (13%)	16,30,33	3.53	3 (18%)
57	5MU	BA	1939	57	13,22,23	1.01	1 (7%)	16,32,35	4.36	3 (18%)
57	5MC	BA	1962	57	14,22,23	1.11	1 (7%)	17,32,35	1.46	3 (17%)
57	6MZ	BA	2030	57	17,25,26	0.85	0	15,36,39	1.35	2 (13%)
57	7MG	BA	2069	57	20,26,27	2.14	3 (15%)	23,39,42	2.20	2 (8%)
57	OMG	BA	2251	57	18,26,27	1.11	1 (5%)	21,38,41	2.54	5 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	2MG	BA	2445	57	18,26,27	1.02	1 (5%)	21,38,41	2.59	6 (28%)
57	H2U	BA	2449	57	17,21,22	1.20	2 (11%)	23,30,33	1.02	0
57	PSU	BA	2457	57	15,21,22	1.10	2 (13%)	16,30,33	3.49	3 (18%)
57	OMC	BA	2498	57	15,22,23	1.11	1 (6%)	20,31,34	0.90	0
57	2MA	BA	2503	57	17,25,26	0.95	0	18,37,40	2.28	4 (22%)
57	PSU	BA	2504	57	15,21,22	1.06	2 (13%)	16,30,33	3.44	2 (12%)
57	OMU	BA	2552	57	14,22,23	1.09	2 (14%)	19,31,34	2.70	3 (15%)
57	PSU	BA	2580	57	15,21,22	1.09	2 (13%)	16,30,33	3.83	4 (25%)
57	PSU	BA	2605	57	15,21,22	1.03	2 (13%)	16,30,33	3.90	5 (31%)
57	1MG	BA	745	57	17,26,27	1.00	0	19,39,42	1.54	2 (10%)
57	PSU	BA	746	57	15,21,22	1.08	2 (13%)	16,30,33	3.57	4 (25%)
57	5MU	BA	747	57	13,22,23	1.05	1 (7%)	16,32,35	4.34	3 (18%)
57	PSU	BA	955	57	15,21,22	1.08	2 (13%)	16,30,33	3.34	4 (25%)

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
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
22	2MG	AA	1207	22	-	0/5/27/28	0/3/3/3
22	4OC	AA	1402	22	-	0/7/29/30	0/2/2/2
22	5MC	AA	1407	22	-	0/3/25/26	0/2/2/2
22	UR3	AA	1498	22	-	0/3/25/26	0/2/2/2
22	2MG	AA	1516	22	-	0/5/27/28	0/3/3/3
22	MA6	AA	1518	22	-	0/7/29/30	0/3/3/3
22	MA6	AA	1519	22	-	0/7/29/30	0/3/3/3
22	PSU	AA	516	22	-	0/7/25/26	0/2/2/2
22	7MG	AA	527	22	-	0/7/37/38	0/3/3/3
22	2MG	AA	966	22	-	0/5/27/28	0/3/3/3
22	5MC	AA	967	22	-	0/3/25/26	0/2/2/2
57	6MZ	BA	1618	57	-	0/5/27/28	0/3/3/3
57	2MG	BA	1835	57	-	0/5/27/28	0/3/3/3
57	PSU	BA	1911	57	-	0/7/25/26	0/2/2/2
57	3TD	BA	1915	57	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PSU	BA	1917	57	-	0/7/25/26	0/2/2/2
57	5MU	BA	1939	57	-	0/3/25/26	0/2/2/2
57	5MC	BA	1962	57	-	0/3/25/26	0/2/2/2
57	6MZ	BA	2030	57	-	0/5/27/28	0/3/3/3
57	7MG	BA	2069	57	-	0/7/37/38	0/3/3/3
57	OMG	BA	2251	57	-	0/5/27/28	0/3/3/3
57	2MG	BA	2445	57	-	0/5/27/28	0/3/3/3
57	H2U	BA	2449	57	-	0/7/38/39	0/2/2/2
57	PSU	BA	2457	57	-	0/7/25/26	0/2/2/2
57	OMC	BA	2498	57	-	0/5/27/28	0/2/2/2
57	2MA	BA	2503	57	-	0/3/25/26	0/3/3/3
57	PSU	BA	2504	57	-	0/7/25/26	0/2/2/2
57	OMU	BA	2552	57	-	0/5/27/28	0/2/2/2
57	PSU	BA	2580	57	-	0/7/25/26	0/2/2/2
57	PSU	BA	2605	57	-	0/7/25/26	0/2/2/2
57	1MG	BA	745	57	-	0/3/25/26	0/3/3/3
57	PSU	BA	746	57	-	0/7/25/26	0/2/2/2
57	5MU	BA	747	57	-	0/3/25/26	0/2/2/2
57	PSU	BA	955	57	-	0/7/25/26	0/2/2/2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	2069	7MG	C8-N9	-7.87	1.34	1.45
22	AA	527	7MG	C8-N9	-7.74	1.34	1.45
57	BA	2449	H2U	C4-N3	-3.25	1.32	1.37
24	A3	21	H2U	C4-N3	-2.88	1.33	1.37
57	BA	2449	H2U	C2-N3	-2.82	1.32	1.38
57	BA	2069	7MG	C8-N7	-2.69	1.31	1.43
22	AA	527	7MG	C8-N7	-2.61	1.31	1.43
24	A3	21	H2U	C2-N3	-2.47	1.33	1.38
57	BA	2498	OMC	C4-N3	-2.34	1.31	1.35
24	A3	33	OMC	C4-N3	-2.15	1.31	1.35
22	AA	1518	MA6	C8-N7	-2.06	1.30	1.34
22	AA	1519	MA6	C8-N7	-2.02	1.30	1.34
57	BA	2457	PSU	C6-N1	2.02	1.38	1.34
57	BA	1917	PSU	C6-N1	2.07	1.38	1.34
22	AA	1402	4OC	C5-C4	2.08	1.44	1.39
57	BA	2504	PSU	C6-N1	2.09	1.38	1.34
57	BA	2552	OMU	C6-N1	2.10	1.38	1.35
57	BA	2605	PSU	C4-N3	2.10	1.36	1.33
57	BA	955	PSU	C6-N1	2.11	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	746	PSU	C6-N1	2.12	1.38	1.34
24	A3	8	4SU	C6-N1	2.15	1.38	1.35
22	AA	516	PSU	C6-N1	2.15	1.38	1.34
57	BA	2580	PSU	C6-N1	2.16	1.39	1.34
24	A3	56	PSU	C6-N1	2.16	1.39	1.34
57	BA	1911	PSU	C6-N1	2.17	1.39	1.34
22	AA	527	7MG	C4-N3	2.26	1.37	1.34
57	BA	1911	PSU	C4-N3	2.32	1.37	1.33
57	BA	2605	PSU	C6-N1	2.32	1.39	1.34
24	A3	56	PSU	C4-N3	2.42	1.37	1.33
22	AA	516	PSU	C4-N3	2.48	1.37	1.33
57	BA	1917	PSU	C4-N3	2.50	1.37	1.33
57	BA	955	PSU	C4-N3	2.53	1.37	1.33
57	BA	2580	PSU	C4-N3	2.55	1.37	1.33
24	A3	55	5MU	C4-N3	2.59	1.37	1.33
22	AA	967	5MC	C5-C4	2.60	1.45	1.41
57	BA	746	PSU	C4-N3	2.62	1.37	1.33
57	BA	2504	PSU	C4-N3	2.66	1.37	1.33
22	AA	1407	5MC	C5-C4	2.67	1.45	1.41
22	AA	1516	2MG	C6-N1	2.67	1.37	1.33
57	BA	747	5MU	C4-N3	2.69	1.37	1.33
57	BA	2457	PSU	C4-N3	2.69	1.37	1.33
57	BA	2445	2MG	C6-N1	2.69	1.37	1.33
22	AA	1207	2MG	C6-N1	2.72	1.37	1.33
57	BA	1939	5MU	C4-N3	2.74	1.38	1.33
57	BA	2069	7MG	C6-N1	2.78	1.38	1.33
57	BA	2552	OMU	C4-N3	2.78	1.38	1.33
57	BA	1835	2MG	C6-N1	2.78	1.38	1.33
57	BA	2251	OMG	C6-N1	2.79	1.38	1.33
57	BA	1962	5MC	C5-C4	2.82	1.45	1.41
22	AA	527	7MG	C6-N1	2.82	1.38	1.33
22	AA	966	2MG	C6-N1	3.02	1.38	1.33

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	55	5MU	C5-C4-N3	-12.66	114.73	125.35
57	BA	1939	5MU	C5-C4-N3	-12.14	115.16	125.35
57	BA	747	5MU	C5-C4-N3	-12.11	115.18	125.35
57	BA	2251	OMG	C5-C6-N1	-7.74	113.40	123.52
22	AA	1516	2MG	C5-C6-N1	-7.54	113.67	123.52
22	AA	1207	2MG	C5-C6-N1	-7.44	113.80	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2445	2MG	C5-C6-N1	-7.34	113.92	123.52
57	BA	1835	2MG	C5-C6-N1	-7.28	114.00	123.52
57	BA	2503	2MA	C2-N3-C4	-7.28	111.78	115.29
22	AA	966	2MG	C5-C6-N1	-7.22	114.08	123.52
57	BA	2069	7MG	C5-C6-N1	-7.00	112.96	123.39
22	AA	527	7MG	C5-C6-N1	-6.71	113.39	123.39
24	A3	8	4SU	C5-C4-N3	-5.45	117.78	123.56
22	AA	516	PSU	C5-C6-N1	-4.31	118.36	124.38
57	BA	2605	PSU	C5-C6-N1	-4.27	118.42	124.38
57	BA	1915	3TD	C5-C6-N1	-4.21	118.51	124.38
57	BA	745	1MG	C5-C6-N1	-4.21	112.84	118.35
57	BA	955	PSU	C5-C6-N1	-4.21	118.51	124.38
57	BA	2504	PSU	C5-C6-N1	-4.18	118.55	124.38
57	BA	2580	PSU	C5-C6-N1	-4.12	118.63	124.38
24	A3	56	PSU	C5-C6-N1	-4.11	118.65	124.38
57	BA	1917	PSU	C5-C6-N1	-4.00	118.80	124.38
57	BA	1911	PSU	C5-C6-N1	-3.90	118.94	124.38
57	BA	746	PSU	C5-C6-N1	-3.87	118.98	124.38
57	BA	2457	PSU	C5-C6-N1	-3.81	119.07	124.38
57	BA	2552	OMU	C5-C4-N3	-3.60	114.44	123.28
57	BA	2605	PSU	C5-C1'-C2'	-3.37	109.71	115.44
57	BA	2503	2MA	C6-C5-C4	-3.28	113.78	119.67
57	BA	1962	5MC	N4-C4-N3	-3.04	112.46	116.92
57	BA	1915	3TD	C4'-O4'-C1'	-2.99	106.46	109.54
57	BA	2445	2MG	C6-C5-C4	-2.96	117.47	120.86
22	AA	966	2MG	C6-C5-C4	-2.87	117.58	120.86
22	AA	1516	2MG	N2-C2-N1	-2.86	113.62	116.94
22	AA	1516	2MG	C6-C5-C4	-2.78	117.68	120.86
22	AA	1207	2MG	C6-C5-C4	-2.75	117.72	120.86
57	BA	1835	2MG	C6-C5-C4	-2.58	117.91	120.86
57	BA	1915	3TD	C5-C4-N3	-2.39	116.70	118.65
57	BA	1939	5MU	C4'-O4'-C1'	-2.39	107.11	109.64
57	BA	2251	OMG	C6-C5-C4	-2.38	118.14	120.86
57	BA	2605	PSU	C4-C5-C1'	-2.37	117.23	121.22
57	BA	1911	PSU	C5-C1'-C2'	-2.27	111.57	115.44
22	AA	1516	2MG	C1'-N9-C4	-2.27	124.28	126.81
57	BA	2445	2MG	C1'-N9-C4	-2.25	124.29	126.81
24	A3	21	H2U	C5-C6-N1	-2.17	108.38	110.76
57	BA	955	PSU	C5-C1'-C2'	-2.12	111.84	115.44
57	BA	2030	6MZ	C4'-O4'-C1'	-2.09	107.43	109.64
22	AA	967	5MC	N4-C4-N3	-2.09	113.86	116.92
22	AA	516	PSU	O2'-C2'-C1'	-2.08	107.40	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1917	PSU	O2'-C2'-C1'	-2.06	107.45	111.93
57	BA	2503	2MA	C2'-C3'-C4'	-2.01	98.52	102.64
24	A3	56	PSU	C5-C1'-C2'	-2.00	112.03	115.44
57	BA	2251	OMG	O3'-C3'-C2'	2.04	117.03	111.13
57	BA	746	PSU	C3'-C2'-C1'	2.05	104.14	101.71
57	BA	955	PSU	O4'-C1'-C2'	2.19	107.06	104.69
57	BA	1962	5MC	O4'-C1'-N1	2.22	112.32	108.10
57	BA	747	5MU	O4'-C1'-N1	2.23	112.34	108.10
22	AA	967	5MC	CM5-C5-C4	2.32	123.92	121.47
57	BA	1835	2MG	CM2-N2-C2	2.38	125.71	123.03
57	BA	2445	2MG	O4'-C1'-N9	2.38	112.60	108.11
57	BA	2552	OMU	C6-C5-C4	2.39	121.72	117.30
24	A3	56	PSU	O4'-C1'-C2'	2.39	107.28	104.69
57	BA	2251	OMG	O4'-C1'-N9	2.44	112.72	108.11
22	AA	1498	UR3	C6-C5-C4	2.46	121.85	117.30
22	AA	1207	2MG	CM2-N2-C2	2.51	125.86	123.03
22	AA	1407	5MC	CM5-C5-C4	2.54	124.16	121.47
57	BA	2457	PSU	O4'-C1'-C2'	2.56	107.46	104.69
22	AA	1402	4OC	O4'-C1'-N1	2.60	113.03	108.10
22	AA	516	PSU	O4'-C1'-C2'	2.60	107.50	104.69
57	BA	2580	PSU	C3'-C2'-C1'	2.63	104.83	101.71
57	BA	1618	6MZ	O4'-C1'-N9	2.63	113.08	108.11
24	A3	21	H2U	C1'-N1-C2	2.69	121.95	118.19
22	AA	1402	4OC	C6-C5-C4	2.75	118.50	117.42
57	BA	746	PSU	O4'-C1'-C2'	3.01	107.94	104.69
22	AA	1516	2MG	CM2-N2-C2	3.10	126.52	123.03
57	BA	1962	5MC	CM5-C5-C4	3.18	124.83	121.47
57	BA	745	1MG	N2-C2-N1	3.19	122.02	118.26
22	AA	966	2MG	N2-C2-N3	3.25	120.72	116.94
22	AA	1402	4OC	C2-N3-C4	3.28	119.61	115.43
57	BA	2445	2MG	N2-C2-N3	3.35	120.83	116.94
57	BA	2605	PSU	O4'-C1'-C2'	3.39	108.36	104.69
57	BA	2580	PSU	O4'-C1'-C2'	3.47	108.44	104.69
57	BA	2503	2MA	O4'-C1'-N9	3.57	114.84	108.11
57	BA	1835	2MG	N2-C2-N3	3.58	121.09	116.94
57	BA	2030	6MZ	C2-N1-C6	3.59	119.05	116.47
22	AA	1519	MA6	C2-N1-C6	3.60	120.12	111.64
57	BA	1618	6MZ	C2-N1-C6	3.77	119.18	116.47
22	AA	1518	MA6	C2-N1-C6	3.87	120.77	111.64
22	AA	1207	2MG	N2-C2-N3	3.93	121.51	116.94
22	AA	1402	4OC	CM4-N4-C4	4.06	126.30	122.87
22	AA	1516	2MG	N2-C2-N3	4.42	122.08	116.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	966	2MG	C6-N1-C2	6.08	123.95	115.24
57	BA	1835	2MG	C6-N1-C2	6.10	123.98	115.24
22	AA	1516	2MG	C6-N1-C2	6.19	124.11	115.24
57	BA	2445	2MG	C6-N1-C2	6.28	124.24	115.24
22	AA	527	7MG	C6-N1-C2	6.40	123.38	115.88
22	AA	1207	2MG	C6-N1-C2	6.40	124.41	115.24
57	BA	2251	OMG	C6-N1-C2	6.61	123.63	115.88
57	BA	2069	7MG	C6-N1-C2	6.85	123.91	115.88
57	BA	2552	OMU	C4-N3-C2	10.47	125.24	114.21
57	BA	747	5MU	C4-N3-C2	11.84	125.04	115.16
57	BA	1939	5MU	C4-N3-C2	11.86	125.05	115.16
57	BA	955	PSU	C4-N3-C2	11.94	125.12	115.16
22	AA	516	PSU	C4-N3-C2	12.27	125.40	115.16
24	A3	56	PSU	C4-N3-C2	12.29	125.41	115.16
57	BA	2457	PSU	C4-N3-C2	12.72	125.77	115.16
57	BA	2504	PSU	C4-N3-C2	12.74	125.79	115.16
57	BA	746	PSU	C4-N3-C2	12.76	125.80	115.16
57	BA	1917	PSU	C4-N3-C2	12.89	125.91	115.16
24	A3	55	5MU	C4-N3-C2	13.04	126.04	115.16
57	BA	1911	PSU	C4-N3-C2	13.42	126.36	115.16
57	BA	2580	PSU	C4-N3-C2	13.52	126.44	115.16
57	BA	2605	PSU	C4-N3-C2	13.82	126.69	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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.