



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:01 PM BST

PDB ID : 4V71  
EMDB ID: : EMD-1717  
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate pre-translocation state (pre2)  
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.  
Deposited on : 2013-10-14  
Resolution : 20.00 Å(reported)  
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a 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>

---

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

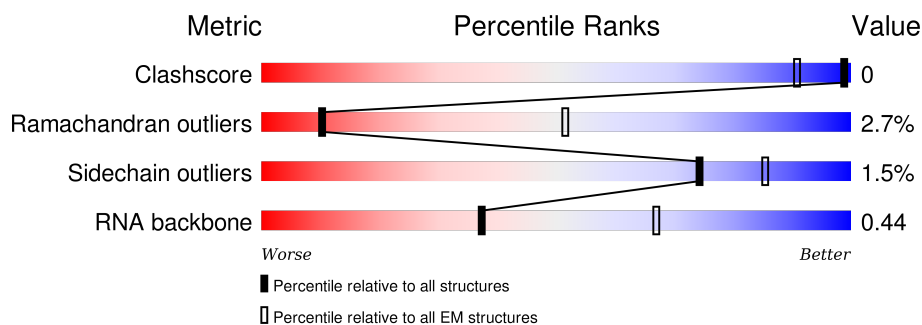
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 20.00 Å.

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














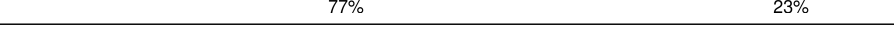
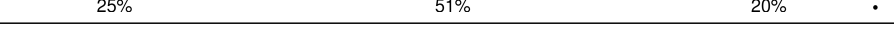
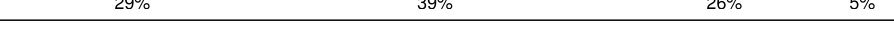
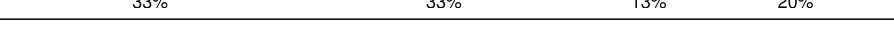
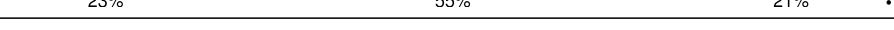



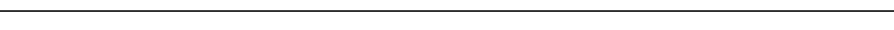

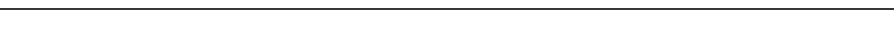
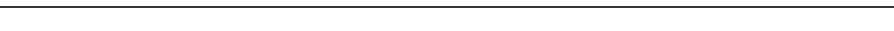


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AB	220	92% 7%
2	AC	208	89% 11%
3	AD	206	90% 9%
4	AE	152	90% 10%
5	AF	101	90% 10%
6	AG	152	89% 11%
7	AH	130	90% 9% .
8	AI	128	86% 13% .












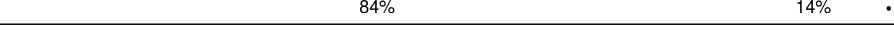

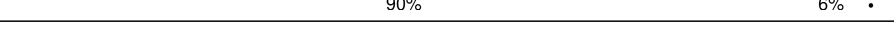







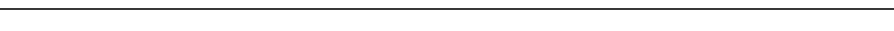

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	AJ	100	 85% 12% .
10	AK	118	 86% 13% .
11	AL	124	 87% 12% .
12	AM	115	 85% 14% .
13	AN	101	 88% 11% .
14	AO	89	 87% 12% .
15	AP	81	 85% 15%
16	AQ	82	 88% 12%
17	AR	57	 88% 12%
18	AS	81	 89% 9% .
19	AT	86	 91% 9%
20	AU	53	 77% 23%
21	AA	1533	 25% 51% 20% .
22	A1	76	 29% 39% 26% 5%
23	A2	15	 33% 33% 13% 20%
24	A3	77	 23% 55% 21% .
25	BC	273	 88% 11%
26	BD	209	 89% 11%
27	BE	201	 92% 8%
28	BF	179	 88% 11% .
29	BG	177	 92% 7% ..
30	BH	149	 95% 5%
31	BI	142	 95% . ..
32	BJ	142	 89% 11%
33	BK	123	 90% 9% .

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
34	BL	144	 90% 9% .
35	BM	136	 85% 15%
36	BN	121	 83% 17% .
37	BO	117	 89% 9% ..
38	BP	115	 82% 17% ..
39	BQ	118	 85% 13% ..
40	BR	103	 90% 10%
41	BS	110	 90% 9% .
42	BT	94	 86% 14%
43	BU	104	 90% 7% ..
44	BV	94	 89% 11%
45	BW	80	 84% 14% .
46	BX	79	 84% 13% ..
47	BY	63	 90% 6% .
48	BZ	59	 88% 10% .
49	B0	57	 84% 14% .
50	B1	52	 92% 8%
51	B2	46	 76% 22% .
52	B3	65	 91% 8% .
53	B4	38	 82% 18%
54	BA	2903	 23% 50% 23% .
55	BB	118	 25% 49% 22% ..
56	B5	234	 89% 6% 5%

## 2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

*Continued on next page...*



*Continued from previous page...*

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

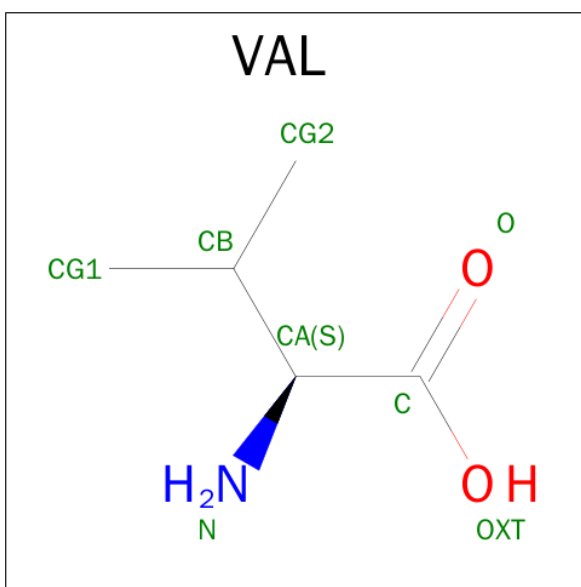
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

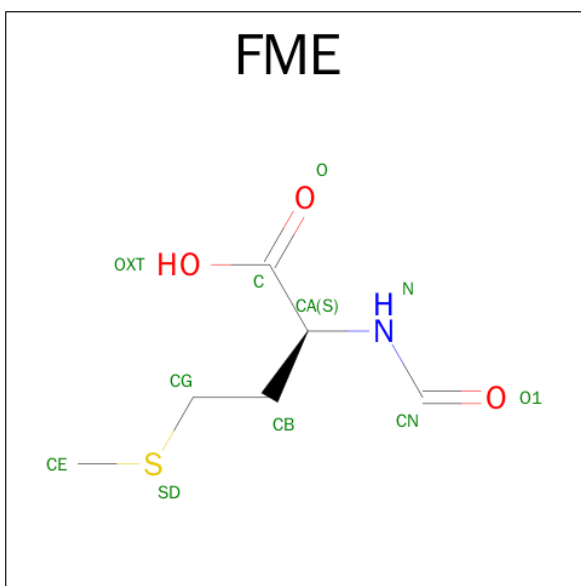
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



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

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ).



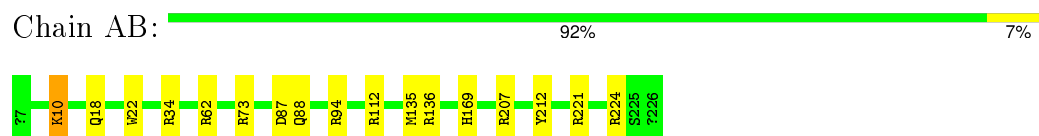
Mol	Chain	Residues	Atoms					AltConf
58	A1	1	Total	C	N	O	S	0
			10	6	1	2	1	



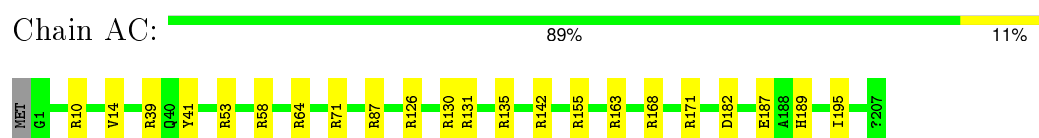
### 3 Residue-property plots [i](#)

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

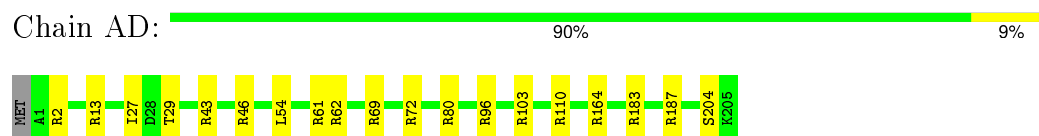
- Molecule 1: 30S ribosomal protein S2



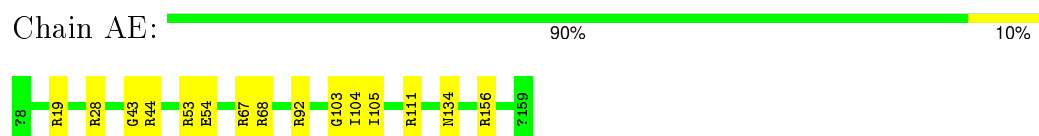
- Molecule 2: 30S ribosomal protein S3



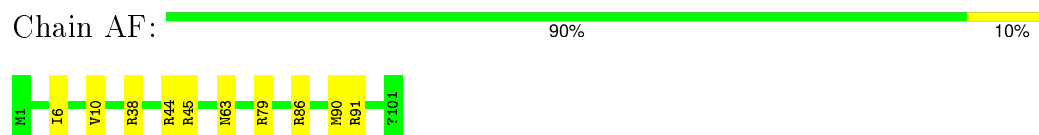
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



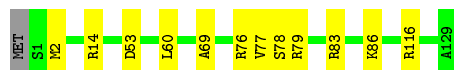
- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 90% 9%



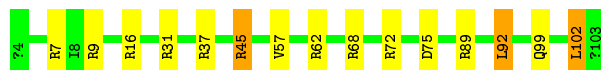
- Molecule 8: 30S ribosomal protein S9

Chain AI: 86% 13%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 85% 12%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 86% 13%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 87% 12%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%




- Molecule 13: 30S ribosomal protein S14

Chain AN: 88% 11%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  87% 12%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  85% 15%



- Molecule 16: 30S ribosomal protein S17

Chain AQ:  88% 12%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  88% 12%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  89% 9%




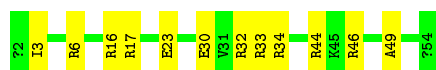
- Molecule 19: 30S ribosomal protein S20

Chain AT:  91% 9%



- Molecule 20: 30S ribosomal protein S21

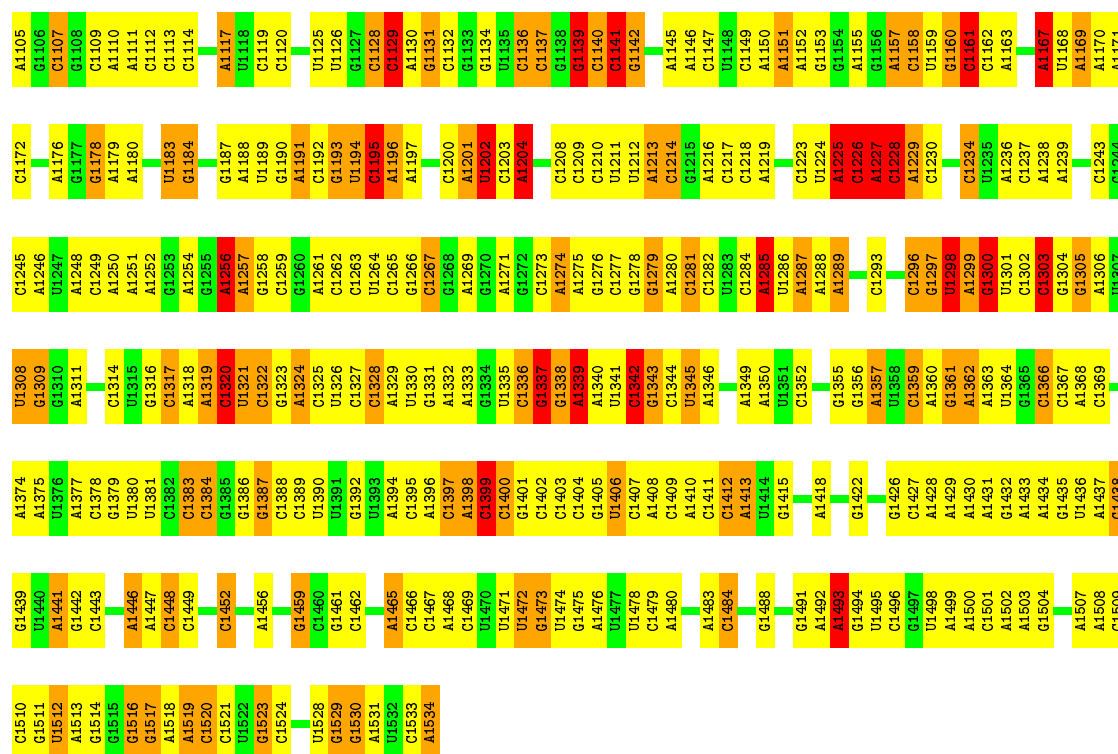
Chain AU:  77% 23%



- Molecule 21: 16S ribosomal RNA

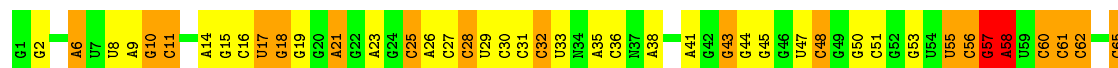
Chain AA:  25% 51% 20%

G1034	A969	U905	U843	C778	G711	U644	A579	C513	A451	U587	A327	G265	G200	C136	G67	A
A1035	C970	A906	G844	C779	A712	G845	C580	C514	A452	G388	C328	G266	G201	U137	G68	A
A1036	G971	A907	A845	A780	G713	G846	G581		A453	A389	A329	C267	G202	U138	G69	U
C1037	C972	A908	G846	A781	G714	G847	C582	G517	A454	U390	C330	U268	G203	A139	U70	G6
C1038	G973	A909	G847	A782	A715	A648	A583	C518	A455	G391	G331	C269	G204	U140	A71	G6
	G974	C910	C848	A783	A716	A649	A584	C519	A456	C392	G332	A270	G205		A72	A7
A1042	A975	U911		A784	U717	G850	G585	A520	A457	A393	U333	C271	C206	A143	C73	A8
G1043	G976	C912	G851	G785	A718	C851	C586	G521	U458	G394	C334	C272	C207		A74	A9
A1044	A977	A913	G852	G786	C719	U852	G587	C522	A459	C395	C335	U273	U208	G148	G75	A10
C1045	A978	A914	C853	A787	C720	U853	G588	A523	A460	C396	A336	U274	U209	A149	A76	G11
A1046	C979	A915		U788		G854	U589	G524	A461	C397	G337		C210	U150	A77	U12
G1047	G980	U916	C856	U789	U723	A655		C525	A462	U398	A338	C277	G211	A151	A78	
G1048	U981	C917	C857	A790	G724		G592	C526	U463	G399	C339	G278	G212	A152	A79	A16
U1049	U982	A918	G858	G791	G725	C858		G527	U464	C400	U340	A279	G213	C153	A80	U17
G1050	A983	A919	G859	A792	G726	U859	A595	C528	U465	C401	C341	C280	C214	C154	A81	C18
C1051	C984		A860	U793	G727	G860	A596	G529	A466	G402	C342	G281	C215	U154	G82	A19
U1052	C985	A923	G861	A794	A728	U861	G597	C530	U467	C403	C343	A282	C216	C156	U83	U20
G1053	U986	C924	C862	C795	A729	U862	U598	U531	G404	G404	A344	U283	C217	U157	U84	G21
C1054	G987	G925	U863	C796		A863	C599	A532	C469	U405	C345	C284		G158	U85	G22
A1055	G988	G926	A864	C797	C732	G864	A600	A533	C470	U406	G346	C285	G220	G159	G86	C23
U1056	U989	G927	A865	U798	G733	A665	G601	A534		G407	G347	C286	C221	A160	G87	C24
G1057	C990	G928	C866		G734	G866	A602	A535	U473	A408	A348	C287	C222	A161	C88	C25
U1058	U991	G929	U867	C735	G735		U603	C536	C474	U409	A349	A288	C223	A162	A26	A26
C1059	U992	C930	G868	C736	C736	U672	G604	G537	C475	G410	G350	G289	U224	G163	G94	G27
U1060	G993	C931	C869	C737	C737	A673		G538	U476	A411	G351	C290		G164	G95	U29
G1061	A994	C932	U870	C738	C738	G874	A607	A539	C477	A412	C352	U291	G226	G165	U96	U30
U1062	C995	G933	U871	C739		A675	A608	G540	U478	G413	G353	G292	G227	U166	G97	G31
C1063	A996	C934	A872	U740	U740	A676	A609	A545	U479	A414	G354	G293	A228	A167	G98	A32
G1064	U997	A935	A873	C908	G741	U677	U610	C546	U480	G415	C355	U294		G168	C99	A33
	C998	G936	G874	G909	G742	U678	C611	A546	G481	G416	A356	C295		C169	G100	
A1067	U999	A937	U875	C810	A743	C679	C612	A547	A482	G417	G357	U296	G232	U170	G101	C34
G1068	A1000	A938	C876	C744	C744	C680	C613	G548	G483	C418	U358	G297	G233	A171	A101	G35
C1069	C1001	C940	G877	G745	G745	A681	G614	C549	G484	G420	G359	A298		A172		C36
U1070	G1002	C941	U878	U746	A747	G682				U421	G360	G299	C235	U173	G105	U37
C1071	G1003	C942	G880	G683	G683	G683	G617	U552	A487	A422	G361	A300	A236	C174	C106	G38
G1072	A1004	U943	U886	U748		U886	U619	A553	C488	G423	G362	G301		C175	G107	G39
U1073	A1005	G944	A881	A749	C750	A887	G620	U554	C489	G424	A363	A303	A238	G176	G108	
	G1006	G945	C882	C817		G888	A621	C556	C490	G425	A364	U304	U239	G177	A109	
G1077		A946	C883	G818	U751	C889	A622	G557	G491	U426	U365	G305	G240	C178	C110	C43
		G947	U884	A819	G752	G691	C623	G558	A492	G428	U367	A306	G241	A179	G111	C44
A1080	C1011	U948	G885	C823	A753		C624	A559	A493	G429	U368	A307	A243	A181	G112	
A1081	A1012	A949	G886	G824	C754	G691	C625	A560	A494	U430	G369	C308	U244	A182	G113	C47
A1082	G1013	G950	G887	A825	C755	A894	U625	U561	A495	A431	C370	A309	U245	C183	U114	C48
U1083	A1014	G951	G888	G826	C756		G626	U562	A496	A432	A371	G310	A246	G184	U49	
G1084	G1015		A889	U757	U757	A895	G627	U563	G497		C372	G247		U185	A50	A51
U1085	A1016	G954	G890	C758		A896	G628	A563	A498	A435	A373	C312	C248	C186	A119	C52
A1092	A1019	U955	U891	A759	G760	U697	A629	C564	A499		A374	U249	G187	A120	A53	
A1093	G1020	U956	A892	G829		G698	A630	U565	C500	C436	U375	C314	A250	G188	U121	C54
G1094	A1021	C957	C893	G760		C699	C631	G566	G501		G376	A315	G251	A189	G122	A55
U1095	A1022	A958	C894	G763		G700	U632	G567	A502	C440	G377	C316	U252	A190	U123	
C1096			G895	C764		U701	G633	G568	C503	A441	G378	U317		G191	C124	C58
U1097	U1025	U960	C896	G765		A702	C634	C569	G504	A442	C379	A320	A253	A192	U125	A59
C1098	G1026	U961	C897	A766		G703	A635	G505	G505	C443	C379	G321	G255	C193	U126	A60
G1099	C1027	C962	G898	A767		A704	U636	G506	C443		G376	A322	U256	G194	A129	G61
C1100	C1028	G963	U899	G768		G705	C637	A574	U508	G446	C381	A321	G257	A195	U130	U62
		A964	A900	G769		A706		A575		G447	A382	U323		A196	A131	C63
A1101		U965	A901	C770		U707	A640	G575	A509	G448	A383	G324	A262	A197	G64	
A1102	C1031	G966	G902	C840		U708	U641	C576	A510	G449	G384	G325	A263	G198	A65	
C1103	G1032	C967	G903	C841		U709	A642	G577	C511		C385	A326				
G1104	G1033	A968	U904	U842		G710	C643	C578	U512		C386	G326	C264	A199	C135	



• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 29% 39% 26% 5%



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

Chain A2: 33% 33% 13% 20%

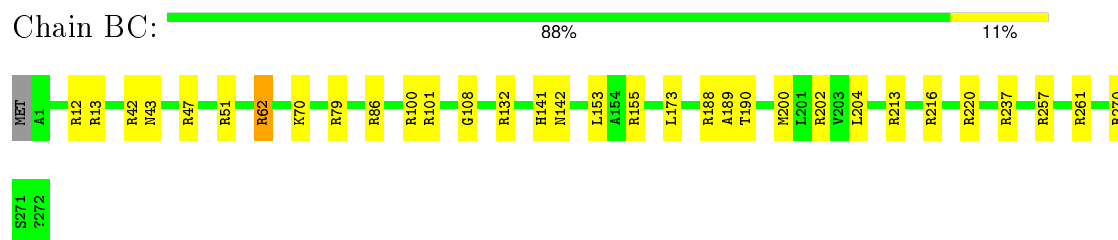


• Molecule 24: tRNA-fMet

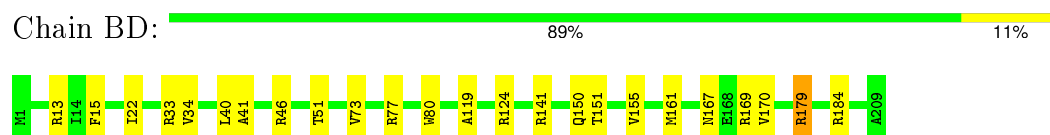
Chain A3: 23% 55% 21%



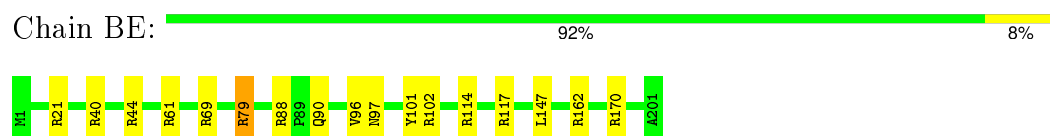
• Molecule 25: 50S ribosomal protein L2



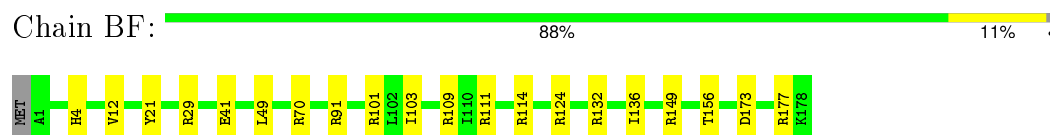
- Molecule 26: 50S ribosomal protein L3



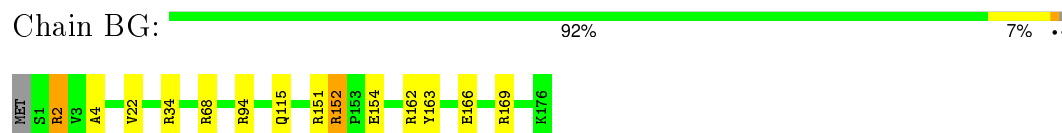
- Molecule 27: 50S ribosomal protein L4



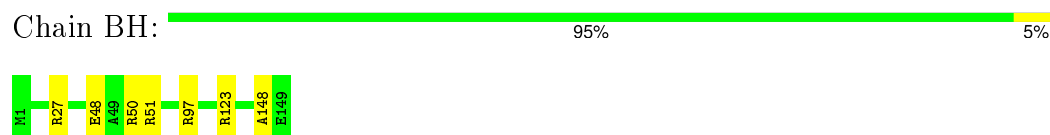
- Molecule 28: 50S ribosomal protein L5



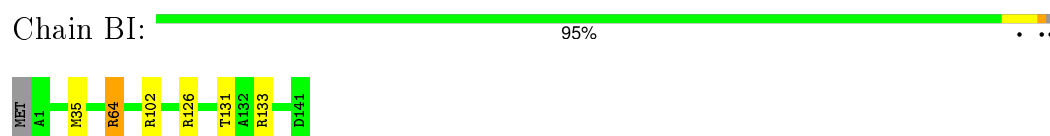
- Molecule 29: 50S ribosomal protein L6



- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L11



- Molecule 32: 50S ribosomal protein L13

Chain BJ:  89% 11%



- Molecule 33: 50S ribosomal protein L14

Chain BK:  90% 9%



- Molecule 34: 50S ribosomal protein L15

Chain BL:  90% 9%




- Molecule 35: 50S ribosomal protein L16

Chain BM:  85% 15%



- Molecule 36: 50S ribosomal protein L17

Chain BN:  83% 17%




- Molecule 37: 50S ribosomal protein L18

Chain BO:  89% 9%



- Molecule 38: 50S ribosomal protein L19

Chain BP:  82% 17%



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  85% 13%



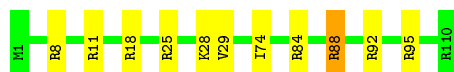
- Molecule 40: 50S ribosomal protein L21

Chain BR: 90% 10%



- Molecule 41: 50S ribosomal protein L22

Chain BS: 90% 9% .



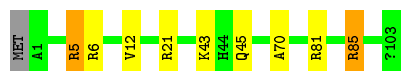
- Molecule 42: 50S ribosomal protein L23

Chain BT: 86% 14%



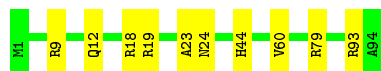
- Molecule 43: 50S ribosomal protein L24

Chain BU: 90% 7% ..



- Molecule 44: 50S ribosomal protein L25

Chain BV: 89% 11%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 84% 14% .



- Molecule 46: 50S ribosomal protein L28

Chain BX: 84% 13% . .





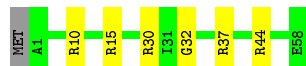
- Molecule 47: 50S ribosomal protein L29

Chain BY:  90% 6%




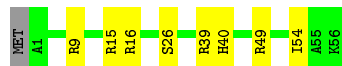
- Molecule 48: 50S ribosomal protein L30

Chain BZ:  88% 10%



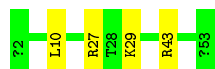
- Molecule 49: 50S ribosomal protein L32

Chain B0:  84% 14%




- Molecule 50: 50S ribosomal protein L33

Chain B1:  92% 8%



- Molecule 51: 50S ribosomal protein L34

Chain B2:  76% 22%




- Molecule 52: 50S ribosomal protein L35

Chain B3:  91% 8%

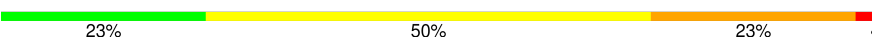


- Molecule 53: 50S ribosomal protein L36

Chain B4:  82% 18%



- Molecule 54: 23S ribosomal RNA


Chain BA:  23% 50% 23%

U1035	A973	A911	U846	A783	C717	G648	A586	G518	G452	G388	C323	A256	G194	A131	G68	G1
G1036	G974	C912	U847	G784	A718	G649	C587	A522	A453	G389	A324	C257	A195	G132	C69	G2
A1039	A975	U913	C848	G785	C719	G851	U589	A523	A454	U390	G325	G258	A196	U133	C70	A5
A1040	G976	C915	A849	G786	U720	U652	C523	C524	C455	U392	G326		A197	G134	A71	A6
G1041	A979	G916	C850	C787	A721	U653	U591	U525	A456	C393	G329	G263	C198	U135	A72	A7
G1042	A880	A917	U852	A788	A722	A854	A592	A526	G458	C394	A330	C264	U200	U138	A74	C8
C1043	C981	A918	C853	A789	C723	A855		C527	U459	U395	C331	A265	C201	U139	G75	G9
C1044	C982	U919	C854	U790	U724		C595	A328	A460	C398	A332	G266	U202	U140	C76	A10
C1045	A983	A920		A792	G726		U596	A529	C461	C399	G333	C267	A203	G141	C77	C11
A1046	A984	C921		A793	G727		G597	G330	C462	U399	C334	C268	A204	A142	U78	U12
G1047	C985	C922		A794	G728		U598	C531	C463	G400	C335	C269	G205	C143	U13	C13
A1048	C986			A795	G729		A599	A532	U464	A401	C336	A270	U206	A144	A14	A14
C1049	C987	A925		C796	A730	G664	G600	G533	G465	A402	C337	G271	A207	C145	G15	
A1050	A988	G926	U865		C731	U665	C601		A466	U403		A272	C208	A146	C16	
G1051	G989	A927	A862		C732	A666	A602		A470	A404	A340	G273	C209	C147	G17	
C1052	A990	A928	C863		C733	U667	G603	A538	A471	U405	A341	C274	C210	U148	U18	U18
C1053	C991	G929	C864		A734	A668	A604	G539	A472	G406	A342	C275	C211	A149	A19	A19
A1054	C992	G930	C865		A735	G669	G605	C540	A473	G407	C343	U276	G212	U150	C20	C20
G1055	G993	U931	C866		C736	U670	U606	C541	G473		A344	G277	A213	C151	A21	A21
C994	C994	U932	U868		C737	C671	U607	C542	G474	G410	A345	A278		A152	C22	C22
C995	A996	U933	C869		G738	C672	A608	G543	C475	G411	A346	A279	A216	U153	G26	G26
A996		U934	U870		C739	C673	A609	C544	C476	A412	A347	U280	A217	U154	A91	A91
C997	C997	C935	U871		C740	A674	C610	U545	A477	C413	A348	C281	A218	A155	G93	G93
C998	C998	A936	U872		G741	A675	C611	U546	A478	C414	U349	A282	A219	A156	A94	A94
U999	U999	C937	C873		A742	A676	G612	A547	A479	A415	G350	G283	G220	C157	A28	A28
A1000	A1000	G938	C874		C743	A677	A613	G548	A480	U416	C351	U284	A221	U158	C96	C96
U1001	A1001	C812	C875		A744	C678	A614	G549	C481	G417	A352		A222	U159	C97	C97
U1006	G1002	U813	C876		G745	C679	U615	C549	A482	C418	C353		A223	A160	G98	G98
A1007	G1003	C814	C877		U746	A679	U616	C550	A483	U419	A354		A224	A161	U99	U99
G1008	U1004	A943	A878		U747		C624	G551	C484	C420			C225	U162	U100	U100
A1009	C1005	C944	C879		G748		G695	U554	C485	C421	C357	G291	A226	C163	C37	C37
C1006	U1006	A945	C880		A749	A885	G620	G555	C486	A422	U358		A227	C164	A38	A38
C1007	A1007	C946	U886		C750	U886	A621	A556	C487	A423	G359	A294	C228	U165	U102	U102
C1071	C1071	A947	C887		A751	U888	G622	C557	C488	G424	U360	G295	C229	A166	A103	A103
A1072	A1008	C948	A888		A752	A889	C623	U558	G489		C361		C230	A167	A104	A104
A1073	A1009	G949	U887		C753		G624	G559	C490	U427	A362		A231	U170	G42	G42
G1074	A1010	C950	C888		U754		G695	C560	C491	A428	C363	A300	C232	U171	A44	A44
C1075	G1011	G951	C889		C755	A893	A626	A563	A492	A429	C364	G301	A233	U172	G45	G45
C1076	U1012	G952	C890		U756	U894	A627	A563		A430	U365	C302	U234	A172	G46	G46
A1077	C1013	G953	C891		G757	G895	G628	C564	A497	U431	C366	G303	U235	A173	C47	C47
U1078	A1014	G954	C892		C758	G896	G629	C565		A432	G367	U304	C236		G48	G48
C1079	U1015	U955	C893		G759	G897	G630	U566	G500	C433	U368	C305	C237	A176	A49	A49
A1080	G1016	U956	U894		C760	C898	A631	U567	A501	U434	U369	U306	C238		U50	U50
U1081	G1017	C956	U895		A761	A899	A632	U568	A502	C435	G370		C239	G177	U113	U113
		C957	C896		U762		A633	A503	A503	C436	A371	G307	C240	G178	U114	G51
A1084	A1020	U958	A896		C763	U702	C634	A572		A439	G372	G308	A241	C179	C115	A52
A1085	A1021	C959	C897		G764	U703	C635	U573	A504	U440	U373	A310	G242	G180	C116	A53
A1086	G1022	A960	C898		C765	G704	G636	A574	G506	C443	U374	A311	A244	A181	G117	G54
G1087	U1023	C961	A899		U766	A705	A637	A575	A507	U441	A374	G312	C245	A182	G55	G55
A1088	G1024	G962	C900			A706	G638	U576	A508	G442		G313	C246	C183	A56	A56
A1089	G1025	U963	C901		G771	G707	U639	U577	C509	C444	C378	G314	G247	C184	U57	C57
A1090	G1026	C964	C902		C772		U640	G577	A509	C445	G379	G315	G248	G185	G121	
C1092	A1027	G965	C903		U773	U710	C641	G578	C510	C446	G380	G316	C249	G186	G124	G124
	A1028	G966	G904		C774	G711	U642	G579	U511	C447	G381	C316	G250	G187	A62	A62
	A1029	U967	A905		C775	G712	U643	U580	G512	G446	A382	G317	G251	G188	U63	U63
U1095	C1030	C968	U906		G776	G713	A644	C581	A513	U448	C383	G318	A251	G189	A126	A126
A1096	G1031	G969	C907			G714	A645	A582	A514	U449	C384	G319	G252	A190	A127	A64
U1097	A1032	U970	C908			A715	C646	G583	A515	G450	C385	A320	C253	A191	C128	U65
A1098	U1033	G971	A909		A781	A716	U646	C584	A516	G451	G386	U321	C254	C192	C129	C66
G1099	G1034	A972	A910		A782	A716	G647	G585	C517		U387	A322	A255	U193	U67	U67

A2054	C1994	A1932	G1869	A1802	G1738	U1671	A1610	A1549	A1419	G1355	C1293	A1226	G1162	C1100
C2055	U1995	G1933	C1870	A1803	A1739	A1672	C1611	C1550	A1420	G1356	U1294	G1227	G1163	U1101
G2056	C1996	A1871	A1872	C1804	G1740	G1673	C1612	A1551		G1357	C1295	G1228	C1164	C1102
C2057	C1997	G1875	A1876	A1805	C1741	G1674	G1613	A1552	G1423	G1358	G1296	A1230	A1165	A1103
A2058	A1998	G1876	G1877	C1806	U1742	C1675	A1614	A1553	G1424	G1359	C1297		G1166	C1104
A2059	C1999	G1877	G1878	G1807	G1743	A1676	C1615	U1554	G1425	G1360	C1298		C1167	U1105
A2060	C2000	G1878	A1879	A1808	A1744	A1677	A1616	G1555	G1426	G1361	C1299		G1168	G1106
G2061	C2001	A1876	A1877	A1809	A1745	A1678	C1617	C1556	A1427	G1362	G1300		A1169	G1107
A2062	G2002	A1877	A1878	A1810	A1746	A1679	A1618	C1557	A1428	G1363	A1301		C1170	U1108
C2063	A2003	G1878	G1879	U1811	U1747	U1680	G1619	C1558		G1364	A1302		G1171	C1109
C2064	G2004	U1812	C1879	U1812	C1748	G1681	G1620	U1559	A1431	A1365	G1303		C1172	G1110
C2065	A2005	U1813	U1880	G1813	A1749	G1682	U1621	G1560	G1432	A1366	A1304		U1173	A1111
C2066	C2006	G1814	C1881	G1814		G1683	G1622	C1498	A1433	A1367	C1305		U1174	G1112
G2067	U2007	A1815	U1882	A1815	C1752	G1684	G1623	C1499	A1434	G1368	C1306		A1175	U1113
U2068	C2008	C1816	U1883	C1816	G1753	C1685	U1624	U1563		G1369	A1307		U1176	C1114
G2069	A2009	G1817	A1884	G1817	A1754	C1686	C1625	C1564	C1437	C1370	A1308		G1177	G1115
A2070	G2010	U1818	A1885	U1818	A1755	G1687	A1626	C1565		G1371	C1309		C1178	G1116
A2071	U2011	A1819	U1886	A1819	G1756	U1688		A1566	U1438	G1372	G1310		C1179	C1117
C2072	G2012	U1820	C1887	U1820	A1757	A1689	U1629	G1567	U1440	A1373	G1311		U1180	C1118
C2073	A2013	A1821	G1888	A1821	U1758	A1690	A1630	U1568	G1441	G1374	U1312			U1119
U2074	C2014	C1822	G1889	C1822	A1759	C1691	G1631	U1569	U1442	U1375	C1313		U1183	G1120
U2075	A2015	G1823	A1890	G1823	C1760		A1632	A1570	U1443	C1376	C1314		U1184	C1121
U2076	U2016	G1824	G1891	G1824	C1761	G1694	G1633	A1571	U1444	G1377	C1315		G1185	G1122
A2077	U2017	U1825	C1892	U1825	A1762	G1695	A1634	A1572	G1445	A1378	U1316		G1186	C1123
C2078	G2018	G1826	C1893	G1826	G1763		A1635	G1573	C1446	A1379	G1317			G1124
U2079	A2019	U1827	C1894	U1827	C1764		U1636	C1574	C1447	G1380	U1318		A1189	C1125
A2080	A2020	G1828	C1895	G1828	G1765	A1698	A1637	C1575		G1381	C1319		G1190	A1126
U2081	C2021	U1829	G1896	A1829	G1766	A1700	C1638	U1576	G1448	G1382	G1320		G1191	A1127
A2082	U2022	C1830	G1897	C1830	G1767	A1701	C1639	C1577	G1449	A1383	A1321			G1128
G2083	C2023	U1831	U1898	G1831	C1768		A1640	C1578	G1450	A1384	A1322		A1194	A1129
C2084	G2024	C1832	C1899	C1832	U1769	C1704	A1641	A1579	G1452	A1385	C1323		G1195	
U2085	C2025	A1833	A1900	G1833	G1770	A1705	G1642	A1580	U1483	C1386	G1324		C1196	U1132
U2086	U2026	U1834	A1901	U1834	C1771	C1706	G1643	U1581	C1454	A1387	U1325		U1197	A1133
G2087	G2027	G1835	C1902	G1835	A1772	G1707	C1644	C1582	G1455	U1388	U1326		U1198	A1134
C2088	U2028	C1836		C1836	A1773	C1708	G1645	A1583	G1456	G1389	A1327		U1199	C1135
C2089	G2029	C1837	U1905	C1837	C1774	U1709	C1646	U1584		C1390	A1328		C1200	G1136
C2091	A2030	C1838	G1906		U1775	G1710	U1647	U1585	G1459	U1391			U1201	G1137
	A2031		G1907			A1711	U1648	A1586	U1460	A1392			G1202	G1138
	G2032	G1908	U1907	G1908	U1779	U1712	G1649	G1587	C1461	U1393	G1331		G1203	G1139
	A2033	C1909		C1909	A1780	U1713	A1650		C1462	A1394	G1332		A1204	C1140
	U2034		A1912			U1714	G1651	A1590	C1463	A1395	C1335		A1205	U1141
	G2035	A1846	A1913	G1846	A1783	A1717	A1652	A1591	G1464	U1396	A1336		G1206	A1142
	C2036	C1847	C1914	A1847	A1784		G1653	C1592	G1465	U1397	G1337		C1207	A1143
	A2037	U1915	A1914	A1848	A1785	U1720	A1654	A1593	U1466	U1398	G1338		C1208	A1144
	G2038		U1916	A1849	A1786	G1721	A1655	U1594	U1467	C1399	G1339		U1209	C1145
	U2039	A1853	A1916		A1787	U1722	C1656	C1595	U1468		U1340		G1210	C1146
	G2040	C1854	U1917	A1854	C1788	A1723	U1657	U1596	A1469	A1403	G1341		A1211	A1147
	A2101		A1918		A1789	G1724	C1658	A1597	A1470	C1404	A1276		G1212	U1148
	C2042		A1919		C1790		G1659	A1598	G1471		G1277		A1213	G1149
	G2043		C1920		A1791		G1660	U1599	C1472	G1343	U1344		A1214	C1150
	C2044				G1792	C1727	G1661	C1600		G1408			G1215	A1151
	U2105	U1923		A1858	G1793	C1728	U1662	G1538	G1473	U1409	C1345		G1216	G1152
	G2046	C1924		G1861	C1794	U1729	G1663	U1539	U1474	U1410	G1346		U1217	C1153
	C2047	C1925		G1862	C1795	A1603	A1604	G1540	U1475	U1411	A1285		G1154	G1154
	G2048	G1863		G1863	U1796	C1730	A1665	C1541	U1476	U1412	A1286			
	U2109	C1926		G1864	G1731	G1732	A1666	A1477	A1413	C1349	G1349		G1220	A1155
	G2049	A1927		U1865	C1732		G1667	C1605	G1478	G1283	A1287		C1221	A1156
	C2050	A1928		U1866	U1798		G1668	C1606	U1479	C1289	G1288		U1222	G1157
	U2111	G1929		A1866	G1799	U1735	A1668	C1607	C1480	C1290	G1289		U1223	C1158
	A2052	G1930		G1867	U1736	A1736	A1669	U1481	U1416	C1291	G1290		U1224	C1159
	G2053	U1931		C1868	G1737		C1670	A1609	G1492	A1354	A1354		G1225	



- Molecule 56: 50S ribosomal protein L1

Chain B5:  89% 6% 5%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	1904	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	161000	Depositor
Image detector	4k CCD camera (TVIPS)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	AB	0.71	0/1736	1.09	15/2340 (0.6%)
10	AK	0.75	0/894	1.23	11/1207 (0.9%)
11	AL	0.75	0/969	1.25	14/1300 (1.1%)
12	AM	0.73	0/884	1.22	11/1181 (0.9%)
13	AN	0.78	0/817	1.22	9/1088 (0.8%)
14	AO	0.71	0/722	1.15	8/964 (0.8%)
15	AP	0.74	0/648	1.35	12/870 (1.4%)
16	AQ	0.70	0/658	1.19	8/883 (0.9%)
17	AR	0.80	0/463	1.21	6/623 (1.0%)
18	AS	0.76	0/653	1.15	9/879 (1.0%)
19	AT	0.68	0/672	1.11	4/890 (0.4%)
2	AC	0.72	0/1651	1.15	16/2225 (0.7%)
20	AU	0.83	0/431	1.66	13/572 (2.3%)
21	AA	1.53	1/36759 (0.0%)	2.22	1937/57346 (3.4%)
22	A1	1.54	0/1668	2.21	86/2595 (3.3%)
23	A2	1.54	0/343	2.22	16/531 (3.0%)
24	A3	1.54	0/1722	2.22	99/2685 (3.7%)
25	BC	0.73	0/2121	1.23	23/2852 (0.8%)
26	BD	0.68	0/1586	1.12	8/2134 (0.4%)
27	BE	0.67	0/1571	1.16	12/2113 (0.6%)
28	BF	0.74	0/1444	1.17	11/1937 (0.6%)
29	BG	0.69	0/1343	1.14	9/1816 (0.5%)
3	AD	0.76	0/1665	1.19	16/2227 (0.7%)
30	BH	0.66	0/1122	1.11	5/1515 (0.3%)
31	BI	0.65	0/1046	1.07	4/1410 (0.3%)
32	BJ	0.73	0/1152	1.25	12/1551 (0.8%)
33	BK	0.70	0/947	1.21	9/1268 (0.7%)
34	BL	0.72	0/1054	1.22	10/1403 (0.7%)
35	BM	0.75	0/1093	1.27	11/1460 (0.8%)
36	BN	0.75	0/973	1.38	18/1301 (1.4%)
37	BO	0.72	0/902	1.26	13/1209 (1.1%)
38	BP	0.74	0/929	1.34	15/1242 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BQ	0.78	0/960	1.30	14/1278 (1.1%)
4	AE	0.71	0/1119	1.11	10/1506 (0.7%)
40	BR	0.70	0/829	1.19	6/1107 (0.5%)
41	BS	0.66	0/864	1.22	10/1156 (0.9%)
42	BT	0.64	0/744	1.18	6/994 (0.6%)
43	BU	0.68	0/787	1.07	5/1051 (0.5%)
44	BV	0.70	0/766	1.13	5/1025 (0.5%)
45	BW	0.75	0/604	1.32	8/799 (1.0%)
46	BX	0.73	0/635	1.34	10/848 (1.2%)
47	BY	0.69	0/510	1.23	4/677 (0.6%)
48	BZ	0.68	0/453	1.23	7/605 (1.2%)
49	B0	0.74	0/450	1.28	5/599 (0.8%)
5	AF	0.73	0/835	1.12	7/1128 (0.6%)
50	B1	0.73	0/417	1.05	2/556 (0.4%)
51	B2	0.81	0/380	1.62	11/498 (2.2%)
52	B3	0.72	0/513	1.15	5/676 (0.7%)
53	B4	0.67	0/303	1.36	6/397 (1.5%)
54	BA	1.40	1/69796 (0.0%)	2.21	4031/108888 (3.7%)
55	BB	1.42	0/2800	2.15	146/4367 (3.3%)
56	B5	0.64	0/1673	1.09	11/2255 (0.5%)
6	AG	0.74	0/1188	1.23	14/1593 (0.9%)
7	AH	0.69	0/989	1.02	5/1326 (0.4%)
8	AI	0.81	0/1035	1.33	17/1377 (1.2%)
9	AJ	0.71	0/797	1.28	10/1079 (0.9%)
All	All	1.28	2/160085 (0.0%)	2.00	6805/239402 (2.8%)

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
14	AO	0	1
21	AA	0	372
22	A1	0	21
23	A2	0	5
24	A3	0	7
27	BE	0	1
3	AD	0	1
37	BO	0	1
39	BQ	0	1
45	BW	0	1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
54	BA	0	726
55	BB	0	20
8	AI	0	1
All	All	0	1158

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1060	U	C5'-C4'	5.13	1.57	1.51
54	BA	2428	G	C2-N2	-5.06	1.29	1.34

All (6805) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	982	C	N3-C2-O2	-13.80	112.24	121.90
54	BA	574	A	N1-C6-N6	-13.05	110.77	118.60
21	AA	676	A	N1-C6-N6	-12.48	111.11	118.60
21	AA	964	A	N1-C6-N6	-12.38	111.17	118.60
54	BA	1932	A	N1-C6-N6	-12.22	111.27	118.60
54	BA	643	A	O4'-C1'-N9	12.01	117.81	108.20
21	AA	845	A	N1-C6-N6	-11.90	111.46	118.60
54	BA	666	A	N1-C6-N6	-11.89	111.47	118.60
54	BA	219	A	N1-C6-N6	-11.86	111.48	118.60
54	BA	119	A	N1-C6-N6	-11.84	111.50	118.60
54	BA	1352	U	O4'-C1'-N1	11.83	117.66	108.20
21	AA	630	A	N1-C6-N6	-11.71	111.57	118.60
54	BA	2654	A	N1-C6-N6	-11.64	111.61	118.60
54	BA	1780	A	N1-C6-N6	-11.64	111.61	118.60
54	BA	789	A	N1-C6-N6	-11.61	111.63	118.60
54	BA	1287	A	N1-C6-N6	-11.56	111.66	118.60
54	BA	2369	A	N1-C6-N6	-11.54	111.67	118.60
54	BA	1080	A	N1-C6-N6	-11.49	111.71	118.60
54	BA	1096	A	N1-C6-N6	-11.48	111.71	118.60
54	BA	932	U	O4'-C1'-N1	11.44	117.35	108.20
54	BA	2753	A	N1-C6-N6	-11.43	111.74	118.60
54	BA	481	G	O4'-C1'-N9	11.43	117.34	108.20
21	AA	493	A	N1-C6-N6	-11.40	111.76	118.60
54	BA	2435	A	N1-C6-N6	-11.38	111.77	118.60
21	AA	389	A	N1-C6-N6	-11.37	111.78	118.60
54	BA	2030	A	N1-C6-N6	-11.29	111.83	118.60
21	AA	109	A	N1-C6-N6	-11.28	111.83	118.60
55	BB	78	A	N1-C6-N6	-11.24	111.86	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	430	A	N1-C6-N6	-11.23	111.86	118.60
54	BA	982	C	N1-C2-O2	11.22	125.63	118.90
54	BA	1569	A	N1-C6-N6	-11.21	111.87	118.60
54	BA	699	A	N1-C6-N6	-11.21	111.87	118.60
54	BA	311	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	1004	A	N1-C6-N6	-11.13	111.92	118.60
54	BA	2810	A	N1-C6-N6	-11.13	111.92	118.60
21	AA	432	A	N1-C6-N6	-11.09	111.95	118.60
54	BA	2850	A	N1-C6-N6	-11.07	111.96	118.60
21	AA	171	A	N1-C6-N6	-11.03	111.98	118.60
21	AA	1339	A	N1-C6-N6	-11.03	111.98	118.60
54	BA	1413	A	N1-C6-N6	-11.02	111.99	118.60
54	BA	1392	A	N1-C6-N6	-11.01	112.00	118.60
54	BA	2893	A	N1-C6-N6	-10.99	112.00	118.60
54	BA	2577	A	N1-C6-N6	-10.98	112.01	118.60
54	BA	1637	A	N1-C6-N6	-10.97	112.02	118.60
54	BA	1134	A	N1-C6-N6	-10.96	112.02	118.60
21	AA	1288	A	N1-C6-N6	-10.95	112.03	118.60
54	BA	2211	A	N1-C6-N6	-10.93	112.04	118.60
21	AA	1434	A	N1-C6-N6	-10.92	112.05	118.60
21	AA	1289	A	N1-C6-N6	-10.87	112.08	118.60
21	AA	1447	A	N1-C6-N6	-10.85	112.09	118.60
54	BA	2247	A	N1-C6-N6	-10.85	112.09	118.60
54	BA	1241	A	N1-C6-N6	-10.84	112.09	118.60
9	AJ	62	ARG	NE-CZ-NH1	10.79	125.69	120.30
54	BA	1494	A	N1-C6-N6	-10.79	112.13	118.60
21	AA	288	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	739	A	N1-C6-N6	-10.77	112.14	118.60
54	BA	747	U	O4'-C1'-N1	10.75	116.80	108.20
54	BA	1634	A	N1-C6-N6	-10.75	112.15	118.60
54	BA	1610	A	N1-C6-N6	-10.71	112.17	118.60
54	BA	2386	A	N1-C6-N6	-10.66	112.20	118.60
54	BA	280	U	O4'-C1'-N1	10.66	116.72	108.20
54	BA	947	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1755	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	497	A	N1-C6-N6	-10.64	112.21	118.60
54	BA	83	A	N1-C6-N6	-10.64	112.22	118.60
21	AA	1105	A	N1-C6-N6	-10.63	112.22	118.60
3	AD	110	ARG	NE-CZ-NH1	10.63	125.61	120.30
54	BA	71	A	N1-C6-N6	-10.62	112.22	118.60
54	BA	1027	A	N1-C6-N6	-10.62	112.23	118.60
21	AA	282	A	N1-C6-N6	-10.62	112.23	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2634	A	N1-C6-N6	-10.62	112.23	118.60
54	BA	507	A	N1-C6-N6	-10.60	112.24	118.60
47	BY	47	ARG	NE-CZ-NH1	10.59	125.60	120.30
54	BA	1175	A	N1-C6-N6	-10.57	112.26	118.60
21	AA	994	A	N1-C6-N6	-10.57	112.26	118.60
54	BA	1284	A	N1-C6-N6	-10.57	112.26	118.60
54	BA	2868	A	N1-C6-N6	-10.57	112.26	118.60
21	AA	98	A	N1-C6-N6	-10.56	112.27	118.60
54	BA	181	A	N1-C6-N6	-10.55	112.27	118.60
54	BA	1570	A	N1-C6-N6	-10.55	112.27	118.60
21	AA	461	A	N1-C6-N6	-10.54	112.28	118.60
54	BA	1260	A	N1-C6-N6	-10.53	112.28	118.60
54	BA	165	A	N1-C6-N6	-10.52	112.29	118.60
54	BA	592	A	N1-C6-N6	-10.51	112.29	118.60
54	BA	972	A	N1-C6-N6	-10.51	112.29	118.60
54	BA	2530	A	N1-C6-N6	-10.51	112.30	118.60
54	BA	984	A	N1-C6-N6	-10.51	112.30	118.60
54	BA	1046	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	2473	U	O4'-C1'-N1	10.49	116.59	108.20
21	AA	270	A	N1-C6-N6	-10.49	112.31	118.60
38	BP	52	ARG	NE-CZ-NH1	10.47	125.54	120.30
54	BA	342	A	N1-C6-N6	-10.47	112.32	118.60
21	AA	1431	A	N1-C6-N6	-10.47	112.32	118.60
21	AA	1368	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	2097	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	1272	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	1301	A	N1-C6-N6	-10.44	112.34	118.60
21	AA	1446	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	456	C	O4'-C1'-N1	10.44	116.55	108.20
54	BA	2346	A	N1-C6-N6	-10.44	112.34	118.60
21	AA	8	A	N1-C6-N6	-10.43	112.34	118.60
54	BA	613	A	O4'-C1'-N9	10.43	116.54	108.20
21	AA	328	C	N3-C2-O2	-10.42	114.61	121.90
54	BA	1754	A	N1-C6-N6	-10.41	112.35	118.60
54	BA	125	A	N1-C6-N6	-10.41	112.35	118.60
54	BA	2867	G	O4'-C1'-N9	10.41	116.53	108.20
54	BA	2287	A	N1-C6-N6	-10.39	112.36	118.60
21	AA	179	A	N1-C6-N6	-10.38	112.37	118.60
54	BA	1086	A	N1-C6-N6	-10.38	112.37	118.60
21	AA	327	A	N1-C6-N6	-10.38	112.38	118.60
21	AA	579	A	N1-C6-N6	-10.37	112.38	118.60
21	AA	456	A	N1-C6-N6	-10.36	112.38	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	34	A	N1-C6-N6	-10.36	112.39	118.60
21	AA	1468	A	N1-C6-N6	-10.35	112.39	118.60
24	A3	73	A	N1-C6-N6	-10.34	112.40	118.60
21	AA	1201	A	N1-C6-N6	-10.33	112.40	118.60
21	AA	535	A	N1-C6-N6	-10.33	112.40	118.60
21	AA	621	A	N1-C6-N6	-10.32	112.41	118.60
54	BA	142	A	N1-C6-N6	-10.32	112.41	118.60
54	BA	2727	A	N1-C6-N6	-10.32	112.41	118.60
54	BA	74	A	N1-C6-N6	-10.29	112.42	118.60
15	AP	51	ARG	NE-CZ-NH1	10.29	125.44	120.30
54	BA	911	A	N1-C6-N6	-10.29	112.43	118.60
54	BA	2090	A	N1-C6-N6	-10.28	112.43	118.60
21	AA	236	A	N1-C6-N6	-10.27	112.44	118.60
21	AA	583	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	750	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	1789	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	2170	A	N1-C6-N6	-10.26	112.45	118.60
54	BA	2478	A	N1-C6-N6	-10.26	112.45	118.60
54	BA	1439	A	N1-C6-N6	-10.25	112.45	118.60
24	A3	60	A	N1-C6-N6	-10.23	112.46	118.60
54	BA	892	A	N1-C6-N6	-10.21	112.47	118.60
54	BA	983	A	N1-C6-N6	-10.21	112.47	118.60
24	A3	36	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	1632	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	2267	A	N1-C6-N6	-10.18	112.49	118.60
21	AA	975	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	602	A	N1-C6-N6	-10.16	112.51	118.60
21	AA	1374	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	1916	A	N1-C6-N6	-10.14	112.52	118.60
21	AA	860	A	N1-C6-N6	-10.13	112.52	118.60
21	AA	681	A	N1-C6-N6	-10.13	112.52	118.60
21	AA	937	A	N1-C6-N6	-10.12	112.53	118.60
54	BA	2734	A	N1-C6-N6	-10.12	112.53	118.60
54	BA	1791	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	2432	A	N1-C6-N6	-10.11	112.53	118.60
21	AA	766	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	1328	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	1591	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	532	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	1085	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	1126	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	2513	A	N1-C6-N6	-10.09	112.54	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1502	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	2005	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	2503	A	O4'-C1'-N9	10.08	116.27	108.20
21	AA	889	A	N1-C6-N6	-10.07	112.56	118.60
21	AA	1188	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	1359	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	2198	A	N1-C6-N6	-10.06	112.56	118.60
54	BA	1090	A	N1-C6-N6	-10.06	112.56	118.60
12	AM	97	ARG	NE-CZ-NH2	10.05	125.32	120.30
37	BO	25	ARG	NE-CZ-NH1	10.05	125.32	120.30
54	BA	1641	A	N1-C6-N6	-10.04	112.58	118.60
21	AA	19	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	1395	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	2564	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	2134	A	N1-C6-N6	-10.01	112.59	118.60
21	AA	573	A	N1-C6-N6	-10.01	112.60	118.60
54	BA	1640	A	N1-C6-N6	-10.01	112.59	118.60
21	AA	50	A	N1-C6-N6	-10.01	112.60	118.60
8	AI	122	ARG	NE-CZ-NH2	10.00	125.30	120.30
21	AA	452	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	933	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	2307	G	O4'-C1'-N9	9.99	116.19	108.20
10	AK	55	ARG	NE-CZ-NH1	9.99	125.30	120.30
54	BA	2411	A	N1-C6-N6	-9.99	112.61	118.60
54	BA	1509	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	78	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	631	A	N1-C6-N6	-9.96	112.62	118.60
54	BA	309	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	510	A	N1-C6-N6	-9.96	112.63	118.60
54	BA	144	A	N1-C6-N6	-9.96	112.63	118.60
21	AA	609	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	2173	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	2225	A	N1-C6-N6	-9.94	112.63	118.60
54	BA	2126	A	O4'-C1'-N9	9.94	116.15	108.20
54	BA	300	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	2814	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	959	A	N1-C6-N6	-9.92	112.65	118.60
39	BQ	69	ARG	NE-CZ-NH1	9.91	125.26	120.30
21	AA	279	A	N1-C6-N6	-9.91	112.65	118.60
54	BA	346	A	N1-C6-N6	-9.91	112.65	118.60
54	BA	1810	A	N1-C6-N6	-9.91	112.66	118.60
54	BA	800	A	N1-C6-N6	-9.90	112.66	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1829	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	1227	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	474	G	O4'-C1'-N9	9.90	116.12	108.20
21	AA	383	A	N1-C6-N6	-9.89	112.66	118.60
54	BA	2700	A	N1-C6-N6	-9.89	112.67	118.60
21	AA	665	A	N1-C6-N6	-9.89	112.67	118.60
21	AA	819	A	N1-C6-N6	-9.89	112.67	118.60
21	AA	325	A	N1-C6-N6	-9.89	112.67	118.60
21	AA	767	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	861	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	443	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	936	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	1459	G	O4'-C1'-N9	9.88	116.11	108.20
21	AA	408	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	1427	A	N1-C6-N6	-9.87	112.68	118.60
21	AA	1067	A	N1-C6-N6	-9.86	112.68	118.60
21	AA	80	A	N1-C6-N6	-9.86	112.69	118.60
11	AL	8	ARG	NE-CZ-NH1	9.85	125.22	120.30
46	BX	27	ARG	NE-CZ-NH1	9.84	125.22	120.30
21	AA	116	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	1084	A	N1-C6-N6	-9.84	112.70	118.60
21	AA	574	A	N1-C6-N6	-9.83	112.70	118.60
13	AN	53	ARG	NE-CZ-NH1	9.82	125.21	120.30
54	BA	1515	A	N1-C6-N6	-9.82	112.71	118.60
54	BA	1929	G	O4'-C1'-N9	9.82	116.06	108.20
54	BA	1378	A	C1'-O4'-C4'	-9.82	102.05	109.90
21	AA	1169	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	182	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	988	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	2009	A	N1-C6-N6	-9.81	112.71	118.60
20	AU	44	ARG	NE-CZ-NH1	9.80	125.20	120.30
10	AK	126	ARG	NE-CZ-NH2	9.80	125.20	120.30
54	BA	2104	C	N3-C2-O2	-9.79	115.04	121.90
54	BA	1387	A	N1-C6-N6	-9.79	112.73	118.60
54	BA	1387	A	O4'-C1'-N9	9.78	116.02	108.20
21	AA	600	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	915	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	728	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	28	A	N1-C6-N6	-9.76	112.74	118.60
54	BA	10	A	N1-C6-N6	-9.76	112.74	118.60
21	AA	841	C	N3-C2-O2	-9.76	115.07	121.90
21	AA	1014	A	N1-C6-N6	-9.76	112.74	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	747	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	931	U	O4'-C1'-N1	9.75	116.00	108.20
21	AA	1396	A	N1-C6-N6	-9.74	112.76	118.60
21	AA	706	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	1705	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2284	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	404	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	927	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	1194	A	N1-C6-N6	-9.72	112.77	118.60
21	AA	782	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	371	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	1583	A	N1-C6-N6	-9.71	112.78	118.60
19	AT	59	ARG	NE-CZ-NH1	9.70	125.15	120.30
54	BA	213	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	352	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1496	A	N1-C6-N6	-9.69	112.78	118.60
54	BA	2872	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	161	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	1597	A	N1-C6-N6	-9.69	112.79	118.60
21	AA	1280	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	914	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	55	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	845	A	N1-C6-N6	-9.67	112.80	118.60
21	AA	815	A	N1-C6-N6	-9.66	112.80	118.60
32	BJ	95	ARG	NE-CZ-NH1	9.66	125.13	120.30
54	BA	1938	A	O4'-C1'-N9	9.66	115.92	108.20
21	AA	640	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	1722	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	155	A	N1-C6-N6	-9.64	112.81	118.60
54	BA	2792	A	N1-C6-N6	-9.64	112.82	118.60
21	AA	1251	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	1746	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	1927	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	465	A	C1'-O4'-C4'	-9.62	102.21	109.90
54	BA	782	A	N1-C6-N6	-9.61	112.83	118.60
1	AB	207	ARG	NE-CZ-NH2	9.61	125.11	120.30
54	BA	1067	A	O4'-C1'-N9	9.61	115.89	108.20
21	AA	1152	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	781	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	241	A	N1-C6-N6	-9.59	112.85	118.60
9	AJ	7	ARG	NE-CZ-NH1	9.59	125.09	120.30
54	BA	821	A	N1-C6-N6	-9.58	112.85	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	831	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	371	A	N1-C6-N6	-9.58	112.86	118.60
21	AA	1519	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	532	A	O4'-C1'-N9	9.57	115.86	108.20
54	BA	878	A	N1-C6-N6	-9.57	112.86	118.60
21	AA	1239	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1504	A	N1-C6-N6	-9.57	112.86	118.60
21	AA	1269	A	N1-C6-N6	-9.56	112.86	118.60
21	AA	1060	U	P-O3'-C3'	9.56	131.17	119.70
21	AA	1311	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	1365	A	N1-C6-N6	-9.56	112.87	118.60
54	BA	1142	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	354	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	432	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	1081	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	675	A	N1-C6-N6	-9.55	112.87	118.60
55	BB	50	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	1214	C	N3-C2-O2	-9.54	115.22	121.90
54	BA	1739	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	945	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	223	A	N1-C6-N6	-9.53	112.88	118.60
34	BL	2	ARG	NE-CZ-NH1	9.52	125.06	120.30
54	BA	1089	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	504	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	752	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	1819	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	365	U	C1'-O4'-C4'	-9.51	102.29	109.90
54	BA	715	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	969	A	N1-C6-N6	-9.50	112.90	118.60
55	BB	87	U	O4'-C1'-N1	9.50	115.80	108.20
54	BA	1230	A	N1-C6-N6	-9.49	112.90	118.60
54	BA	2199	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	285	C	N3-C2-O2	-9.48	115.26	121.90
21	AA	1036	A	N1-C6-N6	-9.48	112.91	118.60
22	A1	6	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	56	A	N1-C6-N6	-9.48	112.91	118.60
22	A1	38	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	429	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	941	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	909	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1103	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1244	A	N1-C6-N6	-9.47	112.92	118.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1246	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1626	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	73	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	1403	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	1580	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	2309	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	348	A	N1-C6-N6	-9.46	112.93	118.60
54	BA	2851	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	1157	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	975	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	2274	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	412	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	1914	C	N3-C2-O2	-9.44	115.29	121.90
54	BA	1552	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	1204	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	74	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	788	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	2430	A	C5-C6-N1	9.43	122.42	117.70
54	BA	1630	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	2051	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	1889	A	N1-C6-N6	-9.42	112.94	118.60
54	BA	1953	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	143	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	2089	C	O4'-C1'-N1	9.41	115.73	108.20
6	AG	110	ARG	NE-CZ-NH1	9.41	125.00	120.30
21	AA	1100	C	N3-C2-O2	-9.41	115.31	121.90
21	AA	872	A	N1-C6-N6	-9.41	112.96	118.60
14	AO	71	ARG	NE-CZ-NH1	9.40	125.00	120.30
54	BA	1678	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	1256	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	14	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	151	A	N1-C6-N6	-9.39	112.96	118.60
54	BA	1378	A	N1-C6-N6	-9.39	112.96	118.60
21	AA	1493	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	1690	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	1410	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	559	A	N1-C6-N6	-9.37	112.97	118.60
21	AA	784	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	807	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	787	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	841	C	N1-C2-O2	9.37	124.52	118.90
21	AA	16	A	N1-C6-N6	-9.37	112.98	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	AJ	37	ARG	NE-CZ-NH1	9.36	124.98	120.30
54	BA	1383	A	N1-C6-N6	-9.36	112.98	118.60
21	AA	1250	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	1854	A	N1-C6-N6	-9.36	112.98	118.60
21	AA	792	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	1586	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	2335	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	2448	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	587	C	O4'-C1'-N1	9.34	115.67	108.20
21	AA	539	A	N1-C6-N6	-9.34	113.00	118.60
21	AA	900	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	514	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	439	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	730	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	118	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	1610	A	O4'-C1'-N9	9.32	115.65	108.20
21	AA	60	A	N1-C6-N6	-9.31	113.01	118.60
22	A1	73	A	C5-C6-N1	9.31	122.35	117.70
54	BA	1608	A	N1-C6-N6	-9.31	113.02	118.60
54	BA	299	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1327	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	743	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1420	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	2311	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	2317	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	2288	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	1858	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	391	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	728	A	C5-C6-N1	9.28	122.34	117.70
51	B2	21	ARG	NE-CZ-NH1	9.28	124.94	120.30
2	AC	131	ARG	NE-CZ-NH1	9.27	124.94	120.30
54	BA	84	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	910	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	63	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1593	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	702	A	N1-C6-N6	-9.27	113.04	118.60
51	B2	12	ARG	NE-CZ-NH1	9.27	124.93	120.30
54	BA	2088	A	N1-C6-N6	-9.27	113.04	118.60
25	BC	51	ARG	NE-CZ-NH1	9.26	124.93	120.30
54	BA	218	A	N1-C6-N6	-9.26	113.04	118.60
54	BA	1490	A	N1-C6-N6	-9.26	113.05	118.60
54	BA	2879	A	O4'-C1'-N9	9.25	115.60	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2145	C	N3-C2-O2	-9.25	115.42	121.90
54	BA	1981	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	522	A	N1-C6-N6	-9.24	113.05	118.60
54	BA	2330	G	O4'-C1'-N9	9.24	115.59	108.20
54	BA	21	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	761	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	847	U	O4'-C1'-N1	9.24	115.59	108.20
21	AA	10	A	N1-C6-N6	-9.23	113.06	118.60
22	A1	58	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	1333	A	N1-C6-N6	-9.23	113.06	118.60
28	BF	111	ARG	NE-CZ-NH1	9.23	124.92	120.30
25	BC	62	ARG	NE-CZ-NH1	9.23	124.91	120.30
54	BA	478	A	N1-C6-N6	-9.23	113.06	118.60
54	BA	1057	A	N1-C6-N6	-9.23	113.06	118.60
54	BA	49	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	272	A	N1-C6-N6	-9.22	113.07	118.60
24	A3	11	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	382	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1067	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	2281	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	320	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	2268	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	2327	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	397	A	N1-C6-N6	-9.21	113.08	118.60
55	BB	115	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	1191	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	575	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	1180	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	2614	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	1418	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	734	A	N1-C6-N6	-9.19	113.08	118.60
21	AA	1257	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	1853	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	925	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1677	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1654	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	2541	A	N1-C6-N6	-9.17	113.09	118.60
54	BA	1919	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	1132	C	N3-C2-O2	-9.16	115.49	121.90
21	AA	1429	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	1871	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	2761	A	N1-C6-N6	-9.16	113.11	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AC	135	ARG	NE-CZ-NH1	9.15	124.88	120.30
54	BA	2412	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1262	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2142	A	N1-C6-N6	-9.15	113.11	118.60
55	BB	52	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1784	A	N1-C6-N6	-9.14	113.11	118.60
19	AT	23	ARG	NE-CZ-NH1	9.14	124.87	120.30
54	BA	1505	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	554	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	1219	A	N1-C6-N6	-9.14	113.12	118.60
21	AA	139	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	1966	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	2033	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	2450	A	N1-C6-N6	-9.14	113.12	118.60
21	AA	315	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	783	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	825	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	2298	A	N1-C6-N6	-9.13	113.12	118.60
22	A1	69	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	1783	A	N1-C6-N6	-9.13	113.12	118.60
35	BM	16	ARG	NE-CZ-NH1	9.12	124.86	120.30
2	AC	53	ARG	NE-CZ-NH1	9.12	124.86	120.30
54	BA	896	A	N1-C6-N6	-9.12	113.13	118.60
55	BB	104	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	181	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	1664	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	1322	C	N3-C2-O2	-9.11	115.52	121.90
54	BA	1848	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	1302	A	N1-C6-N6	-9.11	113.14	118.60
21	AA	353	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	1111	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	1808	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	718	A	N1-C6-N6	-9.10	113.14	118.60
11	AL	82	ARG	NE-CZ-NH1	9.10	124.85	120.30
54	BA	626	A	N1-C6-N6	-9.09	113.14	118.60
54	BA	2158	A	N1-C6-N6	-9.09	113.14	118.60
21	AA	1492	A	N1-C6-N6	-9.09	113.14	118.60
54	BA	572	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	1786	A	N1-C6-N6	-9.09	113.14	118.60
21	AA	1055	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	368	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	1353	A	N1-C6-N6	-9.08	113.15	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1534	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	101	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	1216	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	529	A	N1-C6-N6	-9.08	113.15	118.60
55	BB	94	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	1532	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	1987	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	2095	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	2407	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	1133	A	N1-C6-N6	-9.07	113.16	118.60
53	B4	19	ARG	NE-CZ-NH1	9.06	124.83	120.30
54	BA	1701	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	414	A	N1-C6-N6	-9.06	113.17	118.60
27	BE	114	ARG	NE-CZ-NH1	9.06	124.83	120.30
21	AA	1080	A	N1-C6-N6	-9.05	113.17	118.60
24	A3	22	A	N1-C6-N6	-9.05	113.17	118.60
48	BZ	44	ARG	NE-CZ-NH1	9.05	124.83	120.30
54	BA	1126	A	C5-C6-N1	9.05	122.23	117.70
21	AA	1299	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	2809	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	960	A	N1-C6-N6	-9.04	113.18	118.60
21	AA	913	A	N1-C6-N6	-9.04	113.18	118.60
21	AA	1428	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2060	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	749	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2518	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2062	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1111	A	N1-C6-N6	-9.03	113.18	118.60
36	BN	118	ARG	NE-CZ-NH1	9.03	124.81	120.30
54	BA	503	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	2392	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1900	A	N1-C6-N6	-9.02	113.19	118.60
4	AE	111	ARG	NE-CZ-NH1	9.02	124.81	120.30
54	BA	1714	U	O4'-C1'-N1	9.02	115.42	108.20
54	BA	2418	A	N1-C6-N6	-9.02	113.19	118.60
6	AG	69	ARG	NE-CZ-NH1	9.01	124.81	120.30
54	BA	1008	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	2471	A	N1-C6-N6	-9.01	113.19	118.60
55	BB	109	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	586	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	1169	A	N1-C6-N6	-9.01	113.19	118.60
21	AA	328	C	N1-C2-O2	9.00	124.30	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	655	A	N1-C6-N6	-9.00	113.20	118.60
22	A1	21	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1866	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1606	C	N3-C2-O2	-9.00	115.60	121.90
55	BB	45	A	N1-C6-N6	-8.99	113.20	118.60
6	AG	77	ARG	NE-CZ-NH1	8.99	124.80	120.30
31	BI	64	ARG	NE-CZ-NH1	8.99	124.80	120.30
21	AA	563	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	849	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	1431	A	N1-C6-N6	-8.98	113.22	118.60
21	AA	1155	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	2117	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	696	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	1329	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	965	C	N3-C2-O2	-8.96	115.63	121.90
21	AA	1513	A	N1-C6-N6	-8.96	113.23	118.60
21	AA	958	A	N1-C6-N6	-8.96	113.23	118.60
21	AA	1179	A	N1-C6-N6	-8.95	113.23	118.60
21	AA	802	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	1815	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	1070	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1847	A	N1-C6-N6	-8.94	113.24	118.60
22	A1	23	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	2757	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	2675	A	N1-C6-N6	-8.93	113.25	118.60
8	AI	118	ARG	NE-CZ-NH1	8.92	124.76	120.30
21	AA	1360	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	1009	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	1021	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	2820	A	N1-C6-N6	-8.92	113.25	118.60
21	AA	1319	A	N1-C6-N6	-8.91	113.25	118.60
22	A1	41	A	N1-C6-N6	-8.91	113.25	118.60
21	AA	520	A	N1-C6-N6	-8.91	113.26	118.60
54	BA	160	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	1093	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	1101	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1885	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2212	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2665	A	N1-C6-N6	-8.90	113.26	118.60
24	A3	44	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1635	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	262	A	N1-C6-N6	-8.89	113.26	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1156	A	N1-C6-N6	-8.89	113.26	118.60
10	AK	92	ARG	NE-CZ-NH1	8.89	124.75	120.30
54	BA	980	A	N1-C6-N6	-8.88	113.28	118.60
54	BA	693	A	N1-C6-N6	-8.87	113.28	118.60
45	BW	24	ARG	NE-CZ-NH1	8.87	124.74	120.30
21	AA	959	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	487	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	727	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1728	C	N3-C2-O2	-8.87	115.69	121.90
35	BM	55	ARG	NE-CZ-NH2	8.87	124.73	120.30
54	BA	156	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	454	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1274	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	509	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	207	A	N1-C6-N6	-8.85	113.29	118.60
55	BB	46	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	6	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	195	A	N1-C6-N6	-8.84	113.30	118.60
21	AA	33	A	N1-C6-N6	-8.83	113.30	118.60
2	AC	71	ARG	NE-CZ-NH1	8.83	124.71	120.30
21	AA	946	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	1073	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	53	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	345	C	N3-C2-O2	-8.82	115.73	121.90
16	AQ	5	ARG	NE-CZ-NH1	8.82	124.71	120.30
54	BA	2352	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	1499	A	N1-C6-N6	-8.81	113.31	118.60
6	AG	91	ARG	NE-CZ-NH1	8.81	124.70	120.30
21	AA	546	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	918	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	1266	G	O4'-C1'-N9	8.80	115.24	108.20
54	BA	2070	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	627	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	1759	A	N1-C6-N6	-8.79	113.32	118.60
54	BA	2600	A	N1-C6-N6	-8.80	113.32	118.60
38	BP	100	ARG	NE-CZ-NH1	8.79	124.70	120.30
21	AA	1021	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2077	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	919	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	435	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	523	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1077	A	N1-C6-N6	-8.77	113.34	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1020	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1729	U	O4'-C1'-N1	8.77	115.22	108.20
21	AA	243	A	N1-C6-N6	-8.77	113.34	118.60
51	B2	14	ARG	NE-CZ-NH1	8.76	124.68	120.30
54	BA	582	A	N1-C6-N6	-8.76	113.35	118.60
54	BA	1307	A	N1-C6-N6	-8.76	113.35	118.60
54	BA	2184	A	N1-C6-N6	-8.76	113.35	118.60
54	BA	1761	C	N3-C2-O2	-8.75	115.78	121.90
20	AU	6	ARG	NE-CZ-NH1	8.75	124.67	120.30
21	AA	983	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	53	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	1000	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	1502	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	1054	C	N3-C2-O2	-8.74	115.78	121.90
21	AA	1254	A	N1-C6-N6	-8.74	113.35	118.60
54	BA	199	A	N1-C6-N6	-8.74	113.35	118.60
40	BR	79	ARG	NE-CZ-NH1	8.74	124.67	120.30
54	BA	2565	A	N1-C6-N6	-8.74	113.36	118.60
21	AA	161	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	441	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	1363	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	1102	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1821	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	2733	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	349	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1288	G	O4'-C1'-N9	8.73	115.18	108.20
54	BA	1668	A	N1-C6-N6	-8.72	113.36	118.60
55	BB	66	A	C5-C6-N1	8.72	122.06	117.70
23	A2	79	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	2376	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	2461	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	1238	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	415	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	532	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	1614	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	1650	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	71	A	C5-C6-N1	8.71	122.06	117.70
54	BA	979	A	C5-C6-N1	8.71	122.05	117.70
54	BA	197	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	609	A	N1-C6-N6	-8.69	113.38	118.60
21	AA	466	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	1367	A	N1-C6-N6	-8.69	113.38	118.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1489	C	N3-C2-O2	-8.69	115.82	121.90
54	BA	1872	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1451	C	N3-C2-O2	-8.68	115.82	121.90
54	BA	2119	A	N1-C6-N6	-8.68	113.39	118.60
51	B2	19	ARG	NE-CZ-NH1	8.68	124.64	120.30
9	AJ	89	ARG	NE-CZ-NH1	8.68	124.64	120.30
33	BK	105	ARG	NE-CZ-NH1	8.68	124.64	120.30
36	BN	90	ARG	NE-CZ-NH1	8.67	124.64	120.30
22	A1	73	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	983	A	C5-C6-N1	8.66	122.03	117.70
54	BA	1914	C	N1-C2-O2	8.66	124.10	118.90
54	BA	2439	A	N1-C6-N6	-8.66	113.40	118.60
21	AA	373	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	794	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	2426	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	2534	A	C5-C6-N1	8.65	122.02	117.70
10	AK	105	ARG	NE-CZ-NH1	8.64	124.62	120.30
21	AA	1060	U	O4'-C1'-N1	8.64	115.12	108.20
54	BA	2333	A	N1-C6-N6	-8.64	113.42	118.60
55	BB	101	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	2476	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	129	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	2213	U	O4'-C1'-N1	8.63	115.11	108.20
54	BA	2358	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	344	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	1042	A	N1-C6-N6	-8.62	113.42	118.60
21	AA	1274	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	1318	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	329	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	977	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	1322	C	N1-C2-O2	8.62	124.07	118.90
21	AA	704	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	1960	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	130	A	C5-C6-N1	8.61	122.00	117.70
27	BE	170	ARG	NE-CZ-NH1	8.60	124.60	120.30
54	BA	2712	C	N3-C2-O2	-8.60	115.88	121.90
41	BS	18	ARG	NE-CZ-NH1	8.60	124.60	120.30
54	BA	2497	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	573	A	C5-C6-N1	8.59	122.00	117.70
21	AA	1342	C	P-O3'-C3'	8.59	130.01	119.70
54	BA	2448	A	C5-C6-N1	8.59	122.00	117.70
9	AJ	68	ARG	NE-CZ-NH1	8.59	124.59	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	515	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	616	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	1354	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	816	A	N1-C6-N6	-8.59	113.45	118.60
36	BN	8	ARG	NE-CZ-NH1	8.59	124.59	120.30
36	BN	17	ARG	NE-CZ-NH1	8.58	124.59	120.30
54	BA	10	A	C5-C6-N1	8.58	121.99	117.70
35	BM	44	ARG	NE-CZ-NH1	8.58	124.59	120.30
54	BA	2266	A	C5-C6-N1	8.58	121.99	117.70
21	AA	759	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	2736	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	1264	A	C5-C6-N1	8.57	121.99	117.70
54	BA	391	A	C5-C6-N1	8.57	121.98	117.70
54	BA	1246	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	1749	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2287	A	O4'-C1'-N9	8.57	115.06	108.20
21	AA	1499	A	C5-C6-N1	8.56	121.98	117.70
54	BA	1936	A	N1-C6-N6	-8.56	113.46	118.60
44	BV	9	ARG	NE-CZ-NH1	8.56	124.58	120.30
54	BA	2741	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	2406	A	N1-C6-N6	-8.56	113.47	118.60
40	BR	90	ARG	NE-CZ-NH1	8.56	124.58	120.30
54	BA	172	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	790	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	526	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2021	C	N3-C2-O2	-8.55	115.92	121.90
54	BA	2171	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	1287	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	502	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	1937	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	2312	U	O4'-C1'-N1	8.54	115.04	108.20
15	AP	14	ARG	NE-CZ-NH1	8.54	124.57	120.30
54	BA	64	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	2749	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	513	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	456	C	N3-C2-O2	-8.53	115.93	121.90
54	BA	637	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	1347	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	1167	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	1522	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	975	A	C5-C6-N1	8.53	121.96	117.70
53	B4	12	ARG	NE-CZ-NH1	8.52	124.56	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	483	A	N1-C6-N6	-8.52	113.49	118.60
55	BB	58	A	N1-C6-N6	-8.52	113.49	118.60
4	AE	19	ARG	NE-CZ-NH1	8.52	124.56	120.30
21	AA	152	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	715	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	356	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	44	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1237	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1816	C	N3-C2-O2	-8.51	115.94	121.90
54	BA	2900	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1762	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	2154	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	366	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	1012	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	2705	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1014	A	N1-C6-N6	-8.50	113.50	118.60
8	AI	11	ARG	NE-CZ-NH1	8.50	124.55	120.30
21	AA	1225	A	N1-C6-N6	-8.50	113.50	118.60
25	BC	216	ARG	NE-CZ-NH2	8.50	124.55	120.30
54	BA	139	U	O4'-C1'-N1	8.49	114.99	108.20
54	BA	2639	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	1163	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	964	A	C5-C6-N1	8.47	121.94	117.70
54	BA	443	A	C5-C6-N1	8.47	121.94	117.70
54	BA	1089	A	C5-C6-N1	8.47	121.93	117.70
54	BA	1590	A	N1-C6-N6	-8.47	113.52	118.60
24	A3	58	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	233	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	1548	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1728	C	O4'-C1'-N1	8.46	114.97	108.20
15	AP	8	ARG	NE-CZ-NH2	-8.46	116.07	120.30
54	BA	750	A	C5-C6-N1	8.46	121.93	117.70
21	AA	892	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	1652	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2679	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	533	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2748	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	262	A	C5-C6-N1	8.44	121.92	117.70
54	BA	2241	A	N1-C6-N6	-8.44	113.53	118.60
21	AA	648	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	729	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	1829	A	C5-C6-N1	8.44	121.92	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	393	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	2071	A	N1-C6-N6	-8.43	113.54	118.60
21	AA	363	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	2886	A	C5-C6-N1	8.43	121.91	117.70
1	AB	221	ARG	NE-CZ-NH1	8.42	124.51	120.30
54	BA	1711	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2758	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	981	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	1745	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2667	C	N3-C2-O2	-8.42	116.00	121.90
21	AA	1441	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	28	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	621	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	1571	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	303	A	N1-C6-N6	-8.41	113.55	118.60
39	BQ	29	ARG	NE-CZ-NH1	8.41	124.50	120.30
21	AA	382	A	N1-C6-N6	-8.41	113.56	118.60
56	B5	71	ARG	NE-CZ-NH1	8.41	124.50	120.30
21	AA	397	A	C5-C6-N1	8.40	121.90	117.70
54	BA	1276	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2860	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	768	A	C5-C6-N1	8.40	121.90	117.70
54	BA	1301	A	C5-C6-N1	8.40	121.90	117.70
21	AA	865	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	131	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2020	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2711	A	N1-C6-N6	-8.39	113.56	118.60
47	BY	48	ARG	NE-CZ-NH1	8.38	124.49	120.30
21	AA	765	G	O4'-C1'-N9	8.38	114.91	108.20
54	BA	1001	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	1572	A	C5-C6-N1	8.38	121.89	117.70
54	BA	2654	A	C5-C6-N1	8.38	121.89	117.70
54	BA	742	A	N1-C6-N6	-8.38	113.58	118.60
8	AI	79	ARG	NE-CZ-NH1	8.37	124.48	120.30
21	AA	149	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	428	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	607	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1700	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1871	A	O4'-C1'-N9	8.37	114.89	108.20
54	BA	2781	A	C5-C6-N1	8.37	121.88	117.70
54	BA	1616	A	C5-C6-N1	8.37	121.88	117.70
21	AA	1229	A	N1-C6-N6	-8.36	113.58	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	933	A	O4'-C1'-N9	8.36	114.89	108.20
21	AA	274	A	N1-C6-N6	-8.36	113.58	118.60
24	A3	59	A	N1-C6-N6	-8.36	113.58	118.60
21	AA	131	A	N1-C6-N6	-8.36	113.59	118.60
21	AA	499	A	N1-C6-N6	-8.36	113.59	118.60
54	BA	802	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	877	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	1265	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	2829	A	N1-C6-N6	-8.35	113.59	118.60
24	A3	75	C	N3-C2-O2	-8.35	116.05	121.90
54	BA	347	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1508	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	167	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	384	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	1999	C	O4'-C1'-N1	8.34	114.87	108.20
12	AM	69	ARG	NE-CZ-NH1	8.34	124.47	120.30
20	AU	46	ARG	NE-CZ-NH1	8.34	124.47	120.30
21	AA	1480	A	N1-C6-N6	-8.34	113.60	118.60
39	BQ	91	ARG	NE-CZ-NH1	8.34	124.47	120.30
21	AA	1056	U	O4'-C1'-N1	8.33	114.87	108.20
54	BA	1063	G	C1'-O4'-C4'	-8.33	103.23	109.90
55	BB	66	A	N1-C6-N6	-8.33	113.60	118.60
35	BM	114	ARG	NE-CZ-NH1	8.33	124.46	120.30
54	BA	532	A	C5-C6-N1	8.33	121.86	117.70
54	BA	1286	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	129	A	C5-C6-N1	8.33	121.86	117.70
54	BA	1040	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	2657	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1385	A	N1-C6-N6	-8.33	113.61	118.60
21	AA	1285	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	2541	A	C5-C6-N1	8.32	121.86	117.70
21	AA	1275	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	2646	C	N3-C2-O2	-8.32	116.08	121.90
54	BA	2825	G	O4'-C1'-N9	8.32	114.86	108.20
54	BA	322	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	364	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	1213	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	2340	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	1167	A	C5-C6-N1	8.31	121.86	117.70
21	AA	152	A	C5-C6-N1	8.31	121.85	117.70
21	AA	1336	C	N3-C2-O2	-8.31	116.09	121.90
54	BA	490	C	N3-C2-O2	-8.30	116.09	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1597	A	C5-C6-N1	8.30	121.85	117.70
54	BA	344	A	N1-C6-N6	-8.30	113.62	118.60
24	A3	39	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	204	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	1805	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	477	A	N1-C6-N6	-8.29	113.62	118.60
55	BB	29	A	N1-C6-N6	-8.29	113.62	118.60
21	AA	465	A	N1-C6-N6	-8.29	113.63	118.60
21	AA	572	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	514	A	C5-C6-N1	8.29	121.84	117.70
54	BA	1535	A	O4'-C1'-N9	8.29	114.83	108.20
44	BV	93	ARG	NE-CZ-NH1	8.29	124.44	120.30
54	BA	602	A	C5-C6-N1	8.29	121.84	117.70
54	BA	2205	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	119	A	C5-C6-N1	8.28	121.84	117.70
21	AA	1357	A	N1-C6-N6	-8.28	113.63	118.60
21	AA	1016	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	1196	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	1400	C	N3-C2-O2	-8.27	116.11	121.90
54	BA	943	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	190	A	N1-C6-N6	-8.27	113.64	118.60
32	BJ	34	ARG	NE-CZ-NH1	8.27	124.44	120.30
54	BA	1382	G	O4'-C1'-N9	8.27	114.81	108.20
12	AM	89	ARG	NE-CZ-NH1	8.27	124.43	120.30
54	BA	2270	A	N1-C6-N6	-8.26	113.64	118.60
21	AA	1092	A	N1-C6-N6	-8.26	113.64	118.60
21	AA	1492	A	C5-C6-N1	8.26	121.83	117.70
21	AA	1005	A	N1-C6-N6	-8.26	113.64	118.60
21	AA	352	C	N3-C2-O2	-8.26	116.12	121.90
54	BA	131	A	C5-C6-N1	8.26	121.83	117.70
21	AA	938	A	N1-C6-N6	-8.26	113.65	118.60
54	BA	716	A	N1-C6-N6	-8.26	113.65	118.60
54	BA	996	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	1371	G	O4'-C1'-N9	8.25	114.80	108.20
21	AA	889	A	C5-C6-N1	8.25	121.83	117.70
21	AA	938	A	C5-C6-N1	8.25	121.83	117.70
54	BA	1508	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	1618	A	N1-C6-N6	-8.25	113.65	118.60
21	AA	167	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2170	A	C5-C6-N1	8.25	121.83	117.70
21	AA	246	A	N1-C6-N6	-8.25	113.65	118.60
21	AA	373	A	C5-C6-N1	8.25	121.82	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	649	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	984	A	C5-C6-N1	8.25	121.82	117.70
21	AA	279	A	C5-C6-N1	8.24	121.82	117.70
54	BA	95	A	N1-C6-N6	-8.24	113.65	118.60
21	AA	1000	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	643	A	C5-C6-N1	8.24	121.82	117.70
54	BA	482	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	1791	A	C5-C6-N1	8.24	121.82	117.70
54	BA	479	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	1744	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	50	A	C5-C6-N1	8.23	121.82	117.70
54	BA	38	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	346	A	C5-C6-N1	8.23	121.82	117.70
54	BA	1665	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	1978	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2778	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2799	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	1095	A	O4'-C1'-N9	8.23	114.78	108.20
54	BA	1809	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	216	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	456	C	N1-C2-O2	8.22	123.83	118.90
54	BA	2154	A	C5-C6-N1	8.22	121.81	117.70
21	AA	1054	C	O4'-C1'-N1	8.22	114.78	108.20
51	B2	34	ARG	NE-CZ-NH1	8.22	124.41	120.30
54	BA	2706	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1085	A	C5-C6-N1	8.22	121.81	117.70
54	BA	1583	A	C5-C6-N1	8.22	121.81	117.70
54	BA	2114	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	1393	A	C5-C6-N1	8.21	121.81	117.70
54	BA	482	A	C5-C6-N1	8.21	121.80	117.70
21	AA	71	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1952	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	2721	A	N1-C6-N6	-8.20	113.68	118.60
9	AJ	16	ARG	NE-CZ-NH2	8.20	124.40	120.30
54	BA	928	A	N1-C6-N6	-8.20	113.68	118.60
9	AJ	31	ARG	NE-CZ-NH1	8.20	124.40	120.30
54	BA	1815	A	C5-C6-N1	8.20	121.80	117.70
21	AA	1252	A	C5-C6-N1	8.19	121.80	117.70
54	BA	61	C	N3-C2-O2	-8.19	116.16	121.90
54	BA	2468	A	N1-C6-N6	-8.19	113.68	118.60
21	AA	482	A	N1-C6-N6	-8.19	113.68	118.60
54	BA	1342	A	N1-C6-N6	-8.19	113.69	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1349	A	N1-C6-N6	-8.19	113.69	118.60
37	BO	94	ARG	NE-CZ-NH1	8.19	124.39	120.30
54	BA	527	C	N1-C2-O2	8.19	123.81	118.90
54	BA	528	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	1928	A	C5-C6-N1	8.19	121.79	117.70
54	BA	2800	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	614	A	N1-C6-N6	-8.19	113.69	118.60
3	AD	62	ARG	NE-CZ-NH1	8.18	124.39	120.30
11	AL	30	ARG	NE-CZ-NH1	8.18	124.39	120.30
54	BA	1544	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	2117	A	C5-C6-N1	8.18	121.79	117.70
54	BA	422	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	621	A	C5-C6-N1	8.18	121.79	117.70
54	BA	2392	A	C5-C6-N1	8.18	121.79	117.70
21	AA	263	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	1265	A	C5-C6-N1	8.17	121.79	117.70
54	BA	2309	A	C5-C6-N1	8.17	121.79	117.70
21	AA	906	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	753	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	103	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	689	A	C5-C6-N1	8.16	121.78	117.70
54	BA	722	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	65	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1551	A	N1-C6-N6	-8.16	113.71	118.60
54	BA	2821	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	906	A	C5-C6-N1	8.15	121.78	117.70
21	AA	970	C	N3-C2-O2	-8.15	116.19	121.90
54	BA	863	A	C5-C6-N1	8.15	121.78	117.70
54	BA	1155	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	227	A	N1-C6-N6	-8.15	113.71	118.60
2	AC	168	ARG	NE-CZ-NH1	8.15	124.37	120.30
15	AP	28	ARG	NE-CZ-NH1	8.15	124.37	120.30
21	AA	196	A	N1-C6-N6	-8.14	113.71	118.60
54	BA	2080	A	N1-C6-N6	-8.14	113.72	118.60
21	AA	182	A	N1-C6-N6	-8.14	113.72	118.60
21	AA	915	A	C5-C6-N1	8.14	121.77	117.70
21	AA	1158	C	N3-C2-O2	-8.14	116.20	121.90
54	BA	294	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	911	A	C5-C6-N1	8.14	121.77	117.70
21	AA	1430	A	N1-C6-N6	-8.14	113.72	118.60
13	AN	81	ARG	NE-CZ-NH1	8.13	124.37	120.30
54	BA	2381	A	N1-C6-N6	-8.13	113.72	118.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	45	A	C5-C6-N1	8.13	121.77	117.70
54	BA	311	A	C5-C6-N1	8.13	121.76	117.70
54	BA	829	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	2655	G	O4'-C1'-N9	8.13	114.70	108.20
12	AM	108	ARG	NE-CZ-NH1	8.13	124.36	120.30
54	BA	126	A	C5-C6-N1	8.13	121.76	117.70
1	AB	136	ARG	NE-CZ-NH1	8.13	124.36	120.30
54	BA	1384	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1434	A	O4'-C1'-N9	8.12	114.70	108.20
21	AA	814	A	N1-C6-N6	-8.12	113.73	118.60
24	A3	77	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	527	C	N3-C2-O2	-8.12	116.22	121.90
54	BA	149	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1757	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	2169	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2346	A	C5-C6-N1	8.12	121.76	117.70
54	BA	804	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2385	C	O4'-C1'-N1	8.11	114.69	108.20
21	AA	430	A	N1-C6-N6	-8.11	113.74	118.60
21	AA	451	A	C5-C6-N1	8.11	121.75	117.70
21	AA	978	A	N1-C6-N6	-8.11	113.74	118.60
30	BH	50	ARG	NE-CZ-NH1	8.11	124.35	120.30
54	BA	371	A	C5-C6-N1	8.11	121.75	117.70
54	BA	2003	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	743	A	C5-C6-N1	8.10	121.75	117.70
54	BA	1773	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	718	A	C5-C6-N1	8.09	121.75	117.70
54	BA	1938	A	N1-C6-N6	-8.09	113.75	118.60
21	AA	282	A	C5-C6-N1	8.09	121.74	117.70
54	BA	449	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2660	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	1465	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	2314	A	C5-C6-N1	8.08	121.74	117.70
54	BA	666	A	C4-C5-C6	-8.08	112.96	117.00
21	AA	1346	A	C5-C6-N1	8.07	121.74	117.70
45	BW	38	ARG	NE-CZ-NH1	8.07	124.34	120.30
21	AA	214	C	N3-C2-O2	-8.07	116.25	121.90
3	AD	61	ARG	NE-CZ-NH1	8.07	124.33	120.30
21	AA	1204	A	N1-C6-N6	-8.07	113.76	118.60
49	B0	15	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	AB	224	ARG	NE-CZ-NH1	8.07	124.33	120.30
21	AA	712	A	N1-C6-N6	-8.07	113.76	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	262	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	2058	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	300	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	1397	C	N3-C2-O2	-8.06	116.26	121.90
54	BA	1286	A	C5-C6-N1	8.06	121.73	117.70
21	AA	466	A	C5-C6-N1	8.06	121.73	117.70
21	AA	663	A	N1-C6-N6	-8.06	113.77	118.60
21	AA	228	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	694	A	C5-C6-N1	8.05	121.73	117.70
54	BA	603	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	1469	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	2873	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	1646	C	N3-C2-O2	-8.05	116.26	121.90
54	BA	676	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	2879	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	320	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	510	A	C5-C6-N1	8.05	121.72	117.70
21	AA	547	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	1453	A	N1-C6-N6	-8.04	113.77	118.60
54	BA	2369	A	C4-C5-C6	-8.05	112.98	117.00
32	BJ	96	ARG	NE-CZ-NH1	8.04	124.32	120.30
21	AA	1467	C	N3-C2-O2	-8.04	116.27	121.90
40	BR	13	ARG	NE-CZ-NH1	8.04	124.32	120.30
54	BA	2297	A	O4'-C1'-N9	8.04	114.63	108.20
54	BA	756	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	423	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	189	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	1890	A	N1-C6-N6	-8.03	113.78	118.60
55	BB	108	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2590	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	171	A	C5-C6-N1	8.02	121.71	117.70
54	BA	676	A	C5-C6-N1	8.02	121.71	117.70
54	BA	2740	A	N1-C6-N6	-8.02	113.79	118.60
22	A1	35	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	2191	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	833	A	N1-C6-N6	-8.01	113.79	118.60
21	AA	119	A	N1-C6-N6	-8.01	113.79	118.60
21	AA	1170	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	1254	A	N1-C6-N6	-8.01	113.79	118.60
21	AA	777	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	2781	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	2814	A	C5-C6-N1	8.00	121.70	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	602	A	N1-C6-N6	-8.00	113.80	118.60
25	BC	12	ARG	NE-CZ-NH2	8.00	124.30	120.30
54	BA	2171	A	C5-C6-N1	8.00	121.70	117.70
55	BB	53	A	C5-C6-N1	8.00	121.70	117.70
25	BC	220	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	1451	C	N1-C2-O2	8.00	123.70	118.90
54	BA	613	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	77	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	460	A	N1-C6-N6	-7.99	113.81	118.60
16	AQ	39	ARG	NE-CZ-NH1	7.99	124.29	120.30
54	BA	1953	A	C5-C6-N1	7.99	121.69	117.70
55	BB	89	U	O4'-C1'-N1	7.99	114.59	108.20
24	A3	74	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	501	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	1165	A	N1-C6-N6	-7.99	113.81	118.60
16	AQ	61	ARG	NE-CZ-NH1	7.98	124.29	120.30
54	BA	2750	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	752	A	C5-C6-N1	7.98	121.69	117.70
13	AN	65	ARG	NE-CZ-NH1	7.97	124.29	120.30
21	AA	819	A	C5-C6-N1	7.97	121.69	117.70
24	A3	39	A	C5-C6-N1	7.97	121.69	117.70
54	BA	1477	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	2660	A	C5-C6-N1	7.97	121.69	117.70
54	BA	2835	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	560	A	C5-C6-N1	7.97	121.68	117.70
54	BA	497	A	C5-C6-N1	7.97	121.68	117.70
54	BA	2635	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	663	A	C5-C6-N1	7.97	121.68	117.70
21	AA	878	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	265	A	C5-C6-N1	7.97	121.68	117.70
54	BA	2425	A	C5-C6-N1	7.97	121.68	117.70
21	AA	72	A	C5-C6-N1	7.96	121.68	117.70
22	A1	26	A	C5-C6-N1	7.96	121.68	117.70
49	B0	49	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	614	A	C5-C6-N1	7.96	121.68	117.70
21	AA	77	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1287	A	C5-C6-N1	7.96	121.68	117.70
21	AA	1433	A	C5-C6-N1	7.96	121.68	117.70
21	AA	1197	A	N1-C6-N6	-7.96	113.83	118.60
54	BA	608	A	N1-C6-N6	-7.96	113.82	118.60
22	A1	76	A	O4'-C1'-N9	7.96	114.56	108.20
54	BA	2758	A	C5-C6-N1	7.96	121.68	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1129	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1871	A	C5-C6-N1	7.95	121.68	117.70
21	AA	1046	A	N1-C6-N6	-7.95	113.83	118.60
32	BJ	13	ARG	NE-CZ-NH1	7.95	124.28	120.30
54	BA	213	A	C5-C6-N1	7.95	121.67	117.70
54	BA	223	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1272	A	C5-C6-N1	7.95	121.67	117.70
54	BA	1537	G	O4'-C1'-N9	7.95	114.56	108.20
54	BA	574	A	C4-C5-C6	-7.95	113.03	117.00
54	BA	1392	A	C5-C6-N1	7.95	121.67	117.70
54	BA	632	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1785	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	1044	A	N1-C6-N6	-7.94	113.83	118.60
14	AO	88	ARG	NE-CZ-NH1	7.94	124.27	120.30
21	AA	749	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	1048	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	2670	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	558	U	O4'-C1'-N1	7.94	114.55	108.20
21	AA	937	A	C5-C6-N1	7.94	121.67	117.70
54	BA	84	A	C5-C6-N1	7.93	121.67	117.70
54	BA	2101	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	560	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	845	A	C4-C5-C6	-7.93	113.03	117.00
22	A1	26	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	1531	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	718	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	899	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	613	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1189	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	344	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1336	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1515	A	C5-C6-N1	7.92	121.66	117.70
54	BA	547	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	982	C	O4'-C1'-N1	7.91	114.53	108.20
54	BA	1434	A	C5-C6-N1	7.91	121.66	117.70
54	BA	2560	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	670	A	C5-C6-N1	7.91	121.65	117.70
54	BA	13	A	N1-C6-N6	-7.91	113.86	118.60
21	AA	1214	C	N1-C2-O2	7.91	123.64	118.90
54	BA	1918	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	1069	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	1404	C	N3-C2-O2	-7.90	116.37	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2425	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	2453	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2037	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	2587	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	816	A	C5-C6-N1	7.89	121.65	117.70
21	AA	825	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	1285	A	N1-C6-N6	-7.89	113.86	118.60
21	AA	1054	C	N1-C2-O2	7.89	123.64	118.90
54	BA	910	A	C5-C6-N1	7.89	121.65	117.70
21	AA	1082	A	N1-C6-N6	-7.89	113.86	118.60
24	A3	1	C	N3-C2-O2	-7.89	116.38	121.90
54	BA	49	A	C5-C6-N1	7.89	121.65	117.70
54	BA	2030	A	C4-C5-C6	-7.89	113.05	117.00
21	AA	792	A	C5-C6-N1	7.89	121.64	117.70
54	BA	685	A	C5-C6-N1	7.89	121.64	117.70
54	BA	2762	C	O4'-C1'-N1	7.88	114.51	108.20
21	AA	8	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1775	U	O4'-C1'-N1	7.88	114.50	108.20
54	BA	1784	A	C5-C6-N1	7.88	121.64	117.70
54	BA	784	G	O4'-C1'-N9	7.88	114.50	108.20
54	BA	1545	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	1847	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1490	A	C5-C6-N1	7.87	121.64	117.70
54	BA	2267	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1009	A	C5-C6-N1	7.87	121.64	117.70
21	AA	1261	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	1054	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	583	A	C5-C6-N1	7.87	121.63	117.70
54	BA	1126	A	C4-C5-C6	-7.87	113.07	117.00
21	AA	495	A	C5-C6-N1	7.87	121.63	117.70
21	AA	174	A	C5-C6-N1	7.86	121.63	117.70
27	BE	40	ARG	NE-CZ-NH1	7.86	124.23	120.30
54	BA	654	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	1028	A	N1-C6-N6	-7.86	113.89	118.60
21	AA	51	A	C5-C6-N1	7.86	121.63	117.70
21	AA	253	A	N1-C6-N6	-7.86	113.89	118.60
21	AA	1534	A	C5-C6-N1	7.86	121.63	117.70
55	BB	41	G	O4'-C1'-N9	7.85	114.48	108.20
16	AQ	26	ARG	NE-CZ-NH1	7.85	124.23	120.30
21	AA	574	A	C5-C6-N1	7.85	121.62	117.70
54	BA	599	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2503	A	C5-C6-N1	7.85	121.63	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1456	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2598	A	C5-C6-N1	7.85	121.62	117.70
21	AA	964	A	C4-C5-C6	-7.84	113.08	117.00
54	BA	1773	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2887	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	1552	A	C5-C6-N1	7.84	121.62	117.70
21	AA	7	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	196	A	N1-C6-N6	-7.84	113.90	118.60
21	AA	1256	A	C5-C6-N1	7.84	121.62	117.70
21	AA	197	A	C5-C6-N1	7.84	121.62	117.70
54	BA	1133	A	C5-C6-N1	7.84	121.62	117.70
54	BA	1147	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	99	U	O4'-C1'-N1	7.83	114.47	108.20
46	BX	2	ARG	NE-CZ-NH1	7.83	124.22	120.30
54	BA	2682	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1264	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	1110	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	979	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	2513	A	C5-C6-N1	7.82	121.61	117.70
54	BA	2872	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1675	C	N3-C2-O2	-7.82	116.42	121.90
21	AA	468	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	1008	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1713	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	2478	A	C5-C6-N1	7.82	121.61	117.70
54	BA	126	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	226	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1913	A	C5-C6-N1	7.82	121.61	117.70
54	BA	2381	A	C5-C6-N1	7.82	121.61	117.70
21	AA	1352	C	N3-C2-O2	-7.82	116.43	121.90
54	BA	718	A	O4'-C1'-N9	7.82	114.45	108.20
21	AA	33	A	C5-C6-N1	7.81	121.61	117.70
54	BA	472	A	C5-C6-N1	7.81	121.61	117.70
54	BA	844	A	N1-C6-N6	-7.81	113.91	118.60
21	AA	1377	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	675	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	2108	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	111	A	C5-C6-N1	7.81	121.61	117.70
3	AD	187	ARG	NE-CZ-NH1	7.81	124.20	120.30
21	AA	687	A	N1-C6-N6	-7.81	113.92	118.60
54	BA	1669	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	2738	A	N1-C6-N6	-7.81	113.91	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	547	A	C5-C6-N1	7.81	121.60	117.70
54	BA	972	A	C5-C6-N1	7.81	121.60	117.70
54	BA	278	A	C5-C6-N1	7.81	121.60	117.70
54	BA	2031	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	2751	G	O4'-C1'-N9	7.80	114.44	108.20
21	AA	1329	A	C5-C6-N1	7.80	121.60	117.70
21	AA	1320	C	N3-C2-O2	-7.80	116.44	121.90
54	BA	2531	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	1219	A	C5-C6-N1	7.79	121.60	117.70
54	BA	522	A	C5-C6-N1	7.79	121.60	117.70
54	BA	2278	A	C5-C6-N1	7.79	121.60	117.70
21	AA	702	A	C5-C6-N1	7.79	121.59	117.70
33	BK	71	ARG	NE-CZ-NH1	7.79	124.19	120.30
3	AD	183	ARG	NE-CZ-NH1	7.78	124.19	120.30
20	AU	16	ARG	NE-CZ-NH1	7.78	124.19	120.30
21	AA	1468	A	C5-C6-N1	7.78	121.59	117.70
54	BA	750	A	C4-C5-C6	-7.78	113.11	117.00
54	BA	988	A	C5-C6-N1	7.78	121.59	117.70
21	AA	980	C	N3-C2-O2	-7.78	116.45	121.90
54	BA	1354	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1137	C	N3-C2-O2	-7.78	116.45	121.90
54	BA	104	A	C5-C6-N1	7.78	121.59	117.70
54	BA	751	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	2211	A	C5-C6-N1	7.78	121.59	117.70
54	BA	5	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	792	A	N1-C6-N6	-7.78	113.94	118.60
21	AA	413	G	O4'-C1'-N9	7.77	114.42	108.20
21	AA	451	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	1110	A	C5-C6-N1	7.77	121.59	117.70
31	BI	102	ARG	NE-CZ-NH1	7.77	124.19	120.30
54	BA	1029	A	N1-C6-N6	-7.77	113.94	118.60
40	BR	78	ARG	NE-CZ-NH1	7.77	124.19	120.30
54	BA	740	C	N3-C2-O2	-7.77	116.46	121.90
54	BA	886	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1596	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	1213	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	2602	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1611	C	N3-C2-O2	-7.76	116.47	121.90
54	BA	1919	A	C5-C6-N1	7.76	121.58	117.70
21	AA	130	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	279	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	342	A	C4-C5-C6	-7.76	113.12	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1010	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1912	A	N1-C6-N6	-7.76	113.94	118.60
55	BB	109	A	C5-C6-N1	7.76	121.58	117.70
44	BV	19	ARG	NE-CZ-NH1	7.76	124.18	120.30
54	BA	2273	A	C5-C6-N1	7.76	121.58	117.70
54	BA	177	G	O4'-C1'-N9	7.76	114.41	108.20
54	BA	2435	A	C5-C6-N1	7.76	121.58	117.70
21	AA	572	A	C5-C6-N1	7.75	121.58	117.70
54	BA	668	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2411	A	C5-C6-N1	7.75	121.58	117.70
54	BA	1522	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2453	A	N1-C6-N6	-7.75	113.95	118.60
22	A1	58	A	C5-C6-N1	7.75	121.58	117.70
21	AA	1126	U	O4'-C1'-N1	7.75	114.40	108.20
22	A1	11	C	N3-C2-O2	-7.75	116.48	121.90
37	BO	81	ARG	NE-CZ-NH1	7.75	124.17	120.30
54	BA	140	C	N3-C2-O2	-7.75	116.48	121.90
54	BA	203	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	644	A	C5-C6-N1	7.75	121.57	117.70
54	BA	1050	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2173	A	C5-C6-N1	7.75	121.57	117.70
54	BA	73	A	C5-C6-N1	7.75	121.57	117.70
54	BA	103	A	C5-C6-N1	7.75	121.57	117.70
54	BA	412	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	945	A	C5-C6-N1	7.75	121.57	117.70
54	BA	2054	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1100	C	N1-C2-O2	7.74	123.55	118.90
4	AE	67	ARG	NE-CZ-NH1	7.74	124.17	120.30
21	AA	1022	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1610	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1377	A	C5-C6-N1	7.74	121.57	117.70
24	A3	16	C	N3-C2-O2	-7.74	116.48	121.90
54	BA	2015	A	C5-C6-N1	7.74	121.57	117.70
21	AA	872	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1632	A	C5-C6-N1	7.74	121.57	117.70
54	BA	64	A	C5-C6-N1	7.74	121.57	117.70
21	AA	498	A	C5-C6-N1	7.74	121.57	117.70
29	BG	162	ARG	NE-CZ-NH1	7.74	124.17	120.30
54	BA	1970	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	866	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	553	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	1226	C	N3-C2-O2	-7.73	116.49	121.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	BP	50	ARG	NE-CZ-NH1	7.73	124.17	120.30
21	AA	1433	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	1503	A	C5-C6-N1	7.73	121.56	117.70
54	BA	631	A	C5-C6-N1	7.73	121.56	117.70
54	BA	1127	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	499	A	C5-C6-N1	7.73	121.56	117.70
21	AA	1218	C	N3-C2-O2	-7.73	116.49	121.90
54	BA	2882	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	2542	A	C5-C6-N1	7.73	121.56	117.70
7	AH	76	ARG	NE-CZ-NH1	7.72	124.16	120.30
54	BA	1151	A	C5-C6-N1	7.72	121.56	117.70
56	B5	12	ARG	NE-CZ-NH1	7.72	124.16	120.30
21	AA	192	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	1598	A	C5-C6-N1	7.72	121.56	117.70
21	AA	60	A	C5-C6-N1	7.72	121.56	117.70
21	AA	160	A	N1-C6-N6	-7.72	113.97	118.60
22	A1	75	C	N3-C2-O2	-7.72	116.50	121.90
54	BA	1789	A	C5-C6-N1	7.72	121.56	117.70
54	BA	2634	A	C5-C6-N1	7.72	121.56	117.70
21	AA	746	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	1151	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	2434	A	C5-C6-N1	7.72	121.56	117.70
21	AA	120	A	C5-C6-N1	7.71	121.56	117.70
21	AA	553	A	C5-C6-N1	7.71	121.56	117.70
54	BA	91	A	C5-C6-N1	7.71	121.56	117.70
54	BA	2826	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	802	A	C5-C6-N1	7.71	121.56	117.70
21	AA	923	A	C5-C6-N1	7.71	121.56	117.70
21	AA	1246	A	C5-C6-N1	7.71	121.56	117.70
54	BA	2388	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	320	A	C5-C6-N1	7.71	121.56	117.70
54	BA	889	C	N3-C2-O2	-7.71	116.50	121.90
54	BA	5	A	C5-C6-N1	7.71	121.55	117.70
54	BA	1230	A	C4-C5-C6	-7.71	113.15	117.00
54	BA	2019	A	N1-C6-N6	-7.71	113.98	118.60
54	BA	973	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	2435	A	C4-C5-C6	-7.70	113.15	117.00
26	BD	179	ARG	NE-CZ-NH1	7.70	124.15	120.30
54	BA	1571	A	C5-C6-N1	7.70	121.55	117.70
30	BH	27	ARG	NE-CZ-NH1	7.70	124.15	120.30
21	AA	767	A	C5-C6-N1	7.70	121.55	117.70
24	A3	22	A	C5-C6-N1	7.70	121.55	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	356	A	C5-C6-N1	7.69	121.55	117.70
21	AA	1014	A	C5-C6-N1	7.69	121.55	117.70
54	BA	402	A	N1-C6-N6	-7.69	113.98	118.60
54	BA	689	A	N1-C6-N6	-7.69	113.98	118.60
21	AA	784	A	C5-C6-N1	7.69	121.54	117.70
54	BA	531	C	N3-C2-O2	-7.69	116.52	121.90
21	AA	523	A	C5-C6-N1	7.69	121.54	117.70
54	BA	2311	A	C5-C6-N1	7.69	121.54	117.70
21	AA	338	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	502	A	C5-C6-N1	7.68	121.54	117.70
54	BA	716	A	C5-C6-N1	7.68	121.54	117.70
54	BA	2482	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	1918	A	C5-C6-N1	7.68	121.54	117.70
54	BA	320	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1096	A	C5-C6-N1	7.68	121.54	117.70
54	BA	161	A	C5-C6-N1	7.68	121.54	117.70
8	AI	48	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	1876	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1050	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	1211	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	1324	G	O4'-C1'-N9	7.67	114.34	108.20
21	AA	1252	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	222	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	739	A	C5-C6-N1	7.67	121.54	117.70
21	AA	907	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2092	U	O4'-C1'-N1	7.67	114.33	108.20
21	AA	1418	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1096	A	C4-C5-C6	-7.67	113.17	117.00
54	BA	1275	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2158	A	C5-C6-N1	7.67	121.53	117.70
54	BA	2468	A	C5-C6-N1	7.67	121.53	117.70
54	BA	447	A	N1-C6-N6	-7.66	114.00	118.60
21	AA	1398	A	N1-C6-N6	-7.66	114.00	118.60
21	AA	1476	A	N1-C6-N6	-7.66	114.00	118.60
39	BQ	5	ARG	NE-CZ-NH1	7.66	124.13	120.30
54	BA	1070	A	C5-C6-N1	7.66	121.53	117.70
54	BA	1237	A	C5-C6-N1	7.66	121.53	117.70
54	BA	749	A	C5-C6-N1	7.66	121.53	117.70
54	BA	1713	A	C5-C6-N1	7.66	121.53	117.70
21	AA	364	A	C5-C6-N1	7.66	121.53	117.70
54	BA	167	A	C5-C6-N1	7.66	121.53	117.70
54	BA	1998	A	N1-C6-N6	-7.66	114.01	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1503	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	125	A	C5-C6-N1	7.66	121.53	117.70
21	AA	345	C	N1-C2-O2	7.65	123.49	118.90
56	B5	7	ARG	NE-CZ-NH1	7.65	124.12	120.30
21	AA	909	A	N1-C6-N6	-7.64	114.01	118.60
21	AA	1364	U	O4'-C1'-N1	7.64	114.31	108.20
54	BA	705	A	C5-C6-N1	7.64	121.52	117.70
21	AA	32	A	C5-C6-N1	7.64	121.52	117.70
30	BH	51	ARG	NE-CZ-NH1	7.64	124.12	120.30
54	BA	1759	A	C5-C6-N1	7.64	121.52	117.70
54	BA	453	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	655	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2169	A	C5-C6-N1	7.64	121.52	117.70
21	AA	336	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	1188	A	C5-C6-N1	7.64	121.52	117.70
54	BA	793	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	233	A	C5-C6-N1	7.63	121.52	117.70
54	BA	1698	A	C5-C6-N1	7.63	121.52	117.70
21	AA	196	A	C5-C6-N1	7.63	121.52	117.70
54	BA	661	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	1383	A	C5-C6-N1	7.63	121.52	117.70
21	AA	1203	C	N3-C2-O2	-7.63	116.56	121.90
42	BT	69	ARG	NE-CZ-NH1	7.63	124.11	120.30
54	BA	1226	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	1005	A	C5-C6-N1	7.63	121.51	117.70
54	BA	1626	A	C5-C6-N1	7.63	121.51	117.70
21	AA	794	A	C5-C6-N1	7.62	121.51	117.70
54	BA	219	A	C5-C6-N1	7.62	121.51	117.70
54	BA	362	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	633	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	838	C	N3-C2-O2	-7.62	116.56	121.90
21	AA	415	A	C5-C6-N1	7.62	121.51	117.70
54	BA	330	A	C5-C6-N1	7.62	121.51	117.70
54	BA	515	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2015	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	101	A	C5-C6-N1	7.62	121.51	117.70
54	BA	251	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2267	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	1314	C	N3-C2-O2	-7.62	116.57	121.90
21	AA	1299	A	C5-C6-N1	7.61	121.51	117.70
21	AA	1447	A	C5-C6-N1	7.61	121.51	117.70
21	AA	712	A	C5-C6-N1	7.61	121.50	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1758	U	O4'-C1'-N1	7.61	114.29	108.20
28	BF	70	ARG	NE-CZ-NH1	7.61	124.10	120.30
54	BA	1453	A	O4'-C1'-N9	7.61	114.28	108.20
54	BA	1509	A	C5-C6-N1	7.61	121.50	117.70
54	BA	2883	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1489	C	N1-C2-O2	7.60	123.46	118.90
54	BA	2761	A	C5-C6-N1	7.60	121.50	117.70
54	BA	961	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	981	A	C5-C6-N1	7.60	121.50	117.70
54	BA	1420	A	C5-C6-N1	7.60	121.50	117.70
54	BA	526	A	C5-C6-N1	7.60	121.50	117.70
54	BA	1205	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	1145	A	C5-C6-N1	7.60	121.50	117.70
21	AA	1196	A	C5-C6-N1	7.59	121.50	117.70
54	BA	2614	A	C5-C6-N1	7.59	121.50	117.70
24	A3	45	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	1308	A	N1-C6-N6	-7.59	114.04	118.60
24	A3	38	A	C5-C6-N1	7.59	121.50	117.70
54	BA	2275	C	N3-C2-O2	-7.59	116.59	121.90
6	AG	94	ARG	NE-CZ-NH1	7.59	124.09	120.30
54	BA	614	A	O4'-C1'-N9	7.59	114.27	108.20
54	BA	1854	A	C5-C6-N1	7.59	121.49	117.70
21	AA	371	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2376	A	C5-C6-N1	7.58	121.49	117.70
21	AA	923	A	N1-C6-N6	-7.58	114.05	118.60
21	AA	996	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1332	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	592	A	C4-C5-C6	-7.58	113.21	117.00
54	BA	1585	C	N3-C2-O2	-7.58	116.59	121.90
54	BA	1596	A	C5-C6-N1	7.58	121.49	117.70
21	AA	181	A	C5-C6-N1	7.58	121.49	117.70
21	AA	210	C	N3-C2-O2	-7.58	116.59	121.90
21	AA	768	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	2126	A	C5-C6-N1	7.58	121.49	117.70
11	AL	113	ARG	NE-CZ-NH1	7.58	124.09	120.30
54	BA	374	A	N1-C6-N6	-7.58	114.06	118.60
54	BA	1269	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1677	A	C5-C6-N1	7.58	121.49	117.70
38	BP	20	ARG	NE-CZ-NH1	7.57	124.09	120.30
54	BA	892	A	C4-C5-C6	-7.57	113.21	117.00
54	BA	1247	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	1365	A	C5-C6-N1	7.57	121.49	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1470	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	249	C	N3-C2-O2	-7.57	116.60	121.90
54	BA	1579	A	N1-C6-N6	-7.57	114.06	118.60
21	AA	635	A	N1-C6-N6	-7.57	114.06	118.60
37	BO	10	ARG	NE-CZ-NH1	7.57	124.08	120.30
54	BA	1757	A	C5-C6-N1	7.57	121.48	117.70
54	BA	2851	A	C5-C6-N1	7.57	121.48	117.70
54	BA	2858	C	N3-C2-O2	-7.57	116.60	121.90
54	BA	83	A	C5-C6-N1	7.56	121.48	117.70
54	BA	104	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	582	A	C5-C6-N1	7.56	121.48	117.70
21	AA	640	A	C5-C6-N1	7.56	121.48	117.70
8	AI	129	ARG	NE-CZ-NH1	7.56	124.08	120.30
54	BA	1630	A	C5-C6-N1	7.56	121.48	117.70
21	AA	151	A	C5-C6-N1	7.55	121.48	117.70
54	BA	480	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1791	A	C4-C5-C6	-7.55	113.22	117.00
54	BA	2134	A	C5-C6-N1	7.55	121.48	117.70
21	AA	298	A	C5-C6-N1	7.55	121.48	117.70
54	BA	42	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2432	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2534	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1274	A	C5-C6-N1	7.55	121.47	117.70
21	AA	78	A	C4-C5-C6	-7.54	113.23	117.00
21	AA	320	A	C4-C5-C6	-7.54	113.23	117.00
21	AA	374	A	C5-C6-N1	7.54	121.47	117.70
21	AA	1011	C	N3-C2-O2	-7.54	116.62	121.90
54	BA	119	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	988	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	1508	A	C5-C6-N1	7.54	121.47	117.70
54	BA	693	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1021	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1739	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	1803	A	C5-C6-N1	7.53	121.47	117.70
39	BQ	63	ARG	NE-CZ-NH1	7.53	124.07	120.30
54	BA	806	C	O4'-C1'-N1	7.53	114.23	108.20
21	AA	205	A	C5-C6-N1	7.53	121.47	117.70
54	BA	144	A	C5-C6-N1	7.53	121.47	117.70
54	BA	1378	A	C5-C6-N1	7.53	121.47	117.70
54	BA	2297	A	C5-C6-N1	7.53	121.47	117.70
54	BA	219	A	C4-C5-C6	-7.53	113.24	117.00
17	AR	62	ARG	NE-CZ-NH1	7.53	124.06	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1281	C	N3-C2-O2	-7.53	116.63	121.90
24	A3	73	A	C5-C6-N1	7.53	121.46	117.70
21	AA	728	A	C4-C5-C6	-7.53	113.24	117.00
54	BA	1808	A	C5-C6-N1	7.53	121.46	117.70
54	BA	2322	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	2560	A	C5-C6-N1	7.53	121.46	117.70
54	BA	2753	A	C4-C5-C6	-7.53	113.24	117.00
21	AA	969	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1029	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1250	A	C5-C6-N1	7.52	121.46	117.70
54	BA	331	C	N3-C2-O2	-7.52	116.64	121.90
54	BA	1241	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1694	C	O4'-C1'-N1	7.52	114.22	108.20
54	BA	1728	C	N1-C2-O2	7.52	123.41	118.90
54	BA	1634	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1501	C	N3-C2-O2	-7.52	116.64	121.90
24	A3	60	A	C5-C6-N1	7.52	121.46	117.70
54	BA	936	A	C5-C6-N1	7.52	121.46	117.70
54	BA	2565	A	C5-C6-N1	7.52	121.46	117.70
54	BA	2856	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1394	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1394	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2104	C	N1-C2-O2	7.52	123.41	118.90
54	BA	2165	C	N3-C2-O2	-7.52	116.64	121.90
24	A3	36	A	C4-C5-C6	-7.51	113.24	117.00
54	BA	430	A	C4-C5-C6	-7.51	113.24	117.00
54	BA	706	A	N1-C6-N6	-7.51	114.09	118.60
51	B2	33	ARG	NE-CZ-NH1	7.51	124.06	120.30
54	BA	1269	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2054	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	1502	A	C5-C6-N1	7.51	121.46	117.70
54	BA	917	A	C5-C6-N1	7.51	121.45	117.70
21	AA	596	A	C5-C6-N1	7.51	121.45	117.70
23	A2	79	A	C5-C6-N1	7.51	121.45	117.70
54	BA	1213	A	C5-C6-N1	7.51	121.45	117.70
54	BA	1618	A	C5-C6-N1	7.51	121.45	117.70
24	A3	49	C	N3-C2-O2	-7.50	116.65	121.90
25	BC	101	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	324	A	C5-C6-N1	7.50	121.45	117.70
54	BA	429	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1553	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	1152	A	C5-C6-N1	7.50	121.45	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1608	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2412	A	C5-C6-N1	7.50	121.45	117.70
21	AA	48	C	N3-C2-O2	-7.50	116.65	121.90
21	AA	363	A	C5-C6-N1	7.50	121.45	117.70
21	AA	431	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	1700	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2163	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	101	A	C5-C6-N1	7.49	121.45	117.70
54	BA	207	A	C5-C6-N1	7.49	121.45	117.70
54	BA	226	A	N1-C6-N6	-7.49	114.10	118.60
54	BA	415	A	N1-C6-N6	-7.49	114.10	118.60
54	BA	1801	A	N1-C6-N6	-7.49	114.10	118.60
22	A1	9	A	C5-C6-N1	7.49	121.45	117.70
54	BA	1142	A	C5-C6-N1	7.49	121.45	117.70
21	AA	78	A	C5-C6-N1	7.49	121.44	117.70
54	BA	196	A	C5-C6-N1	7.49	121.44	117.70
54	BA	1347	A	C5-C6-N1	7.49	121.44	117.70
54	BA	2611	C	N3-C2-O2	-7.49	116.66	121.90
54	BA	933	A	C5-C6-N1	7.49	121.44	117.70
53	B4	24	ARG	NE-CZ-NH1	7.49	124.04	120.30
54	BA	1321	A	C5-C6-N1	7.48	121.44	117.70
55	BB	101	A	C5-C6-N1	7.48	121.44	117.70
54	BA	1304	A	N1-C6-N6	-7.48	114.11	118.60
2	AC	10	ARG	NE-CZ-NH1	7.48	124.04	120.30
54	BA	1672	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2147	A	N1-C6-N6	-7.48	114.11	118.60
21	AA	169	C	O4'-C1'-N1	7.48	114.18	108.20
54	BA	2868	A	C5-C6-N1	7.48	121.44	117.70
32	BJ	69	ARG	NE-CZ-NH1	7.47	124.04	120.30
54	BA	1913	A	N1-C6-N6	-7.47	114.11	118.60
54	BA	2476	A	C5-C6-N1	7.47	121.44	117.70
10	AK	97	ARG	NE-CZ-NH1	7.47	124.04	120.30
54	BA	2297	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	2620	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	1495	A	N1-C6-N6	-7.47	114.12	118.60
38	BP	61	ARG	NE-CZ-NH1	7.47	124.03	120.30
54	BA	752	A	O4'-C1'-N9	7.47	114.18	108.20
21	AA	382	A	C5-C6-N1	7.47	121.43	117.70
54	BA	176	A	C5-C6-N1	7.47	121.43	117.70
54	BA	574	A	C5-C6-N1	7.47	121.43	117.70
48	BZ	10	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	1275	A	C5-C6-N1	7.46	121.43	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AF	79	ARG	NE-CZ-NH1	7.46	124.03	120.30
21	AA	573	A	C4-C5-C6	-7.46	113.27	117.00
54	BA	1032	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	1754	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1403	C	N3-C2-O2	-7.46	116.68	121.90
21	AA	26	A	N1-C6-N6	-7.46	114.12	118.60
21	AA	209	U	O4'-C1'-N1	7.46	114.17	108.20
21	AA	432	A	C5-C6-N1	7.46	121.43	117.70
54	BA	788	A	C5-C6-N1	7.46	121.43	117.70
54	BA	897	C	N3-C2-O2	-7.46	116.68	121.90
21	AA	59	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1362	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	1780	A	C5-C6-N1	7.45	121.43	117.70
54	BA	2634	A	C4-C5-C6	-7.45	113.27	117.00
21	AA	814	A	C5-C6-N1	7.45	121.42	117.70
24	A3	36	A	C5-C6-N1	7.45	121.42	117.70
54	BA	71	A	O4'-C1'-N9	7.45	114.16	108.20
54	BA	508	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2101	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2059	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	1044	C	N3-C2-O2	-7.45	116.69	121.90
56	B5	74	ARG	NE-CZ-NH1	7.45	124.02	120.30
54	BA	1247	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2461	A	C5-C6-N1	7.44	121.42	117.70
21	AA	174	A	N1-C6-N6	-7.44	114.13	118.60
54	BA	1080	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	2813	A	N1-C6-N6	-7.44	114.14	118.60
21	AA	468	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1155	A	C5-C6-N1	7.44	121.42	117.70
55	BB	36	C	N3-C2-O2	-7.44	116.69	121.90
21	AA	611	C	N3-C2-O2	-7.44	116.69	121.90
21	AA	1251	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1566	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	2366	A	C5-C6-N1	7.44	121.42	117.70
21	AA	994	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1819	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2503	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	1135	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	1654	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2060	A	C5-C6-N1	7.43	121.42	117.70
54	BA	1046	A	C5-C6-N1	7.43	121.41	117.70
54	BA	1389	G	O4'-C1'-N9	7.43	114.14	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1694	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	685	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	532	A	C5-C6-N1	7.42	121.41	117.70
54	BA	423	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1387	A	C5-C6-N1	7.42	121.41	117.70
54	BA	2214	C	N3-C2-O2	-7.42	116.70	121.90
54	BA	2430	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	2590	A	C5-C6-N1	7.42	121.41	117.70
21	AA	109	A	C5-C6-N1	7.42	121.41	117.70
21	AA	900	A	C5-C6-N1	7.42	121.41	117.70
54	BA	222	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1236	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	374	A	C5-C6-N1	7.42	121.41	117.70
21	AA	53	A	C4-C5-C6	-7.42	113.29	117.00
21	AA	574	A	C4-C5-C6	-7.42	113.29	117.00
21	AA	937	A	C4-C5-C6	-7.42	113.29	117.00
54	BA	1088	A	C5-C6-N1	7.42	121.41	117.70
21	AA	5	U	P-O3'-C3'	7.42	128.60	119.70
54	BA	1088	A	O4'-C1'-N9	7.42	114.13	108.20
21	AA	1136	C	N3-C2-O2	-7.41	116.71	121.90
54	BA	2706	A	C5-C6-N1	7.41	121.41	117.70
54	BA	447	A	C5-C6-N1	7.41	121.41	117.70
13	AN	9	ARG	NE-CZ-NH1	7.41	124.00	120.30
54	BA	228	C	N3-C2-O2	-7.41	116.71	121.90
54	BA	282	A	N1-C6-N6	-7.41	114.15	118.60
54	BA	422	A	C5-C6-N1	7.41	121.41	117.70
21	AA	59	A	N1-C6-N6	-7.41	114.16	118.60
21	AA	1251	A	C4-C5-C6	-7.41	113.30	117.00
21	AA	1410	A	C4-C5-C6	-7.41	113.30	117.00
54	BA	2516	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2530	A	C5-C6-N1	7.41	121.40	117.70
54	BA	172	A	C5-C6-N1	7.41	121.40	117.70
23	A2	91	A	C5-C6-N1	7.41	121.40	117.70
54	BA	404	A	C5-C6-N1	7.41	121.40	117.70
54	BA	1103	A	C5-C6-N1	7.40	121.40	117.70
11	AL	13	ARG	NE-CZ-NH1	7.40	124.00	120.30
21	AA	1346	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	1360	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1014	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2900	A	C5-C6-N1	7.40	121.40	117.70
54	BA	819	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2762	C	N3-C2-O2	-7.40	116.72	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1525	A	N1-C6-N6	-7.40	114.16	118.60
3	AD	43	ARG	NE-CZ-NH1	7.40	124.00	120.30
21	AA	753	A	N1-C6-N6	-7.40	114.16	118.60
27	BE	162	ARG	NE-CZ-NH1	7.40	124.00	120.30
54	BA	644	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	705	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	2115	G	O4'-C1'-N9	7.40	114.12	108.20
21	AA	16	A	C4-C5-C6	-7.39	113.30	117.00
21	AA	595	A	N1-C6-N6	-7.39	114.16	118.60
21	AA	1195	C	N3-C2-O2	-7.39	116.72	121.90
21	AA	1288	A	C5-C6-N1	7.39	121.40	117.70
54	BA	470	A	C5-C6-N1	7.39	121.40	117.70
54	BA	666	A	C5-C6-N1	7.39	121.40	117.70
54	BA	1640	A	C5-C6-N1	7.39	121.40	117.70
54	BA	2284	A	C4-C5-C6	-7.39	113.30	117.00
21	AA	353	A	C5-C6-N1	7.39	121.40	117.70
21	AA	1158	C	N1-C2-O2	7.39	123.34	118.90
42	BT	12	ARG	NE-CZ-NH1	7.39	124.00	120.30
54	BA	2602	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	626	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1722	A	C5-C6-N1	7.39	121.40	117.70
21	AA	1271	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1431	A	C5-C6-N1	7.39	121.39	117.70
21	AA	747	A	C4-C5-C6	-7.39	113.31	117.00
54	BA	101	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	1936	A	C5-C6-N1	7.39	121.39	117.70
21	AA	493	A	C5-C6-N1	7.38	121.39	117.70
21	AA	1269	A	C5-C6-N1	7.38	121.39	117.70
54	BA	173	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	1785	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2452	C	N3-C2-O2	-7.38	116.73	121.90
21	AA	934	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	586	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1689	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	927	A	C5-C6-N1	7.38	121.39	117.70
23	A2	82	A	N1-C6-N6	-7.38	114.17	118.60
32	BJ	99	ARG	NE-CZ-NH1	7.38	123.99	120.30
54	BA	2266	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	2378	A	N1-C6-N6	-7.38	114.17	118.60
13	AN	75	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	1219	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	1885	A	C5-C6-N1	7.38	121.39	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	195	A	C5-C6-N1	7.37	121.39	117.70
21	AA	1374	A	C5-C6-N1	7.37	121.39	117.70
21	AA	1409	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	596	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	794	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1744	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2336	A	N1-C6-N6	-7.37	114.18	118.60
33	BK	17	ARG	NE-CZ-NH1	7.37	123.98	120.30
54	BA	528	A	C5-C6-N1	7.37	121.38	117.70
54	BA	2577	A	C5-C6-N1	7.37	121.38	117.70
54	BA	2823	A	C5-C6-N1	7.37	121.38	117.70
54	BA	2879	A	C5-C6-N1	7.37	121.38	117.70
21	AA	66	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	2612	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	885	C	N3-C2-O2	-7.36	116.75	121.90
21	AA	1004	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1783	A	C5-C6-N1	7.36	121.38	117.70
21	AA	44	A	N1-C6-N6	-7.36	114.18	118.60
21	AA	1216	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1739	A	C5-C6-N1	7.36	121.38	117.70
55	BB	8	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	1874	C	N3-C2-O2	-7.36	116.75	121.90
21	AA	914	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1238	A	C5-C6-N1	7.36	121.38	117.70
24	A3	45	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1606	C	N1-C2-O2	7.36	123.31	118.90
54	BA	57	C	O4'-C1'-N1	7.36	114.08	108.20
54	BA	2459	A	C5-C6-N1	7.36	121.38	117.70
21	AA	182	A	C5-C6-N1	7.35	121.38	117.70
21	AA	183	C	C1'-O4'-C4'	-7.35	104.02	109.90
54	BA	2163	A	C5-C6-N1	7.35	121.38	117.70
21	AA	55	A	C4-C5-C6	-7.35	113.33	117.00
54	BA	74	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2274	A	C5-C6-N1	7.35	121.38	117.70
21	AA	250	A	C5-C6-N1	7.35	121.37	117.70
54	BA	909	A	C5-C6-N1	7.35	121.37	117.70
54	BA	990	A	C5-C6-N1	7.35	121.37	117.70
21	AA	321	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	977	A	C5-C6-N1	7.34	121.37	117.70
54	BA	99	U	N3-C2-O2	-7.34	117.06	122.20
54	BA	1762	A	C5-C6-N1	7.34	121.37	117.70
54	BA	829	A	C5-C6-N1	7.34	121.37	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1603	A	N1-C6-N6	-7.34	114.19	118.60
15	AP	8	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	241	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1147	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1568	G	O4'-C1'-N9	7.34	114.07	108.20
54	BA	2080	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	2352	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2893	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1803	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	2071	A	C5-C6-N1	7.34	121.37	117.70
21	AA	1430	A	C5-C6-N1	7.34	121.37	117.70
16	AQ	64	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	1084	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1672	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	2440	C	N3-C2-O2	-7.34	116.76	121.90
28	BF	101	ARG	NE-CZ-NH1	7.33	123.97	120.30
54	BA	184	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	430	A	C5-C6-N1	7.33	121.37	117.70
25	BC	155	ARG	NE-CZ-NH1	7.33	123.97	120.30
54	BA	457	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	109	A	C1'-O4'-C4'	-7.33	104.04	109.90
21	AA	1180	A	C5-C6-N1	7.33	121.36	117.70
22	A1	76	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	503	A	C5-C6-N1	7.33	121.36	117.70
54	BA	492	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	1363	A	C5-C6-N1	7.33	121.36	117.70
21	AA	250	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	414	A	C5-C6-N1	7.33	121.36	117.70
21	AA	1111	A	C5-C6-N1	7.33	121.36	117.70
21	AA	1395	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	330	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	1635	A	C5-C6-N1	7.33	121.36	117.70
56	B5	122	ARG	NE-CZ-NH1	7.33	123.96	120.30
55	BB	15	A	C5-C6-N1	7.32	121.36	117.70
54	BA	225	C	O4'-C1'-N1	7.32	114.06	108.20
54	BA	229	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	599	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1534	U	N3-C2-O2	-7.32	117.08	122.20
21	AA	864	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	197	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	576	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	1439	A	C5-C6-N1	7.32	121.36	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AC	58	ARG	NE-CZ-NH1	7.32	123.96	120.30
21	AA	729	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2198	A	C5-C6-N1	7.32	121.36	117.70
55	BB	52	A	C5-C6-N1	7.32	121.36	117.70
54	BA	943	A	C5-C6-N1	7.31	121.36	117.70
54	BA	984	A	C4-C5-C6	-7.31	113.34	117.00
54	BA	1668	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2572	A	C5-C6-N1	7.31	121.36	117.70
38	BP	88	ARG	NE-CZ-NH1	7.31	123.96	120.30
41	BS	92	ARG	NE-CZ-NH1	7.31	123.95	120.30
54	BA	2094	A	N1-C6-N6	-7.31	114.21	118.60
21	AA	478	A	N1-C6-N6	-7.31	114.22	118.60
21	AA	1016	A	C5-C6-N1	7.31	121.35	117.70
54	BA	550	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	920	A	N1-C6-N6	-7.31	114.22	118.60
54	BA	2482	A	C5-C6-N1	7.31	121.35	117.70
54	BA	1001	A	C5-C6-N1	7.31	121.35	117.70
54	BA	2328	A	N1-C6-N6	-7.31	114.22	118.60
21	AA	808	C	N3-C2-O2	-7.30	116.79	121.90
21	AA	1236	A	C5-C6-N1	7.30	121.35	117.70
54	BA	632	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1156	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2322	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2598	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	300	A	C5-C6-N1	7.30	121.35	117.70
54	BA	727	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2097	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	2327	A	C5-C6-N1	7.30	121.35	117.70
21	AA	629	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	715	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	1040	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1546	G	O4'-C1'-N9	7.30	114.04	108.20
5	AF	45	ARG	NE-CZ-NH1	7.29	123.95	120.30
21	AA	968	A	O4'-C1'-N9	7.29	114.04	108.20
24	A3	77	A	C5-C6-N1	7.29	121.35	117.70
54	BA	125	A	O4'-C1'-N9	7.29	114.04	108.20
54	BA	1938	A	C5-C6-N1	7.29	121.35	117.70
21	AA	629	A	C5-C6-N1	7.29	121.35	117.70
21	AA	970	C	N1-C2-O2	7.29	123.28	118.90
21	AA	1274	A	C5-C6-N1	7.29	121.35	117.70
24	A3	14	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1118	C	N3-C2-O2	-7.29	116.80	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1480	C	O4'-C1'-N1	7.29	114.03	108.20
54	BA	1603	A	C5-C6-N1	7.29	121.35	117.70
21	AA	892	A	C5-C6-N1	7.29	121.35	117.70
21	AA	1069	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	1214	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	1242	U	O4'-C1'-N1	7.29	114.03	108.20
21	AA	460	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	1098	A	N1-C6-N6	-7.29	114.23	118.60
21	AA	749	A	C5-C6-N1	7.29	121.34	117.70
54	BA	309	A	C5-C6-N1	7.29	121.34	117.70
54	BA	2225	A	C5-C6-N1	7.29	121.34	117.70
54	BA	2564	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1146	A	C5-C6-N1	7.29	121.34	117.70
21	AA	509	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1004	A	C4-C5-C6	-7.29	113.36	117.00
21	AA	1067	A	C5-C6-N1	7.29	121.34	117.70
24	A3	58	A	C5-C6-N1	7.29	121.34	117.70
54	BA	715	A	C5-C6-N1	7.29	121.34	117.70
54	BA	2366	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	2727	A	C5-C6-N1	7.28	121.34	117.70
22	A1	38	A	C5-C6-N1	7.28	121.34	117.70
54	BA	231	A	C5-C6-N1	7.28	121.34	117.70
54	BA	504	A	C5-C6-N1	7.28	121.34	117.70
54	BA	563	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	802	A	C5-C6-N1	7.28	121.34	117.70
54	BA	457	A	C5-C6-N1	7.28	121.34	117.70
54	BA	529	A	C5-C6-N1	7.28	121.34	117.70
21	AA	673	A	C5-C6-N1	7.28	121.34	117.70
22	A1	16	C	N3-C2-O2	-7.28	116.81	121.90
28	BF	124	ARG	NE-CZ-NH1	7.28	123.94	120.30
54	BA	127	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	782	A	C5-C6-N1	7.27	121.34	117.70
54	BA	197	A	C5-C6-N1	7.27	121.34	117.70
54	BA	781	A	C5-C6-N1	7.27	121.34	117.70
54	BA	1566	A	C5-C6-N1	7.27	121.34	117.70
21	AA	975	A	C5-C6-N1	7.27	121.33	117.70
54	BA	255	A	N1-C6-N6	-7.27	114.24	118.60
54	BA	2515	C	N3-C2-O2	-7.27	116.81	121.90
21	AA	263	A	C5-C6-N1	7.27	121.33	117.70
21	AA	374	A	C4-C5-C6	-7.27	113.37	117.00
55	BB	12	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	213	A	C4-C5-C6	-7.26	113.37	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1428	C	N3-C2-O2	-7.26	116.82	121.90
21	AA	81	A	N1-C6-N6	-7.26	114.24	118.60
24	A3	14	A	N1-C6-N6	-7.26	114.24	118.60
54	BA	1310	G	O4'-C1'-N9	7.26	114.01	108.20
54	BA	2287	A	C5-C6-N1	7.26	121.33	117.70
21	AA	7	A	C5-C6-N1	7.26	121.33	117.70
21	AA	478	A	C5-C6-N1	7.26	121.33	117.70
21	AA	687	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2749	A	C5-C6-N1	7.26	121.33	117.70
21	AA	958	A	C5-C6-N1	7.26	121.33	117.70
56	B5	162	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	1378	A	C4-C5-C6	-7.25	113.37	117.00
21	AA	313	A	C5-C6-N1	7.25	121.33	117.70
21	AA	313	A	N1-C6-N6	-7.25	114.25	118.60
21	AA	1246	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	1802	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	2590	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	2632	A	C5-C6-N1	7.25	121.33	117.70
54	BA	2880	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	607	A	C5-C6-N1	7.25	121.33	117.70
21	AA	696	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	279	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1794	A	N1-C6-N6	-7.25	114.25	118.60
21	AA	1022	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	340	A	C5-C6-N1	7.25	121.33	117.70
54	BA	352	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1609	A	O4'-C1'-N9	7.25	114.00	108.20
54	BA	2135	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	2705	A	C5-C6-N1	7.25	121.32	117.70
21	AA	1155	A	C5-C6-N1	7.25	121.32	117.70
54	BA	262	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1005	C	N3-C2-O2	-7.25	116.83	121.90
54	BA	2030	A	C5-C6-N1	7.25	121.32	117.70
54	BA	2126	A	N1-C6-N6	-7.25	114.25	118.60
1	AB	112	ARG	NE-CZ-NH1	7.24	123.92	120.30
21	AA	33	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	1655	A	N1-C6-N6	-7.24	114.25	118.60
21	AA	80	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2542	A	N1-C6-N6	-7.24	114.25	118.60
21	AA	119	A	C5-C6-N1	7.24	121.32	117.70
54	BA	794	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	1786	A	C5-C6-N1	7.24	121.32	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2170	A	C4-C5-C6	-7.24	113.38	117.00
55	BB	73	A	N1-C6-N6	-7.24	114.25	118.60
54	BA	627	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1393	A	N1-C6-N6	-7.24	114.26	118.60
16	AQ	10	ARG	NE-CZ-NH1	7.24	123.92	120.30
21	AA	1413	A	N1-C6-N6	-7.24	114.26	118.60
21	AA	889	A	C4-C5-C6	-7.23	113.38	117.00
54	BA	1536	C	N3-C2-O2	-7.23	116.84	121.90
56	B5	164	ARG	NE-CZ-NH1	7.23	123.92	120.30
21	AA	1410	A	C5-C6-N1	7.23	121.32	117.70
54	BA	111	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	911	A	C4-C5-C6	-7.23	113.38	117.00
54	BA	1858	A	C5-C6-N1	7.23	121.32	117.70
54	BA	2589	A	C5-C6-N1	7.23	121.32	117.70
54	BA	176	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	947	A	C4-C5-C6	-7.23	113.39	117.00
54	BA	2666	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	2042	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2764	A	N1-C6-N6	-7.23	114.26	118.60
3	AD	164	ARG	NE-CZ-NH1	7.23	123.91	120.30
21	AA	794	A	C4-C5-C6	-7.23	113.39	117.00
54	BA	2005	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2063	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	789	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1324	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	941	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1600	C	N3-C2-O2	-7.22	116.84	121.90
54	BA	2662	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	265	A	N1-C6-N6	-7.22	114.27	118.60
21	AA	609	A	C4-C5-C6	-7.22	113.39	117.00
21	AA	1383	C	N3-C2-O2	-7.22	116.85	121.90
38	BP	102	ARG	NE-CZ-NH1	7.22	123.91	120.30
54	BA	146	A	C5-C6-N1	7.22	121.31	117.70
24	A3	74	A	C5-C6-N1	7.22	121.31	117.70
54	BA	382	A	C5-C6-N1	7.22	121.31	117.70
54	BA	787	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	695	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1093	A	C5-C6-N1	7.21	121.31	117.70
34	BL	18	ARG	NE-CZ-NH1	7.21	123.91	120.30
21	AA	412	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1155	A	C4-C5-C6	-7.21	113.39	117.00
21	AA	1368	A	C5-C6-N1	7.21	121.31	117.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	270	A	C5-C6-N1	7.21	121.30	117.70
21	AA	300	A	C5-C6-N1	7.21	121.30	117.70
38	BP	112	ARG	NE-CZ-NH1	7.21	123.91	120.30
11	AL	109	ARG	NE-CZ-NH1	7.21	123.90	120.30
20	AU	32	ARG	NE-CZ-NH1	7.21	123.90	120.30
21	AA	162	A	C5-C6-N1	7.21	121.30	117.70
21	AA	630	A	C5-C6-N1	7.21	121.30	117.70
21	AA	959	A	C5-C6-N1	7.21	121.30	117.70
54	BA	1698	A	N1-C6-N6	-7.21	114.28	118.60
21	AA	900	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	1126	A	O4'-C1'-N9	7.20	113.96	108.20
54	BA	1336	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2114	A	C5-C6-N1	7.20	121.30	117.70
21	AA	38	G	N1-C6-O6	-7.20	115.58	119.90
22	A1	76	A	O4'-C1'-C2'	-7.20	98.60	105.80
54	BA	1284	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1496	A	C5-C6-N1	7.20	121.30	117.70
7	AH	14	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	947	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1847	A	O4'-C1'-N9	7.20	113.96	108.20
54	BA	1924	C	O4'-C1'-N1	7.20	113.96	108.20
54	BA	2703	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	2733	A	C5-C6-N1	7.20	121.30	117.70
54	BA	507	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1469	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1544	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2388	A	C5-C6-N1	7.19	121.30	117.70
21	AA	495	A	N1-C6-N6	-7.19	114.28	118.60
21	AA	1306	A	C5-C6-N1	7.19	121.30	117.70
21	AA	1434	A	C5-C6-N1	7.19	121.30	117.70
41	BS	88	ARG	NE-CZ-NH1	7.19	123.90	120.30
54	BA	2321	U	O4'-C1'-N1	7.19	113.95	108.20
54	BA	2406	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2518	A	C5-C6-N1	7.19	121.30	117.70
21	AA	1476	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1899	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1932	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2090	A	C4-C5-C6	-7.19	113.41	117.00
54	BA	2288	A	C5-C6-N1	7.19	121.30	117.70
54	BA	2358	A	C5-C6-N1	7.19	121.30	117.70
21	AA	665	A	C5-C6-N1	7.19	121.30	117.70
54	BA	964	C	N3-C2-O2	-7.19	116.87	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2426	A	C5-C6-N1	7.19	121.29	117.70
21	AA	498	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	1353	A	C5-C6-N1	7.19	121.29	117.70
54	BA	1676	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	1965	C	N3-C2-O2	-7.19	116.87	121.90
21	AA	845	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1398	A	C5-C6-N1	7.18	121.29	117.70
21	AA	298	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	1327	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1035	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2082	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	2497	A	C5-C6-N1	7.18	121.29	117.70
21	AA	968	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1483	A	C5-C6-N1	7.18	121.29	117.70
54	BA	633	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2135	A	C5-C6-N1	7.18	121.29	117.70
54	BA	973	A	C5-C6-N1	7.18	121.29	117.70
21	AA	754	C	N3-C2-O2	-7.18	116.88	121.90
21	AA	1082	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1170	A	C5-C6-N1	7.18	121.29	117.70
54	BA	190	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	191	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	792	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1359	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1678	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1396	A	C5-C6-N1	7.17	121.29	117.70
34	BL	41	ARG	NE-CZ-NH1	7.17	123.89	120.30
54	BA	322	A	C5-C6-N1	7.17	121.29	117.70
54	BA	362	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1010	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2314	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2847	U	O4'-C1'-N1	7.17	113.94	108.20
54	BA	513	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1204	A	C5-C6-N1	7.17	121.29	117.70
24	A3	35	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	556	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	751	A	C5-C6-N1	7.17	121.29	117.70
54	BA	788	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	1579	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2278	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2589	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	844	A	C5-C6-N1	7.17	121.28	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	482	A	C5-C6-N1	7.17	121.28	117.70
21	AA	1227	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1705	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1932	A	C4-C5-C6	-7.17	113.42	117.00
24	A3	40	C	N3-C2-O2	-7.17	116.89	121.90
21	AA	1259	C	N3-C2-O2	-7.16	116.89	121.90
35	BM	81	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	1032	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2483	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	2820	A	C5-C6-N1	7.16	121.28	117.70
54	BA	985	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	374	A	N1-C6-N6	-7.16	114.30	118.60
21	AA	673	A	N1-C6-N6	-7.16	114.31	118.60
21	AA	747	A	C5-C6-N1	7.16	121.28	117.70
54	BA	756	A	C5-C6-N1	7.16	121.28	117.70
54	BA	980	A	O4'-C1'-N9	7.16	113.93	108.20
54	BA	1679	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	1830	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	152	A	N1-C6-N6	-7.16	114.31	118.60
9	AJ	9	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	218	A	C5-C6-N1	7.16	121.28	117.70
54	BA	730	A	C5-C6-N1	7.16	121.28	117.70
54	BA	1641	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2531	A	C5-C6-N1	7.16	121.28	117.70
21	AA	309	A	C5-C6-N1	7.15	121.28	117.70
21	AA	349	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1879	C	N3-C2-O2	-7.15	116.89	121.90
21	AA	1201	A	P-O3'-C3'	7.15	128.28	119.70
25	BC	47	ARG	NE-CZ-NH1	7.15	123.87	120.30
55	BB	115	A	C5-C6-N1	7.15	121.28	117.70
21	AA	609	A	C5-C6-N1	7.15	121.27	117.70
54	BA	2433	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	223	A	C5-C6-N1	7.14	121.27	117.70
21	AA	267	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	909	A	C5-C6-N1	7.14	121.27	117.70
54	BA	91	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	717	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	2258	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	2778	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1340	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	936	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1570	A	C4-C5-C6	-7.14	113.43	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1916	A	C5-C6-N1	7.14	121.27	117.70
54	BA	546	U	N3-C2-O2	-7.14	117.20	122.20
20	AU	6	ARG	NE-CZ-NH2	-7.14	116.73	120.30
21	AA	314	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	413	G	C1'-O4'-C4'	-7.14	104.19	109.90
54	BA	481	G	C1'-O4'-C4'	-7.14	104.19	109.90
54	BA	1971	U	C1'-O4'-C4'	-7.14	104.19	109.90
54	BA	2020	A	C5-C6-N1	7.14	121.27	117.70
21	AA	665	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	873	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1151	A	N1-C6-N6	-7.14	114.32	118.60
46	BX	17	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	21	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2386	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2533	U	O4'-C1'-N1	7.14	113.91	108.20
54	BA	2766	A	N1-C6-N6	-7.14	114.32	118.60
21	AA	1171	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	587	C	N3-C2-O2	-7.13	116.91	121.90
10	AK	36	ARG	NE-CZ-NH1	7.13	123.87	120.30
21	AA	149	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2013	A	C5-C6-N1	7.13	121.27	117.70
21	AA	282	A	C4-C5-C6	-7.13	113.44	117.00
21	AA	419	C	N3-C2-O2	-7.13	116.91	121.90
21	AA	676	A	C5-C6-N1	7.13	121.27	117.70
54	BA	347	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1100	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	1347	A	C4-C5-C6	-7.13	113.44	117.00
21	AA	1336	C	N1-C2-O2	7.13	123.18	118.90
54	BA	1591	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	256	A	C5-C6-N1	7.13	121.26	117.70
54	BA	1892	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	806	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	959	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1630	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	2727	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	1144	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	1570	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1597	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	1877	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2000	C	O4'-C1'-N1	7.12	113.90	108.20
54	BA	2145	C	N1-C2-O2	7.12	123.17	118.90
5	AF	38	ARG	NE-CZ-NH1	7.12	123.86	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1378	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	1397	C	N1-C2-O2	7.12	123.17	118.90
54	BA	2776	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	1872	A	C5-C6-N1	7.12	121.26	117.70
55	BB	34	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	1456	A	C5-C6-N1	7.12	121.26	117.70
54	BA	668	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2439	A	C5-C6-N1	7.12	121.26	117.70
55	BB	97	C	N3-C2-O2	-7.12	116.92	121.90
25	BC	261	ARG	NE-CZ-NH1	7.11	123.86	120.30
54	BA	94	A	C5-C6-N1	7.11	121.26	117.70
54	BA	466	A	N1-C6-N6	-7.11	114.33	118.60
54	BA	1553	A	C5-C6-N1	7.11	121.26	117.70
54	BA	2652	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	2821	A	C5-C6-N1	7.11	121.26	117.70
54	BA	1447	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	2247	A	C4-C5-C6	-7.11	113.44	117.00
54	BA	2451	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	422	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	759	A	C5-C6-N1	7.11	121.25	117.70
21	AA	880	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	1339	A	C5-C6-N1	7.11	121.25	117.70
54	BA	223	A	C5-C6-N1	7.11	121.25	117.70
54	BA	761	A	C5-C6-N1	7.11	121.25	117.70
54	BA	1952	A	C5-C6-N1	7.11	121.25	117.70
21	AA	131	A	C5-C6-N1	7.11	121.25	117.70
21	AA	383	A	C5-C6-N1	7.11	121.25	117.70
54	BA	637	A	C5-C6-N1	7.11	121.25	117.70
55	BB	39	A	C5-C6-N1	7.11	121.25	117.70
54	BA	231	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	2513	A	C4-C5-C6	-7.10	113.45	117.00
11	AL	49	ARG	NE-CZ-NH1	7.10	123.85	120.30
21	AA	781	A	C5-C6-N1	7.10	121.25	117.70
54	BA	743	A	C4-C5-C6	-7.10	113.45	117.00
21	AA	805	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	124	C	N3-C2-O2	-7.10	116.93	121.90
22	A1	21	A	C5-C6-N1	7.10	121.25	117.70
54	BA	886	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	2062	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1146	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	1170	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	345	A	C5-C6-N1	7.10	121.25	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	899	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1669	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1987	A	C5-C6-N1	7.10	121.25	117.70
21	AA	496	A	C1'-O4'-C4'	-7.10	104.22	109.90
21	AA	1408	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1302	A	C5-C6-N1	7.10	121.25	117.70
21	AA	608	A	N1-C6-N6	-7.09	114.34	118.60
23	A2	80	C	N3-C2-O2	-7.09	116.93	121.90
54	BA	603	A	C5-C6-N1	7.09	121.25	117.70
54	BA	979	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	1049	C	N3-C2-O2	-7.09	116.93	121.90
54	BA	1404	C	N1-C2-O2	7.09	123.16	118.90
54	BA	300	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2281	A	C5-C6-N1	7.09	121.25	117.70
21	AA	74	A	C4-C5-C6	-7.09	113.45	117.00
22	A1	14	A	N1-C6-N6	-7.09	114.34	118.60
54	BA	1342	A	C5-C6-N1	7.09	121.25	117.70
21	AA	303	A	C5-C6-N1	7.09	121.24	117.70
54	BA	190	A	C5-C6-N1	7.09	121.24	117.70
54	BA	2104	C	O4'-C1'-N1	7.09	113.87	108.20
17	AR	47	ARG	NE-CZ-NH1	7.08	123.84	120.30
21	AA	460	A	C5-C6-N1	7.08	121.24	117.70
54	BA	753	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1140	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	1441	A	C5-C6-N1	7.08	121.24	117.70
54	BA	719	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	2386	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	2591	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	559	A	C5-C6-N1	7.08	121.24	117.70
21	AA	1298	U	N3-C2-O2	-7.08	117.25	122.20
54	BA	2654	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	811	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	2411	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	1549	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	514	A	C4-C5-C6	-7.07	113.46	117.00
54	BA	735	A	C5-C6-N1	7.07	121.24	117.70
54	BA	1569	A	C4-C5-C6	-7.07	113.46	117.00
54	BA	1690	A	C5-C6-N1	7.07	121.24	117.70
54	BA	2089	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	2119	A	C5-C6-N1	7.07	121.24	117.70
55	BB	26	C	N3-C2-O2	-7.07	116.95	121.90
10	AK	126	ARG	NE-CZ-NH1	-7.07	116.77	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	238	A	C5-C6-N1	7.07	121.23	117.70
21	AA	325	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2377	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	2776	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2734	A	C5-C6-N1	7.07	121.23	117.70
8	AI	108	ARG	NE-CZ-NH1	7.07	123.83	120.30
21	AA	51	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	53	A	C5-C6-N1	7.07	121.23	117.70
21	AA	758	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	1311	A	C5-C6-N1	7.07	121.23	117.70
21	AA	1437	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	1901	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	2042	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	2541	A	C4-C5-C6	-7.07	113.47	117.00
21	AA	602	A	C5-C6-N1	7.07	121.23	117.70
54	BA	1569	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2883	A	N1-C6-N6	-7.06	114.36	118.60
55	BB	78	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1679	A	C5-C6-N1	7.06	121.23	117.70
21	AA	637	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	2178	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	1055	A	C5-C6-N1	7.06	121.23	117.70
21	AA	1150	A	N1-C6-N6	-7.06	114.36	118.60
21	AA	1197	A	C5-C6-N1	7.06	121.23	117.70
54	BA	76	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	900	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1614	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2392	A	C4-C5-C6	-7.06	113.47	117.00
55	BB	115	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	1228	C	N3-C2-O2	-7.06	116.96	121.90
55	BB	27	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	189	A	C5-C6-N1	7.05	121.23	117.70
21	AA	315	A	C5-C6-N1	7.05	121.23	117.70
54	BA	282	A	C5-C6-N1	7.05	121.23	117.70
54	BA	2336	A	C5-C6-N1	7.05	121.23	117.70
54	BA	2657	A	C5-C6-N1	7.05	121.23	117.70
54	BA	2733	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	2741	A	C5-C6-N1	7.05	121.23	117.70
39	BQ	12	ARG	NE-CZ-NH1	7.05	123.83	120.30
54	BA	6	A	C5-C6-N1	7.05	121.23	117.70
54	BA	983	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1960	A	C5-C6-N1	7.05	121.23	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	462	G	N3-C2-N2	-7.05	114.96	119.90
21	AA	1229	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1350	A	N1-C6-N6	-7.05	114.37	118.60
24	A3	38	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	262	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	765	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	821	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	1000	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1453	A	C5-C6-N1	7.05	121.23	117.70
54	BA	2310	C	N3-C2-O2	-7.05	116.96	121.90
54	BA	990	A	N1-C6-N6	-7.05	114.37	118.60
21	AA	408	A	C5-C6-N1	7.05	121.22	117.70
54	BA	118	A	C5-C6-N1	7.05	121.22	117.70
54	BA	910	A	C4-C5-C6	-7.05	113.48	117.00
54	BA	1308	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1395	A	C5-C6-N1	7.05	121.22	117.70
21	AA	199	A	N1-C6-N6	-7.04	114.37	118.60
33	BK	64	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	2675	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2704	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	2887	A	C5-C6-N1	7.04	121.22	117.70
54	BA	608	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2082	A	C5-C6-N1	7.04	121.22	117.70
21	AA	80	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	2212	A	O4'-C1'-N9	7.04	113.83	108.20
21	AA	172	A	N1-C6-N6	-7.04	114.38	118.60
49	B0	9	ARG	NE-CZ-NH1	7.04	123.82	120.30
21	AA	1107	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	1302	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	1446	A	C5-C6-N1	7.04	121.22	117.70
29	BG	2	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	1027	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1200	C	N3-C2-O2	-7.04	116.98	121.90
54	BA	1322	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	2823	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	807	A	C5-C6-N1	7.03	121.22	117.70
21	AA	1105	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	6	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	643	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	2711	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2809	A	C5-C6-N1	7.03	121.22	117.70
8	AI	98	ARG	NE-CZ-NH1	7.03	123.81	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1134	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1340	U	O4'-C1'-N1	7.03	113.83	108.20
54	BA	1413	A	C4-C5-C6	-7.03	113.48	117.00
21	AA	1169	A	C5-C6-N1	7.03	121.21	117.70
21	AA	1328	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1755	A	C5-C6-N1	7.03	121.21	117.70
54	BA	1900	A	C5-C6-N1	7.03	121.21	117.70
21	AA	465	A	C5-C6-N1	7.03	121.21	117.70
22	A1	14	A	C5-C6-N1	7.03	121.21	117.70
54	BA	890	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1020	A	C5-C6-N1	7.03	121.21	117.70
22	A1	66	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1535	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	1717	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	2516	A	N1-C6-N6	-7.02	114.39	118.60
21	AA	595	A	C5-C6-N1	7.02	121.21	117.70
54	BA	782	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	900	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	2129	C	N3-C2-O2	-7.02	116.98	121.90
21	AA	341	C	N3-C2-O2	-7.02	116.99	121.90
21	AA	583	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	631	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	1102	C	N3-C2-O2	-7.02	116.99	121.90
21	AA	610	U	O4'-C1'-N1	7.02	113.81	108.20
54	BA	2579	C	N3-C2-O2	-7.02	116.99	121.90
21	AA	766	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1320	C	N1-C2-O2	7.02	123.11	118.90
23	A2	80	C	C1'-O4'-C4'	-7.02	104.29	109.90
54	BA	270	A	C5-C6-N1	7.02	121.21	117.70
54	BA	920	A	C5-C6-N1	7.02	121.21	117.70
54	BA	2581	G	O4'-C1'-N9	7.02	113.81	108.20
21	AA	643	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	1296	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	730	A	C4-C5-C6	-7.01	113.49	117.00
21	AA	179	A	C5-C6-N1	7.01	121.21	117.70
54	BA	155	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2700	A	C4-C5-C6	-7.01	113.49	117.00
21	AA	288	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1927	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2814	A	C4-C5-C6	-7.01	113.49	117.00
36	BN	63	ARG	NE-CZ-NH1	7.01	123.80	120.30
54	BA	1305	C	N3-C2-O2	-7.01	116.99	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2566	A	N1-C6-N6	-7.01	114.39	118.60
21	AA	129	A	C4-C5-C6	-7.01	113.50	117.00
55	BB	15	A	O4'-C1'-N9	7.01	113.81	108.20
54	BA	675	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2748	A	C5-C6-N1	7.01	121.20	117.70
54	BA	199	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1367	A	C5-C6-N1	7.00	121.20	117.70
21	AA	489	C	N3-C2-O2	-7.00	117.00	121.90
24	A3	60	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	352	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1253	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	2268	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2628	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	1411	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	654	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1073	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1652	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1787	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	298	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	946	A	C5-C6-N1	7.00	121.20	117.70
51	B2	28	ARG	NE-CZ-NH1	7.00	123.80	120.30
54	BA	127	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2443	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	448	U	O4'-C1'-N1	7.00	113.80	108.20
54	BA	1080	A	C5-C6-N1	7.00	121.20	117.70
54	BA	181	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1307	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	217	A	C5-C6-N1	6.99	121.20	117.70
54	BA	678	C	O4'-C1'-N1	6.99	113.80	108.20
54	BA	863	A	N1-C6-N6	-6.99	114.40	118.60
50	B1	43	ARG	NE-CZ-NH1	6.99	123.80	120.30
54	BA	699	A	C5-C6-N1	6.99	121.20	117.70
21	AA	681	A	C5-C6-N1	6.99	121.19	117.70
22	A1	73	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	348	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1580	A	C5-C6-N1	6.99	121.20	117.70
54	BA	602	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	1593	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1737	G	O4'-C1'-N9	6.99	113.79	108.20
54	BA	945	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	2632	A	N1-C6-N6	-6.99	114.41	118.60
55	BB	30	C	O4'-C1'-N1	6.99	113.79	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	72	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	277	G	O4'-C1'-N9	6.99	113.79	108.20
54	BA	660	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	1641	A	C4-C5-C6	-6.99	113.51	117.00
55	BB	78	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	89	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	170	U	O4'-C1'-N1	6.98	113.79	108.20
21	AA	19	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1095	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1260	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1320	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	2077	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2467	C	N3-C2-O2	-6.98	117.01	121.90
24	A3	42	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	195	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1175	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2052	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	2417	C	N3-C2-O2	-6.98	117.01	121.90
21	AA	448	A	C5-C6-N1	6.98	121.19	117.70
54	BA	820	A	N1-C6-N6	-6.98	114.41	118.60
21	AA	1179	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1650	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1752	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	1760	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	2312	U	N3-C2-O2	-6.98	117.31	122.20
54	BA	2799	A	C5-C6-N1	6.98	121.19	117.70
22	A1	23	A	C5-C6-N1	6.98	121.19	117.70
21	AA	228	A	C5-C6-N1	6.97	121.19	117.70
54	BA	368	A	C5-C6-N1	6.97	121.19	117.70
54	BA	428	A	C5-C6-N1	6.97	121.19	117.70
54	BA	505	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2427	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	547	A	C5-C6-N1	6.97	121.19	117.70
21	AA	1375	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2019	A	C5-C6-N1	6.97	121.19	117.70
41	BS	11	ARG	NE-CZ-NH1	6.97	123.79	120.30
52	B3	41	ARG	NE-CZ-NH1	6.97	123.78	120.30
54	BA	342	A	C5-C6-N1	6.97	121.18	117.70
54	BA	2903	U	O4'-C1'-N1	6.97	113.78	108.20
54	BA	19	A	C5-C6-N1	6.97	121.18	117.70
21	AA	160	A	C5-C6-N1	6.97	121.18	117.70
21	AA	1369	C	N3-C2-O2	-6.97	117.02	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2198	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	2717	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2810	A	C5-C6-N1	6.97	121.18	117.70
54	BA	146	A	N1-C6-N6	-6.96	114.42	118.60
54	BA	323	C	N3-C2-O2	-6.96	117.03	121.90
55	BB	91	C	N3-C2-O2	-6.96	117.02	121.90
54	BA	203	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1810	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2498	C	O4'-C1'-N1	6.96	113.77	108.20
34	BL	59	ARG	NE-CZ-NH1	6.96	123.78	120.30
54	BA	251	A	C5-C6-N1	6.96	121.18	117.70
54	BA	819	A	N1-C6-N6	-6.96	114.42	118.60
54	BA	2815	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	622	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1551	A	C5-C6-N1	6.96	121.18	117.70
6	AG	2	ARG	NE-CZ-NH1	6.95	123.78	120.30
54	BA	471	A	C5-C6-N1	6.95	121.18	117.70
54	BA	1352	U	N3-C2-O2	-6.95	117.33	122.20
54	BA	2700	A	C5-C6-N1	6.95	121.18	117.70
54	BA	2176	A	N1-C6-N6	-6.95	114.43	118.60
16	AQ	76	ARG	NE-CZ-NH1	6.95	123.78	120.30
21	AA	1080	A	C5-C6-N1	6.95	121.17	117.70
21	AA	1277	C	N3-C2-O2	-6.95	117.04	121.90
21	AA	1483	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	386	G	O4'-C1'-N9	6.95	113.76	108.20
54	BA	2333	A	C5-C6-N1	6.95	121.17	117.70
54	BA	131	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	2740	A	C5-C6-N1	6.95	121.17	117.70
21	AA	325	A	C4-C5-C6	-6.95	113.53	117.00
22	A1	71	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	1853	A	C5-C6-N1	6.95	121.17	117.70
54	BA	157	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	1535	A	C5-C6-N1	6.94	121.17	117.70
21	AA	327	A	C4-C5-C6	-6.94	113.53	117.00
21	AA	718	A	C5-C6-N1	6.94	121.17	117.70
21	AA	1394	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	42	A	N1-C6-N6	-6.94	114.43	118.60
54	BA	1165	A	C4-C5-C6	-6.94	113.53	117.00
21	AA	535	A	C5-C6-N1	6.94	121.17	117.70
36	BN	64	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	44	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	2614	A	C4-C5-C6	-6.94	113.53	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	172	A	C5-C6-N1	6.94	121.17	117.70
36	BN	86	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	2547	A	C5-C6-N1	6.94	121.17	117.70
21	AA	777	A	C5-C6-N1	6.94	121.17	117.70
54	BA	2270	A	C5-C6-N1	6.94	121.17	117.70
51	B2	39	ARG	NE-CZ-NH1	6.94	123.77	120.30
21	AA	807	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	872	A	C1'-O4'-C4'	-6.93	104.35	109.90
26	BD	33	ARG	NE-CZ-NH1	6.93	123.77	120.30
54	BA	492	A	C5-C6-N1	6.93	121.17	117.70
54	BA	2090	A	C5-C6-N1	6.93	121.17	117.70
14	AO	63	ARG	NE-CZ-NH1	6.93	123.77	120.30
21	AA	908	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	1157	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	432	A	C5-C6-N1	6.93	121.17	117.70
55	BB	35	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	221	A	C5-C6-N1	6.93	121.17	117.70
54	BA	655	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	1253	A	C5-C6-N1	6.93	121.16	117.70
54	BA	182	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	749	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	1383	A	C4-C5-C6	-6.93	113.54	117.00
54	BA	271	G	O4'-C1'-N9	6.93	113.74	108.20
54	BA	56	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2035	G	O4'-C1'-N9	6.92	113.74	108.20
54	BA	2070	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2369	A	C5-C6-N1	6.92	121.16	117.70
21	AA	1375	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	2705	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	924	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	1263	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	138	U	O4'-C1'-N1	6.92	113.74	108.20
54	BA	1085	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1780	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	1101	A	P-O3'-C3'	6.92	128.00	119.70
54	BA	2726	A	N1-C6-N6	-6.92	114.45	118.60
21	AA	1036	A	C4-C5-C6	-6.92	113.54	117.00
37	BO	15	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	208	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	2146	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	2726	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2736	A	C5-C6-N1	6.92	121.16	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1289	A	C5-C6-N1	6.92	121.16	117.70
54	BA	865	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	1503	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	1665	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2899	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	1194	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2858	C	N1-C2-O2	6.92	123.05	118.90
22	A1	66	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	236	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	915	A	C4-C5-C6	-6.91	113.54	117.00
21	AA	162	A	N1-C6-N6	-6.91	114.45	118.60
21	AA	622	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1307	A	C5-C6-N1	6.91	121.16	117.70
21	AA	526	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	2052	A	C5-C6-N1	6.91	121.15	117.70
22	A1	69	A	C5-C6-N1	6.91	121.15	117.70
24	A3	26	C	N3-C2-O2	-6.91	117.07	121.90
54	BA	32	C	N3-C2-O2	-6.91	117.07	121.90
54	BA	1548	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2639	A	C5-C6-N1	6.91	121.15	117.70
22	A1	72	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	1434	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	1276	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1322	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1866	A	C5-C6-N1	6.90	121.15	117.70
54	BA	540	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2428	G	N1-C6-O6	-6.90	115.76	119.90
12	AM	92	ARG	NE-CZ-NH1	6.90	123.75	120.30
21	AA	161	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1225	A	C5-C6-N1	6.90	121.15	117.70
21	AA	815	A	C5-C6-N1	6.89	121.15	117.70
21	AA	1429	A	C5-C6-N1	6.89	121.15	117.70
24	A3	22	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	155	A	C5-C6-N1	6.89	121.15	117.70
54	BA	927	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	928	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1518	A	N1-C6-N6	-6.89	114.47	118.60
54	BA	783	A	C5-C6-N1	6.89	121.14	117.70
54	BA	1366	A	C5-C6-N1	6.89	121.14	117.70
54	BA	2080	A	C5-C6-N1	6.89	121.14	117.70
54	BA	2510	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	694	A	N1-C6-N6	-6.89	114.47	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2665	A	C4-C5-C6	-6.89	113.56	117.00
21	AA	136	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	1332	A	C5-C6-N1	6.88	121.14	117.70
54	BA	63	A	C5-C6-N1	6.88	121.14	117.70
54	BA	541	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1981	A	C5-C6-N1	6.88	121.14	117.70
21	AA	784	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1439	A	O4'-C1'-N9	6.88	113.71	108.20
54	BA	2496	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	2837	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	510	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1686	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	288	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1492	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2142	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2147	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2835	A	C5-C6-N1	6.88	121.14	117.70
54	BA	160	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1609	A	C5-C6-N1	6.88	121.14	117.70
21	AA	1500	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	1327	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	227	A	C5-C6-N1	6.87	121.14	117.70
54	BA	451	U	O4'-C1'-N1	6.87	113.70	108.20
54	BA	983	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	2041	U	O4'-C1'-N1	6.87	113.70	108.20
54	BA	2573	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	1117	A	N1-C6-N6	-6.87	114.48	118.60
21	AA	1480	A	C5-C6-N1	6.87	121.14	117.70
45	BW	13	ARG	NE-CZ-NH1	6.87	123.73	120.30
54	BA	351	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	460	A	C5-C6-N1	6.87	121.14	117.70
21	AA	379	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	53	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1254	A	C5-C6-N1	6.87	121.13	117.70
21	AA	32	A	N1-C6-N6	-6.87	114.48	118.60
21	AA	860	A	C4-C5-C6	-6.87	113.57	117.00
50	B1	27	ARG	NE-CZ-NH1	6.87	123.73	120.30
54	BA	1167	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	152	A	C5-C6-N1	6.87	121.13	117.70
54	BA	905	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1015	U	O4'-C1'-N1	6.87	113.69	108.20
54	BA	2254	C	N3-C2-O2	-6.87	117.09	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1191	A	C5-C6-N1	6.86	121.13	117.70
54	BA	382	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	2850	A	C5-C6-N1	6.86	121.13	117.70
21	AA	1396	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	878	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2031	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2503	A	C1'-O4'-C4'	-6.86	104.41	109.90
21	AA	19	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	974	A	C5-C6-N1	6.86	121.13	117.70
21	AA	1035	A	N1-C6-N6	-6.86	114.48	118.60
22	A1	26	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	310	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1704	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2830	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	706	A	C5-C6-N1	6.86	121.13	117.70
21	AA	1519	A	C5-C6-N1	6.86	121.13	117.70
54	BA	804	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1593	A	C4-C5-C6	-6.86	113.57	117.00
19	AT	73	ARG	NE-CZ-NH1	6.86	123.73	120.30
21	AA	67	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	441	A	C5-C6-N1	6.86	121.13	117.70
22	A1	35	A	C5-C6-N1	6.86	121.13	117.70
24	A3	11	A	C5-C6-N1	6.86	121.13	117.70
54	BA	699	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	1265	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	2404	U	O4'-C1'-N1	6.85	113.68	108.20
36	BN	2	ARG	NE-CZ-NH1	6.85	123.73	120.30
21	AA	16	A	C5-C6-N1	6.85	121.12	117.70
21	AA	225	C	N3-C2-O2	-6.85	117.10	121.90
54	BA	2003	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	2827	C	N3-C2-O2	-6.85	117.10	121.90
21	AA	1339	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	466	A	C5-C6-N1	6.85	121.12	117.70
54	BA	1616	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	969	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	1583	A	C4-C5-C6	-6.85	113.58	117.00
18	AS	31	ARG	NE-CZ-NH1	6.85	123.72	120.30
21	AA	1418	A	C4-C5-C6	-6.84	113.58	117.00
21	AA	370	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1086	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1230	A	C5-C6-N1	6.84	121.12	117.70
54	BA	590	A	N1-C6-N6	-6.84	114.50	118.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	918	A	N1-C6-N6	-6.84	114.50	118.60
55	BB	52	A	C4-C5-C6	-6.84	113.58	117.00
21	AA	1054	C	C1'-O4'-C4'	-6.84	104.43	109.90
21	AA	716	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1042	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1093	A	C1'-O4'-C4'	-6.84	104.43	109.90
21	AA	1128	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	2546	U	O4'-C1'-N1	6.84	113.67	108.20
21	AA	750	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	1114	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	52	A	N1-C6-N6	-6.84	114.50	118.60
54	BA	443	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	845	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1705	A	C4-C5-C6	-6.84	113.58	117.00
20	AU	34	ARG	NE-CZ-NH1	6.83	123.72	120.30
21	AA	502	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	1434	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	2142	A	C5-C6-N1	6.83	121.12	117.70
21	AA	8	A	O4'-C1'-N9	6.83	113.67	108.20
21	AA	270	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	1090	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2600	A	C5-C6-N1	6.83	121.12	117.70
54	BA	1977	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	487	A	C5-C6-N1	6.83	121.11	117.70
21	AA	322	C	C1'-O4'-C4'	-6.83	104.44	109.90
21	AA	1092	A	C5-C6-N1	6.83	121.11	117.70
54	BA	441	U	O4'-C1'-N1	6.83	113.66	108.20
54	BA	1088	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	1549	A	C5-C6-N1	6.83	121.11	117.70
21	AA	712	A	C4-C5-C6	-6.83	113.59	117.00
21	AA	1257	A	C5-C6-N1	6.83	121.11	117.70
54	BA	239	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	849	A	C5-C6-N1	6.83	121.11	117.70
54	BA	1926	U	O4'-C1'-N1	6.82	113.66	108.20
54	BA	2669	G	O4'-C1'-N9	6.82	113.66	108.20
54	BA	739	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	1325	U	O4'-C1'-N1	6.82	113.66	108.20
21	AA	411	A	C5-C6-N1	6.82	121.11	117.70
21	AA	634	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	1027	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	523	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1362	A	C5-C6-N1	6.82	121.11	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	BT	73	ARG	NE-CZ-NH1	6.82	123.71	120.30
21	AA	264	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	470	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	1351	C	O4'-C1'-N1	6.82	113.65	108.20
54	BA	1876	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	2101	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	932	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	544	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	459	A	C5-C6-N1	6.81	121.11	117.70
54	BA	2222	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	2813	A	C5-C6-N1	6.81	121.11	117.70
6	AG	118	ARG	NE-CZ-NH1	6.81	123.71	120.30
21	AA	1318	A	C5-C6-N1	6.81	121.11	117.70
54	BA	676	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	2028	U	O4'-C1'-N1	6.81	113.65	108.20
54	BA	2665	A	C5-C6-N1	6.81	121.11	117.70
54	BA	601	C	N3-C2-O2	-6.81	117.13	121.90
55	BB	3	C	N3-C2-O2	-6.81	117.13	121.90
42	BT	77	ARG	NE-CZ-NH1	6.81	123.70	120.30
21	AA	1067	A	C4-C5-C6	-6.81	113.60	117.00
55	BB	50	A	C4-C5-C6	-6.81	113.60	117.00
21	AA	1031	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	2227	A	C5-C6-N1	6.80	121.10	117.70
54	BA	244	A	N1-C6-N6	-6.80	114.52	118.60
54	BA	1528	A	C5-C6-N1	6.80	121.10	117.70
21	AA	882	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	1101	U	O4'-C1'-N1	6.80	113.64	108.20
20	AU	46	ARG	NE-CZ-NH2	-6.80	116.90	120.30
46	BX	56	ARG	NE-CZ-NH1	6.80	123.70	120.30
54	BA	201	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	448	A	N1-C6-N6	-6.80	114.52	118.60
21	AA	546	A	C5-C6-N1	6.80	121.10	117.70
54	BA	128	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	294	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2622	U	O4'-C1'-N1	6.80	113.64	108.20
21	AA	1046	A	C5-C6-N1	6.79	121.10	117.70
23	A2	92	U	C5'-C4'-C3'	-6.79	105.13	116.00
54	BA	623	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	2266	A	N1-C6-N6	-6.79	114.52	118.60
54	BA	2317	A	C5-C6-N1	6.79	121.10	117.70
21	AA	364	A	C4-C5-C6	-6.79	113.60	117.00
21	AA	790	A	C5-C6-N1	6.79	121.10	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	114	ARG	NE-CZ-NH1	6.79	123.70	120.30
21	AA	840	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	1306	A	N1-C6-N6	-6.79	114.53	118.60
21	AA	1357	A	C5-C6-N1	6.79	121.09	117.70
24	A3	58	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	616	A	C5-C6-N1	6.79	121.09	117.70
54	BA	1941	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	2676	C	N3-C2-O2	-6.79	117.15	121.90
24	A3	57	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	1306	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	2725	A	N1-C6-N6	-6.79	114.53	118.60
10	AK	127	ARG	NE-CZ-NH1	6.79	123.69	120.30
21	AA	149	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	743	A	C5-C6-N1	6.79	121.09	117.70
21	AA	1465	A	C5-C6-N1	6.79	121.09	117.70
22	A1	9	A	N1-C6-N6	-6.79	114.53	118.60
54	BA	1398	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	1890	A	C5-C6-N1	6.79	121.09	117.70
54	BA	2442	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	55	A	C5-C6-N1	6.78	121.09	117.70
21	AA	152	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	327	A	C5-C6-N1	6.78	121.09	117.70
21	AA	502	A	N1-C6-N6	-6.78	114.53	118.60
21	AA	696	A	C5-C6-N1	6.78	121.09	117.70
21	AA	753	A	C5-C6-N1	6.78	121.09	117.70
54	BA	38	A	C5-C6-N1	6.78	121.09	117.70
54	BA	888	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	501	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1966	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2298	A	C5-C6-N1	6.78	121.09	117.70
54	BA	443	A	C1'-O4'-C4'	-6.78	104.47	109.90
54	BA	892	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1129	A	C5-C6-N1	6.78	121.09	117.70
55	BB	31	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	2013	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	508	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	609	A	C5-C6-N1	6.78	121.09	117.70
55	BB	104	A	C5-C6-N1	6.78	121.09	117.70
21	AA	356	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	648	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	781	A	N1-C6-N6	-6.78	114.53	118.60
21	AA	1140	C	N3-C2-O2	-6.78	117.16	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1226	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1328	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1504	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2092	U	N3-C2-O2	-6.77	117.46	122.20
54	BA	2247	A	C5-C6-N1	6.77	121.09	117.70
1	AB	94	ARG	NE-CZ-NH1	6.77	123.69	120.30
54	BA	182	A	C5-C6-N1	6.77	121.09	117.70
54	BA	1057	A	C5-C6-N1	6.77	121.09	117.70
21	AA	465	A	O4'-C1'-N9	6.77	113.62	108.20
21	AA	579	A	C5-C6-N1	6.77	121.08	117.70
28	BF	109	ARG	NE-CZ-NH1	6.77	123.68	120.30
54	BA	1962	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	2059	A	C5-C6-N1	6.77	121.08	117.70
21	AA	1012	A	C5-C6-N1	6.77	121.08	117.70
32	BJ	95	ARG	NE-CZ-NH2	-6.77	116.92	120.30
54	BA	2284	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2723	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	802	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	1342	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	433	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	980	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1095	A	N1-C6-N6	-6.76	114.54	118.60
21	AA	1280	A	C5-C6-N1	6.76	121.08	117.70
6	AG	142	ARG	NE-CZ-NH1	6.76	123.68	120.30
11	AL	49	ARG	NE-CZ-NH2	-6.76	116.92	120.30
21	AA	373	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	1103	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	485	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	502	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1505	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1626	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	2484	G	O4'-C1'-N9	6.76	113.61	108.20
21	AA	1229	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	1248	A	C5-C6-N1	6.76	121.08	117.70
54	BA	439	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	2730	C	N3-C2-O2	-6.76	117.17	121.90
55	BB	70	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	408	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	545	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	753	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	849	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	1019	A	C5-C6-N1	6.75	121.08	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1012	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	311	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	1241	A	O4'-C1'-N9	6.75	113.60	108.20
54	BA	2767	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	1180	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	1287	A	C5-C6-N1	6.75	121.08	117.70
54	BA	998	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	1532	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1805	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	913	A	C5-C6-N1	6.75	121.08	117.70
55	BB	108	A	C5-C6-N1	6.75	121.08	117.70
21	AA	383	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	746	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1503	A	C5-C6-N1	6.75	121.07	117.70
21	AA	120	A	N1-C6-N6	-6.75	114.55	118.60
21	AA	207	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	520	A	C5-C6-N1	6.75	121.07	117.70
21	AA	1234	C	N3-C2-O2	-6.75	117.18	121.90
23	A2	82	A	C5-C6-N1	6.75	121.07	117.70
54	BA	975	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	199	A	C5-C6-N1	6.75	121.07	117.70
21	AA	190	A	C5-C6-N1	6.74	121.07	117.70
21	AA	469	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	1101	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1676	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2014	A	N1-C6-N6	-6.74	114.55	118.60
54	BA	2771	C	N3-C2-O2	-6.74	117.18	121.90
55	BB	8	C	O4'-C1'-N1	6.74	113.59	108.20
21	AA	841	C	O4'-C1'-N1	6.74	113.59	108.20
54	BA	1533	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	511	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	546	A	C4-C5-C6	-6.74	113.63	117.00
24	A3	1	C	N1-C2-O2	6.74	122.94	118.90
55	BB	57	A	C5-C6-N1	6.74	121.07	117.70
21	AA	231	U	O4'-C1'-N1	6.74	113.59	108.20
21	AA	918	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1141	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	908	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	918	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1067	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1470	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1477	A	C5-C6-N1	6.74	121.07	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2450	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2753	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1081	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1113	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1639	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1504	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1617	C	N3-C2-O2	-6.74	117.19	121.90
54	BA	1900	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1431	A	C5-C6-N1	6.73	121.07	117.70
21	AA	1507	A	C5-C6-N1	6.73	121.07	117.70
54	BA	1244	A	C4-C5-C6	-6.73	113.63	117.00
54	BA	620	G	O4'-C1'-N9	6.73	113.59	108.20
54	BA	661	A	C5-C6-N1	6.73	121.07	117.70
54	BA	1165	A	C5-C6-N1	6.73	121.07	117.70
54	BA	241	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	1636	U	O4'-C1'-N1	6.73	113.58	108.20
54	BA	2469	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	1502	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	2716	C	N3-C2-O2	-6.73	117.19	121.90
18	AS	2	ARG	NE-CZ-NH1	6.73	123.66	120.30
21	AA	279	A	C4-C5-C6	-6.73	113.64	117.00
21	AA	1412	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	613	A	C1'-O4'-C4'	-6.73	104.52	109.90
54	BA	1967	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1969	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	2014	A	C5-C6-N1	6.73	121.06	117.70
54	BA	2682	A	C5-C6-N1	6.73	121.06	117.70
21	AA	194	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	432	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	255	A	C5-C6-N1	6.73	121.06	117.70
21	AA	222	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	1403	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2070	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2459	A	N1-C6-N6	-6.72	114.56	118.60
55	BB	109	A	C4-C5-C6	-6.72	113.64	117.00
41	BS	84	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	14	A	C5-C6-N1	6.72	121.06	117.70
54	BA	915	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	118	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	272	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	896	A	C5-C6-N1	6.72	121.06	117.70
54	BA	1028	A	C5-C6-N1	6.72	121.06	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	397	A	O4'-C1'-N9	6.72	113.58	108.20
21	AA	1384	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	909	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1205	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2281	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	436	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	1987	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	354	A	C5-C6-N1	6.71	121.06	117.70
54	BA	483	A	C5-C6-N1	6.71	121.06	117.70
54	BA	540	C	O4'-C1'-N1	6.71	113.57	108.20
54	BA	563	A	C5-C6-N1	6.71	121.06	117.70
54	BA	702	U	O4'-C1'-N1	6.71	113.57	108.20
54	BA	1048	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2547	A	N1-C6-N6	-6.71	114.57	118.60
54	BA	2901	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	329	A	C5-C6-N1	6.71	121.06	117.70
54	BA	11	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	2211	A	C4-C5-C6	-6.71	113.64	117.00
21	AA	1150	A	C5-C6-N1	6.71	121.06	117.70
37	BO	16	ARG	NE-CZ-NH1	6.71	123.66	120.30
54	BA	218	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1335	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	1529	G	O4'-C1'-N9	6.71	113.57	108.20
54	BA	281	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	706	A	C5-C6-N1	6.71	121.05	117.70
21	AA	47	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	878	A	C5-C6-N1	6.71	121.05	117.70
54	BA	320	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	732	C	N3-C2-O2	-6.71	117.21	121.90
54	BA	1054	A	C5-C6-N1	6.71	121.05	117.70
54	BA	2089	C	C1'-O4'-C4'	-6.71	104.53	109.90
54	BA	348	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	1711	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	2388	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	1169	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1572	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	1809	A	C5-C6-N1	6.70	121.05	117.70
21	AA	435	A	C5-C6-N1	6.70	121.05	117.70
54	BA	432	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	81	A	C5-C6-N1	6.70	121.05	117.70
21	AA	1239	A	C5-C6-N1	6.70	121.05	117.70
21	AA	1469	C	N3-C2-O2	-6.70	117.21	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1794	A	C5-C6-N1	6.70	121.05	117.70
21	AA	431	A	C5-C6-N1	6.70	121.05	117.70
54	BA	28	A	C5-C6-N1	6.70	121.05	117.70
54	BA	163	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1698	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2451	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1689	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2610	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1349	C	N3-C2-O2	-6.69	117.21	121.90
1	AB	221	ARG	NE-CZ-NH2	-6.69	116.95	120.30
21	AA	676	A	C4-C5-C6	-6.69	113.65	117.00
22	A1	6	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	786	C	N3-C2-O2	-6.69	117.22	121.90
15	AP	56	ARG	NE-CZ-NH2	6.69	123.64	120.30
54	BA	742	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1832	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2058	A	C5-C6-N1	6.69	121.05	117.70
54	BA	204	A	C5-C6-N1	6.69	121.04	117.70
54	BA	216	A	C5-C6-N1	6.69	121.04	117.70
54	BA	278	A	N1-C6-N6	-6.69	114.59	118.60
54	BA	332	A	N1-C6-N6	-6.69	114.59	118.60
54	BA	1744	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	2327	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	949	A	C5-C6-N1	6.69	121.04	117.70
21	AA	1274	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	1145	C	N3-C2-O2	-6.68	117.22	121.90
55	BB	58	A	C5-C6-N1	6.68	121.04	117.70
24	A3	72	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	972	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1650	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2025	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	2635	A	C4-C5-C6	-6.68	113.66	117.00
24	A3	67	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	257	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	670	A	N1-C6-N6	-6.68	114.59	118.60
6	AG	9	ARG	NE-CZ-NH1	6.68	123.64	120.30
54	BA	639	U	O4'-C1'-N1	6.68	113.54	108.20
21	AA	766	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	368	A	C4-C5-C6	-6.68	113.66	117.00
55	BB	55	U	O4'-C1'-N1	6.68	113.54	108.20
21	AA	248	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	271	C	N3-C2-O2	-6.67	117.23	121.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1300	G	O4'-C1'-N9	6.67	113.54	108.20
21	AA	1320	C	O4'-C1'-N1	6.67	113.54	108.20
54	BA	332	A	C5-C6-N1	6.67	121.04	117.70
54	BA	401	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1304	A	C5-C6-N1	6.67	121.04	117.70
54	BA	2471	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	2886	A	O4'-C1'-N9	6.67	113.54	108.20
54	BA	1013	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2176	A	C5-C6-N1	6.67	121.04	117.70
54	BA	435	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	472	A	N1-C6-N6	-6.67	114.60	118.60
54	BA	2051	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2882	A	C5-C6-N1	6.67	121.04	117.70
21	AA	1449	C	N3-C2-O2	-6.67	117.23	121.90
24	A3	72	C	O3'-P-O5'	6.67	116.67	104.00
12	AM	100	ARG	NE-CZ-NH1	6.67	123.63	120.30
21	AA	130	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	478	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2160	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2521	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	306	A	C5-C6-N1	6.67	121.03	117.70
54	BA	156	A	C5-C6-N1	6.66	121.03	117.70
54	BA	572	A	C5-C6-N1	6.66	121.03	117.70
54	BA	825	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1357	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	2088	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2765	A	C5-C6-N1	6.66	121.03	117.70
36	BN	96	ARG	NE-CZ-NH1	6.66	123.63	120.30
54	BA	722	A	C5-C6-N1	6.66	121.03	117.70
21	AA	1342	C	O4'-C1'-N1	6.66	113.53	108.20
54	BA	1213	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1993	U	O4'-C1'-N1	6.66	113.53	108.20
54	BA	156	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1870	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	2009	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2855	C	N3-C2-O2	-6.66	117.24	121.90
8	AI	123	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	1368	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	105	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	648	A	C5-C6-N1	6.65	121.03	117.70
21	AA	1340	A	C5-C6-N1	6.65	121.03	117.70
54	BA	902	C	N3-C2-O2	-6.65	117.24	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	76	A	C8-N9-C4	-6.65	103.14	105.80
54	BA	142	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1868	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	879	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	1000	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	310	A	N1-C6-N6	-6.65	114.61	118.60
54	BA	1039	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1433	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1991	U	O4'-C1'-N1	6.65	113.52	108.20
54	BA	2065	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	71	A	C5-C6-N1	6.65	121.03	117.70
21	AA	998	C	N3-C2-O2	-6.65	117.25	121.90
22	A1	61	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	2097	A	C5-C6-N1	6.65	121.02	117.70
54	BA	2738	A	C5-C6-N1	6.65	121.02	117.70
21	AA	1303	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1592	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1787	A	C5-C6-N1	6.65	121.02	117.70
54	BA	2406	A	O4'-C1'-N9	6.65	113.52	108.20
54	BA	727	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	1701	A	C5-C6-N1	6.65	121.02	117.70
54	BA	2679	A	C5-C6-N1	6.65	121.02	117.70
21	AA	901	A	N1-C6-N6	-6.64	114.61	118.60
54	BA	384	A	C5-C6-N1	6.64	121.02	117.70
54	BA	522	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	272	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	554	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	649	A	C5-C6-N1	6.64	121.02	117.70
21	AA	1022	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	299	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	412	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1392	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1547	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2009	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2164	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	461	A	C5-C6-N1	6.64	121.02	117.70
21	AA	1060	U	C5'-C4'-O4'	6.64	117.07	109.10
21	AA	1081	A	C5-C6-N1	6.64	121.02	117.70
21	AA	549	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	1446	A	C4-C5-C6	-6.64	113.68	117.00
24	A3	24	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1384	A	C5-C6-N1	6.64	121.02	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2725	A	C5-C6-N1	6.64	121.02	117.70
21	AA	355	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1708	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1363	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2469	A	C5-C6-N1	6.64	121.02	117.70
4	AE	44	ARG	NE-CZ-NH1	6.63	123.62	120.30
21	AA	178	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	315	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	436	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	1201	A	C5-C6-N1	6.63	121.02	117.70
54	BA	2534	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	642	A	C5-C6-N1	6.63	121.02	117.70
32	BJ	37	ARG	NE-CZ-NH1	6.63	123.62	120.30
54	BA	2199	A	C5-C6-N1	6.63	121.02	117.70
54	BA	1244	A	C5-C6-N1	6.63	121.02	117.70
21	AA	1193	G	O4'-C1'-N9	6.63	113.50	108.20
21	AA	825	A	C5-C6-N1	6.63	121.01	117.70
21	AA	1230	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1938	A	C1'-O4'-C4'	-6.63	104.60	109.90
21	AA	866	C	N3-C2-O2	-6.62	117.26	121.90
48	BZ	15	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	675	A	C5-C6-N1	6.62	121.01	117.70
21	AA	883	C	N3-C2-O2	-6.62	117.26	121.90
48	BZ	37	ARG	NE-CZ-NH1	6.62	123.61	120.30
54	BA	471	A	N1-C6-N6	-6.62	114.63	118.60
54	BA	477	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1143	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1257	C	N3-C2-O2	-6.62	117.26	121.90
21	AA	695	A	N1-C6-N6	-6.62	114.63	118.60
54	BA	426	C	N3-C2-O2	-6.62	117.26	121.90
54	BA	2766	A	C5-C6-N1	6.62	121.01	117.70
21	AA	253	A	C5-C6-N1	6.62	121.01	117.70
21	AA	958	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1189	A	C5-C6-N1	6.62	121.01	117.70
21	AA	280	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	960	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2346	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	2893	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	68	G	N1-C6-O6	-6.62	115.93	119.90
21	AA	1314	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	1327	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	575	A	C4-C5-C6	-6.62	113.69	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1207	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	2899	A	C5-C6-N1	6.62	121.01	117.70
55	BB	19	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	994	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	1262	A	C5-C6-N1	6.61	121.01	117.70
38	BP	92	ARG	NE-CZ-NH1	6.61	123.61	120.30
21	AA	303	A	C4-C5-C6	-6.61	113.69	117.00
21	AA	1059	C	N3-C2-O2	-6.61	117.27	121.90
39	BQ	2	ARG	NE-CZ-NH2	6.61	123.61	120.30
54	BA	429	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	734	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1194	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	2667	C	N1-C2-O2	6.61	122.87	118.90
54	BA	1144	A	C5-C6-N1	6.61	121.00	117.70
24	A3	49	C	N1-C2-O2	6.61	122.86	118.90
54	BA	49	A	O4'-C1'-N9	6.61	113.49	108.20
54	BA	309	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	1146	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1632	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	1677	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	311	C	N3-C2-O2	-6.61	117.28	121.90
21	AA	1217	C	N3-C2-O2	-6.61	117.28	121.90
21	AA	1531	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1591	A	C5-C6-N1	6.61	121.00	117.70
54	BA	764	A	C5-C6-N1	6.60	121.00	117.70
54	BA	877	A	C5-C6-N1	6.60	121.00	117.70
54	BA	2153	C	N3-C2-O2	-6.60	117.28	121.90
3	AD	80	ARG	NE-CZ-NH1	6.60	123.60	120.30
21	AA	578	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	819	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	95	A	C5-C6-N1	6.60	121.00	117.70
54	BA	538	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	1021	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1454	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	2173	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	2342	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	872	A	O4'-C1'-N9	6.60	113.48	108.20
54	BA	455	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	898	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1772	A	N1-C6-N6	-6.60	114.64	118.60
55	BB	29	A	C5-C6-N1	6.60	121.00	117.70
15	AP	31	ARG	NE-CZ-NH1	6.60	123.60	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1176	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1745	A	C5-C6-N1	6.60	121.00	117.70
54	BA	839	U	O4'-C1'-N1	6.60	113.48	108.20
54	BA	2072	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	2241	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1805	A	C5-C6-N1	6.60	121.00	117.70
21	AA	366	A	C5-C6-N1	6.59	121.00	117.70
21	AA	635	A	C5-C6-N1	6.59	121.00	117.70
54	BA	1345	C	N3-C2-O2	-6.59	117.28	121.90
21	AA	1102	A	C5-C6-N1	6.59	121.00	117.70
54	BA	449	A	C5-C6-N1	6.59	121.00	117.70
55	BB	90	C	N3-C2-O2	-6.59	117.28	121.90
21	AA	764	C	N3-C2-O2	-6.59	117.29	121.90
22	A1	56	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	453	A	C5-C6-N1	6.59	121.00	117.70
54	BA	1321	A	N1-C6-N6	-6.59	114.64	118.60
54	BA	2183	A	C5-C6-N1	6.59	121.00	117.70
54	BA	2711	A	C4-C5-C6	-6.59	113.70	117.00
41	BS	8	ARG	NE-CZ-NH1	6.59	123.59	120.30
54	BA	191	A	C5-C6-N1	6.59	121.00	117.70
54	BA	1735	A	C5-C6-N1	6.59	121.00	117.70
54	BA	1759	A	C4-C5-C6	-6.59	113.71	117.00
54	BA	1575	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	962	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	1021	A	C5-C6-N1	6.59	120.99	117.70
22	A1	76	A	C5-C6-N1	6.59	120.99	117.70
54	BA	2171	A	C4-C5-C6	-6.59	113.71	117.00
54	BA	2670	A	C5-C6-N1	6.59	120.99	117.70
21	AA	179	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1077	A	C5-C6-N1	6.58	120.99	117.70
21	AA	26	A	C5-C6-N1	6.58	120.99	117.70
21	AA	1324	A	C5-C6-N1	6.58	120.99	117.70
22	A1	25	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	1264	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2231	U	O4'-C1'-N1	6.58	113.47	108.20
54	BA	2468	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2873	A	C5-C6-N1	6.58	120.99	117.70
21	AA	1014	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1092	A	C4-C5-C6	-6.58	113.71	117.00
26	BD	124	ARG	NE-CZ-NH1	6.58	123.59	120.30
32	BJ	120	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	272	A	C5-C6-N1	6.58	120.99	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	465	G	O4'-C1'-N9	6.58	113.47	108.20
54	BA	2317	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	100	G	N1-C6-O6	-6.58	115.95	119.90
54	BA	637	A	O4'-C1'-N9	6.58	113.46	108.20
54	BA	2430	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1045	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	764	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	937	C	N3-C2-O2	-6.58	117.30	121.90
21	AA	1279	G	N3-C4-C5	-6.58	125.31	128.60
21	AA	1508	A	C5-C6-N1	6.58	120.99	117.70
54	BA	917	A	N1-C6-N6	-6.58	114.66	118.60
54	BA	1431	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	171	A	C4-C5-C6	-6.57	113.71	117.00
21	AA	1063	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	209	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	385	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	440	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2326	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	715	A	C5-C6-N1	6.57	120.99	117.70
21	AA	335	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	796	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1577	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2169	A	O4'-C1'-N9	6.57	113.46	108.20
21	AA	277	C	N3-C2-O2	-6.57	117.30	121.90
20	AU	33	ARG	NE-CZ-NH1	6.57	123.58	120.30
21	AA	736	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	892	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	634	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	794	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	1048	A	C5-C6-N1	6.57	120.98	117.70
54	BA	1848	A	C5-C6-N1	6.57	120.98	117.70
21	AA	857	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	1287	A	C4-C5-C6	-6.57	113.72	117.00
22	A1	58	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	41	C	N3-C2-O2	-6.57	117.31	121.90
54	BA	986	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1558	C	N3-C2-O2	-6.57	117.31	121.90
54	BA	1942	C	N3-C2-O2	-6.57	117.30	121.90
36	BN	30	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	1268	A	N1-C6-N6	-6.56	114.66	118.60
54	BA	1502	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1793	C	N3-C2-O2	-6.56	117.31	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	554	A	C5-C6-N1	6.56	120.98	117.70
21	AA	1273	C	N3-C2-O2	-6.56	117.31	121.90
22	A1	41	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	269	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2212	A	C5-C6-N1	6.56	120.98	117.70
54	BA	582	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	835	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1274	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2601	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	501	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	978	A	C5-C6-N1	6.56	120.98	117.70
54	BA	237	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	270	A	N1-C6-N6	-6.56	114.66	118.60
55	BB	113	C	N3-C2-O2	-6.56	117.31	121.90
43	BU	85	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	1494	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2095	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	1239	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	143	A	C5-C6-N1	6.55	120.98	117.70
21	AA	188	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1236	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	60	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1970	A	C5-C6-N1	6.55	120.98	117.70
3	AD	72	ARG	NE-CZ-NH1	6.55	123.58	120.30
54	BA	1901	A	C5-C6-N1	6.55	120.98	117.70
21	AA	181	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	533	A	C5-C6-N1	6.55	120.97	117.70
21	AA	1308	U	C3'-C2'-C1'	-6.55	96.26	101.50
54	BA	502	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1109	C	N3-C4-N4	-6.55	113.42	118.00
54	BA	2088	A	C5-C6-N1	6.55	120.97	117.70
21	AA	1223	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	1916	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	2378	A	C5-C6-N1	6.55	120.97	117.70
21	AA	349	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	142	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	223	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	505	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	1522	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	2033	A	C5-C6-N1	6.55	120.97	117.70
55	BB	108	A	C4-C5-C6	-6.55	113.73	117.00
21	AA	1534	A	O4'-C1'-N9	6.54	113.44	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1427	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1609	A	N1-C6-N6	-6.54	114.67	118.60
54	BA	1885	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	1176	A	N1-C6-N6	-6.54	114.67	118.60
21	AA	1404	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	556	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1800	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1958	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	2795	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	876	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	1271	A	N1-C6-N6	-6.54	114.67	118.60
24	A3	29	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	407	G	N1-C6-O6	-6.54	115.97	119.90
54	BA	1077	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	1518	A	C5-C6-N1	6.54	120.97	117.70
36	BN	22	ARG	NE-CZ-NH1	6.54	123.57	120.30
54	BA	2792	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	61	C	N1-C2-O2	6.54	122.82	118.90
54	BA	1742	U	O4'-C1'-N1	6.54	113.43	108.20
54	BA	2860	A	C5-C6-N1	6.54	120.97	117.70
21	AA	913	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	1468	A	C4-C5-C6	-6.54	113.73	117.00
27	BE	61	ARG	NE-CZ-NH1	6.54	123.57	120.30
54	BA	421	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	1691	C	O4'-C1'-N1	6.54	113.43	108.20
38	BP	108	ARG	NE-CZ-NH2	6.53	123.57	120.30
54	BA	820	A	C5-C6-N1	6.53	120.97	117.70
54	BA	1399	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	2418	A	C5-C6-N1	6.53	120.97	117.70
21	AA	1265	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	513	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	602	A	C4-C5-C6	-6.53	113.73	117.00
51	B2	3	ARG	NE-CZ-NH2	6.53	123.56	120.30
54	BA	575	A	C5-C6-N1	6.53	120.97	117.70
21	AA	823	C	N3-C2-O2	-6.53	117.33	121.90
24	A3	59	A	C5-C6-N1	6.53	120.97	117.70
54	BA	1385	A	C5-C6-N1	6.53	120.97	117.70
2	AC	163	ARG	NE-CZ-NH1	6.53	123.56	120.30
21	AA	856	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1038	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1117	A	C5-C6-N1	6.53	120.96	117.70
21	AA	1428	A	C5-C6-N1	6.53	120.96	117.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	149	ARG	NE-CZ-NH1	6.53	123.56	120.30
54	BA	147	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1607	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1655	A	C5-C6-N1	6.53	120.96	117.70
22	A1	32	C	N3-C2-O2	-6.53	117.33	121.90
32	BJ	27	ARG	NE-CZ-NH1	6.53	123.56	120.30
54	BA	584	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	921	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1404	C	O4'-C1'-N1	6.53	113.42	108.20
54	BA	1804	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	2091	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	2712	C	N1-C2-O2	6.52	122.81	118.90
17	AR	60	ARG	NE-CZ-NH1	6.52	123.56	120.30
21	AA	393	A	C5-C6-N1	6.52	120.96	117.70
21	AA	1237	C	N3-C2-O2	-6.52	117.33	121.90
21	AA	1248	A	N1-C6-N6	-6.52	114.69	118.60
23	A2	91	A	O4'-C1'-N9	6.52	113.42	108.20
21	AA	1429	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	149	A	C5-C6-N1	6.52	120.96	117.70
54	BA	793	A	C5-C6-N1	6.52	120.96	117.70
55	BB	95	U	O4'-C1'-N1	6.52	113.42	108.20
54	BA	688	U	O4'-C1'-N1	6.52	113.42	108.20
54	BA	1784	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2205	A	C5-C6-N1	6.52	120.96	117.70
21	AA	389	A	C5-C6-N1	6.52	120.96	117.70
21	AA	716	A	N1-C6-N6	-6.52	114.69	118.60
21	AA	735	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	907	A	C5-C6-N1	6.52	120.96	117.70
54	BA	2501	C	O4'-C1'-C2'	-6.52	99.28	105.80
54	BA	2522	U	O4'-C1'-N1	6.52	113.41	108.20
54	BA	2731	G	O4'-C1'-N9	6.52	113.41	108.20
21	AA	163	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	2471	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1722	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	1833	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	2019	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	2635	A	C5-C6-N1	6.51	120.96	117.70
54	BA	538	A	C5-C6-N1	6.51	120.96	117.70
54	BA	1069	A	C5-C6-N1	6.51	120.96	117.70
54	BA	1366	A	N1-C6-N6	-6.51	114.69	118.60
54	BA	2403	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	984	C	N3-C2-O2	-6.51	117.34	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	84	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1446	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1882	U	O4'-C1'-N1	6.51	113.41	108.20
21	AA	553	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	439	A	C5-C6-N1	6.51	120.95	117.70
54	BA	721	A	C5-C6-N1	6.51	120.95	117.70
54	BA	742	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1790	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	1278	G	N3-C2-N2	-6.51	115.34	119.90
54	BA	83	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1912	A	C5-C6-N1	6.51	120.95	117.70
21	AA	28	A	C4-C5-C6	-6.51	113.75	117.00
21	AA	1071	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	1163	A	C5-C6-N1	6.51	120.95	117.70
54	BA	1735	A	N1-C6-N6	-6.51	114.70	118.60
55	BB	62	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	919	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1877	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	2175	C	N3-C2-O2	-6.50	117.35	121.90
37	BO	9	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	2888	C	N3-C2-O2	-6.50	117.35	121.90
24	A3	77	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	186	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	974	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	1090	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1226	C	N1-C2-O2	6.50	122.80	118.90
54	BA	632	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	791	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1472	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1749	A	C5-C6-N1	6.50	120.95	117.70
21	AA	401	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	647	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	1036	A	C5-C6-N1	6.50	120.95	117.70
8	AI	84	ARG	NE-CZ-NH1	6.49	123.55	120.30
21	AA	468	A	O4'-C1'-N9	6.49	113.39	108.20
21	AA	1282	C	N3-C2-O2	-6.49	117.35	121.90
54	BA	1637	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	65	A	C5-C6-N1	6.49	120.95	117.70
21	AA	1318	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1111	A	C5-C6-N1	6.49	120.95	117.70
4	AE	53	ARG	NE-CZ-NH1	6.49	123.55	120.30
21	AA	394	G	N3-C2-N2	-6.49	115.36	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	613	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	756	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	184	C	N1-C2-O2	6.49	122.79	118.90
54	BA	721	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	781	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	833	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1634	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	10	A	C4-C5-C6	-6.49	113.76	117.00
21	AA	1194	U	P-O3'-C3'	6.49	127.49	119.70
54	BA	497	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	546	U	O4'-C1'-N1	6.49	113.39	108.20
55	BB	43	C	N3-C2-O2	-6.49	117.36	121.90
18	AS	36	ARG	NE-CZ-NH1	6.49	123.54	120.30
54	BA	517	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	1204	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	16	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2377	A	C5-C6-N1	6.49	120.94	117.70
9	AJ	45	ARG	NE-CZ-NH1	6.48	123.54	120.30
54	BA	371	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	1080	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	1465	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	403	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	767	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	831	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	635	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1022	G	O4'-C1'-N9	6.48	113.38	108.20
54	BA	2456	C	N3-C2-O2	-6.48	117.36	121.90
55	BB	99	A	C5-C6-N1	6.48	120.94	117.70
21	AA	642	A	N1-C6-N6	-6.48	114.71	118.60
24	A3	44	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1757	A	C4-C5-C6	-6.48	113.76	117.00
24	A3	63	C	N3-C2-O2	-6.48	117.37	121.90
54	BA	1152	C	N3-C2-O2	-6.48	117.37	121.90
54	BA	2501	C	O4'-C1'-N1	6.48	113.38	108.20
21	AA	780	A	N1-C6-N6	-6.48	114.71	118.60
29	BG	68	ARG	NE-CZ-NH1	6.48	123.54	120.30
21	AA	556	C	N3-C2-O2	-6.47	117.37	121.90
46	BX	17	ARG	NE-CZ-NH2	-6.47	117.06	120.30
54	BA	756	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	2646	C	O4'-C1'-N1	6.47	113.38	108.20
21	AA	139	A	C5-C6-N1	6.47	120.94	117.70
54	BA	1717	A	C5-C6-N1	6.47	120.94	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2416	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	83	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	313	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	344	A	C5-C6-N1	6.47	120.94	117.70
54	BA	222	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1678	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	411	A	N1-C6-N6	-6.47	114.72	118.60
21	AA	739	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	865	A	C5-C6-N1	6.47	120.94	117.70
21	AA	985	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1188	A	C4-C5-C6	-6.47	113.77	117.00
24	A3	36	A	C1'-O4'-C4'	-6.47	104.72	109.90
54	BA	462	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	848	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2207	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	516	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1127	A	C5-C6-N1	6.47	120.93	117.70
21	AA	246	A	C5-C6-N1	6.47	120.93	117.70
21	AA	312	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	274	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1214	A	C5-C6-N1	6.47	120.93	117.70
54	BA	2826	A	C5-C6-N1	6.47	120.93	117.70
55	BB	88	C	N3-C2-O2	-6.47	117.37	121.90
3	AD	13	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	1319	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2824	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	853	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1019	A	N1-C6-N6	-6.46	114.72	118.60
22	A1	41	A	C5-C6-N1	6.46	120.93	117.70
37	BO	13	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	101	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1403	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1098	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2285	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2734	A	C4-C5-C6	-6.46	113.77	117.00
55	BB	87	U	N3-C2-O2	-6.46	117.68	122.20
21	AA	381	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	782	A	O4'-C1'-N9	6.46	113.37	108.20
54	BA	2764	A	C5-C6-N1	6.46	120.93	117.70
21	AA	655	A	C5-C6-N1	6.46	120.93	117.70
54	BA	283	G	N1-C6-O6	-6.46	116.03	119.90
54	BA	541	A	N1-C6-N6	-6.46	114.73	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	586	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	692	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1801	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2306	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	274	A	C5-C6-N1	6.46	120.93	117.70
52	B3	7	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	1076	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	50	A	C4-C5-C6	-6.45	113.77	117.00
21	AA	108	G	O4'-C1'-N9	6.45	113.36	108.20
21	AA	167	A	C5-C6-N1	6.45	120.93	117.70
21	AA	221	C	N3-C2-O2	-6.45	117.38	121.90
32	BJ	75	TYR	CB-CG-CD2	-6.45	117.13	121.00
21	AA	1493	A	C5-C6-N1	6.45	120.93	117.70
21	AA	1516	G	N3-C2-N2	-6.45	115.38	119.90
54	BA	996	A	C5-C6-N1	6.45	120.93	117.70
54	BA	2433	A	C5-C6-N1	6.45	120.93	117.70
21	AA	95	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	321	A	C5-C6-N1	6.45	120.93	117.70
21	AA	503	C	O4'-C1'-N1	6.45	113.36	108.20
54	BA	1293	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1151	A	C5-C6-N1	6.45	120.92	117.70
25	BC	42	ARG	NE-CZ-NH1	6.45	123.52	120.30
49	B0	39	ARG	NE-CZ-NH1	6.45	123.52	120.30
54	BA	104	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	401	A	N1-C6-N6	-6.45	114.73	118.60
54	BA	1598	A	N1-C6-N6	-6.45	114.73	118.60
54	BA	2577	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	2851	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	564	C	N3-C2-O2	-6.45	117.39	121.90
22	A1	36	C	N3-C2-O2	-6.45	117.39	121.90
39	BQ	23	TYR	CB-CG-CD2	-6.45	117.13	121.00
54	BA	2902	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	233	C	N3-C2-O2	-6.44	117.39	121.90
33	BK	17	ARG	NE-CZ-NH2	-6.44	117.08	120.30
54	BA	1768	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2374	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	1755	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	336	A	C5-C6-N1	6.44	120.92	117.70
21	AA	780	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1145	A	N1-C6-N6	-6.44	114.74	118.60
21	AA	1157	A	C5-C6-N1	6.44	120.92	117.70
54	BA	792	A	C4-C5-C6	-6.44	113.78	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2196	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2305	U	O4'-C1'-N1	6.44	113.35	108.20
54	BA	2381	A	C4-C5-C6	-6.44	113.78	117.00
55	BB	73	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1925	C	O4'-C1'-N1	6.44	113.35	108.20
21	AA	174	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	1105	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1308	U	P-O3'-C3'	6.44	127.43	119.70
54	BA	21	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	948	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2765	A	N1-C6-N6	-6.44	114.74	118.60
54	BA	541	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1793	C	C4'-C3'-C2'	-6.44	96.16	102.60
54	BA	2350	C	O4'-C1'-N1	6.44	113.35	108.20
54	BA	2853	C	N3-C2-O2	-6.44	117.39	121.90
3	AD	96	ARG	NE-CZ-NH1	6.43	123.52	120.30
31	BI	126	ARG	NE-CZ-NH1	6.43	123.52	120.30
54	BA	161	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1287	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1304	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1545	A	C5-C6-N1	6.43	120.92	117.70
21	AA	529	G	N1-C6-O6	-6.43	116.04	119.90
21	AA	1408	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	1507	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	557	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	783	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1802	A	C5-C6-N1	6.43	120.92	117.70
24	A3	44	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1586	A	C5-C6-N1	6.43	120.92	117.70
54	BA	2385	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2566	A	C5-C6-N1	6.43	120.92	117.70
54	BA	37	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1789	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	10	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	334	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	398	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1312	U	P-O3'-C3'	6.43	127.41	119.70
1	AB	62	ARG	NE-CZ-NH1	6.42	123.51	120.30
21	AA	1152	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	640	C	N3-C2-O2	-6.42	117.40	121.90
54	BA	1918	A	C4-C5-C6	-6.42	113.79	117.00
55	BB	94	A	C5-C6-N1	6.42	120.91	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	253	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	944	C	N3-C2-O2	-6.42	117.40	121.90
12	AM	28	ARG	NE-CZ-NH1	6.42	123.51	120.30
21	AA	630	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	167	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	486	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1969	A	C5-C6-N1	6.42	120.91	117.70
21	AA	967	C	N3-C2-O2	-6.42	117.41	121.90
44	BV	79	ARG	NE-CZ-NH1	6.42	123.51	120.30
54	BA	549	G	N3-C2-N2	-6.42	115.41	119.90
54	BA	1350	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1819	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	243	A	C5-C6-N1	6.41	120.91	117.70
21	AA	935	A	C5-C6-N1	6.41	120.91	117.70
54	BA	173	A	C5-C6-N1	6.41	120.91	117.70
54	BA	935	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1996	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	475	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	759	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	1214	C	O4'-C1'-N1	6.41	113.33	108.20
46	BX	71	ARG	NE-CZ-NH1	6.41	123.51	120.30
54	BA	606	U	O4'-C1'-N1	6.41	113.33	108.20
54	BA	1086	A	C4-C5-C6	-6.41	113.79	117.00
14	AO	52	ARG	NE-CZ-NH1	6.41	123.50	120.30
54	BA	807	U	O4'-C1'-N1	6.41	113.33	108.20
54	BA	1126	A	P-O3'-C3'	6.41	127.39	119.70
54	BA	1608	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1749	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	587	C	N3-C4-C5	6.41	124.46	121.90
54	BA	2354	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	611	C	O4'-C1'-N1	6.40	113.32	108.20
54	BA	734	A	C4-C5-C6	-6.40	113.80	117.00
8	AI	32	ARG	NE-CZ-NH1	6.40	123.50	120.30
54	BA	221	A	N1-C6-N6	-6.40	114.76	118.60
54	BA	1014	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1354	A	C4-C5-C6	-6.40	113.80	117.00
56	B5	60	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	AB	10	LYS	C-N-CA	6.40	137.70	121.70
6	AG	101	ARG	NE-CZ-NH1	6.40	123.50	120.30
21	AA	1300	G	N3-C4-C5	-6.40	125.40	128.60
54	BA	1233	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1246	A	C5-C6-N1	6.40	120.90	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1260	A	C5-C6-N1	6.40	120.90	117.70
54	BA	1821	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2208	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2868	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	155	A	C5-C6-N1	6.40	120.90	117.70
21	AA	430	A	C5-C6-N1	6.40	120.90	117.70
21	AA	1484	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1298	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2094	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	223	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	658	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	777	A	C4-C5-C6	-6.39	113.80	117.00
22	A1	47	U	O4'-C1'-N1	6.39	113.32	108.20
54	BA	8	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	58	C	O4'-C1'-N1	6.39	113.31	108.20
21	AA	73	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	148	G	N3-C2-N2	-6.39	115.42	119.90
54	BA	60	G	N3-C2-N2	-6.39	115.42	119.90
54	BA	916	G	N1-C6-O6	-6.39	116.06	119.90
54	BA	1821	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	299	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2422	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2821	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	480	A	C5-C6-N1	6.39	120.89	117.70
54	BA	1836	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2646	C	N1-C2-O2	6.39	122.73	118.90
23	A2	79	A	C4-C5-C6	-6.38	113.81	117.00
35	BM	18	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BA	179	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2020	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2810	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	539	A	C5-C6-N1	6.38	120.89	117.70
54	BA	461	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2352	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2547	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2750	A	C5-C6-N1	6.38	120.89	117.70
54	BA	89	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1662	U	O4'-C1'-N1	6.38	113.30	108.20
55	BB	93	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	389	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1150	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	2261	C	N3-C2-O2	-6.38	117.44	121.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2774	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	499	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	579	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	796	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	995	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	2736	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	726	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1044	A	C5-C6-N1	6.37	120.89	117.70
21	AA	1513	A	C5-C6-N1	6.37	120.89	117.70
54	BA	528	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	592	A	C5-C6-N1	6.37	120.89	117.70
54	BA	687	C	N3-C2-O2	-6.37	117.44	121.90
3	AD	2	ARG	NE-CZ-NH1	6.37	123.48	120.30
21	AA	139	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	276	U	O4'-C1'-N1	6.37	113.29	108.20
54	BA	2340	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2559	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1978	A	C5-C6-N1	6.37	120.88	117.70
6	AG	3	ARG	NE-CZ-NH1	6.37	123.48	120.30
33	BK	78	ARG	NE-CZ-NH1	6.37	123.48	120.30
54	BA	1268	A	C5-C6-N1	6.37	120.88	117.70
54	BA	1889	A	C5-C6-N1	6.37	120.88	117.70
54	BA	2362	C	O4'-C1'-N1	6.37	113.29	108.20
54	BA	2757	A	C5-C6-N1	6.37	120.88	117.70
21	AA	496	A	O4'-C1'-N9	6.36	113.29	108.20
22	A1	68	C	N3-C2-O2	-6.36	117.44	121.90
24	A3	73	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2498	C	N3-C2-O2	-6.36	117.44	121.90
54	BA	2887	A	C4-C5-C6	-6.36	113.82	117.00
12	AM	2	ARG	NE-CZ-NH2	6.36	123.48	120.30
55	BB	59	A	C5-C6-N1	6.36	120.88	117.70
21	AA	1055	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	981	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1151	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1997	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2616	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2649	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	680	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	566	U	O4'-C1'-N1	6.36	113.29	108.20
54	BA	1161	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	946	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2732	G	N3-C4-C5	-6.36	125.42	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2314	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	286	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	496	A	C5-C6-N1	6.35	120.88	117.70
54	BA	607	U	O4'-C1'-N1	6.35	113.28	108.20
54	BA	2191	A	C5-C6-N1	6.35	120.88	117.70
54	BA	2200	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	98	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	797	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	2773	C	N3-C2-O2	-6.35	117.45	121.90
14	AO	53	ARG	NE-CZ-NH1	6.35	123.47	120.30
54	BA	1089	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	1189	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	1619	G	N3-C2-N2	-6.35	115.46	119.90
54	BA	1672	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	2274	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	2347	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2636	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	845	A	C6-C5-N7	6.35	136.74	132.30
54	BA	815	C	N3-C2-O2	-6.35	117.46	121.90
15	AP	35	ARG	NE-CZ-NH1	6.35	123.47	120.30
45	BW	74	LYS	C-N-CA	6.35	137.56	121.70
54	BA	420	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	951	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	1299	G	O4'-C1'-N9	6.35	113.28	108.20
54	BA	2263	C	N3-C2-O2	-6.35	117.46	121.90
17	AR	52	ARG	NE-CZ-NH1	6.34	123.47	120.30
46	BX	44	ARG	NE-CZ-NH1	6.34	123.47	120.30
54	BA	94	A	N1-C6-N6	-6.34	114.79	118.60
54	BA	2861	U	O4'-C1'-N1	6.34	113.28	108.20
54	BA	903	C	N3-C2-O2	-6.34	117.46	121.90
2	AC	39	ARG	NE-CZ-NH1	6.34	123.47	120.30
21	AA	363	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	2713	U	O4'-C1'-N1	6.34	113.27	108.20
3	AD	46	ARG	NE-CZ-NH1	6.34	123.47	120.30
21	AA	580	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	1250	A	C4-C5-C6	-6.34	113.83	117.00
11	AL	30	ARG	NE-CZ-NH2	-6.34	117.13	120.30
21	AA	873	A	N1-C6-N6	-6.34	114.80	118.60
21	AA	968	A	N1-C6-N6	-6.34	114.80	118.60
54	BA	572	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	610	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	1101	A	C4-C5-C6	-6.34	113.83	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1137	C	N1-C2-O2	6.34	122.70	118.90
54	BA	1656	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2789	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	116	A	C5-C6-N1	6.33	120.87	117.70
54	BA	238	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1204	A	C5-C6-N1	6.33	120.87	117.70
54	BA	337	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1359	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	1386	C	O4'-C1'-N1	6.33	113.27	108.20
54	BA	1495	A	C5-C6-N1	6.33	120.87	117.70
54	BA	1670	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2512	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1389	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	84	A	O4'-C1'-N9	6.33	113.27	108.20
54	BA	2203	U	N3-C2-O2	-6.33	117.77	122.20
21	AA	316	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1774	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1378	A	O4'-C1'-N9	6.33	113.26	108.20
21	AA	1366	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	644	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	528	C	N3-C2-O2	-6.32	117.47	121.90
21	AA	635	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	923	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	1350	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1565	C	N3-C2-O2	-6.32	117.47	121.90
21	AA	704	A	C5-C6-N1	6.32	120.86	117.70
21	AA	908	A	C5-C6-N1	6.32	120.86	117.70
21	AA	1254	A	C5-C6-N1	6.32	120.86	117.70
54	BA	302	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	1211	C	N1-C2-O2	6.32	122.69	118.90
54	BA	1413	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1548	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1586	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	2187	U	O4'-C1'-N1	6.32	113.26	108.20
54	BA	2395	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	637	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	723	U	N3-C2-O2	-6.32	117.78	122.20
21	AA	1413	A	C5-C6-N1	6.32	120.86	117.70
54	BA	38	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	54	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	1499	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1262	A	C4-C5-C6	-6.31	113.84	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	914	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	1001	C	N3-C2-O2	-6.31	117.48	121.90
32	BJ	116	ARG	NE-CZ-NH1	6.31	123.46	120.30
33	BK	70	ARG	NE-CZ-NH1	6.31	123.46	120.30
54	BA	372	G	O4'-C1'-N9	6.31	113.25	108.20
54	BA	1902	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2720	U	O4'-C1'-N1	6.31	113.25	108.20
54	BA	2813	A	C4-C5-C6	-6.31	113.84	117.00
55	BB	114	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	192	A	C5-C6-N1	6.31	120.86	117.70
54	BA	204	A	C4-C5-C6	-6.31	113.84	117.00
3	AD	69	ARG	NE-CZ-NH1	6.31	123.45	120.30
21	AA	135	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	518	C	N3-C2-O2	-6.31	117.48	121.90
52	B3	12	ARG	NE-CZ-NH1	6.31	123.45	120.30
54	BA	1294	U	O4'-C1'-N1	6.31	113.25	108.20
21	AA	63	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	616	A	C4-C5-C6	-6.31	113.85	117.00
54	BA	1974	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2527	C	N3-C2-O2	-6.31	117.48	121.90
55	BB	51	G	O4'-C1'-N9	6.31	113.25	108.20
21	AA	729	A	C4-C5-C6	-6.31	113.85	117.00
21	AA	631	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1311	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1908	C	O4'-C1'-N1	6.30	113.24	108.20
54	BA	2448	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2896	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	948	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	164	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2806	C	N3-C2-O2	-6.30	117.49	121.90
55	BB	80	U	O4'-C1'-N1	6.30	113.24	108.20
21	AA	1179	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	458	G	O4'-C1'-N9	6.30	113.24	108.20
54	BA	1541	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1609	A	C1'-O4'-C4'	-6.30	104.86	109.90
27	BE	88	ARG	NE-CZ-NH1	6.30	123.45	120.30
21	AA	938	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	1329	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1045	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2215	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2691	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	182	A	C4-C5-C6	-6.29	113.85	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	624	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	1131	G	N3-C2-N2	-6.29	115.49	119.90
54	BA	71	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	910	C	N3-C2-O2	-6.29	117.50	121.90
25	BC	86	ARG	NE-CZ-NH1	6.29	123.45	120.30
54	BA	216	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	946	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1419	A	C5-C6-N1	6.29	120.85	117.70
54	BA	1746	A	C5-C6-N1	6.29	120.85	117.70
54	BA	2043	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2829	A	C5-C6-N1	6.29	120.85	117.70
55	BB	104	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	44	A	C5-C6-N1	6.29	120.84	117.70
21	AA	1171	A	C5-C6-N1	6.29	120.84	117.70
54	BA	1494	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	2402	U	O4'-C1'-N1	6.29	113.23	108.20
54	BA	503	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1039	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1512	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2564	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	2636	C	O4'-C1'-N1	6.29	113.23	108.20
54	BA	2825	G	N3-C2-N2	-6.29	115.50	119.90
21	AA	43	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	177	G	O4'-C1'-N9	6.28	113.23	108.20
21	AA	536	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1216	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	611	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2800	A	C5-C6-N1	6.28	120.84	117.70
54	BA	2818	U	O4'-C1'-N1	6.28	113.23	108.20
21	AA	262	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	1243	C	N3-C2-O2	-6.28	117.50	121.90
22	A1	38	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1043	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1285	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1571	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2006	C	N3-C2-O2	-6.28	117.50	121.90
55	BB	45	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	624	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1564	C	N3-C2-O2	-6.28	117.50	121.90
2	AC	171	ARG	NE-CZ-NH1	6.28	123.44	120.30
21	AA	435	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	1431	A	C4-C5-C6	-6.28	113.86	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AP	70	ARG	NE-CZ-NH1	6.28	123.44	120.30
22	A1	31	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	2179	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	2368	C	O4'-C1'-N1	6.28	113.22	108.20
21	AA	1082	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	1936	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	58	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1028	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1346	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	166	U	O4'-C1'-N1	6.27	113.22	108.20
54	BA	1986	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1053	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1437	A	C5-C6-N1	6.27	120.83	117.70
27	BE	79	ARG	NE-CZ-NH1	6.27	123.43	120.30
54	BA	165	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	2199	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	295	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	74	A	C5-C6-N1	6.26	120.83	117.70
21	AA	461	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1158	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1773	A	C4-C5-C6	-6.26	113.87	117.00
55	BB	68	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	800	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2154	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2184	A	C5-C6-N1	6.26	120.83	117.70
54	BA	144	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1960	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	1433	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1923	U	O4'-C1'-N1	6.26	113.21	108.20
54	BA	1977	A	C5-C6-N1	6.26	120.83	117.70
10	AK	68	ARG	NE-CZ-NH1	6.25	123.43	120.30
21	AA	611	C	N1-C2-O2	6.25	122.65	118.90
34	BL	60	ARG	NE-CZ-NH2	6.25	123.43	120.30
54	BA	1373	A	C5-C6-N1	6.25	120.83	117.70
54	BA	2278	A	C4-C5-C6	-6.25	113.87	117.00
21	AA	106	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	664	G	O4'-C1'-N9	6.25	113.20	108.20
39	BQ	91	ARG	NE-CZ-NH2	-6.25	117.17	120.30
54	BA	1928	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	2462	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	2520	C	N3-C2-O2	-6.25	117.52	121.90
20	AU	30	GLU	C-N-CA	6.25	137.33	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	189	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	2003	A	C5-C6-N1	6.25	120.83	117.70
55	BB	28	C	N3-C2-O2	-6.25	117.52	121.90
55	BB	66	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	968	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	269	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	394	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1937	A	C5-C6-N1	6.25	120.82	117.70
6	AG	4	ARG	C-N-CA	6.25	137.31	121.70
21	AA	878	A	C4-C5-C6	-6.25	113.88	117.00
22	A1	48	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	861	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	1246	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2088	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	2264	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	2482	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	609	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2600	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	706	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1510	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1322	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1330	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	1685	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	681	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	702	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	860	A	C5-C6-N1	6.24	120.82	117.70
21	AA	1226	C	C5'-C4'-O4'	6.24	116.59	109.10
54	BA	325	G	N3-C2-N2	-6.24	115.53	119.90
54	BA	633	A	C4-C5-C6	-6.24	113.88	117.00
55	BB	69	G	N1-C6-O6	-6.24	116.16	119.90
21	AA	1400	C	N1-C2-O2	6.24	122.64	118.90
54	BA	861	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1255	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	73	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	415	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1367	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	108	G	N3-C2-N2	-6.24	115.54	119.90
54	BA	1057	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1386	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1748	C	N3-C2-O2	-6.24	117.54	121.90
54	BA	2539	C	N3-C2-O2	-6.24	117.54	121.90
54	BA	2662	A	C5-C6-N1	6.24	120.82	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	793	A	O4'-C1'-N9	6.23	113.19	108.20
54	BA	1746	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	1225	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2060	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	600	A	C5-C6-N1	6.23	120.82	117.70
21	AA	1213	A	C5-C6-N1	6.23	120.82	117.70
54	BA	1806	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1924	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1408	A	N1-C6-N6	-6.23	114.86	118.60
54	BA	645	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	789	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	823	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	845	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	2071	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	243	A	C4-C5-C6	-6.23	113.89	117.00
24	A3	45	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	901	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2837	A	C5-C6-N1	6.23	120.81	117.70
55	BB	71	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	69	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	828	U	N3-C2-O2	-6.23	117.84	122.20
54	BA	832	U	O4'-C1'-N1	6.23	113.18	108.20
54	BA	2587	A	C5-C6-N1	6.23	120.81	117.70
21	AA	87	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	677	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1009	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1144	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1745	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1818	U	O4'-C1'-N1	6.22	113.18	108.20
24	A3	11	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	22	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	527	C	O4'-C1'-N1	6.22	113.18	108.20
21	AA	621	A	C5-C6-N1	6.22	120.81	117.70
21	AA	655	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	2380	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2886	A	N1-C6-N6	-6.22	114.87	118.60
55	BB	60	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	1184	G	N3-C2-N2	-6.22	115.55	119.90
54	BA	378	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1953	A	C4-C5-C6	-6.22	113.89	117.00
37	BO	102	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	680	C	N3-C2-O2	-6.22	117.55	121.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	795	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	873	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2699	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	618	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1398	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1319	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1761	C	N1-C2-O2	6.21	122.63	118.90
54	BA	1919	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1998	A	C5-C6-N1	6.21	120.81	117.70
21	AA	1262	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1668	A	C4-C5-C6	-6.21	113.89	117.00
35	BM	10	ARG	NE-CZ-NH1	6.21	123.41	120.30
54	BA	1164	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2134	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2226	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2463	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2863	C	N3-C2-O2	-6.21	117.55	121.90
38	BP	87	ARG	NE-CZ-NH1	6.21	123.41	120.30
54	BA	91	A	O4'-C1'-N9	6.21	113.17	108.20
54	BA	2066	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1520	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	203	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1072	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1109	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	1971	U	O4'-C1'-N1	6.21	113.17	108.20
21	AA	996	A	N1-C6-N6	-6.21	114.88	118.60
29	BG	169	ARG	NE-CZ-NH1	6.21	123.40	120.30
54	BA	2706	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	246	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	1208	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1093	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	302	C	O4'-C1'-N1	6.20	113.16	108.20
54	BA	547	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1084	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1834	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1895	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2359	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2850	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	817	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1050	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	459	A	N1-C6-N6	-6.20	114.88	118.60
21	AA	629	A	C4-C5-C6	-6.20	113.90	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	782	A	C5-C6-N1	6.20	120.80	117.70
21	AA	977	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1261	A	C5-C6-N1	6.20	120.80	117.70
54	BA	346	A	O4'-C1'-N9	6.20	113.16	108.20
54	BA	1353	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1952	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1982	U	C5'-C4'-O4'	6.20	116.54	109.10
21	AA	338	A	C5-C6-N1	6.20	120.80	117.70
54	BA	737	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2362	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	79	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1711	A	C5-C6-N1	6.20	120.80	117.70
54	BA	1838	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	478	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	693	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	878	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1092	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1387	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1694	C	N1-C2-O2	6.20	122.62	118.90
21	AA	290	C	N3-C2-O2	-6.19	117.56	121.90
21	AA	1149	C	N3-C2-O2	-6.19	117.56	121.90
54	BA	649	G	O4'-C1'-N9	6.19	113.16	108.20
54	BA	838	C	O4'-C1'-N1	6.19	113.16	108.20
54	BA	2117	A	O4'-C1'-N9	6.19	113.16	108.20
54	BA	885	C	O4'-C1'-N1	6.19	113.15	108.20
54	BA	2889	C	N3-C2-O2	-6.19	117.56	121.90
54	BA	1284	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	1427	A	P-O3'-C3'	6.19	127.13	119.70
54	BA	1498	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	2407	A	C5-C6-N1	6.19	120.80	117.70
21	AA	336	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	414	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	590	A	C5-C6-N1	6.19	120.80	117.70
54	BA	2062	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	226	G	N3-C2-N2	-6.19	115.57	119.90
21	AA	1275	A	C5-C6-N1	6.19	120.79	117.70
54	BA	821	A	C5-C6-N1	6.19	120.79	117.70
54	BA	1169	A	C5-C6-N1	6.19	120.79	117.70
54	BA	1357	C	O4'-C1'-N1	6.19	113.15	108.20
54	BA	2773	C	O4'-C1'-N1	6.19	113.15	108.20
55	BB	99	A	N1-C6-N6	-6.19	114.89	118.60
54	BA	1532	A	C4-C5-C6	-6.19	113.91	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	264	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	197	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	490	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1771	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	2350	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	651	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	839	C	N3-C2-O2	-6.18	117.57	121.90
36	BN	12	ARG	NE-CZ-NH1	6.18	123.39	120.30
54	BA	490	C	N1-C2-O2	6.18	122.61	118.90
4	AE	92	ARG	NE-CZ-NH1	6.18	123.39	120.30
54	BA	1611	C	N1-C2-O2	6.18	122.61	118.90
55	BB	94	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	236	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	211	C	O4'-C1'-N1	6.18	113.14	108.20
54	BA	1331	G	N1-C6-O6	-6.18	116.19	119.90
54	BA	1990	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	285	C	N1-C2-O2	6.17	122.61	118.90
21	AA	371	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	253	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1104	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1686	C	O4'-C1'-N1	6.17	113.14	108.20
54	BA	2340	A	C5-C6-N1	6.17	120.79	117.70
54	BA	2632	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	400	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	1046	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	2900	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	1466	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2637	U	O4'-C1'-N1	6.17	113.14	108.20
55	BB	53	A	N1-C6-N6	-6.17	114.90	118.60
54	BA	1054	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	1176	U	O4'-C1'-N1	6.17	113.14	108.20
54	BA	1615	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2184	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	2793	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	145	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1302	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	936	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1270	C	N3-C2-O2	-6.17	117.58	121.90
10	AK	12	ARG	NE-CZ-NH1	6.16	123.38	120.30
21	AA	143	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	663	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	323	C	C1'-O4'-C4'	-6.16	104.97	109.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	196	A	O4'-C1'-N9	6.16	113.13	108.20
10	AK	121	ARG	NE-CZ-NH2	6.16	123.38	120.30
21	AA	77	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	172	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	612	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	343	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	724	U	O4'-C1'-N1	6.16	113.13	108.20
54	BA	2787	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	1428	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	227	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	581	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	877	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1175	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1999	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	412	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	1000	A	C5-C6-N1	6.16	120.78	117.70
54	BA	318	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1638	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1772	A	C5-C6-N1	6.16	120.78	117.70
54	BA	126	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1007	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1556	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	18	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	456	A	C4-C5-C6	-6.15	113.92	117.00
21	AA	507	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	1293	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2078	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	523	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	800	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	1397	U	O4'-C1'-N1	6.15	113.12	108.20
21	AA	339	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	1008	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	1674	G	O4'-C1'-N9	6.15	113.12	108.20
55	BB	47	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	548	G	O4'-C1'-N9	6.15	113.12	108.20
21	AA	151	A	C4-C5-C6	-6.14	113.93	117.00
47	BY	7	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	482	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1866	A	C4-C5-C6	-6.14	113.93	117.00
22	A1	11	C	N1-C2-O2	6.14	122.59	118.90
21	AA	101	A	C4-C5-C6	-6.14	113.93	117.00
22	A1	74	C	N3-C2-O2	-6.14	117.60	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	346	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	526	A	O4'-C1'-N9	6.14	113.11	108.20
54	BA	574	A	C1'-O4'-C4'	-6.14	104.99	109.90
54	BA	752	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1204	A	O4'-C1'-N9	6.14	113.11	108.20
54	BA	2332	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2760	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	34	C	N3-C2-O2	-6.14	117.60	121.90
55	BB	46	A	C5-C6-N1	6.14	120.77	117.70
21	AA	382	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	520	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	723	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1644	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2715	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	1197	A	C4-C5-C6	-6.13	113.93	117.00
55	BB	39	A	N1-C6-N6	-6.13	114.92	118.60
21	AA	393	A	C4-C5-C6	-6.13	113.93	117.00
21	AA	935	A	N1-C6-N6	-6.13	114.92	118.60
54	BA	652	U	O4'-C1'-N1	6.13	113.11	108.20
54	BA	1480	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1985	C	O4'-C1'-N1	6.13	113.11	108.20
54	BA	2077	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	2766	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	197	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	572	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2800	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	1267	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	614	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2000	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	284	C	N3-C2-O2	-6.12	117.61	121.90
22	A1	35	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1605	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	2119	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2602	A	C1'-O4'-C4'	-6.12	105.00	109.90
21	AA	1333	A	C5-C6-N1	6.12	120.76	117.70
24	A3	68	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	603	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	854	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1162	G	N1-C6-O6	-6.12	116.23	119.90
54	BA	1286	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1579	A	C4-C5-C6	-6.12	113.94	117.00
30	BH	97	ARG	NE-CZ-NH1	6.12	123.36	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	66	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2678	C	O4'-C1'-N1	6.12	113.10	108.20
14	AO	76	ARG	NE-CZ-NH1	6.12	123.36	120.30
21	AA	743	A	N1-C6-N6	-6.12	114.93	118.60
54	BA	2205	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2418	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	1513	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1342	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2465	C	N3-C2-O2	-6.12	117.62	121.90
1	AB	212	TYR	CB-CG-CD1	-6.11	117.33	121.00
54	BA	1595	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1879	C	N1-C2-O2	6.11	122.57	118.90
54	BA	2313	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1301	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	1765	U	O4'-C1'-N1	6.11	113.09	108.20
21	AA	660	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	1479	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	931	U	C1'-O4'-C4'	-6.11	105.01	109.90
54	BA	995	C	N1-C2-O2	6.11	122.57	118.90
54	BA	2602	A	O4'-C1'-N9	6.11	113.09	108.20
8	AI	94	ARG	NE-CZ-NH1	6.11	123.36	120.30
21	AA	732	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	1257	A	C4-C5-C6	-6.11	113.95	117.00
36	BN	69	ARG	NE-CZ-NH1	6.11	123.35	120.30
54	BA	2342	C	O4'-C1'-N1	6.11	113.09	108.20
21	AA	217	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1654	A	C4-C5-C6	-6.11	113.95	117.00
21	AA	575	G	N1-C6-O6	-6.11	116.24	119.90
24	A3	52	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	804	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	1551	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	2052	A	C4-C5-C6	-6.11	113.95	117.00
21	AA	959	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	141	G	N3-C2-N2	-6.10	115.63	119.90
54	BA	1920	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	2448	A	O4'-C1'-N9	6.10	113.08	108.20
54	BA	896	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	960	A	O4'-C1'-N9	6.10	113.08	108.20
54	BA	2336	A	O4'-C1'-N9	6.10	113.08	108.20
54	BA	2376	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	930	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1524	C	N3-C2-O2	-6.10	117.63	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1111	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1706	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1894	C	N3-C2-O2	-6.10	117.63	121.90
55	BB	42	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	241	G	C1'-O4'-C4'	-6.10	105.02	109.90
21	AA	1110	A	C4-C5-C6	-6.10	113.95	117.00
55	BB	29	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	509	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	983	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	505	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	670	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	673	C	O4'-C1'-N1	6.09	113.08	108.20
54	BA	2792	A	C5-C6-N1	6.09	120.75	117.70
21	AA	1132	C	N1-C2-O2	6.09	122.56	118.90
21	AA	896	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	1664	A	C5-C6-N1	6.09	120.75	117.70
54	BA	1247	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	175	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	238	A	N1-C6-N6	-6.09	114.95	118.60
54	BA	391	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	422	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	1822	C	N3-C2-O2	-6.09	117.64	121.90
25	BC	237	ARG	NE-CZ-NH1	6.09	123.34	120.30
26	BD	141	ARG	NE-CZ-NH1	6.09	123.34	120.30
54	BA	282	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	515	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	147	C	C1'-O4'-C4'	-6.08	105.03	109.90
54	BA	1783	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	344	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2161	C	N3-C2-O2	-6.08	117.64	121.90
39	BQ	50	ARG	NE-CZ-NH1	6.08	123.34	120.30
21	AA	498	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	1269	A	C4-C5-C6	-6.08	113.96	117.00
28	BF	91	ARG	NE-CZ-NH1	6.08	123.34	120.30
21	AA	209	U	N3-C2-O2	-6.08	117.95	122.20
21	AA	608	A	C5-C6-N1	6.08	120.74	117.70
21	AA	1320	C	C6-N1-C2	-6.08	117.87	120.30
54	BA	504	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	965	C	N1-C2-O2	6.08	122.55	118.90
54	BA	1561	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	2096	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	2678	C	N3-C2-O2	-6.08	117.65	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2785	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	452	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	547	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	1876	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	2033	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	2300	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2740	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	1367	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	146	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	671	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	905	A	N1-C6-N6	-6.07	114.96	118.60
55	BB	15	A	N1-C6-N6	-6.07	114.96	118.60
38	BP	38	ARG	NE-CZ-NH1	6.07	123.33	120.30
21	AA	539	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	1344	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	1352	C	N1-C2-O2	6.07	122.54	118.90
54	BA	1837	C	N3-C2-O2	-6.07	117.65	121.90
55	BB	4	C	O4'-C1'-N1	6.07	113.05	108.20
21	AA	525	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1610	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	819	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1552	A	O4'-C1'-N9	6.06	113.05	108.20
54	BA	1744	A	O4'-C1'-N9	6.06	113.05	108.20
54	BA	2054	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2890	G	N1-C6-O6	-6.06	116.26	119.90
54	BA	2158	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2268	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	309	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	687	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	968	A	C1'-O4'-C4'	-6.06	105.05	109.90
54	BA	192	C	O4'-C1'-N1	6.06	113.05	108.20
54	BA	866	A	C5-C6-N1	6.06	120.73	117.70
54	BA	1488	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1574	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2143	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	48	C	N1-C2-O2	6.06	122.53	118.90
21	AA	334	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1156	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1376	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1732	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2174	C	N3-C2-O2	-6.06	117.66	121.90
22	A1	62	C	C1'-O4'-C4'	-6.06	105.06	109.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	37	C	N3-C2-O2	-6.06	117.66	121.90
3	AD	103	ARG	NE-CZ-NH1	6.05	123.33	120.30
21	AA	116	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	1097	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	1448	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	689	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1117	C	N3-C2-O2	-6.05	117.66	121.90
15	AP	5	ARG	NE-CZ-NH1	6.05	123.33	120.30
54	BA	47	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	812	C	N3-C2-O2	-6.05	117.66	121.90
55	BB	77	U	O4'-C1'-N1	6.05	113.04	108.20
21	AA	999	C	N3-C2-O2	-6.05	117.67	121.90
46	BX	73	ARG	NE-CZ-NH1	6.05	123.32	120.30
54	BA	97	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1241	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2882	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	473	U	O4'-C1'-N1	6.05	113.04	108.20
54	BA	793	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	2805	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1995	U	O4'-C1'-N1	6.05	113.04	108.20
21	AA	990	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	1162	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	13	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	787	C	N1-C2-O2	6.04	122.53	118.90
54	BA	1557	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	456	A	C5-C6-N1	6.04	120.72	117.70
54	BA	1499	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2742	G	O4'-C1'-N9	6.04	113.03	108.20
21	AA	28	A	C5-C6-N1	6.04	120.72	117.70
21	AA	1427	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1328	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1596	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2273	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2772	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	972	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	668	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1515	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	71	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	532	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	737	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	28	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	961	C	O4'-C1'-N1	6.04	113.03	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	3	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1496	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2051	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2538	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2672	U	O4'-C1'-N1	6.04	113.03	108.20
21	AA	877	G	N1-C6-O6	-6.04	116.28	119.90
54	BA	1499	C	O4'-C1'-N1	6.04	113.03	108.20
21	AA	621	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	294	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	324	A	N1-C6-N6	-6.03	114.98	118.60
54	BA	529	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	967	U	O4'-C1'-N1	6.03	113.03	108.20
54	BA	1700	A	C4-C5-C6	-6.03	113.98	117.00
8	AI	40	ARG	NE-CZ-NH1	6.03	123.32	120.30
23	A2	91	A	N1-C6-N6	-6.03	114.98	118.60
24	A3	39	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	10	A	C5-C6-N1	6.03	120.72	117.70
21	AA	23	C	N3-C2-O2	-6.03	117.68	121.90
22	A1	70	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	152	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	1493	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1419	A	N1-C6-N6	-6.03	114.98	118.60
55	BB	51	G	N1-C6-O6	-6.03	116.28	119.90
21	AA	306	A	N1-C6-N6	-6.03	114.98	118.60
54	BA	942	G	N3-C2-N2	-6.03	115.68	119.90
54	BA	989	G	C3'-C2'-C1'	6.03	106.32	101.50
54	BA	1170	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1652	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	2165	C	N1-C2-O2	6.03	122.52	118.90
54	BA	2288	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	454	A	C5-C6-N1	6.03	120.71	117.70
1	AB	73	ARG	NE-CZ-NH1	6.02	123.31	120.30
21	AA	720	C	N3-C2-O2	-6.02	117.68	121.90
31	BI	133	ARG	NE-CZ-NH1	6.02	123.31	120.30
54	BA	2055	C	N3-C2-O2	-6.02	117.68	121.90
21	AA	1213	A	C4-C5-C6	-6.02	113.99	117.00
24	A3	17	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	916	U	O4'-C1'-N1	6.02	113.02	108.20
24	A3	9	G	N1-C6-O6	-6.02	116.29	119.90
54	BA	550	C	N1-C2-O2	6.02	122.51	118.90
54	BA	1508	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2368	C	N3-C2-O2	-6.02	117.69	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	120	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	595	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1079	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1172	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1269	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2619	C	N3-C2-O2	-6.02	117.69	121.90
41	BS	11	ARG	NE-CZ-NH2	-6.02	117.29	120.30
21	AA	1172	C	N3-C2-O2	-6.01	117.69	121.90
22	A1	18	G	O4'-C1'-N9	6.01	113.01	108.20
45	BW	54	ARG	NE-CZ-NH1	6.01	123.31	120.30
54	BA	244	A	C5-C6-N1	6.01	120.71	117.70
54	BA	650	C	N3-C2-O2	-6.01	117.69	121.90
37	BO	81	ARG	NH1-CZ-NH2	-6.01	112.79	119.40
54	BA	574	A	C6-C5-N7	6.01	136.51	132.30
54	BA	919	U	O4'-C1'-N1	6.01	113.01	108.20
54	BA	2687	U	O4'-C1'-N1	6.01	113.01	108.20
21	AA	792	A	O4'-C1'-N9	6.01	113.01	108.20
54	BA	1912	A	O4'-C1'-N9	6.01	113.01	108.20
21	AA	397	A	C2-N3-C4	6.01	113.61	110.60
21	AA	1285	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	455	C	N1-C2-O2	6.01	122.50	118.90
54	BA	2008	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2225	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2657	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	1278	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2856	A	N1-C6-N6	-6.01	115.00	118.60
21	AA	443	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1113	U	O4'-C1'-N1	6.01	113.00	108.20
54	BA	1495	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2339	C	N3-C2-O2	-6.01	117.70	121.90
21	AA	192	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	322	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	52	A	C5-C6-N1	6.00	120.70	117.70
54	BA	833	A	C5-C6-N1	6.00	120.70	117.70
54	BA	1795	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2606	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	1947	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2565	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1590	A	C5-C6-N1	6.00	120.70	117.70
54	BA	2829	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	1349	A	C5-C6-N1	6.00	120.70	117.70
21	AA	1360	A	C4-C5-C6	-6.00	114.00	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	22	C	C1'-O4'-C4'	-6.00	105.10	109.90
54	BA	2150	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2163	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2551	C	N3-C2-O2	-6.00	117.70	121.90
55	BB	49	C	N3-C2-O2	-6.00	117.70	121.90
55	BB	110	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1238	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1297	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1500	A	C5-C6-N1	5.99	120.70	117.70
54	BA	64	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	2011	U	O4'-C1'-N1	5.99	113.00	108.20
54	BA	1899	A	N1-C6-N6	-5.99	115.00	118.60
54	BA	2428	G	O4'-C1'-N9	5.99	112.99	108.20
54	BA	994	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1540	G	O4'-C1'-N9	5.99	112.99	108.20
54	BA	1614	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	2501	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2710	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	205	G	N3-C4-C5	-5.99	125.61	128.60
54	BA	2227	A	N1-C6-N6	-5.99	115.01	118.60
5	AF	91	ARG	NE-CZ-NH1	5.99	123.29	120.30
40	BR	21	ARG	NE-CZ-NH1	5.99	123.29	120.30
54	BA	758	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1340	U	N3-C2-O2	-5.99	118.01	122.20
54	BA	278	A	N9-C1'-C2'	5.99	121.78	114.00
54	BA	1736	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	2802	G	N1-C6-O6	-5.99	116.31	119.90
54	BA	1323	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	533	A	C4-C5-C6	-5.98	114.01	117.00
24	A3	69	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	844	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1509	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1889	A	C4-C5-C6	-5.98	114.01	117.00
18	AS	78	THR	C-N-CA	5.98	136.65	121.70
21	AA	321	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1893	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	384	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1385	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	36	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	195	A	N1-C6-N6	-5.98	115.01	118.60
54	BA	2202	U	O4'-C1'-N1	5.98	112.98	108.20
54	BA	747	U	N3-C2-O2	-5.97	118.02	122.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2507	C	N3-C2-O2	-5.97	117.72	121.90
16	AQ	26	ARG	NE-CZ-NH2	-5.97	117.31	120.30
54	BA	2283	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2359	C	O4'-C1'-N1	5.97	112.98	108.20
21	AA	190	A	C4-C5-C6	-5.97	114.01	117.00
22	A1	6	A	C5-C6-N1	5.97	120.69	117.70
21	AA	156	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	76	C	N1-C2-O2	5.97	122.48	118.90
54	BA	165	A	C5-C6-N1	5.97	120.68	117.70
54	BA	532	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	1121	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1531	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1927	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2749	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	309	A	N1-C6-N6	-5.97	115.02	118.60
2	AC	87	ARG	NE-CZ-NH1	5.97	123.28	120.30
54	BA	1068	G	N1-C6-O6	-5.97	116.32	119.90
54	BA	1272	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	1767	G	O4'-C1'-N9	5.97	112.97	108.20
21	AA	353	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	518	G	N1-C6-O6	-5.96	116.32	119.90
54	BA	1978	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	199	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	415	A	O4'-C1'-N9	5.96	112.97	108.20
54	BA	2500	U	C1'-O4'-C4'	-5.96	105.13	109.90
54	BA	2675	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	385	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	826	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	899	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	106	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	526	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2179	C	O4'-C1'-N1	5.96	112.97	108.20
27	BE	44	ARG	NE-CZ-NH1	5.96	123.28	120.30
21	AA	396	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	1430	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1461	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1787	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2874	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	933	G	N1-C6-O6	-5.96	116.33	119.90
21	AA	1508	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2516	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2461	A	C4-C5-C6	-5.96	114.02	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2530	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1109	C	N1-C2-O2	5.95	122.47	118.90
54	BA	1816	C	N1-C2-O2	5.95	122.47	118.90
54	BA	2815	C	O4'-C1'-N1	5.95	112.96	108.20
21	AA	1261	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	2037	A	C5-C6-N1	5.95	120.68	117.70
54	BA	2067	G	P-O3'-C3'	5.95	126.84	119.70
54	BA	2626	C	N3-C2-O2	-5.95	117.73	121.90
2	AC	142	ARG	NE-CZ-NH1	5.95	123.28	120.30
21	AA	1192	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	1447	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	428	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1103	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	1456	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	749	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	206	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	1906	G	N1-C6-O6	-5.95	116.33	119.90
21	AA	365	U	O4'-C1'-N1	5.94	112.96	108.20
39	BQ	57	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	2021	C	N1-C2-O2	5.94	122.47	118.90
21	AA	868	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	305	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	574	A	O4'-C1'-N9	5.94	112.95	108.20
21	AA	738	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	160	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1874	C	N1-C2-O2	5.94	122.46	118.90
55	BB	118	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	1357	A	C4-C5-C6	-5.94	114.03	117.00
25	BC	13	ARG	NE-CZ-NH1	5.94	123.27	120.30
46	BX	49	ARG	NE-CZ-NH1	5.94	123.27	120.30
35	BM	50	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	641	U	O4'-C1'-N1	5.94	112.95	108.20
54	BA	1808	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2273	A	N1-C6-N6	-5.94	115.04	118.60
54	BA	2761	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	164	G	N3-C4-C5	-5.94	125.63	128.60
21	AA	600	A	C4-C5-C6	-5.93	114.03	117.00
27	BE	21	ARG	NE-CZ-NH1	5.93	123.27	120.30
54	BA	154	U	O4'-C1'-N1	5.93	112.95	108.20
54	BA	710	U	O4'-C1'-N1	5.93	112.95	108.20
54	BA	1119	U	O4'-C1'-N1	5.93	112.95	108.20
54	BA	1669	A	C4-C5-C6	-5.93	114.03	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	623	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1037	C	N3-C2-O2	-5.93	117.75	121.90
24	A3	37	U	O4'-C1'-N1	5.93	112.95	108.20
54	BA	147	C	O4'-C1'-N1	5.93	112.95	108.20
54	BA	1169	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1801	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2005	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1252	G	N1-C6-O6	-5.93	116.34	119.90
54	BA	2578	G	N1-C6-O6	-5.93	116.34	119.90
21	AA	1324	A	C4-C5-C6	-5.93	114.03	117.00
33	BK	18	ARG	NE-CZ-NH1	5.93	123.27	120.30
54	BA	840	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	1073	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1966	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	762	U	C1'-O4'-C4'	-5.93	105.16	109.90
54	BA	825	A	C4-C5-C6	-5.93	114.04	117.00
54	BA	2047	C	N3-C2-O2	-5.93	117.75	121.90
2	AC	130	ARG	NE-CZ-NH1	5.93	123.26	120.30
21	AA	535	A	C4-C5-C6	-5.93	114.04	117.00
21	AA	918	A	C4-C5-C6	-5.93	114.04	117.00
22	A1	21	A	C4-C5-C6	-5.93	114.04	117.00
54	BA	1172	C	O4'-C1'-N1	5.93	112.94	108.20
54	BA	2271	G	N1-C6-O6	-5.93	116.34	119.90
21	AA	176	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	20	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	460	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1202	G	N3-C2-N2	-5.92	115.75	119.90
54	BA	1427	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1507	C	N3-C2-O2	-5.92	117.75	121.90
55	BB	57	A	N1-C6-N6	-5.92	115.05	118.60
54	BA	130	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	176	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2746	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2758	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	483	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	466	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1764	C	N3-C2-O2	-5.92	117.76	121.90
35	BM	51	ARG	NE-CZ-NH1	5.92	123.26	120.30
54	BA	225	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	2183	A	N1-C6-N6	-5.92	115.05	118.60
54	BA	2558	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	1120	C	N3-C2-O2	-5.92	117.76	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1833	C	O4'-C1'-N1	5.92	112.93	108.20
54	BA	2721	A	C5-C6-N1	5.92	120.66	117.70
21	AA	183	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	181	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	210	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	1679	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2020	A	O4'-C1'-N9	5.92	112.93	108.20
21	AA	162	A	C4-C5-C6	-5.91	114.04	117.00
21	AA	205	A	C4-C5-C6	-5.91	114.04	117.00
21	AA	779	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	900	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	1064	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1426	G	O4'-C1'-N9	5.91	112.93	108.20
54	BA	1446	C	N1-C2-O2	5.91	122.45	118.90
54	BA	2884	U	O4'-C1'-N1	5.91	112.93	108.20
21	AA	234	C	P-O3'-C3'	5.91	126.80	119.70
21	AA	357	G	C3'-C2'-C1'	5.91	106.23	101.50
21	AA	599	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	1111	A	C4-C5-C6	-5.91	114.05	117.00
22	A1	72	C	C5'-C4'-C3'	-5.91	106.54	116.00
42	BT	3	ARG	NE-CZ-NH2	5.91	123.26	120.30
54	BA	479	A	C5-C6-N1	5.91	120.66	117.70
54	BA	1226	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	2103	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2738	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	1016	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	56	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	587	C	C1'-O4'-C4'	-5.91	105.17	109.90
54	BA	965	C	C6-N1-C2	-5.91	117.94	120.30
54	BA	2497	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	1208	C	N3-C2-O2	-5.91	117.77	121.90
21	AA	1134	G	N3-C2-N2	-5.91	115.77	119.90
54	BA	973	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1029	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1617	C	N1-C2-O2	5.91	122.44	118.90
8	AI	48	ARG	NE-CZ-NH2	-5.90	117.35	120.30
54	BA	1118	C	N1-C2-O2	5.90	122.44	118.90
54	BA	991	C	N3-C2-O2	-5.90	117.77	121.90
55	BB	34	A	C5-C6-N1	5.90	120.65	117.70
8	AI	105	ARG	NE-CZ-NH1	5.90	123.25	120.30
21	AA	566	G	N1-C6-O6	-5.90	116.36	119.90
54	BA	342	A	C6-C5-N7	5.90	136.43	132.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1070	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1114	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	504	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	607	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	864	A	C5-C6-N1	5.90	120.65	117.70
21	AA	906	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	982	U	P-O3'-C3'	5.90	126.78	119.70
21	AA	1363	A	O4'-C1'-N9	5.90	112.92	108.20
21	AA	1374	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	507	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1489	C	O4'-C1'-N1	5.90	112.92	108.20
55	BB	63	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	477	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1127	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	949	A	N1-C6-N6	-5.89	115.06	118.60
54	BA	2037	A	C4-C5-C6	-5.89	114.05	117.00
17	AR	42	ARG	NE-CZ-NH1	5.89	123.25	120.30
21	AA	576	C	N1-C2-O2	5.89	122.44	118.90
54	BA	627	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	1221	C	O4'-C1'-N1	5.89	112.91	108.20
54	BA	1938	A	C4-C5-C6	-5.89	114.05	117.00
55	BB	96	G	N1-C6-O6	-5.89	116.36	119.90
21	AA	1245	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	198	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	685	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	465	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	503	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1917	U	O4'-C1'-N1	5.89	112.91	108.20
54	BA	2476	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	1227	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	22	C	O4'-C1'-N1	5.89	112.91	108.20
54	BA	335	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	886	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	2232	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2835	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	912	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	231	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	922	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1479	G	O4'-C1'-N9	5.88	112.91	108.20
54	BA	1969	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2883	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	1248	A	C4-C5-C6	-5.88	114.06	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	565	C	N3-C2-O2	-5.88	117.78	121.90
12	AM	112	ARG	NE-CZ-NH1	5.88	123.24	120.30
21	AA	873	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2051	A	C3'-C2'-C1'	5.88	106.20	101.50
54	BA	2328	A	C5-C6-N1	5.88	120.64	117.70
55	BB	36	C	N1-C2-O2	5.88	122.43	118.90
55	BB	82	U	P-O3'-C3'	5.88	126.76	119.70
21	AA	729	A	O4'-C1'-N9	5.88	112.90	108.20
21	AA	901	A	C5-C6-N1	5.88	120.64	117.70
21	AA	909	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	931	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1069	C	N1-C2-O2	5.88	122.43	118.90
54	BA	336	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	1305	C	O4'-C1'-N1	5.88	112.90	108.20
54	BA	1477	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1690	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2506	U	O4'-C1'-N1	5.88	112.90	108.20
54	BA	2870	C	N3-C2-O2	-5.88	117.79	121.90
21	AA	649	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	116	C	N3-C2-O2	-5.88	117.79	121.90
21	AA	169	C	C1'-O4'-C4'	-5.88	105.20	109.90
21	AA	340	U	O4'-C1'-N1	5.88	112.90	108.20
54	BA	2871	U	O4'-C1'-N1	5.88	112.90	108.20
5	AF	44	ARG	NE-CZ-NH1	5.87	123.24	120.30
15	AP	25	ARG	NE-CZ-NH1	5.87	123.24	120.30
54	BA	57	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	587	C	C3'-C2'-C1'	-5.87	96.80	101.50
54	BA	1762	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2094	A	C5-C6-N1	5.87	120.64	117.70
54	BA	2099	U	N3-C2-O2	-5.87	118.09	122.20
54	BA	2872	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	467	U	N3-C2-O2	-5.87	118.09	122.20
21	AA	640	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	1234	U	O4'-C1'-N1	5.87	112.90	108.20
54	BA	2369	A	C6-C5-N7	5.87	136.41	132.30
14	AO	16	ARG	NE-CZ-NH1	5.87	123.23	120.30
21	AA	897	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1160	G	O4'-C1'-N9	5.87	112.89	108.20
54	BA	217	A	N1-C6-N6	-5.87	115.08	118.60
54	BA	1315	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2745	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1079	C	O4'-C1'-N1	5.87	112.89	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	451	A	C4-C5-C6	-5.87	114.07	117.00
21	AA	743	A	C4-C5-C6	-5.87	114.07	117.00
24	A3	40	C	N1-C2-O2	5.87	122.42	118.90
24	A3	42	C	N1-C2-O2	5.87	122.42	118.90
54	BA	2036	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2014	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	2860	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1096	A	C6-C5-N7	5.86	136.40	132.30
54	BA	2045	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	13	A	C5-C6-N1	5.86	120.63	117.70
54	BA	96	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	974	G	O4'-C1'-N9	5.86	112.89	108.20
54	BA	1727	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2845	U	O4'-C1'-N1	5.86	112.89	108.20
21	AA	99	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	1129	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1505	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1957	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	40	C	N3-C2-O2	-5.85	117.80	121.90
21	AA	1130	A	C5-C6-N1	5.85	120.63	117.70
21	AA	1462	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	115	C	N3-C2-O2	-5.85	117.80	121.90
23	A2	79	A	O4'-C1'-N9	5.85	112.88	108.20
46	BX	26	ARG	NE-CZ-NH1	5.85	123.23	120.30
54	BA	87	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	1133	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	1323	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2726	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	493	A	C3'-C2'-C1'	5.85	106.18	101.50
54	BA	1934	C	N3-C2-O2	-5.85	117.80	121.90
55	BB	58	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	715	A	C4-C5-C6	-5.85	114.08	117.00
24	A3	16	C	N1-C2-O2	5.85	122.41	118.90
25	BC	188	ARG	NE-CZ-NH1	5.85	123.22	120.30
54	BA	353	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	893	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	1891	G	N3-C2-N2	-5.85	115.81	119.90
54	BA	2245	U	O4'-C1'-N1	5.85	112.88	108.20
21	AA	488	C	N3-C2-O2	-5.85	117.81	121.90
21	AA	787	A	C5-C6-N1	5.85	120.62	117.70
21	AA	1345	U	N3-C2-O2	-5.85	118.11	122.20
54	BA	417	C	N3-C2-O2	-5.85	117.81	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	472	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1001	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1209	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	1289	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	1810	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	2084	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	366	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	716	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1431	A	O4'-C1'-N9	5.85	112.88	108.20
55	BB	92	C	N3-C2-O2	-5.85	117.81	121.90
21	AA	1035	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	1051	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	1285	A	C5-C6-N1	5.84	120.62	117.70
54	BA	1243	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2322	A	C4-C5-C6	-5.84	114.08	117.00
55	BB	50	A	C5-C6-N1	5.84	120.62	117.70
21	AA	351	G	O4'-C1'-N9	5.84	112.87	108.20
21	AA	927	G	O4'-C1'-N9	5.84	112.87	108.20
54	BA	718	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1439	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1965	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	2424	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2741	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	608	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1550	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2478	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	2820	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1653	G	N1-C6-O6	-5.84	116.40	119.90
54	BA	2251	G	N3-C2-N2	-5.84	115.81	119.90
54	BA	2287	A	C2-N3-C4	5.84	113.52	110.60
21	AA	1289	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	957	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2335	A	C5-C6-N1	5.84	120.62	117.70
54	BA	430	A	C6-C5-N7	5.83	136.38	132.30
54	BA	1410	G	O4'-C1'-N9	5.83	112.87	108.20
54	BA	1881	C	N3-C2-O2	-5.83	117.81	121.90
54	BA	2517	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	164	G	O4'-C1'-N9	5.83	112.87	108.20
21	AA	429	U	P-O3'-C3'	5.83	126.70	119.70
44	BV	18	ARG	NE-CZ-NH1	5.83	123.22	120.30
54	BA	111	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	2108	A	C4-C5-C6	-5.83	114.08	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2319	G	O4'-C1'-N9	5.83	112.87	108.20
54	BA	2788	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	210	C	N1-C2-O2	5.83	122.40	118.90
54	BA	393	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1395	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	1637	A	C5-C6-N1	5.83	120.62	117.70
21	AA	1359	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	1443	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	493	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	1252	A	C4-C5-C6	-5.83	114.09	117.00
22	A1	27	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	928	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	1006	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1052	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1221	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2039	U	O4'-C1'-N1	5.83	112.86	108.20
21	AA	790	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	310	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	2108	A	C5-C6-N1	5.83	120.61	117.70
54	BA	2572	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	643	A	C3'-C2'-C1'	5.83	106.16	101.50
54	BA	992	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	366	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	452	A	C5-C6-N1	5.82	120.61	117.70
21	AA	1388	C	N3-C2-O2	-5.82	117.82	121.90
54	BA	2540	C	N3-C2-O2	-5.82	117.82	121.90
21	AA	87	C	C1'-O4'-C4'	-5.82	105.24	109.90
54	BA	600	G	N1-C6-O6	-5.82	116.41	119.90
54	BA	1261	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2206	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2328	A	C4-C5-C6	-5.82	114.09	117.00
55	BB	30	C	N3-C2-O2	-5.82	117.83	121.90
55	BB	89	U	N3-C2-O2	-5.82	118.13	122.20
21	AA	357	G	O4'-C1'-N9	5.82	112.85	108.20
22	A1	65	C	N3-C2-O2	-5.82	117.83	121.90
24	A3	7	G	O4'-C1'-N9	5.82	112.85	108.20
27	BE	69	ARG	NE-CZ-NH1	5.82	123.21	120.30
54	BA	516	C	O4'-C1'-N1	5.82	112.86	108.20
54	BA	810	U	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2117	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2602	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	1306	A	C4-C5-C6	-5.82	114.09	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2074	U	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2150	C	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2752	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	52	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	1139	G	N3-C2-N2	-5.81	115.83	119.90
22	A1	23	A	C4-C5-C6	-5.81	114.09	117.00
34	BL	48	ARG	NE-CZ-NH1	5.81	123.21	120.30
11	AL	82	ARG	NE-CZ-NH2	-5.81	117.39	120.30
54	BA	2397	G	N1-C6-O6	-5.81	116.41	119.90
21	AA	1288	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	1476	A	C4-C5-C6	-5.81	114.09	117.00
24	A3	72	C	C3'-C2'-C1'	-5.81	96.85	101.50
28	BF	177	ARG	NE-CZ-NH2	5.81	123.20	120.30
54	BA	1925	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2579	C	N1-C2-O2	5.81	122.39	118.90
54	BA	666	A	C6-C5-N7	5.81	136.37	132.30
54	BA	980	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	2044	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	723	U	O4'-C1'-N1	5.81	112.85	108.20
22	A1	69	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	510	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	772	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1994	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2050	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	7	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	44	A	C5-C6-N1	5.81	120.60	117.70
21	AA	995	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1132	U	P-O3'-C3'	5.80	126.67	119.70
54	BA	2335	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2655	G	N1-C6-O6	-5.80	116.42	119.90
54	BA	2681	C	N3-C2-O2	-5.80	117.84	121.90
13	AN	41	ARG	NE-CZ-NH1	5.80	123.20	120.30
21	AA	474	G	N1-C6-O6	-5.80	116.42	119.90
21	AA	768	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1475	G	N3-C2-N2	-5.80	115.84	119.90
54	BA	2653	U	O4'-C1'-N1	5.80	112.84	108.20
22	A1	60	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	1218	C	N1-C2-O2	5.80	122.38	118.90
54	BA	5	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	177	G	N1-C6-O6	-5.80	116.42	119.90
54	BA	806	C	C1'-O4'-C4'	-5.80	105.26	109.90
54	BA	811	U	O4'-C1'-N1	5.80	112.84	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	890	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2473	U	N3-C2-O2	-5.80	118.14	122.20
21	AA	675	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	63	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	1129	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	1905	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	98	A	C5-C6-N1	5.79	120.60	117.70
21	AA	622	A	C4-C5-C6	-5.79	114.10	117.00
52	B3	39	ARG	NE-CZ-NH1	5.79	123.20	120.30
54	BA	82	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2496	C	N1-C2-O2	5.79	122.38	118.90
21	AA	397	A	C4-C5-C6	-5.79	114.10	117.00
21	AA	1183	U	O4'-C1'-N1	5.79	112.83	108.20
21	AA	1480	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	316	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	418	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	741	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2172	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2336	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	228	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2135	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	404	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	672	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1941	C	N1-C2-O2	5.79	122.37	118.90
55	BB	90	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	192	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	679	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	2260	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	2366	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	1069	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2512	C	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2658	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	1203	C	N1-C2-O2	5.78	122.37	118.90
21	AA	441	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	689	C	N3-C2-O2	-5.78	117.85	121.90
22	A1	72	C	N1-C2-O2	5.78	122.37	118.90
54	BA	19	A	N1-C6-N6	-5.78	115.13	118.60
54	BA	590	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	853	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2425	A	P-O3'-C3'	5.78	126.64	119.70
21	AA	195	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1590	A	C4-C5-C6	-5.78	114.11	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	4	C	N3-C2-O2	-5.78	117.86	121.90
21	AA	51	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1451	C	P-O3'-C3'	5.78	126.63	119.70
54	BA	1829	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	945	G	N3-C4-C5	-5.78	125.71	128.60
21	AA	1044	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1201	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	673	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	694	U	N3-C2-O2	-5.78	118.16	122.20
54	BA	2809	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1210	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	660	C	N1-C2-O2	5.77	122.36	118.90
54	BA	1134	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	661	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	2096	C	O4'-C1'-N1	5.77	112.82	108.20
54	BA	2743	U	O4'-C1'-N1	5.77	112.82	108.20
21	AA	250	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	1290	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1586	A	O4'-C1'-N9	5.77	112.82	108.20
21	AA	478	A	C4-C5-C6	-5.77	114.11	117.00
21	AA	514	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	108	G	N3-C4-C5	-5.77	125.72	128.60
54	BA	722	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	1075	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1908	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	2364	C	N3-C2-O2	-5.77	117.86	121.90
55	BB	113	C	N1-C2-O2	5.77	122.36	118.90
21	AA	808	C	N1-C2-O2	5.77	122.36	118.90
21	AA	1325	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1255	U	C3'-C2'-C1'	5.77	106.11	101.50
54	BA	1658	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1909	C	N3-C2-O2	-5.77	117.86	121.90
5	AF	45	ARG	NE-CZ-NH2	-5.76	117.42	120.30
54	BA	1251	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	1664	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	444	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	731	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	1040	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2378	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	31	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	907	G	N1-C6-O6	-5.76	116.44	119.90
21	AA	109	A	O4'-C1'-N9	5.76	112.81	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2115	G	N3-C4-C5	-5.76	125.72	128.60
54	BA	2407	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	1214	C	N3-C4-N4	-5.76	113.97	118.00
21	AA	1228	C	O4'-C1'-N1	5.76	112.81	108.20
54	BA	1646	C	N1-C2-O2	5.76	122.36	118.90
21	AA	137	U	O4'-C1'-N1	5.76	112.81	108.20
54	BA	1254	A	C3'-C2'-C1'	5.76	106.11	101.50
54	BA	1830	C	N1-C2-O2	5.76	122.35	118.90
54	BA	2001	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2594	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2781	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	14	A	C3'-C2'-C1'	5.75	106.10	101.50
22	A1	17	U	N3-C2-O2	-5.75	118.17	122.20
54	BA	492	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	1518	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	1629	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	1640	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	1196	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	1509	C	N3-C2-O2	-5.75	117.87	121.90
24	A3	66	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	446	G	O4'-C4'-C3'	5.75	110.70	106.10
54	BA	670	A	P-O3'-C3'	5.75	126.60	119.70
21	AA	1297	G	O4'-C1'-N9	5.75	112.80	108.20
21	AA	1438	G	N3-C2-N2	-5.75	115.88	119.90
54	BA	125	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2338	C	N3-C2-O2	-5.75	117.88	121.90
7	AH	83	ARG	NE-CZ-NH1	5.75	123.17	120.30
21	AA	25	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	235	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	1021	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	887	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	1714	U	N3-C2-O2	-5.75	118.18	122.20
54	BA	2755	C	N3-C2-O2	-5.75	117.88	121.90
13	AN	61	ARG	NE-CZ-NH1	5.75	123.17	120.30
21	AA	975	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	2301	C	N3-C2-O2	-5.75	117.88	121.90
36	BN	4	ARG	NE-CZ-NH1	5.75	123.17	120.30
54	BA	599	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	889	C	N1-C2-O2	5.75	122.35	118.90
21	AA	177	G	N3-C4-C5	-5.74	125.73	128.60
54	BA	1287	A	O4'-C1'-N9	5.74	112.80	108.20
54	BA	1378	A	C5'-C4'-O4'	5.74	115.99	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2177	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	2358	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	487	A	C4-C5-C6	-5.74	114.13	117.00
22	A1	44	G	N1-C6-O6	-5.74	116.46	119.90
54	BA	941	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2486	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	132	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	825	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	1042	A	C4-C5-C6	-5.74	114.13	117.00
55	BB	39	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	1300	G	C8-N9-C4	-5.74	104.11	106.40
54	BA	268	C	O4'-C1'-N1	5.74	112.79	108.20
54	BA	925	A	C5-C6-N1	5.74	120.57	117.70
54	BA	1604	C	N3-C2-O2	-5.74	117.89	121.90
21	AA	460	A	C4-C5-C6	-5.73	114.13	117.00
21	AA	614	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1398	C	N1-C2-O2	5.73	122.34	118.90
21	AA	338	A	C4-C5-C6	-5.73	114.13	117.00
21	AA	586	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	929	G	N1-C6-O6	-5.73	116.46	119.90
21	AA	1027	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	275	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	487	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1528	A	N1-C6-N6	-5.73	115.16	118.60
54	BA	2451	A	C4-C5-C6	-5.73	114.13	117.00
54	BA	446	G	C3'-C2'-C1'	5.73	106.08	101.50
54	BA	838	C	N1-C2-O2	5.73	122.34	118.90
54	BA	1123	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	35	G	N3-C4-C5	-5.73	125.74	128.60
21	AA	234	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	1258	G	N3-C2-N2	-5.73	115.89	119.90
54	BA	1503	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	601	C	N1-C2-O2	5.72	122.33	118.90
36	BN	45	ARG	NE-CZ-NH1	5.72	123.16	120.30
54	BA	1032	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1351	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	1441	G	N1-C6-O6	-5.72	116.47	119.90
54	BA	2309	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2799	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	559	A	O4'-C1'-N9	5.72	112.78	108.20
21	AA	1362	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1487	U	O4'-C1'-N1	5.72	112.78	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	459	A	C4-C5-C6	-5.72	114.14	117.00
24	A3	59	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	544	C	O4'-C1'-N1	5.72	112.78	108.20
54	BA	1616	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2030	A	C6-C5-N7	5.72	136.30	132.30
21	AA	1187	G	N1-C6-O6	-5.72	116.47	119.90
54	BA	249	C	N1-C2-O2	5.72	122.33	118.90
54	BA	820	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	1461	G	N1-C6-O6	-5.71	116.47	119.90
43	BU	21	ARG	NE-CZ-NH1	5.71	123.16	120.30
54	BA	95	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	560	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	634	C	O4'-C1'-N1	5.71	112.77	108.20
54	BA	847	U	N3-C2-O2	-5.71	118.20	122.20
54	BA	943	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1000	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1142	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1525	A	C5-C6-N1	5.71	120.56	117.70
54	BA	2238	G	C3'-C2'-C1'	5.71	106.07	101.50
55	BB	68	C	O4'-C1'-N1	5.71	112.77	108.20
21	AA	575	G	P-O3'-C3'	5.71	126.56	119.70
54	BA	643	A	C1'-O4'-C4'	-5.71	105.33	109.90
54	BA	1854	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2518	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2542	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2561	U	O4'-C1'-N1	5.71	112.77	108.20
21	AA	131	A	C4-C5-C6	-5.71	114.15	117.00
21	AA	919	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	445	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	1607	C	O4'-C1'-N1	5.71	112.77	108.20
54	BA	1619	G	N1-C6-O6	-5.71	116.48	119.90
54	BA	1809	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	2439	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	362	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1196	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	2123	G	O4'-C1'-N9	5.70	112.76	108.20
54	BA	1786	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1788	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	1947	C	O4'-C1'-N1	5.70	112.76	108.20
21	AA	6	G	N1-C6-O6	-5.70	116.48	119.90
21	AA	281	G	N1-C6-O6	-5.70	116.48	119.90
54	BA	354	A	C4-C5-C6	-5.70	114.15	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	719	C	N1-C2-O2	5.70	122.32	118.90
54	BA	2267	A	O4'-C1'-N9	5.70	112.76	108.20
54	BA	2326	C	C1'-O4'-C4'	-5.70	105.34	109.90
55	BB	53	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	402	A	C5-C6-N1	5.70	120.55	117.70
54	BA	675	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	945	A	O4'-C1'-N9	5.70	112.76	108.20
54	BA	1525	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1558	C	N1-C2-O2	5.70	122.32	118.90
54	BA	2311	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	492	C	N3-C2-O2	-5.69	117.91	121.90
21	AA	1237	C	N1-C2-O2	5.69	122.31	118.90
54	BA	1735	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2880	C	N1-C2-O2	5.69	122.31	118.90
55	BB	71	C	O4'-C1'-N1	5.69	112.75	108.20
21	AA	44	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	162	U	O4'-C1'-N1	5.69	112.75	108.20
55	BB	17	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	341	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1858	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	2511	U	O4'-C1'-N1	5.69	112.75	108.20
5	AF	86	ARG	NE-CZ-NH1	5.69	123.14	120.30
21	AA	1263	C	N1-C2-O2	5.69	122.31	118.90
24	A3	62	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	109	C	N3-C2-O2	-5.69	117.92	121.90
55	BB	101	A	C4-C5-C6	-5.69	114.16	117.00
25	BC	202	ARG	NE-CZ-NH1	5.69	123.14	120.30
54	BA	2268	A	O4'-C1'-N9	5.69	112.75	108.20
21	AA	1407	C	N3-C2-O2	-5.68	117.92	121.90
21	AA	1413	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	173	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	694	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1204	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1612	C	N3-C2-O2	-5.68	117.92	121.90
2	AC	64	ARG	NE-CZ-NH1	5.68	123.14	120.30
21	AA	1533	C	N3-C2-O2	-5.68	117.92	121.90
25	BC	270	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	386	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	1362	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	1785	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	960	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1363	C	O4'-C1'-N1	5.68	112.74	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1002	G	N1-C6-O6	-5.68	116.49	119.90
21	AA	1107	C	N1-C2-O2	5.68	122.31	118.90
25	BC	216	ARG	NE-CZ-NH1	-5.68	117.46	120.30
54	BA	423	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1372	U	O4'-C1'-N1	5.68	112.74	108.20
54	BA	2639	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	872	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	1098	C	N3-C2-O2	-5.68	117.93	121.90
22	A1	57	G	C3'-C2'-C1'	5.68	106.04	101.50
47	BY	23	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	1853	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	2097	A	C6-C5-N7	5.68	136.27	132.30
54	BA	2254	C	N1-C2-O2	5.68	122.31	118.90
54	BA	2308	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	2611	C	N1-C2-O2	5.68	122.31	118.90
21	AA	215	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	1032	G	N3-C4-C5	-5.67	125.76	128.60
54	BA	2105	U	O4'-C1'-N1	5.67	112.74	108.20
21	AA	519	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2159	G	C5'-C4'-O4'	5.67	115.91	109.10
21	AA	522	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	1191	A	C4-C5-C6	-5.67	114.17	117.00
21	AA	1254	A	C4-C5-C6	-5.67	114.17	117.00
25	BC	100	ARG	NE-CZ-NH1	5.67	123.14	120.30
54	BA	2440	C	N1-C2-O2	5.67	122.30	118.90
21	AA	1096	C	N3-C2-O2	-5.67	117.93	121.90
35	BM	59	ARG	NE-CZ-NH1	5.67	123.14	120.30
21	AA	300	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	453	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	1266	G	N3-C4-C5	-5.67	125.77	128.60
54	BA	2022	U	O4'-C1'-N1	5.67	112.73	108.20
55	BB	118	C	O4'-C1'-N1	5.67	112.73	108.20
54	BA	457	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	996	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	2191	A	C4-C5-C6	-5.67	114.17	117.00
21	AA	795	C	N3-C2-O2	-5.67	117.94	121.90
22	A1	28	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1752	C	N1-C2-O2	5.67	122.30	118.90
54	BA	2765	A	O4'-C1'-N9	5.67	112.73	108.20
55	BB	26	C	N1-C2-O2	5.67	122.30	118.90
21	AA	739	C	N1-C2-O2	5.66	122.30	118.90
21	AA	1502	A	C4-C5-C6	-5.66	114.17	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	196	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	315	G	O4'-C1'-N9	5.66	112.73	108.20
54	BA	626	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2270	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	1437	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	1521	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	827	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1318	U	O4'-C1'-N1	5.66	112.73	108.20
36	BN	46	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	1153	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1928	A	N1-C6-N6	-5.66	115.20	118.60
54	BA	315	G	N1-C6-O6	-5.66	116.50	119.90
54	BA	933	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	66	A	C5-C6-N1	5.66	120.53	117.70
21	AA	470	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	195	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	689	C	O4'-C1'-N1	5.66	112.72	108.20
21	AA	770	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	2732	G	C8-N9-C4	-5.66	104.14	106.40
21	AA	196	A	C4-C5-C6	-5.65	114.17	117.00
21	AA	993	G	N3-C4-C5	-5.65	125.77	128.60
21	AA	1340	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1771	C	O4'-C1'-N1	5.65	112.72	108.20
24	A3	76	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	740	C	N1-C2-O2	5.65	122.29	118.90
21	AA	67	C	N1-C2-O2	5.65	122.29	118.90
21	AA	392	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	708	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	190	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	764	A	C4-C5-C6	-5.65	114.17	117.00
21	AA	1195	C	N1-C2-O2	5.65	122.29	118.90
54	BA	129	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	274	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	592	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	165	A	C6-C5-N7	5.65	136.25	132.30
54	BA	323	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1366	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	1649	G	O4'-C1'-N9	5.65	112.72	108.20
18	AS	77	ARG	NE-CZ-NH1	5.65	123.12	120.30
21	AA	193	C	N3-C2-O2	-5.65	117.95	121.90
21	AA	160	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	718	A	C4-C5-C6	-5.64	114.18	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1150	A	C4-C5-C6	-5.64	114.18	117.00
24	A3	70	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	233	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	374	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1291	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	205	G	O4'-C1'-N9	5.64	112.71	108.20
54	BA	509	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1254	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1275	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1961	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2296	U	O4'-C1'-N1	5.64	112.72	108.20
54	BA	2587	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2606	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2670	A	C4-C5-C6	-5.64	114.18	117.00
55	BB	11	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2794	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	1275	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	1467	C	N1-C2-O2	5.64	122.28	118.90
54	BA	269	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	345	A	N1-C6-N6	-5.64	115.22	118.60
54	BA	1135	C	N1-C2-O2	5.64	122.28	118.90
54	BA	2546	U	O3'-P-O5'	-5.64	93.28	104.00
54	BA	507	A	O4'-C1'-N9	5.64	112.71	108.20
54	BA	829	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1174	U	O4'-C1'-N1	5.64	112.71	108.20
54	BA	2598	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	355	C	N1-C2-O2	5.64	122.28	118.90
22	A1	51	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	650	C	C2-N3-C4	-5.64	117.08	119.90
54	BA	2073	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2250	G	N1-C6-O6	-5.64	116.52	119.90
21	AA	1377	A	C4-C5-C6	-5.63	114.18	117.00
22	A1	71	C	N1-C2-O2	5.63	122.28	118.90
24	A3	26	C	N1-C2-O2	5.63	122.28	118.90
54	BA	149	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	267	C	O4'-C1'-N1	5.63	112.71	108.20
54	BA	765	C	N1-C2-O2	5.63	122.28	118.90
54	BA	2241	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	2258	C	N1-C2-O2	5.63	122.28	118.90
54	BA	2790	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	2837	A	C4-C5-C6	-5.63	114.18	117.00
21	AA	665	A	C6-C5-N7	5.63	136.24	132.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	746	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	573	U	N3-C2-O2	-5.63	118.26	122.20
54	BA	2147	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	211	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	433	C	N1-C2-O2	5.63	122.28	118.90
21	AA	203	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	11	C	N1-C2-O2	5.63	122.28	118.90
54	BA	1931	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	2617	U	O4'-C1'-N1	5.63	112.70	108.20
21	AA	805	C	N1-C2-O2	5.63	122.28	118.90
54	BA	388	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	912	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	989	G	O4'-C4'-C3'	5.63	110.60	106.10
21	AA	1402	C	N3-C2-O2	-5.62	117.96	121.90
25	BC	257	ARG	NE-CZ-NH1	5.62	123.11	120.30
54	BA	143	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	564	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	2229	U	C5'-C4'-C3'	-5.62	107.00	116.00
54	BA	2656	U	O4'-C1'-N1	5.62	112.70	108.20
21	AA	744	C	N3-C2-O2	-5.62	117.96	121.90
21	AA	1161	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	761	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	987	C	N3-C2-O2	-5.62	117.96	121.90
18	AS	54	ARG	NE-CZ-NH1	5.62	123.11	120.30
54	BA	821	A	C6-C5-N7	5.62	136.24	132.30
55	BB	59	A	N1-C6-N6	-5.62	115.23	118.60
21	AA	205	A	N1-C6-N6	-5.62	115.23	118.60
21	AA	372	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	386	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	620	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1080	A	C6-C5-N7	5.62	136.23	132.30
54	BA	1474	U	O4'-C1'-N1	5.62	112.70	108.20
21	AA	169	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	858	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	240	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1975	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	2333	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1387	G	O4'-C1'-N9	5.62	112.69	108.20
54	BA	226	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	784	G	N3-C4-C5	-5.62	125.79	128.60
21	AA	227	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	673	A	C4-C5-C6	-5.62	114.19	117.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2899	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	74	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	135	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1046	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	2651	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	816	A	C4-C5-C6	-5.61	114.19	117.00
21	AA	1281	C	C1'-O4'-C4'	-5.61	105.41	109.90
54	BA	2412	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	127	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	159	G	N7-C8-N9	5.61	115.91	113.10
54	BA	608	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	2207	C	N1-C2-O2	5.61	122.27	118.90
54	BA	91	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	1730	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1998	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	2307	G	N1-C6-O6	-5.61	116.54	119.90
21	AA	395	C	N3-C2-O2	-5.61	117.98	121.90
21	AA	482	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	1004	A	C6-C5-N7	5.61	136.22	132.30
54	BA	89	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	1229	C	N3-C2-O2	-5.61	117.98	121.90
54	BA	2526	G	N1-C6-O6	-5.61	116.54	119.90
55	BB	3	C	O4'-C1'-N1	5.61	112.69	108.20
21	AA	1209	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	597	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	749	A	C6-C5-N7	5.60	136.22	132.30
54	BA	53	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	268	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1276	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	240	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	538	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1769	U	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2615	U	O4'-C1'-N1	5.60	112.68	108.20
55	BB	40	U	O4'-C1'-N1	5.60	112.68	108.20
21	AA	512	U	O4'-C1'-N1	5.60	112.68	108.20
54	BA	655	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	2056	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	474	G	P-O3'-C3'	5.60	126.42	119.70
54	BA	1796	U	O4'-C1'-N1	5.60	112.68	108.20
21	AA	297	G	N1-C6-O6	-5.59	116.54	119.90
21	AA	563	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	1141	C	N1-C2-O2	5.59	122.26	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	BQ	50	ARG	NE-CZ-NH2	-5.59	117.50	120.30
54	BA	288	U	O4'-C1'-N1	5.59	112.68	108.20
54	BA	1887	C	N3-C2-O2	-5.59	117.98	121.90
21	AA	634	C	N1-C2-O2	5.59	122.26	118.90
21	AA	664	G	C3'-C2'-C1'	5.59	105.97	101.50
54	BA	357	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	1428	C	N1-C2-O2	5.59	122.25	118.90
54	BA	1454	C	N1-C2-O2	5.59	122.25	118.90
21	AA	783	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1183	U	N3-C2-O2	-5.59	118.29	122.20
25	BC	79	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	AB	10	LYS	CA-C-N	5.59	129.49	117.20
54	BA	872	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	2296	U	C3'-C2'-C1'	5.59	105.97	101.50
54	BA	2480	C	O4'-C1'-N1	5.59	112.67	108.20
54	BA	2666	C	N1-C2-O2	5.59	122.25	118.90
21	AA	440	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	1147	A	C4-C5-C6	-5.58	114.21	117.00
55	BB	56	G	C3'-C2'-C1'	5.58	105.97	101.50
54	BA	698	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	814	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	2459	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2753	A	O4'-C1'-N9	5.58	112.67	108.20
21	AA	569	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	1472	U	O4'-C1'-N1	5.58	112.67	108.20
54	BA	302	C	C1'-O4'-C4'	-5.58	105.44	109.90
54	BA	717	C	N1-C2-O2	5.58	122.25	118.90
54	BA	1398	C	N3-C4-C5	5.58	124.13	121.90
54	BA	1695	G	N3-C4-C5	-5.58	125.81	128.60
54	BA	1625	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	355	C	N3-C4-C5	5.58	124.13	121.90
54	BA	167	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	865	C	N1-C2-O2	5.58	122.25	118.90
54	BA	1437	C	N3-C2-O2	-5.58	118.00	121.90
4	AE	68	ARG	NE-CZ-NH1	5.58	123.09	120.30
20	AU	33	ARG	NE-CZ-NH2	-5.58	117.51	120.30
54	BA	1417	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	1463	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	1162	G	O4'-C1'-N9	5.58	112.66	108.20
54	BA	1384	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	342	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1754	A	C4-C5-C6	-5.57	114.21	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2279	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	2717	C	N1-C2-O2	5.57	122.24	118.90
54	BA	2504	U	N3-C2-O2	-5.57	118.30	122.20
4	AE	92	ARG	NE-CZ-NH2	-5.57	117.52	120.30
21	AA	172	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	194	C	N1-C2-O2	5.57	122.24	118.90
21	AA	8	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	1151	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	526	A	C5'-C4'-O4'	5.56	115.78	109.10
24	A3	13	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	45	G	C3'-C2'-C1'	5.56	105.95	101.50
54	BA	219	A	C6-C5-N7	5.56	136.19	132.30
54	BA	345	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	729	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	2114	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	1005	A	C4-C5-C6	-5.56	114.22	117.00
25	BC	132	ARG	NE-CZ-NH1	5.56	123.08	120.30
54	BA	1642	G	O4'-C1'-N9	5.56	112.65	108.20
21	AA	1305	G	N1-C6-O6	-5.56	116.56	119.90
21	AA	1452	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	119	A	C6-C5-N7	5.56	136.19	132.30
54	BA	816	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1576	U	O4'-C1'-N1	5.56	112.65	108.20
21	AA	65	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	765	G	N3-C4-C5	-5.56	125.82	128.60
54	BA	1676	A	C4-C5-C6	-5.56	114.22	117.00
55	BB	18	G	N3-C2-N2	-5.56	116.01	119.90
21	AA	563	A	C5-C6-N1	5.55	120.48	117.70
21	AA	1338	G	N3-C2-N2	-5.55	116.01	119.90
54	BA	267	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	1313	U	N3-C2-O2	-5.55	118.31	122.20
54	BA	1442	U	O4'-C1'-N1	5.55	112.64	108.20
21	AA	530	G	N3-C4-C5	-5.55	125.82	128.60
21	AA	1296	C	N1-C2-O2	5.55	122.23	118.90
54	BA	314	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	746	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1175	A	O4'-C1'-N9	5.55	112.64	108.20
21	AA	109	A	C4-C5-C6	-5.55	114.22	117.00
21	AA	940	C	N3-C2-O2	-5.55	118.02	121.90
21	AA	754	C	N1-C2-O2	5.55	122.23	118.90
54	BA	103	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	966	G	N1-C6-O6	-5.55	116.57	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1324	G	N1-C6-O6	-5.55	116.57	119.90
21	AA	679	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2585	U	O4'-C1'-N1	5.54	112.64	108.20
24	A3	74	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	821	A	O4'-C1'-N9	5.54	112.64	108.20
54	BA	1462	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	1890	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2182	U	O4'-C1'-N1	5.54	112.63	108.20
21	AA	1523	G	N1-C6-O6	-5.54	116.58	119.90
21	AA	704	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	316	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	540	C	N1-C2-O2	5.54	122.22	118.90
54	BA	1440	U	O4'-C1'-N1	5.54	112.63	108.20
54	BA	2247	A	C6-C5-N7	5.54	136.18	132.30
54	BA	2499	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2840	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	265	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1140	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1691	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	1848	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	699	C	N3-C2-O2	-5.54	118.03	121.90
21	AA	865	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	1112	C	N3-C2-O2	-5.54	118.03	121.90
21	AA	1493	A	C4-C5-C6	-5.54	114.23	117.00
24	A3	34	U	C1'-O4'-C4'	-5.54	105.47	109.90
27	BE	102	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	267	C	N1-C2-O2	5.53	122.22	118.90
21	AA	723	U	C1'-O4'-C4'	-5.53	105.47	109.90
54	BA	1758	U	N3-C2-O2	-5.53	118.33	122.20
54	BA	2842	G	N1-C6-O6	-5.53	116.58	119.90
2	AC	126	ARG	NE-CZ-NH1	5.53	123.07	120.30
54	BA	990	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	351	G	P-O3'-C3'	5.53	126.34	119.70
21	AA	496	A	N1-C6-N6	-5.53	115.28	118.60
24	A3	19	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	256	A	N1-C6-N6	-5.53	115.28	118.60
54	BA	876	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2160	C	N1-C2-O2	5.53	122.22	118.90
6	AG	4	ARG	NE-CZ-NH2	5.53	123.06	120.30
21	AA	495	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	577	G	C8-N9-C4	-5.53	104.19	106.40
54	BA	1363	C	N1-C2-O2	5.53	122.22	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	88	C	N1-C2-O2	5.53	122.22	118.90
21	AA	272	C	N1-C2-O2	5.53	122.22	118.90
54	BA	157	C	O4'-C1'-N1	5.53	112.62	108.20
21	AA	728	A	C6-C5-N7	5.52	136.17	132.30
21	AA	811	C	N1-C2-O2	5.52	122.21	118.90
21	AA	1317	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	1519	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1005	C	N1-C2-O2	5.52	122.21	118.90
54	BA	1665	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	1256	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	341	C	O4'-C1'-N1	5.52	112.62	108.20
54	BA	473	G	N1-C6-O6	-5.52	116.59	119.90
54	BA	477	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1022	G	C8-N9-C4	-5.52	104.19	106.40
54	BA	1152	C	O4'-C1'-N1	5.52	112.62	108.20
54	BA	1393	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1974	C	N1-C2-O2	5.52	122.21	118.90
54	BA	1981	A	C4-C5-C6	-5.52	114.24	117.00
20	AU	30	GLU	O-C-N	-5.52	113.87	122.70
54	BA	147	C	N1-C2-O2	5.52	122.21	118.90
54	BA	1102	C	O4'-C1'-N1	5.52	112.61	108.20
54	BA	253	C	O4'-C1'-N1	5.52	112.61	108.20
8	AI	79	ARG	NE-CZ-NH2	-5.51	117.54	120.30
45	BW	40	ARG	NE-CZ-NH1	5.51	123.06	120.30
54	BA	133	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	2575	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	559	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	16	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	1055	A	P-O3'-C3'	5.51	126.31	119.70
54	BA	622	G	N1-C6-O6	-5.51	116.59	119.90
54	BA	888	C	O4'-C1'-N1	5.51	112.61	108.20
54	BA	1180	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	1955	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	2042	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	2453	A	C4-C5-C6	-5.51	114.24	117.00
21	AA	72	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	2082	A	C4-C5-C6	-5.51	114.25	117.00
22	A1	9	A	O4'-C1'-N9	5.51	112.61	108.20
54	BA	92	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	340	A	N1-C6-N6	-5.51	115.30	118.60
54	BA	2456	C	N1-C2-O2	5.51	122.20	118.90
54	BA	542	C	N3-C2-O2	-5.50	118.05	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2620	C	N1-C2-O2	5.50	122.20	118.90
21	AA	431	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	584	G	N3-C4-C5	-5.50	125.85	128.60
54	BA	50	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1553	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	2419	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	2435	A	C6-C5-N7	5.50	136.15	132.30
25	BC	213	ARG	NE-CZ-NH1	5.50	123.05	120.30
54	BA	395	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	413	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1790	C	N1-C2-O2	5.50	122.20	118.90
54	BA	1373	A	N1-C6-N6	-5.50	115.30	118.60
22	A1	18	G	N3-C4-C5	-5.50	125.85	128.60
54	BA	258	G	O4'-C1'-N9	5.50	112.60	108.20
54	BA	754	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	33	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1306	C	N1-C2-O2	5.50	122.20	118.90
54	BA	330	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	330	A	O4'-C1'-N9	5.50	112.60	108.20
21	AA	810	C	N3-C2-O2	-5.49	118.05	121.90
54	BA	158	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	1344	U	N3-C2-O2	-5.49	118.35	122.20
54	BA	1382	G	N3-C4-C5	-5.49	125.85	128.60
55	BB	90	C	N1-C2-O2	5.49	122.20	118.90
21	AA	1167	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	126	A	C5'-C4'-C3'	-5.49	107.21	116.00
54	BA	1877	A	C4-C5-C6	-5.49	114.25	117.00
21	AA	1249	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	1794	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	79	C	O4'-C1'-N1	5.49	112.59	108.20
54	BA	182	A	C6-C5-N7	5.49	136.14	132.30
54	BA	803	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	2267	A	C6-C5-N7	5.48	136.14	132.30
55	BB	82	U	O4'-C1'-N1	5.48	112.59	108.20
21	AA	59	A	C4-C5-C6	-5.48	114.26	117.00
41	BS	25	ARG	NE-CZ-NH1	5.48	123.04	120.30
54	BA	284	U	O4'-C1'-N1	5.48	112.59	108.20
54	BA	337	C	N1-C2-O2	5.48	122.19	118.90
54	BA	1115	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	1981	A	O4'-C1'-N9	5.48	112.59	108.20
54	BA	2396	G	N1-C6-O6	-5.48	116.61	119.90
21	AA	932	C	N1-C2-O2	5.48	122.19	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	38	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	626	G	N3-C2-N2	-5.48	116.06	119.90
54	BA	1335	C	N1-C2-O2	5.48	122.19	118.90
21	AA	978	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	421	C	N1-C2-O2	5.48	122.19	118.90
54	BA	1368	G	O4'-C1'-N9	5.48	112.58	108.20
54	BA	447	A	C4-C5-C6	-5.48	114.26	117.00
45	BW	24	ARG	NE-CZ-NH2	-5.47	117.56	120.30
54	BA	337	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	846	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	2732	G	N1-C6-O6	-5.47	116.62	119.90
21	AA	589	U	O4'-C1'-N1	5.47	112.58	108.20
39	BQ	47	ARG	NE-CZ-NH1	5.47	123.03	120.30
54	BA	1022	G	N3-C4-C5	-5.47	125.86	128.60
54	BA	1783	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	2238	G	N3-C4-C5	-5.47	125.86	128.60
54	BA	108	G	O4'-C1'-N9	5.47	112.58	108.20
54	BA	736	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	271	C	O4'-C1'-N1	5.47	112.57	108.20
54	BA	289	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	925	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	2750	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	2770	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	2894	G	N1-C6-O6	-5.47	116.62	119.90
56	B5	53	ARG	NE-CZ-NH1	5.47	123.03	120.30
13	AN	24	ARG	NE-CZ-NH1	5.46	123.03	120.30
36	BN	71	ARG	NE-CZ-NH1	5.46	123.03	120.30
41	BS	18	ARG	NE-CZ-NH2	-5.46	117.57	120.30
54	BA	2401	U	O4'-C1'-N1	5.46	112.57	108.20
55	BB	75	G	N1-C6-O6	-5.46	116.62	119.90
21	AA	1441	A	C3'-C2'-C1'	5.46	105.87	101.50
25	BC	101	ARG	NE-CZ-NH2	-5.46	117.57	120.30
54	BA	991	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	48	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	469	C	N1-C2-O2	5.46	122.18	118.90
54	BA	587	C	N1-C2-O2	5.46	122.18	118.90
21	AA	242	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	935	C	N1-C2-O2	5.46	122.17	118.90
54	BA	1253	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1348	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	1937	A	O4'-C1'-N9	5.46	112.57	108.20
21	AA	1369	C	N1-C2-O2	5.46	122.17	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	B3	7	ARG	NE-CZ-NH2	-5.46	117.57	120.30
54	BA	28	A	O4'-C1'-N9	5.46	112.56	108.20
54	BA	1635	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2337	G	N3-C2-N2	-5.46	116.08	119.90
21	AA	741	G	N1-C6-O6	-5.46	116.63	119.90
21	AA	1223	C	N1-C2-O2	5.46	122.17	118.90
21	AA	415	A	C4-C5-C6	-5.45	114.27	117.00
21	AA	462	G	N9-C4-C5	5.45	107.58	105.40
54	BA	1544	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	1982	U	N3-C2-O2	-5.45	118.38	122.20
54	BA	2200	C	O4'-C1'-N1	5.45	112.56	108.20
21	AA	411	A	O4'-C1'-N9	5.45	112.56	108.20
21	AA	1284	C	N3-C2-O2	-5.45	118.08	121.90
37	BO	81	ARG	NE-CZ-NH2	5.45	123.03	120.30
54	BA	114	U	O4'-C1'-N1	5.45	112.56	108.20
54	BA	331	C	N1-C2-O2	5.45	122.17	118.90
21	AA	1049	U	O4'-C1'-N1	5.45	112.56	108.20
22	A1	62	C	N3-C2-O2	-5.45	118.09	121.90
34	BL	2	ARG	NE-CZ-NH2	-5.45	117.58	120.30
54	BA	94	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2086	U	O4'-C1'-N1	5.45	112.56	108.20
21	AA	1145	A	C4-C5-C6	-5.45	114.28	117.00
36	BN	64	ARG	NE-CZ-NH2	-5.45	117.58	120.30
54	BA	102	U	N3-C2-O2	-5.45	118.39	122.20
54	BA	999	U	O4'-C1'-N1	5.45	112.56	108.20
54	BA	1701	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2284	A	C6-C5-N7	5.45	136.11	132.30
54	BA	826	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	2458	G	N3-C4-C5	-5.44	125.88	128.60
54	BA	2589	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	484	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	2676	C	N1-C2-O2	5.44	122.17	118.90
21	AA	105	G	N1-C6-O6	-5.44	116.64	119.90
21	AA	1397	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	186	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	516	C	C5'-C4'-O4'	5.44	115.63	109.10
54	BA	1321	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1572	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	2153	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	1109	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	1451	C	C2'-C3'-O3'	5.44	122.40	113.70
54	BA	2279	G	O4'-C1'-N9	5.44	112.55	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2621	G	N3-C2-N2	-5.44	116.09	119.90
21	AA	1019	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	1102	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	1126	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	2422	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	60	A	P-O3'-C3'	5.44	126.22	119.70
21	AA	1171	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	1184	G	C5-C6-N1	5.44	114.22	111.50
54	BA	2730	C	N1-C2-O2	5.44	122.16	118.90
21	AA	1530	G	C1'-O4'-C4'	-5.43	105.55	109.90
29	BG	163	TYR	CB-CG-CD1	-5.43	117.74	121.00
54	BA	318	C	O4'-C1'-N1	5.43	112.55	108.20
54	BA	1490	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	1643	G	C5'-C4'-O4'	5.43	115.62	109.10
11	AL	82	ARG	CD-NE-CZ	5.43	131.21	123.60
21	AA	806	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	980	C	N1-C2-O2	5.43	122.16	118.90
54	BA	140	C	N1-C2-O2	5.43	122.16	118.90
54	BA	2438	U	C3'-C2'-C1'	5.43	105.85	101.50
21	AA	1363	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	449	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	1346	G	O4'-C1'-N9	5.43	112.54	108.20
54	BA	2695	U	O4'-C1'-N1	5.43	112.54	108.20
21	AA	1441	A	O4'-C1'-N9	5.43	112.54	108.20
54	BA	721	A	C4-C5-C6	-5.43	114.29	117.00
8	AI	98	ARG	NH1-CZ-NH2	-5.42	113.43	119.40
21	AA	360	G	N3-C2-N2	-5.42	116.10	119.90
21	AA	1224	U	N3-C2-O2	-5.42	118.40	122.20
54	BA	723	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	899	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1603	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2026	U	O4'-C1'-N1	5.42	112.54	108.20
54	BA	2317	A	O4'-C1'-N9	5.42	112.54	108.20
54	BA	2875	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	2016	U	N3-C2-O2	-5.42	118.40	122.20
54	BA	2183	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2572	A	N1-C6-N6	-5.42	115.35	118.60
21	AA	232	G	N1-C6-O6	-5.42	116.65	119.90
21	AA	1361	G	N3-C4-C5	-5.42	125.89	128.60
54	BA	1565	C	N1-C2-O2	5.42	122.15	118.90
54	BA	2556	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	592	A	C6-C5-N7	5.42	136.09	132.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1375	U	O4'-C1'-N1	5.42	112.54	108.20
54	BA	1937	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1298	U	O4'-C1'-N1	5.42	112.53	108.20
54	BA	254	G	N1-C6-O6	-5.42	116.65	119.90
21	AA	595	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1105	A	C6-C5-N7	5.42	136.09	132.30
54	BA	1863	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	860	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1872	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	2679	A	C4-C5-C6	-5.41	114.29	117.00
4	AE	156	ARG	NE-CZ-NH1	5.41	123.01	120.30
21	AA	307	C	N3-C2-O2	-5.41	118.11	121.90
21	AA	1277	C	N1-C2-O2	5.41	122.15	118.90
54	BA	443	A	C5'-C4'-O4'	5.41	115.59	109.10
21	AA	358	U	O4'-C1'-N1	5.41	112.53	108.20
21	AA	644	U	O4'-C1'-N1	5.41	112.53	108.20
21	AA	792	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	188	G	N3-C2-N2	-5.41	116.11	119.90
54	BA	959	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1348	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2753	A	C6-C5-N7	5.41	136.09	132.30
21	AA	90	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	324	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	833	G	N1-C6-O6	-5.41	116.66	119.90
54	BA	1243	C	O4'-C1'-N1	5.41	112.52	108.20
54	BA	2553	G	C3'-C2'-C1'	5.41	105.83	101.50
54	BA	557	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	817	C	N1-C2-O2	5.40	122.14	118.90
21	AA	512	U	C5-C6-N1	-5.40	120.00	122.70
21	AA	609	A	C6-C5-N7	5.40	136.08	132.30
21	AA	1193	G	N1-C6-O6	-5.40	116.66	119.90
22	A1	9	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	124	C	N1-C2-O2	5.40	122.14	118.90
21	AA	428	G	N1-C6-O6	-5.40	116.66	119.90
21	AA	449	G	N3-C2-N2	-5.40	116.12	119.90
54	BA	1370	C	N3-C2-O2	-5.40	118.12	121.90
24	A3	57	C	N1-C2-O2	5.40	122.14	118.90
54	BA	892	A	C6-C5-N7	5.40	136.08	132.30
54	BA	2652	C	N1-C2-O2	5.40	122.14	118.90
54	BA	2295	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	419	C	N1-C2-O2	5.40	122.14	118.90
54	BA	1528	A	C4-C5-C6	-5.40	114.30	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	64	G	N1-C6-O6	-5.39	116.66	119.90
21	AA	110	C	N3-C2-O2	-5.39	118.12	121.90
21	AA	220	G	N1-C6-O6	-5.39	116.66	119.90
21	AA	1267	C	N1-C2-O2	5.39	122.14	118.90
24	A3	9	G	N3-C4-C5	-5.39	125.90	128.60
24	A3	27	G	N1-C6-O6	-5.39	116.66	119.90
54	BA	1128	G	N1-C6-O6	-5.39	116.66	119.90
54	BA	2432	A	O4'-C1'-N9	5.39	112.52	108.20
54	BA	2521	C	N1-C2-O2	5.39	122.14	118.90
30	BH	123	ARG	NE-CZ-NH1	5.39	123.00	120.30
54	BA	454	A	C4-C5-C6	-5.39	114.31	117.00
21	AA	1109	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1332	G	N3-C2-N2	-5.39	116.13	119.90
54	BA	1470	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	1847	A	C5'-C4'-C3'	-5.39	107.38	116.00
21	AA	782	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	921	C	N1-C2-O2	5.39	122.13	118.90
54	BA	2023	C	O4'-C1'-N1	5.39	112.51	108.20
55	BB	35	C	N1-C2-O2	5.39	122.13	118.90
21	AA	998	C	N1-C2-O2	5.38	122.13	118.90
21	AA	1322	C	N3-C4-N4	-5.38	114.23	118.00
54	BA	11	C	O4'-C1'-N1	5.38	112.51	108.20
54	BA	715	A	C6-C5-N7	5.38	136.07	132.30
54	BA	1414	C	N3-C2-O2	-5.38	118.13	121.90
54	BA	1843	C	N3-C2-O2	-5.38	118.13	121.90
21	AA	578	C	N1-C2-O2	5.38	122.13	118.90
21	AA	814	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	383	C	N3-C2-O2	-5.38	118.13	121.90
54	BA	654	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	1179	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1245	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1625	C	O4'-C1'-N1	5.38	112.51	108.20
21	AA	815	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	112	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	1469	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	2462	C	N1-C2-O2	5.38	122.13	118.90
55	BB	78	A	C6-C5-N7	5.38	136.07	132.30
54	BA	1203	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	1378	A	C6-C5-N7	5.38	136.06	132.30
54	BA	2728	U	O4'-C1'-N1	5.38	112.50	108.20
21	AA	831	A	C5-C6-N1	5.38	120.39	117.70
21	AA	1271	A	C4-C5-C6	-5.38	114.31	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	399	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	2248	C	N3-C2-O2	-5.38	118.14	121.90
21	AA	1411	C	N1-C2-O2	5.38	122.12	118.90
21	AA	466	A	C4-C5-C6	-5.37	114.31	117.00
41	BS	95	ARG	NE-CZ-NH1	5.37	122.99	120.30
54	BA	1049	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2275	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2520	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2721	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	1365	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	2215	C	O4'-C1'-N1	5.37	112.50	108.20
24	A3	44	A	O4'-C1'-N9	5.37	112.50	108.20
43	BU	5	ARG	NE-CZ-NH1	5.37	122.98	120.30
54	BA	1816	C	N3-C4-N4	-5.37	114.24	118.00
54	BA	1871	A	C4-C5-C6	-5.37	114.31	117.00
21	AA	765	G	C1'-O4'-C4'	-5.37	105.61	109.90
27	BE	117	ARG	NE-CZ-NH1	5.37	122.98	120.30
37	BO	111	ARG	NE-CZ-NH1	5.37	122.98	120.30
54	BA	426	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2514	U	O4'-C1'-N1	5.37	112.50	108.20
21	AA	163	C	N1-C2-O2	5.37	122.12	118.90
21	AA	848	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	2248	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	614	A	C1'-O4'-C4'	-5.37	105.61	109.90
54	BA	1173	U	O4'-C1'-N1	5.37	112.49	108.20
54	BA	1663	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	308	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	329	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	579	A	O4'-C1'-N9	5.36	112.49	108.20
54	BA	2146	C	N1-C2-O2	5.36	122.12	118.90
54	BA	2427	C	N1-C2-O2	5.36	122.12	118.90
54	BA	2492	U	N3-C2-O2	-5.36	118.45	122.20
17	AR	50	TYR	CB-CG-CD1	-5.36	117.78	121.00
21	AA	114	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	359	G	N1-C6-O6	-5.36	116.68	119.90
54	BA	585	G	C5'-C4'-O4'	5.36	115.53	109.10
56	B5	134	ARG	NE-CZ-NH1	5.36	122.98	120.30
21	AA	395	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	485	C	N1-C2-O2	5.36	122.11	118.90
21	AA	254	G	C5'-C4'-O4'	5.36	115.53	109.10
21	AA	418	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	1977	A	C4-C5-C6	-5.36	114.32	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2757	A	C5'-C4'-C3'	-5.36	107.43	116.00
54	BA	2833	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	1582	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	1815	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2420	C	N3-C2-O2	-5.36	118.15	121.90
24	A3	48	U	P-O3'-C3'	5.35	126.12	119.70
34	BL	21	ARG	NE-CZ-NH1	5.35	122.98	120.30
54	BA	601	C	C4'-C3'-C2'	-5.35	97.25	102.60
54	BA	705	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	2525	G	N3-C2-N2	-5.35	116.15	119.90
21	AA	1119	C	N3-C2-O2	-5.35	118.15	121.90
22	A1	76	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	49	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	347	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	828	U	N1-C1'-C2'	5.35	120.96	114.00
21	AA	422	C	N1-C2-O2	5.35	122.11	118.90
21	AA	427	U	N3-C2-O2	-5.35	118.45	122.20
54	BA	183	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	895	U	N3-C2-O2	-5.35	118.46	122.20
54	BA	1552	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	1792	G	N1-C6-O6	-5.35	116.69	119.90
51	B2	34	ARG	NE-CZ-NH2	-5.35	117.63	120.30
54	BA	2063	C	C1'-O4'-C4'	-5.35	105.62	109.90
20	AU	30	GLU	CA-C-N	5.34	128.96	117.20
29	BG	152	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BA	20	C	O4'-C1'-N1	5.34	112.48	108.20
54	BA	545	U	N3-C2-O2	-5.34	118.46	122.20
54	BA	961	C	N1-C2-O2	5.34	122.11	118.90
54	BA	2825	G	N3-C4-C5	-5.34	125.93	128.60
54	BA	2704	C	O4'-C1'-N1	5.34	112.47	108.20
24	A3	43	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	824	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1177	G	N3-C2-N2	-5.34	116.16	119.90
54	BA	1580	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2122	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2185	U	O4'-C1'-N1	5.34	112.47	108.20
21	AA	66	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	151	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	598	U	N3-C2-O2	-5.34	118.46	122.20
54	BA	713	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	1675	C	N1-C2-O2	5.34	122.10	118.90
54	BA	2621	G	N1-C6-O6	-5.34	116.70	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1251	A	C6-C5-N7	5.34	136.04	132.30
54	BA	1066	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2757	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	795	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1185	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	1901	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	1168	U	N3-C2-O2	-5.33	118.47	122.20
21	AA	411	A	C4-C5-C6	-5.33	114.33	117.00
48	BZ	30	ARG	NE-CZ-NH2	-5.33	117.63	120.30
54	BA	678	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	730	A	C6-C5-N7	5.33	136.03	132.30
54	BA	2148	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	555	U	C1'-O4'-C4'	-5.33	105.64	109.90
21	AA	1459	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	270	A	C4-C5-C6	-5.33	114.34	117.00
38	BP	52	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
21	AA	501	C	N1-C2-O2	5.33	122.09	118.90
54	BA	1029	A	C4'-C3'-C2'	-5.33	97.28	102.60
54	BA	1587	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	625	U	N3-C2-O2	-5.32	118.47	122.20
54	BA	37	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	228	C	N1-C2-O2	5.32	122.09	118.90
54	BA	2244	U	N3-C2-O2	-5.32	118.47	122.20
54	BA	2583	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	1113	C	N1-C2-O2	5.32	122.09	118.90
54	BA	2697	G	N1-C6-O6	-5.32	116.71	119.90
55	BB	14	U	O4'-C1'-N1	5.32	112.46	108.20
21	AA	1449	C	N1-C2-O2	5.32	122.09	118.90
24	A3	50	G	N3-C2-N2	-5.32	116.18	119.90
54	BA	696	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	2023	C	N3-C2-O2	-5.32	118.18	121.90
54	BA	2498	C	N1-C2-O2	5.32	122.09	118.90
21	AA	816	A	O4'-C1'-N9	5.32	112.45	108.20
54	BA	1205	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	1704	C	O4'-C1'-N1	5.32	112.45	108.20
54	BA	2507	C	N1-C2-O2	5.32	122.09	118.90
54	BA	2612	C	N1-C2-O2	5.32	122.09	118.90
21	AA	1342	C	C5'-C4'-O4'	5.32	115.48	109.10
21	AA	1474	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	249	C	P-O3'-C3'	5.32	126.08	119.70
54	BA	1010	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	2434	A	N1-C6-N6	-5.32	115.41	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1468	A	C6-C5-N7	5.31	136.02	132.30
54	BA	1325	U	N3-C2-O2	-5.31	118.48	122.20
21	AA	406	G	N3-C4-C5	-5.31	125.94	128.60
54	BA	650	C	N3-C4-C5	5.31	124.03	121.90
54	BA	1844	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	2460	U	O4'-C1'-N1	5.31	112.45	108.20
21	AA	493	A	O4'-C1'-N9	5.31	112.45	108.20
21	AA	658	C	N1-C2-O2	5.31	122.09	118.90
54	BA	513	A	C4-C5-C6	-5.31	114.34	117.00
21	AA	251	G	O4'-C1'-N9	5.31	112.45	108.20
21	AA	355	C	N3-C4-N4	-5.31	114.28	118.00
21	AA	1426	G	N3-C2-N2	-5.31	116.18	119.90
54	BA	2237	G	N1-C6-O6	-5.31	116.72	119.90
54	BA	1413	A	C6-C5-N7	5.31	136.01	132.30
54	BA	2634	A	C6-C5-N7	5.31	136.01	132.30
54	BA	2194	U	O4'-C1'-N1	5.31	112.44	108.20
54	BA	2841	C	N3-C2-O2	-5.31	118.19	121.90
21	AA	124	C	C3'-C2'-C1'	5.30	105.74	101.50
21	AA	949	A	C4-C5-C6	-5.30	114.35	117.00
55	BB	46	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	2245	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	2426	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	862	C	N3-C2-O2	-5.30	118.19	121.90
21	AA	1406	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	584	C	N1-C2-O2	5.30	122.08	118.90
21	AA	119	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	894	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	968	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1739	A	C6-C5-N7	5.30	136.01	132.30
54	BA	34	U	N1-C2-N3	5.30	118.08	114.90
54	BA	159	G	C8-N9-C4	-5.30	104.28	106.40
54	BA	1594	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2178	C	N1-C2-O2	5.30	122.08	118.90
18	AS	78	THR	CA-C-N	5.30	128.85	117.20
54	BA	1847	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	2133	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	2214	C	N1-C2-O2	5.30	122.08	118.90
21	AA	168	G	N1-C6-O6	-5.29	116.72	119.90
21	AA	719	C	N3-C2-O2	-5.29	118.19	121.90
54	BA	1720	U	O4'-C1'-N1	5.29	112.44	108.20
54	BA	1773	A	O4'-C1'-N9	5.29	112.44	108.20
54	BA	2628	C	N1-C2-O2	5.29	122.08	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	677	A	N1-C6-N6	-5.29	115.43	118.60
54	BA	870	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2029	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	2711	A	P-O3'-C3'	5.29	126.05	119.70
24	A3	18	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1035	U	O4'-C1'-N1	5.29	112.43	108.20
22	A1	31	C	N1-C2-O2	5.29	122.07	118.90
54	BA	479	A	O4'-C1'-N9	5.29	112.43	108.20
54	BA	1088	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	1713	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	2386	A	C6-C5-N7	5.29	136.00	132.30
55	BB	90	C	N3-C4-C5	5.29	124.01	121.90
1	AB	34	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	AA	390	U	N1-C2-N3	5.28	118.07	114.90
21	AA	1049	U	C1'-O4'-C4'	-5.28	105.67	109.90
21	AA	1176	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1828	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	2175	C	N1-C2-O2	5.28	122.07	118.90
54	BA	2425	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	2748	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	694	A	C4-C5-C6	-5.28	114.36	117.00
22	A1	10	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	1030	C	N3-C2-O2	-5.28	118.20	121.90
21	AA	893	C	N3-C2-O2	-5.28	118.20	121.90
54	BA	97	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	109	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	642	U	N3-C2-O2	-5.28	118.50	122.20
54	BA	2702	G	N3-C2-N2	-5.28	116.20	119.90
54	BA	2826	A	C4-C5-C6	-5.28	114.36	117.00
55	BB	34	A	C6-C5-N7	5.28	136.00	132.30
14	AO	57	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	AA	951	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	1210	G	N3-C4-C5	-5.28	125.96	128.60
7	AH	116	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	AA	111	G	N3-C2-N2	-5.28	116.21	119.90
54	BA	2660	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	2707	U	O4'-C1'-N1	5.28	112.42	108.20
49	B0	16	ARG	NE-CZ-NH1	5.28	122.94	120.30
54	BA	2776	A	O4'-C1'-N9	5.28	112.42	108.20
21	AA	239	U	N3-C2-O2	-5.27	118.51	122.20
21	AA	1202	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	837	C	N3-C2-O2	-5.27	118.21	121.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2332	C	O4'-C1'-N1	5.27	112.42	108.20
21	AA	728	A	C2-N3-C4	5.27	113.24	110.60
54	BA	640	C	N1-C2-O2	5.27	122.06	118.90
54	BA	775	G	O4'-C1'-N9	5.27	112.42	108.20
54	BA	1386	C	C5'-C4'-O4'	5.27	115.43	109.10
21	AA	817	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	34	U	N3-C2-O2	-5.27	118.51	122.20
54	BA	516	C	N1-C2-O2	5.27	122.06	118.90
21	AA	628	G	N1-C6-O6	-5.27	116.74	119.90
35	BM	66	ARG	NE-CZ-NH1	5.27	122.93	120.30
54	BA	971	G	C5-C6-N1	5.27	114.14	111.50
54	BA	1184	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	1399	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	1668	A	O4'-C1'-N9	5.27	112.42	108.20
54	BA	1825	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	1892	C	N1-C2-O2	5.27	122.06	118.90
54	BA	2475	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	2638	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	737	C	O4'-C1'-N1	5.27	112.41	108.20
54	BA	2343	U	O4'-C1'-N1	5.27	112.42	108.20
21	AA	483	C	N1-C2-O2	5.27	122.06	118.90
21	AA	1280	A	C4-C5-C6	-5.27	114.37	117.00
21	AA	1507	A	C4-C5-C6	-5.27	114.37	117.00
54	BA	635	C	C5'-C4'-O4'	5.27	115.42	109.10
54	BA	718	A	C2-N3-C4	5.27	113.23	110.60
54	BA	2889	C	O4'-C1'-N1	5.27	112.41	108.20
21	AA	735	C	N1-C2-O2	5.26	122.06	118.90
21	AA	985	C	N1-C2-O2	5.26	122.06	118.90
21	AA	1130	A	N1-C6-N6	-5.26	115.44	118.60
54	BA	1724	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	1729	U	N3-C2-O2	-5.26	118.52	122.20
55	BB	100	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	2013	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2342	C	N1-C2-O2	5.26	122.06	118.90
54	BA	2771	C	N1-C2-O2	5.26	122.06	118.90
21	AA	271	C	C3'-C2'-C1'	5.26	105.71	101.50
21	AA	1333	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1441	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2406	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2823	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	934	C	N1-C2-O2	5.26	122.06	118.90
21	AA	1163	A	C4-C5-C6	-5.26	114.37	117.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1256	A	C2-N3-C4	5.26	113.23	110.60
54	BA	2089	C	C5'-C4'-O4'	5.26	115.41	109.10
54	BA	2286	G	C3'-C2'-C1'	5.26	105.71	101.50
54	BA	2703	C	N1-C2-O2	5.26	122.06	118.90
21	AA	238	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	534	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	2394	C	N3-C2-O2	-5.26	118.22	121.90
29	BG	94	ARG	NE-CZ-NH1	5.26	122.93	120.30
54	BA	695	G	N3-C2-N2	-5.26	116.22	119.90
54	BA	958	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	1652	A	O4'-C1'-N9	5.26	112.41	108.20
54	BA	2063	C	N1-C2-O2	5.26	122.05	118.90
21	AA	552	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	556	A	C4-C5-C6	-5.25	114.37	117.00
21	AA	78	A	C6-C5-N7	5.25	135.98	132.30
54	BA	1779	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1932	A	C6-C5-N7	5.25	135.98	132.30
54	BA	2244	U	C3'-C2'-C1'	5.25	105.70	101.50
54	BA	970	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1385	A	O4'-C1'-N9	5.25	112.40	108.20
54	BA	2195	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2472	G	N3-C4-C5	-5.25	125.97	128.60
21	AA	278	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	886	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	664	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	301	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	302	C	N3-C4-C5	5.25	124.00	121.90
54	BA	885	C	N1-C2-O2	5.25	122.05	118.90
54	BA	1220	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	2059	A	C4-C5-C6	-5.25	114.38	117.00
21	AA	1502	A	O4'-C1'-N9	5.25	112.40	108.20
54	BA	1618	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	2855	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	579	A	C3'-C2'-C1'	5.25	105.70	101.50
54	BA	902	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1443	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	279	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	920	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1039	A	N1-C6-N6	-5.24	115.45	118.60
54	BA	1570	A	C6-C5-N7	5.24	135.97	132.30
54	BA	1670	C	O4'-C1'-N1	5.24	112.39	108.20
21	AA	330	C	N3-C2-O2	-5.24	118.23	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BW	76	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BA	262	A	C6-C5-N7	5.24	135.97	132.30
54	BA	2795	C	N1-C2-O2	5.24	122.05	118.90
11	AL	98	ARG	NE-CZ-NH1	5.24	122.92	120.30
21	AA	80	A	C6-C5-N7	5.24	135.97	132.30
21	AA	630	A	C6-C5-N7	5.24	135.97	132.30
51	B2	35	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BA	531	C	N1-C2-O2	5.24	122.05	118.90
54	BA	1072	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2046	G	C5-C6-N1	5.24	114.12	111.50
21	AA	236	A	C5-C6-N1	5.24	120.32	117.70
21	AA	1200	C	N3-C2-O2	-5.24	118.23	121.90
21	AA	1528	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	461	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1805	A	C4'-C3'-C2'	-5.24	97.36	102.60
21	AA	993	G	C5-C6-N1	5.24	114.12	111.50
21	AA	1141	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	19	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1802	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	2621	G	N9-C4-C5	5.24	107.49	105.40
54	BA	621	A	C4-C5-C6	-5.23	114.38	117.00
54	BA	1217	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2828	G	N3-C2-N2	-5.23	116.24	119.90
21	AA	1501	C	N1-C2-O2	5.23	122.04	118.90
54	BA	191	A	C4-C5-C6	-5.23	114.38	117.00
54	BA	1944	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2313	C	O4'-C1'-N1	5.23	112.39	108.20
21	AA	428	G	N3-C2-N2	-5.23	116.24	119.90
54	BA	2469	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	2570	G	N3-C2-N2	-5.23	116.24	119.90
21	AA	200	G	N3-C4-C5	-5.23	125.98	128.60
23	A2	87	U	O4'-C1'-N1	5.23	112.38	108.20
54	BA	751	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	998	C	C4'-C3'-C2'	-5.23	97.37	102.60
54	BA	2601	C	N1-C2-O2	5.23	122.04	118.90
54	BA	732	C	O4'-C1'-N1	5.23	112.38	108.20
54	BA	2084	C	O4'-C1'-N1	5.23	112.38	108.20
4	AE	28	ARG	NE-CZ-NH1	5.22	122.91	120.30
21	AA	26	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	129	A	C6-C5-N7	5.22	135.96	132.30
53	B4	24	ARG	NE-CZ-NH2	-5.22	117.69	120.30
54	BA	528	A	O4'-C1'-N9	5.22	112.38	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2298	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	2443	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	173	U	O4'-C1'-N1	5.22	112.38	108.20
21	AA	851	G	C5-C6-N1	5.22	114.11	111.50
55	BB	92	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	481	G	N3-C4-C5	-5.22	125.99	128.60
21	AA	714	G	N3-C4-C5	-5.22	125.99	128.60
21	AA	1077	G	C1'-O4'-C4'	-5.22	105.72	109.90
21	AA	1209	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	905	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	1055	A	O4'-C1'-N9	5.22	112.37	108.20
21	AA	1136	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2058	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	312	C	N1-C2-O2	5.22	122.03	118.90
21	AA	856	C	O4'-C1'-N1	5.22	112.37	108.20
21	AA	1299	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	1399	C	N3-C2-O2	-5.22	118.25	121.90
21	AA	1534	A	C1'-O4'-C4'	-5.22	105.73	109.90
54	BA	2450	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	385	C	N1-C2-O2	5.21	122.03	118.90
54	BA	703	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2867	G	N3-C4-C5	-5.21	125.99	128.60
21	AA	1341	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	863	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	1028	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	41	C	N1-C2-O2	5.21	122.03	118.90
54	BA	1396	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	1933	G	C4'-C3'-C2'	-5.21	97.39	102.60
54	BA	2192	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2236	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	867	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	1002	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	1423	G	O4'-C1'-N9	5.21	112.37	108.20
34	BL	132	ARG	NE-CZ-NH1	5.21	122.90	120.30
54	BA	926	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	1687	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	2048	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	2063	C	O4'-C1'-N1	5.21	112.37	108.20
21	AA	157	U	N3-C2-O2	-5.21	118.56	122.20
21	AA	311	C	N1-C2-O2	5.21	122.02	118.90
24	A3	21	H2U	O3'-P-O5'	-5.21	94.11	104.00
54	BA	280	U	N3-C2-O2	-5.21	118.56	122.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	745	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	1585	C	N1-C2-O2	5.21	122.02	118.90
54	BA	2509	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	2684	U	O4'-C1'-N1	5.21	112.36	108.20
21	AA	803	G	C8-N9-C4	-5.21	104.32	106.40
54	BA	300	A	C6-C5-N7	5.21	135.94	132.30
54	BA	2131	U	N3-C2-O2	-5.21	118.56	122.20
24	A3	29	C	N1-C2-O2	5.20	122.02	118.90
42	BT	6	ARG	NE-CZ-NH1	5.20	122.90	120.30
54	BA	1336	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	1621	U	C3'-C2'-C1'	5.20	105.66	101.50
54	BA	2226	C	O4'-C1'-N1	5.20	112.36	108.20
21	AA	1146	A	C4-C5-C6	-5.20	114.40	117.00
21	AA	328	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	102	U	C3'-C2'-C1'	5.20	105.66	101.50
21	AA	811	C	C1'-O4'-C4'	-5.20	105.74	109.90
54	BA	398	C	N1-C2-O2	5.20	122.02	118.90
54	BA	475	C	N3-C4-C5	5.20	123.98	121.90
54	BA	613	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	992	C	O4'-C1'-N1	5.20	112.36	108.20
55	BB	8	C	N1-C2-O2	5.20	122.02	118.90
21	AA	1049	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	27	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	766	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1676	A	O4'-C1'-N9	5.20	112.36	108.20
21	AA	323	U	N3-C2-O2	-5.19	118.56	122.20
21	AA	1279	G	C8-N9-C4	-5.19	104.32	106.40
54	BA	462	C	O4'-C1'-N1	5.19	112.36	108.20
54	BA	2810	A	C6-C5-N7	5.19	135.94	132.30
21	AA	824	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	1591	A	C6-C5-N7	5.19	135.94	132.30
21	AA	528	C	N1-C2-O2	5.19	122.01	118.90
21	AA	1409	C	N1-C2-O2	5.19	122.01	118.90
40	BR	84	ARG	NE-CZ-NH1	5.19	122.89	120.30
54	BA	539	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	1230	A	C6-C5-N7	5.19	135.93	132.30
54	BA	2237	G	O4'-C1'-N9	5.19	112.35	108.20
21	AA	864	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	2739	U	O4'-C1'-N1	5.19	112.35	108.20
21	AA	880	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	1126	A	C6-C5-N7	5.19	135.93	132.30
54	BA	1200	C	N1-C2-O2	5.19	122.01	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2464	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	2888	C	N1-C2-O2	5.19	122.01	118.90
21	AA	19	A	C6-C5-N7	5.19	135.93	132.30
21	AA	757	U	N3-C2-O2	-5.19	118.57	122.20
54	BA	1738	G	N3-C2-N2	-5.19	116.27	119.90
21	AA	6	G	O4'-C1'-N9	5.18	112.35	108.20
21	AA	204	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	871	U	O4'-C1'-N1	5.18	112.35	108.20
21	AA	1129	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1194	U	N1-C2-N3	5.18	118.01	114.90
24	A3	9	G	C3'-C2'-C1'	5.18	105.65	101.50
26	BD	13	ARG	NE-CZ-NH1	5.18	122.89	120.30
54	BA	2539	C	N1-C2-O2	5.18	122.01	118.90
54	BA	2650	U	O4'-C1'-N1	5.18	112.35	108.20
54	BA	2896	C	N1-C2-O2	5.18	122.01	118.90
55	BB	12	C	N1-C2-O2	5.18	122.01	118.90
2	AC	155	ARG	NE-CZ-NH1	5.18	122.89	120.30
29	BG	151	ARG	NE-CZ-NH1	5.18	122.89	120.30
54	BA	380	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	738	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	1568	G	N3-C4-C5	-5.18	126.01	128.60
54	BA	2015	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2064	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	2742	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	528	C	N3-C4-C5	5.18	123.97	121.90
28	BF	29	ARG	NE-CZ-NH1	5.18	122.89	120.30
54	BA	491	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	677	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2663	G	O4'-C1'-N9	5.18	112.34	108.20
21	AA	29	U	O4'-C1'-N1	5.18	112.34	108.20
24	A3	35	C	N1-C2-O2	5.18	122.01	118.90
54	BA	116	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	465	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	2402	U	N3-C2-O2	-5.18	118.57	122.20
18	AS	78	THR	O-C-N	-5.18	114.42	122.70
21	AA	658	C	N3-C4-C5	5.18	123.97	121.90
54	BA	1639	C	N1-C2-O2	5.18	122.01	118.90
21	AA	38	G	C5'-C4'-C3'	-5.18	107.72	116.00
54	BA	1104	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	1827	U	O4'-C1'-N1	5.18	112.34	108.20
21	AA	597	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	1225	A	C3'-C2'-C1'	5.17	105.64	101.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A2	80	C	P-O3'-C3'	5.17	125.91	119.70
54	BA	2088	A	C6-C5-N7	5.17	135.92	132.30
21	AA	846	G	C5-C6-N1	5.17	114.09	111.50
54	BA	2260	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	2831	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	191	G	N3-C4-C5	-5.17	126.01	128.60
21	AA	1364	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	1100	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1155	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	1191	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	2638	G	N3-C4-C5	-5.17	126.01	128.60
54	BA	2808	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	85	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	1541	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1985	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	2466	C	N3-C2-O2	-5.17	118.28	121.90
21	AA	161	A	C4-C5-C6	-5.17	114.42	117.00
21	AA	686	U	O4'-C1'-N1	5.17	112.33	108.20
54	BA	1624	U	O4'-C1'-N1	5.17	112.33	108.20
54	BA	1800	C	N1-C2-O2	5.17	122.00	118.90
54	BA	2344	U	N3-C2-O2	-5.17	118.58	122.20
3	AD	46	ARG	NE-CZ-NH2	-5.17	117.72	120.30
21	AA	99	C	N1-C2-O2	5.17	122.00	118.90
21	AA	179	A	C6-C5-N7	5.17	135.92	132.30
21	AA	353	A	O4'-C1'-N9	5.17	112.33	108.20
21	AA	1488	G	N1-C6-O6	-5.17	116.80	119.90
22	A1	16	C	N1-C2-O2	5.17	122.00	118.90
54	BA	2586	U	O4'-C1'-N1	5.17	112.33	108.20
18	AS	22	VAL	C-N-CA	5.17	134.61	121.70
54	BA	2626	C	O4'-C1'-N1	5.17	112.33	108.20
1	AB	136	ARG	NE-CZ-NH2	-5.16	117.72	120.30
7	AH	79	ARG	NE-CZ-NH1	5.16	122.88	120.30
21	AA	926	G	C3'-C2'-C1'	5.16	105.63	101.50
34	BL	47	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BA	503	A	C3'-C2'-C1'	5.16	105.63	101.50
54	BA	686	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1044	C	O4'-C1'-N1	5.16	112.33	108.20
54	BA	2061	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	2164	C	N1-C2-O2	5.16	122.00	118.90
54	BA	2434	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	2769	U	O4'-C1'-N1	5.16	112.33	108.20
22	A1	58	A	C6-C5-N7	5.16	135.91	132.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	47	C	C3'-C2'-C1'	5.16	105.63	101.50
54	BA	735	A	N1-C6-N6	-5.16	115.50	118.60
54	BA	2480	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	11	G	N1-C6-O6	-5.16	116.80	119.90
21	AA	314	C	N1-C2-O2	5.16	122.00	118.90
54	BA	253	C	N1-C2-O2	5.16	122.00	118.90
54	BA	786	C	N1-C2-O2	5.16	122.00	118.90
54	BA	1453	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	453	G	C5-C6-N1	5.16	114.08	111.50
21	AA	827	U	N3-C2-O2	-5.16	118.59	122.20
21	AA	924	C	N1-C2-O2	5.16	122.00	118.90
29	BG	34	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BA	841	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	2527	C	N1-C2-O2	5.16	122.00	118.90
21	AA	1099	G	C5-C6-N1	5.16	114.08	111.50
15	AP	8	ARG	CD-NE-CZ	5.16	130.82	123.60
21	AA	1473	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	2334	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	2491	U	O4'-C1'-N1	5.16	112.32	108.20
21	AA	1200	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	157	C	N1-C2-O2	5.15	121.99	118.90
54	BA	164	C	C4'-C3'-C2'	-5.15	97.45	102.60
54	BA	2176	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	2858	C	O4'-C1'-N1	5.15	112.32	108.20
21	AA	964	A	C6-C5-N7	5.15	135.91	132.30
21	AA	1117	A	C4-C5-C6	-5.15	114.42	117.00
26	BD	184	ARG	NE-CZ-NH1	5.15	122.88	120.30
54	BA	70	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	2145	C	C6-N1-C2	-5.15	118.24	120.30
21	AA	113	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	791	C	N1-C2-O2	5.15	121.99	118.90
6	AG	137	ARG	NE-CZ-NH2	-5.15	117.72	120.30
54	BA	2295	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	138	G	N1-C6-O6	-5.15	116.81	119.90
21	AA	468	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	742	G	N1-C6-O6	-5.15	116.81	119.90
21	AA	1387	G	C1'-O4'-C4'	-5.15	105.78	109.90
23	A2	80	C	N3-C4-N4	-5.15	114.40	118.00
54	BA	239	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	624	C	N1-C2-O2	5.15	121.99	118.90
54	BA	866	A	C4-C5-C6	-5.15	114.43	117.00
54	BA	1708	C	N1-C2-O2	5.15	121.99	118.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	206	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	199	A	C4-C5-C6	-5.15	114.43	117.00
54	BA	851	C	N3-C2-O2	-5.14	118.30	121.90
54	BA	2463	C	O4'-C1'-N1	5.14	112.32	108.20
54	BA	2515	C	N1-C2-O2	5.14	121.99	118.90
21	AA	683	G	N1-C6-O6	-5.14	116.81	119.90
21	AA	716	A	C4-C5-C6	-5.14	114.43	117.00
21	AA	947	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	1146	C	N1-C2-O2	5.14	121.98	118.90
54	BA	1964	G	N3-C4-C5	-5.14	126.03	128.60
54	BA	2581	G	N3-C2-N2	-5.14	116.30	119.90
21	AA	331	G	C5-C6-N1	5.14	114.07	111.50
21	AA	1303	C	N1-C2-O2	5.14	121.98	118.90
54	BA	759	G	C5'-C4'-O4'	5.14	115.27	109.10
22	A1	53	G	N3-C2-N2	-5.14	116.30	119.90
54	BA	898	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	1730	C	N1-C2-O2	5.14	121.98	118.90
54	BA	2422	C	N3-C4-C5	5.14	123.96	121.90
54	BA	2607	G	N3-C2-N2	-5.14	116.30	119.90
21	AA	408	A	C6-C5-N7	5.14	135.90	132.30
54	BA	421	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	1067	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	1699	G	C5-C6-N1	5.14	114.07	111.50
54	BA	2006	C	N1-C2-O2	5.14	121.98	118.90
21	AA	214	C	N1-C2-O2	5.14	121.98	118.90
24	A3	9	G	C5'-C4'-C3'	-5.14	107.78	116.00
54	BA	151	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	334	C	N1-C2-O2	5.14	121.98	118.90
54	BA	508	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	1161	C	C4'-C3'-C2'	-5.14	97.46	102.60
54	BA	1185	G	C3'-C2'-C1'	5.14	105.61	101.50
54	BA	2396	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	2560	A	C4-C5-C6	-5.14	114.43	117.00
21	AA	1099	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	1228	C	N1-C2-O2	5.13	121.98	118.90
54	BA	163	C	N1-C2-O2	5.13	121.98	118.90
54	BA	322	A	C4-C5-C6	-5.13	114.43	117.00
13	AN	81	ARG	NH1-CZ-NH2	-5.13	113.75	119.40
21	AA	16	A	C6-C5-N7	5.13	135.89	132.30
21	AA	832	G	C5-C6-N1	5.13	114.07	111.50
54	BA	290	U	O4'-C1'-N1	5.13	112.31	108.20
54	BA	1046	A	O4'-C1'-N9	5.13	112.31	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1339	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	40	C	C1'-O4'-C4'	-5.13	105.80	109.90
24	A3	41	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	998	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2406	A	C2-N3-C4	5.13	113.17	110.60
21	AA	461	A	O4'-C1'-N9	5.13	112.30	108.20
21	AA	1142	G	N3-C4-C5	-5.13	126.03	128.60
54	BA	2002	G	C5-C6-N1	5.13	114.06	111.50
19	AT	28	ARG	NE-CZ-NH1	5.13	122.86	120.30
21	AA	96	U	O4'-C1'-N1	5.13	112.30	108.20
21	AA	792	A	C1'-O4'-C4'	-5.13	105.80	109.90
21	AA	1406	U	C5-C6-N1	-5.13	120.14	122.70
54	BA	281	C	O4'-C1'-N1	5.13	112.30	108.20
54	BA	547	A	O4'-C4'-C3'	5.13	110.20	106.10
54	BA	2300	C	N1-C2-O2	5.13	121.98	118.90
21	AA	631	C	N1-C2-O2	5.13	121.98	118.90
55	BB	17	C	O4'-C1'-N1	5.13	112.30	108.20
21	AA	788	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	31	C	N1-C2-O2	5.12	121.97	118.90
54	BA	440	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	479	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1214	A	O4'-C1'-N9	5.12	112.30	108.20
54	BA	2503	A	C5'-C4'-O4'	5.12	115.25	109.10
54	BA	623	C	N1-C2-O2	5.12	121.97	118.90
54	BA	796	C	N3-C4-N4	-5.12	114.42	118.00
54	BA	1639	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1864	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	2025	C	N1-C2-O2	5.12	121.97	118.90
21	AA	1152	A	C6-C5-N7	5.12	135.88	132.30
54	BA	54	G	N3-C2-N2	-5.12	116.32	119.90
54	BA	1468	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1634	A	C6-C5-N7	5.12	135.88	132.30
55	BB	23	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	870	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	331	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	486	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1263	U	C3'-C2'-C1'	5.12	105.59	101.50
21	AA	240	G	C1'-O4'-C4'	-5.12	105.81	109.90
54	BA	364	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2103	C	O4'-C1'-N1	5.12	112.29	108.20
26	BD	169	ARG	NE-CZ-NH1	5.12	122.86	120.30
54	BA	1015	U	N3-C2-O2	-5.12	118.62	122.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2559	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2658	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2757	A	C5'-C4'-O4'	5.12	115.24	109.10
21	AA	405	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	416	G	C5-C6-N1	5.11	114.06	111.50
21	AA	955	U	O4'-C1'-N1	5.11	112.29	108.20
22	A1	50	G	N3-C2-N2	-5.11	116.32	119.90
24	A3	17	C	N1-C2-O2	5.11	121.97	118.90
54	BA	32	C	N1-C2-O2	5.11	121.97	118.90
54	BA	458	G	C3'-C2'-C1'	-5.11	97.41	101.50
54	BA	1080	A	O4'-C1'-N9	5.11	112.29	108.20
54	BA	2783	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	2840	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	646	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	306	A	C4-C5-C6	-5.11	114.44	117.00
24	A3	30	G	N3-C4-C5	-5.11	126.05	128.60
54	BA	574	A	C5-C6-N6	5.11	127.79	123.70
54	BA	859	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	987	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	1105	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	2842	G	O4'-C1'-N9	5.11	112.29	108.20
21	AA	785	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	9	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	1186	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	1842	G	N3-C2-N2	-5.11	116.32	119.90
54	BA	2291	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	676	A	C6-C5-N7	5.11	135.88	132.30
54	BA	706	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	1238	G	N1-C6-O6	-5.11	116.84	119.90
54	BA	1314	C	C6-N1-C2	-5.11	118.26	120.30
21	AA	1007	U	N3-C2-O2	-5.11	118.63	122.20
54	BA	501	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	1549	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	2090	A	C6-C5-N7	5.11	135.87	132.30
21	AA	1259	C	N1-C2-O2	5.10	121.96	118.90
54	BA	947	A	C6-C5-N7	5.10	135.87	132.30
54	BA	1051	G	N3-C2-N2	-5.10	116.33	119.90
54	BA	1846	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	2699	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1422	G	N3-C2-N2	-5.10	116.33	119.90
21	AA	818	G	N3-C2-N2	-5.10	116.33	119.90
21	AA	1114	C	N1-C2-O2	5.10	121.96	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	804	A	C3'-C2'-C1'	5.10	105.58	101.50
54	BA	911	A	C6-C5-N7	5.10	135.87	132.30
54	BA	1526	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	1981	A	C3'-C2'-C1'	5.10	105.58	101.50
54	BA	2181	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2297	A	C1'-O4'-C4'	-5.10	105.82	109.90
21	AA	911	U	N1-C2-N3	5.10	117.96	114.90
21	AA	927	G	C5-C6-N1	5.10	114.05	111.50
54	BA	112	U	C5-C6-N1	-5.10	120.15	122.70
54	BA	645	C	N1-C2-O2	5.10	121.96	118.90
54	BA	699	A	C6-C5-N7	5.10	135.87	132.30
54	BA	2119	A	O4'-C1'-N9	5.10	112.28	108.20
33	BK	108	ARG	NE-CZ-NH1	5.10	122.85	120.30
54	BA	2727	A	C6-C5-N7	5.10	135.87	132.30
21	AA	794	A	C6-C5-N7	5.09	135.87	132.30
21	AA	1302	C	N1-C2-O2	5.09	121.96	118.90
48	BZ	15	ARG	NE-CZ-NH2	-5.09	117.75	120.30
54	BA	201	C	N3-C4-C5	5.09	123.94	121.90
54	BA	1183	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1335	C	C3'-C2'-C1'	5.09	105.58	101.50
21	AA	295	C	N1-C2-O2	5.09	121.96	118.90
21	AA	557	G	N1-C6-O6	-5.09	116.84	119.90
21	AA	588	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	1178	C	N3-C2-O2	-5.09	118.33	121.90
54	BA	1566	A	C4-C5-C6	-5.09	114.45	117.00
21	AA	1006	G	N3-C2-N2	-5.09	116.33	119.90
21	AA	1239	A	C3'-C2'-C1'	5.09	105.57	101.50
54	BA	2432	A	C4-C5-C6	-5.09	114.45	117.00
21	AA	1281	C	N1-C2-O2	5.09	121.95	118.90
22	A1	57	G	N7-C8-N9	5.09	115.64	113.10
24	A3	23	G	C1'-O4'-C4'	-5.09	105.83	109.90
54	BA	1036	G	N3-C4-C5	-5.09	126.06	128.60
54	BA	1779	U	C5'-C4'-O4'	5.09	115.21	109.10
54	BA	2566	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	2759	G	C3'-C2'-C1'	5.09	105.57	101.50
1	AB	10	LYS	O-C-N	-5.09	114.56	122.70
21	AA	344	A	C4-C5-C6	-5.09	114.46	117.00
21	AA	860	A	C6-C5-N7	5.09	135.86	132.30
54	BA	712	G	N3-C2-N2	-5.09	116.34	119.90
54	BA	2714	G	N3-C2-N2	-5.09	116.34	119.90
56	B5	71	ARG	NE-CZ-NH2	-5.09	117.76	120.30
21	AA	379	C	N1-C2-O2	5.09	121.95	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1337	G	P-O3'-C3'	5.09	125.80	119.70
21	AA	1434	A	C6-C5-N7	5.09	135.86	132.30
24	A3	16	C	N3-C4-C5	5.09	123.93	121.90
54	BA	786	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1609	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	1931	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	2591	C	N1-C2-O2	5.09	121.95	118.90
54	BA	1136	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	1207	C	N1-C2-O2	5.08	121.95	118.90
54	BA	1434	A	C4'-C3'-C2'	-5.08	97.52	102.60
21	AA	903	G	O4'-C1'-N9	5.08	112.27	108.20
21	AA	1342	C	C3'-C2'-C1'	-5.08	97.43	101.50
21	AA	53	A	C6-C5-N7	5.08	135.86	132.30
54	BA	366	C	N3-C2-O2	-5.08	118.34	121.90
54	BA	372	G	C8-N9-C4	-5.08	104.37	106.40
54	BA	414	C	N3-C2-O2	-5.08	118.34	121.90
54	BA	2095	A	C5-C6-N1	5.08	120.24	117.70
54	BA	2212	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	2435	A	O4'-C1'-N9	5.08	112.27	108.20
21	AA	99	C	N3-C4-C5	5.08	123.93	121.90
54	BA	440	C	N1-C2-O2	5.08	121.95	118.90
54	BA	1020	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	346	G	N3-C4-C5	-5.08	126.06	128.60
21	AA	974	A	C4-C5-C6	-5.08	114.46	117.00
53	B4	19	ARG	NE-CZ-NH2	-5.08	117.76	120.30
54	BA	1523	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	2285	C	O4'-C1'-N1	5.08	112.26	108.20
21	AA	756	C	N1-C2-O2	5.08	121.94	118.90
54	BA	1420	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	2106	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	2804	U	O4'-C1'-N1	5.08	112.26	108.20
11	AL	30	ARG	CD-NE-CZ	5.07	130.70	123.60
21	AA	582	C	N3-C2-O2	-5.07	118.35	121.90
21	AA	697	U	O4'-C1'-N1	5.07	112.26	108.20
21	AA	1286	U	N3-C2-O2	-5.07	118.65	122.20
21	AA	1415	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	349	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	773	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	1592	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1736	U	C5-C6-N1	-5.07	120.16	122.70
54	BA	2170	A	C6-C5-N7	5.07	135.85	132.30
54	BA	2543	G	N3-C2-N2	-5.07	116.35	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2674	G	N3-C2-N2	-5.07	116.35	119.90
54	BA	2824	C	O4'-C1'-N1	5.07	112.26	108.20
54	BA	2856	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	1741	C	O4'-C1'-N1	5.07	112.26	108.20
54	BA	2596	U	C5-C6-N1	-5.07	120.16	122.70
21	AA	271	C	N1-C2-O2	5.07	121.94	118.90
21	AA	446	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	1447	A	C5'-C4'-C3'	-5.07	107.89	116.00
54	BA	281	C	N1-C2-O2	5.07	121.94	118.90
54	BA	930	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1292	G	C3'-C2'-C1'	5.07	105.56	101.50
54	BA	1695	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	1067	A	C6-C5-N7	5.07	135.85	132.30
43	BU	6	ARG	NE-CZ-NH1	5.07	122.83	120.30
54	BA	914	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1295	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	2331	G	N3-C4-C5	-5.07	126.07	128.60
54	BA	2430	A	C6-N1-C2	-5.07	115.56	118.60
54	BA	2649	C	N1-C2-O2	5.07	121.94	118.90
12	AM	70	ARG	NE-CZ-NH1	5.07	122.83	120.30
21	AA	6	G	N3-C4-C5	-5.07	126.07	128.60
21	AA	560	A	C4-C5-C6	-5.07	114.47	117.00
21	AA	1496	C	N3-C2-O2	-5.07	118.35	121.90
54	BA	602	A	C6-C5-N7	5.07	135.85	132.30
54	BA	806	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1520	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1806	C	C5'-C4'-O4'	5.07	115.18	109.10
54	BA	2474	U	N3-C2-O2	-5.07	118.65	122.20
21	AA	1308	U	C5'-C4'-O4'	5.06	115.18	109.10
21	AA	1410	A	C6-C5-N7	5.06	135.84	132.30
23	A2	83	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	2306	C	N1-C2-O2	5.06	121.94	118.90
21	AA	410	G	N1-C6-O6	-5.06	116.86	119.90
21	AA	653	U	N3-C2-O2	-5.06	118.66	122.20
43	BU	81	ARG	NE-CZ-NH1	5.06	122.83	120.30
54	BA	512	G	O4'-C1'-N9	5.06	112.25	108.20
21	AA	973	G	N1-C6-O6	-5.06	116.86	119.90
21	AA	282	A	C6-C5-N7	5.06	135.84	132.30
54	BA	949	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	988	A	C6-C5-N7	5.06	135.84	132.30
21	AA	165	G	N7-C8-N9	5.06	115.63	113.10
21	AA	284	C	N1-C2-O2	5.06	121.94	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BO	7	ARG	NE-CZ-NH1	5.06	122.83	120.30
54	BA	917	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	1004	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1091	G	N1-C6-O6	-5.06	116.87	119.90
54	BA	1791	A	C6-C5-N7	5.06	135.84	132.30
54	BA	1940	U	C1'-O4'-C4'	-5.06	105.85	109.90
54	BA	2091	C	N1-C2-O2	5.06	121.94	118.90
54	BA	2214	C	O4'-C1'-N1	5.06	112.25	108.20
21	AA	148	G	C5-C6-N1	5.06	114.03	111.50
21	AA	677	U	O4'-C1'-N1	5.06	112.25	108.20
21	AA	1512	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	667	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	750	A	C6-C5-N7	5.06	135.84	132.30
54	BA	2220	U	O4'-C1'-N1	5.06	112.25	108.20
21	AA	270	A	C6-C5-N7	5.05	135.84	132.30
21	AA	584	G	C5-C6-N1	5.05	114.03	111.50
54	BA	2017	U	C3'-C2'-C1'	5.05	105.54	101.50
54	BA	2287	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	2326	C	N1-C2-O2	5.05	121.93	118.90
21	AA	879	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1155	A	C6-C5-N7	5.05	135.84	132.30
54	BA	141	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	1267	C	C3'-C2'-C1'	5.05	105.54	101.50
22	A1	66	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	271	G	O4'-C4'-C3'	5.05	110.14	106.10
54	BA	619	G	N3-C4-C5	-5.05	126.08	128.60
54	BA	1992	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	2354	C	O4'-C1'-N1	5.05	112.24	108.20
21	AA	240	G	N3-C2-N2	-5.05	116.36	119.90
21	AA	945	G	C8-N9-C4	-5.05	104.38	106.40
21	AA	1479	C	N1-C2-O2	5.05	121.93	118.90
54	BA	985	C	N1-C2-O2	5.05	121.93	118.90
54	BA	994	C	O4'-C4'-C3'	5.05	110.14	106.10
54	BA	2643	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	2698	U	N3-C2-O2	-5.05	118.67	122.20
21	AA	748	G	C5-C6-N1	5.05	114.02	111.50
54	BA	1107	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1731	G	N1-C6-O6	-5.05	116.87	119.90
11	AL	120	ARG	NE-CZ-NH2	5.05	122.82	120.30
21	AA	28	A	C6-C5-N7	5.05	135.83	132.30
21	AA	619	U	N3-C2-O2	-5.05	118.67	122.20
54	BA	351	C	N1-C2-O2	5.05	121.93	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2380	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2696	U	O4'-C1'-N1	5.05	112.24	108.20
21	AA	1503	A	C4-C5-C6	-5.04	114.48	117.00
55	BB	73	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	341	C	N1-C2-O2	5.04	121.93	118.90
54	BA	217	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	390	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	554	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	878	A	O4'-C1'-N9	5.04	112.23	108.20
54	BA	1017	G	N1-C6-O6	-5.04	116.87	119.90
54	BA	1455	G	C5'-C4'-C3'	-5.04	107.93	116.00
55	BB	38	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	43	G	C3'-C2'-C1'	5.04	105.53	101.50
54	BA	1349	C	N1-C2-O2	5.04	121.92	118.90
22	A1	45	G	C5-C6-N1	5.04	114.02	111.50
54	BA	841	G	C4'-C3'-C2'	-5.04	97.56	102.60
54	BA	1044	C	N1-C2-O2	5.04	121.92	118.90
12	AM	56	ARG	NE-CZ-NH1	5.04	122.82	120.30
54	BA	986	C	N1-C2-O2	5.04	121.92	118.90
21	AA	348	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	1467	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	171	A	C6-C5-N7	5.04	135.82	132.30
21	AA	263	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	666	G	N3-C2-N2	-5.04	116.38	119.90
21	AA	1511	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2716	C	N1-C2-O2	5.04	121.92	118.90
54	BA	861	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1857	G	N3-C4-C5	-5.03	126.08	128.60
54	BA	2120	G	N3-C4-C5	-5.03	126.08	128.60
54	BA	2416	C	N1-C2-O2	5.03	121.92	118.90
21	AA	277	C	N1-C2-O2	5.03	121.92	118.90
54	BA	185	G	O4'-C1'-N9	5.03	112.23	108.20
21	AA	173	U	N3-C2-O2	-5.03	118.68	122.20
48	BZ	30	ARG	NE-CZ-NH1	5.03	122.81	120.30
54	BA	479	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1168	G	N3-C4-C5	-5.03	126.08	128.60
54	BA	2307	G	N3-C4-C5	-5.03	126.08	128.60
54	BA	2331	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	2433	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	1331	G	C5-C6-N1	5.03	114.01	111.50
54	BA	2126	A	C4-C5-C6	-5.03	114.48	117.00
21	AA	1518	A	C4-C5-C6	-5.03	114.49	117.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	908	C	O4'-C1'-N1	5.03	112.22	108.20
38	BP	71	ARG	NE-CZ-NH1	5.03	122.81	120.30
38	BP	102	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
54	BA	307	G	N3-C2-N2	-5.03	116.38	119.90
54	BA	1270	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	2022	U	N3-C2-O2	-5.03	118.68	122.20
55	BB	114	C	N1-C2-O2	5.03	121.92	118.90
22	A1	53	G	N9-C4-C5	5.02	107.41	105.40
28	BF	111	ARG	NE-CZ-NH2	-5.02	117.79	120.30
54	BA	869	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	1220	G	O4'-C1'-N9	5.02	112.22	108.20
54	BA	1943	U	N3-C2-O2	-5.02	118.68	122.20
21	AA	596	A	C4-C5-C6	-5.02	114.49	117.00
53	B4	4	ARG	NE-CZ-NH1	5.02	122.81	120.30
54	BA	506	G	O4'-C1'-N9	5.02	112.22	108.20
54	BA	2099	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	2321	U	N3-C2-O2	-5.02	118.68	122.20
54	BA	2391	G	C5-C6-N1	5.02	114.01	111.50
54	BA	2759	G	N1-C6-O6	-5.02	116.89	119.90
55	BB	24	G	O4'-C4'-C3'	5.02	110.12	106.10
55	BB	103	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	725	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	945	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	26	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	643	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	964	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1630	A	C6-C5-N7	5.02	135.81	132.30
54	BA	2729	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	268	U	C5-C6-N1	-5.02	120.19	122.70
21	AA	346	G	C5-C6-N1	5.02	114.01	111.50
21	AA	697	U	N3-C2-O2	-5.02	118.69	122.20
26	BD	46	ARG	NE-CZ-NH1	5.02	122.81	120.30
54	BA	873	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1638	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2244	U	O4'-C4'-C3'	5.02	110.12	106.10
21	AA	287	U	O4'-C1'-N1	5.02	112.22	108.20
21	AA	1020	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	62	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	159	G	N3-C2-N2	-5.02	116.39	119.90
54	BA	1514	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	1593	A	O4'-C1'-N9	5.02	112.21	108.20
54	BA	1651	G	N1-C6-O6	-5.02	116.89	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1500	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	1547	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	2137	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	2265	U	O4'-C1'-N1	5.02	112.21	108.20
54	BA	2374	C	N1-C2-O2	5.02	121.91	118.90
21	AA	184	G	C8-N9-C4	-5.01	104.39	106.40
21	AA	610	U	N3-C2-O2	-5.01	118.69	122.20
39	BQ	27	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	179	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1660	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	2613	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	293	G	N7-C8-N9	5.01	115.61	113.10
54	BA	405	U	O4'-C1'-N1	5.01	112.21	108.20
55	BB	9	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	660	C	C3'-C2'-C1'	5.01	105.51	101.50
54	BA	1225	G	C5-C6-N1	5.01	114.01	111.50
54	BA	1667	G	N1-C6-O6	-5.01	116.89	119.90
9	AJ	72	ARG	NE-CZ-NH2	5.01	122.81	120.30
21	AA	995	C	O4'-C1'-N1	5.01	112.21	108.20
24	A3	75	C	N1-C2-O2	5.01	121.91	118.90
54	BA	364	C	N3-C2-O2	-5.01	118.39	121.90
54	BA	1314	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1357	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1493	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1520	U	C5-C6-N1	-5.01	120.19	122.70
54	BA	2157	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	2618	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	811	C	O4'-C1'-N1	5.01	112.21	108.20
54	BA	373	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	1434	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	1668	A	C6-C5-N7	5.01	135.81	132.30
54	BA	2167	U	C5-C6-N1	-5.01	120.20	122.70
54	BA	999	U	C5-C6-N1	-5.01	120.20	122.70
54	BA	1301	A	C1'-O4'-C4'	-5.01	105.89	109.90
54	BA	1306	C	O4'-C1'-N1	5.01	112.20	108.20
54	BA	1706	C	N1-C2-O2	5.01	121.90	118.90
54	BA	2065	C	N1-C2-O2	5.01	121.90	118.90
54	BA	2377	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	1475	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	1738	G	O4'-C4'-C3'	5.00	110.10	106.10
54	BA	1798	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1836	C	N3-C4-C5	5.00	123.90	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1528	U	N3-C2-O2	-5.00	118.70	122.20
54	BA	127	A	O4'-C1'-N9	5.00	112.20	108.20
54	BA	303	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	1148	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1256	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	1408	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	1813	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	2308	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	2870	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	787	A	C4-C5-C6	-5.00	114.50	117.00
21	AA	948	C	N1-C2-O2	5.00	121.90	118.90
21	AA	1107	C	N3-C4-C5	5.00	123.90	121.90
24	A3	23	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	796	C	N1-C2-O2	5.00	121.90	118.90
54	BA	2735	G	C5-C6-N1	5.00	114.00	111.50

There are no chirality outliers.

All (1158) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	11	C	Sidechain
22	A1	15	G	Sidechain
22	A1	18	G	Sidechain
22	A1	19	G	Sidechain
22	A1	2	G	Sidechain
22	A1	25	C	Sidechain
22	A1	28	C	Sidechain
22	A1	29	U	Sidechain
22	A1	30	C	Sidechain
22	A1	33	U	Sidechain
22	A1	43	G	Sidechain
22	A1	58	A	Sidechain
22	A1	6	A	Sidechain
22	A1	65	C	Sidechain
22	A1	66	A	Sidechain
22	A1	67	U	Sidechain
22	A1	70	C	Sidechain
22	A1	73	A	Sidechain
22	A1	74	C	Sidechain
22	A1	76	A	Sidechain
22	A1	8	U	Sidechain
23	A2	80	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
23	A2	83	U	Sidechain
23	A2	84	G	Sidechain
23	A2	85	G	Sidechain
23	A2	92	U	Sidechain
24	A3	11	A	Sidechain
24	A3	2	G	Sidechain
24	A3	34	U	Sidechain
24	A3	46	G	Sidechain
24	A3	54	G	Sidechain
24	A3	60	A	Sidechain
24	A3	66	C	Sidechain
21	AA	10	A	Sidechain
21	AA	1000	A	Sidechain
21	AA	1012	A	Sidechain
21	AA	1013	G	Sidechain
21	AA	1019	A	Sidechain
21	AA	1021	A	Sidechain
21	AA	1025	U	Sidechain
21	AA	1033	G	Sidechain
21	AA	1048	G	Sidechain
21	AA	1049	U	Sidechain
21	AA	1052	U	Sidechain
21	AA	1055	A	Sidechain
21	AA	1057	G	Sidechain
21	AA	1058	G	Sidechain
21	AA	1060	U	Sidechain
21	AA	1061	G	Sidechain
21	AA	1064	G	Sidechain
21	AA	1069	C	Sidechain
21	AA	1073	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	108	G	Sidechain
21	AA	1080	A	Sidechain
21	AA	1083	U	Sidechain
21	AA	1084	G	Sidechain
21	AA	1085	U	Sidechain
21	AA	109	A	Sidechain
21	AA	1101	A	Sidechain
21	AA	1107	C	Sidechain
21	AA	1117	A	Sidechain
21	AA	1125	U	Sidechain
21	AA	1128	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
21	AA	1129	C	Sidechain
21	AA	1131	G	Sidechain
21	AA	1139	G	Sidechain
21	AA	114	U	Sidechain
21	AA	1141	C	Sidechain
21	AA	1147	C	Sidechain
21	AA	1153	G	Sidechain
21	AA	1158	C	Sidechain
21	AA	1161	C	Sidechain
21	AA	1167	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1184	G	Sidechain
21	AA	1193	G	Sidechain
21	AA	1195	C	Sidechain
21	AA	12	U	Sidechain
21	AA	1202	U	Sidechain
21	AA	1204	A	Sidechain
21	AA	121	U	Sidechain
21	AA	1211	U	Sidechain
21	AA	1212	U	Sidechain
21	AA	1225	A	Sidechain
21	AA	1226	C	Sidechain
21	AA	1227	A	Sidechain
21	AA	1228	C	Sidechain
21	AA	123	U	Sidechain
21	AA	1234	C	Sidechain
21	AA	125	U	Sidechain
21	AA	1256	A	Sidechain
21	AA	1264	U	Sidechain
21	AA	1266	G	Sidechain
21	AA	1276	G	Sidechain
21	AA	1279	G	Sidechain
21	AA	1285	A	Sidechain
21	AA	1289	A	Sidechain
21	AA	129	A	Sidechain
21	AA	1297	G	Sidechain
21	AA	1298	U	Sidechain
21	AA	1300	G	Sidechain
21	AA	1301	U	Sidechain
21	AA	1303	C	Sidechain
21	AA	1304	G	Sidechain
21	AA	1309	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
21	AA	1316	G	Sidechain
21	AA	1320	C	Sidechain
21	AA	1321	U	Sidechain
21	AA	1324	A	Sidechain
21	AA	1326	U	Sidechain
21	AA	1328	C	Sidechain
21	AA	1331	G	Sidechain
21	AA	1335	U	Sidechain
21	AA	1336	C	Sidechain
21	AA	1337	G	Sidechain
21	AA	1339	A	Sidechain
21	AA	1342	C	Sidechain
21	AA	1343	G	Sidechain
21	AA	1356	G	Sidechain
21	AA	1357	A	Sidechain
21	AA	1359	C	Sidechain
21	AA	1361	G	Sidechain
21	AA	1366	C	Sidechain
21	AA	1386	G	Sidechain
21	AA	1387	G	Sidechain
21	AA	1390	U	Sidechain
21	AA	1392	G	Sidechain
21	AA	1397	C	Sidechain
21	AA	1398	A	Sidechain
21	AA	1399	C	Sidechain
21	AA	140	U	Sidechain
21	AA	1400	C	Sidechain
21	AA	1405	G	Sidechain
21	AA	1406	U	Sidechain
21	AA	1432	G	Sidechain
21	AA	1435	G	Sidechain
21	AA	1436	U	Sidechain
21	AA	1438	G	Sidechain
21	AA	1439	G	Sidechain
21	AA	1441	A	Sidechain
21	AA	1442	G	Sidechain
21	AA	1448	C	Sidechain
21	AA	1452	C	Sidechain
21	AA	1459	G	Sidechain
21	AA	1465	A	Sidechain
21	AA	1473	G	Sidechain
21	AA	1478	U	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
21	AA	148	G	Sidechain
21	AA	1484	C	Sidechain
21	AA	1491	G	Sidechain
21	AA	1493	A	Sidechain
21	AA	1494	G	Sidechain
21	AA	1495	U	Sidechain
21	AA	1498	U	Sidechain
21	AA	1504	G	Sidechain
21	AA	1512	U	Sidechain
21	AA	1514	G	Sidechain
21	AA	1516	G	Sidechain
21	AA	1517	G	Sidechain
21	AA	1519	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1523	G	Sidechain
21	AA	153	C	Sidechain
21	AA	159	G	Sidechain
21	AA	163	C	Sidechain
21	AA	168	G	Sidechain
21	AA	173	U	Sidechain
21	AA	175	C	Sidechain
21	AA	184	G	Sidechain
21	AA	187	G	Sidechain
21	AA	195	A	Sidechain
21	AA	197	A	Sidechain
21	AA	198	G	Sidechain
21	AA	20	U	Sidechain
21	AA	200	G	Sidechain
21	AA	201	G	Sidechain
21	AA	204	G	Sidechain
21	AA	206	C	Sidechain
21	AA	208	U	Sidechain
21	AA	211	G	Sidechain
21	AA	215	C	Sidechain
21	AA	223	A	Sidechain
21	AA	236	A	Sidechain
21	AA	238	A	Sidechain
21	AA	239	U	Sidechain
21	AA	240	G	Sidechain
21	AA	241	G	Sidechain
21	AA	254	G	Sidechain
21	AA	257	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
21	AA	26	A	Sidechain
21	AA	263	A	Sidechain
21	AA	266	G	Sidechain
21	AA	282	A	Sidechain
21	AA	284	C	Sidechain
21	AA	29	U	Sidechain
21	AA	292	G	Sidechain
21	AA	294	U	Sidechain
21	AA	295	C	Sidechain
21	AA	296	U	Sidechain
21	AA	298	A	Sidechain
21	AA	299	G	Sidechain
21	AA	304	U	Sidechain
21	AA	305	G	Sidechain
21	AA	308	C	Sidechain
21	AA	31	G	Sidechain
21	AA	314	C	Sidechain
21	AA	315	A	Sidechain
21	AA	316	C	Sidechain
21	AA	317	U	Sidechain
21	AA	324	G	Sidechain
21	AA	328	C	Sidechain
21	AA	331	G	Sidechain
21	AA	333	U	Sidechain
21	AA	336	A	Sidechain
21	AA	337	G	Sidechain
21	AA	340	U	Sidechain
21	AA	346	G	Sidechain
21	AA	349	A	Sidechain
21	AA	359	G	Sidechain
21	AA	36	C	Sidechain
21	AA	362	G	Sidechain
21	AA	363	A	Sidechain
21	AA	368	U	Sidechain
21	AA	373	A	Sidechain
21	AA	376	G	Sidechain
21	AA	377	G	Sidechain
21	AA	380	G	Sidechain
21	AA	381	C	Sidechain
21	AA	382	A	Sidechain
21	AA	383	A	Sidechain
21	AA	384	G	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
21	AA	388	G	Sidechain
21	AA	391	G	Sidechain
21	AA	397	A	Sidechain
21	AA	403	C	Sidechain
21	AA	404	G	Sidechain
21	AA	408	A	Sidechain
21	AA	409	U	Sidechain
21	AA	412	A	Sidechain
21	AA	413	G	Sidechain
21	AA	421	U	Sidechain
21	AA	423	G	Sidechain
21	AA	425	G	Sidechain
21	AA	427	U	Sidechain
21	AA	428	G	Sidechain
21	AA	429	U	Sidechain
21	AA	430	A	Sidechain
21	AA	436	C	Sidechain
21	AA	442	G	Sidechain
21	AA	446	G	Sidechain
21	AA	448	A	Sidechain
21	AA	450	G	Sidechain
21	AA	453	G	Sidechain
21	AA	454	G	Sidechain
21	AA	459	A	Sidechain
21	AA	461	A	Sidechain
21	AA	464	U	Sidechain
21	AA	466	A	Sidechain
21	AA	467	U	Sidechain
21	AA	47	C	Sidechain
21	AA	476	U	Sidechain
21	AA	480	U	Sidechain
21	AA	481	G	Sidechain
21	AA	483	C	Sidechain
21	AA	487	A	Sidechain
21	AA	494	G	Sidechain
21	AA	499	A	Sidechain
21	AA	5	U	Sidechain
21	AA	50	A	Sidechain
21	AA	500	G	Sidechain
21	AA	503	C	Sidechain
21	AA	504	C	Sidechain
21	AA	505	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
21	AA	506	G	Sidechain
21	AA	513	C	Sidechain
21	AA	517	G	Sidechain
21	AA	519	C	Sidechain
21	AA	524	G	Sidechain
21	AA	530	G	Sidechain
21	AA	535	A	Sidechain
21	AA	536	C	Sidechain
21	AA	537	G	Sidechain
21	AA	538	G	Sidechain
21	AA	540	G	Sidechain
21	AA	558	G	Sidechain
21	AA	564	C	Sidechain
21	AA	568	G	Sidechain
21	AA	572	A	Sidechain
21	AA	575	G	Sidechain
21	AA	583	A	Sidechain
21	AA	597	G	Sidechain
21	AA	60	A	Sidechain
21	AA	600	A	Sidechain
21	AA	604	G	Sidechain
21	AA	608	A	Sidechain
21	AA	61	G	Sidechain
21	AA	610	U	Sidechain
21	AA	612	C	Sidechain
21	AA	613	C	Sidechain
21	AA	614	C	Sidechain
21	AA	617	G	Sidechain
21	AA	618	C	Sidechain
21	AA	620	C	Sidechain
21	AA	621	A	Sidechain
21	AA	623	C	Sidechain
21	AA	626	G	Sidechain
21	AA	628	G	Sidechain
21	AA	633	G	Sidechain
21	AA	640	A	Sidechain
21	AA	641	U	Sidechain
21	AA	642	A	Sidechain
21	AA	646	G	Sidechain
21	AA	652	U	Sidechain
21	AA	662	U	Sidechain
21	AA	672	U	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
21	AA	675	A	Sidechain
21	AA	676	A	Sidechain
21	AA	677	U	Sidechain
21	AA	678	U	Sidechain
21	AA	682	G	Sidechain
21	AA	69	G	Sidechain
21	AA	690	G	Sidechain
21	AA	691	G	Sidechain
21	AA	695	A	Sidechain
21	AA	698	G	Sidechain
21	AA	700	G	Sidechain
21	AA	703	G	Sidechain
21	AA	710	G	Sidechain
21	AA	714	G	Sidechain
21	AA	715	A	Sidechain
21	AA	717	U	Sidechain
21	AA	727	G	Sidechain
21	AA	739	C	Sidechain
21	AA	740	U	Sidechain
21	AA	741	G	Sidechain
21	AA	752	G	Sidechain
21	AA	754	C	Sidechain
21	AA	76	G	Sidechain
21	AA	760	G	Sidechain
21	AA	763	G	Sidechain
21	AA	764	C	Sidechain
21	AA	766	A	Sidechain
21	AA	771	G	Sidechain
21	AA	79	G	Sidechain
21	AA	790	A	Sidechain
21	AA	795	C	Sidechain
21	AA	798	U	Sidechain
21	AA	803	G	Sidechain
21	AA	804	U	Sidechain
21	AA	805	C	Sidechain
21	AA	811	C	Sidechain
21	AA	816	A	Sidechain
21	AA	819	A	Sidechain
21	AA	824	G	Sidechain
21	AA	826	C	Sidechain
21	AA	827	U	Sidechain
21	AA	829	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
21	AA	833	G	Sidechain
21	AA	836	G	Sidechain
21	AA	838	G	Sidechain
21	AA	840	C	Sidechain
21	AA	842	U	Sidechain
21	AA	844	G	Sidechain
21	AA	846	G	Sidechain
21	AA	865	A	Sidechain
21	AA	873	A	Sidechain
21	AA	875	U	Sidechain
21	AA	881	G	Sidechain
21	AA	884	U	Sidechain
21	AA	887	G	Sidechain
21	AA	891	U	Sidechain
21	AA	895	G	Sidechain
21	AA	898	G	Sidechain
21	AA	899	C	Sidechain
21	AA	90	C	Sidechain
21	AA	900	A	Sidechain
21	AA	903	G	Sidechain
21	AA	904	U	Sidechain
21	AA	905	U	Sidechain
21	AA	909	A	Sidechain
21	AA	917	G	Sidechain
21	AA	926	G	Sidechain
21	AA	928	G	Sidechain
21	AA	931	C	Sidechain
21	AA	933	G	Sidechain
21	AA	94	G	Sidechain
21	AA	943	U	Sidechain
21	AA	944	G	Sidechain
21	AA	947	G	Sidechain
21	AA	949	A	Sidechain
21	AA	954	G	Sidechain
21	AA	957	U	Sidechain
21	AA	961	U	Sidechain
21	AA	966	G	Sidechain
21	AA	97	G	Sidechain
21	AA	978	A	Sidechain
21	AA	981	U	Sidechain
21	AA	982	U	Sidechain
21	AA	986	U	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
21	AA	988	G	Sidechain
21	AA	990	C	Sidechain
21	AA	991	U	Sidechain
21	AA	994	A	Sidechain
21	AA	999	C	Sidechain
3	AD	204	SER	Mainchain
8	AI	105	ARG	Sidechain
14	AO	87	ARG	Sidechain
54	BA	1000	A	Sidechain
54	BA	101	A	Sidechain
54	BA	1025	G	Sidechain
54	BA	1026	G	Sidechain
54	BA	1027	A	Sidechain
54	BA	1030	C	Sidechain
54	BA	1034	G	Sidechain
54	BA	1040	A	Sidechain
54	BA	1042	G	Sidechain
54	BA	1047	G	Sidechain
54	BA	1055	G	Sidechain
54	BA	106	C	Sidechain
54	BA	1061	U	Sidechain
54	BA	1064	C	Sidechain
54	BA	1068	G	Sidechain
54	BA	1070	A	Sidechain
54	BA	1071	G	Sidechain
54	BA	1076	C	Sidechain
54	BA	1081	U	Sidechain
54	BA	1095	A	Sidechain
54	BA	1099	G	Sidechain
54	BA	11	C	Sidechain
54	BA	110	G	Sidechain
54	BA	1106	G	Sidechain
54	BA	1109	C	Sidechain
54	BA	1112	G	Sidechain
54	BA	1114	C	Sidechain
54	BA	112	U	Sidechain
54	BA	1124	G	Sidechain
54	BA	1128	G	Sidechain
54	BA	113	U	Sidechain
54	BA	1132	U	Sidechain
54	BA	1135	C	Sidechain
54	BA	1138	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	1139	G	Sidechain
54	BA	1143	A	Sidechain
54	BA	1144	A	Sidechain
54	BA	1148	U	Sidechain
54	BA	1149	G	Sidechain
54	BA	1151	A	Sidechain
54	BA	1157	G	Sidechain
54	BA	1158	C	Sidechain
54	BA	1171	G	Sidechain
54	BA	1175	A	Sidechain
54	BA	1178	C	Sidechain
54	BA	1179	G	Sidechain
54	BA	1186	G	Sidechain
54	BA	1190	G	Sidechain
54	BA	1198	U	Sidechain
54	BA	1202	G	Sidechain
54	BA	121	G	Sidechain
54	BA	1210	G	Sidechain
54	BA	1212	G	Sidechain
54	BA	1216	G	Sidechain
54	BA	1220	G	Sidechain
54	BA	1223	G	Sidechain
54	BA	1224	U	Sidechain
54	BA	1236	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	1239	G	Sidechain
54	BA	124	G	Sidechain
54	BA	1246	A	Sidechain
54	BA	1251	C	Sidechain
54	BA	1262	A	Sidechain
54	BA	1263	U	Sidechain
54	BA	1265	A	Sidechain
54	BA	1266	G	Sidechain
54	BA	1270	C	Sidechain
54	BA	1273	U	Sidechain
54	BA	1283	G	Sidechain
54	BA	1287	A	Sidechain
54	BA	1289	C	Sidechain
54	BA	1290	C	Sidechain
54	BA	1293	C	Sidechain
54	BA	1307	A	Sidechain
54	BA	1309	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	1313	U	Sidechain
54	BA	1315	C	Sidechain
54	BA	1316	U	Sidechain
54	BA	1318	U	Sidechain
54	BA	1319	C	Sidechain
54	BA	1320	C	Sidechain
54	BA	1323	C	Sidechain
54	BA	1331	G	Sidechain
54	BA	1338	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1350	C	Sidechain
54	BA	1352	U	Sidechain
54	BA	1355	G	Sidechain
54	BA	1360	G	Sidechain
54	BA	1361	G	Sidechain
54	BA	1369	G	Sidechain
54	BA	1370	C	Sidechain
54	BA	1376	C	Sidechain
54	BA	1378	A	Sidechain
54	BA	138	U	Sidechain
54	BA	1386	C	Sidechain
54	BA	1387	A	Sidechain
54	BA	1389	G	Sidechain
54	BA	1391	U	Sidechain
54	BA	1393	A	Sidechain
54	BA	1395	A	Sidechain
54	BA	1396	U	Sidechain
54	BA	1397	U	Sidechain
54	BA	1399	C	Sidechain
54	BA	140	C	Sidechain
54	BA	1404	C	Sidechain
54	BA	1408	G	Sidechain
54	BA	141	G	Sidechain
54	BA	1412	U	Sidechain
54	BA	1414	C	Sidechain
54	BA	1415	U	Sidechain
54	BA	1416	G	Sidechain
54	BA	1417	C	Sidechain
54	BA	1419	A	Sidechain
54	BA	1424	G	Sidechain
54	BA	143	C	Sidechain
54	BA	1432	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	1433	A	Sidechain
54	BA	1439	A	Sidechain
54	BA	1442	U	Sidechain
54	BA	1445	G	Sidechain
54	BA	1448	G	Sidechain
54	BA	1449	G	Sidechain
54	BA	1450	G	Sidechain
54	BA	1454	C	Sidechain
54	BA	1456	G	Sidechain
54	BA	1460	U	Sidechain
54	BA	1465	G	Sidechain
54	BA	1478	G	Sidechain
54	BA	1480	C	Sidechain
54	BA	1487	U	Sidechain
54	BA	1488	C	Sidechain
54	BA	1489	C	Sidechain
54	BA	1492	G	Sidechain
54	BA	1494	A	Sidechain
54	BA	1495	A	Sidechain
54	BA	1507	C	Sidechain
54	BA	1509	A	Sidechain
54	BA	1519	G	Sidechain
54	BA	152	A	Sidechain
54	BA	1525	A	Sidechain
54	BA	153	U	Sidechain
54	BA	1530	G	Sidechain
54	BA	1535	A	Sidechain
54	BA	1536	C	Sidechain
54	BA	1538	G	Sidechain
54	BA	1539	U	Sidechain
54	BA	154	U	Sidechain
54	BA	1540	G	Sidechain
54	BA	1544	A	Sidechain
54	BA	1546	G	Sidechain
54	BA	155	A	Sidechain
54	BA	1554	U	Sidechain
54	BA	1555	G	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1564	C	Sidechain
54	BA	1567	G	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	1568	G	Sidechain
54	BA	1569	A	Sidechain
54	BA	1586	A	Sidechain
54	BA	1587	G	Sidechain
54	BA	1595	C	Sidechain
54	BA	1596	A	Sidechain
54	BA	1597	A	Sidechain
54	BA	1599	U	Sidechain
54	BA	160	A	Sidechain
54	BA	1601	G	Sidechain
54	BA	1602	U	Sidechain
54	BA	1604	C	Sidechain
54	BA	1606	C	Sidechain
54	BA	1610	A	Sidechain
54	BA	1621	U	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1634	A	Sidechain
54	BA	1638	C	Sidechain
54	BA	1646	C	Sidechain
54	BA	1649	G	Sidechain
54	BA	165	A	Sidechain
54	BA	1657	U	Sidechain
54	BA	1662	U	Sidechain
54	BA	1664	A	Sidechain
54	BA	1666	G	Sidechain
54	BA	1671	U	Sidechain
54	BA	1672	A	Sidechain
54	BA	1674	G	Sidechain
54	BA	1677	A	Sidechain
54	BA	1681	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1683	U	Sidechain
54	BA	1684	G	Sidechain
54	BA	1698	A	Sidechain
54	BA	17	G	Sidechain
54	BA	1700	A	Sidechain
54	BA	1704	C	Sidechain
54	BA	1705	A	Sidechain
54	BA	1709	U	Sidechain
54	BA	1710	G	Sidechain
54	BA	1724	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	1727	C	Sidechain
54	BA	1730	C	Sidechain
54	BA	1731	G	Sidechain
54	BA	1732	C	Sidechain
54	BA	1741	C	Sidechain
54	BA	1743	G	Sidechain
54	BA	1747	U	Sidechain
54	BA	1752	C	Sidechain
54	BA	1753	G	Sidechain
54	BA	1756	G	Sidechain
54	BA	1758	U	Sidechain
54	BA	1759	A	Sidechain
54	BA	1762	A	Sidechain
54	BA	177	G	Sidechain
54	BA	1773	A	Sidechain
54	BA	1774	C	Sidechain
54	BA	1788	C	Sidechain
54	BA	1790	C	Sidechain
54	BA	1797	G	Sidechain
54	BA	180	G	Sidechain
54	BA	1807	G	Sidechain
54	BA	1816	C	Sidechain
54	BA	1820	U	Sidechain
54	BA	1823	G	Sidechain
54	BA	1827	U	Sidechain
54	BA	1830	C	Sidechain
54	BA	1831	G	Sidechain
54	BA	1832	C	Sidechain
54	BA	1844	C	Sidechain
54	BA	1847	A	Sidechain
54	BA	1853	A	Sidechain
54	BA	1857	G	Sidechain
54	BA	1861	G	Sidechain
54	BA	1866	A	Sidechain
54	BA	1867	G	Sidechain
54	BA	1871	A	Sidechain
54	BA	1874	C	Sidechain
54	BA	1876	A	Sidechain
54	BA	1884	G	Sidechain
54	BA	1888	G	Sidechain
54	BA	189	G	Sidechain
54	BA	1891	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	1894	C	Sidechain
54	BA	1897	G	Sidechain
54	BA	19	A	Sidechain
54	BA	1902	C	Sidechain
54	BA	1912	A	Sidechain
54	BA	1915	U	Sidechain
54	BA	1929	G	Sidechain
54	BA	1931	U	Sidechain
54	BA	1932	A	Sidechain
54	BA	1933	G	Sidechain
54	BA	1935	G	Sidechain
54	BA	1938	A	Sidechain
54	BA	1940	U	Sidechain
54	BA	1942	C	Sidechain
54	BA	1943	U	Sidechain
54	BA	1944	U	Sidechain
54	BA	1945	G	Sidechain
54	BA	195	A	Sidechain
54	BA	1950	G	Sidechain
54	BA	196	A	Sidechain
54	BA	1960	A	Sidechain
54	BA	1961	C	Sidechain
54	BA	1962	C	Sidechain
54	BA	197	A	Sidechain
54	BA	1971	U	Sidechain
54	BA	1972	G	Sidechain
54	BA	1974	C	Sidechain
54	BA	1977	A	Sidechain
54	BA	1980	G	Sidechain
54	BA	1982	U	Sidechain
54	BA	1989	G	Sidechain
54	BA	1993	U	Sidechain
54	BA	1997	C	Sidechain
54	BA	2	G	Sidechain
54	BA	2002	G	Sidechain
54	BA	2014	A	Sidechain
54	BA	2017	U	Sidechain
54	BA	2018	G	Sidechain
54	BA	2020	A	Sidechain
54	BA	2022	U	Sidechain
54	BA	203	A	Sidechain
54	BA	2030	A	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	2037	A	Sidechain
54	BA	2038	G	Sidechain
54	BA	2046	G	Sidechain
54	BA	205	G	Sidechain
54	BA	2056	G	Sidechain
54	BA	2059	A	Sidechain
54	BA	2064	C	Sidechain
54	BA	2067	G	Sidechain
54	BA	207	A	Sidechain
54	BA	2073	C	Sidechain
54	BA	2074	U	Sidechain
54	BA	2077	A	Sidechain
54	BA	208	C	Sidechain
54	BA	2085	U	Sidechain
54	BA	2097	A	Sidechain
54	BA	2099	U	Sidechain
54	BA	210	C	Sidechain
54	BA	2100	G	Sidechain
54	BA	2101	A	Sidechain
54	BA	2105	U	Sidechain
54	BA	2106	U	Sidechain
54	BA	2109	U	Sidechain
54	BA	2115	G	Sidechain
54	BA	2126	A	Sidechain
54	BA	2130	U	Sidechain
54	BA	2131	U	Sidechain
54	BA	2134	A	Sidechain
54	BA	2136	G	Sidechain
54	BA	2144	G	Sidechain
54	BA	2154	A	Sidechain
54	BA	2164	C	Sidechain
54	BA	2165	C	Sidechain
54	BA	2166	U	Sidechain
54	BA	2168	G	Sidechain
54	BA	2179	C	Sidechain
54	BA	2180	U	Sidechain
54	BA	2181	U	Sidechain
54	BA	2186	G	Sidechain
54	BA	2188	U	Sidechain
54	BA	2193	G	Sidechain
54	BA	2196	C	Sidechain
54	BA	2197	U	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	2199	A	Sidechain
54	BA	2204	G	Sidechain
54	BA	2206	C	Sidechain
54	BA	2207	C	Sidechain
54	BA	221	A	Sidechain
54	BA	2210	U	Sidechain
54	BA	2213	U	Sidechain
54	BA	2216	G	Sidechain
54	BA	2217	G	Sidechain
54	BA	2218	G	Sidechain
54	BA	2225	A	Sidechain
54	BA	2227	A	Sidechain
54	BA	2233	U	Sidechain
54	BA	2235	G	Sidechain
54	BA	2236	U	Sidechain
54	BA	2239	G	Sidechain
54	BA	2241	A	Sidechain
54	BA	2249	U	Sidechain
54	BA	2259	U	Sidechain
54	BA	2266	A	Sidechain
54	BA	2267	A	Sidechain
54	BA	2268	A	Sidechain
54	BA	2271	G	Sidechain
54	BA	2281	A	Sidechain
54	BA	2282	G	Sidechain
54	BA	2283	C	Sidechain
54	BA	2287	A	Sidechain
54	BA	2294	G	Sidechain
54	BA	2296	U	Sidechain
54	BA	2300	C	Sidechain
54	BA	2302	U	Sidechain
54	BA	2305	U	Sidechain
54	BA	2308	G	Sidechain
54	BA	231	A	Sidechain
54	BA	2321	U	Sidechain
54	BA	2323	G	Sidechain
54	BA	2324	U	Sidechain
54	BA	2327	A	Sidechain
54	BA	2328	A	Sidechain
54	BA	2330	G	Sidechain
54	BA	2333	A	Sidechain
54	BA	2336	A	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	2337	G	Sidechain
54	BA	2339	C	Sidechain
54	BA	2340	A	Sidechain
54	BA	2347	C	Sidechain
54	BA	235	U	Sidechain
54	BA	2352	A	Sidechain
54	BA	2357	G	Sidechain
54	BA	2362	C	Sidechain
54	BA	2367	G	Sidechain
54	BA	2369	A	Sidechain
54	BA	2375	G	Sidechain
54	BA	2381	A	Sidechain
54	BA	2385	C	Sidechain
54	BA	2389	G	Sidechain
54	BA	239	C	Sidechain
54	BA	2390	U	Sidechain
54	BA	240	C	Sidechain
54	BA	2406	A	Sidechain
54	BA	2411	A	Sidechain
54	BA	2413	G	Sidechain
54	BA	2425	A	Sidechain
54	BA	2427	C	Sidechain
54	BA	2428	G	Sidechain
54	BA	2429	G	Sidechain
54	BA	2432	A	Sidechain
54	BA	2433	A	Sidechain
54	BA	2439	A	Sidechain
54	BA	244	A	Sidechain
54	BA	2442	C	Sidechain
54	BA	2448	A	Sidechain
54	BA	2450	A	Sidechain
54	BA	2451	A	Sidechain
54	BA	2455	G	Sidechain
54	BA	2456	C	Sidechain
54	BA	2458	G	Sidechain
54	BA	2461	A	Sidechain
54	BA	2462	C	Sidechain
54	BA	2464	G	Sidechain
54	BA	2465	C	Sidechain
54	BA	2466	C	Sidechain
54	BA	2468	A	Sidechain
54	BA	2472	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	2475	C	Sidechain
54	BA	2484	G	Sidechain
54	BA	2485	G	Sidechain
54	BA	2488	G	Sidechain
54	BA	2489	U	Sidechain
54	BA	2498	C	Sidechain
54	BA	2499	C	Sidechain
54	BA	250	G	Sidechain
54	BA	2500	U	Sidechain
54	BA	2503	A	Sidechain
54	BA	2508	G	Sidechain
54	BA	2509	G	Sidechain
54	BA	2517	C	Sidechain
54	BA	2529	G	Sidechain
54	BA	2533	U	Sidechain
54	BA	2536	G	Sidechain
54	BA	2540	C	Sidechain
54	BA	2550	G	Sidechain
54	BA	2557	G	Sidechain
54	BA	2558	C	Sidechain
54	BA	2564	A	Sidechain
54	BA	2566	A	Sidechain
54	BA	2567	G	Sidechain
54	BA	2571	U	Sidechain
54	BA	2573	C	Sidechain
54	BA	2576	G	Sidechain
54	BA	2578	G	Sidechain
54	BA	2581	G	Sidechain
54	BA	2589	A	Sidechain
54	BA	2590	A	Sidechain
54	BA	2592	G	Sidechain
54	BA	2595	G	Sidechain
54	BA	2601	C	Sidechain
54	BA	2607	G	Sidechain
54	BA	2608	G	Sidechain
54	BA	2612	C	Sidechain
54	BA	2613	U	Sidechain
54	BA	2617	U	Sidechain
54	BA	2625	G	Sidechain
54	BA	2626	C	Sidechain
54	BA	2630	G	Sidechain
54	BA	2631	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	2633	G	Sidechain
54	BA	2637	U	Sidechain
54	BA	2638	G	Sidechain
54	BA	2640	G	Sidechain
54	BA	2641	G	Sidechain
54	BA	2643	G	Sidechain
54	BA	2649	C	Sidechain
54	BA	265	A	Sidechain
54	BA	2655	G	Sidechain
54	BA	2656	U	Sidechain
54	BA	2657	A	Sidechain
54	BA	2661	G	Sidechain
54	BA	2663	G	Sidechain
54	BA	2665	A	Sidechain
54	BA	2666	C	Sidechain
54	BA	2674	G	Sidechain
54	BA	2675	A	Sidechain
54	BA	2681	C	Sidechain
54	BA	2682	A	Sidechain
54	BA	2689	U	Sidechain
54	BA	2690	U	Sidechain
54	BA	2698	U	Sidechain
54	BA	27	G	Sidechain
54	BA	2704	C	Sidechain
54	BA	2706	A	Sidechain
54	BA	271	G	Sidechain
54	BA	2718	G	Sidechain
54	BA	272	A	Sidechain
54	BA	2721	A	Sidechain
54	BA	2726	A	Sidechain
54	BA	2729	G	Sidechain
54	BA	2731	G	Sidechain
54	BA	2732	G	Sidechain
54	BA	2738	A	Sidechain
54	BA	2740	A	Sidechain
54	BA	2745	C	Sidechain
54	BA	2756	U	Sidechain
54	BA	2760	C	Sidechain
54	BA	2762	C	Sidechain
54	BA	2765	A	Sidechain
54	BA	2777	G	Sidechain
54	BA	2780	G	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	2784	U	Sidechain
54	BA	279	A	Sidechain
54	BA	2790	U	Sidechain
54	BA	2793	C	Sidechain
54	BA	2794	C	Sidechain
54	BA	2798	U	Sidechain
54	BA	2808	G	Sidechain
54	BA	281	C	Sidechain
54	BA	2810	A	Sidechain
54	BA	2811	G	Sidechain
54	BA	2816	G	Sidechain
54	BA	2819	G	Sidechain
54	BA	2824	C	Sidechain
54	BA	2831	G	Sidechain
54	BA	2832	U	Sidechain
54	BA	2833	U	Sidechain
54	BA	2835	A	Sidechain
54	BA	2836	U	Sidechain
54	BA	2852	G	Sidechain
54	BA	2856	A	Sidechain
54	BA	2859	G	Sidechain
54	BA	2862	G	Sidechain
54	BA	2864	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	2876	G	Sidechain
54	BA	2877	G	Sidechain
54	BA	2886	A	Sidechain
54	BA	2889	C	Sidechain
54	BA	2896	C	Sidechain
54	BA	2899	A	Sidechain
54	BA	2901	C	Sidechain
54	BA	2902	C	Sidechain
54	BA	291	G	Sidechain
54	BA	295	G	Sidechain
54	BA	299	A	Sidechain
54	BA	303	G	Sidechain
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	31	C	Sidechain
54	BA	313	G	Sidechain
54	BA	317	G	Sidechain
54	BA	326	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	33	C	Sidechain
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	336	C	Sidechain
54	BA	337	C	Sidechain
54	BA	347	A	Sidechain
54	BA	354	A	Sidechain
54	BA	361	G	Sidechain
54	BA	362	A	Sidechain
54	BA	363	G	Sidechain
54	BA	369	U	Sidechain
54	BA	370	G	Sidechain
54	BA	378	C	Sidechain
54	BA	389	G	Sidechain
54	BA	392	U	Sidechain
54	BA	394	C	Sidechain
54	BA	395	U	Sidechain
54	BA	410	G	Sidechain
54	BA	418	C	Sidechain
54	BA	419	U	Sidechain
54	BA	422	A	Sidechain
54	BA	426	C	Sidechain
54	BA	428	A	Sidechain
54	BA	43	G	Sidechain
54	BA	431	U	Sidechain
54	BA	433	C	Sidechain
54	BA	436	C	Sidechain
54	BA	440	C	Sidechain
54	BA	446	G	Sidechain
54	BA	449	A	Sidechain
54	BA	450	G	Sidechain
54	BA	454	A	Sidechain
54	BA	456	C	Sidechain
54	BA	458	G	Sidechain
54	BA	459	U	Sidechain
54	BA	463	G	Sidechain
54	BA	47	C	Sidechain
54	BA	472	A	Sidechain
54	BA	474	G	Sidechain
54	BA	475	C	Sidechain
54	BA	476	G	Sidechain
54	BA	48	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	480	A	Sidechain
54	BA	481	G	Sidechain
54	BA	488	G	Sidechain
54	BA	49	A	Sidechain
54	BA	492	A	Sidechain
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain
54	BA	502	A	Sidechain
54	BA	504	A	Sidechain
54	BA	505	A	Sidechain
54	BA	507	A	Sidechain
54	BA	508	A	Sidechain
54	BA	51	G	Sidechain
54	BA	511	U	Sidechain
54	BA	514	A	Sidechain
54	BA	525	U	Sidechain
54	BA	528	A	Sidechain
54	BA	530	G	Sidechain
54	BA	533	G	Sidechain
54	BA	537	G	Sidechain
54	BA	54	G	Sidechain
54	BA	541	A	Sidechain
54	BA	548	G	Sidechain
54	BA	551	G	Sidechain
54	BA	558	U	Sidechain
54	BA	568	U	Sidechain
54	BA	577	G	Sidechain
54	BA	586	A	Sidechain
54	BA	588	U	Sidechain
54	BA	589	U	Sidechain
54	BA	595	C	Sidechain
54	BA	599	A	Sidechain
54	BA	60	G	Sidechain
54	BA	600	G	Sidechain
54	BA	605	G	Sidechain
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	614	A	Sidechain
54	BA	621	A	Sidechain
54	BA	626	A	Sidechain
54	BA	628	G	Sidechain
54	BA	629	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	630	G	Sidechain
54	BA	631	A	Sidechain
54	BA	638	G	Sidechain
54	BA	64	A	Sidechain
54	BA	641	U	Sidechain
54	BA	646	U	Sidechain
54	BA	65	U	Sidechain
54	BA	661	A	Sidechain
54	BA	662	G	Sidechain
54	BA	663	G	Sidechain
54	BA	665	U	Sidechain
54	BA	670	A	Sidechain
54	BA	671	C	Sidechain
54	BA	674	G	Sidechain
54	BA	676	A	Sidechain
54	BA	68	G	Sidechain
54	BA	686	U	Sidechain
54	BA	69	C	Sidechain
54	BA	697	G	Sidechain
54	BA	707	G	Sidechain
54	BA	71	A	Sidechain
54	BA	714	U	Sidechain
54	BA	718	A	Sidechain
54	BA	724	U	Sidechain
54	BA	725	G	Sidechain
54	BA	728	G	Sidechain
54	BA	730	A	Sidechain
54	BA	738	G	Sidechain
54	BA	74	A	Sidechain
54	BA	746	U	Sidechain
54	BA	75	G	Sidechain
54	BA	750	A	Sidechain
54	BA	754	U	Sidechain
54	BA	76	C	Sidechain
54	BA	771	G	Sidechain
54	BA	773	U	Sidechain
54	BA	775	G	Sidechain
54	BA	782	A	Sidechain
54	BA	79	C	Sidechain
54	BA	799	G	Sidechain
54	BA	800	A	Sidechain
54	BA	801	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	802	A	Sidechain
54	BA	803	U	Sidechain
54	BA	804	A	Sidechain
54	BA	810	U	Sidechain
54	BA	811	U	Sidechain
54	BA	816	C	Sidechain
54	BA	822	G	Sidechain
54	BA	823	C	Sidechain
54	BA	827	U	Sidechain
54	BA	828	U	Sidechain
54	BA	831	G	Sidechain
54	BA	832	U	Sidechain
54	BA	837	C	Sidechain
54	BA	848	C	Sidechain
54	BA	849	A	Sidechain
54	BA	851	C	Sidechain
54	BA	853	C	Sidechain
54	BA	858	G	Sidechain
54	BA	862	G	Sidechain
54	BA	864	G	Sidechain
54	BA	869	G	Sidechain
54	BA	87	U	Sidechain
54	BA	874	G	Sidechain
54	BA	880	G	Sidechain
54	BA	886	A	Sidechain
54	BA	887	U	Sidechain
54	BA	889	C	Sidechain
54	BA	902	C	Sidechain
54	BA	906	U	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	914	G	Sidechain
54	BA	928	A	Sidechain
54	BA	934	U	Sidechain
54	BA	937	C	Sidechain
54	BA	938	G	Sidechain
54	BA	94	A	Sidechain
54	BA	942	G	Sidechain
54	BA	946	C	Sidechain
54	BA	947	A	Sidechain
54	BA	950	G	Sidechain
54	BA	951	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
54	BA	952	G	Sidechain
54	BA	954	G	Sidechain
54	BA	955	U	Sidechain
54	BA	957	C	Sidechain
54	BA	959	A	Sidechain
54	BA	96	C	Sidechain
54	BA	966	G	Sidechain
54	BA	968	C	Sidechain
54	BA	969	G	Sidechain
54	BA	975	A	Sidechain
54	BA	976	G	Sidechain
54	BA	980	A	Sidechain
54	BA	981	A	Sidechain
54	BA	982	C	Sidechain
54	BA	984	A	Sidechain
54	BA	986	C	Sidechain
54	BA	989	G	Sidechain
54	BA	99	U	Sidechain
54	BA	992	C	Sidechain
54	BA	993	G	Sidechain
55	BB	100	G	Sidechain
55	BB	108	A	Sidechain
55	BB	109	A	Sidechain
55	BB	11	C	Sidechain
55	BB	12	C	Sidechain
55	BB	14	U	Sidechain
55	BB	18	G	Sidechain
55	BB	27	C	Sidechain
55	BB	33	G	Sidechain
55	BB	34	A	Sidechain
55	BB	40	U	Sidechain
55	BB	41	G	Sidechain
55	BB	60	C	Sidechain
55	BB	62	C	Sidechain
55	BB	65	U	Sidechain
55	BB	69	G	Sidechain
55	BB	73	A	Sidechain
55	BB	75	G	Sidechain
55	BB	83	G	Sidechain
55	BB	93	C	Sidechain
27	BE	101	TYR	Sidechain
37	BO	7	ARG	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
39	BQ	44	TYR	Sidechain
45	BW	54	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	1	0
11	AL	955	0	1019	1	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	1	0
19	AT	668	0	718	2	0
20	AU	429	0	453	0	0
21	AA	32828	0	16522	3	0
22	A1	1627	0	832	1	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	1	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	1	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	1	0
54	BA	62317	0	31343	6	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	A1	10	0	10	0	0
All	All	147653	0	99663	16	0

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

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AT:40:ALA:HB1	19:AT:41:GLY:HA2	1.86	0.57
54:BA:1977:A:H2'	54:BA:1978:A:C8	2.51	0.46
54:BA:1709:U:H2'	54:BA:1710:G:C8	2.52	0.44
18:AS:78:THR:HB	18:AS:79:TYR:HA	1.99	0.44
39:BQ:40:LYS:HE2	39:BQ:44:TYR:CZ	2.53	0.44
53:B4:1:MET:HA	53:B4:34:LYS:O	2.17	0.44

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:AA:1412:C:H2'	21:AA:1413:A:C8	2.53	0.43
10:AK:34:THR:HG21	21:AA:707:U:H1'	1.99	0.43
54:BA:2318:G:H2'	54:BA:2319:G:C8	2.54	0.43
54:BA:889:C:H1'	54:BA:890:C:C6	2.54	0.43
19:AT:40:ALA:HB1	19:AT:41:GLY:CA	2.49	0.42
54:BA:1752:C:H2'	54:BA:1753:G:C8	2.56	0.41
22:A1:55:PSU:HO2'	22:A1:57:G:H8	1.65	0.41
54:BA:152:A:H2'	54:BA:153:U:C6	2.56	0.41
35:BM:119:LEU:H	35:BM:119:LEU:HD23	1.86	0.40
11:AL:47:ALA:HB3	21:AA:529:G:H22	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	201 (92%)	14 (6%)	3 (1%)	14	58
2	AC	205/208 (99%)	189 (92%)	13 (6%)	3 (2%)	13	57
3	AD	203/206 (98%)	188 (93%)	13 (6%)	2 (1%)	19	65
4	AE	150/152 (99%)	135 (90%)	10 (7%)	5 (3%)	5	40
5	AF	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	4	35
6	AG	150/152 (99%)	134 (89%)	13 (9%)	3 (2%)	9	51
7	AH	127/130 (98%)	117 (92%)	5 (4%)	5 (4%)	4	36
8	AI	126/128 (98%)	106 (84%)	16 (13%)	4 (3%)	5	41
9	AJ	98/100 (98%)	91 (93%)	2 (2%)	5 (5%)	2	30
10	AK	116/118 (98%)	109 (94%)	4 (3%)	3 (3%)	7	45
11	AL	121/124 (98%)	109 (90%)	9 (7%)	3 (2%)	7	46
12	AM	112/115 (97%)	93 (83%)	14 (12%)	5 (4%)	3	33

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	AN	98/101 (97%)	88 (90%)	9 (9%)	1 (1%)	19	65
14	AO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	16	61
15	AP	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	7	46
16	AQ	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
17	AR	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	11	53
18	AS	79/81 (98%)	69 (87%)	9 (11%)	1 (1%)	15	60
19	AT	84/86 (98%)	73 (87%)	9 (11%)	2 (2%)	7	47
20	AU	51/53 (96%)	32 (63%)	15 (29%)	4 (8%)	1	20
25	BC	270/273 (99%)	236 (87%)	26 (10%)	8 (3%)	5	42
26	BD	207/209 (99%)	178 (86%)	15 (7%)	14 (7%)	1	23
27	BE	199/201 (99%)	187 (94%)	7 (4%)	5 (2%)	7	46
28	BF	176/179 (98%)	153 (87%)	18 (10%)	5 (3%)	6	44
29	BG	174/177 (98%)	160 (92%)	11 (6%)	3 (2%)	11	55
30	BH	147/149 (99%)	136 (92%)	9 (6%)	2 (1%)	14	58
31	BI	139/142 (98%)	127 (91%)	11 (8%)	1 (1%)	26	71
32	BJ	140/142 (99%)	131 (94%)	7 (5%)	2 (1%)	14	58
33	BK	121/123 (98%)	107 (88%)	10 (8%)	4 (3%)	5	40
34	BL	141/144 (98%)	122 (86%)	15 (11%)	4 (3%)	6	44
35	BM	134/136 (98%)	121 (90%)	8 (6%)	5 (4%)	4	38
36	BN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	11	55
37	BO	114/117 (97%)	105 (92%)	8 (7%)	1 (1%)	21	67
38	BP	112/115 (97%)	94 (84%)	11 (10%)	7 (6%)	2	25
39	BQ	115/118 (98%)	106 (92%)	6 (5%)	3 (3%)	7	45
40	BR	101/103 (98%)	92 (91%)	7 (7%)	2 (2%)	9	51
41	BS	108/110 (98%)	100 (93%)	5 (5%)	3 (3%)	6	44
42	BT	92/94 (98%)	77 (84%)	8 (9%)	7 (8%)	1	20
43	BU	101/104 (97%)	85 (84%)	10 (10%)	6 (6%)	2	27
44	BV	92/94 (98%)	86 (94%)	3 (3%)	3 (3%)	5	40
45	BW	78/80 (98%)	56 (72%)	16 (20%)	6 (8%)	1	20
46	BX	75/79 (95%)	66 (88%)	7 (9%)	2 (3%)	6	45
47	BY	61/63 (97%)	54 (88%)	5 (8%)	2 (3%)	5	40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BZ	56/59 (95%)	50 (89%)	5 (9%)	1 (2%)	11	53
49	B0	54/57 (95%)	44 (82%)	9 (17%)	1 (2%)	10	52
50	B1	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
51	B2	44/46 (96%)	42 (96%)	0	2 (4%)	3	33
52	B3	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	12	56
53	B4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
56	B5	221/234 (94%)	206 (93%)	13 (6%)	2 (1%)	21	67
All	All	5876/6008 (98%)	5254 (89%)	461 (8%)	161 (3%)	10	45

All (161) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	10	LYS
5	AF	90	MET
6	AG	5	VAL
7	AH	77	VAL
10	AK	125	LYS
11	AL	43	LYS
12	AM	85	TYR
26	BD	80	TRP
26	BD	170	VAL
27	BE	79	ARG
33	BK	103	VAL
43	BU	85	ARG
46	BX	43	LYS
1	AB	18	GLN
3	AD	29	THR
4	AE	105	ILE
5	AF	6	ILE
5	AF	10	VAL
6	AG	6	ILE
9	AJ	75	ASP
9	AJ	102	LEU
12	AM	3	ILE
12	AM	42	VAL
12	AM	104	ASN
17	AR	20	ILE
18	AS	5	LYS
20	AU	23	GLU
25	BC	189	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	BD	34	VAL
26	BD	41	ALA
26	BD	77	ARG
26	BD	119	ALA
26	BD	155	VAL
27	BE	90	GLN
27	BE	97	ASN
27	BE	147	LEU
28	BF	12	VAL
28	BF	103	ILE
29	BG	152	ARG
33	BK	25	LEU
34	BL	101	ILE
35	BM	70	ASP
36	BN	47	VAL
37	BO	89	ASP
39	BQ	87	VAL
39	BQ	91	ARG
40	BR	91	GLN
41	BS	88	ARG
42	BT	66	LYS
42	BT	68	LYS
42	BT	88	LYS
43	BU	45	GLN
45	BW	10	ARG
47	BY	23	ARG
48	BZ	32	GLY
51	B2	3	ARG
4	AE	54	GLU
6	AG	113	LYS
8	AI	127	SER
10	AK	126	ARG
11	AL	46	SER
13	AN	63	ARG
14	AO	43	ALA
15	AP	43	ALA
19	AT	3	ILE
19	AT	65	LEU
25	BC	43	ASN
25	BC	141	HIS
25	BC	142	ASN
25	BC	153	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	BD	40	LEU
26	BD	73	VAL
26	BD	150	GLN
28	BF	136	ILE
30	BH	148	ALA
32	BJ	81	ILE
34	BL	13	LYS
34	BL	82	LEU
35	BM	69	PRO
35	BM	110	GLU
38	BP	58	PHE
38	BP	113	LEU
42	BT	11	LEU
43	BU	5	ARG
43	BU	12	VAL
43	BU	43	LYS
45	BW	38	ARG
45	BW	44	PHE
52	B3	3	ILE
56	B5	91	GLY
56	B5	219	GLY
2	AC	195	ILE
7	AH	69	ALA
7	AH	78	SER
8	AI	120	ALA
9	AJ	45	ARG
9	AJ	57	VAL
9	AJ	92	LEU
10	AK	16	SER
20	AU	17	ARG
20	AU	49	ALA
25	BC	70	LYS
25	BC	204	LEU
26	BD	15	PHE
26	BD	51	THR
28	BF	132	ARG
28	BF	156	THR
29	BG	4	ALA
29	BG	22	VAL
30	BH	48	GLU
33	BK	92	GLU
36	BN	2	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
38	BP	74	GLN
41	BS	28	LYS
43	BU	70	ALA
44	BV	23	ALA
44	BV	24	ASN
45	BW	23	LYS
45	BW	56	HIS
46	BX	21	LEU
47	BY	7	ARG
51	B2	4	THR
1	AB	87	ASP
2	AC	189	HIS
5	AF	63	ASN
7	AH	2	MET
8	AI	55	ASP
8	AI	112	ARG
11	AL	117	GLY
12	AM	65	GLU
15	AP	17	TYR
31	BI	64	ARG
32	BJ	25	LEU
38	BP	31	VAL
38	BP	94	ALA
38	BP	110	LYS
41	BS	29	VAL
42	BT	70	HIS
45	BW	75	ASN
49	B0	26	SER
4	AE	103	GLY
7	AH	53	ASP
20	AU	3	ILE
26	BD	22	ILE
26	BD	167	ASN
33	BK	2	ILE
34	BL	24	GLY
35	BM	6	ARG
39	BQ	32	ARG
40	BR	53	PHE
42	BT	78	SER
44	BV	60	VAL
3	AD	27	ILE
4	AE	43	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
42	BT	2	ILE
27	BE	96	VAL
2	AC	14	VAL
4	AE	104	ILE
25	BC	108	GLY
35	BM	36	VAL
38	BP	20	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	176 (98%)	4 (2%)	60	83
2	AC	170/171 (99%)	167 (98%)	3 (2%)	66	87
3	AD	172/173 (99%)	171 (99%)	1 (1%)	90	95
4	AE	113/113 (100%)	112 (99%)	1 (1%)	84	93
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	86	94
7	AH	104/105 (99%)	102 (98%)	2 (2%)	65	86
8	AI	105/105 (100%)	104 (99%)	1 (1%)	82	92
9	AJ	86/86 (100%)	83 (96%)	3 (4%)	43	74
10	AK	90/90 (100%)	87 (97%)	3 (3%)	45	76
11	AL	103/104 (99%)	101 (98%)	2 (2%)	65	86
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	81 (98%)	2 (2%)	57	82
14	AO	76/77 (99%)	75 (99%)	1 (1%)	76	89
15	AP	65/65 (100%)	65 (100%)	0	100	100
16	AQ	74/74 (100%)	71 (96%)	3 (4%)	37	71
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	69 (99%)	1 (1%)	74	89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	212 (98%)	4 (2%)	65	86
26	BD	164/164 (100%)	161 (98%)	3 (2%)	66	87
27	BE	165/165 (100%)	165 (100%)	0	100	100
28	BF	149/150 (99%)	144 (97%)	5 (3%)	44	75
29	BG	137/138 (99%)	133 (97%)	4 (3%)	50	78
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	107 (98%)	2 (2%)	66	87
32	BJ	116/116 (100%)	114 (98%)	2 (2%)	68	87
33	BK	103/103 (100%)	102 (99%)	1 (1%)	82	92
34	BL	102/103 (99%)	102 (100%)	0	100	100
35	BM	109/109 (100%)	106 (97%)	3 (3%)	51	78
36	BN	100/100 (100%)	97 (97%)	3 (3%)	48	77
37	BO	86/87 (99%)	86 (100%)	0	100	100
38	BP	99/100 (99%)	98 (99%)	1 (1%)	82	92
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	80	91
40	BR	84/84 (100%)	82 (98%)	2 (2%)	57	82
41	BS	93/93 (100%)	92 (99%)	1 (1%)	80	91
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	83 (100%)	0	100	100
44	BV	78/78 (100%)	76 (97%)	2 (3%)	54	80
45	BW	59/59 (100%)	58 (98%)	1 (2%)	68	87
46	BX	67/68 (98%)	66 (98%)	1 (2%)	72	88
47	BY	55/55 (100%)	53 (96%)	2 (4%)	42	74
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	45 (96%)	2 (4%)	35	70
50	B1	45/45 (100%)	43 (96%)	2 (4%)	35	69
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	51 (100%)	0	100	100
53	B4	34/34 (100%)	33 (97%)	1 (3%)	50	78

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	B5	173/181 (96%)	170 (98%)	3 (2%)	68 87
All	All	4842/4870 (99%)	4768 (98%)	74 (2%)	74 88

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	22	TRP
1	AB	88	GLN
1	AB	135	MET
1	AB	169	HIS
2	AC	41	TYR
2	AC	182	ASP
2	AC	187	GLU
3	AD	54	LEU
4	AE	134	ASN
6	AG	129	ASN
7	AH	60	LEU
7	AH	86	LYS
8	AI	79	ARG
9	AJ	92	LEU
9	AJ	99	GLN
9	AJ	102	LEU
10	AK	19	VAL
10	AK	37	GLN
10	AK	80	ASN
11	AL	28	GLN
11	AL	93	ARG
13	AN	6	MET
13	AN	26	GLU
14	AO	20	ASP
16	AQ	42	LYS
16	AQ	46	HIS
16	AQ	69	THR
18	AS	54	ARG
25	BC	62	ARG
25	BC	173	LEU
25	BC	190	THR
25	BC	200	MET
26	BD	151	THR
26	BD	161	MET
26	BD	179	ARG
28	BF	4	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
28	BF	21	TYR
28	BF	41	GLU
28	BF	49	LEU
28	BF	173	ASP
29	BG	2	ARG
29	BG	115	GLN
29	BG	154	GLU
29	BG	166	GLU
31	BI	35	MET
31	BI	131	THR
32	BJ	50	THR
32	BJ	84	ILE
33	BK	105	ARG
35	BM	97	GLN
35	BM	108	VAL
35	BM	126	ILE
36	BN	1	MET
36	BN	97	ILE
36	BN	112	TYR
38	BP	64	SER
39	BQ	96	ASP
40	BR	40	MET
40	BR	94	THR
41	BS	74	ILE
44	BV	12	GLN
44	BV	44	HIS
45	BW	63	ASP
46	BX	73	ARG
47	BY	1	MET
47	BY	43	LEU
49	B0	40	HIS
49	B0	54	ILE
50	B1	10	LEU
50	B1	29	LYS
53	B4	35	GLN
56	B5	79	THR
56	B5	97	MET
56	B5	171	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	17	HIS
1	AB	202	ASN
11	AL	45	ASN
36	BN	3	HIS
44	BV	44	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	237 (15%)	85 (5%)
22	A1	73/76 (96%)	12 (16%)	8 (10%)
23	A2	14/15 (93%)	5 (35%)	2 (14%)
24	A3	76/77 (98%)	15 (19%)	6 (7%)
54	BA	2902/2903 (99%)	487 (16%)	135 (4%)
55	BB	116/118 (98%)	17 (14%)	3 (2%)
All	All	4711/4722 (99%)	773 (16%)	239 (5%)

All (773) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	9	G
21	AA	20	U
21	AA	21	G
21	AA	31	G
21	AA	32	A
21	AA	33	A
21	AA	36	C
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	49	U
21	AA	50	A
21	AA	51	A
21	AA	61	G
21	AA	72	A
21	AA	84	U
21	AA	85	U
21	AA	86	G
21	AA	87	C
21	AA	94	G
21	AA	95	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	AA	100	G
21	AA	110	C
21	AA	112	G
21	AA	120	A
21	AA	125	U
21	AA	151	A
21	AA	153	C
21	AA	161	A
21	AA	163	C
21	AA	164	G
21	AA	165	G
21	AA	183	C
21	AA	198	G
21	AA	201	G
21	AA	212	G
21	AA	235	C
21	AA	240	G
21	AA	244	U
21	AA	245	U
21	AA	247	G
21	AA	251	G
21	AA	255	G
21	AA	256	U
21	AA	266	G
21	AA	272	C
21	AA	289	G
21	AA	293	G
21	AA	294	U
21	AA	298	A
21	AA	301	G
21	AA	328	C
21	AA	330	C
21	AA	332	G
21	AA	344	A
21	AA	345	C
21	AA	346	G
21	AA	352	C
21	AA	353	A
21	AA	354	G
21	AA	358	U
21	AA	365	U
21	AA	372	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	AA	381	C
21	AA	384	G
21	AA	389	A
21	AA	398	U
21	AA	406	G
21	AA	412	A
21	AA	413	G
21	AA	414	A
21	AA	415	A
21	AA	421	U
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	452	A
21	AA	457	G
21	AA	463	U
21	AA	465	A
21	AA	466	A
21	AA	467	U
21	AA	468	A
21	AA	474	G
21	AA	482	A
21	AA	483	C
21	AA	484	G
21	AA	493	A
21	AA	495	A
21	AA	497	G
21	AA	509	A
21	AA	511	C
21	AA	524	G
21	AA	527	G
21	AA	532	A
21	AA	547	A
21	AA	559	A
21	AA	562	U
21	AA	566	G
21	AA	572	A
21	AA	573	A
21	AA	576	C
21	AA	580	C
21	AA	618	C
21	AA	619	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	AA	620	C
21	AA	623	C
21	AA	627	G
21	AA	632	U
21	AA	642	A
21	AA	653	U
21	AA	661	G
21	AA	687	A
21	AA	695	A
21	AA	700	G
21	AA	724	G
21	AA	753	A
21	AA	755	G
21	AA	777	A
21	AA	787	A
21	AA	794	A
21	AA	812	G
21	AA	816	A
21	AA	817	C
21	AA	819	A
21	AA	828	U
21	AA	841	C
21	AA	843	U
21	AA	844	G
21	AA	845	A
21	AA	846	G
21	AA	885	G
21	AA	900	A
21	AA	926	G
21	AA	927	G
21	AA	933	G
21	AA	937	A
21	AA	939	G
21	AA	945	G
21	AA	946	A
21	AA	959	A
21	AA	960	U
21	AA	962	C
21	AA	965	U
21	AA	966	G
21	AA	969	A
21	AA	971	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	AA	974	A
21	AA	976	G
21	AA	977	A
21	AA	978	A
21	AA	980	C
21	AA	983	A
21	AA	993	G
21	AA	994	A
21	AA	995	C
21	AA	996	A
21	AA	997	U
21	AA	1004	A
21	AA	1020	G
21	AA	1031	C
21	AA	1032	G
21	AA	1033	G
21	AA	1045	C
21	AA	1050	G
21	AA	1056	U
21	AA	1060	U
21	AA	1061	G
21	AA	1068	G
21	AA	1081	A
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1136	C
21	AA	1137	C
21	AA	1139	G
21	AA	1141	C
21	AA	1142	G
21	AA	1151	A
21	AA	1157	A
21	AA	1159	U
21	AA	1160	G
21	AA	1161	C
21	AA	1169	A
21	AA	1178	G
21	AA	1183	U
21	AA	1189	U
21	AA	1191	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	AA	1194	U
21	AA	1195	C
21	AA	1196	A
21	AA	1202	U
21	AA	1204	A
21	AA	1213	A
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1228	C
21	AA	1229	A
21	AA	1256	A
21	AA	1257	A
21	AA	1274	A
21	AA	1285	A
21	AA	1287	A
21	AA	1300	G
21	AA	1303	C
21	AA	1305	G
21	AA	1308	U
21	AA	1309	G
21	AA	1317	C
21	AA	1320	C
21	AA	1321	U
21	AA	1323	G
21	AA	1337	G
21	AA	1338	G
21	AA	1339	A
21	AA	1342	C
21	AA	1343	G
21	AA	1345	U
21	AA	1355	G
21	AA	1362	A
21	AA	1379	G
21	AA	1381	U
21	AA	1383	C
21	AA	1384	C
21	AA	1399	C
21	AA	1401	G
21	AA	1446	A
21	AA	1472	U
21	AA	1493	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
21	AA	1517	G
21	AA	1520	C
21	AA	1529	G
21	AA	1530	G
21	AA	1534	A
22	A1	10	G
22	A1	17	U
22	A1	21	A
22	A1	32	C
22	A1	48	C
22	A1	56	C
22	A1	57	G
22	A1	58	A
22	A1	61	C
22	A1	62	C
22	A1	73	A
22	A1	74	C
23	A2	81	U
23	A2	82	A
23	A2	83	U
23	A2	91	A
23	A2	92	U
24	A3	2	G
24	A3	9	G
24	A3	16	C
24	A3	18	U
24	A3	19	G
24	A3	20	G
24	A3	22	A
24	A3	48	U
24	A3	49	C
24	A3	55	5MU
24	A3	56	PSU
24	A3	60	A
24	A3	73	A
24	A3	75	C
24	A3	76	C
54	BA	10	A
54	BA	14	A
54	BA	15	G
54	BA	22	C
54	BA	43	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	44	A
54	BA	46	G
54	BA	48	G
54	BA	52	A
54	BA	60	G
54	BA	61	C
54	BA	62	U
54	BA	74	A
54	BA	75	G
54	BA	77	G
54	BA	91	A
54	BA	99	U
54	BA	100	U
54	BA	101	A
54	BA	102	U
54	BA	103	A
54	BA	119	A
54	BA	120	U
54	BA	127	A
54	BA	128	C
54	BA	142	A
54	BA	147	C
54	BA	148	U
54	BA	155	A
54	BA	173	A
54	BA	194	G
54	BA	196	A
54	BA	197	A
54	BA	199	A
54	BA	200	U
54	BA	204	A
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	230	G
54	BA	233	A
54	BA	244	A
54	BA	248	G
54	BA	249	C
54	BA	250	G
54	BA	258	G
54	BA	265	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	266	G
54	BA	278	A
54	BA	279	A
54	BA	280	U
54	BA	299	A
54	BA	301	G
54	BA	302	C
54	BA	316	C
54	BA	322	A
54	BA	323	C
54	BA	329	G
54	BA	330	A
54	BA	331	C
54	BA	346	A
54	BA	370	G
54	BA	371	A
54	BA	373	U
54	BA	374	A
54	BA	386	G
54	BA	387	U
54	BA	388	G
54	BA	389	G
54	BA	404	A
54	BA	411	G
54	BA	428	A
54	BA	443	A
54	BA	446	G
54	BA	447	A
54	BA	448	U
54	BA	451	U
54	BA	457	A
54	BA	458	G
54	BA	475	C
54	BA	481	G
54	BA	482	A
54	BA	491	G
54	BA	504	A
54	BA	509	C
54	BA	512	G
54	BA	527	C
54	BA	529	A
54	BA	530	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	544	C
54	BA	546	U
54	BA	548	G
54	BA	549	G
54	BA	550	C
54	BA	573	U
54	BA	574	A
54	BA	575	A
54	BA	577	G
54	BA	579	G
54	BA	590	A
54	BA	603	A
54	BA	613	A
54	BA	614	A
54	BA	615	U
54	BA	637	A
54	BA	647	G
54	BA	653	U
54	BA	654	A
54	BA	671	C
54	BA	672	C
54	BA	686	U
54	BA	719	C
54	BA	725	G
54	BA	730	A
54	BA	736	C
54	BA	747	U
54	BA	748	G
54	BA	751	A
54	BA	752	A
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	790	U
54	BA	792	A
54	BA	805	G
54	BA	806	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	810	U
54	BA	812	C
54	BA	827	U
54	BA	828	U
54	BA	847	U
54	BA	858	G
54	BA	866	A
54	BA	889	C
54	BA	890	C
54	BA	907	G
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	932	U
54	BA	933	A
54	BA	946	C
54	BA	958	U
54	BA	959	A
54	BA	961	C
54	BA	962	G
54	BA	965	C
54	BA	966	G
54	BA	974	G
54	BA	983	A
54	BA	984	A
54	BA	989	G
54	BA	990	A
54	BA	995	C
54	BA	996	A
54	BA	1012	U
54	BA	1013	C
54	BA	1024	G
54	BA	1025	G
54	BA	1026	G
54	BA	1033	U
54	BA	1046	A
54	BA	1047	G
54	BA	1063	G
54	BA	1068	G
54	BA	1070	A
54	BA	1071	G
54	BA	1073	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	1088	A
54	BA	1089	A
54	BA	1090	A
54	BA	1095	A
54	BA	1096	A
54	BA	1097	U
54	BA	1102	C
54	BA	1112	G
54	BA	1127	A
54	BA	1129	A
54	BA	1132	U
54	BA	1133	A
54	BA	1134	A
54	BA	1135	C
54	BA	1142	A
54	BA	1144	A
54	BA	1155	A
54	BA	1176	U
54	BA	1177	G
54	BA	1186	G
54	BA	1189	A
54	BA	1204	A
54	BA	1211	C
54	BA	1227	G
54	BA	1236	G
54	BA	1237	A
54	BA	1241	A
54	BA	1242	U
54	BA	1252	G
54	BA	1253	A
54	BA	1254	A
54	BA	1255	U
54	BA	1256	G
54	BA	1262	A
54	BA	1263	U
54	BA	1266	G
54	BA	1272	A
54	BA	1273	U
54	BA	1274	A
54	BA	1275	A
54	BA	1276	A
54	BA	1287	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	1300	G
54	BA	1301	A
54	BA	1302	A
54	BA	1303	G
54	BA	1311	G
54	BA	1313	U
54	BA	1328	A
54	BA	1332	G
54	BA	1341	G
54	BA	1342	A
54	BA	1350	C
54	BA	1365	A
54	BA	1366	A
54	BA	1379	U
54	BA	1380	G
54	BA	1384	A
54	BA	1385	A
54	BA	1386	C
54	BA	1388	G
54	BA	1390	U
54	BA	1396	U
54	BA	1416	G
54	BA	1417	C
54	BA	1420	A
54	BA	1427	A
54	BA	1428	C
54	BA	1440	U
54	BA	1452	G
54	BA	1453	A
54	BA	1455	G
54	BA	1459	G
54	BA	1460	U
54	BA	1461	C
54	BA	1482	G
54	BA	1490	A
54	BA	1491	G
54	BA	1493	C
54	BA	1508	A
54	BA	1509	A
54	BA	1523	U
54	BA	1538	G
54	BA	1539	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	1540	G
54	BA	1568	G
54	BA	1569	A
54	BA	1574	C
54	BA	1578	U
54	BA	1585	C
54	BA	1586	A
54	BA	1599	U
54	BA	1604	C
54	BA	1608	A
54	BA	1617	C
54	BA	1618	A
54	BA	1621	U
54	BA	1622	G
54	BA	1626	A
54	BA	1635	A
54	BA	1639	C
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1650	A
54	BA	1653	G
54	BA	1654	A
54	BA	1663	G
54	BA	1666	G
54	BA	1668	A
54	BA	1669	A
54	BA	1674	G
54	BA	1707	G
54	BA	1729	U
54	BA	1738	G
54	BA	1758	U
54	BA	1764	C
54	BA	1773	A
54	BA	1783	A
54	BA	1784	A
54	BA	1785	A
54	BA	1800	C
54	BA	1804	C
54	BA	1808	A
54	BA	1811	G
54	BA	1819	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	1820	U
54	BA	1830	C
54	BA	1835	G
54	BA	1847	A
54	BA	1870	C
54	BA	1871	A
54	BA	1873	G
54	BA	1874	C
54	BA	1900	A
54	BA	1914	C
54	BA	1915	U
54	BA	1930	G
54	BA	1931	U
54	BA	1937	A
54	BA	1938	A
54	BA	1939	U
54	BA	1943	U
54	BA	1944	U
54	BA	1945	G
54	BA	1952	A
54	BA	1953	A
54	BA	1955	U
54	BA	1967	C
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1981	A
54	BA	1982	U
54	BA	1993	U
54	BA	1996	C
54	BA	1997	C
54	BA	2006	C
54	BA	2022	U
54	BA	2023	C
54	BA	2032	G
54	BA	2035	G
54	BA	2044	C
54	BA	2052	A
54	BA	2055	C
54	BA	2060	A
54	BA	2061	G
54	BA	2063	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	2068	U
54	BA	2076	U
54	BA	2077	A
54	BA	2092	U
54	BA	2111	U
54	BA	2112	G
54	BA	2117	A
54	BA	2118	U
54	BA	2119	A
54	BA	2126	A
54	BA	2127	G
54	BA	2157	G
54	BA	2159	G
54	BA	2160	C
54	BA	2165	C
54	BA	2169	A
54	BA	2172	U
54	BA	2203	U
54	BA	2211	A
54	BA	2212	A
54	BA	2213	U
54	BA	2232	C
54	BA	2238	G
54	BA	2245	U
54	BA	2246	G
54	BA	2267	A
54	BA	2269	G
54	BA	2275	C
54	BA	2283	C
54	BA	2297	A
54	BA	2305	U
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2312	U
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2326	C
54	BA	2333	A
54	BA	2334	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	2335	A
54	BA	2347	C
54	BA	2353	G
54	BA	2383	G
54	BA	2385	C
54	BA	2388	A
54	BA	2389	G
54	BA	2390	U
54	BA	2391	G
54	BA	2392	A
54	BA	2394	C
54	BA	2407	A
54	BA	2424	C
54	BA	2425	A
54	BA	2426	A
54	BA	2428	G
54	BA	2429	G
54	BA	2431	U
54	BA	2432	A
54	BA	2433	A
54	BA	2434	A
54	BA	2439	A
54	BA	2440	C
54	BA	2441	U
54	BA	2447	G
54	BA	2448	A
54	BA	2449	U
54	BA	2474	U
54	BA	2478	A
54	BA	2485	G
54	BA	2491	U
54	BA	2496	C
54	BA	2498	C
54	BA	2499	C
54	BA	2500	U
54	BA	2502	G
54	BA	2504	U
54	BA	2505	G
54	BA	2529	G
54	BA	2531	A
54	BA	2532	G
54	BA	2534	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	2540	C
54	BA	2547	A
54	BA	2554	U
54	BA	2556	C
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2573	C
54	BA	2585	U
54	BA	2586	U
54	BA	2589	A
54	BA	2599	G
54	BA	2602	A
54	BA	2603	G
54	BA	2614	A
54	BA	2617	U
54	BA	2629	U
54	BA	2630	G
54	BA	2642	G
54	BA	2655	G
54	BA	2660	A
54	BA	2661	G
54	BA	2663	G
54	BA	2665	A
54	BA	2666	C
54	BA	2669	G
54	BA	2676	C
54	BA	2684	U
54	BA	2689	U
54	BA	2690	U
54	BA	2691	C
54	BA	2707	U
54	BA	2712	C
54	BA	2713	U
54	BA	2718	G
54	BA	2732	G
54	BA	2750	A
54	BA	2751	G
54	BA	2752	C
54	BA	2765	A
54	BA	2778	A
54	BA	2779	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	2780	G
54	BA	2786	U
54	BA	2791	G
54	BA	2797	U
54	BA	2799	A
54	BA	2800	A
54	BA	2801	G
54	BA	2816	G
54	BA	2820	A
54	BA	2821	A
54	BA	2824	C
54	BA	2850	A
54	BA	2858	C
54	BA	2867	G
54	BA	2884	U
54	BA	2885	G
54	BA	2886	A
54	BA	2887	A
54	BA	2893	A
54	BA	2895	G
55	BB	9	G
55	BB	11	C
55	BB	13	G
55	BB	14	U
55	BB	15	A
55	BB	16	G
55	BB	25	U
55	BB	35	C
55	BB	36	C
55	BB	37	C
55	BB	44	G
55	BB	45	A
55	BB	57	A
55	BB	67	G
55	BB	83	G
55	BB	89	U
55	BB	109	A

All (239) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	AA	30	U
21	AA	32	A
21	AA	49	U
21	AA	51	A
21	AA	60	A
21	AA	85	U
21	AA	94	G
21	AA	98	A
21	AA	109	A
21	AA	120	A
21	AA	184	G
21	AA	234	C
21	AA	244	U
21	AA	255	G
21	AA	293	G
21	AA	344	A
21	AA	345	C
21	AA	351	G
21	AA	353	A
21	AA	357	G
21	AA	384	G
21	AA	412	A
21	AA	414	A
21	AA	465	A
21	AA	482	A
21	AA	493	A
21	AA	559	A
21	AA	575	G
21	AA	579	A
21	AA	602	A
21	AA	611	C
21	AA	622	A
21	AA	626	G
21	AA	641	U
21	AA	664	G
21	AA	733	G
21	AA	753	A
21	AA	804	U
21	AA	811	C
21	AA	841	C
21	AA	872	A
21	AA	884	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	AA	926	G
21	AA	932	C
21	AA	945	G
21	AA	958	A
21	AA	975	A
21	AA	982	U
21	AA	983	A
21	AA	992	U
21	AA	994	A
21	AA	996	A
21	AA	1031	C
21	AA	1050	G
21	AA	1060	U
21	AA	1101	A
21	AA	1129	C
21	AA	1140	C
21	AA	1142	G
21	AA	1157	A
21	AA	1167	A
21	AA	1190	G
21	AA	1194	U
21	AA	1196	A
21	AA	1201	A
21	AA	1214	C
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1267	C
21	AA	1281	C
21	AA	1296	C
21	AA	1298	U
21	AA	1299	A
21	AA	1308	U
21	AA	1319	A
21	AA	1322	C
21	AA	1338	G
21	AA	1342	C
21	AA	1355	G
21	AA	1380	U
21	AA	1383	C
21	AA	1399	C
21	AA	1471	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	A1	10	G
22	A1	43	G
22	A1	48	C
22	A1	55	PSU
22	A1	57	G
22	A1	58	A
22	A1	60	C
22	A1	61	C
23	A2	80	C
23	A2	91	A
24	A3	15	G
24	A3	16	C
24	A3	19	G
24	A3	48	U
24	A3	72	C
24	A3	74	A
54	BA	9	G
54	BA	13	A
54	BA	14	A
54	BA	43	G
54	BA	45	G
54	BA	47	C
54	BA	60	G
54	BA	99	U
54	BA	101	A
54	BA	118	A
54	BA	119	A
54	BA	125	A
54	BA	127	A
54	BA	147	C
54	BA	196	A
54	BA	199	A
54	BA	233	A
54	BA	249	C
54	BA	278	A
54	BA	279	A
54	BA	323	C
54	BA	330	A
54	BA	369	U
54	BA	388	G
54	BA	443	A
54	BA	446	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	474	G
54	BA	481	G
54	BA	504	A
54	BA	529	A
54	BA	530	G
54	BA	532	A
54	BA	574	A
54	BA	614	A
54	BA	670	A
54	BA	726	G
54	BA	762	U
54	BA	790	U
54	BA	810	U
54	BA	827	U
54	BA	957	C
54	BA	961	C
54	BA	965	C
54	BA	980	A
54	BA	984	A
54	BA	989	G
54	BA	994	C
54	BA	1067	A
54	BA	1069	A
54	BA	1089	A
54	BA	1096	A
54	BA	1126	A
54	BA	1132	U
54	BA	1141	U
54	BA	1175	A
54	BA	1185	G
54	BA	1236	G
54	BA	1254	A
54	BA	1255	U
54	BA	1262	A
54	BA	1273	U
54	BA	1288	G
54	BA	1300	G
54	BA	1301	A
54	BA	1312	U
54	BA	1379	U
54	BA	1384	A
54	BA	1427	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	1451	C
54	BA	1453	A
54	BA	1490	A
54	BA	1508	A
54	BA	1539	U
54	BA	1552	A
54	BA	1598	A
54	BA	1621	U
54	BA	1634	A
54	BA	1668	A
54	BA	1699	G
54	BA	1706	C
54	BA	1737	G
54	BA	1774	C
54	BA	1779	U
54	BA	1783	A
54	BA	1784	A
54	BA	1816	C
54	BA	1819	A
54	BA	1828	G
54	BA	1869	G
54	BA	1930	G
54	BA	1938	A
54	BA	1941	C
54	BA	1943	U
54	BA	1945	G
54	BA	1952	A
54	BA	1970	A
54	BA	1971	U
54	BA	1980	G
54	BA	2005	A
54	BA	2035	G
54	BA	2076	U
54	BA	2110	G
54	BA	2117	A
54	BA	2141	G
54	BA	2164	C
54	BA	2211	A
54	BA	2227	A
54	BA	2244	U
54	BA	2245	U
54	BA	2275	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	BA	2282	G
54	BA	2286	G
54	BA	2304	G
54	BA	2311	A
54	BA	2352	A
54	BA	2389	G
54	BA	2391	G
54	BA	2402	U
54	BA	2425	A
54	BA	2439	A
54	BA	2473	U
54	BA	2483	C
54	BA	2495	G
54	BA	2565	A
54	BA	2585	U
54	BA	2602	A
54	BA	2641	G
54	BA	2645	G
54	BA	2665	A
54	BA	2690	U
54	BA	2711	A
54	BA	2712	C
54	BA	2780	G
54	BA	2799	A
54	BA	2894	G
55	BB	24	G
55	BB	56	G
55	BB	82	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CM0	A1	34	22,23	15,26,27	1.88	3 (20%)	18,37,40	3.02	3 (16%)
22	6MZ	A1	37	22	17,25,26	0.91	0	15,36,39	1.12	1 (6%)
22	7MG	A1	46	22	20,26,27	2.29	3 (15%)	23,39,42	2.03	2 (8%)
22	5MU	A1	54	22	13,22,23	1.07	1 (7%)	16,32,35	4.62	2 (12%)
22	PSU	A1	55	22	15,21,22	2.04	4 (26%)	16,30,33	4.15	6 (37%)
22	4SU	A1	7	22	12,21,22	0.95	1 (8%)	15,30,33	2.22	2 (13%)
24	H2U	A3	21	24	17,21,22	1.39	2 (11%)	23,30,33	1.34	4 (17%)
24	OMC	A3	33	24	15,22,23	1.11	1 (6%)	20,31,34	0.92	1 (5%)
24	5MU	A3	55	24	13,22,23	0.92	1 (7%)	16,32,35	4.53	3 (18%)
24	PSU	A3	56	24	15,21,22	1.09	1 (6%)	16,30,33	3.30	4 (25%)
24	4SU	A3	8	24	12,21,22	1.10	1 (8%)	15,30,33	2.26	1 (6%)

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

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.61	1.33	1.45
22	A1	34	CM0	O5-C5	-5.90	1.25	1.37
22	A1	55	PSU	C2'-C1'	-4.73	1.49	1.53
24	A3	21	H2U	C4-N3	-3.49	1.32	1.37
24	A3	21	H2U	C2-N3	-3.24	1.31	1.38
22	A1	46	7MG	C8-N7	-2.71	1.31	1.43
22	A1	55	PSU	O4'-C1'	-2.32	1.40	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A3	33	OMC	C4-N3	-2.04	1.31	1.35
22	A1	7	4SU	C6-N1	2.06	1.38	1.35
24	A3	8	4SU	C6-N1	2.10	1.38	1.35
22	A1	55	PSU	C4-N3	2.18	1.37	1.33
24	A3	56	PSU	C4-N3	2.25	1.37	1.33
24	A3	55	5MU	C4-N3	2.36	1.37	1.33
22	A1	34	CM0	C4-C5	2.41	1.47	1.40
22	A1	34	CM0	C4-N3	2.61	1.37	1.33
22	A1	54	5MU	C4-N3	2.71	1.37	1.33
22	A1	46	7MG	C6-N1	2.90	1.38	1.33
22	A1	55	PSU	C5-C1'	4.59	1.56	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C5-C4-N3	-13.20	114.27	125.35
24	A3	55	5MU	C5-C4-N3	-12.30	115.02	125.35
22	A1	55	PSU	C4-C5-C1'	-9.87	104.59	121.22
24	A3	8	4SU	C5-C4-N3	-8.08	114.99	123.56
22	A1	7	4SU	C5-C4-N3	-7.65	115.44	123.56
22	A1	46	7MG	C5-C6-N1	-6.54	113.65	123.39
22	A1	55	PSU	C4'-O4'-C1'	-5.43	103.94	109.54
22	A1	55	PSU	C5-C6-N1	-5.10	117.27	124.38
22	A1	55	PSU	O2'-C2'-C1'	-3.47	104.39	111.93
24	A3	56	PSU	C5-C6-N1	-2.96	120.26	124.38
24	A3	56	PSU	C5-C1'-C2'	-2.41	111.34	115.44
24	A3	21	H2U	O2-C2-N3	-2.31	116.91	121.44
24	A3	33	OMC	C4'-O4'-C1'	-2.12	107.39	109.64
22	A1	34	CM0	O4'-C4'-C3'	2.04	109.30	105.16
22	A1	7	4SU	O4'-C4'-C3'	2.17	109.56	105.16
24	A3	21	H2U	C5-C6-N1	2.27	113.25	110.76
24	A3	55	5MU	O4'-C4'-C3'	2.38	109.99	105.16
24	A3	21	H2U	C5-C4-N3	2.49	119.25	116.62
22	A1	37	6MZ	C2-N1-C6	2.77	118.46	116.47
24	A3	56	PSU	O4'-C1'-C2'	3.12	108.06	104.69
22	A1	34	CM0	C7-O5-C5	3.42	124.12	117.83
24	A3	21	H2U	N3-C2-N1	3.95	120.30	116.64
22	A1	55	PSU	O4'-C1'-C2'	4.31	109.35	104.69
22	A1	46	7MG	C6-N1-C2	6.20	123.15	115.88
22	A1	55	PSU	C4-N3-C2	9.41	123.01	115.16
22	A1	34	CM0	C4-N3-C2	11.66	124.89	115.16
24	A3	56	PSU	C4-N3-C2	11.95	125.13	115.16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	54	5MU	C4-N3-C2	12.63	125.70	115.16
24	A3	55	5MU	C4-N3-C2	12.76	125.80	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	VAL	A1	101	58,22	5,6,7	0.50	0	5,7,9	2.31	2 (40%)
58	FME	A1	102	57	8,9,10	0.83	0	5,9,11	1.20	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	VAL	A1	101	58,22	-	0/4/6/8	0/0/0/0
58	FME	A1	102	57	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
57	A1	101	VAL	O-C-CA	-4.44	113.56	125.69
58	A1	102	FME	O-C-CA	-2.52	118.80	125.69
57	A1	101	VAL	C-CA-N	2.66	115.82	109.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.