Full wwPDB EM Validation Report

Nov 20, 2022 – 02:08 AM EST

PDB ID	:	4V7A
EMDB ID	:	EMD-1724
Title	:	E. coli 70S-fMetVal-tRNAVal post-translocation complex (post4)
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	:	9.00 Å(reported)
Based on initial models	:	2HGP, 3I1O, 2WRI, 2K4C

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

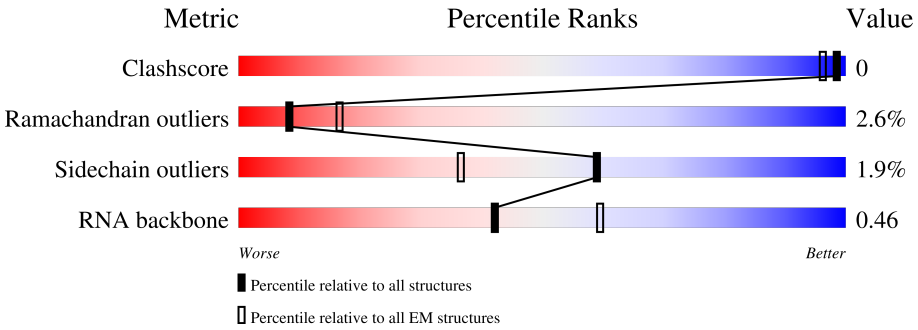
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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.



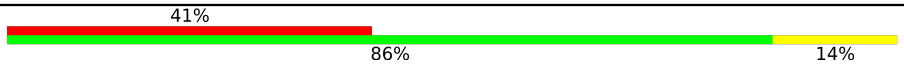
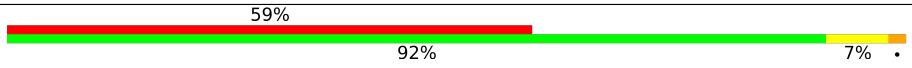
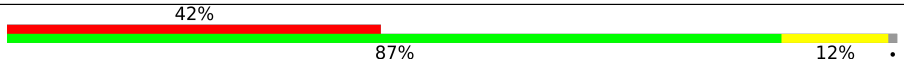
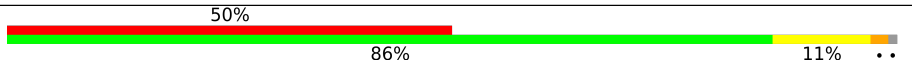
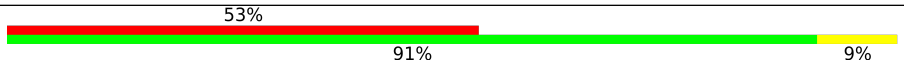
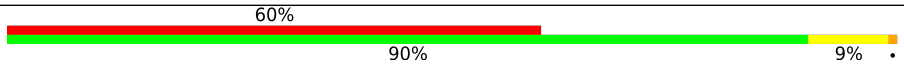
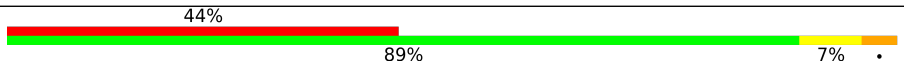
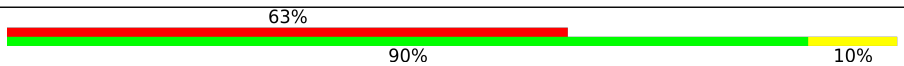
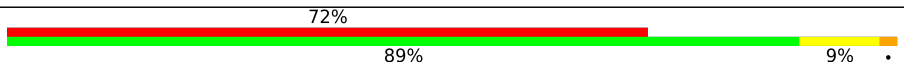
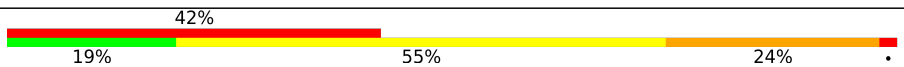
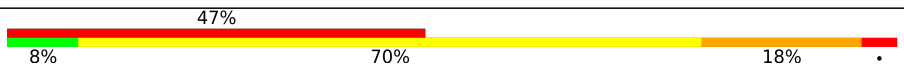
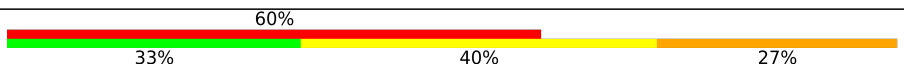
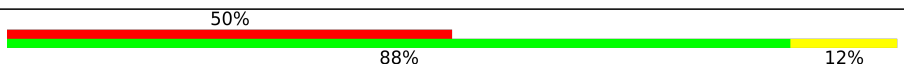
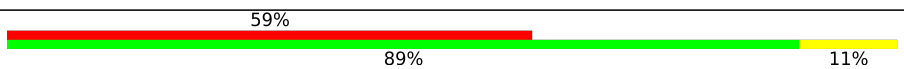
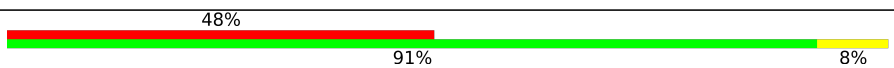
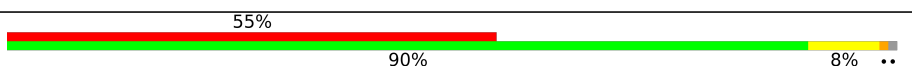
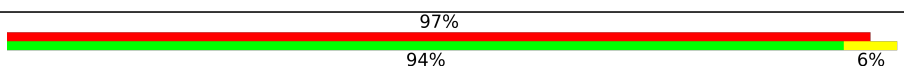
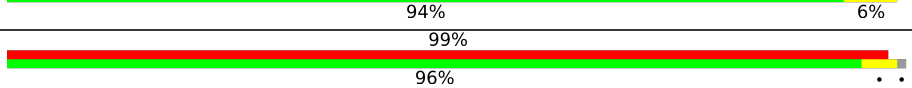
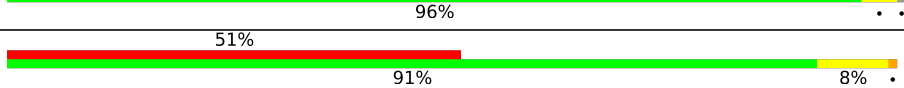
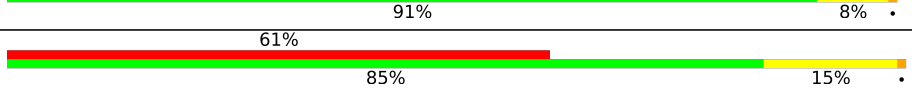
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	220	71% 94% 6%
2	AC	208	62% 87% 12%
3	AD	206	60% 91% 8%
4	AE	152	57% 91% 8%
5	AF	101	70% 90% 10%
6	AG	152	53% 89% 11%
7	AH	130	47% 95%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	AI	128	
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	
28	BG	177	
29	BH	149	
30	BI	142	
31	BJ	142	
32	BK	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	BL	144	51% 83% 15%
34	BM	136	55% 89% 10%
35	BN	121	67% 83% 16%
36	BO	117	39% 91% 9%
37	BP	115	70% 90% 9%
38	BQ	118	53% 87% 12%
39	BR	103	68% 88% 12%
40	BS	110	58% 89% 11%
41	BT	94	67% 85% 15%
42	BU	104	72% 90% 8%
43	BV	94	51% 89% 11%
44	BW	80	58% 79% 20%
45	BX	79	61% 82% 13%
46	BY	63	68% 90% 10%
47	BZ	59	44% 86% 8%
48	B0	57	60% 84% 14%
49	B1	52	79% 87% 13%
50	B2	46	61% 78% 22%
51	B3	65	62% 85% 14%
52	B4	38	55% 87% 11%
53	BA	2903	50% 16% 55% 25%
54	BB	118	46% 21% 53% 19% 5%
55	B5	234	91% 89% 6% 5%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146011 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
			Total	C	N	O	S		
1	AB	220	1708	1083	306	312	7	0	1

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
			Total	C	N	O	S		
2	AC	207	1625	1028	306	288	3	0	1

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
			Total	C	N	O	S		
3	AD	205	1643	1026	315	298	4	0	0

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

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

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

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	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 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	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 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	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 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	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 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	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 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	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 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	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 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
49	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 50 is a protein called 50S ribosomal protein L34.

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

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

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

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

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

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

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

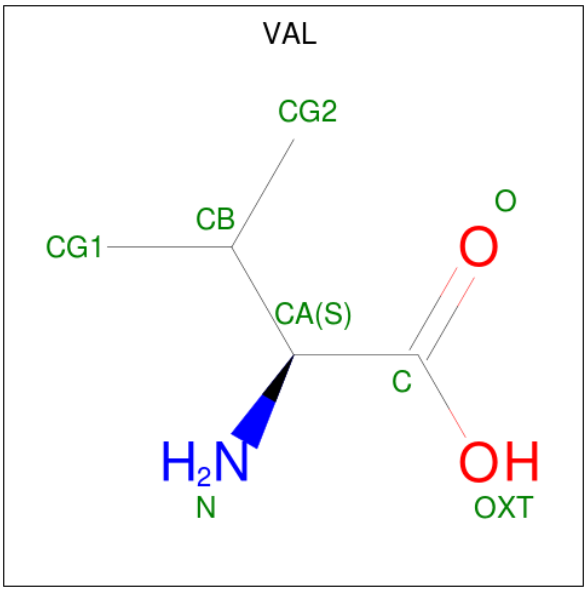
- Molecule 54 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 55 is a protein called 50S ribosomal protein L1.

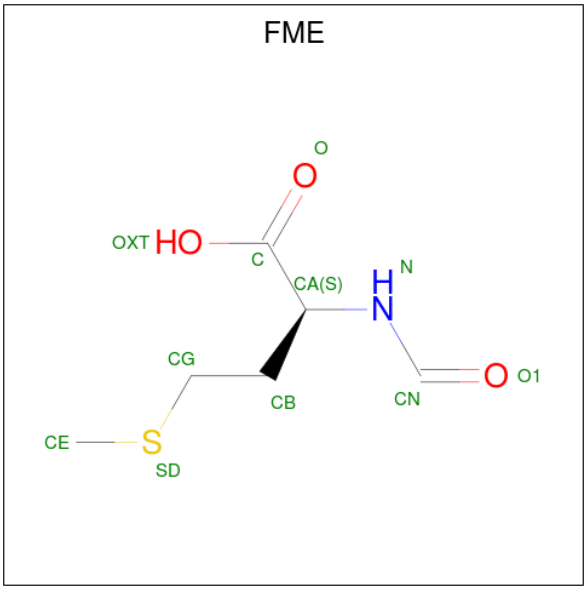
Mol	Chain	Residues	Atoms					AltConf	Trace
55	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 56 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



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

- Molecule 57 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



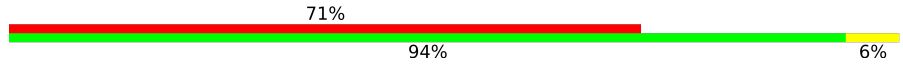
Mol	Chain	Residues	Atoms					AltConf
57	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

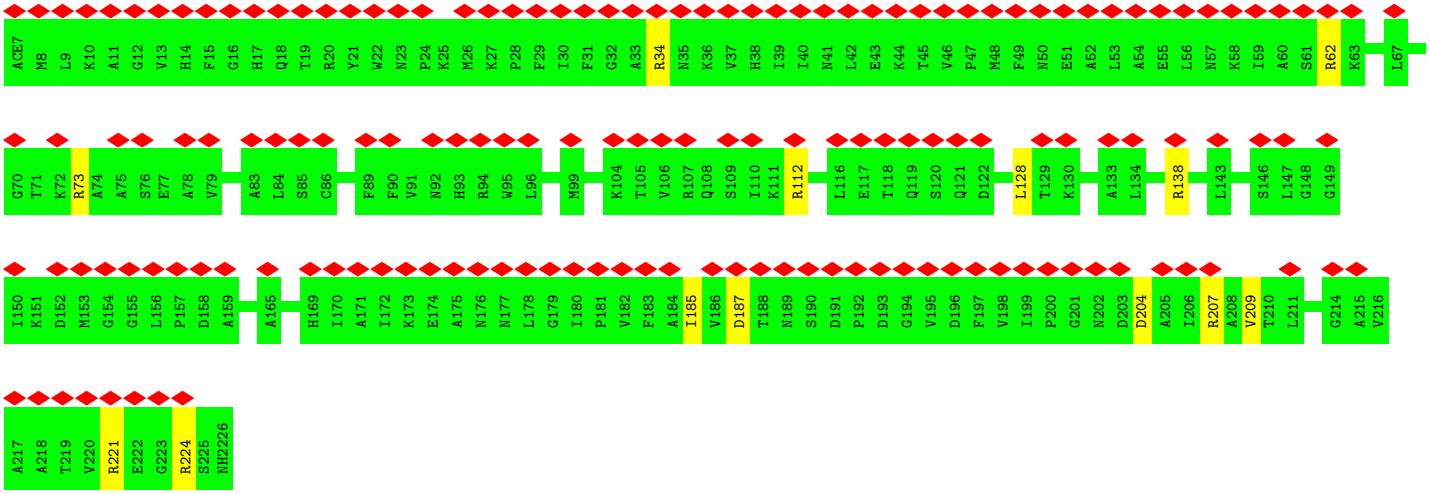
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

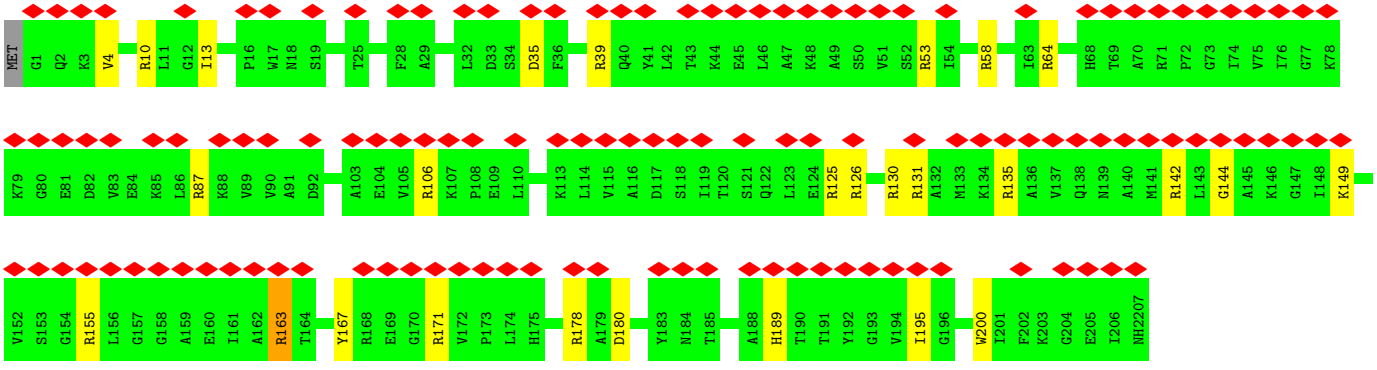
Chain AB:





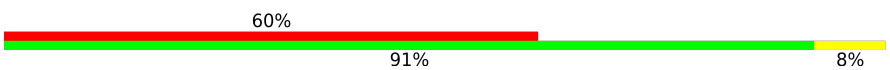
• Molecule 2: 30S ribosomal protein S3

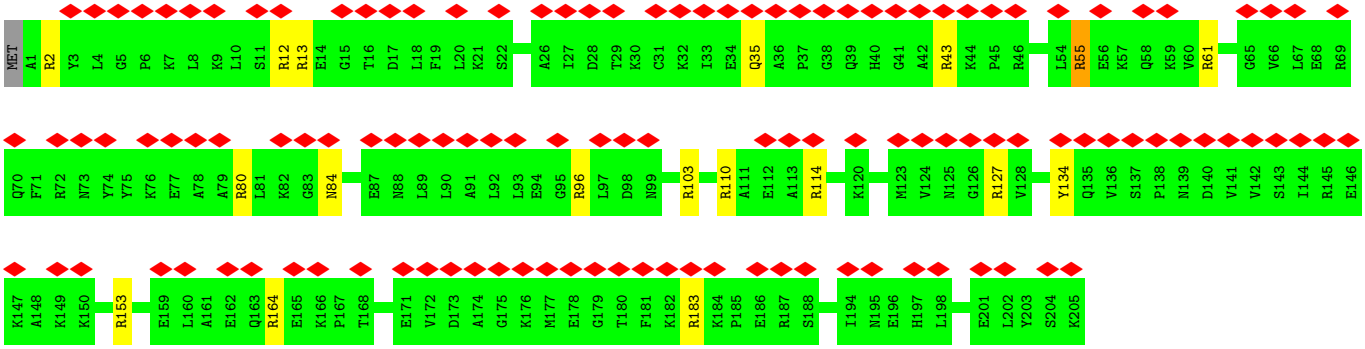
Chain AC:



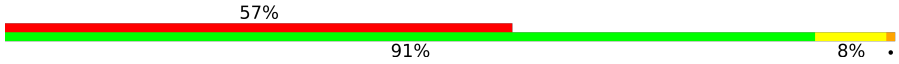
• Molecule 3: 30S ribosomal protein S4

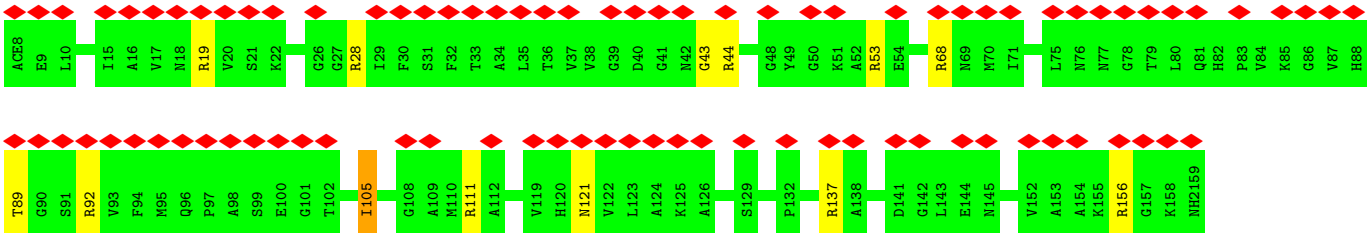
Chain AD:



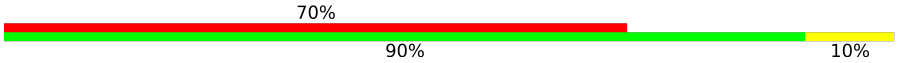


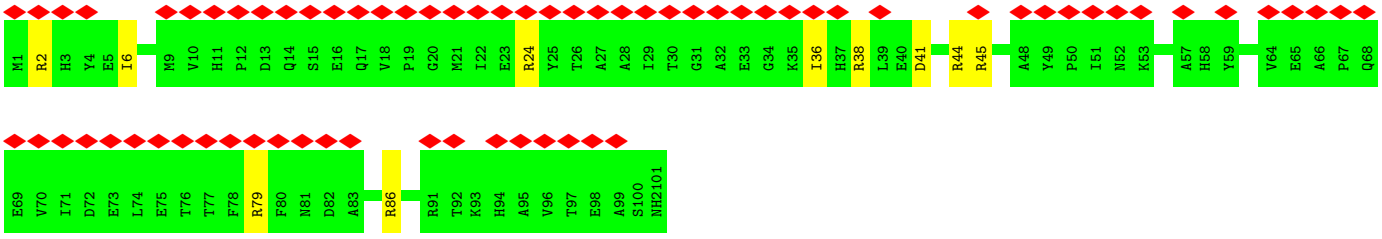
• Molecule 4: 30S ribosomal protein S5



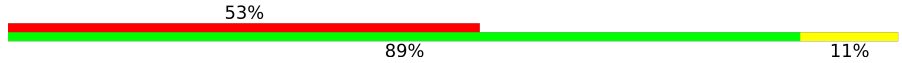


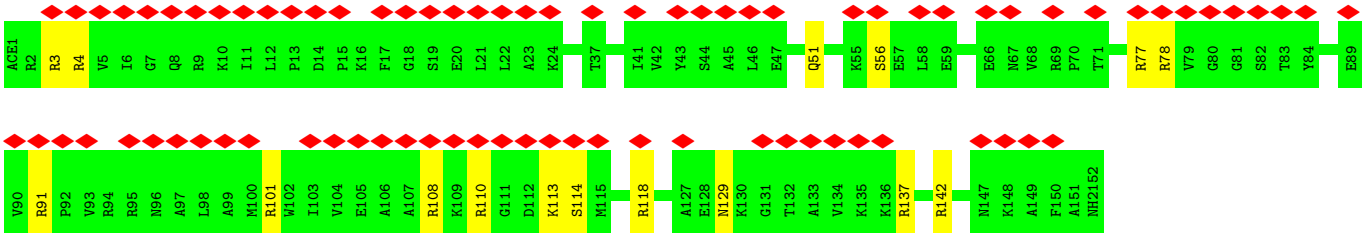
• Molecule 5: 30S ribosomal protein S6



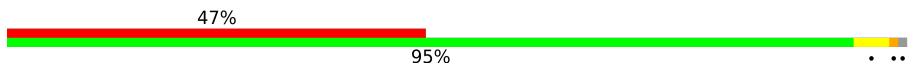


• Molecule 6: 30S ribosomal protein S7

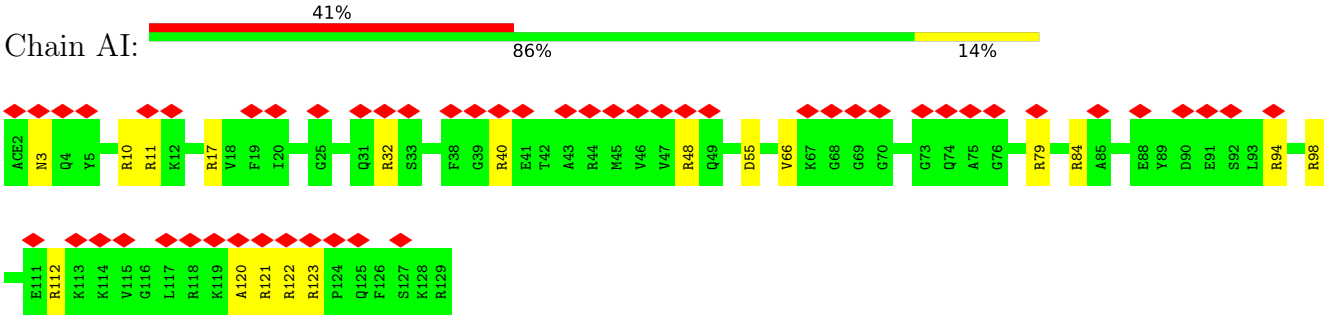




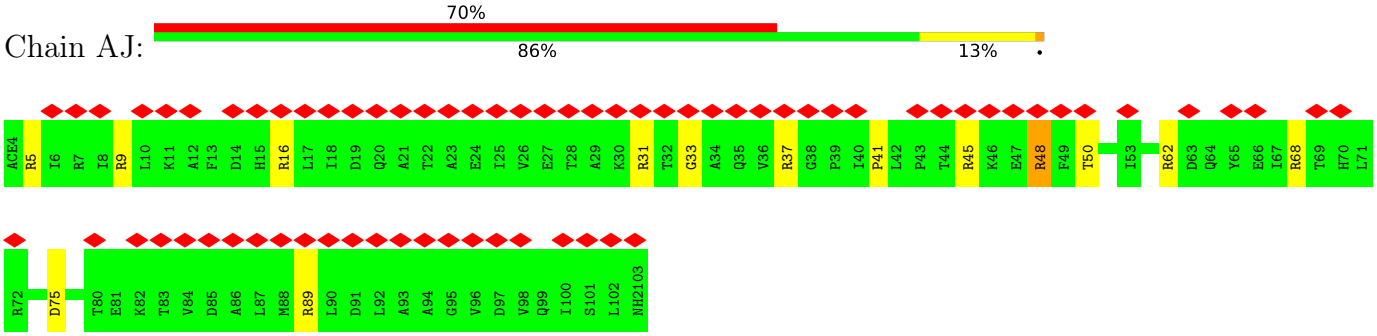
• Molecule 7: 30S ribosomal protein S8



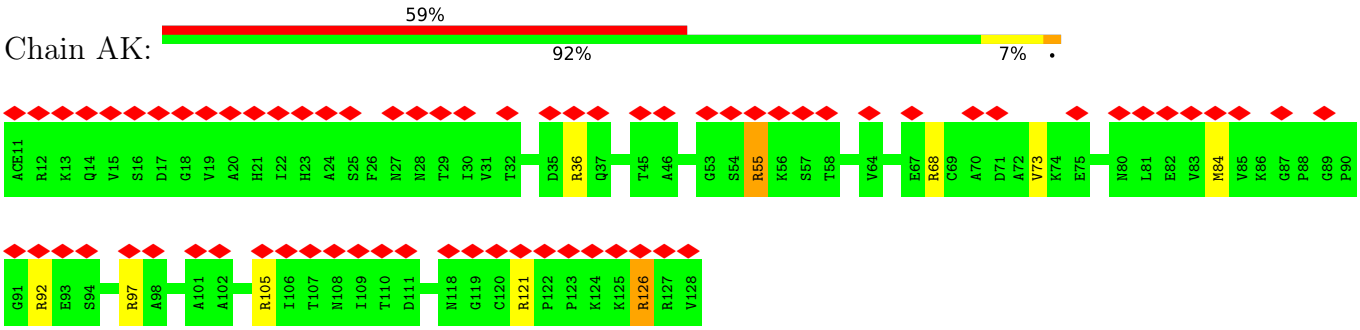
• Molecule 8: 30S ribosomal protein S9



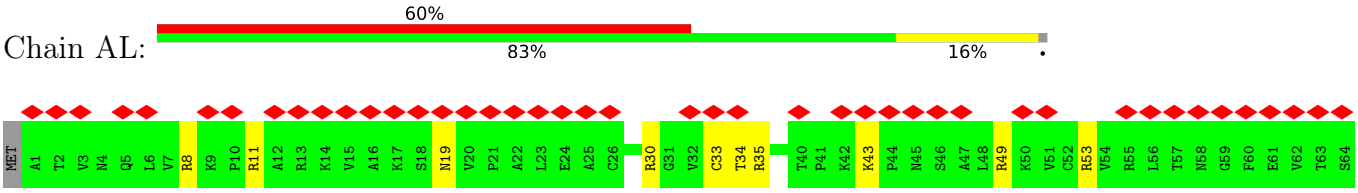
• Molecule 9: 30S ribosomal protein S10

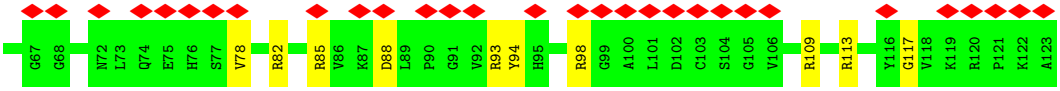


• Molecule 10: 30S ribosomal protein S11

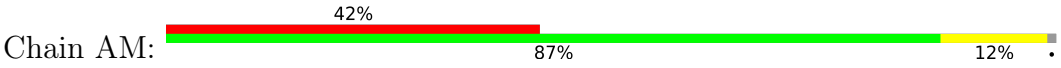


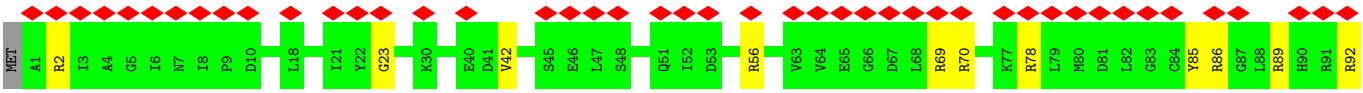
• Molecule 11: 30S ribosomal protein S12

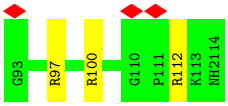




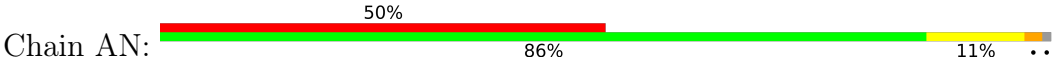
• Molecule 12: 30S ribosomal protein S13

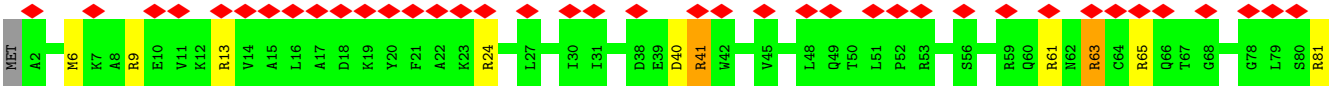


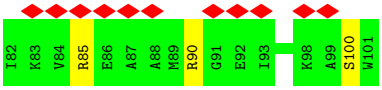




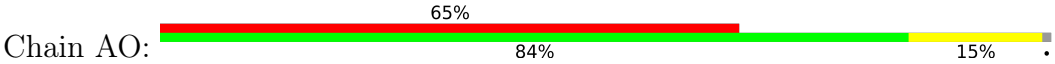
• Molecule 13: 30S ribosomal protein S14

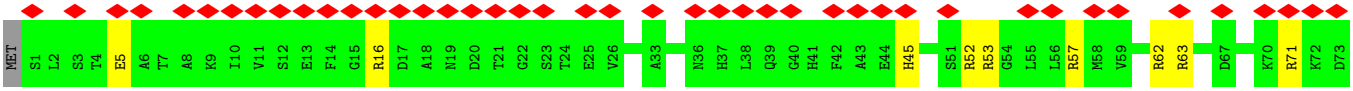


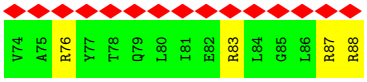




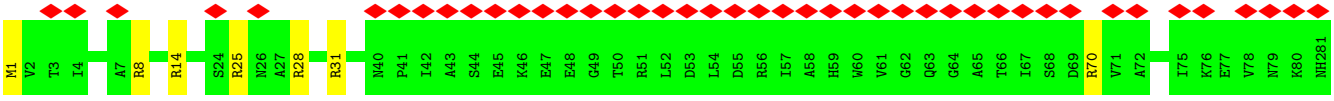
• Molecule 14: 30S ribosomal protein S15



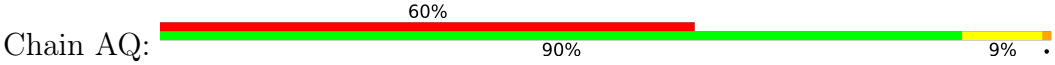


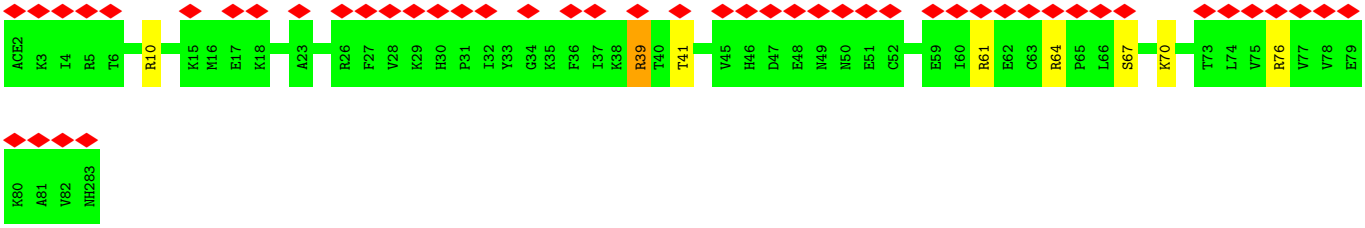


• Molecule 15: 30S ribosomal protein S16

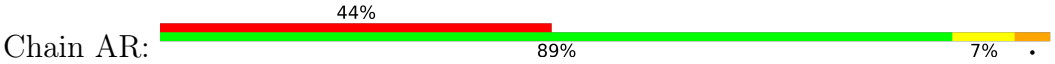


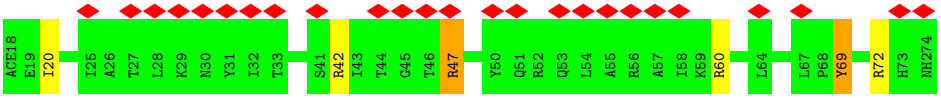
• Molecule 16: 30S ribosomal protein S17



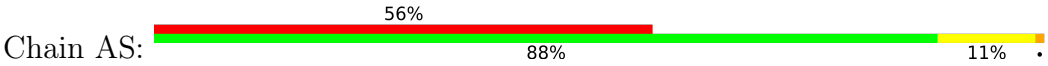


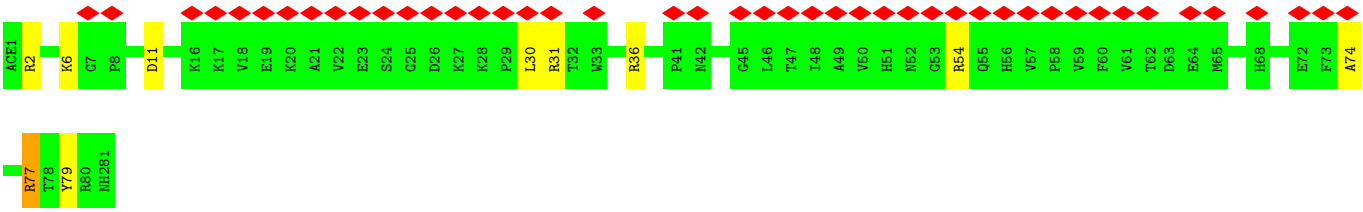
• Molecule 17: 30S ribosomal protein S18



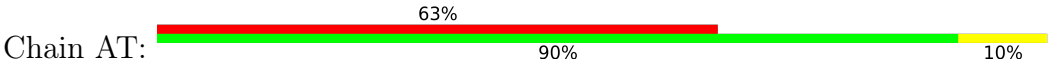


• Molecule 18: 30S ribosomal protein S19

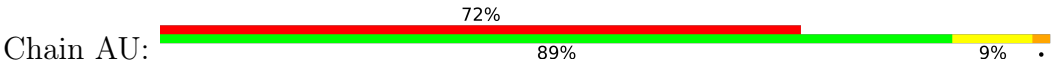


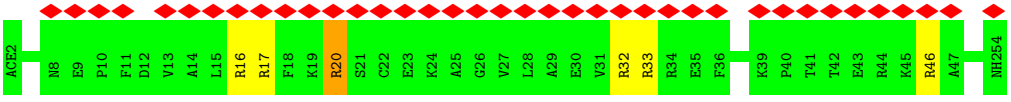


• Molecule 19: 30S ribosomal protein S20

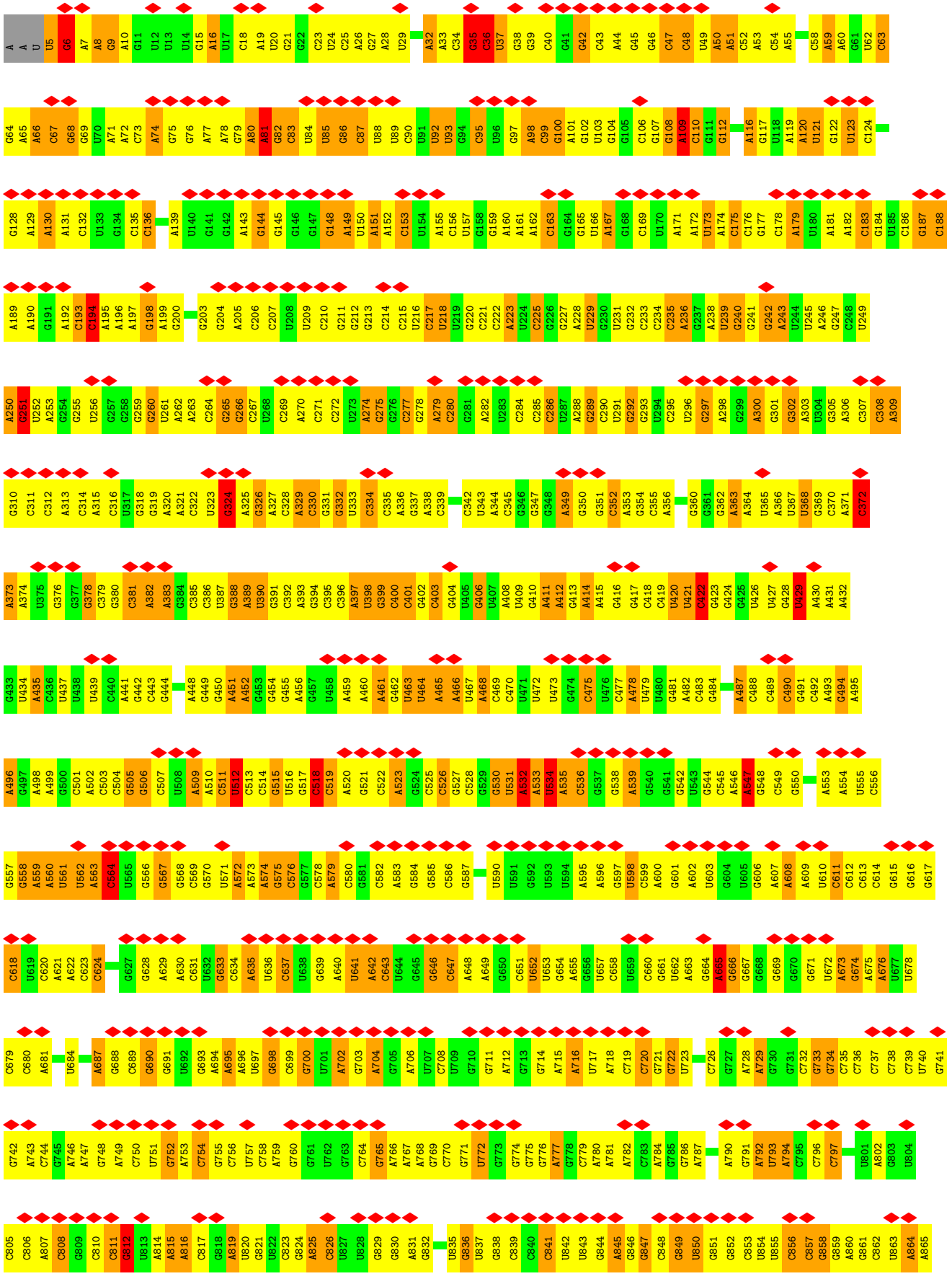


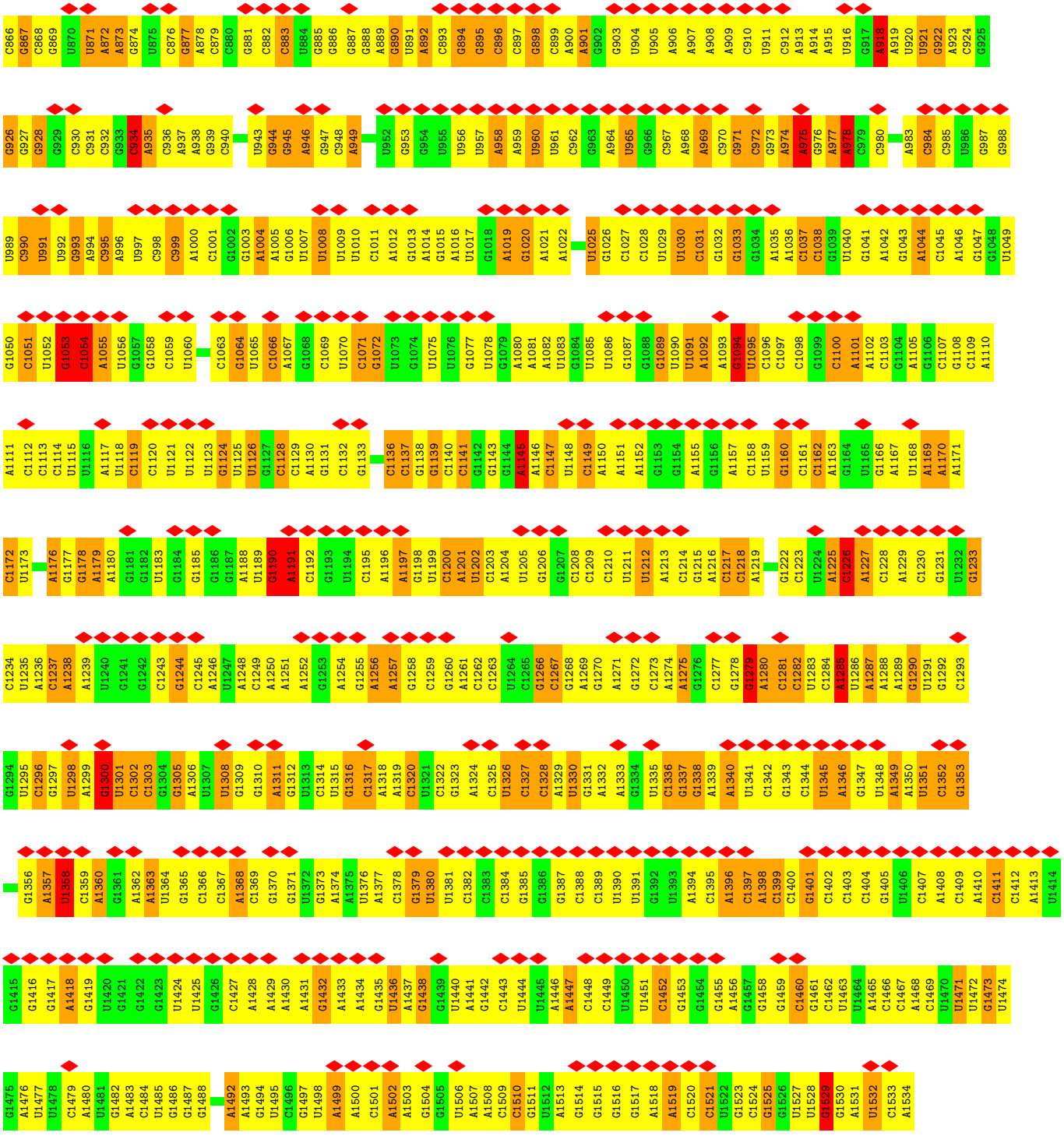
• Molecule 20: 30S ribosomal protein S21



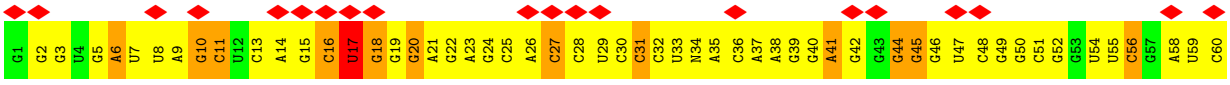


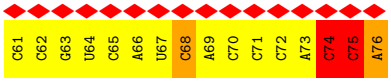
• Molecule 21: 16S ribosomal RNA





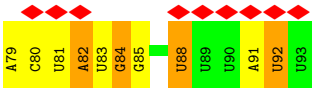
• Molecule 22: fMet-Val-tRNA-Val





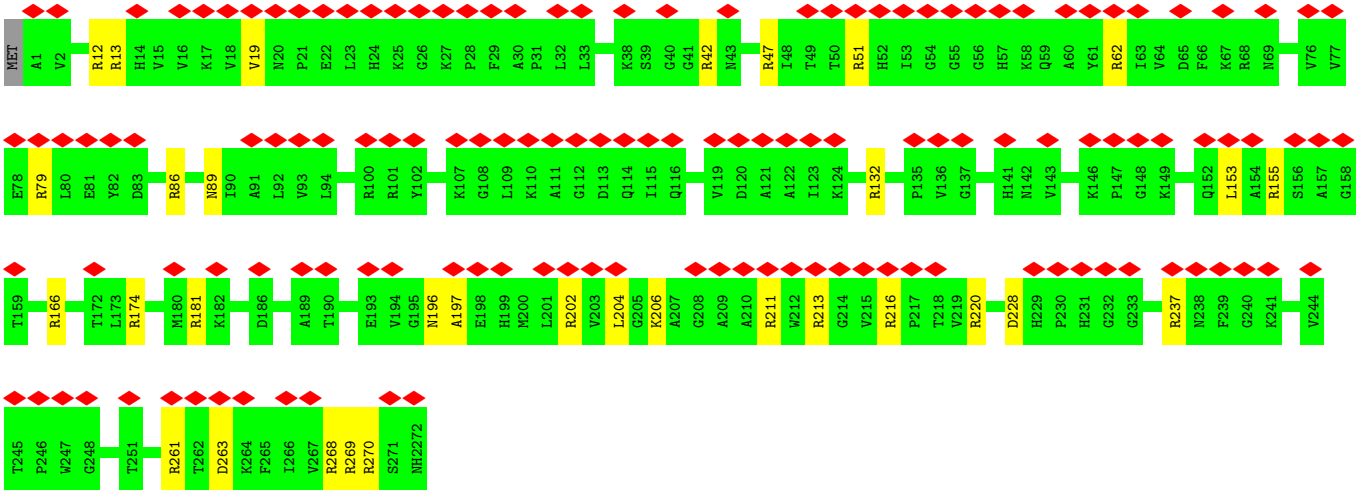
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

Chain A2:



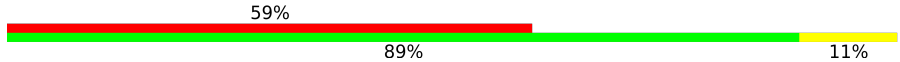
• Molecule 24: 50S ribosomal protein L2

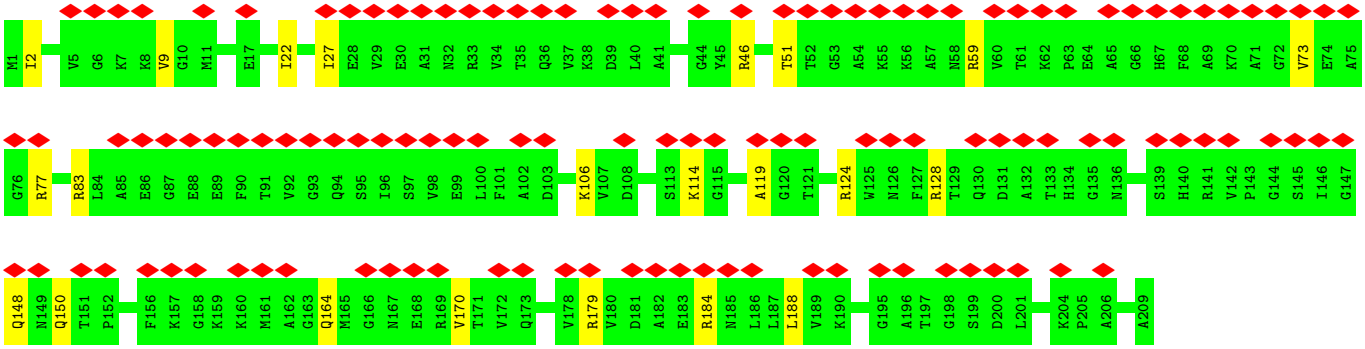
Chain BC:



• Molecule 25: 50S ribosomal protein L3

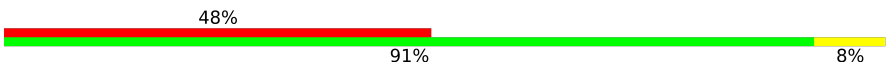
Chain BD:

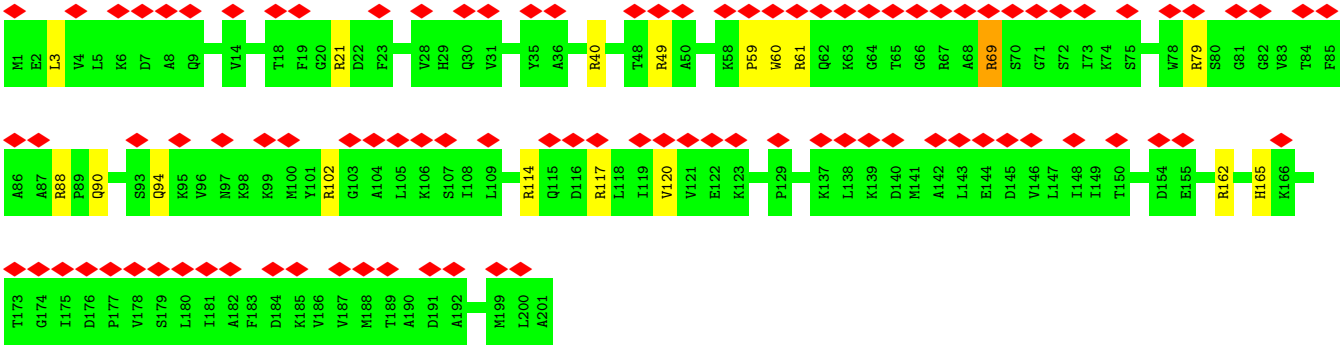




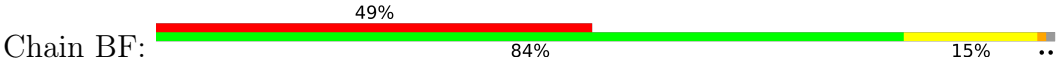
• Molecule 26: 50S ribosomal protein L4

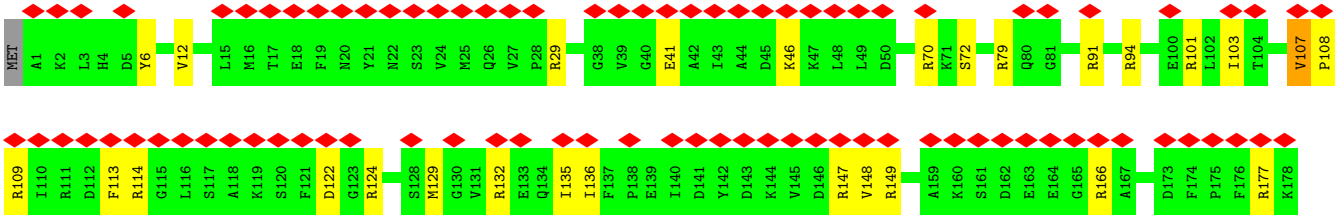
Chain BE:



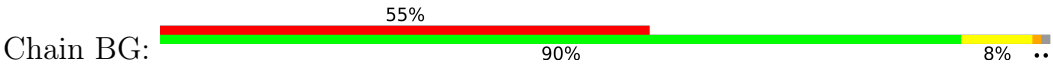


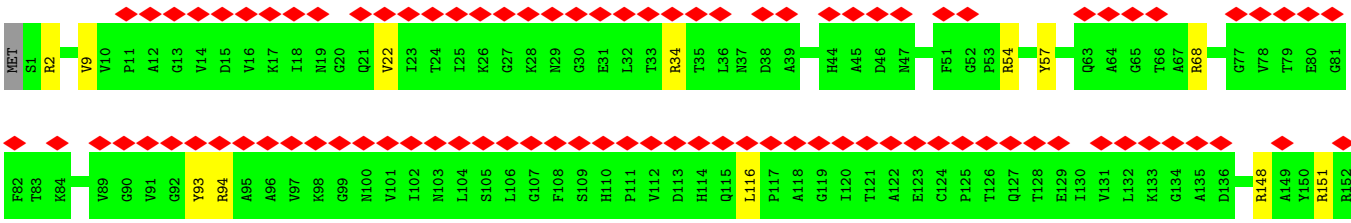
• Molecule 27: 50S ribosomal protein L5



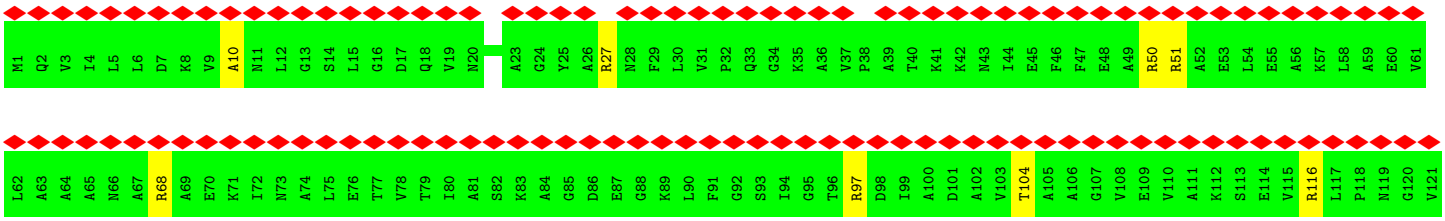


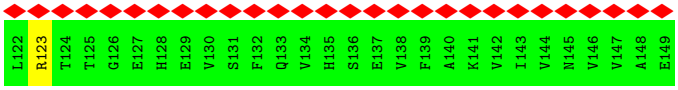
• Molecule 28: 50S ribosomal protein L6





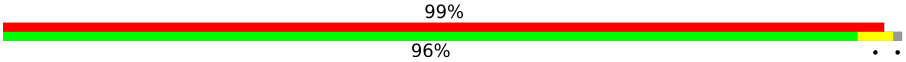
• Molecule 29: 50S ribosomal protein L9

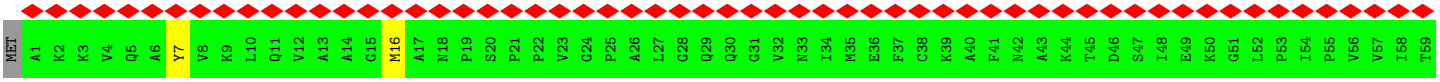


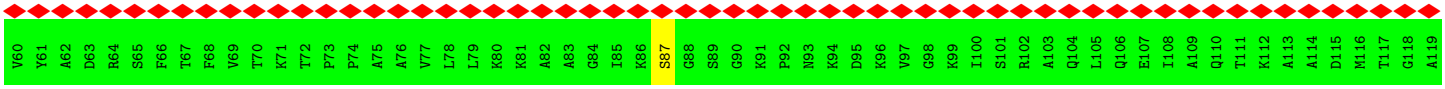


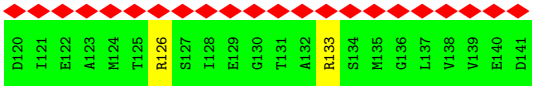
• Molecule 30: 50S ribosomal protein L11

Chain BI:



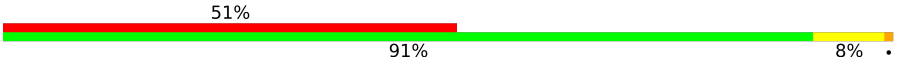


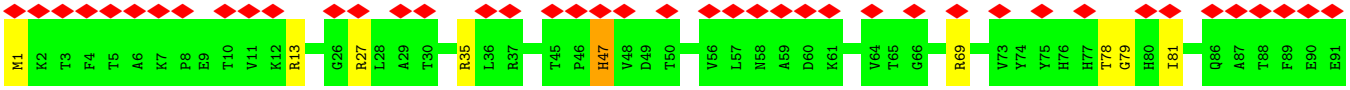


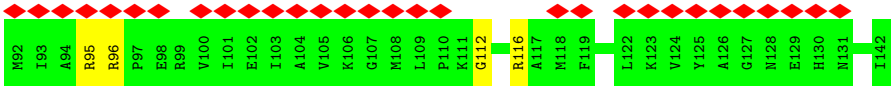


• Molecule 31: 50S ribosomal protein L13

Chain BJ:

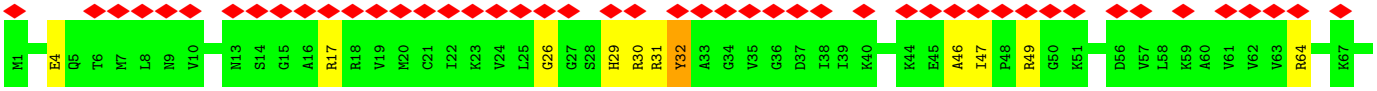


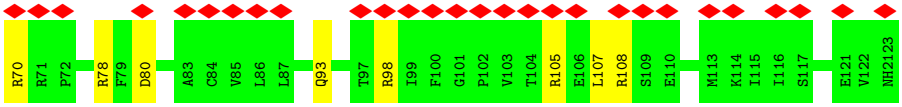




• Molecule 32: 50S ribosomal protein L14

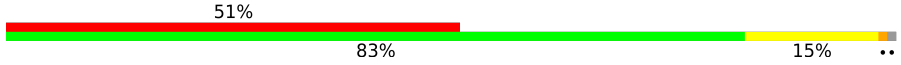
Chain BK:

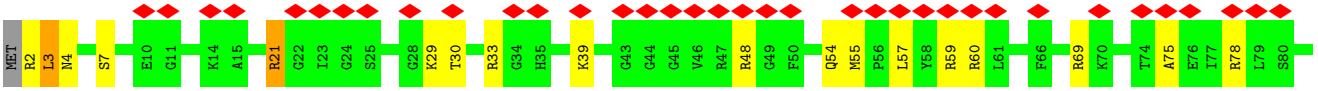


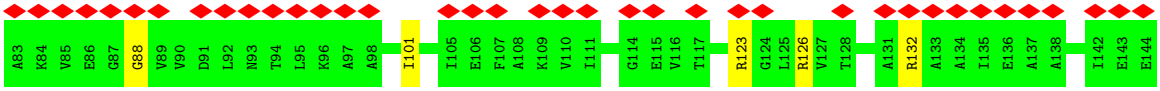


• Molecule 33: 50S ribosomal protein L15

Chain BL:

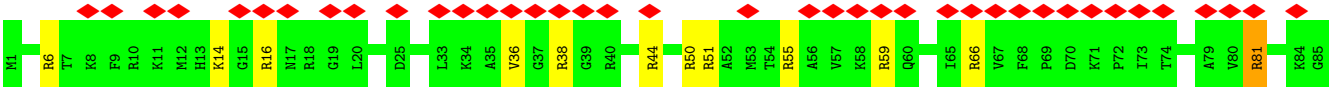


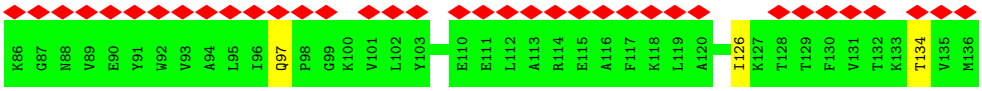




• Molecule 34: 50S ribosomal protein L16

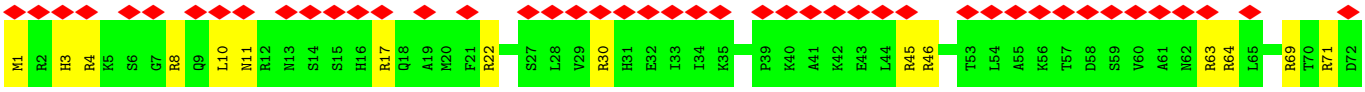
Chain BM:

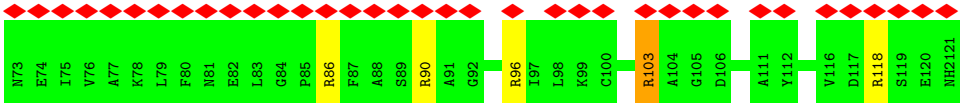




• Molecule 35: 50S ribosomal protein L17

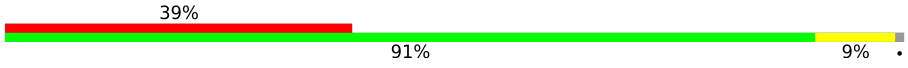
Chain BN:

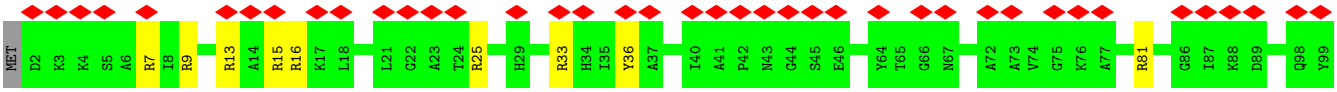


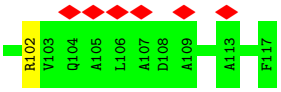


• Molecule 36: 50S ribosomal protein L18

Chain BO:

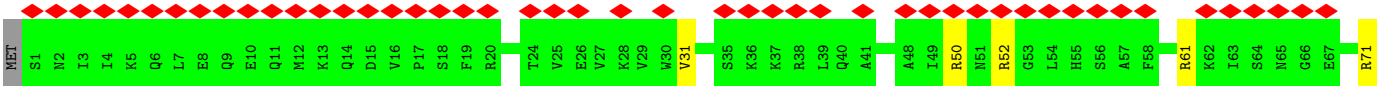


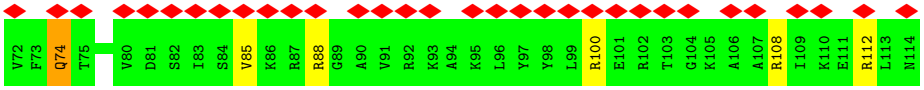




• Molecule 37: 50S ribosomal protein L19

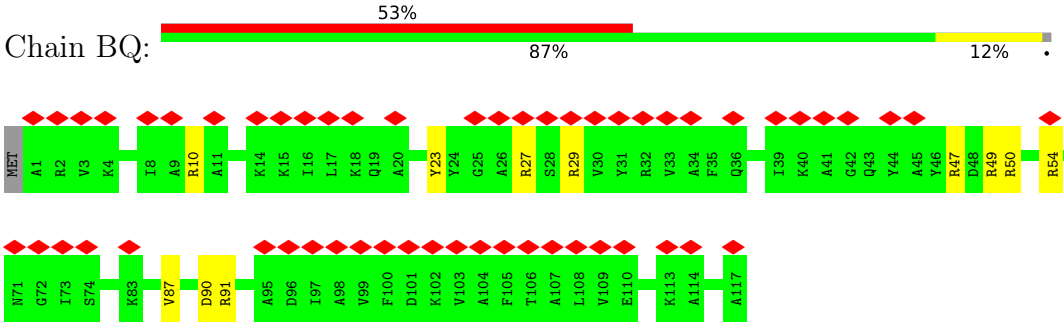
Chain BP:





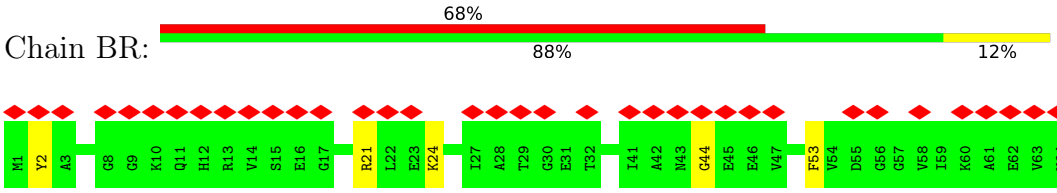
• Molecule 38: 50S ribosomal protein L20

Chain BQ:



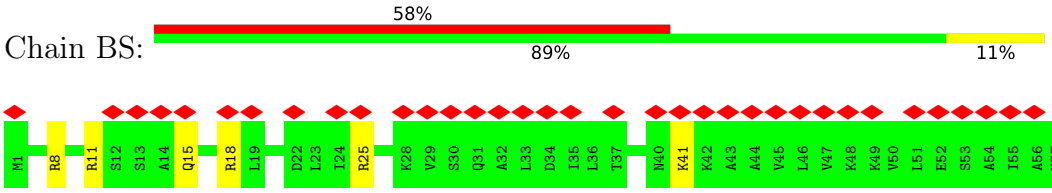
• Molecule 39: 50S ribosomal protein L21

Chain BR:



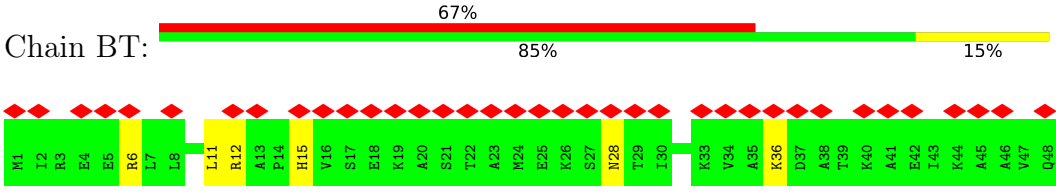
• Molecule 40: 50S ribosomal protein L22

Chain BS:



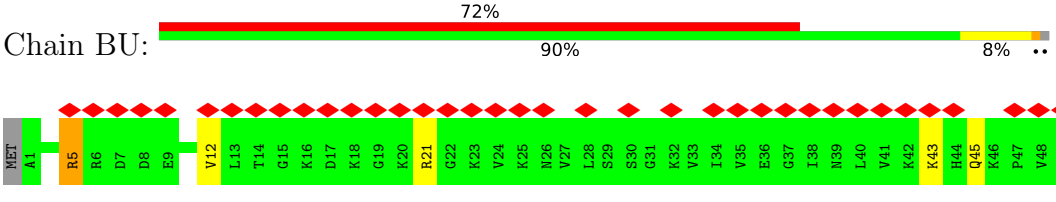
• Molecule 41: 50S ribosomal protein L23

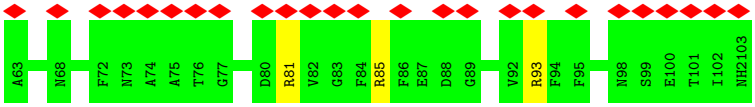
Chain BT:



• Molecule 42: 50S ribosomal protein L24

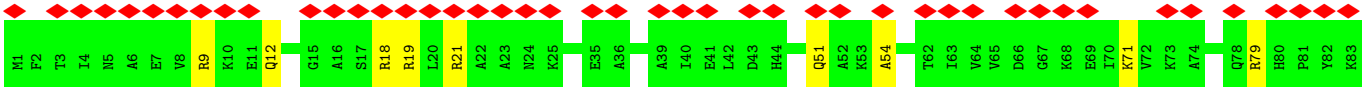
Chain BU:

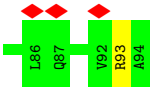




• Molecule 43: 50S ribosomal protein L25

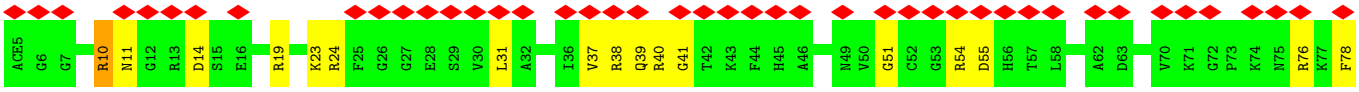
Chain BV:





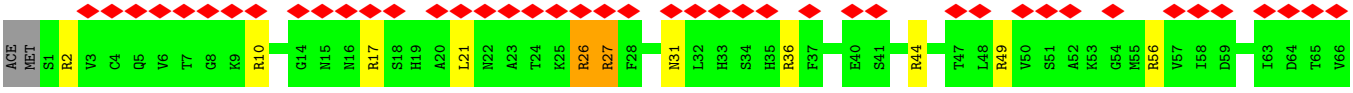
• Molecule 44: 50S ribosomal protein L27

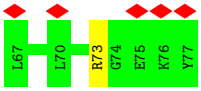
Chain BW:



• Molecule 45: 50S ribosomal protein L28

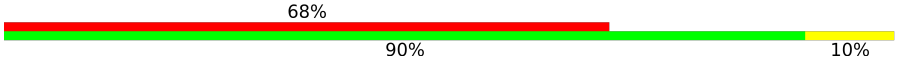
Chain BX:

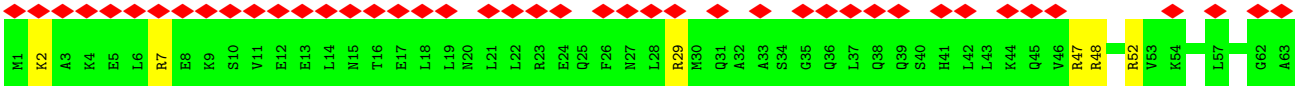




• Molecule 46: 50S ribosomal protein L29

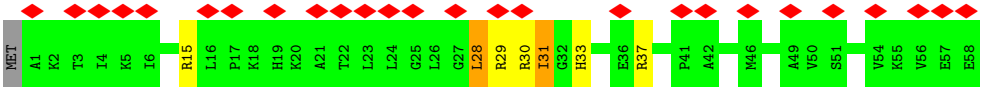
Chain BY:





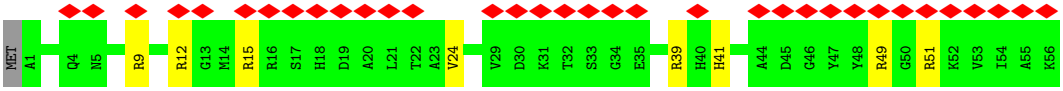
• Molecule 47: 50S ribosomal protein L30

Chain BZ:



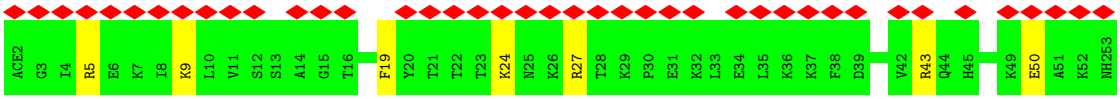
• Molecule 48: 50S ribosomal protein L32

Chain B0:



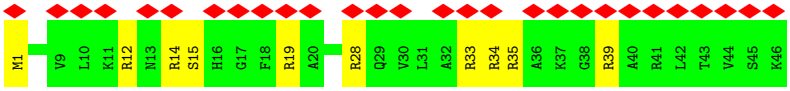
• Molecule 49: 50S ribosomal protein L33

Chain B1:



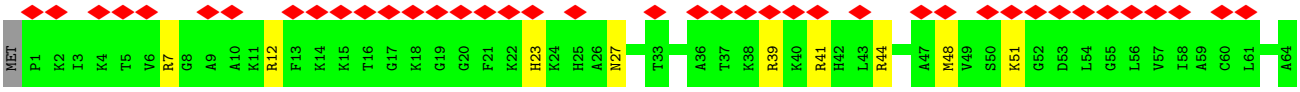
• Molecule 50: 50S ribosomal protein L34

Chain B2:



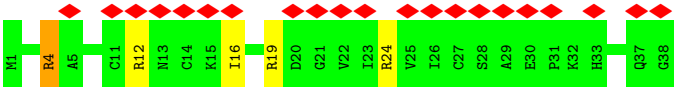
• Molecule 51: 50S ribosomal protein L35

Chain B3:



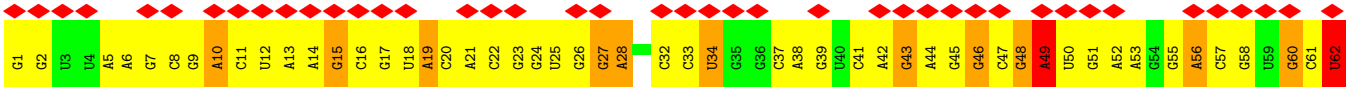
• Molecule 52: 50S ribosomal protein L36

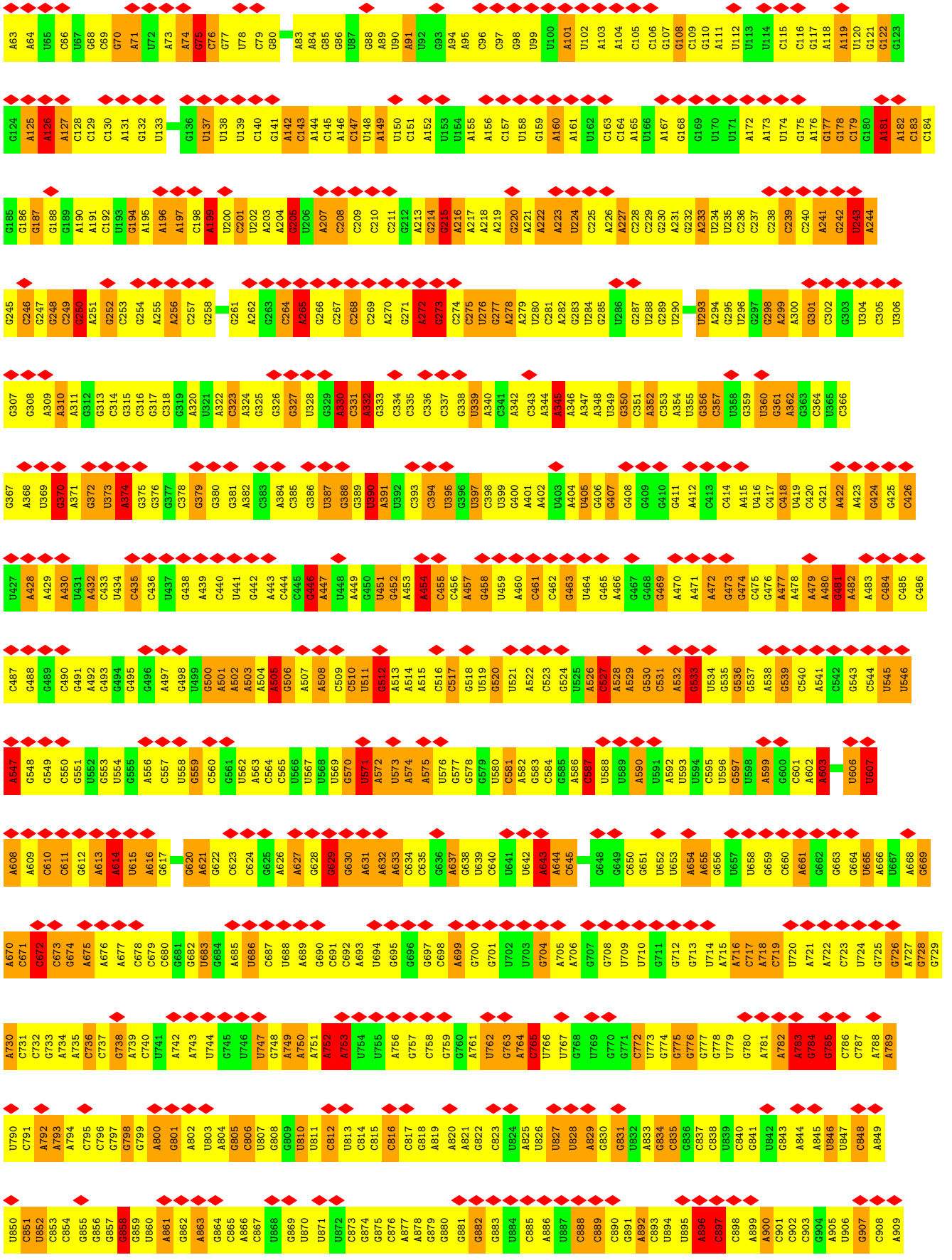
Chain B4:

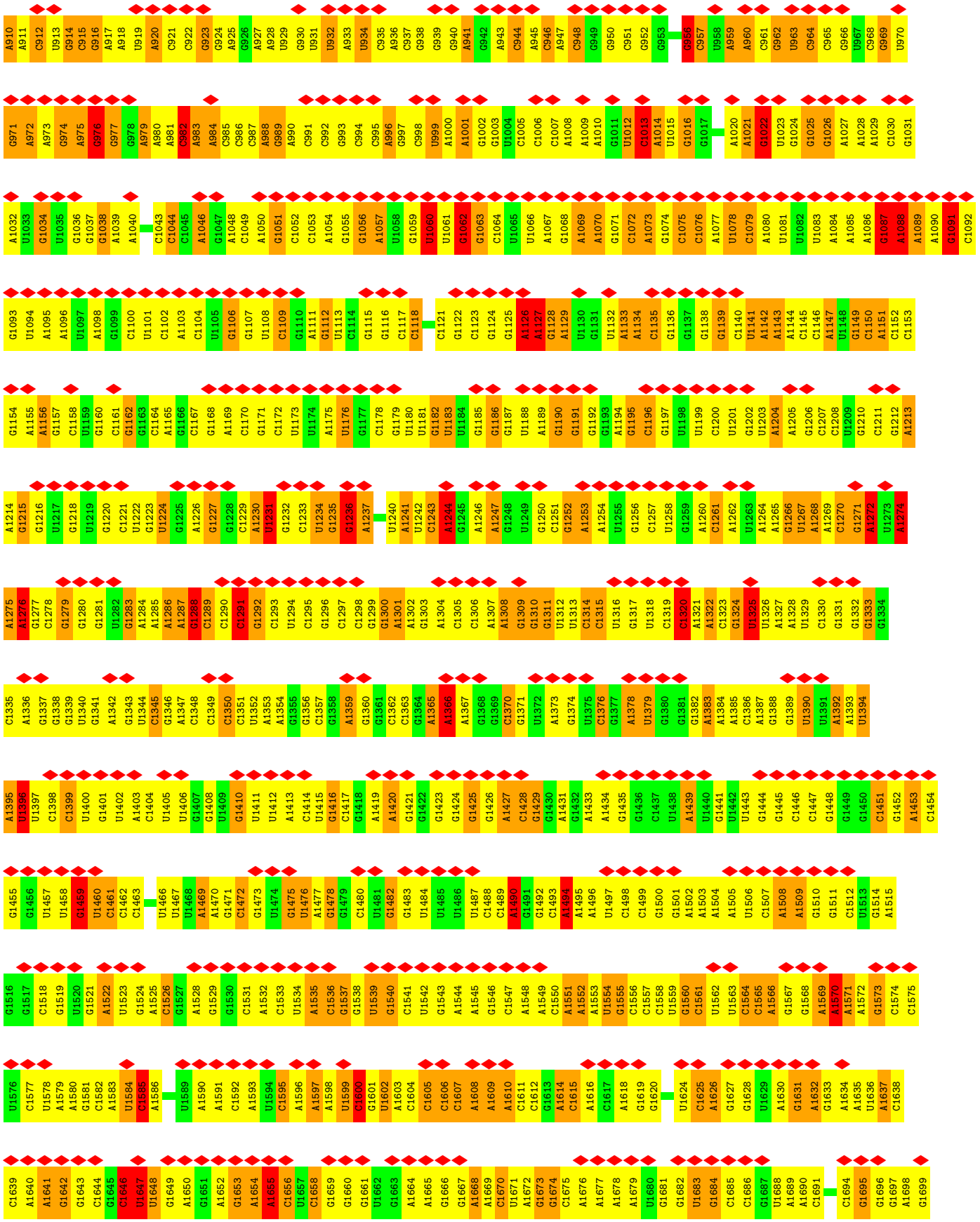


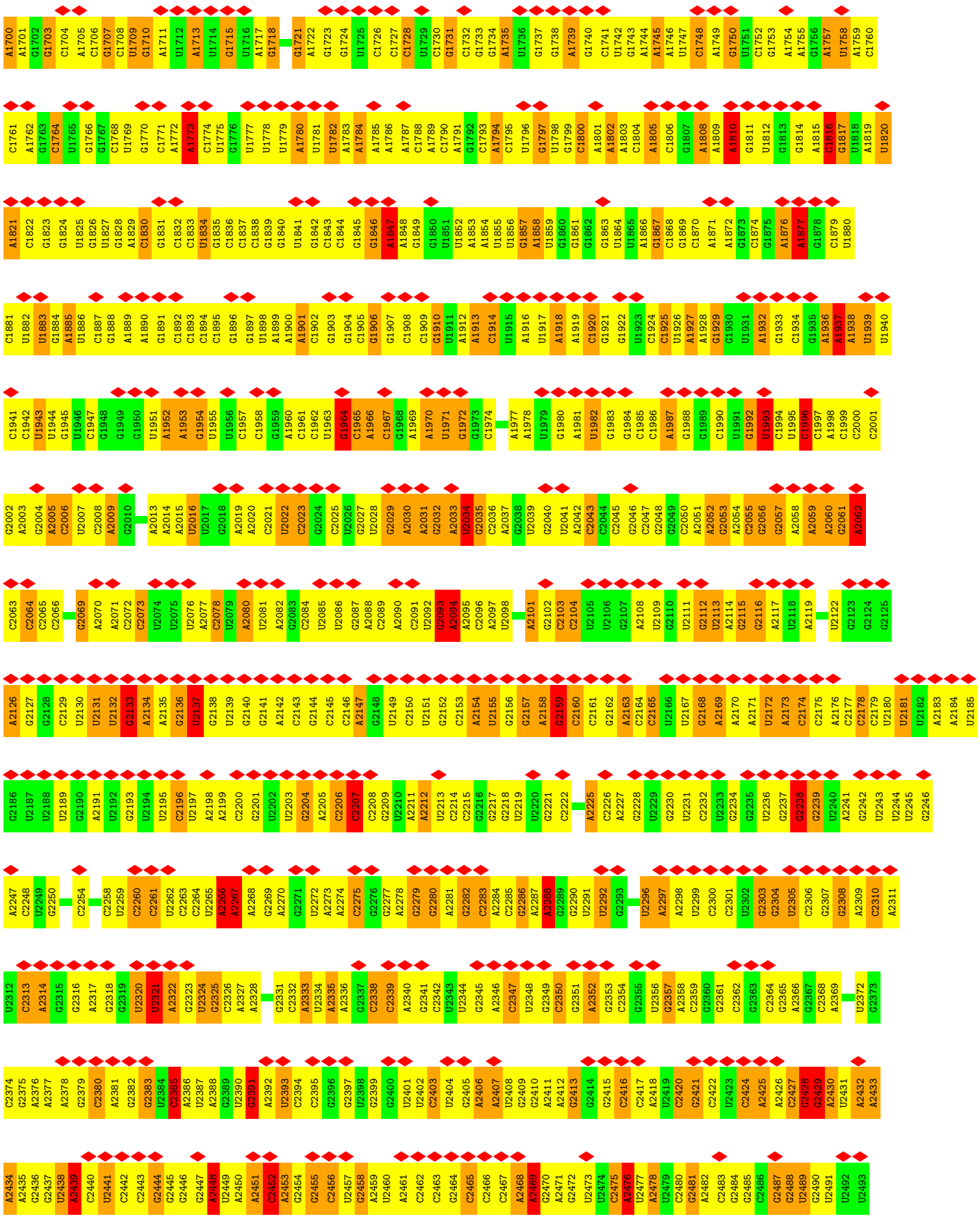
• Molecule 53: 23S ribosomal RNA

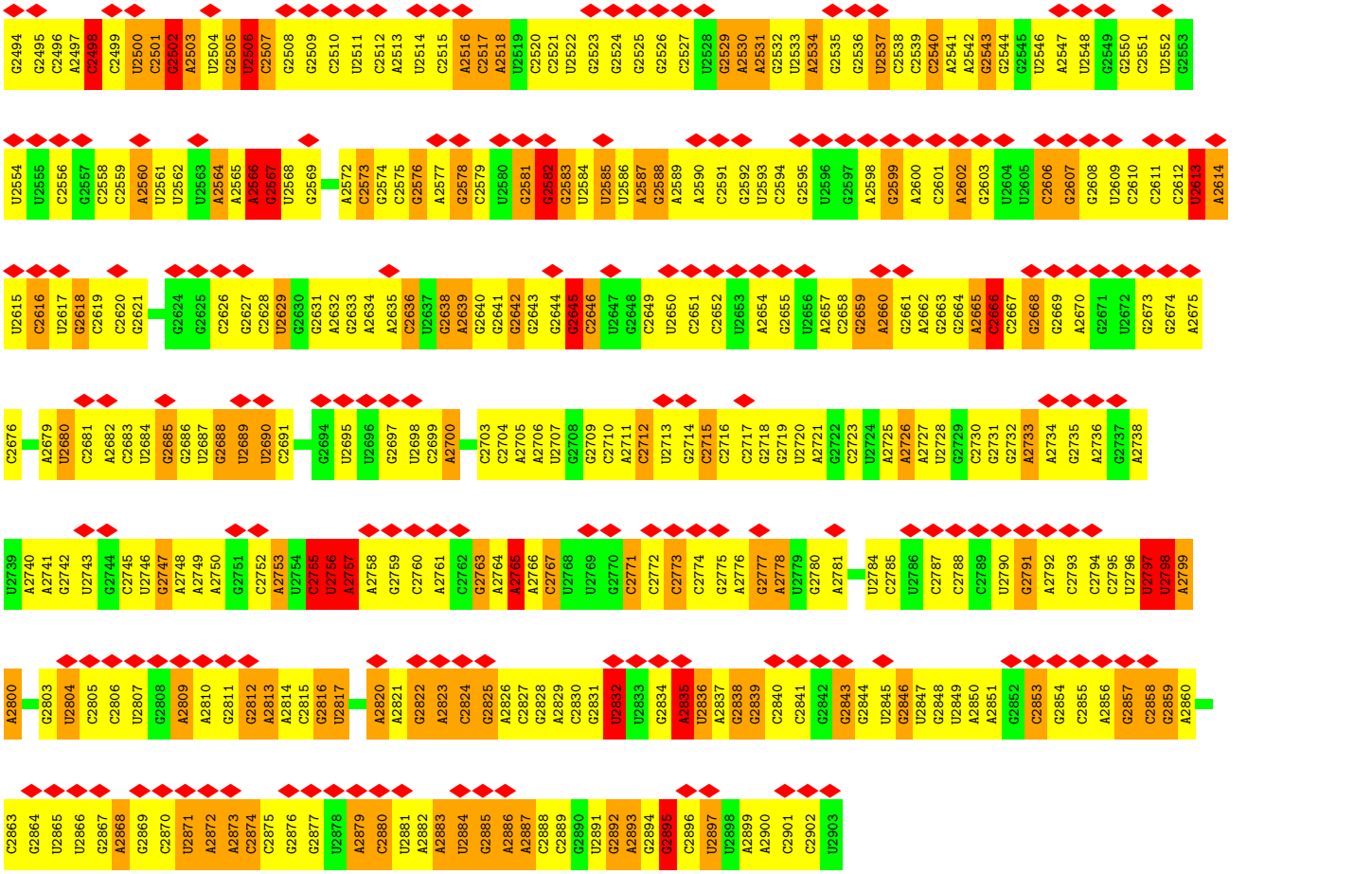
Chain BA:





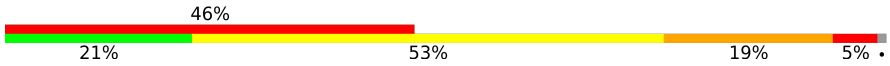


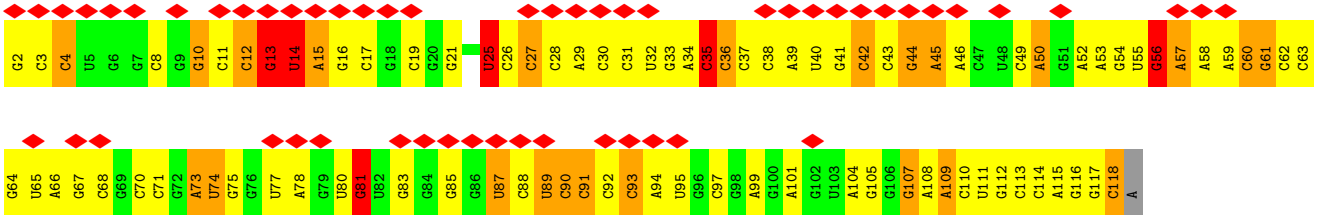

A1700 A1701 G1702 G1703 C1704 A1705 C1706 G1707 C1708 U1709 G1710 A1711 U1712 A1713 U1714 C1715 U1716 A1717 G1718 G1721 A1722 G1723 G1724 U1725 C1726 C1727 C1728 U1729 C1730 G1731 C1732 G1733 G1734 A1735 U1736 G1737 G1738 A1739 G1740 C1741 U1742 G1743 A1744 A1745 A1746 U1747 C1748 A1749 G1750 U1751 C1752 G1753 A1754 A1755 G1756 A1757 U1758 A1759 C1760
C1761 A1762 G1763 C1764 U1765 G1766 G1767 C1768 U1769 G1770 C1771 A1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 U1781 U1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1793 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 C1804 A1805 C1806 G1807 A1808 A1809 A1810 G1811 U1812 G1813 G1814 A1815 C1816 G1817 U1818 A1819 U1820
A1821 C1822 G1823 G1824 U1825 G1826 U1827 G1828 A1829 C1830 G1831 C1832 C1833 U1834 G1835 C1836 C1837 C1838 G1839 G1840 U1841 G1842 C1843 C1844 G1845 G1846 A1847 A1848 G1849 C1850 U1851 U1852 A1853 A1854 U1855 U1856 G1857 A1858 U1859 G1860 G1861 G1862 G1863 U1864 U1865 A1866 G1867 C1868 G1869 C1870 A1871 A1872 G1873 C1874 G1875 A1876 A1877 G1878 C1879 U1880
C1881 U1882 U1883 G1884 A1885 U1886 C1887 G1888 A1889 A1890 G1891 C1892 C1893 C1894 C1895 G1896 G1897 U1898 A1899 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907 C1908 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 U1926 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940
C1941 C1942 U1943 U1944 G1945 U1946 C1947 G1948 G1949 G1950 U1951 A1952 A1953 G1954 U1955 U1956 C1957 C1958 G1959 A1960 C1961 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 U1971 G1972 G1973 C1974 A1977 A1978 U1979 G1980 A1981 U1982 G1983 G1984 C1985 C1986 A1987 G1988 G1989 C1990 U1991 G1992 U1993 C1994 U1995 C1996 C1997 A1998 C1999 C2000 C2001
G2002 A2003 G2004 A2005 C2006 U2007 C2008 A2009 G2010 A2013 A2014 A2015 U2016 U2017 G2018 A2019 A2020 C2021 U2022 C2023 G2024 C2025 U2026 G2027 U2028 G2029 A2030 A2031 C2032 A2033 U2034 G2035 C2036 A2037 G2038 U2039 G2040 U2041 A2042 C2043 C2044 C2045 G2046 C2047 C2048 G2049 C2050 A2051 A2052 G2053 A2054 C2055 C2056 G2057 A2058 A2059 A2060 G2061 A2062
C2063 C2064 C2065 C2066 G2069 A2070 A2071 C2072 C2073 U2074 U2075 U2076 A2077 C2078 U2079 A2080 U2081 A2082 G2083 C2084 U2085 U2086 G2087 A2088 C2089 A2090 C2091 U2092 G2093 A2094 A2095 C2096 A2097 U2098 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 U2122 G2123 G2124 G2125
A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 C2156 G2157 A2158 G2159 C2160 C2161 C2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185
G2186 U2187 U2188 U2189 G2190 A2191 U2192 G2193 U2194 U2195 C2196 U2197 A2198 A2199 C2200 G2201 U2202 U2203 G2204 A2205 C2206 C2207 C2208 G2209 U2210 A2211 A2212 U2213 C2214 C2215 G2216 G2217 G2218 U2219 U2220 G2221 C2222 A2225 C2226 A2227 G2228 U2229 G2230 U2231 C2232 U2233 G2234 G2235 U2236 G2237 G2238 G2239 U2240 A2241 G2242 U2243 U2244 U2245 G2246
A2247 C2248 U2249 G2250 C2254 C2258 U2259 C2260 C2261 U2262 C2263 C2264 U2265 A2266 A2267 A2268 G2269 A2270 G2271 U2272 A2273 A2274 C2275 C2276 G2277 A2278 G2279 G2280 A2281 G2282 C2283 A2284 C2285 G2286 A2287 A2288 G2289 G2290 U2291 U2292 G2293 U2296 A2297 A2298 U2299 C2300 C2301 U2302 G2303 G2304 U2305 C2306 G2307 G2308 A2309 C2310 A2311
U2312 C2313 A2314 G2315 G2316 A2317 G2318 G2319 U2320 U2321 A2322 G2323 U2324 G2325 C2326 A2327 A2328 G2331 C2332 A2333 U2334 A2335 A2336 G2337 C2338 C2339 A2340 G2341 C2342 U2343 U2344 G2345 A2346 C2347 U2348 G2349 C2350 G2351 A2352 G2353 C2354 G2355 U2356 G2357 A2358 C2359 G2360 G2361 C2362 G2363 C2364 G2365 A2366 G2367 C2368 A2369 U2372 G2373
C2374 G2375 A2376 A2377 A2378 G2379 C2380 A2381 G2382 G2383 U2384 C2385 A2386 U2387 A2388 G2389 U2390 G2391 A2392 U2393 C2394 C2395 G2396 G2397 U2398 G2399 G2400 U2401 U2402 C2403 U2404 G2405 A2406 A2407 U2408 G2409 G2410 A2411 A2412 G2413 G2414 G2415 C2416 C2417 A2418 U2419 C2420 G2421 C2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2432 A2433
A2434 A2435 G2436 G2437 U2438 A2439 C2440 U2441 C2442 C2443 G2444 G2445 G2446 G2447 A2448 U2449 A2450 A2451 C2452 A2453 G2454 G2455 C2456 U2457 G2458 A2459 U2460 A2461 C2462 C2463 G2464 C2465 C2466 C2467 A2468 A2469 G2470 A2471 G2472 U2473 U2474 C2475 A2476 U2477 A2478 U2479 C2480 G2481 A2482 C2483 G2484 G2485 C2486 G2487 G2488 U2489 G2490 U2491 U2492 U2493



• Molecule 54: 5S ribosomal RNA

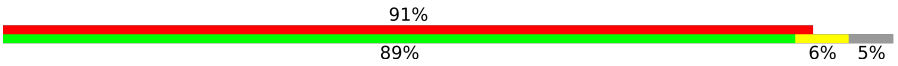
Chain BB:

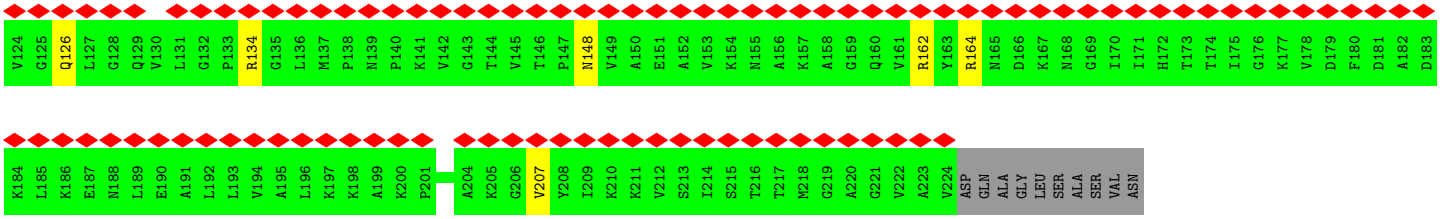




• Molecule 55: 50S ribosomal protein L1

Chain B5:




V124 G125 Q126 L127 G128 Q129 V130 L131 G132 P133 R134 G135 L136 M137 P138 N139 P140 K141 V142 G143 T144 V145 T146 P147 N148 V149 A150 E151 A152 V153 K154 N155 A156 K157 A158 G159 Q160 V161 R162 Y163 R164 N165 D166 K167 N168 G169 I170 I171 H172 T173 T174 I175 G176 K177 V178 D179 F180 D181 A182 D183
K184 L185 K186 E187 N188 L189 E190 A191 L192 L193 V194 A195 L196 K197 K198 A199 K200 P201 A204 K205 G206 V207 Y208 I209 K210 K211 V212 S213 I214 S215 T216 T217 M218 G219 A220 G221 V222 A223 V224 ASP GLN ALA GLY LEU SER ALA SER VAL ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26429	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	223.953	Depositor
Minimum map value	-122.023	Depositor
Average map value	-0.756	Depositor
Map value standard deviation	22.478	Depositor
Recommended contour level	40.0	Depositor
Map size (Å)	359.04, 359.04, 359.04	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.87, 1.87, 1.87	Depositor

5 Model quality

5.1 Standard geometry

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

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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AB	0.69	0/1736	1.15	8/2340 (0.3%)
2	AC	0.77	0/1651	1.28	18/2225 (0.8%)
3	AD	0.80	0/1665	1.26	20/2227 (0.9%)
4	AE	0.72	0/1119	1.20	11/1506 (0.7%)
5	AF	0.76	0/835	1.23	7/1128 (0.6%)
6	AG	0.76	0/1188	1.28	12/1593 (0.8%)
7	AH	0.71	0/989	1.11	5/1326 (0.4%)
8	AI	0.83	0/1035	1.37	14/1377 (1.0%)
9	AJ	0.78	0/797	1.33	11/1079 (1.0%)
10	AK	0.76	0/894	1.26	9/1207 (0.7%)
11	AL	0.77	0/969	1.37	17/1300 (1.3%)
12	AM	0.79	0/884	1.35	11/1181 (0.9%)
13	AN	0.82	0/817	1.41	11/1088 (1.0%)
14	AO	0.72	0/722	1.29	13/964 (1.3%)
15	AP	0.84	0/648	1.28	7/870 (0.8%)
16	AQ	0.73	0/658	1.19	5/883 (0.6%)
17	AR	0.80	0/463	1.21	5/623 (0.8%)
18	AS	0.76	0/653	1.27	4/879 (0.5%)
19	AT	0.71	0/672	1.12	5/890 (0.6%)
20	AU	0.85	0/431	1.31	6/572 (1.0%)
21	AA	1.75	365/36759 (1.0%)	2.28	2447/57346 (4.3%)
22	A1	1.75	20/1668 (1.2%)	2.26	110/2595 (4.2%)
23	A2	1.66	1/343 (0.3%)	2.18	17/531 (3.2%)
24	BC	0.81	0/2121	1.35	26/2852 (0.9%)
25	BD	0.71	0/1586	1.18	9/2134 (0.4%)
26	BE	0.72	0/1571	1.19	11/2113 (0.5%)
27	BF	0.77	0/1444	1.26	16/1937 (0.8%)
28	BG	0.71	0/1343	1.18	10/1816 (0.6%)
29	BH	0.68	0/1122	1.16	7/1515 (0.5%)
30	BI	0.68	0/1046	1.07	5/1410 (0.4%)
31	BJ	0.75	0/1152	1.23	9/1551 (0.6%)
32	BK	0.76	0/947	1.23	10/1268 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BL	0.79	0/1054	1.29	12/1403 (0.9%)
34	BM	0.80	0/1093	1.22	10/1460 (0.7%)
35	BN	0.83	0/973	1.44	18/1301 (1.4%)
36	BO	0.77	0/902	1.29	9/1209 (0.7%)
37	BP	0.78	0/929	1.25	9/1242 (0.7%)
38	BQ	0.81	0/960	1.36	14/1278 (1.1%)
39	BR	0.72	0/829	1.13	6/1107 (0.5%)
40	BS	0.70	0/864	1.28	10/1156 (0.9%)
41	BT	0.72	0/744	1.22	4/994 (0.4%)
42	BU	0.72	0/787	1.15	5/1051 (0.5%)
43	BV	0.74	0/766	1.27	8/1025 (0.8%)
44	BW	0.78	0/604	1.24	6/799 (0.8%)
45	BX	0.84	0/635	1.35	10/848 (1.2%)
46	BY	0.71	0/510	1.24	4/677 (0.6%)
47	BZ	0.73	0/453	1.31	6/605 (1.0%)
48	B0	0.80	0/450	1.26	8/599 (1.3%)
49	B1	0.73	0/417	1.14	3/556 (0.5%)
50	B2	0.89	0/380	1.58	10/498 (2.0%)
51	B3	0.79	0/513	1.23	6/676 (0.9%)
52	B4	0.80	0/303	1.35	6/397 (1.5%)
53	BA	1.77	819/69796 (1.2%)	2.30	4869/108888 (4.5%)
54	BB	1.74	17/2800 (0.6%)	2.24	176/4367 (4.0%)
55	B5	0.69	0/1673	1.11	8/2255 (0.4%)
All	All	1.54	1222/158363 (0.8%)	2.07	8093/236717 (3.4%)

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
18	AS	0	1
21	AA	0	328
22	A1	0	18
23	A2	0	2
53	BA	0	652
54	BB	0	27
All	All	0	1028

All (1222) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2078	C	C4-N4	-7.15	1.27	1.33
21	AA	1521	C	C4-N4	-7.01	1.27	1.33
53	BA	897	C	C4-N4	-6.68	1.27	1.33
21	AA	1214	C	C4-N4	-6.67	1.27	1.33
21	AA	637	C	C4-N4	-6.64	1.27	1.33
53	BA	787	C	C4-N4	-6.62	1.27	1.33
53	BA	1059	G	C2-N2	-6.60	1.27	1.34
53	BA	2336	A	C6-N1	-6.59	1.30	1.35
53	BA	635	C	C4-N4	-6.59	1.28	1.33
53	BA	1410	G	C2-N2	-6.59	1.27	1.34
21	AA	1366	C	C4-N4	-6.57	1.28	1.33
21	AA	1293	C	C4-N4	-6.55	1.28	1.33
53	BA	2000	C	C4-N4	-6.54	1.28	1.33
53	BA	1507	C	C4-N4	-6.54	1.28	1.33
53	BA	2681	C	C4-N4	-6.53	1.28	1.33
21	AA	1266	G	C2-N2	-6.51	1.28	1.34
53	BA	2841	C	C4-N4	-6.50	1.28	1.33
21	AA	36	C	C4-N4	-6.49	1.28	1.33
53	BA	236	C	C4-N4	-6.48	1.28	1.33
53	BA	908	C	C4-N4	-6.47	1.28	1.33
53	BA	1158	C	C4-N4	-6.46	1.28	1.33
53	BA	1656	C	C4-N4	-6.45	1.28	1.33
53	BA	1659	G	C2-N2	-6.45	1.28	1.34
21	AA	207	C	C4-N4	-6.42	1.28	1.33
22	A1	11	C	C4-N4	-6.42	1.28	1.33
21	AA	569	C	C4-N4	-6.41	1.28	1.33
21	AA	1332	A	C6-N1	-6.41	1.31	1.35
53	BA	2646	C	C4-N4	-6.38	1.28	1.33
53	BA	786	C	C4-N4	-6.35	1.28	1.33
53	BA	1410	G	C6-N1	-6.35	1.35	1.39
53	BA	2496	C	C4-N4	-6.35	1.28	1.33
53	BA	835	C	C4-N4	-6.33	1.28	1.33
53	BA	1271	G	C2-N2	-6.33	1.28	1.34
21	AA	699	C	C4-N4	-6.33	1.28	1.33
21	AA	866	C	C4-N4	-6.33	1.28	1.33
53	BA	1298	C	C4-N4	-6.32	1.28	1.33
53	BA	452	G	C2-N2	-6.32	1.28	1.34
53	BA	1536	C	C4-N4	-6.31	1.28	1.33
53	BA	2463	C	C4-N4	-6.30	1.28	1.33
53	BA	817	C	C4-N4	-6.29	1.28	1.33
53	BA	2335	A	C6-N1	-6.28	1.31	1.35
53	BA	179	C	C4-N4	-6.27	1.28	1.33
53	BA	2525	G	C2-N2	-6.27	1.28	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	324	G	C2-N2	-6.27	1.28	1.34
21	AA	1331	G	C2-N2	-6.26	1.28	1.34
53	BA	2452	C	N3-C4	-6.25	1.29	1.33
21	AA	1197	A	C6-N1	-6.25	1.31	1.35
21	AA	1516	G	N1-C2	-6.25	1.32	1.37
53	BA	751	A	C6-N1	-6.24	1.31	1.35
53	BA	1814	G	C2-N2	-6.24	1.28	1.34
21	AA	1263	C	C4-N4	-6.24	1.28	1.33
53	BA	1104	C	C4-N4	-6.24	1.28	1.33
21	AA	898	G	C2-N2	-6.24	1.28	1.34
21	AA	912	C	C4-N4	-6.24	1.28	1.33
21	AA	86	G	C2-N2	-6.23	1.28	1.34
53	BA	2261	C	C4-N4	-6.23	1.28	1.33
21	AA	1309	G	C2-N2	-6.23	1.28	1.34
53	BA	1789	A	C6-N1	-6.22	1.31	1.35
21	AA	83	C	C4-N4	-6.22	1.28	1.33
53	BA	8	C	C4-N4	-6.22	1.28	1.33
53	BA	1153	C	C4-N4	-6.21	1.28	1.33
53	BA	2317	A	C6-N1	-6.21	1.31	1.35
53	BA	426	C	C4-N4	-6.21	1.28	1.33
53	BA	1293	C	C4-N4	-6.20	1.28	1.33
21	AA	1328	C	C4-N4	-6.20	1.28	1.33
53	BA	1644	C	C4-N4	-6.20	1.28	1.33
53	BA	1853	A	C6-N1	-6.20	1.31	1.35
53	BA	1215	G	C2-N2	-6.19	1.28	1.34
21	AA	896	C	C4-N4	-6.19	1.28	1.33
21	AA	856	C	C4-N4	-6.19	1.28	1.33
53	BA	201	C	C4-N4	-6.18	1.28	1.33
53	BA	1934	C	C4-N4	-6.18	1.28	1.33
53	BA	2391	G	C2-N2	-6.16	1.28	1.34
21	AA	849	G	C2-N2	-6.16	1.28	1.34
53	BA	742	A	C6-N1	-6.16	1.31	1.35
53	BA	1706	C	C4-N4	-6.16	1.28	1.33
53	BA	2278	A	C6-N1	-6.16	1.31	1.35
53	BA	560	C	C4-N4	-6.16	1.28	1.33
53	BA	2055	C	C4-N4	-6.15	1.28	1.33
53	BA	192	C	C4-N4	-6.15	1.28	1.33
53	BA	1894	C	C4-N4	-6.14	1.28	1.33
53	BA	2536	G	C2-N2	-6.14	1.28	1.34
53	BA	1233	C	C4-N4	-6.14	1.28	1.33
53	BA	111	A	C6-N1	-6.13	1.31	1.35
21	AA	1282	C	C4-N4	-6.12	1.28	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	543	G	C2-N2	-6.12	1.28	1.34
53	BA	2001	C	C4-N4	-6.12	1.28	1.33
21	AA	351	G	C2-N2	-6.12	1.28	1.34
53	BA	406	G	C2-N2	-6.11	1.28	1.34
53	BA	1021	A	C6-N1	-6.11	1.31	1.35
53	BA	1168	G	N1-C2	-6.11	1.32	1.37
21	AA	570	G	C2-N2	-6.10	1.28	1.34
53	BA	1052	C	C4-N4	-6.10	1.28	1.33
53	BA	2857	G	C2-N2	-6.10	1.28	1.34
53	BA	1236	G	C2-N2	-6.10	1.28	1.34
53	BA	1731	G	C2-N2	-6.10	1.28	1.34
53	BA	2575	C	N3-C4	-6.10	1.29	1.33
53	BA	2806	C	C4-N4	-6.10	1.28	1.33
53	BA	240	C	C4-N4	-6.10	1.28	1.33
21	AA	882	C	N3-C4	-6.09	1.29	1.33
53	BA	208	C	C4-N4	-6.09	1.28	1.33
21	AA	857	C	C4-N4	-6.09	1.28	1.33
53	BA	533	G	C2-N2	-6.09	1.28	1.34
53	BA	863	A	C6-N1	-6.09	1.31	1.35
53	BA	1235	G	C2-N2	-6.09	1.28	1.34
22	A1	30	C	C4-N4	-6.09	1.28	1.33
53	BA	1682	G	C2-N2	-6.08	1.28	1.34
53	BA	2003	A	C6-N1	-6.08	1.31	1.35
21	AA	1158	C	C4-N4	-6.08	1.28	1.33
53	BA	2763	G	C2-N2	-6.07	1.28	1.34
54	BB	30	C	C4-N4	-6.07	1.28	1.33
21	AA	99	C	C4-N4	-6.07	1.28	1.33
53	BA	1007	C	C4-N4	-6.07	1.28	1.33
53	BA	1924	C	C4-N4	-6.07	1.28	1.33
21	AA	328	C	C4-N4	-6.06	1.28	1.33
53	BA	1454	C	N3-C4	-6.06	1.29	1.33
53	BA	1721	G	C2-N2	-6.06	1.28	1.34
53	BA	1480	C	C4-N4	-6.06	1.28	1.33
53	BA	1799	G	C2-N2	-6.06	1.28	1.34
53	BA	421	C	C4-N4	-6.05	1.28	1.33
53	BA	512	G	C2-N2	-6.05	1.28	1.34
53	BA	109	C	C4-N4	-6.04	1.28	1.33
54	BB	88	C	C4-N4	-6.04	1.28	1.33
53	BA	2405	G	N1-C2	-6.04	1.32	1.37
53	BA	2848	G	C2-N2	-6.04	1.28	1.34
21	AA	265	G	C2-N2	-6.04	1.28	1.34
53	BA	916	G	C2-N2	-6.04	1.28	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2487	G	C2-N2	-6.04	1.28	1.34
53	BA	1843	C	C4-N4	-6.03	1.28	1.33
21	AA	286	C	C4-N4	-6.03	1.28	1.33
21	AA	1028	C	N3-C4	-6.02	1.29	1.33
53	BA	1296	G	C2-N2	-6.02	1.28	1.34
53	BA	1838	C	C4-N4	-6.02	1.28	1.33
53	BA	2538	C	C4-N4	-6.02	1.28	1.33
53	BA	1079	C	C4-N4	-6.01	1.28	1.33
21	AA	1271	A	C6-N1	-6.01	1.31	1.35
53	BA	2146	C	C4-N4	-6.01	1.28	1.33
53	BA	2250	G	C2-N2	-6.01	1.28	1.34
22	A1	16	C	N3-C4	-6.01	1.29	1.33
53	BA	971	G	N1-C2	-6.01	1.32	1.37
53	BA	469	G	C2-N2	-6.00	1.28	1.34
53	BA	634	C	C4-N4	-6.00	1.28	1.33
53	BA	436	C	C4-N4	-6.00	1.28	1.33
22	A1	24	G	C2-N2	-6.00	1.28	1.34
53	BA	2811	G	C2-N2	-6.00	1.28	1.34
53	BA	298	G	C6-N1	-5.99	1.35	1.39
53	BA	2839	G	C2-N2	-5.99	1.28	1.34
21	AA	1400	C	C4-N4	-5.99	1.28	1.33
53	BA	1903	G	C2-N2	-5.98	1.28	1.34
21	AA	556	C	C4-N4	-5.98	1.28	1.33
21	AA	1352	C	C4-N4	-5.98	1.28	1.33
53	BA	540	C	C4-N4	-5.98	1.28	1.33
53	BA	2787	C	C4-N4	-5.98	1.28	1.33
21	AA	388	G	C2-N2	-5.97	1.28	1.34
53	BA	2521	C	N3-C4	-5.97	1.29	1.33
53	BA	1521	G	C2-N2	-5.97	1.28	1.34
53	BA	1006	C	N3-C4	-5.97	1.29	1.33
21	AA	383	A	C6-N1	-5.96	1.31	1.35
53	BA	1540	G	C2-N2	-5.96	1.28	1.34
21	AA	940	C	C4-N4	-5.96	1.28	1.33
21	AA	643	C	C4-N4	-5.96	1.28	1.33
53	BA	778	G	C6-N1	-5.96	1.35	1.39
53	BA	1323	C	C4-N4	-5.95	1.28	1.33
53	BA	1575	C	C4-N4	-5.95	1.28	1.33
53	BA	812	C	C4-N4	-5.95	1.28	1.33
53	BA	298	G	C2-N2	-5.95	1.28	1.34
53	BA	869	G	C6-N1	-5.95	1.35	1.39
53	BA	2517	C	C4-N4	-5.94	1.28	1.33
53	BA	723	C	C4-N4	-5.94	1.28	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	212	G	C2-N2	-5.94	1.28	1.34
53	BA	965	C	N3-C4	-5.94	1.29	1.33
53	BA	2153	C	C4-N4	-5.94	1.28	1.33
53	BA	1022	G	C2-N2	-5.94	1.28	1.34
21	AA	67	C	C4-N4	-5.94	1.28	1.33
53	BA	1889	A	C6-N1	-5.94	1.31	1.35
54	BB	35	C	C4-N4	-5.94	1.28	1.33
21	AA	322	C	C4-N4	-5.93	1.28	1.33
53	BA	156	A	C6-N1	-5.93	1.31	1.35
21	AA	640	A	C6-N1	-5.93	1.31	1.35
21	AA	1343	G	C2-N2	-5.93	1.28	1.34
53	BA	898	C	C4-N4	-5.93	1.28	1.33
53	BA	1893	C	N3-C4	-5.93	1.29	1.33
21	AA	702	A	C6-N1	-5.93	1.31	1.35
53	BA	957	C	C4-N4	-5.92	1.28	1.33
21	AA	1327	C	C4-N4	-5.92	1.28	1.33
53	BA	269	C	C4-N4	-5.92	1.28	1.33
53	BA	2567	G	C2-N2	-5.92	1.28	1.34
53	BA	2304	G	C2-N2	-5.92	1.28	1.34
21	AA	549	C	N3-C4	-5.92	1.29	1.33
53	BA	1161	C	N3-C4	-5.92	1.29	1.33
21	AA	601	G	C6-N1	-5.92	1.35	1.39
53	BA	822	G	C6-N1	-5.92	1.35	1.39
53	BA	783	A	C6-N1	-5.91	1.31	1.35
53	BA	2895	G	C2-N2	-5.91	1.28	1.34
21	AA	739	C	C4-N4	-5.91	1.28	1.33
53	BA	1574	C	C4-N4	-5.91	1.28	1.33
53	BA	989	G	C2-N2	-5.91	1.28	1.34
21	AA	611	C	C4-N4	-5.89	1.28	1.33
53	BA	1994	C	C4-N4	-5.89	1.28	1.33
22	A1	74	C	C4-N4	-5.89	1.28	1.33
21	AA	862	C	C4-N4	-5.89	1.28	1.33
53	BA	406	G	C6-N1	-5.89	1.35	1.39
21	AA	339	C	C4-N4	-5.89	1.28	1.33
53	BA	2043	C	C4-N4	-5.89	1.28	1.33
21	AA	597	G	C2-N2	-5.89	1.28	1.34
53	BA	439	A	C6-N1	-5.89	1.31	1.35
53	BA	2501	C	C4-N4	-5.88	1.28	1.33
53	BA	2072	C	C4-N4	-5.88	1.28	1.33
21	AA	1046	A	C6-N1	-5.88	1.31	1.35
21	AA	1037	C	N3-C4	-5.87	1.29	1.33
21	AA	601	G	C2-N2	-5.87	1.28	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	264	C	C4-N4	-5.87	1.28	1.33
21	AA	60	A	C6-N1	-5.86	1.31	1.35
21	AA	206	C	C4-N4	-5.86	1.28	1.33
53	BA	370	G	C2-N2	-5.86	1.28	1.34
53	BA	822	G	C2-N2	-5.86	1.28	1.34
53	BA	1761	C	C4-N4	-5.86	1.28	1.33
53	BA	2502	G	C2-N2	-5.86	1.28	1.34
54	BB	54	G	C2-N2	-5.86	1.28	1.34
53	BA	2594	C	C4-N4	-5.85	1.28	1.33
53	BA	823	C	C4-N4	-5.85	1.28	1.33
21	AA	182	A	C6-N1	-5.85	1.31	1.35
53	BA	2864	G	C2-N2	-5.85	1.28	1.34
21	AA	885	G	C2-N2	-5.85	1.28	1.34
21	AA	646	G	C2-N2	-5.84	1.28	1.34
21	AA	1369	C	N3-C4	-5.84	1.29	1.33
21	AA	69	G	C2-N2	-5.84	1.28	1.34
21	AA	169	C	C4-N4	-5.84	1.28	1.33
21	AA	1012	A	C6-N1	-5.84	1.31	1.35
53	BA	1116	G	C2-N2	-5.84	1.28	1.34
53	BA	379	G	C2-N2	-5.84	1.28	1.34
53	BA	981	A	C6-N1	-5.84	1.31	1.35
21	AA	770	C	N3-C4	-5.83	1.29	1.33
21	AA	27	G	C2-N2	-5.83	1.28	1.34
53	BA	758	C	N3-C4	-5.83	1.29	1.33
53	BA	1055	G	C2-N2	-5.82	1.28	1.34
21	AA	1344	C	N3-C4	-5.82	1.29	1.33
21	AA	1524	C	N3-C4	-5.82	1.29	1.33
53	BA	2525	G	C6-N1	-5.82	1.35	1.39
53	BA	1031	G	C2-N2	-5.82	1.28	1.34
53	BA	97	C	N3-C4	-5.82	1.29	1.33
21	AA	1251	A	C6-N1	-5.82	1.31	1.35
53	BA	1691	C	C4-N4	-5.82	1.28	1.33
53	BA	1086	A	C6-N1	-5.81	1.31	1.35
21	AA	667	G	C2-N2	-5.81	1.28	1.34
21	AA	948	C	C4-N4	-5.81	1.28	1.33
53	BA	1115	G	C2-N2	-5.81	1.28	1.34
53	BA	1314	C	N3-C4	-5.81	1.29	1.33
21	AA	1200	C	C4-N4	-5.80	1.28	1.33
53	BA	553	G	C2-N2	-5.80	1.28	1.34
53	BA	795	C	C4-N4	-5.80	1.28	1.33
21	AA	1336	C	C4-N4	-5.80	1.28	1.33
53	BA	2467	C	N3-C4	-5.80	1.29	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	548	G	C2-N2	-5.79	1.28	1.34
53	BA	1196	C	N3-C4	-5.79	1.29	1.33
21	AA	75	G	C2-N2	-5.79	1.28	1.34
53	BA	1666	G	C2-N2	-5.79	1.28	1.34
53	BA	2726	A	C6-N1	-5.79	1.31	1.35
21	AA	381	C	C4-N4	-5.79	1.28	1.33
21	AA	345	C	C4-N4	-5.78	1.28	1.33
53	BA	66	C	C4-N4	-5.78	1.28	1.33
53	BA	168	G	C2-N2	-5.78	1.28	1.34
53	BA	650	C	C4-N4	-5.78	1.28	1.33
53	BA	706	A	C6-N6	-5.78	1.29	1.33
21	AA	1501	C	C4-N4	-5.77	1.28	1.33
21	AA	1021	A	C6-N1	-5.77	1.31	1.35
21	AA	1059	C	C4-N4	-5.77	1.28	1.33
53	BA	342	A	C6-N1	-5.77	1.31	1.35
53	BA	1659	G	C6-N1	-5.77	1.35	1.39
53	BA	1190	G	C2-N2	-5.77	1.28	1.34
53	BA	1592	C	C4-N4	-5.77	1.28	1.33
21	AA	885	G	C6-N1	-5.76	1.35	1.39
21	AA	829	G	C2-N2	-5.76	1.28	1.34
53	BA	1854	A	C6-N1	-5.76	1.31	1.35
53	BA	2839	G	C6-N1	-5.76	1.35	1.39
53	BA	1292	G	N1-C2	-5.76	1.33	1.37
53	BA	2771	C	C4-N4	-5.76	1.28	1.33
53	BA	2461	A	C6-N1	-5.75	1.31	1.35
53	BA	960	A	C6-N1	-5.75	1.31	1.35
53	BA	1962	C	C4-N4	-5.75	1.28	1.33
53	BA	1277	G	C2-N2	-5.75	1.28	1.34
21	AA	864	A	C6-N1	-5.75	1.31	1.35
22	A1	24	G	C6-N1	-5.75	1.35	1.39
53	BA	2212	A	C6-N1	-5.74	1.31	1.35
21	AA	1031	C	C4-N4	-5.74	1.28	1.33
53	BA	1152	C	N3-C4	-5.74	1.29	1.33
21	AA	1272	G	C2-N2	-5.74	1.28	1.34
53	BA	1660	G	C2-N2	-5.74	1.28	1.34
21	AA	87	C	N3-C4	-5.74	1.29	1.33
21	AA	95	C	C4-N4	-5.74	1.28	1.33
53	BA	2089	C	C4-N4	-5.74	1.28	1.33
21	AA	881	G	C2-N2	-5.73	1.28	1.34
53	BA	2543	G	C2-N2	-5.73	1.28	1.34
21	AA	198	G	C2-N2	-5.73	1.28	1.34
53	BA	2876	G	C2-N2	-5.73	1.28	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1069	A	C6-N1	-5.73	1.31	1.35
21	AA	82	G	N1-C2	-5.73	1.33	1.37
21	AA	836	G	C2-N2	-5.72	1.28	1.34
53	BA	1202	G	C2-N2	-5.72	1.28	1.34
53	BA	2652	C	C4-N4	-5.72	1.28	1.33
53	BA	367	G	C2-N2	-5.72	1.28	1.34
53	BA	708	G	C2-N2	-5.72	1.28	1.34
21	AA	1514	G	C2-N2	-5.72	1.28	1.34
53	BA	1107	G	C2-N2	-5.72	1.28	1.34
53	BA	1638	C	N3-C4	-5.72	1.29	1.33
53	BA	2456	C	N3-C4	-5.72	1.29	1.33
53	BA	2526	G	C2-N2	-5.72	1.28	1.34
22	A1	40	G	C2-N2	-5.72	1.28	1.34
53	BA	2424	C	C4-N4	-5.72	1.28	1.33
53	BA	628	G	C2-N2	-5.71	1.28	1.34
53	BA	2298	A	C6-N1	-5.71	1.31	1.35
53	BA	2859	G	C2-N2	-5.71	1.28	1.34
21	AA	194	C	C4-N4	-5.71	1.28	1.33
53	BA	948	C	C4-N4	-5.71	1.28	1.33
53	BA	687	C	C4-N4	-5.71	1.28	1.33
53	BA	2263	C	C4-N4	-5.71	1.28	1.33
21	AA	1288	A	C6-N1	-5.71	1.31	1.35
53	BA	2579	C	C4-N4	-5.70	1.28	1.33
21	AA	210	C	N3-C4	-5.70	1.29	1.33
53	BA	484	C	C4-N4	-5.70	1.28	1.33
53	BA	2442	C	C4-N4	-5.70	1.28	1.33
53	BA	2599	G	C2-N2	-5.70	1.28	1.34
21	AA	595	A	C6-N1	-5.70	1.31	1.35
21	AA	1368	A	C6-N1	-5.70	1.31	1.35
21	AA	886	G	C2-N2	-5.70	1.28	1.34
21	AA	1006	G	C2-N2	-5.69	1.28	1.34
21	AA	984	C	C4-N4	-5.69	1.28	1.33
21	AA	1356	G	C2-N2	-5.69	1.28	1.34
53	BA	510	C	C4-N4	-5.69	1.28	1.33
21	AA	1245	C	C4-N4	-5.69	1.28	1.33
53	BA	336	C	C4-N4	-5.69	1.28	1.33
53	BA	2287	A	C6-N1	-5.69	1.31	1.35
53	BA	21	A	C6-N1	-5.69	1.31	1.35
53	BA	800	A	C6-N1	-5.69	1.31	1.35
53	BA	901	C	N3-C4	-5.69	1.29	1.33
53	BA	1633	G	C2-N2	-5.69	1.28	1.34
53	BA	2551	C	N3-C4	-5.69	1.29	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	934	C	C4-N4	-5.68	1.28	1.33
21	AA	212	G	C6-N1	-5.68	1.35	1.39
53	BA	935	C	C4-N4	-5.68	1.28	1.33
53	BA	2515	C	N3-C4	-5.68	1.29	1.33
53	BA	2144	G	C2-N2	-5.67	1.28	1.34
53	BA	522	A	C6-N1	-5.67	1.31	1.35
53	BA	640	C	C4-N4	-5.67	1.28	1.33
53	BA	1932	A	C6-N1	-5.67	1.31	1.35
53	BA	2668	G	C2-N2	-5.67	1.28	1.34
54	BB	31	C	N3-C4	-5.67	1.29	1.33
53	BA	1311	G	C2-N2	-5.67	1.28	1.34
53	BA	629	G	C6-N1	-5.67	1.35	1.39
53	BA	2674	G	C2-N2	-5.67	1.28	1.34
53	BA	533	G	C6-N1	-5.67	1.35	1.39
53	BA	778	G	C2-N2	-5.66	1.28	1.34
53	BA	2066	C	C4-N4	-5.66	1.28	1.33
53	BA	2560	A	C6-N1	-5.66	1.31	1.35
21	AA	998	C	N3-C4	-5.66	1.29	1.33
53	BA	1642	G	C2-N2	-5.66	1.28	1.34
53	BA	2853	C	C4-N4	-5.66	1.28	1.33
21	AA	599	C	C4-N4	-5.66	1.28	1.33
53	BA	440	C	N3-C4	-5.66	1.29	1.33
53	BA	777	G	C2-N2	-5.66	1.28	1.34
53	BA	2342	C	C4-N4	-5.66	1.28	1.33
53	BA	2412	A	C6-N1	-5.65	1.31	1.35
53	BA	865	C	C4-N4	-5.65	1.28	1.33
53	BA	912	C	N3-C4	-5.65	1.29	1.33
53	BA	1014	A	C6-N1	-5.65	1.31	1.35
53	BA	994	C	C4-N4	-5.65	1.28	1.33
53	BA	2164	C	C4-N4	-5.65	1.28	1.33
21	AA	688	G	C2-N2	-5.65	1.28	1.34
53	BA	1482	G	C2-N2	-5.65	1.28	1.34
53	BA	902	C	C4-N4	-5.65	1.28	1.33
21	AA	615	G	C2-N2	-5.64	1.28	1.34
21	AA	883	C	C4-N4	-5.64	1.28	1.33
53	BA	1500	G	C2-N2	-5.64	1.28	1.34
53	BA	1685	C	C4-N4	-5.64	1.28	1.33
53	BA	2481	G	C2-N2	-5.64	1.28	1.34
53	BA	1076	C	C4-N4	-5.64	1.28	1.33
53	BA	2876	G	C6-N1	-5.64	1.35	1.39
53	BA	880	G	C2-N2	-5.64	1.28	1.34
21	AA	187	G	C2-N2	-5.64	1.28	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1310	G	C2-N2	-5.64	1.28	1.34
53	BA	1791	A	C6-N1	-5.64	1.31	1.35
22	A1	25	C	C4-N4	-5.64	1.28	1.33
21	AA	1357	A	C6-N1	-5.63	1.31	1.35
53	BA	46	G	C2-N2	-5.63	1.28	1.34
53	BA	854	C	C4-N4	-5.63	1.28	1.33
53	BA	1905	C	C4-N4	-5.63	1.28	1.33
53	BA	2444	G	C2-N2	-5.63	1.28	1.34
53	BA	2509	G	C2-N2	-5.63	1.28	1.34
53	BA	2840	C	C4-N4	-5.63	1.28	1.33
53	BA	1243	C	C4-N4	-5.63	1.28	1.33
53	BA	1817	G	C2-N2	-5.63	1.28	1.34
21	AA	769	G	C2-N2	-5.63	1.28	1.34
53	BA	1337	G	C2-N2	-5.63	1.28	1.34
53	BA	1780	A	C6-N1	-5.63	1.31	1.35
53	BA	2004	G	C2-N2	-5.63	1.28	1.34
21	AA	311	C	C4-N4	-5.62	1.28	1.33
53	BA	869	G	C2-N2	-5.62	1.28	1.34
54	BB	28	C	C4-N4	-5.62	1.28	1.33
53	BA	327	G	C2-N2	-5.62	1.28	1.34
53	BA	2844	G	C2-N2	-5.62	1.28	1.34
53	BA	452	G	C6-N1	-5.62	1.35	1.39
21	AA	1096	C	C4-N4	-5.62	1.28	1.33
53	BA	1059	G	C6-N1	-5.62	1.35	1.39
53	BA	1315	C	C4-N4	-5.62	1.28	1.33
53	BA	1489	C	C4-N4	-5.62	1.28	1.33
53	BA	257	C	N3-C4	-5.62	1.30	1.33
53	BA	792	A	C6-N1	-5.62	1.31	1.35
53	BA	943	A	C6-N1	-5.62	1.31	1.35
21	AA	1350	A	C6-N1	-5.62	1.31	1.35
53	BA	2683	C	C4-N4	-5.62	1.28	1.33
53	BA	985	C	C4-N4	-5.61	1.28	1.33
53	BA	1117	C	N3-C4	-5.61	1.30	1.33
21	AA	195	A	C5-C4	-5.61	1.34	1.38
21	AA	1136	C	C4-N4	-5.61	1.28	1.33
53	BA	1336	A	C6-N1	-5.61	1.31	1.35
53	BA	2857	G	C6-N1	-5.61	1.35	1.39
53	BA	213	A	C6-N1	-5.61	1.31	1.35
21	AA	350	G	C2-N2	-5.61	1.28	1.34
53	BA	876	C	C4-N4	-5.61	1.28	1.33
53	BA	1897	G	C6-N1	-5.61	1.35	1.39
21	AA	97	G	C2-N2	-5.60	1.28	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1531	C	C4-N4	-5.60	1.28	1.33
21	AA	859	G	C2-N2	-5.60	1.28	1.34
53	BA	867	C	C4-N4	-5.60	1.28	1.33
53	BA	1633	G	C6-N1	-5.60	1.35	1.39
53	BA	2411	A	C6-N1	-5.60	1.31	1.35
53	BA	463	G	C2-N2	-5.59	1.28	1.34
53	BA	2268	A	C6-N1	-5.59	1.31	1.35
21	AA	836	G	C6-N1	-5.59	1.35	1.39
21	AA	646	G	C6-N1	-5.59	1.35	1.39
53	BA	1909	C	C4-N4	-5.59	1.28	1.33
21	AA	149	A	C6-N1	-5.59	1.31	1.35
21	AA	612	C	C4-N4	-5.59	1.28	1.33
53	BA	80	G	N1-C2	-5.59	1.33	1.37
53	BA	2290	G	C2-N2	-5.59	1.28	1.34
21	AA	1395	C	N3-C4	-5.59	1.30	1.33
53	BA	689	A	C6-N1	-5.59	1.31	1.35
21	AA	102	G	C2-N2	-5.58	1.28	1.34
21	AA	647	C	N3-C4	-5.58	1.30	1.33
21	AA	903	G	C2-N2	-5.58	1.28	1.34
21	AA	1281	C	C4-N4	-5.58	1.28	1.33
53	BA	353	C	C4-N4	-5.58	1.28	1.33
53	BA	2242	G	C2-N2	-5.58	1.28	1.34
53	BA	2662	A	C6-N1	-5.58	1.31	1.35
21	AA	549	C	C4-N4	-5.58	1.28	1.33
53	BA	858	G	C2-N2	-5.58	1.28	1.34
21	AA	756	C	C4-N4	-5.58	1.28	1.33
21	AA	865	A	C5-C4	-5.58	1.34	1.38
53	BA	266	G	C2-N2	-5.58	1.28	1.34
53	BA	1311	G	C6-N1	-5.58	1.35	1.39
21	AA	1244	G	C2-N2	-5.57	1.28	1.34
53	BA	2004	G	C6-N1	-5.57	1.35	1.39
21	AA	867	G	C2-N2	-5.57	1.28	1.34
53	BA	1321	A	C6-N1	-5.57	1.31	1.35
53	BA	2279	G	C2-N2	-5.57	1.28	1.34
21	AA	332	G	C2-N2	-5.57	1.28	1.34
53	BA	1068	G	C2-N2	-5.57	1.28	1.34
53	BA	2273	A	C6-N1	-5.57	1.31	1.35
21	AA	240	G	C2-N2	-5.56	1.28	1.34
21	AA	715	A	C6-N1	-5.56	1.31	1.35
21	AA	1523	G	C2-N2	-5.56	1.28	1.34
53	BA	261	G	C2-N2	-5.56	1.28	1.34
53	BA	173	A	C6-N1	-5.56	1.31	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	923	G	C2-N2	-5.56	1.28	1.34
53	BA	456	C	C4-N4	-5.55	1.28	1.33
53	BA	1490	A	C6-N1	-5.55	1.31	1.35
53	BA	2440	C	C4-N4	-5.55	1.28	1.33
53	BA	1524	G	C2-N2	-5.55	1.28	1.34
22	A1	10	G	C6-N1	-5.55	1.35	1.39
53	BA	1927	A	C6-N1	-5.55	1.31	1.35
53	BA	903	C	C4-N4	-5.55	1.28	1.33
53	BA	2316	G	C2-N2	-5.55	1.29	1.34
21	AA	752	G	C2-N2	-5.54	1.29	1.34
53	BA	2527	C	C4-N4	-5.54	1.28	1.33
53	BA	2902	C	C4-N4	-5.54	1.28	1.33
21	AA	73	C	C4-N4	-5.54	1.28	1.33
21	AA	76	G	C2-N2	-5.54	1.29	1.34
21	AA	568	G	N1-C2	-5.54	1.33	1.37
53	BA	1123	C	C4-N4	-5.54	1.28	1.33
21	AA	282	A	C6-N6	-5.54	1.29	1.33
21	AA	174	A	C6-N6	-5.54	1.29	1.33
53	BA	1125	G	C2-N2	-5.54	1.29	1.34
53	BA	1135	C	C4-N4	-5.54	1.28	1.33
53	BA	1210	G	C2-N2	-5.54	1.29	1.34
53	BA	2104	C	N3-C4	-5.54	1.30	1.33
53	BA	2506	U	C4'-C3'	-5.54	1.47	1.52
53	BA	848	C	N3-C4	-5.54	1.30	1.33
53	BA	1136	G	C2-N2	-5.54	1.29	1.34
53	BA	1837	C	C4-N4	-5.54	1.28	1.33
53	BA	2614	A	C6-N1	-5.54	1.31	1.35
21	AA	1043	G	N1-C2	-5.54	1.33	1.37
53	BA	364	C	C4-N4	-5.54	1.28	1.33
53	BA	1151	A	C6-N1	-5.54	1.31	1.35
53	BA	1423	G	C2-N2	-5.53	1.29	1.34
53	BA	2512	C	C4-N4	-5.53	1.28	1.33
53	BA	1179	G	C2-N2	-5.53	1.29	1.34
53	BA	157	C	N3-C4	-5.53	1.30	1.33
53	BA	402	A	C6-N6	-5.53	1.29	1.33
53	BA	374	A	C6-N1	-5.53	1.31	1.35
53	BA	1050	A	C6-N1	-5.53	1.31	1.35
53	BA	1847	A	C6-N1	-5.53	1.31	1.35
53	BA	43	G	C2-N2	-5.53	1.29	1.34
53	BA	79	C	N3-C4	-5.53	1.30	1.33
53	BA	1164	C	C4-N4	-5.53	1.28	1.33
53	BA	122	G	C2-N2	-5.52	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	476	G	C2-N2	-5.52	1.29	1.34
53	BA	2260	C	N3-C4	-5.52	1.30	1.33
53	BA	1965	C	N3-C4	-5.52	1.30	1.33
53	BA	1288	G	C2-N2	-5.52	1.29	1.34
53	BA	1717	A	C6-N1	-5.52	1.31	1.35
53	BA	1715	G	C2-N2	-5.52	1.29	1.34
53	BA	2455	G	C2-N2	-5.52	1.29	1.34
53	BA	1006	C	C4-N4	-5.51	1.28	1.33
53	BA	1771	C	C4-N4	-5.51	1.28	1.33
53	BA	2171	A	C6-N1	-5.51	1.31	1.35
21	AA	326	G	C2-N2	-5.51	1.29	1.34
21	AA	572	A	C6-N1	-5.51	1.31	1.35
21	AA	1038	C	C4-N4	-5.51	1.28	1.33
53	BA	935	C	N3-C4	-5.51	1.30	1.33
21	AA	573	A	C6-N1	-5.51	1.31	1.35
21	AA	1504	G	C2-N2	-5.51	1.29	1.34
22	A1	15	G	C2-N2	-5.51	1.29	1.34
53	BA	524	G	N1-C2	-5.51	1.33	1.37
53	BA	1190	G	C6-N1	-5.51	1.35	1.39
53	BA	1805	A	C6-N1	-5.51	1.31	1.35
21	AA	45	G	C2-N2	-5.51	1.29	1.34
21	AA	808	C	C4-N4	-5.51	1.28	1.33
53	BA	1823	G	C2-N2	-5.51	1.29	1.34
21	AA	879	C	C4-N4	-5.50	1.28	1.33
21	AA	1196	A	C5-C4	-5.50	1.34	1.38
53	BA	1998	A	C6-N1	-5.50	1.31	1.35
53	BA	225	C	C4-N4	-5.50	1.28	1.33
53	BA	915	C	C4-N4	-5.50	1.28	1.33
53	BA	2896	C	N3-C4	-5.50	1.30	1.33
53	BA	2087	G	N1-C2	-5.50	1.33	1.37
53	BA	221	A	C5-C4	-5.50	1.34	1.38
53	BA	796	C	C4-N4	-5.50	1.28	1.33
53	BA	2882	A	C6-N1	-5.50	1.31	1.35
53	BA	2531	A	C6-N1	-5.50	1.31	1.35
53	BA	2642	G	C2-N2	-5.50	1.29	1.34
53	BA	2448	A	C6-N1	-5.50	1.31	1.35
53	BA	2815	C	N3-C4	-5.50	1.30	1.33
21	AA	195	A	C6-N6	-5.49	1.29	1.33
21	AA	967	C	C4-N4	-5.49	1.29	1.33
21	AA	1037	C	C4-N4	-5.49	1.29	1.33
21	AA	1297	G	N1-C2	-5.49	1.33	1.37
53	BA	256	A	C6-N1	-5.49	1.31	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	230	G	C2-N2	-5.49	1.29	1.34
53	BA	237	C	C4-N4	-5.49	1.29	1.33
53	BA	488	G	C2-N2	-5.49	1.29	1.34
21	AA	823	C	N3-C4	-5.49	1.30	1.33
53	BA	433	C	N3-C4	-5.49	1.30	1.33
53	BA	1844	C	C4-N4	-5.49	1.29	1.33
53	BA	2834	G	N1-C2	-5.49	1.33	1.37
21	AA	1255	G	C2-N2	-5.49	1.29	1.34
53	BA	76	C	C4-N4	-5.49	1.29	1.33
53	BA	110	G	C2-N2	-5.49	1.29	1.34
53	BA	1008	A	C6-N1	-5.49	1.31	1.35
53	BA	46	G	C6-N1	-5.49	1.35	1.39
53	BA	1521	G	C6-N1	-5.48	1.35	1.39
53	BA	1062	G	C2-N2	-5.48	1.29	1.34
53	BA	2529	G	C2-N2	-5.48	1.29	1.34
53	BA	2651	C	C4-N4	-5.48	1.29	1.33
21	AA	1292	G	C2-N2	-5.48	1.29	1.34
53	BA	194	G	C2-N2	-5.48	1.29	1.34
53	BA	916	G	C6-N1	-5.48	1.35	1.39
53	BA	1118	C	C4-N4	-5.48	1.29	1.33
53	BA	1967	C	N3-C4	-5.48	1.30	1.33
53	BA	791	C	N3-C4	-5.48	1.30	1.33
53	BA	2274	A	C6-N6	-5.48	1.29	1.33
21	AA	1063	C	N3-C4	-5.47	1.30	1.33
21	AA	1067	A	C5-C4	-5.47	1.34	1.38
53	BA	2466	C	N3-C4	-5.47	1.30	1.33
21	AA	860	A	C6-N1	-5.47	1.31	1.35
53	BA	959	A	C6-N1	-5.47	1.31	1.35
53	BA	1319	C	N3-C4	-5.47	1.30	1.33
53	BA	2844	G	C6-N1	-5.47	1.35	1.39
53	BA	995	C	C4-N4	-5.46	1.29	1.33
53	BA	1005	C	N3-C4	-5.46	1.30	1.33
53	BA	1908	C	N3-C4	-5.46	1.30	1.33
21	AA	831	A	C5-C4	-5.46	1.34	1.38
53	BA	716	A	C6-N1	-5.46	1.31	1.35
53	BA	2300	C	C4-N4	-5.46	1.29	1.33
53	BA	2581	G	C2-N2	-5.46	1.29	1.34
53	BA	420	C	C4-N4	-5.46	1.29	1.33
53	BA	1331	G	C2-N2	-5.46	1.29	1.34
53	BA	1541	C	N3-C4	-5.46	1.30	1.33
53	BA	1002	G	C2-N2	-5.46	1.29	1.34
53	BA	1473	G	C2-N2	-5.46	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	690	G	N1-C2	-5.45	1.33	1.37
53	BA	1469	A	C5-C4	-5.45	1.34	1.38
53	BA	523	C	N3-C4	-5.45	1.30	1.33
53	BA	914	G	C2-N2	-5.45	1.29	1.34
53	BA	1745	A	C6-N6	-5.45	1.29	1.33
53	BA	446	G	C2-N2	-5.45	1.29	1.34
53	BA	1064	C	C4-N4	-5.45	1.29	1.33
53	BA	2772	C	C4-N4	-5.45	1.29	1.33
54	BB	29	A	C6-N6	-5.45	1.29	1.33
53	BA	1728	C	C4-N4	-5.45	1.29	1.33
53	BA	253	C	C4-N4	-5.45	1.29	1.33
21	AA	313	A	C6-N1	-5.44	1.31	1.35
21	AA	1252	A	C5-C4	-5.44	1.34	1.38
53	BA	2088	A	C6-N6	-5.44	1.29	1.33
53	BA	2462	C	C4-N4	-5.44	1.29	1.33
21	AA	399	G	C2-N2	-5.44	1.29	1.34
53	BA	2277	G	C2-N2	-5.44	1.29	1.34
53	BA	268	C	C4-N4	-5.44	1.29	1.33
53	BA	986	C	C4-N4	-5.44	1.29	1.33
53	BA	2436	G	C2-N2	-5.44	1.29	1.34
22	A1	48	C	C4-N4	-5.43	1.29	1.33
53	BA	338	G	C2-N2	-5.43	1.29	1.34
53	BA	732	C	N3-C4	-5.43	1.30	1.33
53	BA	922	C	N3-C4	-5.43	1.30	1.33
53	BA	1160	G	C2-N2	-5.43	1.29	1.34
53	BA	1274	A	C6-N1	-5.43	1.31	1.35
53	BA	1300	G	C2-N2	-5.43	1.29	1.34
22	A1	31	C	C4-N4	-5.43	1.29	1.33
53	BA	61	C	N3-C4	-5.43	1.30	1.33
54	BB	61	G	C2-N2	-5.43	1.29	1.34
21	AA	1051	C	N3-C4	-5.43	1.30	1.33
53	BA	335	C	C4-N4	-5.43	1.29	1.33
53	BA	340	A	C6-N6	-5.43	1.29	1.33
53	BA	672	C	N3-C4	-5.43	1.30	1.33
21	AA	316	C	C4-N4	-5.42	1.29	1.33
21	AA	334	C	C4-N4	-5.42	1.29	1.33
53	BA	1795	C	C4-N4	-5.42	1.29	1.33
53	BA	1417	C	C4-N4	-5.42	1.29	1.33
53	BA	2532	G	C2-N2	-5.42	1.29	1.34
21	AA	814	A	C6-N1	-5.42	1.31	1.35
21	AA	894	G	C2-N2	-5.42	1.29	1.34
21	AA	791	G	C2-N2	-5.42	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1879	C	C4-N4	-5.42	1.29	1.33
53	BA	2065	C	C4-N4	-5.42	1.29	1.33
53	BA	2416	C	N3-C4	-5.42	1.30	1.33
21	AA	266	G	C2-N2	-5.42	1.29	1.34
53	BA	517	C	N3-C4	-5.42	1.30	1.33
53	BA	679	C	C4-N4	-5.42	1.29	1.33
53	BA	2008	C	N3-C4	-5.42	1.30	1.33
21	AA	750	C	C4-N4	-5.41	1.29	1.33
53	BA	1178	C	C4-N4	-5.41	1.29	1.33
53	BA	1459	G	C2-N2	-5.41	1.29	1.34
21	AA	689	C	N3-C4	-5.41	1.30	1.33
53	BA	1307	A	C6-N1	-5.41	1.31	1.35
21	AA	1497	G	C2-N2	-5.41	1.29	1.34
53	BA	108	G	N1-C2	-5.41	1.33	1.37
53	BA	550	C	C4-N4	-5.41	1.29	1.33
53	BA	1322	A	C5-C4	-5.41	1.34	1.38
53	BA	438	G	C2-N2	-5.41	1.29	1.34
53	BA	1518	C	C4-N4	-5.41	1.29	1.33
21	AA	1531	A	C6-N1	-5.40	1.31	1.35
53	BA	704	G	C2-N2	-5.40	1.29	1.34
53	BA	2230	G	C2-N2	-5.40	1.29	1.34
22	A1	45	G	C2-N2	-5.40	1.29	1.34
53	BA	1100	C	C4-N4	-5.40	1.29	1.33
53	BA	1247	A	C6-N1	-5.40	1.31	1.35
53	BA	1305	C	C4-N4	-5.40	1.29	1.33
53	BA	2437	G	C2-N2	-5.40	1.29	1.34
53	BA	879	G	C2-N2	-5.40	1.29	1.34
53	BA	2033	A	C5-C4	-5.40	1.34	1.38
53	BA	2313	C	C4-N4	-5.40	1.29	1.33
21	AA	1160	G	C2-N2	-5.40	1.29	1.34
22	A1	28	C	N3-C4	-5.39	1.30	1.33
21	AA	576	C	C4-N4	-5.39	1.29	1.33
53	BA	783	A	O3'-P	-5.39	1.54	1.61
53	BA	706	A	C5-C4	-5.39	1.34	1.38
53	BA	725	G	C2-N2	-5.39	1.29	1.34
53	BA	997	G	C2-N2	-5.39	1.29	1.34
53	BA	1091	G	C2-N2	-5.39	1.29	1.34
21	AA	100	G	N1-C2	-5.39	1.33	1.37
21	AA	1309	G	C6-N1	-5.39	1.35	1.39
53	BA	969	G	C2-N2	-5.39	1.29	1.34
53	BA	1469	A	C6-N6	-5.39	1.29	1.33
53	BA	1639	C	N3-C4	-5.39	1.30	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1424	G	C2-N2	-5.39	1.29	1.34
53	BA	2676	C	C4-N4	-5.39	1.29	1.33
53	BA	2816	G	C2-N2	-5.39	1.29	1.34
53	BA	1600	C	C4-N4	-5.38	1.29	1.33
53	BA	2227	A	C6-N1	-5.38	1.31	1.35
53	BA	2530	A	C6-N1	-5.38	1.31	1.35
53	BA	677	A	C6-N1	-5.38	1.31	1.35
53	BA	1498	C	C4-N4	-5.38	1.29	1.33
53	BA	1835	G	C2-N2	-5.38	1.29	1.34
53	BA	859	G	N1-C2	-5.38	1.33	1.37
53	BA	1025	G	C2-N2	-5.38	1.29	1.34
21	AA	792	A	C6-N1	-5.37	1.31	1.35
21	AA	1192	C	C4-N4	-5.37	1.29	1.33
21	AA	1356	G	C6-N1	-5.37	1.35	1.39
53	BA	1581	G	C2-N2	-5.37	1.29	1.34
54	BB	26	C	C4-N4	-5.37	1.29	1.33
53	BA	209	C	C4-N4	-5.37	1.29	1.33
53	BA	2855	C	C4-N4	-5.37	1.29	1.33
21	AA	714	G	C2-N2	-5.37	1.29	1.34
53	BA	1846	G	C2-N2	-5.37	1.29	1.34
21	AA	1493	A	C6-N6	-5.37	1.29	1.33
53	BA	1668	A	C5-C4	-5.37	1.34	1.38
53	BA	2628	C	C4-N4	-5.37	1.29	1.33
21	AA	624	C	C4-N4	-5.37	1.29	1.33
21	AA	1252	A	C6-N6	-5.37	1.29	1.33
21	AA	738	C	C4-N4	-5.36	1.29	1.33
21	AA	824	G	N1-C2	-5.36	1.33	1.37
21	AA	796	C	N3-C4	-5.36	1.30	1.33
53	BA	1694	C	N3-C4	-5.36	1.30	1.33
54	BB	41	G	N1-C2	-5.36	1.33	1.37
21	AA	509	A	C6-N1	-5.36	1.31	1.35
53	BA	1522	A	C5-C4	-5.36	1.34	1.38
21	AA	1020	G	C2-N2	-5.36	1.29	1.34
21	AA	1373	G	C6-N1	-5.36	1.35	1.39
53	BA	638	G	C2-N2	-5.36	1.29	1.34
53	BA	1722	A	C6-N1	-5.36	1.31	1.35
53	BA	2616	C	N3-C4	-5.36	1.30	1.33
53	BA	1907	G	C2-N2	-5.35	1.29	1.34
53	BA	2260	C	C4-N4	-5.35	1.29	1.33
21	AA	1246	A	C6-N6	-5.35	1.29	1.33
53	BA	465	G	C2-N2	-5.35	1.29	1.34
53	BA	2116	G	C2-N2	-5.35	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2467	C	C4-N4	-5.35	1.29	1.33
53	BA	1170	C	C4-N4	-5.35	1.29	1.33
53	BA	2685	G	C2-N2	-5.35	1.29	1.34
53	BA	1625	C	N3-C4	-5.35	1.30	1.33
21	AA	693	G	C2-N2	-5.35	1.29	1.34
21	AA	698	G	N1-C2	-5.35	1.33	1.37
53	BA	261	G	C6-N1	-5.35	1.35	1.39
22	A1	36	C	N3-C4	-5.34	1.30	1.33
53	BA	128	C	C4-N4	-5.34	1.29	1.33
53	BA	2892	G	C2-N2	-5.34	1.29	1.34
21	AA	1487	G	C2-N2	-5.34	1.29	1.34
53	BA	544	C	N3-C4	-5.34	1.30	1.33
53	BA	782	A	C6-N1	-5.34	1.31	1.35
53	BA	2080	A	C6-N1	-5.34	1.31	1.35
21	AA	1022	A	C5-C4	-5.34	1.35	1.38
53	BA	2147	A	C5-C4	-5.34	1.35	1.38
53	BA	2318	G	N1-C2	-5.34	1.33	1.37
53	BA	2539	C	C4-N4	-5.34	1.29	1.33
21	AA	1262	C	C4-N4	-5.34	1.29	1.33
21	AA	631	C	C4-N4	-5.34	1.29	1.33
53	BA	1897	G	C2-N2	-5.34	1.29	1.34
53	BA	1957	C	N3-C4	-5.34	1.30	1.33
21	AA	900	A	C6-N1	-5.33	1.31	1.35
53	BA	1652	A	C6-N1	-5.33	1.31	1.35
21	AA	1016	A	C6-N1	-5.33	1.31	1.35
53	BA	1296	G	C6-N1	-5.33	1.35	1.39
53	BA	1739	A	C5-C4	-5.33	1.35	1.38
54	BB	29	A	C5-C4	-5.33	1.35	1.38
21	AA	574	A	C5-C4	-5.33	1.35	1.38
53	BA	2445	G	C2-N2	-5.33	1.29	1.34
53	BA	1511	G	C2-N2	-5.33	1.29	1.34
21	AA	1128	C	O3'-P	-5.33	1.54	1.61
53	BA	266	G	C6-N1	-5.33	1.35	1.39
53	BA	2483	C	C4-N4	-5.33	1.29	1.33
53	BA	356	G	C6-N1	-5.32	1.35	1.39
53	BA	918	A	C6-N1	-5.32	1.31	1.35
21	AA	1520	C	C4-N4	-5.32	1.29	1.33
53	BA	923	G	C6-N1	-5.32	1.35	1.39
53	BA	324	A	C6-N6	-5.32	1.29	1.33
53	BA	2641	G	C2-N2	-5.32	1.29	1.34
21	AA	267	C	C4-N4	-5.31	1.29	1.33
21	AA	1058	G	C2-N2	-5.31	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1325	C	N3-C4	-5.31	1.30	1.33
53	BA	273	G	C2-N2	-5.31	1.29	1.34
53	BA	414	C	N3-C4	-5.31	1.30	1.33
53	BA	2232	C	C4-N4	-5.31	1.29	1.33
53	BA	2270	A	N9-C4	-5.31	1.34	1.37
53	BA	2325	G	C2-N2	-5.31	1.29	1.34
53	BA	1328	A	C5-C4	-5.31	1.35	1.38
21	AA	694	A	C5-C4	-5.30	1.35	1.38
21	AA	1306	A	C6-N1	-5.30	1.31	1.35
21	AA	1404	C	C4-N4	-5.30	1.29	1.33
53	BA	1399	C	N3-C4	-5.30	1.30	1.33
53	BA	1512	C	C4-N4	-5.30	1.29	1.33
53	BA	1642	G	C6-N1	-5.30	1.35	1.39
53	BA	2447	G	C2-N2	-5.30	1.29	1.34
53	BA	1106	G	C2-N2	-5.30	1.29	1.34
21	AA	1191	A	C6-N1	-5.30	1.31	1.35
21	AA	1249	C	N3-C4	-5.30	1.30	1.33
21	AA	1446	A	C6-N1	-5.30	1.31	1.35
53	BA	444	C	C4-N4	-5.30	1.29	1.33
53	BA	2084	C	C4-N4	-5.30	1.29	1.33
53	BA	2775	G	C2-N2	-5.30	1.29	1.34
53	BA	254	G	C2-N2	-5.29	1.29	1.34
53	BA	1914	C	C4-N4	-5.29	1.29	1.33
53	BA	2429	G	C2-N2	-5.29	1.29	1.34
21	AA	858	G	C2-N2	-5.29	1.29	1.34
53	BA	2226	C	C4-N4	-5.29	1.29	1.33
53	BA	2527	C	N3-C4	-5.29	1.30	1.33
53	BA	1928	A	C6-N1	-5.29	1.31	1.35
21	AA	582	C	C4-N4	-5.29	1.29	1.33
53	BA	343	C	N3-C4	-5.29	1.30	1.33
53	BA	1404	C	N3-C4	-5.29	1.30	1.33
21	AA	34	C	N3-C4	-5.29	1.30	1.33
21	AA	1033	G	N1-C2	-5.29	1.33	1.37
21	AA	211	G	N1-C2	-5.29	1.33	1.37
21	AA	342	C	N3-C4	-5.29	1.30	1.33
21	AA	829	G	C6-N1	-5.29	1.35	1.39
53	BA	966	G	N1-C2	-5.29	1.33	1.37
53	BA	1424	G	C6-N1	-5.29	1.35	1.39
53	BA	2516	A	C6-N1	-5.28	1.31	1.35
21	AA	679	C	N3-C4	-5.28	1.30	1.33
21	AA	946	A	C6-N1	-5.28	1.31	1.35
21	AA	38	G	C2-N2	-5.28	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	98	G	C2-N2	-5.28	1.29	1.34
53	BA	1848	A	C6-N1	-5.28	1.31	1.35
53	BA	2165	C	C4-N4	-5.28	1.29	1.33
21	AA	1403	C	C4-N4	-5.28	1.29	1.33
53	BA	1990	C	C4-N4	-5.28	1.29	1.33
53	BA	2682	A	C6-N6	-5.28	1.29	1.33
53	BA	823	C	N3-C4	-5.28	1.30	1.33
53	BA	2874	C	C4-N4	-5.27	1.29	1.33
21	AA	282	A	C5-C4	-5.27	1.35	1.38
21	AA	1083	U	O3'-P	-5.27	1.54	1.61
53	BA	1921	G	C2-N2	-5.27	1.29	1.34
53	BA	864	G	N1-C2	-5.27	1.33	1.37
53	BA	2507	C	C4-N4	-5.27	1.29	1.33
21	AA	744	C	C4-N4	-5.27	1.29	1.33
21	AA	536	C	C4-N4	-5.27	1.29	1.33
21	AA	553	A	C6-N1	-5.27	1.31	1.35
53	BA	1483	G	C2-N2	-5.27	1.29	1.34
21	AA	117	G	C2-N2	-5.26	1.29	1.34
21	AA	1237	C	C4-N4	-5.26	1.29	1.33
53	BA	267	C	N3-C4	-5.26	1.30	1.33
53	BA	1185	G	C2-N2	-5.26	1.29	1.34
53	BA	1903	G	C6-N1	-5.26	1.35	1.39
53	BA	713	G	C2-N2	-5.26	1.29	1.34
53	BA	1842	G	C2-N2	-5.26	1.29	1.34
53	BA	2767	C	C4-N4	-5.26	1.29	1.33
21	AA	314	C	N3-C4	-5.26	1.30	1.33
21	AA	647	C	C4-N4	-5.26	1.29	1.33
53	BA	663	G	C2-N2	-5.26	1.29	1.34
53	BA	2788	C	C4-N4	-5.26	1.29	1.33
21	AA	1260	G	C2-N2	-5.26	1.29	1.34
21	AA	1432	G	C2-N2	-5.26	1.29	1.34
53	BA	838	C	C4-N4	-5.26	1.29	1.33
53	BA	1596	A	C6-N1	-5.26	1.31	1.35
53	BA	2506	U	O3'-P	-5.26	1.54	1.61
21	AA	1041	G	C2-N2	-5.25	1.29	1.34
53	BA	71	A	C6-N1	-5.25	1.31	1.35
21	AA	596	A	C6-N1	-5.25	1.31	1.35
53	BA	844	A	C6-N6	-5.25	1.29	1.33
53	BA	326	G	C2-N2	-5.25	1.29	1.34
21	AA	1244	G	C6-N1	-5.25	1.35	1.39
21	AA	72	A	C5-C4	-5.25	1.35	1.38
21	AA	1233	G	C2-N2	-5.25	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1054	A	C6-N1	-5.25	1.31	1.35
53	BA	1062	G	C6-N1	-5.25	1.35	1.39
53	BA	1389	G	N1-C2	-5.25	1.33	1.37
53	BA	2510	C	N3-C4	-5.25	1.30	1.33
21	AA	1013	G	N1-C2	-5.25	1.33	1.37
53	BA	1322	A	C6-N6	-5.25	1.29	1.33
53	BA	2158	A	C5-C4	-5.25	1.35	1.38
53	BA	2830	C	C4-N4	-5.25	1.29	1.33
53	BA	372	G	C2-N2	-5.25	1.29	1.34
53	BA	1346	G	C2-N2	-5.25	1.29	1.34
53	BA	1896	G	C2-N2	-5.25	1.29	1.34
53	BA	2582	G	C2-N2	-5.25	1.29	1.34
53	BA	1140	C	N3-C4	-5.24	1.30	1.33
53	BA	245	G	C2-N2	-5.24	1.29	1.34
53	BA	2542	A	C6-N1	-5.24	1.31	1.35
53	BA	232	G	N1-C2	-5.24	1.33	1.37
53	BA	874	G	C2-N2	-5.24	1.29	1.34
53	BA	1738	G	N1-C2	-5.24	1.33	1.37
53	BA	1999	C	C4-N4	-5.24	1.29	1.33
53	BA	2145	C	N3-C4	-5.24	1.30	1.33
21	AA	48	C	C4-N4	-5.24	1.29	1.33
21	AA	832	G	N1-C2	-5.24	1.33	1.37
53	BA	881	G	C2-N2	-5.24	1.29	1.34
53	BA	2073	C	C4-N4	-5.24	1.29	1.33
21	AA	338	A	C5-C4	-5.23	1.35	1.38
21	AA	1418	A	O3'-P	-5.23	1.54	1.61
53	BA	2239	G	N1-C2	-5.23	1.33	1.37
53	BA	2070	A	C6-N1	-5.23	1.31	1.35
53	BA	2510	C	C4-N4	-5.23	1.29	1.33
21	AA	86	G	C6-N1	-5.23	1.35	1.39
53	BA	1744	A	C6-N1	-5.23	1.31	1.35
53	BA	1964	G	C2-N2	-5.23	1.29	1.34
53	BA	2870	C	N3-C4	-5.23	1.30	1.33
53	BA	1	G	C2-N2	-5.23	1.29	1.34
21	AA	570	G	C6-N1	-5.23	1.35	1.39
53	BA	85	G	N1-C2	-5.23	1.33	1.37
53	BA	1139	G	C2-N2	-5.23	1.29	1.34
53	BA	1920	C	N3-C4	-5.23	1.30	1.33
53	BA	685	A	C6-N6	-5.23	1.29	1.33
53	BA	2303	G	C2-N2	-5.23	1.29	1.34
53	BA	1752	C	C4-N4	-5.22	1.29	1.33
53	BA	2052	A	C5-C4	-5.22	1.35	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2606	C	C4-N4	-5.22	1.29	1.33
21	AA	1399	C	C4-N4	-5.22	1.29	1.33
53	BA	402	A	C5-C4	-5.22	1.35	1.38
53	BA	1279	G	N1-C2	-5.22	1.33	1.37
53	BA	1969	A	C6-N1	-5.22	1.31	1.35
53	BA	2535	G	C2-N2	-5.22	1.29	1.34
53	BA	1002	G	C6-N1	-5.22	1.35	1.39
53	BA	183	C	C4-N4	-5.22	1.29	1.33
53	BA	891	G	N1-C2	-5.22	1.33	1.37
53	BA	2397	G	C2-N2	-5.22	1.29	1.34
21	AA	830	G	C2-N2	-5.21	1.29	1.34
21	AA	1407	C	N3-C4	-5.21	1.30	1.33
53	BA	1509	A	C6-N1	-5.21	1.31	1.35
53	BA	1625	C	C4-N4	-5.21	1.29	1.33
53	BA	394	C	C4-N4	-5.21	1.29	1.33
22	A1	35	A	C6-N1	-5.21	1.31	1.35
53	BA	495	G	C2-N2	-5.21	1.29	1.34
21	AA	81	A	C6-N1	-5.21	1.31	1.35
21	AA	232	G	C2-N2	-5.21	1.29	1.34
21	AA	75	G	C6-N1	-5.21	1.35	1.39
21	AA	242	G	N1-C2	-5.21	1.33	1.37
21	AA	766	A	C6-N1	-5.21	1.31	1.35
23	A2	82	A	C5-C4	-5.21	1.35	1.38
53	BA	2727	A	C5-C4	-5.21	1.35	1.38
21	AA	47	C	C4-N4	-5.21	1.29	1.33
53	BA	380	G	C2-N2	-5.21	1.29	1.34
21	AA	382	A	C6-N1	-5.21	1.31	1.35
53	BA	430	A	C6-N1	-5.21	1.31	1.35
53	BA	1737	G	C2-N2	-5.21	1.29	1.34
53	BA	2612	C	C4-N4	-5.21	1.29	1.33
54	BB	37	C	N3-C4	-5.21	1.30	1.33
53	BA	1297	C	C4-N4	-5.20	1.29	1.33
21	AA	944	G	C2-N2	-5.20	1.29	1.34
53	BA	1210	G	C6-N1	-5.20	1.35	1.39
53	BA	262	A	C6-N1	-5.20	1.31	1.35
53	BA	1300	G	C6-N1	-5.20	1.35	1.39
53	BA	1639	C	C4-N4	-5.20	1.29	1.33
21	AA	958	A	C5-C4	-5.20	1.35	1.38
53	BA	1288	G	C6-N1	-5.20	1.35	1.39
53	BA	1727	C	N3-C4	-5.20	1.30	1.33
21	AA	1365	G	N1-C2	-5.20	1.33	1.37
53	BA	471	A	C6-N1	-5.20	1.31	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	1271	G	C6-N1	-5.20	1.35	1.39
53	BA	2879	A	C5-C4	-5.20	1.35	1.38
21	AA	33	A	C6-N1	-5.19	1.31	1.35
53	BA	2046	G	C2-N2	-5.19	1.29	1.34
53	BA	1537	G	C2-N2	-5.19	1.29	1.34
53	BA	1707	G	C2-N2	-5.19	1.29	1.34
21	AA	847	G	C2-N2	-5.19	1.29	1.34
21	AA	962	C	C4-N4	-5.19	1.29	1.33
53	BA	2082	A	C6-N1	-5.19	1.31	1.35
53	BA	1748	C	N3-C4	-5.19	1.30	1.33
53	BA	1906	G	C2-N2	-5.19	1.29	1.34
21	AA	732	C	C4-N4	-5.18	1.29	1.33
53	BA	57	C	C4-N4	-5.18	1.29	1.33
53	BA	623	C	C4-N4	-5.18	1.29	1.33
21	AA	974	A	C5-C4	-5.18	1.35	1.38
53	BA	629	G	C2-N2	-5.18	1.29	1.34
53	BA	950	G	C2-N2	-5.18	1.29	1.34
21	AA	887	G	N1-C2	-5.18	1.33	1.37
21	AA	1006	G	C6-N1	-5.18	1.35	1.39
53	BA	997	G	C6-N1	-5.18	1.35	1.39
21	AA	260	G	C2-N2	-5.18	1.29	1.34
21	AA	767	A	C5-C4	-5.18	1.35	1.38
53	BA	2626	C	N3-C4	-5.18	1.30	1.33
21	AA	888	G	C2-N2	-5.18	1.29	1.34
53	BA	250	G	C2-N2	-5.18	1.29	1.34
53	BA	1628	G	N1-C2	-5.18	1.33	1.37
21	AA	1311	A	C5-C4	-5.18	1.35	1.38
53	BA	417	C	C4-N4	-5.18	1.29	1.33
53	BA	1616	A	C6-N1	-5.18	1.31	1.35
53	BA	2140	G	C2-N2	-5.18	1.29	1.34
53	BA	2469	A	C5-C4	-5.18	1.35	1.38
53	BA	572	A	C6-N1	-5.17	1.31	1.35
53	BA	1526	C	C4-N4	-5.17	1.29	1.33
53	BA	1824	G	C2-N2	-5.17	1.29	1.34
53	BA	2069	G	C2-N2	-5.17	1.29	1.34
53	BA	2417	C	C4-N4	-5.17	1.29	1.33
21	AA	999	C	C4-N4	-5.17	1.29	1.33
53	BA	164	C	N3-C4	-5.17	1.30	1.33
53	BA	2036	C	N3-C4	-5.17	1.30	1.33
53	BA	2201	G	O3'-P	-5.17	1.54	1.61
53	BA	2550	G	C2-N2	-5.17	1.29	1.34
21	AA	64	G	C2-N2	-5.17	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	628	G	C2-N2	-5.17	1.29	1.34
21	AA	1515	G	C2-N2	-5.17	1.29	1.34
53	BA	643	A	C6-N1	-5.16	1.31	1.35
53	BA	1669	A	C5-C4	-5.16	1.35	1.38
53	BA	1760	C	C4-N4	-5.16	1.29	1.33
21	AA	172	A	C6-N1	-5.16	1.31	1.35
21	AA	550	G	N1-C2	-5.16	1.33	1.37
21	AA	1260	G	C6-N1	-5.16	1.35	1.39
53	BA	331	C	N3-C4	-5.16	1.30	1.33
53	BA	485	C	C4-N4	-5.16	1.29	1.33
53	BA	798	G	C2-N2	-5.16	1.29	1.34
53	BA	1828	G	C2-N2	-5.16	1.29	1.34
53	BA	2556	C	N3-C4	-5.16	1.30	1.33
53	BA	2793	C	C4-N4	-5.16	1.29	1.33
21	AA	810	C	C4-N4	-5.16	1.29	1.33
21	AA	1047	G	N1-C2	-5.16	1.33	1.37
53	BA	1655	A	C6-N1	-5.16	1.31	1.35
53	BA	1028	A	C5-C4	-5.15	1.35	1.38
53	BA	1216	G	C2-N2	-5.15	1.29	1.34
21	AA	278	G	C2-N2	-5.15	1.29	1.34
21	AA	694	A	C6-N6	-5.15	1.29	1.33
22	A1	39	G	C2-N2	-5.15	1.29	1.34
53	BA	407	G	C2-N2	-5.15	1.29	1.34
53	BA	928	A	C6-N1	-5.15	1.31	1.35
53	BA	2115	G	C2-N2	-5.15	1.29	1.34
21	AA	305	G	C2-N2	-5.15	1.29	1.34
53	BA	274	C	C4-N4	-5.15	1.29	1.33
53	BA	2682	A	C5-C4	-5.15	1.35	1.38
22	A1	44	G	C2-N2	-5.15	1.29	1.34
21	AA	1373	G	C2-N2	-5.15	1.29	1.34
53	BA	41	C	C4-N4	-5.15	1.29	1.33
53	BA	1001	A	N9-C4	-5.15	1.34	1.37
53	BA	2487	G	C6-N1	-5.15	1.35	1.39
21	AA	563	A	C6-N6	-5.15	1.29	1.33
21	AA	1208	C	C4-N4	-5.15	1.29	1.33
53	BA	899	A	C6-N1	-5.15	1.31	1.35
21	AA	1198	G	C2-N2	-5.14	1.29	1.34
53	BA	400	G	N1-C2	-5.14	1.33	1.37
53	BA	806	C	N3-C4	-5.14	1.30	1.33
53	BA	1278	C	N3-C4	-5.14	1.30	1.33
53	BA	1423	G	C6-N1	-5.14	1.35	1.39
53	BA	1721	G	C6-N1	-5.14	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	61	C	C4-N4	-5.14	1.29	1.33
53	BA	1028	A	C6-N6	-5.14	1.29	1.33
53	BA	1577	C	N3-C4	-5.14	1.30	1.33
53	BA	2088	A	C5-C4	-5.14	1.35	1.38
21	AA	1510	C	C4-N4	-5.14	1.29	1.33
53	BA	379	G	C6-N1	-5.14	1.35	1.39
53	BA	939	G	C2-N2	-5.14	1.29	1.34
53	BA	833	A	C6-N1	-5.14	1.31	1.35
53	BA	875	G	C2-N2	-5.14	1.29	1.34
21	AA	1089	G	C2-N2	-5.14	1.29	1.34
53	BA	132	G	C2-N2	-5.14	1.29	1.34
53	BA	1327	A	C6-N1	-5.14	1.31	1.35
21	AA	696	A	C6-N1	-5.13	1.31	1.35
21	AA	450	G	C2-N2	-5.13	1.29	1.34
21	AA	1318	A	C6-N1	-5.13	1.31	1.35
53	BA	740	C	C4-N4	-5.13	1.29	1.33
53	BA	1631	G	C2-N2	-5.13	1.29	1.34
53	BA	843	G	C2-N2	-5.13	1.29	1.34
53	BA	537	G	C2-N2	-5.13	1.29	1.34
53	BA	628	G	C6-N1	-5.13	1.35	1.39
53	BA	2578	G	N1-C2	-5.13	1.33	1.37
53	BA	2610	C	C4-N4	-5.13	1.29	1.33
21	AA	974	A	C6-N6	-5.13	1.29	1.33
21	AA	1204	A	C6-N1	-5.13	1.31	1.35
53	BA	673	C	C4-N4	-5.13	1.29	1.33
53	BA	2247	A	C6-N1	-5.13	1.31	1.35
53	BA	691	C	C4-N4	-5.12	1.29	1.33
53	BA	708	G	C6-N1	-5.12	1.35	1.39
53	BA	885	C	N3-C4	-5.12	1.30	1.33
21	AA	910	C	N3-C4	-5.12	1.30	1.33
53	BA	2883	A	C6-N1	-5.12	1.31	1.35
21	AA	1317	C	C4-N4	-5.12	1.29	1.33
53	BA	2304	G	C6-N1	-5.12	1.35	1.39
21	AA	79	G	C2-N2	-5.12	1.29	1.34
21	AA	554	A	C6-N1	-5.12	1.31	1.35
53	BA	2674	G	C6-N1	-5.12	1.35	1.39
21	AA	716	A	C6-N1	-5.12	1.31	1.35
21	AA	945	G	C2-N2	-5.12	1.29	1.34
53	BA	2742	G	C2-N2	-5.12	1.29	1.34
53	BA	2446	G	N1-C2	-5.11	1.33	1.37
53	BA	401	A	C5-C4	-5.11	1.35	1.38
53	BA	587	C	N3-C4	-5.11	1.30	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	726	C	C4-N4	-5.11	1.29	1.33
53	BA	22	C	N3-C4	-5.11	1.30	1.33
53	BA	1749	A	C5-C4	-5.11	1.35	1.38
53	BA	678	C	C4-N4	-5.11	1.29	1.33
21	AA	241	G	N1-C2	-5.11	1.33	1.37
53	BA	2421	G	C2-N2	-5.11	1.29	1.34
53	BA	2803	G	C2-N2	-5.11	1.29	1.34
53	BA	2879	A	C6-N6	-5.11	1.29	1.33
53	BA	729	G	N1-C2	-5.11	1.33	1.37
53	BA	1126	A	C5-C4	-5.10	1.35	1.38
53	BA	1236	G	C6-N1	-5.10	1.35	1.39
53	BA	1525	A	C6-N1	-5.10	1.31	1.35
53	BA	2509	G	C6-N1	-5.10	1.35	1.39
53	BA	1640	A	C5-C4	-5.10	1.35	1.38
53	BA	127	A	C6-N1	-5.10	1.31	1.35
53	BA	866	A	C6-N6	-5.10	1.29	1.33
53	BA	1612	C	C4-N4	-5.10	1.29	1.33
53	BA	2673	G	C2-N2	-5.10	1.29	1.34
21	AA	148	G	C2-N2	-5.10	1.29	1.34
21	AA	295	C	N3-C4	-5.10	1.30	1.33
53	BA	2658	C	C4-N4	-5.10	1.29	1.33
54	BB	36	C	C4-N4	-5.10	1.29	1.33
53	BA	1665	A	C6-N1	-5.10	1.31	1.35
53	BA	1895	C	C4-N4	-5.10	1.29	1.33
53	BA	1116	G	C6-N1	-5.09	1.35	1.39
53	BA	393	C	N3-C4	-5.09	1.30	1.33
53	BA	241	A	C6-N1	-5.09	1.31	1.35
53	BA	1907	G	C6-N1	-5.09	1.35	1.39
53	BA	1980	G	C2-N2	-5.09	1.29	1.34
53	BA	1674	G	C2-N2	-5.09	1.29	1.34
53	BA	1715	G	C6-N1	-5.09	1.35	1.39
21	AA	771	G	C2-N2	-5.09	1.29	1.34
53	BA	279	A	C6-N6	-5.09	1.29	1.33
21	AA	513	C	C4-N4	-5.09	1.29	1.33
21	AA	1013	G	C2-N2	-5.09	1.29	1.34
21	AA	1333	A	C5-C4	-5.09	1.35	1.38
53	BA	1244	A	C6-N6	-5.09	1.29	1.33
21	AA	184	G	N1-C2	-5.08	1.33	1.37
53	BA	1420	A	C6-N1	-5.08	1.31	1.35
53	BA	819	A	C5-C4	-5.08	1.35	1.38
53	BA	1192	G	N1-C2	-5.08	1.33	1.37
53	BA	2339	C	N3-C4	-5.08	1.30	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1196	A	C6-N6	-5.08	1.29	1.33
53	BA	1324	G	C2-N2	-5.08	1.29	1.34
53	BA	2168	G	C2-N2	-5.08	1.29	1.34
21	AA	160	A	C6-N1	-5.08	1.31	1.35
21	AA	1268	G	C2-N2	-5.08	1.29	1.34
21	AA	175	C	C4-N4	-5.08	1.29	1.33
53	BA	1703	G	C2-N2	-5.08	1.29	1.34
53	BA	2895	G	C6-N1	-5.08	1.35	1.39
21	AA	284	C	N3-C4	-5.08	1.30	1.33
53	BA	1783	A	C6-N1	-5.08	1.31	1.35
21	AA	144	G	N1-C2	-5.07	1.33	1.37
53	BA	508	A	C5-C4	-5.07	1.35	1.38
53	BA	1175	A	C5-C4	-5.07	1.35	1.38
21	AA	77	A	C6-N6	-5.07	1.29	1.33
21	AA	1397	C	C4-N4	-5.07	1.29	1.33
53	BA	2138	G	C2-N2	-5.07	1.29	1.34
21	AA	259	G	C2-N2	-5.07	1.29	1.34
21	AA	584	G	C2-N2	-5.07	1.29	1.34
53	BA	371	A	C5-C4	-5.07	1.35	1.38
53	BA	2483	C	N3-C4	-5.07	1.30	1.33
53	BA	2902	C	N3-C4	-5.07	1.30	1.33
21	AA	1289	A	C6-N1	-5.07	1.32	1.35
53	BA	1999	C	N3-C4	-5.07	1.30	1.33
54	BB	81	G	O3'-P	-5.07	1.55	1.61
21	AA	839	C	C4-N4	-5.07	1.29	1.33
21	AA	1514	G	C6-N1	-5.07	1.36	1.39
22	A1	48	C	N3-C4	-5.07	1.30	1.33
53	BA	1511	G	C6-N1	-5.07	1.36	1.39
53	BA	1710	G	N1-C2	-5.07	1.33	1.37
53	BA	2638	G	N1-C2	-5.07	1.33	1.37
53	BA	1595	C	N3-C4	-5.06	1.30	1.33
53	BA	1958	C	C4-N4	-5.06	1.29	1.33
53	BA	1985	C	C4-N4	-5.06	1.29	1.33
53	BA	1171	G	C2-N2	-5.06	1.29	1.34
53	BA	1332	G	C2-N2	-5.06	1.29	1.34
53	BA	1686	C	C4-N4	-5.06	1.29	1.33
53	BA	2417	C	N3-C4	-5.06	1.30	1.33
53	BA	2478	A	C5-C4	-5.06	1.35	1.38
53	BA	2495	G	N1-C2	-5.06	1.33	1.37
53	BA	368	A	C6-N1	-5.06	1.32	1.35
53	BA	624	C	C4-N4	-5.06	1.29	1.33
53	BA	996	A	C6-N1	-5.06	1.32	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	43	G	C6-N1	-5.06	1.36	1.39
53	BA	47	C	C4-N4	-5.06	1.29	1.33
53	BA	1136	G	C6-N1	-5.06	1.36	1.39
53	BA	1637	A	C6-N1	-5.06	1.32	1.35
21	AA	505	G	N1-C2	-5.06	1.33	1.37
21	AA	574	A	C6-N6	-5.06	1.29	1.33
21	AA	742	G	C2-N2	-5.06	1.29	1.34
21	AA	1370	G	C2-N2	-5.06	1.29	1.34
21	AA	192	A	C6-N1	-5.05	1.32	1.35
21	AA	1273	C	C4-N4	-5.05	1.29	1.33
53	BA	2631	G	C2-N2	-5.05	1.29	1.34
21	AA	152	A	C6-N6	-5.05	1.29	1.33
53	BA	2333	A	C5-C4	-5.05	1.35	1.38
21	AA	1337	G	C2-N2	-5.05	1.29	1.34
53	BA	672	C	C4-N4	-5.05	1.29	1.33
53	BA	776	G	C2-N2	-5.05	1.29	1.34
54	BB	68	C	C4-N4	-5.05	1.29	1.33
21	AA	1379	G	C2-N2	-5.04	1.29	1.34
53	BA	637	A	C5-C4	-5.04	1.35	1.38
21	AA	200	G	N1-C2	-5.04	1.33	1.37
21	AA	1210	C	N3-C4	-5.04	1.30	1.33
53	BA	559	G	C2-N2	-5.04	1.29	1.34
53	BA	1261	C	C4-N4	-5.04	1.29	1.33
53	BA	2813	A	C5-C4	-5.04	1.35	1.38
21	AA	301	G	C2-N2	-5.04	1.29	1.34
53	BA	175	G	N1-C2	-5.04	1.33	1.37
53	BA	785	G	C2-N2	-5.04	1.29	1.34
53	BA	380	G	N1-C2	-5.04	1.33	1.37
53	BA	1597	A	C5-C4	-5.04	1.35	1.38
53	BA	2444	G	C6-N1	-5.04	1.36	1.39
53	BA	1315	C	N3-C4	-5.04	1.30	1.33
21	AA	396	C	C4-N4	-5.03	1.29	1.33
21	AA	1036	A	C6-N1	-5.03	1.32	1.35
53	BA	757	G	C2-N2	-5.03	1.29	1.34
53	BA	1790	C	N3-C4	-5.03	1.30	1.33
21	AA	849	G	C6-N1	-5.03	1.36	1.39
53	BA	194	G	C6-N1	-5.03	1.36	1.39
53	BA	1808	A	C6-N1	-5.03	1.32	1.35
54	BB	44	G	N1-C2	-5.03	1.33	1.37
21	AA	1312	G	N1-C2	-5.03	1.33	1.37
53	BA	1669	A	C6-N6	-5.03	1.29	1.33
53	BA	2047	C	C4-N4	-5.03	1.29	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	2854	G	N1-C2	-5.03	1.33	1.37
21	AA	90	C	C4-N4	-5.03	1.29	1.33
21	AA	1452	C	N3-C4	-5.03	1.30	1.33
21	AA	124	C	C4-N4	-5.03	1.29	1.33
21	AA	1239	A	C6-N1	-5.03	1.32	1.35
53	BA	1598	A	C6-N1	-5.03	1.32	1.35
21	AA	824	G	C2-N2	-5.03	1.29	1.34
21	AA	153	C	N3-C4	-5.02	1.30	1.33
21	AA	1305	G	N1-C2	-5.02	1.33	1.37
53	BA	1125	G	C6-N1	-5.02	1.36	1.39
21	AA	351	G	C6-N1	-5.02	1.36	1.39
53	BA	344	A	C5-C4	-5.02	1.35	1.38
53	BA	1387	A	C6-N1	-5.02	1.32	1.35
21	AA	1305	G	C2-N2	-5.02	1.29	1.34
53	BA	147	C	C4-N4	-5.02	1.29	1.33
53	BA	743	A	C6-N1	-5.02	1.32	1.35
53	BA	2425	A	C5-C4	-5.02	1.35	1.38
22	A1	9	A	C6-N1	-5.02	1.32	1.35
53	BA	880	G	C6-N1	-5.02	1.36	1.39
53	BA	1337	G	N1-C2	-5.02	1.33	1.37
53	BA	424	G	C2-N2	-5.01	1.29	1.34
53	BA	2242	G	C6-N1	-5.01	1.36	1.39
21	AA	285	C	N3-C4	-5.01	1.30	1.33
53	BA	1500	G	C6-N1	-5.01	1.36	1.39
53	BA	2006	C	C4-C5	-5.01	1.39	1.43
54	BB	63	C	C4-N4	-5.01	1.29	1.33
53	BA	705	A	C6-N1	-5.01	1.32	1.35
53	BA	924	G	N1-C2	-5.01	1.33	1.37
53	BA	988	A	C6-N1	-5.01	1.32	1.35
53	BA	1287	A	C6-N6	-5.01	1.29	1.33
53	BA	1290	C	N3-C4	-5.01	1.30	1.33
53	BA	502	A	C6-N1	-5.01	1.32	1.35
53	BA	2574	G	C2-N2	-5.01	1.29	1.34
21	AA	27	G	C6-N1	-5.01	1.36	1.39
53	BA	198	C	C4-N4	-5.01	1.29	1.33
21	AA	1045	C	N3-C4	-5.00	1.30	1.33
53	BA	1138	G	N1-C2	-5.00	1.33	1.37
21	AA	901	A	C5-C4	-5.00	1.35	1.38
53	BA	15	G	C2-N2	-5.00	1.29	1.34
53	BA	838	C	N3-C4	-5.00	1.30	1.33
53	BA	2505	G	N1-C2	-5.00	1.33	1.37
21	AA	69	G	C6-N1	-5.00	1.36	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	BA	94	A	C6-N6	-5.00	1.29	1.33
53	BA	2472	G	C2-N2	-5.00	1.29	1.34
53	BA	2828	G	C2-N2	-5.00	1.29	1.34

All (8093) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	323	C	O4'-C1'-N1	14.98	120.18	108.20
53	BA	1932	A	N1-C6-N6	-13.12	110.73	118.60
53	BA	800	A	N1-C6-N6	-12.78	110.93	118.60
21	AA	1502	A	N1-C6-N6	-12.44	111.14	118.60
53	BA	219	A	N1-C6-N6	-12.42	111.15	118.60
53	BA	344	A	N1-C6-N6	-12.40	111.16	118.60
22	A1	59	U	O4'-C1'-N1	12.38	118.10	108.20
21	AA	1257	A	N1-C6-N6	-12.30	111.22	118.60
53	BA	2889	C	O4'-C1'-N1	12.30	118.04	108.20
53	BA	1791	A	N1-C6-N6	-12.28	111.23	118.60
53	BA	2388	A	N1-C6-N6	-12.21	111.27	118.60
53	BA	1591	A	N1-C6-N6	-12.21	111.27	118.60
53	BA	2212	A	N1-C6-N6	-12.17	111.30	118.60
53	BA	1469	A	N1-C6-N6	-12.11	111.34	118.60
54	BB	37	C	O4'-C1'-N1	12.11	117.88	108.20
53	BA	752	A	O4'-C1'-N9	12.02	117.82	108.20
21	AA	195	A	N1-C6-N6	-12.01	111.39	118.60
21	AA	1534	A	N1-C6-N6	-11.96	111.43	118.60
53	BA	38	A	N1-C6-N6	-11.85	111.49	118.60
53	BA	165	A	N1-C6-N6	-11.85	111.49	118.60
53	BA	1969	A	N1-C6-N6	-11.84	111.49	118.60
21	AA	621	A	N1-C6-N6	-11.84	111.50	118.60
18	AS	2	ARG	NE-CZ-NH2	11.84	126.22	120.30
53	BA	2033	A	N1-C6-N6	-11.82	111.51	118.60
53	BA	412	A	N1-C6-N6	-11.81	111.51	118.60
53	BA	743	A	N1-C6-N6	-11.81	111.51	118.60
21	AA	383	A	N1-C6-N6	-11.80	111.52	118.60
53	BA	2516	A	N1-C6-N6	-11.79	111.53	118.60
53	BA	1453	A	N1-C6-N6	-11.73	111.56	118.60
21	AA	865	A	N1-C6-N6	-11.67	111.60	118.60
53	BA	103	A	N1-C6-N6	-11.65	111.61	118.60
21	AA	194	C	N1-C2-O2	11.59	125.85	118.90
21	AA	190	A	N1-C6-N6	-11.57	111.66	118.60
21	AA	1360	A	N1-C6-N6	-11.56	111.67	118.60
21	AA	630	A	N1-C6-N6	-11.52	111.69	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	886	A	N1-C6-N6	-11.50	111.70	118.60
53	BA	1890	A	N1-C6-N6	-11.50	111.70	118.60
53	BA	2448	A	N1-C6-N6	-11.50	111.70	118.60
21	AA	1311	A	N1-C6-N6	-11.48	111.71	118.60
53	BA	1275	A	N1-C6-N6	-11.48	111.71	118.60
21	AA	1288	A	N1-C6-N6	-11.48	111.71	118.60
53	BA	2882	A	N1-C6-N6	-11.47	111.72	118.60
21	AA	389	A	N1-C6-N6	-11.47	111.72	118.60
21	AA	468	A	N1-C6-N6	-11.46	111.73	118.60
53	BA	514	A	N1-C6-N6	-11.44	111.73	118.60
21	AA	602	A	N1-C6-N6	-11.44	111.74	118.60
53	BA	1569	A	N1-C6-N6	-11.44	111.74	118.60
53	BA	119	A	N1-C6-N6	-11.44	111.74	118.60
53	BA	199	A	N1-C6-N6	-11.42	111.75	118.60
21	AA	937	A	N1-C6-N6	-11.40	111.76	118.60
21	AA	499	A	N1-C6-N6	-11.38	111.77	118.60
53	BA	666	A	N1-C6-N6	-11.37	111.78	118.60
53	BA	2009	A	N1-C6-N6	-11.37	111.78	118.60
21	AA	635	A	N1-C6-N6	-11.34	111.80	118.60
53	BA	2278	A	N1-C6-N6	-11.33	111.80	118.60
53	BA	2600	A	N1-C6-N6	-11.33	111.80	118.60
53	BA	415	A	N1-C6-N6	-11.32	111.81	118.60
53	BA	1010	A	N1-C6-N6	-11.30	111.82	118.60
53	BA	2406	A	N1-C6-N6	-11.30	111.82	118.60
53	BA	1319	C	O4'-C1'-N1	11.29	117.23	108.20
21	AA	1021	A	N1-C6-N6	-11.26	111.84	118.60
53	BA	2147	A	N1-C6-N6	-11.25	111.85	118.60
53	BA	984	A	N1-C6-N6	-11.22	111.87	118.60
21	AA	1213	A	N1-C6-N6	-11.21	111.87	118.60
54	BB	50	A	N1-C6-N6	-11.21	111.87	118.60
53	BA	2425	A	N1-C6-N6	-11.21	111.88	118.60
53	BA	1274	A	N1-C6-N6	-11.21	111.88	118.60
53	BA	1378	A	N1-C6-N6	-11.21	111.88	118.60
53	BA	849	A	N1-C6-N6	-11.20	111.88	118.60
21	AA	1394	A	N1-C6-N6	-11.19	111.89	118.60
53	BA	479	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	610	U	O4'-C1'-N1	11.16	117.13	108.20
53	BA	56	A	N1-C6-N6	-11.15	111.91	118.60
24	BC	237	ARG	NE-CZ-NH1	11.15	125.88	120.30
53	BA	508	A	N1-C6-N6	-11.14	111.91	118.60
21	AA	1030	U	O4'-C1'-N1	11.14	117.11	108.20
53	BA	705	A	N1-C6-N6	-11.14	111.92	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1086	A	N1-C6-N6	-11.13	111.92	118.60
21	AA	831	A	N1-C6-N6	-11.12	111.93	118.60
53	BA	1854	A	N1-C6-N6	-11.11	111.93	118.60
53	BA	2418	A	N1-C6-N6	-11.10	111.94	118.60
53	BA	2476	A	N1-C6-N6	-11.08	111.95	118.60
21	AA	1046	A	N1-C6-N6	-11.07	111.96	118.60
21	AA	1363	A	N1-C6-N6	-11.06	111.96	118.60
21	AA	1531	A	N1-C6-N6	-11.06	111.97	118.60
53	BA	2033	A	O4'-C1'-N9	11.02	117.02	108.20
53	BA	2266	A	N1-C6-N6	-11.02	111.99	118.60
21	AA	814	A	N1-C6-N6	-11.01	111.99	118.60
53	BA	668	A	N1-C6-N6	-11.01	111.99	118.60
21	AA	320	A	N1-C6-N6	-11.00	112.00	118.60
31	BJ	27	ARG	NE-CZ-NH1	10.98	125.79	120.30
54	BB	94	A	N1-C6-N6	-10.98	112.01	118.60
21	AA	718	A	N1-C6-N6	-10.97	112.02	118.60
21	AA	8	A	N1-C6-N6	-10.96	112.02	118.60
53	BA	574	A	N1-C6-N6	-10.96	112.03	118.60
53	BA	127	A	N1-C6-N6	-10.95	112.03	118.60
53	BA	1241	A	N1-C6-N6	-10.94	112.03	118.60
53	BA	2589	A	N1-C6-N6	-10.94	112.03	118.60
21	AA	182	A	N1-C6-N6	-10.91	112.06	118.60
21	AA	1067	A	N1-C6-N6	-10.91	112.06	118.60
53	BA	1640	A	N1-C6-N6	-10.89	112.06	118.60
21	AA	994	A	N1-C6-N6	-10.89	112.07	118.60
53	BA	2590	A	N1-C6-N6	-10.88	112.07	118.60
53	BA	160	A	N1-C6-N6	-10.83	112.10	118.60
53	BA	2478	A	N1-C6-N6	-10.82	112.11	118.60
53	BA	784	G	O4'-C1'-N9	10.82	116.85	108.20
21	AA	152	A	N1-C6-N6	-10.81	112.11	118.60
53	BA	2675	A	N1-C6-N6	-10.80	112.12	118.60
21	AA	282	A	N1-C6-N6	-10.80	112.12	118.60
54	BB	45	A	N1-C6-N6	-10.80	112.12	118.60
21	AA	520	A	N1-C6-N6	-10.79	112.12	118.60
53	BA	751	A	N1-C6-N6	-10.79	112.12	118.60
21	AA	1093	A	N1-C6-N6	-10.79	112.13	118.60
53	BA	1940	U	O4'-C1'-N1	10.79	116.83	108.20
53	BA	1387	A	N1-C6-N6	-10.78	112.13	118.60
53	BA	2639	A	N1-C6-N6	-10.77	112.14	118.60
4	AE	28	ARG	NE-CZ-NH1	10.76	125.68	120.30
53	BA	572	A	N1-C6-N6	-10.75	112.15	118.60
21	AA	706	A	N1-C6-N6	-10.74	112.15	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	554	A	N1-C6-N6	-10.73	112.16	118.60
53	BA	1690	A	N1-C6-N6	-10.72	112.17	118.60
53	BA	1590	A	N1-C6-N6	-10.71	112.17	118.60
21	AA	151	A	N1-C6-N6	-10.69	112.19	118.60
21	AA	1251	A	N1-C6-N6	-10.69	112.19	118.60
53	BA	1103	A	N1-C6-N6	-10.68	112.19	118.60
53	BA	497	A	N1-C6-N6	-10.65	112.21	118.60
53	BA	1021	A	N1-C6-N6	-10.65	112.21	118.60
21	AA	194	C	N3-C2-O2	-10.64	114.45	121.90
54	BB	37	C	N3-C2-O2	-10.64	114.45	121.90
53	BA	49	A	O4'-C1'-N9	10.63	116.70	108.20
53	BA	1535	A	N1-C6-N6	-10.63	112.22	118.60
53	BA	1717	A	N1-C6-N6	-10.62	112.23	118.60
21	AA	28	A	N1-C6-N6	-10.62	112.23	118.60
21	AA	452	A	N1-C6-N6	-10.61	112.23	118.60
53	BA	2352	A	N1-C6-N6	-10.61	112.23	118.60
53	BA	453	A	N1-C6-N6	-10.60	112.24	118.60
53	BA	1308	A	N1-C6-N6	-10.60	112.24	118.60
21	AA	179	A	N1-C6-N6	-10.59	112.25	118.60
53	BA	1889	A	N1-C6-N6	-10.59	112.25	118.60
11	AL	93	ARG	NE-CZ-NH1	10.58	125.59	120.30
21	AA	704	A	N1-C6-N6	-10.58	112.25	118.60
40	BS	99	ARG	NE-CZ-NH1	10.56	125.58	120.30
21	AA	155	A	N1-C6-N6	-10.55	112.27	118.60
24	BC	181	ARG	NE-CZ-NH1	10.55	125.57	120.30
23	A2	82	A	N1-C6-N6	-10.54	112.27	118.60
21	AA	968	A	N1-C6-N6	-10.54	112.28	118.60
53	BA	2126	A	O4'-C1'-N9	10.54	116.63	108.20
53	BA	1937	A	N1-C6-N6	-10.53	112.28	118.60
53	BA	422	A	N1-C6-N6	-10.53	112.28	118.60
53	BA	300	A	N1-C6-N6	-10.52	112.29	118.60
21	AA	1227	A	N1-C6-N6	-10.52	112.29	118.60
53	BA	1496	A	N1-C6-N6	-10.52	112.29	118.60
53	BA	1265	A	N1-C6-N6	-10.49	112.30	118.60
53	BA	1505	A	N1-C6-N6	-10.49	112.30	118.60
21	AA	1004	A	N1-C6-N6	-10.49	112.31	118.60
21	AA	749	A	N1-C6-N6	-10.49	112.31	118.60
50	B2	34	ARG	NE-CZ-NH1	10.48	125.54	120.30
53	BA	941	A	N1-C6-N6	-10.47	112.31	118.60
21	AA	183	C	O4'-C1'-N1	10.47	116.58	108.20
53	BA	2727	A	N1-C6-N6	-10.47	112.32	118.60
21	AA	223	A	N1-C6-N6	-10.46	112.32	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2071	A	N1-C6-N6	-10.46	112.32	118.60
21	AA	629	A	N1-C6-N6	-10.46	112.32	118.60
21	AA	98	A	N1-C6-N6	-10.45	112.33	118.60
53	BA	556	A	N1-C6-N6	-10.41	112.36	118.60
53	BA	2850	A	N1-C6-N6	-10.41	112.36	118.60
53	BA	2336	A	N1-C6-N6	-10.40	112.36	118.60
53	BA	988	A	N1-C6-N6	-10.39	112.37	118.60
53	BA	1384	A	N1-C6-N6	-10.38	112.37	118.60
53	BA	1610	A	O4'-C1'-N9	10.38	116.50	108.20
13	AN	63	ARG	NE-CZ-NH1	10.36	125.48	120.30
21	AA	915	A	N1-C6-N6	-10.36	112.39	118.60
53	BA	181	A	N1-C6-N6	-10.35	112.39	118.60
53	BA	1755	A	N1-C6-N6	-10.35	112.39	118.60
53	BA	401	A	N1-C6-N6	-10.34	112.39	118.60
53	BA	44	A	N1-C6-N6	-10.32	112.41	118.60
39	BR	80	ARG	NE-CZ-NH2	10.32	125.46	120.30
53	BA	322	A	N1-C6-N6	-10.31	112.41	118.60
21	AA	1499	A	N1-C6-N6	-10.31	112.42	118.60
21	AA	777	A	N1-C6-N6	-10.29	112.42	118.60
21	AA	1433	A	N1-C6-N6	-10.29	112.43	118.60
53	BA	2700	A	N1-C6-N6	-10.29	112.43	118.60
27	BF	124	ARG	NE-CZ-NH2	10.28	125.44	120.30
11	AL	82	ARG	NE-CZ-NH1	10.28	125.44	120.30
21	AA	1430	A	N1-C6-N6	-10.27	112.44	118.60
53	BA	449	A	N1-C6-N6	-10.26	112.44	118.60
53	BA	1253	A	N1-C6-N6	-10.26	112.44	118.60
53	BA	2738	A	N1-C6-N6	-10.26	112.44	118.60
3	AD	127	ARG	NE-CZ-NH1	10.26	125.43	120.30
23	A2	79	A	N1-C6-N6	-10.26	112.45	118.60
21	AA	329	A	N1-C6-N6	-10.25	112.45	118.60
53	BA	2564	A	N1-C6-N6	-10.25	112.45	118.60
53	BA	2679	A	N1-C6-N6	-10.25	112.45	118.60
36	BO	81	ARG	NE-CZ-NH1	10.25	125.42	120.30
21	AA	1171	A	N1-C6-N6	-10.23	112.46	118.60
53	BA	1046	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1508	A	N1-C6-N6	-10.22	112.47	118.60
53	BA	2468	A	N1-C6-N6	-10.22	112.47	118.60
21	AA	1287	A	N1-C6-N6	-10.22	112.47	118.60
53	BA	2665	A	N1-C6-N6	-10.22	112.47	118.60
53	BA	1805	A	N1-C6-N6	-10.21	112.47	118.60
53	BA	1439	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	2542	A	N1-C6-N6	-10.20	112.48	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1858	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	223	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	677	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	753	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	222	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	1392	A	N1-C6-N6	-10.20	112.48	118.60
53	BA	685	A	C5-C6-N1	10.19	122.80	117.70
53	BA	928	A	N1-C6-N6	-10.19	112.49	118.60
53	BA	1586	A	N1-C6-N6	-10.16	112.50	118.60
53	BA	1783	A	N1-C6-N6	-10.14	112.51	118.60
21	AA	415	A	N1-C6-N6	-10.14	112.51	118.60
21	AA	802	A	N1-C6-N6	-10.14	112.52	118.60
21	AA	199	A	N1-C6-N6	-10.14	112.52	118.60
21	AA	1042	A	N1-C6-N6	-10.14	112.52	118.60
53	BA	1759	A	N1-C6-N6	-10.13	112.52	118.60
21	AA	965	U	O4'-C1'-N1	10.12	116.30	108.20
53	BA	1580	A	N1-C6-N6	-10.13	112.53	118.60
53	BA	156	A	N1-C6-N6	-10.12	112.53	118.60
53	BA	63	A	N1-C6-N6	-10.12	112.53	118.60
21	AA	1256	A	N1-C6-N6	-10.12	112.53	118.60
53	BA	2135	A	N1-C6-N6	-10.12	112.53	118.60
53	BA	1583	A	N1-C6-N6	-10.11	112.54	118.60
22	A1	73	A	N1-C6-N6	-10.10	112.54	118.60
53	BA	1901	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	560	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	864	A	N1-C6-N6	-10.10	112.54	118.60
53	BA	111	A	N1-C6-N6	-10.09	112.54	118.60
53	BA	2003	A	N1-C6-N6	-10.08	112.55	118.60
53	BA	2750	A	N1-C6-N6	-10.08	112.55	118.60
53	BA	207	A	N1-C6-N6	-10.08	112.55	118.60
53	BA	1912	A	N1-C6-N6	-10.08	112.55	118.60
53	BA	2211	A	N1-C6-N6	-10.07	112.56	118.60
53	BA	2117	A	N1-C6-N6	-10.06	112.56	118.60
21	AA	532	A	N1-C6-N6	-10.06	112.56	118.60
34	BM	55	ARG	NE-CZ-NH1	10.06	125.33	120.30
53	BA	1287	A	N1-C6-N6	-10.05	112.57	118.60
53	BA	721	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	1289	A	N1-C6-N6	-10.05	112.57	118.60
53	BA	2267	A	N1-C6-N6	-10.04	112.58	118.60
53	BA	1205	A	N1-C6-N6	-10.04	112.58	118.60
2	AC	171	ARG	NE-CZ-NH1	10.03	125.31	120.30
21	AA	1169	A	N1-C6-N6	-10.03	112.58	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1230	A	N1-C6-N6	-10.03	112.58	118.60
21	AA	1396	A	N1-C6-N6	-10.02	112.59	118.60
53	BA	614	A	O4'-C1'-N9	10.02	116.22	108.20
53	BA	1606	C	N3-C2-O2	-10.02	114.89	121.90
21	AA	573	A	N1-C6-N6	-10.02	112.59	118.60
53	BA	866	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	1332	A	N1-C6-N6	-10.01	112.60	118.60
24	BC	269	ARG	NE-CZ-NH1	10.01	125.30	120.30
53	BA	1451	C	N3-C2-O2	-10.01	114.90	121.90
53	BA	83	A	N1-C6-N6	-10.00	112.60	118.60
53	BA	2820	A	N1-C6-N6	-9.99	112.60	118.60
53	BA	1469	A	C5-C6-N1	9.99	122.69	117.70
53	BA	2309	A	N1-C6-N6	-9.99	112.61	118.60
53	BA	1454	C	N3-C2-O2	-9.98	114.92	121.90
21	AA	681	A	N1-C6-N6	-9.98	112.61	118.60
53	BA	21	A	N1-C6-N6	-9.97	112.61	118.60
53	BA	1502	A	N1-C6-N6	-9.97	112.61	118.60
53	BA	2461	A	N1-C6-N6	-9.97	112.61	118.60
53	BA	197	A	N1-C6-N6	-9.97	112.62	118.60
21	AA	1204	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	572	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	10	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	642	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	493	A	O4'-C1'-N9	9.94	116.15	108.20
53	BA	504	A	N1-C6-N6	-9.94	112.63	118.60
53	BA	1603	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	815	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	33	A	N1-C6-N6	-9.93	112.64	118.60
53	BA	547	A	N1-C6-N6	-9.93	112.64	118.60
21	AA	648	A	N1-C6-N6	-9.92	112.65	118.60
21	AA	1346	A	N1-C6-N6	-9.92	112.65	118.60
53	BA	457	A	N1-C6-N6	-9.92	112.64	118.60
31	BJ	116	ARG	NE-CZ-NH1	9.92	125.26	120.30
21	AA	306	A	N1-C6-N6	-9.91	112.65	118.60
53	BA	685	A	N1-C6-N6	-9.91	112.65	118.60
53	BA	1383	A	N1-C6-N6	-9.91	112.66	118.60
21	AA	675	A	N1-C6-N6	-9.91	112.66	118.60
53	BA	1952	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	71	A	N1-C6-N6	-9.90	112.66	118.60
8	AI	11	ARG	NE-CZ-NH1	9.90	125.25	120.30
53	BA	793	A	N1-C6-N6	-9.89	112.66	118.60
21	AA	974	A	C5-C6-N1	9.89	122.64	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	101	A	N1-C6-N6	-9.88	112.67	118.60
21	AA	1252	A	C5-C6-N1	9.88	122.64	117.70
21	AA	1216	A	N1-C6-N6	-9.87	112.68	118.60
53	BA	2333	A	N1-C6-N6	-9.87	112.68	118.60
53	BA	311	A	N1-C6-N6	-9.87	112.68	118.60
21	AA	983	A	N1-C6-N6	-9.87	112.68	118.60
53	BA	1794	A	N1-C6-N6	-9.87	112.68	118.60
53	BA	1749	A	N1-C6-N6	-9.86	112.69	118.60
46	BY	29	ARG	NE-CZ-NH2	9.86	125.23	120.30
53	BA	310	A	N1-C6-N6	-9.86	112.69	118.60
53	BA	1489	C	O4'-C1'-N1	9.86	116.08	108.20
54	BB	73	A	N1-C6-N6	-9.86	112.69	118.60
53	BA	781	A	N1-C6-N6	-9.85	112.69	118.60
6	AG	110	ARG	NE-CZ-NH1	9.85	125.22	120.30
53	BA	173	A	N1-C6-N6	-9.84	112.69	118.60
21	AA	1408	A	N1-C6-N6	-9.84	112.70	118.60
53	BA	2052	A	N1-C6-N6	-9.84	112.70	118.60
53	BA	1353	A	N1-C6-N6	-9.83	112.70	118.60
9	AJ	37	ARG	NE-CZ-NH1	9.82	125.21	120.30
21	AA	1191	A	N1-C6-N6	-9.82	112.70	118.60
21	AA	65	A	N1-C6-N6	-9.82	112.71	118.60
53	BA	439	A	N1-C6-N6	-9.82	112.71	118.60
53	BA	910	A	N1-C6-N6	-9.82	112.71	118.60
53	BA	2052	A	C5-C6-N1	9.82	122.61	117.70
53	BA	348	A	N1-C6-N6	-9.81	112.71	118.60
42	BU	93	ARG	NE-CZ-NH1	9.81	125.20	120.30
54	BB	15	A	N1-C6-N6	-9.81	112.72	118.60
50	B2	28	ARG	NE-CZ-NH1	9.80	125.20	120.30
53	BA	279	A	C5-C6-N1	9.80	122.60	117.70
54	BB	46	A	N1-C6-N6	-9.79	112.72	118.60
21	AA	1492	A	N1-C6-N6	-9.79	112.73	118.60
21	AA	1398	A	N1-C6-N6	-9.78	112.73	118.60
53	BA	1754	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	767	A	N1-C6-N6	-9.77	112.74	118.60
54	BB	29	A	N1-C6-N6	-9.76	112.75	118.60
53	BA	1966	A	N1-C6-N6	-9.75	112.75	118.60
54	BB	34	A	N1-C6-N6	-9.74	112.75	118.60
53	BA	896	A	O4'-C1'-N9	9.74	115.99	108.20
53	BA	1960	A	N1-C6-N6	-9.74	112.76	118.60
53	BA	1301	A	N1-C6-N6	-9.73	112.76	118.60
53	BA	716	A	N1-C6-N6	-9.73	112.76	118.60
53	BA	582	A	N1-C6-N6	-9.72	112.77	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	465	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	195	A	C5-C6-N1	9.71	122.56	117.70
21	AA	609	A	N1-C6-N6	-9.71	112.78	118.60
53	BA	2705	A	N1-C6-N6	-9.71	112.78	118.60
21	AA	766	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	574	A	N1-C6-N6	-9.70	112.78	118.60
53	BA	1525	A	N1-C6-N6	-9.69	112.78	118.60
53	BA	2097	A	N1-C6-N6	-9.69	112.78	118.60
21	AA	1214	C	N1-C2-O2	9.68	124.71	118.90
53	BA	2114	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	1362	A	N1-C6-N6	-9.68	112.79	118.60
50	B2	33	ARG	NE-CZ-NH1	9.68	125.14	120.30
53	BA	1549	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	1214	C	N3-C2-O2	-9.68	115.13	121.90
53	BA	502	A	N1-C6-N6	-9.67	112.80	118.60
53	BA	231	A	N1-C6-N6	-9.66	112.80	118.60
21	AA	563	A	C5-C6-N1	9.66	122.53	117.70
31	BJ	13	ARG	NE-CZ-NH1	9.66	125.13	120.30
53	BA	734	A	N1-C6-N6	-9.66	112.80	118.60
53	BA	2734	A	N1-C6-N6	-9.66	112.80	118.60
53	BA	1395	A	N1-C6-N6	-9.66	112.81	118.60
22	A1	16	C	N3-C2-O2	-9.65	115.14	121.90
21	AA	559	A	O4'-C1'-N9	9.65	115.92	108.20
21	AA	1333	A	N1-C6-N6	-9.65	112.81	118.60
53	BA	655	A	N1-C6-N6	-9.65	112.81	118.60
53	BA	1032	A	N1-C6-N6	-9.64	112.82	118.60
21	AA	1428	A	N1-C6-N6	-9.64	112.82	118.60
53	BA	1067	A	N1-C6-N6	-9.64	112.82	118.60
53	BA	2298	A	N1-C6-N6	-9.64	112.82	118.60
5	AF	86	ARG	NE-CZ-NH1	9.62	125.11	120.30
53	BA	1913	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	448	A	N1-C6-N6	-9.62	112.83	118.60
27	BF	79	ARG	NE-CZ-NH2	9.62	125.11	120.30
53	BA	2598	A	N1-C6-N6	-9.62	112.83	118.60
53	BA	73	A	N1-C6-N6	-9.61	112.83	118.60
53	BA	94	A	N1-C6-N6	-9.61	112.83	118.60
53	BA	2092	U	O4'-C1'-N1	9.61	115.89	108.20
53	BA	279	A	N1-C6-N6	-9.61	112.83	118.60
22	A1	35	A	N1-C6-N6	-9.61	112.84	118.60
53	BA	2518	A	N1-C6-N6	-9.61	112.84	118.60
53	BA	2800	A	N1-C6-N6	-9.60	112.84	118.60
53	BA	2682	A	C5-C6-N1	9.60	122.50	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	368	A	N1-C6-N6	-9.60	112.84	118.60
21	AA	1055	A	N1-C6-N6	-9.60	112.84	118.60
53	BA	1321	A	N1-C6-N6	-9.60	112.84	118.60
53	BA	981	A	N1-C6-N6	-9.60	112.84	118.60
53	BA	2654	A	N1-C6-N6	-9.60	112.84	118.60
53	BA	53	A	N1-C6-N6	-9.59	112.85	118.60
53	BA	1866	A	N1-C6-N6	-9.58	112.85	118.60
8	AI	84	ARG	NE-CZ-NH1	9.57	125.09	120.30
53	BA	1829	A	N1-C6-N6	-9.57	112.86	118.60
53	BA	1302	A	N1-C6-N6	-9.56	112.86	118.60
43	BV	21	ARG	NE-CZ-NH1	9.56	125.08	120.30
53	BA	294	A	N1-C6-N6	-9.56	112.86	118.60
21	AA	754	C	N3-C2-O2	-9.56	115.21	121.90
53	BA	963	U	O4'-C1'-N1	9.56	115.85	108.20
53	BA	1322	A	C5-C6-N1	9.56	122.48	117.70
53	BA	2176	A	N1-C6-N6	-9.56	112.87	118.60
53	BA	1981	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	344	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	1306	A	N1-C6-N6	-9.55	112.87	118.60
53	BA	905	A	N1-C6-N6	-9.55	112.87	118.60
53	BA	2711	A	N1-C6-N6	-9.55	112.87	118.60
53	BA	1677	A	N1-C6-N6	-9.55	112.87	118.60
53	BA	825	A	N1-C6-N6	-9.55	112.87	118.60
53	BA	2825	G	O4'-C1'-N9	9.55	115.84	108.20
53	BA	1848	A	N1-C6-N6	-9.54	112.88	118.60
21	AA	139	A	N1-C6-N6	-9.54	112.88	118.60
53	BA	1453	A	C5-C6-N1	9.54	122.47	117.70
53	BA	2468	A	C5-C6-N1	9.54	122.47	117.70
21	AA	974	A	N1-C6-N6	-9.54	112.88	118.60
53	BA	2425	A	C5-C6-N1	9.53	122.47	117.70
53	BA	1637	A	N1-C6-N6	-9.53	112.88	118.60
21	AA	968	A	C5-C6-N1	9.52	122.46	117.70
21	AA	345	C	N3-C2-O2	-9.52	115.24	121.90
21	AA	1150	A	N1-C6-N6	-9.52	112.89	118.60
14	AO	53	ARG	NE-CZ-NH1	9.51	125.06	120.30
43	BV	93	ARG	NE-CZ-NH1	9.51	125.06	120.30
53	BA	1347	A	N1-C6-N6	-9.50	112.90	118.60
21	AA	246	A	N1-C6-N6	-9.50	112.90	118.60
21	AA	435	A	N1-C6-N6	-9.49	112.90	118.60
21	AA	535	A	N1-C6-N6	-9.49	112.91	118.60
4	AE	19	ARG	NE-CZ-NH1	9.48	125.04	120.30
53	BA	2503	A	N1-C6-N6	-9.48	112.91	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	BQ	69	ARG	NE-CZ-NH1	9.47	125.04	120.30
21	AA	860	A	N1-C6-N6	-9.47	112.92	118.60
53	BA	1156	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	72	A	N1-C6-N6	-9.46	112.92	118.60
22	A1	58	A	N1-C6-N6	-9.46	112.92	118.60
53	BA	2169	A	N1-C6-N6	-9.46	112.92	118.60
53	BA	1579	A	N1-C6-N6	-9.46	112.93	118.60
21	AA	665	A	N1-C6-N6	-9.45	112.93	118.60
53	BA	1853	A	N1-C6-N6	-9.45	112.93	118.60
53	BA	1789	A	N1-C6-N6	-9.45	112.93	118.60
53	BA	613	A	N1-C6-N6	-9.45	112.93	118.60
53	BA	1758	U	O4'-C1'-N1	9.45	115.76	108.20
53	BA	943	A	N1-C6-N6	-9.44	112.93	118.60
53	BA	2886	A	N1-C6-N6	-9.44	112.93	118.60
21	AA	1493	A	C5-C6-N1	9.44	122.42	117.70
53	BA	1679	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	441	A	N1-C6-N6	-9.44	112.94	118.60
53	BA	2453	A	N1-C6-N6	-9.43	112.94	118.60
23	A2	91	A	N1-C6-N6	-9.43	112.94	118.60
49	B1	5	ARG	NE-CZ-NH1	9.43	125.01	120.30
53	BA	1268	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	327	A	N1-C6-N6	-9.43	112.94	118.60
53	BA	152	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	995	C	N3-C2-O2	-9.41	115.31	121.90
14	AO	16	ARG	NE-CZ-NH1	9.40	125.00	120.30
21	AA	845	A	N1-C6-N6	-9.40	112.96	118.60
53	BA	1528	A	N1-C6-N6	-9.40	112.96	118.60
53	BA	637	A	N1-C6-N6	-9.39	112.96	118.60
21	AA	53	A	N1-C6-N6	-9.39	112.96	118.60
53	BA	960	A	N1-C6-N6	-9.39	112.97	118.60
53	BA	2134	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	1500	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	181	A	N1-C6-N6	-9.38	112.97	118.60
22	A1	6	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	466	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	2328	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	1048	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	2560	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	1368	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	592	A	N1-C6-N6	-9.38	112.97	118.60
53	BA	2009	A	C5-C6-N1	9.37	122.38	117.70
53	BA	2634	A	N1-C6-N6	-9.36	112.98	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	BN	45	ARG	NE-CZ-NH1	9.36	124.98	120.30
21	AA	130	A	N1-C6-N6	-9.36	112.98	118.60
21	AA	1440	U	O4'-C1'-N1	9.36	115.69	108.20
53	BA	1780	A	N1-C6-N6	-9.36	112.99	118.60
53	BA	270	A	N1-C6-N6	-9.35	112.99	118.60
53	BA	2058	A	N1-C6-N6	-9.34	112.99	118.60
21	AA	189	A	N1-C6-N6	-9.34	113.00	118.60
53	BA	2748	A	N1-C6-N6	-9.34	113.00	118.60
53	BA	280	U	O4'-C1'-N1	9.34	115.67	108.20
53	BA	412	A	C4-C5-C6	-9.34	112.33	117.00
53	BA	1427	A	N1-C6-N6	-9.34	113.00	118.60
21	AA	1465	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	1377	A	N1-C6-N6	-9.32	113.01	118.60
53	BA	727	A	N1-C6-N6	-9.32	113.01	118.60
4	AE	68	ARG	NE-CZ-NH1	9.32	124.96	120.30
21	AA	1298	U	O4'-C1'-N1	9.32	115.65	108.20
53	BA	6	A	N1-C6-N6	-9.31	113.01	118.60
53	BA	945	A	N1-C6-N6	-9.31	113.01	118.60
53	BA	213	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	663	A	N1-C6-N6	-9.31	113.02	118.60
53	BA	1095	A	N1-C6-N6	-9.30	113.02	118.60
53	BA	1385	A	N1-C6-N6	-9.30	113.02	118.60
21	AA	81	A	N1-C6-N6	-9.29	113.02	118.60
53	BA	456	C	N3-C2-O2	-9.29	115.39	121.90
53	BA	1596	A	N1-C6-N6	-9.29	113.02	118.60
53	BA	2879	A	N1-C6-N6	-9.29	113.02	118.60
21	AA	794	A	N1-C6-N6	-9.29	113.02	118.60
53	BA	1885	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	129	A	N1-C6-N6	-9.29	113.03	118.60
53	BA	472	A	N1-C6-N6	-9.29	113.03	118.60
53	BA	2327	A	N1-C6-N6	-9.29	113.03	118.60
53	BA	2183	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	92	U	O4'-C1'-N1	9.28	115.62	108.20
21	AA	1257	A	C5-C6-N1	9.28	122.34	117.70
53	BA	204	A	N1-C6-N6	-9.28	113.03	118.60
53	BA	1937	A	C4-C5-C6	-9.28	112.36	117.00
53	BA	1998	A	N1-C6-N6	-9.28	113.03	118.60
53	BA	706	A	C5-C6-N1	9.27	122.34	117.70
21	AA	279	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	1111	A	N1-C6-N6	-9.27	113.04	118.60
53	BA	654	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	1155	A	N1-C6-N6	-9.27	113.04	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	420	C	N3-C2-O2	-9.27	115.41	121.90
53	BA	1366	A	N1-C6-N6	-9.26	113.04	118.60
21	AA	174	A	C5-C6-N1	9.26	122.33	117.70
53	BA	742	A	N1-C6-N6	-9.26	113.05	118.60
53	BA	861	A	N1-C6-N6	-9.25	113.05	118.60
10	AK	36	ARG	NE-CZ-NH1	9.25	124.92	120.30
53	BA	94	A	C5-C6-N1	9.25	122.33	117.70
53	BA	1762	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	149	A	N1-C6-N6	-9.24	113.05	118.60
53	BA	345	A	N1-C6-N6	-9.24	113.06	118.60
53	BA	1669	A	C5-C6-N1	9.24	122.32	117.70
53	BA	2358	A	N1-C6-N6	-9.24	113.06	118.60
53	BA	1640	A	C5-C6-N1	9.24	122.32	117.70
53	BA	1652	A	N1-C6-N6	-9.24	113.06	118.60
13	AN	81	ARG	NE-CZ-NH1	9.23	124.92	120.30
53	BA	982	C	N3-C2-O2	-9.23	115.44	121.90
53	BA	802	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	167	A	N1-C6-N6	-9.22	113.07	118.60
53	BA	402	A	C5-C6-N1	9.21	122.31	117.70
21	AA	152	A	C5-C6-N1	9.21	122.31	117.70
21	AA	574	A	C5-C6-N1	9.21	122.31	117.70
21	AA	192	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	1246	A	N1-C6-N6	-9.21	113.07	118.60
53	BA	71	A	N1-C6-N6	-9.21	113.08	118.60
43	BV	9	ARG	NE-CZ-NH1	9.20	124.90	120.30
54	BB	37	C	N1-C2-O2	9.21	124.42	118.90
53	BA	2033	A	O3'-P-O5'	-9.20	86.51	104.00
22	A1	74	C	O4'-C1'-N1	9.20	115.56	108.20
53	BA	2372	U	O4'-C1'-N1	9.20	115.56	108.20
21	AA	408	A	N1-C6-N6	-9.20	113.08	118.60
53	BA	833	A	N1-C6-N6	-9.20	113.08	118.60
53	BA	1618	A	N1-C6-N6	-9.19	113.08	118.60
13	AN	9	ARG	NE-CZ-NH1	9.19	124.89	120.30
32	BK	30	ARG	NE-CZ-NH1	9.19	124.89	120.30
21	AA	1398	A	C5-C6-N1	9.18	122.29	117.70
53	BA	340	A	C5-C6-N1	9.18	122.29	117.70
53	BA	1320	C	N3-C2-O2	-9.18	115.47	121.90
53	BA	1050	A	N1-C6-N6	-9.18	113.09	118.60
21	AA	1101	A	N1-C6-N6	-9.17	113.10	118.60
54	BB	36	C	N3-C2-O2	-9.17	115.48	121.90
21	AA	1004	A	C5-C6-N1	9.17	122.29	117.70
53	BA	2602	A	N1-C6-N6	-9.17	113.10	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	50	A	C5-C6-N1	9.17	122.28	117.70
21	AA	510	A	N1-C6-N6	-9.17	113.10	118.60
53	BA	2821	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	1102	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	901	A	N1-C6-N6	-9.15	113.11	118.60
53	BA	192	C	N3-C2-O2	-9.15	115.49	121.90
53	BA	1977	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	958	A	C5-C6-N1	9.15	122.27	117.70
53	BA	195	A	C5-C6-N1	9.14	122.27	117.70
53	BA	508	A	C5-C6-N1	9.14	122.27	117.70
53	BA	637	A	C5-C6-N1	9.14	122.27	117.70
53	BA	1745	A	C5-C6-N1	9.14	122.27	117.70
53	BA	1815	A	N1-C6-N6	-9.14	113.11	118.60
53	BA	456	C	N1-C2-O2	9.14	124.38	118.90
22	A1	16	C	O4'-C1'-N1	9.13	115.51	108.20
35	BN	17	ARG	NE-CZ-NH1	9.13	124.87	120.30
53	BA	2033	A	C5-C6-N1	9.13	122.27	117.70
26	BE	114	ARG	NE-CZ-NH1	9.13	124.86	120.30
53	BA	821	A	N1-C6-N6	-9.12	113.12	118.60
21	AA	716	A	N1-C6-N6	-9.12	113.13	118.60
53	BA	2482	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	1110	A	N1-C6-N6	-9.12	113.13	118.60
28	BG	54	ARG	NE-CZ-NH1	9.12	124.86	120.30
53	BA	689	A	N1-C6-N6	-9.11	113.13	118.60
53	BA	1322	A	N1-C6-N6	-9.12	113.13	118.60
53	BA	2829	A	N1-C6-N6	-9.11	113.13	118.60
21	AA	1036	A	N1-C6-N6	-9.11	113.13	118.60
53	BA	453	A	C5-C6-N1	9.11	122.25	117.70
21	AA	975	A	N1-C6-N6	-9.11	113.14	118.60
21	AA	1067	A	C5-C6-N1	9.11	122.25	117.70
31	BJ	69	ARG	NE-CZ-NH1	9.10	124.85	120.30
53	BA	160	A	C5-C6-N1	9.10	122.25	117.70
53	BA	146	A	N1-C6-N6	-9.10	113.14	118.60
53	BA	699	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	563	A	N1-C6-N6	-9.10	113.14	118.60
53	BA	1420	A	O4'-C1'-N9	9.10	115.48	108.20
21	AA	575	G	O4'-C1'-N9	9.10	115.48	108.20
53	BA	925	A	N1-C6-N6	-9.10	113.14	118.60
53	BA	1489	C	N3-C2-O2	-9.10	115.53	121.90
53	BA	2158	A	C5-C6-N1	9.10	122.25	117.70
53	BA	2407	A	N1-C6-N6	-9.09	113.14	118.60
53	BA	420	C	N1-C2-O2	9.09	124.35	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2369	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	977	A	N1-C6-N6	-9.08	113.15	118.60
53	BA	706	A	N1-C6-N6	-9.08	113.15	118.60
55	B5	122	ARG	NE-CZ-NH1	9.08	124.84	120.30
21	AA	495	A	N1-C6-N6	-9.08	113.15	118.60
53	BA	933	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	238	A	N1-C6-N6	-9.07	113.16	118.60
53	BA	221	A	C5-C6-N1	9.07	122.24	117.70
15	AP	70	ARG	NE-CZ-NH1	9.07	124.84	120.30
21	AA	371	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1163	A	N1-C6-N6	-9.07	113.16	118.60
53	BA	990	A	C1'-O4'-C4'	-9.07	102.65	109.90
53	BA	1890	A	C5-C6-N1	9.07	122.23	117.70
21	AA	174	A	N1-C6-N6	-9.06	113.16	118.60
53	BA	2835	A	N1-C6-N6	-9.06	113.16	118.60
53	BA	195	A	N1-C6-N6	-9.06	113.17	118.60
53	BA	2321	U	O4'-C1'-N1	9.05	115.44	108.20
15	AP	8	ARG	NE-CZ-NH1	9.05	124.83	120.30
53	BA	613	A	C5-C6-N1	9.05	122.23	117.70
53	BA	2753	A	N1-C6-N6	-9.05	113.17	118.60
35	BN	69	ARG	NE-CZ-NH1	9.04	124.82	120.30
33	BL	21	ARG	NE-CZ-NH2	9.04	124.82	120.30
53	BA	371	A	C5-C6-N1	9.04	122.22	117.70
53	BA	1610	A	C5-C6-N1	9.04	122.22	117.70
21	AA	338	A	C5-C6-N1	9.03	122.22	117.70
38	BQ	91	ARG	NE-CZ-NH1	9.03	124.82	120.30
53	BA	1126	A	C5-C6-N1	9.03	122.22	117.70
21	AA	1283	U	O4'-C1'-N1	9.03	115.42	108.20
21	AA	1434	A	N1-C6-N6	-9.03	113.19	118.60
53	BA	2005	A	C5-C6-N1	9.03	122.21	117.70
53	BA	2395	C	O4'-C1'-N1	9.02	115.42	108.20
21	AA	274	A	N1-C6-N6	-9.02	113.19	118.60
53	BA	1609	A	N1-C6-N6	-9.02	113.19	118.60
53	BA	1551	A	N1-C6-N6	-9.02	113.19	118.60
53	BA	2632	A	N1-C6-N6	-9.02	113.19	118.60
53	BA	947	A	N1-C6-N6	-9.01	113.19	118.60
21	AA	1250	A	N1-C6-N6	-9.01	113.19	118.60
53	BA	196	A	N1-C6-N6	-9.01	113.20	118.60
53	BA	346	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	1318	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	282	A	C5-C6-N1	9.00	122.20	117.70
53	BA	2886	A	C5-C6-N1	9.00	122.20	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2426	A	N1-C6-N6	-8.99	113.20	118.60
5	AF	38	ARG	NE-CZ-NH1	8.99	124.79	120.30
21	AA	782	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	373	A	C5-C6-N1	8.99	122.19	117.70
21	AA	1357	A	N1-C6-N6	-8.99	113.21	118.60
17	AR	72	ARG	NE-CZ-NH2	8.98	124.79	120.30
53	BA	1509	A	N1-C6-N6	-8.98	113.21	118.60
53	BA	1938	A	N1-C6-N6	-8.98	113.21	118.60
53	BA	2860	A	N1-C6-N6	-8.98	113.21	118.60
53	BA	1142	A	N1-C6-N6	-8.98	113.21	118.60
53	BA	2274	A	C5-C6-N1	8.98	122.19	117.70
53	BA	2071	A	C5-C6-N1	8.97	122.19	117.70
54	BB	104	A	N1-C6-N6	-8.97	113.22	118.60
53	BA	1669	A	N1-C6-N6	-8.97	113.22	118.60
53	BA	1928	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	547	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	1016	A	N1-C6-N6	-8.96	113.22	118.60
53	BA	52	A	N1-C6-N6	-8.96	113.22	118.60
53	BA	1301	A	C5-C6-N1	8.96	122.18	117.70
53	BA	1772	A	N1-C6-N6	-8.96	113.22	118.60
53	BA	2093	G	O4'-C1'-N9	8.96	115.37	108.20
22	A1	74	C	N3-C2-O2	-8.96	115.63	121.90
53	BA	982	C	N1-C2-O2	8.96	124.27	118.90
54	BB	66	A	C5-C6-N1	8.95	122.17	117.70
1	AB	224	ARG	NE-CZ-NH1	8.95	124.77	120.30
21	AA	1374	A	N1-C6-N6	-8.94	113.23	118.60
53	BA	1336	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	1429	A	N1-C6-N6	-8.94	113.24	118.60
26	BE	162	ARG	NE-CZ-NH1	8.94	124.77	120.30
21	AA	72	A	C5-C6-N1	8.94	122.17	117.70
21	AA	767	A	C5-C6-N1	8.93	122.17	117.70
21	AA	1146	A	N1-C6-N6	-8.93	113.24	118.60
10	AK	92	ARG	NE-CZ-NH1	8.93	124.77	120.30
21	AA	607	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	1180	A	N1-C6-N6	-8.93	113.24	118.60
25	BD	59	ARG	NE-CZ-NH1	8.93	124.77	120.30
8	AI	121	ARG	NE-CZ-NH1	8.93	124.77	120.30
53	BA	2051	A	N1-C6-N6	-8.93	113.24	118.60
53	BA	2070	A	N1-C6-N6	-8.93	113.24	118.60
53	BA	670	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	900	A	N1-C6-N6	-8.93	113.25	118.60
53	BA	2101	A	N1-C6-N6	-8.93	113.25	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2879	A	C5-C6-N1	8.93	122.16	117.70
21	AA	533	A	N1-C6-N6	-8.92	113.25	118.60
25	BD	77	ARG	NE-CZ-NH1	8.92	124.76	120.30
53	BA	1616	A	N1-C6-N6	-8.92	113.25	118.60
53	BA	1434	A	O4'-C1'-N9	8.92	115.34	108.20
18	AS	77	ARG	NE-CZ-NH1	8.92	124.76	120.30
21	AA	819	A	N1-C6-N6	-8.91	113.25	118.60
21	AA	422	C	O4'-C1'-N1	8.90	115.32	108.20
53	BA	654	A	O4'-C1'-N9	8.90	115.32	108.20
21	AA	509	A	N1-C6-N6	-8.90	113.26	118.60
53	BA	323	C	N3-C2-O2	-8.90	115.67	121.90
53	BA	1978	A	N1-C6-N6	-8.89	113.26	118.60
21	AA	697	U	O4'-C1'-N1	8.89	115.31	108.20
53	BA	1133	A	N1-C6-N6	-8.89	113.27	118.60
53	BA	2377	A	N1-C6-N6	-8.89	113.27	118.60
53	BA	1048	A	C5-C6-N1	8.88	122.14	117.70
21	AA	152	A	C4-C5-C6	-8.88	112.56	117.00
8	AI	10	ARG	NE-CZ-NH1	8.88	124.74	120.30
21	AA	819	A	C5-C6-N1	8.88	122.14	117.70
53	BA	2317	A	N1-C6-N6	-8.88	113.27	118.60
53	BA	227	A	N1-C6-N6	-8.88	113.28	118.60
21	AA	1275	A	N1-C6-N6	-8.87	113.28	118.60
53	BA	1801	A	N1-C6-N6	-8.87	113.28	118.60
53	BA	2883	A	N1-C6-N6	-8.86	113.28	118.60
53	BA	2340	A	N1-C6-N6	-8.86	113.28	118.60
53	BA	103	A	C5-C6-N1	8.86	122.13	117.70
53	BA	1134	A	N1-C6-N6	-8.86	113.29	118.60
53	BA	1431	A	N1-C6-N6	-8.86	113.29	118.60
53	BA	781	A	C5-C6-N1	8.85	122.13	117.70
53	BA	626	A	N1-C6-N6	-8.85	113.29	118.60
54	BB	78	A	N1-C6-N6	-8.85	113.29	118.60
53	BA	631	A	C5-C6-N1	8.85	122.12	117.70
53	BA	2418	A	C4-C5-C6	-8.85	112.58	117.00
53	BA	1014	A	N1-C6-N6	-8.85	113.29	118.60
53	BA	2158	A	N1-C6-N6	-8.84	113.30	118.60
53	BA	2614	A	N1-C6-N6	-8.84	113.30	118.60
53	BA	1000	A	C5-C6-N1	8.84	122.12	117.70
53	BA	1204	A	N1-C6-N6	-8.84	113.30	118.60
53	BA	2889	C	N1-C2-O2	8.84	124.20	118.90
53	BA	89	A	N1-C6-N6	-8.83	113.30	118.60
53	BA	1439	A	O4'-C1'-N9	8.83	115.26	108.20
21	AA	1216	A	C5-C6-N1	8.82	122.11	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	BQ	49	ARG	NE-CZ-NH1	8.82	124.71	120.30
53	BA	845	A	N1-C6-N6	-8.82	113.31	118.60
53	BA	2657	A	N1-C6-N6	-8.82	113.31	118.60
11	AL	85	ARG	NE-CZ-NH1	8.82	124.71	120.30
53	BA	221	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	780	A	N1-C6-N6	-8.81	113.31	118.60
53	BA	633	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	179	A	C5-C6-N1	8.81	122.10	117.70
53	BA	1744	A	N1-C6-N6	-8.81	113.31	118.60
53	BA	1810	A	N1-C6-N6	-8.80	113.32	118.60
53	BA	1490	A	N1-C6-N6	-8.80	113.32	118.60
53	BA	1544	A	C5-C6-N1	8.80	122.10	117.70
21	AA	938	A	N1-C6-N6	-8.79	113.32	118.60
21	AA	98	A	C5-C6-N1	8.79	122.10	117.70
21	AA	466	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	1285	A	N1-C6-N6	-8.79	113.32	118.60
53	BA	783	A	N1-C6-N6	-8.79	113.32	118.60
22	A1	41	A	N1-C6-N6	-8.79	113.33	118.60
12	AM	92	ARG	NE-CZ-NH2	8.79	124.69	120.30
21	AA	1022	A	N1-C6-N6	-8.79	113.33	118.60
53	BA	2668	G	O4'-C1'-N9	8.79	115.23	108.20
21	AA	1377	A	C5-C6-N1	8.79	122.09	117.70
53	BA	1169	A	N1-C6-N6	-8.79	113.33	118.60
53	BA	2451	A	N1-C6-N6	-8.79	113.33	118.60
54	BB	58	A	C5-C6-N1	8.79	122.09	117.70
54	BB	109	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	382	A	N1-C6-N6	-8.79	113.33	118.60
53	BA	2433	A	N1-C6-N6	-8.79	113.33	118.60
53	BA	1287	A	C5-C6-N1	8.78	122.09	117.70
53	BA	2530	A	N1-C6-N6	-8.78	113.33	118.60
8	AI	94	ARG	NE-CZ-NH1	8.77	124.69	120.30
9	AJ	89	ARG	NE-CZ-NH1	8.77	124.68	120.30
21	AA	19	A	N1-C6-N6	-8.77	113.34	118.60
53	BA	2813	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	913	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	210	C	N3-C2-O2	-8.76	115.77	121.90
37	BP	100	ARG	NE-CZ-NH1	8.76	124.68	120.30
53	BA	2126	A	N1-C6-N6	-8.76	113.34	118.60
53	BA	2837	A	C4-C5-C6	-8.76	112.62	117.00
21	AA	174	A	C4-C5-C6	-8.76	112.62	117.00
53	BA	478	A	N1-C6-N6	-8.76	113.34	118.60
53	BA	2333	A	C5-C6-N1	8.76	122.08	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1031	C	N3-C2-O2	-8.76	115.77	121.90
53	BA	1039	A	N1-C6-N6	-8.76	113.35	118.60
21	AA	1311	A	C5-C6-N1	8.76	122.08	117.70
53	BA	1900	A	N1-C6-N6	-8.76	113.35	118.60
2	AC	10	ARG	NE-CZ-NH1	8.75	124.68	120.30
21	AA	1480	A	N1-C6-N6	-8.75	113.35	118.60
53	BA	920	A	C4-C5-C6	-8.75	112.62	117.00
53	BA	2108	A	N1-C6-N6	-8.75	113.35	118.60
53	BA	340	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	171	A	N1-C6-N6	-8.74	113.35	118.60
21	AA	330	C	N3-C2-O2	-8.74	115.78	121.90
21	AA	1093	A	C4-C5-C6	-8.74	112.63	117.00
53	BA	676	A	N1-C6-N6	-8.74	113.35	118.60
53	BA	980	A	N1-C6-N6	-8.74	113.35	118.60
53	BA	2518	A	C5-C6-N1	8.74	122.07	117.70
21	AA	190	A	C5-C6-N1	8.74	122.07	117.70
53	BA	2639	A	C5-C6-N1	8.74	122.07	117.70
53	BA	2721	A	N1-C6-N6	-8.74	113.36	118.60
53	BA	2733	A	N1-C6-N6	-8.74	113.36	118.60
21	AA	959	A	N1-C6-N6	-8.74	113.36	118.60
22	A1	60	C	N3-C2-O2	-8.74	115.78	121.90
53	BA	144	A	N1-C6-N6	-8.73	113.36	118.60
53	BA	449	A	C5-C6-N1	8.73	122.06	117.70
21	AA	949	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	1196	A	C5-C6-N1	8.73	122.06	117.70
53	BA	2666	C	O4'-C1'-N1	8.73	115.18	108.20
53	BA	1286	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	793	U	O4'-C1'-N1	8.72	115.18	108.20
53	BA	1265	A	C5-C6-N1	8.72	122.06	117.70
53	BA	1901	A	C4-C5-C6	-8.72	112.64	117.00
53	BA	73	A	C5-C6-N1	8.72	122.06	117.70
53	BA	344	A	C5-C6-N1	8.71	122.06	117.70
53	BA	1147	A	N1-C6-N6	-8.71	113.37	118.60
53	BA	2541	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	1364	U	O4'-C1'-N1	8.71	115.17	108.20
53	BA	1635	A	N1-C6-N6	-8.71	113.37	118.60
53	BA	1730	C	N3-C2-O2	-8.71	115.80	121.90
53	BA	1579	A	C5-C6-N1	8.71	122.05	117.70
21	AA	199	A	C5-C6-N1	8.71	122.05	117.70
21	AA	648	A	C5-C6-N1	8.71	122.05	117.70
53	BA	2274	A	N1-C6-N6	-8.71	113.38	118.60
53	BA	2042	A	N1-C6-N6	-8.70	113.38	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2889	C	N3-C2-O2	-8.70	115.81	121.90
53	BA	1580	A	C4-C5-C6	-8.70	112.65	117.00
53	BA	2346	A	N1-C6-N6	-8.70	113.38	118.60
53	BA	2682	A	C4-C5-C6	-8.69	112.65	117.00
21	AA	901	A	C5-C6-N1	8.69	122.04	117.70
53	BA	608	A	C5-C6-N1	8.69	122.04	117.70
9	AJ	48	ARG	NE-CZ-NH2	8.68	124.64	120.30
53	BA	1080	A	N1-C6-N6	-8.68	113.39	118.60
53	BA	1073	A	C5-C6-N1	8.68	122.04	117.70
53	BA	2288	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	461	A	C5-C6-N1	8.68	122.04	117.70
53	BA	789	A	N1-C6-N6	-8.67	113.40	118.60
53	BA	1672	A	N1-C6-N6	-8.67	113.40	118.60
53	BA	2273	A	N1-C6-N6	-8.67	113.40	118.60
53	BA	1028	A	C5-C6-N1	8.66	122.03	117.70
38	BQ	27	ARG	NE-CZ-NH1	8.66	124.63	120.30
53	BA	94	A	C4-C5-C6	-8.66	112.67	117.00
53	BA	233	A	N1-C6-N6	-8.66	113.40	118.60
53	BA	44	A	C5-C6-N1	8.66	122.03	117.70
53	BA	1134	A	C5-C6-N1	8.66	122.03	117.70
53	BA	2170	A	N1-C6-N6	-8.66	113.41	118.60
53	BA	2761	A	N1-C6-N6	-8.66	113.41	118.60
53	BA	1609	A	C5-C6-N1	8.65	122.03	117.70
21	AA	205	A	N1-C6-N6	-8.65	113.41	118.60
40	BS	8	ARG	NE-CZ-NH1	8.65	124.62	120.30
53	BA	819	A	C5-C6-N1	8.65	122.03	117.70
21	AA	66	A	N1-C6-N6	-8.65	113.41	118.60
54	BB	39	A	C5-C6-N1	8.65	122.02	117.70
21	AA	1502	A	C5-C6-N1	8.64	122.02	117.70
53	BA	838	C	N3-C2-O2	-8.64	115.85	121.90
21	AA	958	A	N1-C6-N6	-8.64	113.42	118.60
53	BA	256	A	N1-C6-N6	-8.64	113.42	118.60
53	BA	546	U	O4'-C1'-N1	8.64	115.11	108.20
53	BA	1495	A	N1-C6-N6	-8.64	113.42	118.60
53	BA	2281	A	C5-C6-N1	8.64	122.02	117.70
8	AI	79	ARG	NE-CZ-NH1	8.63	124.62	120.30
41	BT	69	ARG	NE-CZ-NH1	8.63	124.62	120.30
53	BA	1937	A	C5-C6-N1	8.63	122.02	117.70
21	AA	59	A	N1-C6-N6	-8.63	113.42	118.60
53	BA	1700	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	412	A	N1-C6-N6	-8.62	113.42	118.60
21	AA	1396	A	C5-C6-N1	8.63	122.01	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1188	A	N1-C6-N6	-8.62	113.43	118.60
53	BA	49	A	N1-C6-N6	-8.62	113.42	118.60
53	BA	74	A	N1-C6-N6	-8.62	113.42	118.60
53	BA	973	A	N1-C6-N6	-8.63	113.42	118.60
24	BC	42	ARG	NE-CZ-NH2	8.62	124.61	120.30
38	BQ	50	ARG	NE-CZ-NH1	8.62	124.61	120.30
53	BA	866	A	C5-C6-N1	8.62	122.01	117.70
53	BA	1630	A	N1-C6-N6	-8.62	113.43	118.60
53	BA	825	A	C4-C5-C6	-8.62	112.69	117.00
6	AG	4	ARG	NE-CZ-NH2	8.62	124.61	120.30
53	BA	1285	A	N1-C6-N6	-8.61	113.43	118.60
21	AA	1022	A	C5-C6-N1	8.61	122.00	117.70
21	AA	1441	A	N1-C6-N6	-8.61	113.43	118.60
53	BA	2821	A	C5-C6-N1	8.61	122.00	117.70
21	AA	1012	A	N1-C6-N6	-8.61	113.44	118.60
53	BA	142	A	C5-C6-N1	8.61	122.00	117.70
53	BA	2062	A	C5-C6-N1	8.61	122.00	117.70
21	AA	270	A	N1-C6-N6	-8.60	113.44	118.60
21	AA	694	A	C5-C6-N1	8.60	122.00	117.70
21	AA	1080	A	N1-C6-N6	-8.60	113.44	118.60
53	BA	1359	A	N1-C6-N6	-8.60	113.44	118.60
53	BA	1067	A	C5-C6-N1	8.60	122.00	117.70
21	AA	934	C	N3-C2-O2	-8.60	115.88	121.90
21	AA	197	A	C5-C6-N1	8.59	122.00	117.70
21	AA	1196	A	N1-C6-N6	-8.59	113.44	118.60
53	BA	845	A	C4-C5-C6	-8.59	112.70	117.00
21	AA	1238	A	N1-C6-N6	-8.59	113.44	118.60
53	BA	2406	A	C5-C6-N1	8.59	121.99	117.70
21	AA	964	A	N1-C6-N6	-8.59	113.45	118.60
53	BA	933	A	C5-C6-N1	8.59	121.99	117.70
53	BA	849	A	C5-C6-N1	8.58	121.99	117.70
53	BA	877	A	C5-C6-N1	8.58	121.99	117.70
53	BA	1916	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	704	A	C5-C6-N1	8.58	121.99	117.70
12	AM	100	ARG	NE-CZ-NH1	8.57	124.59	120.30
53	BA	990	A	O4'-C1'-N9	8.57	115.06	108.20
21	AA	329	A	C5-C6-N1	8.57	121.98	117.70
21	AA	630	A	C5-C6-N1	8.57	121.99	117.70
21	AA	66	A	C5-C6-N1	8.57	121.98	117.70
53	BA	1545	A	N1-C6-N6	-8.57	113.46	118.60
53	BA	2800	A	C5-C6-N1	8.57	121.98	117.70
53	BA	2386	A	N1-C6-N6	-8.57	113.46	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	BL	78	ARG	NE-CZ-NH1	8.56	124.58	120.30
53	BA	324	A	C5-C6-N1	8.56	121.98	117.70
53	BA	2376	A	N1-C6-N6	-8.56	113.46	118.60
53	BA	2749	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	461	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	1441	A	C4-C5-C6	-8.56	112.72	117.00
23	A2	82	A	C5-C6-N1	8.55	121.98	117.70
47	BZ	15	ARG	NE-CZ-NH1	8.55	124.58	120.30
53	BA	1061	U	O4'-C1'-N1	8.55	115.04	108.20
45	BX	49	ARG	NE-CZ-NH1	8.55	124.58	120.30
53	BA	983	A	N1-C6-N6	-8.55	113.47	118.60
53	BA	794	A	N1-C6-N6	-8.55	113.47	118.60
53	BA	2564	A	C5-C6-N1	8.55	121.97	117.70
8	AI	40	ARG	NE-CZ-NH1	8.54	124.57	120.30
21	AA	364	A	N1-C6-N6	-8.54	113.47	118.60
53	BA	2765	A	O4'-C1'-N9	8.54	115.03	108.20
11	AL	85	ARG	NE-CZ-NH2	-8.54	116.03	120.30
53	BA	909	A	C4-C5-C6	-8.54	112.73	117.00
21	AA	160	A	N1-C6-N6	-8.54	113.48	118.60
53	BA	563	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	1176	A	N1-C6-N6	-8.53	113.48	118.60
23	A2	79	A	C5-C6-N1	8.54	121.97	117.70
21	AA	1110	A	C5-C6-N1	8.53	121.97	117.70
21	AA	459	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	1269	A	N1-C6-N6	-8.53	113.48	118.60
53	BA	1133	A	C5-C6-N1	8.53	121.97	117.70
53	BA	1175	A	C5-C6-N1	8.53	121.96	117.70
21	AA	1229	A	N1-C6-N6	-8.53	113.48	118.60
53	BA	2675	A	C5-C6-N1	8.53	121.96	117.70
54	BB	57	A	N1-C6-N6	-8.53	113.48	118.60
53	BA	222	A	C5-C6-N1	8.52	121.96	117.70
53	BA	1384	A	C5-C6-N1	8.52	121.96	117.70
54	BB	34	A	C4-C5-C6	-8.52	112.74	117.00
53	BA	1489	C	N1-C2-O2	8.52	124.01	118.90
21	AA	16	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	695	A	C5-C6-N1	8.52	121.96	117.70
53	BA	2547	A	C5-C6-N1	8.52	121.96	117.70
53	BA	1169	A	C4-C5-C6	-8.52	112.74	117.00
21	AA	1500	A	C5-C6-N1	8.51	121.95	117.70
53	BA	2104	C	N3-C2-O2	-8.51	115.94	121.90
53	BA	693	A	N1-C6-N6	-8.51	113.50	118.60
53	BA	1938	A	O4'-C1'-N9	8.51	115.00	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2395	C	N3-C2-O2	-8.51	115.95	121.90
21	AA	663	A	C5-C6-N1	8.50	121.95	117.70
2	AC	155	ARG	NE-CZ-NH1	8.50	124.55	120.30
53	BA	1096	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	815	A	C5-C6-N1	8.50	121.95	117.70
43	BV	19	ARG	NE-CZ-NH1	8.50	124.55	120.30
53	BA	126	A	O4'-C1'-N9	8.49	115.00	108.20
53	BA	750	A	N1-C6-N6	-8.49	113.50	118.60
53	BA	792	A	N1-C6-N6	-8.49	113.50	118.60
53	BA	1761	C	N3-C2-O2	-8.49	115.96	121.90
51	B3	44	ARG	NE-CZ-NH1	8.49	124.54	120.30
21	AA	356	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	460	A	N1-C6-N6	-8.48	113.51	118.60
53	BA	1451	C	O4'-C1'-N1	8.48	114.98	108.20
53	BA	1307	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	583	A	C5-C6-N1	8.48	121.94	117.70
53	BA	1745	A	C4-C5-C6	-8.47	112.76	117.00
12	AM	86	ARG	NE-CZ-NH1	8.47	124.54	120.30
53	BA	1764	C	O4'-C1'-N1	8.47	114.98	108.20
53	BA	909	A	N1-C6-N6	-8.47	113.52	118.60
21	AA	747	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	1183	U	O4'-C1'-N1	8.47	114.97	108.20
21	AA	1158	C	N3-C2-O2	-8.46	115.97	121.90
53	BA	1515	A	N1-C6-N6	-8.46	113.52	118.60
53	BA	2542	A	C5-C6-N1	8.46	121.93	117.70
2	AC	39	ARG	NE-CZ-NH1	8.46	124.53	120.30
53	BA	781	A	C4-C5-C6	-8.46	112.77	117.00
53	BA	631	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	1410	A	N1-C6-N6	-8.46	113.53	118.60
53	BA	1876	A	C5-C6-N1	8.46	121.93	117.70
21	AA	51	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	970	C	N3-C2-O2	-8.45	115.98	121.90
21	AA	1014	A	C5-C6-N1	8.45	121.93	117.70
53	BA	1070	A	N1-C6-N6	-8.45	113.53	118.60
53	BA	2510	C	N3-C2-O2	-8.45	115.99	121.90
53	BA	637	A	C4-C5-C6	-8.45	112.78	117.00
21	AA	753	A	N1-C6-N6	-8.44	113.53	118.60
53	BA	1213	A	C5-C6-N1	8.44	121.92	117.70
21	AA	704	A	C4-C5-C6	-8.44	112.78	117.00
53	BA	1247	A	N1-C6-N6	-8.44	113.54	118.60
53	BA	1668	A	N1-C6-N6	-8.44	113.54	118.60
53	BA	2117	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(^{o})	Ideal(^{o})
53	BA	2328	A	C4-C5-C6	-8.44	112.78	117.00
53	BA	2088	A	C5-C6-N1	8.44	121.92	117.70
22	A1	76	A	N1-C6-N6	-8.44	113.54	118.60
53	BA	2469	A	N1-C6-N6	-8.44	113.54	118.60
12	AM	97	ARG	NE-CZ-NH1	8.43	124.52	120.30
53	BA	2013	A	N1-C6-N6	-8.43	113.54	118.60
53	BA	2458	G	O4'-C1'-N9	8.43	114.94	108.20
53	BA	910	A	C5-C6-N1	8.43	121.92	117.70
21	AA	914	A	N1-C6-N6	-8.43	113.54	118.60
21	AA	946	A	N1-C6-N6	-8.43	113.55	118.60
53	BA	91	A	N1-C6-N6	-8.43	113.54	118.60
53	BA	1244	A	C5-C6-N1	8.43	121.91	117.70
12	AM	89	ARG	NE-CZ-NH1	8.42	124.51	120.30
21	AA	465	A	O4'-C1'-N9	8.42	114.94	108.20
21	AA	969	A	N1-C6-N6	-8.42	113.55	118.60
53	BA	975	A	C5-C6-N1	8.42	121.91	117.70
53	BA	1635	A	C5-C6-N1	8.42	121.91	117.70
21	AA	77	A	C5-C6-N1	8.42	121.91	117.70
21	AA	865	A	C5-C6-N1	8.42	121.91	117.70
53	BA	176	A	C5-C6-N1	8.42	121.91	117.70
53	BA	1970	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	759	A	N1-C6-N6	-8.41	113.55	118.60
53	BA	718	A	O4'-C1'-N9	8.41	114.93	108.20
21	AA	172	A	N1-C6-N6	-8.41	113.55	118.60
45	BX	44	ARG	NE-CZ-NH1	8.41	124.51	120.30
53	BA	2005	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	48	C	N3-C2-O2	-8.41	116.01	121.90
53	BA	84	A	N1-C6-N6	-8.41	113.55	118.60
53	BA	844	A	C4-C5-C6	-8.41	112.80	117.00
53	BA	2311	A	C5-C6-N1	8.41	121.91	117.70
53	BA	2565	A	C5-C6-N1	8.41	121.91	117.70
21	AA	7	A	C5-C6-N1	8.41	121.90	117.70
21	AA	1157	A	N1-C6-N6	-8.41	113.56	118.60
53	BA	197	A	C5-C6-N1	8.41	121.90	117.70
53	BA	1413	A	N1-C6-N6	-8.41	113.56	118.60
54	BB	101	A	N1-C6-N6	-8.41	113.56	118.60
21	AA	50	A	N1-C6-N6	-8.40	113.56	118.60
26	BE	61	ARG	NE-CZ-NH1	8.40	124.50	120.30
21	AA	1092	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	250	A	O4'-C1'-N9	8.40	114.92	108.20
21	AA	130	A	C4-C5-C6	-8.40	112.80	117.00
24	BC	12	ARG	NE-CZ-NH1	8.40	124.50	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1957	C	N3-C2-O2	-8.40	116.02	121.90
53	BA	2030	A	N1-C6-N6	-8.39	113.56	118.60
53	BA	2147	A	C5-C6-N1	8.39	121.90	117.70
54	BB	29	A	C5-C6-N1	8.39	121.90	117.70
21	AA	872	A	N1-C6-N6	-8.39	113.56	118.60
22	A1	47	U	O4'-C1'-N1	8.39	114.91	108.20
21	AA	321	A	N1-C6-N6	-8.39	113.57	118.60
53	BA	975	A	N1-C6-N6	-8.39	113.56	118.60
53	BA	1668	A	C5-C6-N1	8.39	121.89	117.70
21	AA	1014	A	C4-C5-C6	-8.39	112.81	117.00
21	AA	1340	A	C4-C5-C6	-8.39	112.81	117.00
53	BA	2227	A	N1-C6-N6	-8.39	113.57	118.60
40	BS	11	ARG	NE-CZ-NH1	8.39	124.49	120.30
53	BA	2572	A	N1-C6-N6	-8.39	113.57	118.60
21	AA	298	A	C5-C6-N1	8.38	121.89	117.70
53	BA	28	A	N1-C6-N6	-8.38	113.57	118.60
53	BA	1029	A	N1-C6-N6	-8.38	113.57	118.60
53	BA	886	A	C5-C6-N1	8.38	121.89	117.70
53	BA	1127	A	O4'-C1'-N9	8.38	114.90	108.20
21	AA	794	A	C5-C6-N1	8.38	121.89	117.70
53	BA	203	A	N1-C6-N6	-8.38	113.57	118.60
53	BA	497	A	C5-C6-N1	8.38	121.89	117.70
21	AA	1267	C	N3-C2-O2	-8.37	116.04	121.90
21	AA	109	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	746	A	N1-C6-N6	-8.37	113.58	118.60
53	BA	404	A	C5-C6-N1	8.37	121.88	117.70
53	BA	2660	A	N1-C6-N6	-8.37	113.58	118.60
54	BB	39	A	N1-C6-N6	-8.37	113.58	118.60
53	BA	272	A	O4'-C1'-N9	8.37	114.89	108.20
53	BA	1522	A	N1-C6-N6	-8.36	113.58	118.60
45	BX	36	ARG	NE-CZ-NH2	8.36	124.48	120.30
53	BA	1932	A	C5-C6-N1	8.36	121.88	117.70
21	AA	983	A	C5-C6-N1	8.36	121.88	117.70
8	AI	112	ARG	NE-CZ-NH2	8.36	124.48	120.30
53	BA	2042	A	C5-C6-N1	8.36	121.88	117.70
53	BA	1147	A	C4-C5-C6	-8.36	112.82	117.00
53	BA	621	A	N1-C6-N6	-8.36	113.59	118.60
53	BA	2726	A	N1-C6-N6	-8.36	113.59	118.60
53	BA	1143	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	499	A	C5-C6-N1	8.35	121.88	117.70
53	BA	2163	A	N1-C6-N6	-8.35	113.59	118.60
53	BA	2191	A	N1-C6-N6	-8.35	113.59	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	AQ	39	ARG	NE-CZ-NH1	8.35	124.47	120.30
21	AA	397	A	C5-C6-N1	8.35	121.88	117.70
21	AA	553	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1126	U	O4'-C1'-N1	8.35	114.88	108.20
45	BX	2	ARG	NE-CZ-NH1	8.35	124.47	120.30
53	BA	2095	A	N1-C6-N6	-8.35	113.59	118.60
53	BA	5	A	N1-C6-N6	-8.35	113.59	118.60
53	BA	293	U	O4'-C1'-N1	8.35	114.88	108.20
53	BA	390	U	O4'-C1'-N1	8.35	114.88	108.20
53	BA	1569	A	C5-C6-N1	8.35	121.87	117.70
22	A1	74	C	N1-C2-O2	8.34	123.91	118.90
21	AA	119	A	C5-C6-N1	8.34	121.87	117.70
21	AA	729	A	N1-C6-N6	-8.34	113.59	118.60
21	AA	262	A	N1-C6-N6	-8.34	113.60	118.60
3	AD	80	ARG	NE-CZ-NH1	8.34	124.47	120.30
21	AA	183	C	N3-C2-O2	-8.34	116.06	121.90
21	AA	345	C	O4'-C1'-N1	8.34	114.87	108.20
21	AA	1201	A	N1-C6-N6	-8.34	113.60	118.60
53	BA	602	A	N1-C6-N6	-8.34	113.60	118.60
53	BA	1583	A	C5-C6-N1	8.34	121.87	117.70
35	BN	118	ARG	NE-CZ-NH1	8.33	124.47	120.30
53	BA	1272	A	N1-C6-N6	-8.33	113.60	118.60
47	BZ	37	ARG	NE-CZ-NH1	8.33	124.46	120.30
53	BA	1593	A	C4-C5-C6	-8.33	112.84	117.00
53	BA	2335	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	411	A	N1-C6-N6	-8.32	113.61	118.60
32	BK	70	ARG	NE-CZ-NH1	8.32	124.46	120.30
53	BA	1608	A	N1-C6-N6	-8.32	113.61	118.60
53	BA	1672	A	C5-C6-N1	8.32	121.86	117.70
21	AA	1093	A	C5-C6-N1	8.32	121.86	117.70
21	AA	1280	A	N1-C6-N6	-8.32	113.61	118.60
53	BA	262	A	N1-C6-N6	-8.32	113.61	118.60
53	BA	2135	A	C5-C6-N1	8.32	121.86	117.70
53	BA	2145	C	N3-C2-O2	-8.31	116.08	121.90
21	AA	831	A	C5-C6-N1	8.31	121.86	117.70
53	BA	2311	A	N1-C6-N6	-8.31	113.61	118.60
9	AJ	68	ARG	NE-CZ-NH1	8.31	124.46	120.30
21	AA	1279	G	O4'-C1'-N9	8.31	114.85	108.20
53	BA	1328	A	N1-C6-N6	-8.31	113.61	118.60
26	BE	69	ARG	NE-CZ-NH1	8.31	124.45	120.30
53	BA	1453	A	O4'-C1'-N9	8.31	114.85	108.20
53	BA	2163	A	C5-C6-N1	8.31	121.86	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2309	A	C5-C6-N1	8.31	121.85	117.70
21	AA	1360	A	C5-C6-N1	8.31	121.85	117.70
53	BA	2164	C	N3-C2-O2	-8.31	116.09	121.90
11	AL	53	ARG	NE-CZ-NH1	8.30	124.45	120.30
35	BN	103	ARG	NE-CZ-NH1	8.30	124.45	120.30
53	BA	2711	A	C4-C5-C6	-8.30	112.85	117.00
21	AA	1413	A	N1-C6-N6	-8.30	113.62	118.60
53	BA	1953	A	N1-C6-N6	-8.30	113.62	118.60
53	BA	429	A	N1-C6-N6	-8.29	113.62	118.60
53	BA	2820	A	C5-C6-N1	8.29	121.85	117.70
21	AA	1339	A	N1-C6-N6	-8.29	113.63	118.60
53	BA	279	A	C4-C5-C6	-8.29	112.86	117.00
53	BA	324	A	N1-C6-N6	-8.29	113.63	118.60
53	BA	2517	C	N3-C2-O2	-8.29	116.10	121.90
21	AA	161	A	N1-C6-N6	-8.28	113.63	118.60
53	BA	1439	A	C5-C6-N1	8.28	121.84	117.70
53	BA	1597	A	N1-C6-N6	-8.29	113.63	118.60
21	AA	179	A	C4-C5-C6	-8.28	112.86	117.00
21	AA	196	A	N1-C6-N6	-8.28	113.63	118.60
21	AA	648	A	C4-C5-C6	-8.28	112.86	117.00
53	BA	412	A	C5-C6-N1	8.28	121.84	117.70
53	BA	979	A	N1-C6-N6	-8.28	113.63	118.60
53	BA	1327	A	N1-C6-N6	-8.28	113.63	118.60
53	BA	1496	A	C5-C6-N1	8.28	121.84	117.70
53	BA	199	A	C5-C6-N1	8.28	121.84	117.70
53	BA	526	A	C5-C6-N1	8.28	121.84	117.70
53	BA	1080	A	C4-C5-C6	-8.28	112.86	117.00
21	AA	845	A	C4-C5-C6	-8.27	112.86	117.00
21	AA	622	A	C5-C6-N1	8.27	121.83	117.70
53	BA	514	A	C5-C6-N1	8.27	121.83	117.70
21	AA	1431	A	N1-C6-N6	-8.27	113.64	118.60
53	BA	609	A	N1-C6-N6	-8.27	113.64	118.60
53	BA	1469	A	C4-C5-C6	-8.26	112.87	117.00
10	AK	68	ARG	NE-CZ-NH1	8.26	124.43	120.30
21	AA	1101	A	C5-C6-N1	8.26	121.83	117.70
53	BA	240	C	N3-C2-O2	-8.26	116.12	121.90
21	AA	345	C	N1-C2-O2	8.26	123.85	118.90
21	AA	579	A	N1-C6-N6	-8.26	113.65	118.60
53	BA	176	A	N1-C6-N6	-8.26	113.65	118.60
53	BA	2340	A	C5-C6-N1	8.26	121.83	117.70
21	AA	794	A	C4-C5-C6	-8.25	112.87	117.00
53	BA	216	A	N1-C6-N6	-8.25	113.65	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	907	A	C5-C6-N1	8.25	121.83	117.70
53	BA	204	A	C5-C6-N1	8.25	121.83	117.70
53	BA	1156	A	C5-C6-N1	8.25	121.83	117.70
53	BA	1565	C	O4'-C1'-N1	8.25	114.80	108.20
53	BA	1626	A	C5-C6-N1	8.25	121.82	117.70
21	AA	363	A	N1-C6-N6	-8.24	113.65	118.60
53	BA	2406	A	O4'-C1'-N9	8.24	114.80	108.20
53	BA	2452	C	N3-C2-O2	-8.24	116.13	121.90
53	BA	2154	A	N1-C6-N6	-8.24	113.66	118.60
53	BA	1126	A	N1-C6-N6	-8.24	113.66	118.60
53	BA	2376	A	C5-C6-N1	8.24	121.82	117.70
21	AA	1446	A	N1-C6-N6	-8.23	113.66	118.60
53	BA	1175	A	N1-C6-N6	-8.23	113.66	118.60
53	BA	2388	A	C5-C6-N1	8.23	121.81	117.70
53	BA	492	A	N1-C6-N6	-8.23	113.66	118.60
53	BA	2867	G	O4'-C1'-N9	8.23	114.78	108.20
21	AA	1037	C	N3-C2-O2	-8.22	116.14	121.90
53	BA	920	A	N1-C6-N6	-8.22	113.67	118.60
53	BA	1046	A	C5-C6-N1	8.22	121.81	117.70
53	BA	1553	A	N1-C6-N6	-8.22	113.67	118.60
53	BA	2872	A	N1-C6-N6	-8.22	113.67	118.60
53	BA	794	A	C5-C6-N1	8.22	121.81	117.70
24	BC	62	ARG	NE-CZ-NH1	8.22	124.41	120.30
53	BA	1809	A	N1-C6-N6	-8.21	113.67	118.60
53	BA	2412	A	N1-C6-N6	-8.21	113.67	118.60
21	AA	1447	A	C5-C6-N1	8.21	121.81	117.70
53	BA	265	A	N1-C6-N6	-8.21	113.67	118.60
53	BA	1084	A	N1-C6-N6	-8.21	113.67	118.60
53	BA	1077	A	N1-C6-N6	-8.21	113.67	118.60
21	AA	262	A	C4-C5-C6	-8.21	112.90	117.00
21	AA	1465	A	C5-C6-N1	8.21	121.81	117.70
53	BA	844	A	C5-C6-N1	8.21	121.81	117.70
21	AA	298	A	N1-C6-N6	-8.21	113.68	118.60
21	AA	673	A	N1-C6-N6	-8.21	113.68	118.60
53	BA	53	A	C5-C6-N1	8.21	121.80	117.70
53	BA	1508	A	C5-C6-N1	8.21	121.80	117.70
53	BA	1713	A	C4-C5-C6	-8.21	112.90	117.00
53	BA	2850	A	C4-C5-C6	-8.21	112.90	117.00
53	BA	599	A	N1-C6-N6	-8.21	113.68	118.60
21	AA	1109	C	N3-C2-O2	-8.20	116.16	121.90
21	AA	1378	C	N3-C2-O2	-8.20	116.16	121.90
53	BA	2764	A	N1-C6-N6	-8.20	113.68	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1048	A	C4-C5-C6	-8.20	112.90	117.00
53	BA	2117	A	O4'-C1'-N9	8.20	114.76	108.20
21	AA	1278	G	N3-C2-N2	-8.19	114.16	119.90
53	BA	749	A	N1-C6-N6	-8.19	113.68	118.60
53	BA	1534	U	O4'-C1'-N1	8.19	114.75	108.20
53	BA	2432	A	N1-C6-N6	-8.20	113.68	118.60
53	BA	2766	A	N1-C6-N6	-8.19	113.68	118.60
53	BA	2459	A	N1-C6-N6	-8.19	113.68	118.60
21	AA	1271	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	130	A	C5-C6-N1	8.19	121.80	117.70
53	BA	1039	A	C4-C5-C6	-8.19	112.91	117.00
21	AA	1441	A	C5-C6-N1	8.19	121.79	117.70
53	BA	1077	A	C4-C5-C6	-8.19	112.91	117.00
53	BA	1894	C	N3-C2-O2	-8.19	116.17	121.90
53	BA	2776	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	865	A	C4-C5-C6	-8.19	112.91	117.00
53	BA	1328	A	C5-C6-N1	8.19	121.79	117.70
21	AA	243	A	C4-C5-C6	-8.18	112.91	117.00
53	BA	721	A	C5-C6-N1	8.18	121.79	117.70
53	BA	1095	A	C5-C6-N1	8.18	121.79	117.70
53	BA	1580	A	C5-C6-N1	8.18	121.79	117.70
53	BA	1713	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	228	A	N1-C6-N6	-8.18	113.69	118.60
37	BP	61	ARG	NE-CZ-NH1	8.18	124.39	120.30
53	BA	2670	A	N1-C6-N6	-8.17	113.70	118.60
3	AD	114	ARG	NE-CZ-NH1	8.17	124.39	120.30
9	AJ	9	ARG	NE-CZ-NH1	8.17	124.38	120.30
21	AA	621	A	C5-C6-N1	8.17	121.78	117.70
53	BA	1129	A	N1-C6-N6	-8.17	113.70	118.60
53	BA	2646	C	N3-C2-O2	-8.17	116.18	121.90
21	AA	1157	A	C5-C6-N1	8.16	121.78	117.70
53	BA	861	A	C5-C6-N1	8.16	121.78	117.70
54	BB	29	A	C4-C5-C6	-8.16	112.92	117.00
21	AA	1044	A	C5-C6-N1	8.16	121.78	117.70
21	AA	1246	A	C4-C5-C6	-8.16	112.92	117.00
53	BA	2173	A	N1-C6-N6	-8.16	113.70	118.60
53	BA	119	A	O4'-C1'-N9	8.16	114.73	108.20
53	BA	2217	G	O4'-C1'-N9	8.16	114.73	108.20
53	BA	817	C	N3-C2-O2	-8.16	116.19	121.90
53	BA	1378	A	C5-C6-N1	8.16	121.78	117.70
21	AA	913	A	C5-C6-N1	8.15	121.78	117.70
35	BN	22	ARG	NE-CZ-NH1	8.15	124.38	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1069	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	253	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	765	G	O4'-C1'-N9	8.15	114.72	108.20
21	AA	1227	A	C5-C6-N1	8.15	121.78	117.70
21	AA	1269	A	C5-C6-N1	8.15	121.77	117.70
53	BA	139	U	O4'-C1'-N1	8.15	114.72	108.20
53	BA	1570	A	N1-C6-N6	-8.15	113.71	118.60
53	BA	2868	A	C5-C6-N1	8.15	121.77	117.70
21	AA	1311	A	C4-C5-C6	-8.14	112.93	117.00
21	AA	1456	A	C5-C6-N1	8.14	121.77	117.70
53	BA	920	A	C5-C6-N1	8.14	121.77	117.70
21	AA	1014	A	N1-C6-N6	-8.14	113.72	118.60
53	BA	244	A	N1-C6-N6	-8.14	113.72	118.60
53	BA	572	A	C5-C6-N1	8.14	121.77	117.70
53	BA	2077	A	C5-C6-N1	8.14	121.77	117.70
53	BA	1393	A	C5-C6-N1	8.14	121.77	117.70
21	AA	313	A	N1-C6-N6	-8.13	113.72	118.60
53	BA	118	A	N1-C6-N6	-8.14	113.72	118.60
53	BA	1039	A	C5-C6-N1	8.14	121.77	117.70
53	BA	547	A	C4-C5-C6	-8.13	112.93	117.00
53	BA	1701	A	N1-C6-N6	-8.13	113.72	118.60
53	BA	2547	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	622	A	N1-C6-N6	-8.13	113.72	118.60
53	BA	320	A	N1-C6-N6	-8.13	113.72	118.60
53	BA	705	A	C5-C6-N1	8.13	121.77	117.70
10	AK	55	ARG	NE-CZ-NH2	8.13	124.37	120.30
22	A1	38	A	C4-C5-C6	-8.13	112.93	117.00
53	BA	1885	A	C5-C6-N1	8.13	121.77	117.70
53	BA	2169	A	C5-C6-N1	8.13	121.77	117.70
53	BA	2797	U	O4'-C1'-N1	8.13	114.71	108.20
53	BA	2823	A	N1-C6-N6	-8.13	113.72	118.60
53	BA	1815	A	C4-C5-C6	-8.13	112.94	117.00
53	BA	1639	C	N3-C2-O2	-8.12	116.21	121.90
53	BA	2211	A	C4-C5-C6	-8.12	112.94	117.00
6	AG	101	ARG	NE-CZ-NH1	8.12	124.36	120.30
53	BA	2573	C	N3-C2-O2	-8.12	116.22	121.90
53	BA	608	A	N1-C6-N6	-8.12	113.73	118.60
53	BA	2020	A	C5-C6-N1	8.12	121.76	117.70
53	BA	2090	A	N1-C6-N6	-8.12	113.73	118.60
53	BA	38	A	C5-C6-N1	8.12	121.76	117.70
53	BA	586	A	N1-C6-N6	-8.12	113.73	118.60
53	BA	2114	A	C5-C6-N1	8.12	121.76	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2266	A	C5-C6-N1	8.11	121.76	117.70
21	AA	935	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	1225	A	C5-C6-N1	8.11	121.76	117.70
53	BA	195	A	C4-C5-C6	-8.11	112.95	117.00
53	BA	541	A	C4-C5-C6	-8.11	112.95	117.00
21	AA	1246	A	C5-C6-N1	8.10	121.75	117.70
53	BA	1739	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	807	A	N1-C6-N6	-8.10	113.74	118.60
53	BA	1000	A	N1-C6-N6	-8.10	113.74	118.60
53	BA	1722	A	N1-C6-N6	-8.10	113.74	118.60
28	BG	151	ARG	NE-CZ-NH1	8.10	124.35	120.30
53	BA	265	A	C4-C5-C6	-8.10	112.95	117.00
53	BA	861	A	C4-C5-C6	-8.10	112.95	117.00
21	AA	197	A	C4-C5-C6	-8.09	112.95	117.00
21	AA	414	A	C5-C6-N1	8.09	121.75	117.70
21	AA	743	A	N1-C6-N6	-8.09	113.74	118.60
42	BU	81	ARG	NE-CZ-NH1	8.09	124.35	120.30
53	BA	2211	A	C5-C6-N1	8.09	121.75	117.70
53	BA	1044	C	N3-C2-O2	-8.09	116.24	121.90
53	BA	1451	C	N1-C2-O2	8.09	123.75	118.90
53	BA	2327	A	C5-C6-N1	8.09	121.74	117.70
21	AA	560	A	C5-C6-N1	8.09	121.74	117.70
53	BA	554	U	O4'-C1'-N1	8.09	114.67	108.20
53	BA	1503	A	N1-C6-N6	-8.09	113.75	118.60
53	BA	2483	C	N3-C2-O2	-8.08	116.24	121.90
53	BA	795	C	N3-C2-O2	-8.08	116.24	121.90
53	BA	2572	A	C5-C6-N1	8.08	121.74	117.70
53	BA	829	A	C5-C6-N1	8.08	121.74	117.70
53	BA	2214	C	N3-C2-O2	-8.08	116.24	121.90
53	BA	1728	C	N3-C2-O2	-8.08	116.25	121.90
21	AA	1008	U	O4'-C1'-N1	8.07	114.66	108.20
53	BA	282	A	N1-C6-N6	-8.07	113.76	118.60
53	BA	1912	A	C5-C6-N1	8.07	121.74	117.70
53	BA	1705	A	C5-C6-N1	8.07	121.74	117.70
15	AP	25	ARG	NE-CZ-NH2	8.07	124.33	120.30
21	AA	162	A	C5-C6-N1	8.07	121.74	117.70
21	AA	1005	A	C5-C6-N1	8.07	121.74	117.70
21	AA	65	A	C5-C6-N1	8.07	121.73	117.70
21	AA	119	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	702	A	N1-C6-N6	-8.07	113.76	118.60
53	BA	507	A	C5-C6-N1	8.07	121.73	117.70
53	BA	142	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(^{o})	Ideal(^{o})
54	BB	115	A	C5-C6-N1	8.07	121.73	117.70
53	BA	1029	A	C5-C6-N1	8.06	121.73	117.70
53	BA	2247	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	1163	A	C5-C6-N1	8.06	121.73	117.70
21	AA	371	A	C5-C6-N1	8.06	121.73	117.70
53	BA	1046	A	O4'-C1'-N9	8.06	114.65	108.20
53	BA	1871	A	O4'-C1'-N9	8.06	114.65	108.20
54	BB	50	A	C5-C6-N1	8.06	121.73	117.70
21	AA	109	A	C5-C6-N1	8.05	121.73	117.70
53	BA	2541	A	C5-C6-N1	8.05	121.73	117.70
21	AA	478	A	N1-C6-N6	-8.05	113.77	118.60
53	BA	1204	A	O4'-C1'-N9	8.05	114.64	108.20
53	BA	1532	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	994	A	C5-C6-N1	8.05	121.72	117.70
21	AA	1352	C	N3-C2-O2	-8.05	116.27	121.90
21	AA	535	A	C5-C6-N1	8.05	121.72	117.70
53	BA	945	A	C4-C5-C6	-8.05	112.98	117.00
21	AA	546	A	C5-C6-N1	8.04	121.72	117.70
21	AA	649	A	N1-C6-N6	-8.04	113.78	118.60
53	BA	1678	A	N1-C6-N6	-8.04	113.78	118.60
53	BA	2191	A	C5-C6-N1	8.04	121.72	117.70
53	BA	1535	A	C5-C6-N1	8.04	121.72	117.70
31	BJ	27	ARG	NE-CZ-NH2	-8.04	116.28	120.30
53	BA	2613	U	O4'-C1'-N1	8.03	114.63	108.20
53	BA	2781	A	C5-C6-N1	8.03	121.72	117.70
54	BB	35	C	N3-C2-O2	-8.04	116.28	121.90
11	AL	30	ARG	NE-CZ-NH1	8.03	124.32	120.30
53	BA	219	A	C5-C6-N1	8.03	121.72	117.70
21	AA	815	A	C4-C5-C6	-8.03	112.99	117.00
21	AA	1213	A	C5-C6-N1	8.03	121.71	117.70
53	BA	1073	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	1081	A	N1-C6-N6	-8.03	113.78	118.60
53	BA	466	A	C5-C6-N1	8.03	121.71	117.70
53	BA	2031	A	C5-C6-N1	8.03	121.71	117.70
53	BA	99	U	O4'-C1'-N1	8.02	114.62	108.20
53	BA	1077	A	C5-C6-N1	8.02	121.71	117.70
21	AA	907	A	N1-C6-N6	-8.02	113.79	118.60
46	BY	52	ARG	NE-CZ-NH1	8.02	124.31	120.30
53	BA	1502	A	C4-C5-C6	-8.02	112.99	117.00
53	BA	2060	A	N1-C6-N6	-8.02	113.79	118.60
53	BA	1205	A	C5-C6-N1	8.02	121.71	117.70
53	BA	1821	A	N1-C6-N6	-8.02	113.79	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2850	A	C5-C6-N1	8.02	121.71	117.70
15	AP	31	ARG	NE-CZ-NH1	8.01	124.31	120.30
21	AA	451	A	C5-C6-N1	8.01	121.71	117.70
36	BO	13	ARG	NE-CZ-NH1	8.01	124.31	120.30
52	B4	4	ARG	NE-CZ-NH1	8.01	124.31	120.30
53	BA	1534	U	N3-C2-O2	-8.01	116.59	122.20
13	AN	24	ARG	NE-CZ-NH1	8.01	124.30	120.30
21	AA	363	A	C4-C5-C6	-8.01	113.00	117.00
53	BA	2799	A	O4'-C1'-N9	8.01	114.61	108.20
53	BA	1739	A	C5-C6-N1	8.01	121.70	117.70
21	AA	315	A	N1-C6-N6	-8.01	113.80	118.60
53	BA	1966	A	C5-C6-N1	8.01	121.70	117.70
53	BA	2813	A	C5-C6-N1	8.00	121.70	117.70
53	BA	1147	A	C5-C6-N1	8.00	121.70	117.70
53	BA	1596	A	C5-C6-N1	8.00	121.70	117.70
53	BA	371	A	N1-C6-N6	-7.99	113.80	118.60
53	BA	2422	C	N3-C2-O2	-7.99	116.30	121.90
21	AA	493	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	1518	A	C4-C5-C6	-7.99	113.00	117.00
53	BA	460	A	C5-C6-N1	7.99	121.69	117.70
53	BA	1194	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	415	A	O4'-C1'-N9	7.99	114.59	108.20
21	AA	1336	C	O4'-C1'-N1	7.99	114.59	108.20
21	AA	1503	A	C5-C6-N1	7.99	121.69	117.70
48	B0	12	ARG	NE-CZ-NH2	7.99	124.29	120.30
53	BA	936	A	C5-C6-N1	7.99	121.69	117.70
53	BA	1755	A	C5-C6-N1	7.99	121.69	117.70
7	AH	76	ARG	NE-CZ-NH1	7.99	124.29	120.30
53	BA	265	A	C5-C6-N1	7.99	121.69	117.70
2	AC	53	ARG	NE-CZ-NH1	7.98	124.29	120.30
21	AA	892	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	768	A	C5-C6-N1	7.98	121.69	117.70
53	BA	2281	A	N1-C6-N6	-7.98	113.81	118.60
53	BA	2758	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	1285	A	C4-C5-C6	-7.98	113.01	117.00
53	BA	155	A	N1-C6-N6	-7.98	113.81	118.60
53	BA	2534	A	N1-C6-N6	-7.98	113.81	118.60
53	BA	1899	A	C5-C6-N1	7.98	121.69	117.70
21	AA	131	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	1476	A	N1-C6-N6	-7.97	113.82	118.60
53	BA	2439	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	845	A	C5-C6-N1	7.97	121.68	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1402	C	N3-C2-O2	-7.97	116.32	121.90
24	BC	51	ARG	NE-CZ-NH2	7.97	124.28	120.30
53	BA	531	C	O4'-C1'-N1	7.97	114.57	108.20
21	AA	303	A	C5-C6-N1	7.96	121.68	117.70
21	AA	913	A	C4-C5-C6	-7.96	113.02	117.00
53	BA	28	A	C5-C6-N1	7.96	121.68	117.70
53	BA	1650	A	C5-C6-N1	7.96	121.68	117.70
53	BA	251	A	N1-C6-N6	-7.96	113.82	118.60
13	AN	85	ARG	NE-CZ-NH1	7.96	124.28	120.30
21	AA	7	A	N1-C6-N6	-7.96	113.82	118.60
21	AA	958	A	C4-C5-C6	-7.96	113.02	117.00
53	BA	1304	A	N1-C6-N6	-7.96	113.82	118.60
53	BA	1808	A	N1-C6-N6	-7.96	113.82	118.60
53	BA	2682	A	N1-C6-N6	-7.96	113.82	118.60
53	BA	1395	A	C5-C6-N1	7.96	121.68	117.70
21	AA	303	A	C4-C5-C6	-7.96	113.02	117.00
21	AA	983	A	C4-C5-C6	-7.96	113.02	117.00
53	BA	428	A	C5-C6-N1	7.96	121.68	117.70
53	BA	941	A	C5-C6-N1	7.96	121.68	117.70
53	BA	2051	A	C5-C6-N1	7.96	121.68	117.70
53	BA	2411	A	N1-C6-N6	-7.96	113.83	118.60
53	BA	2851	A	N1-C6-N6	-7.96	113.83	118.60
53	BA	2823	A	C5-C6-N1	7.96	121.68	117.70
53	BA	1927	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	1340	A	N1-C6-N6	-7.95	113.83	118.60
53	BA	2274	A	C4-C5-C6	-7.95	113.03	117.00
53	BA	1899	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	1236	A	C4-C5-C6	-7.95	113.03	117.00
53	BA	311	A	C5-C6-N1	7.95	121.67	117.70
53	BA	505	A	N1-C6-N6	-7.95	113.83	118.60
53	BA	544	C	N3-C2-O2	-7.95	116.34	121.90
53	BA	347	A	N1-C6-N6	-7.94	113.83	118.60
53	BA	299	A	N1-C6-N6	-7.94	113.83	118.60
53	BA	1877	A	N1-C6-N6	-7.94	113.83	118.60
21	AA	1042	A	C5-C6-N1	7.94	121.67	117.70
22	A1	38	A	C5-C6-N1	7.94	121.67	117.70
52	B4	12	ARG	NE-CZ-NH2	7.94	124.27	120.30
53	BA	176	A	C4-C5-C6	-7.94	113.03	117.00
21	AA	937	A	C5-C6-N1	7.94	121.67	117.70
21	AA	1214	C	O4'-C1'-N1	7.94	114.55	108.20
53	BA	866	A	C4-C5-C6	-7.94	113.03	117.00
53	BA	854	C	N3-C2-O2	-7.94	116.34	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BB	91	C	O4'-C1'-N1	7.94	114.55	108.20
21	AA	1170	A	N1-C6-N6	-7.93	113.84	118.60
53	BA	481	G	O4'-C1'-N9	7.93	114.55	108.20
53	BA	1626	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	1197	A	N1-C6-N6	-7.93	113.84	118.60
33	BL	48	ARG	NE-CZ-NH1	7.93	124.27	120.30
53	BA	710	U	O4'-C1'-N1	7.93	114.54	108.20
53	BA	844	A	N1-C6-N6	-7.93	113.84	118.60
53	BA	1602	U	O4'-C1'-N1	7.93	114.54	108.20
53	BA	382	A	C4-C5-C6	-7.93	113.04	117.00
53	BA	2119	A	C4-C5-C6	-7.93	113.04	117.00
53	BA	95	A	N1-C6-N6	-7.93	113.84	118.60
19	AT	24	ARG	NE-CZ-NH1	7.92	124.26	120.30
21	AA	1492	A	C5-C6-N1	7.92	121.66	117.70
22	A1	76	A	C5-C6-N1	7.92	121.66	117.70
53	BA	2114	A	C4-C5-C6	-7.92	113.04	117.00
21	AA	59	A	C5-C6-N1	7.92	121.66	117.70
21	AA	607	A	C5-C6-N1	7.92	121.66	117.70
21	AA	1299	A	N1-C6-N6	-7.92	113.85	118.60
21	AA	196	A	C5-C6-N1	7.92	121.66	117.70
53	BA	2501	C	N3-C2-O2	-7.92	116.36	121.90
54	BB	108	A	N1-C6-N6	-7.92	113.85	118.60
24	BC	79	ARG	NE-CZ-NH1	7.92	124.26	120.30
53	BA	1815	A	C5-C6-N1	7.92	121.66	117.70
53	BA	2171	A	N1-C6-N6	-7.92	113.85	118.60
53	BA	1143	A	C4-C5-C6	-7.91	113.04	117.00
53	BA	44	A	C4-C5-C6	-7.91	113.05	117.00
53	BA	1978	A	C5-C6-N1	7.91	121.66	117.70
21	AA	19	A	C5-C6-N1	7.91	121.66	117.70
21	AA	325	A	N1-C6-N6	-7.91	113.86	118.60
53	BA	804	A	C4-C5-C6	-7.91	113.05	117.00
53	BA	2082	A	N1-C6-N6	-7.91	113.86	118.60
21	AA	161	A	C5-C6-N1	7.91	121.65	117.70
53	BA	423	A	N1-C6-N6	-7.90	113.86	118.60
53	BA	1428	C	N3-C2-O2	-7.90	116.37	121.90
21	AA	1019	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1158	C	N1-C2-O2	7.90	123.64	118.90
53	BA	2778	A	N1-C6-N6	-7.90	113.86	118.60
53	BA	1135	C	N3-C2-O2	-7.90	116.37	121.90
55	B5	7	ARG	NE-CZ-NH1	7.90	124.25	120.30
21	AA	572	A	C5-C6-N1	7.89	121.65	117.70
53	BA	1230	A	C5-C6-N1	7.89	121.65	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1634	A	N1-C6-N6	-7.89	113.86	118.60
21	AA	726	C	N3-C2-O2	-7.89	116.38	121.90
53	BA	644	A	N1-C6-N6	-7.89	113.87	118.60
53	BA	1304	A	C4-C5-C6	-7.89	113.06	117.00
21	AA	1394	A	C5-C6-N1	7.89	121.64	117.70
21	AA	1117	A	N1-C6-N6	-7.88	113.87	118.60
53	BA	332	A	C5-C6-N1	7.88	121.64	117.70
53	BA	1226	A	N1-C6-N6	-7.88	113.87	118.60
53	BA	574	A	C5-C6-N1	7.88	121.64	117.70
53	BA	761	A	N1-C6-N6	-7.88	113.87	118.60
53	BA	1488	C	N3-C2-O2	-7.88	116.39	121.90
21	AA	777	A	C5-C6-N1	7.88	121.64	117.70
53	BA	2893	A	C5-C6-N1	7.88	121.64	117.70
21	AA	487	A	N1-C6-N6	-7.88	113.88	118.60
53	BA	2887	A	N1-C6-N6	-7.88	113.88	118.60
27	BF	101	ARG	NE-CZ-NH1	7.87	124.24	120.30
53	BA	1155	A	N1-C6-N6	-7.87	113.88	118.60
53	BA	2888	C	O4'-C1'-N1	7.87	114.50	108.20
53	BA	973	A	C4-C5-C6	-7.87	113.06	117.00
21	AA	749	A	C4-C5-C6	-7.87	113.06	117.00
53	BA	207	A	C5-C6-N1	7.87	121.64	117.70
21	AA	781	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	1082	A	N1-C6-N6	-7.87	113.88	118.60
53	BA	391	A	C5-C6-N1	7.87	121.63	117.70
53	BA	877	A	C4-C5-C6	-7.87	113.07	117.00
3	AD	61	ARG	NE-CZ-NH1	7.86	124.23	120.30
53	BA	249	C	N3-C2-O2	-7.86	116.40	121.90
53	BA	1470	A	C5-C6-N1	7.86	121.63	117.70
53	BA	1794	A	C5-C6-N1	7.86	121.63	117.70
21	AA	583	A	C4-C5-C6	-7.86	113.07	117.00
53	BA	342	A	N1-C6-N6	-7.86	113.88	118.60
53	BA	1069	A	O4'-C1'-N9	7.86	114.49	108.20
53	BA	2804	U	O4'-C1'-N1	7.86	114.49	108.20
21	AA	274	A	C5-C6-N1	7.86	121.63	117.70
53	BA	480	A	N1-C6-N6	-7.86	113.88	118.60
21	AA	316	C	N3-C2-O2	-7.86	116.40	121.90
21	AA	595	A	N1-C6-N6	-7.86	113.89	118.60
53	BA	101	A	O4'-C1'-N9	7.85	114.48	108.20
53	BA	361	G	O4'-C1'-N9	7.85	114.48	108.20
54	BB	50	A	C4-C5-C6	-7.85	113.07	117.00
47	BZ	30	ARG	NE-CZ-NH1	7.85	124.23	120.30
53	BA	819	A	N1-C6-N6	-7.85	113.89	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2062	A	C4-C5-C6	-7.85	113.07	117.00
53	BA	2062	A	N1-C6-N6	-7.85	113.89	118.60
54	BB	53	A	C5-C6-N1	7.85	121.63	117.70
12	AM	70	ARG	NE-CZ-NH2	7.85	124.22	120.30
55	B5	162	ARG	NE-CZ-NH1	7.85	124.22	120.30
53	BA	2418	A	C5-C6-N1	7.85	121.62	117.70
53	BA	2281	A	C4-C5-C6	-7.84	113.08	117.00
53	BA	2328	A	C5-C6-N1	7.84	121.62	117.70
53	BA	2417	C	N3-C2-O2	-7.84	116.41	121.90
53	BA	165	A	C4-C5-C6	-7.84	113.08	117.00
21	AA	756	C	N3-C2-O2	-7.84	116.41	121.90
21	AA	1493	A	N1-C6-N6	-7.84	113.89	118.60
53	BA	878	A	C5-C6-N1	7.84	121.62	117.70
53	BA	2273	A	C5-C6-N1	7.84	121.62	117.70
53	BA	34	U	O4'-C1'-N1	7.84	114.47	108.20
21	AA	1395	C	N3-C2-O2	-7.84	116.41	121.90
24	BC	166	ARG	NE-CZ-NH1	7.84	124.22	120.30
38	BQ	57	ARG	NE-CZ-NH1	7.84	124.22	120.30
53	BA	1626	A	C4-C5-C6	-7.84	113.08	117.00
21	AA	250	A	C5-C6-N1	7.83	121.62	117.70
21	AA	327	A	C5-C6-N1	7.83	121.62	117.70
53	BA	362	A	N1-C6-N6	-7.83	113.90	118.60
53	BA	2297	A	N1-C6-N6	-7.83	113.90	118.60
53	BA	2440	C	N3-C2-O2	-7.83	116.42	121.90
21	AA	549	C	N3-C2-O2	-7.83	116.42	121.90
21	AA	635	A	C5-C6-N1	7.83	121.61	117.70
21	AA	1333	A	C5-C6-N1	7.83	121.61	117.70
21	AA	238	A	C5-C6-N1	7.83	121.61	117.70
9	AJ	5	ARG	NE-CZ-NH1	7.82	124.21	120.30
53	BA	2781	A	N1-C6-N6	-7.82	113.91	118.60
24	BC	155	ARG	NE-CZ-NH1	7.82	124.21	120.30
53	BA	1243	C	N3-C2-O2	-7.82	116.43	121.90
53	BA	2058	A	C5-C6-N1	7.82	121.61	117.70
55	B5	53	ARG	NE-CZ-NH2	-7.82	116.39	120.30
53	BA	1073	A	C4-C5-C6	-7.82	113.09	117.00
21	AA	1350	A	N1-C6-N6	-7.82	113.91	118.60
53	BA	673	C	N3-C2-O2	-7.81	116.43	121.90
53	BA	1593	A	N1-C6-N6	-7.81	113.91	118.60
21	AA	975	A	C5-C6-N1	7.81	121.61	117.70
53	BA	2241	A	N1-C6-N6	-7.81	113.91	118.60
53	BA	912	C	N3-C2-O2	-7.81	116.43	121.90
53	BA	64	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(^{o})	Ideal(^{o})
53	BA	340	A	C4-C5-C6	-7.81	113.09	117.00
53	BA	1365	A	C5-C6-N1	7.81	121.61	117.70
53	BA	1570	A	C5-C6-N1	7.81	121.61	117.70
53	BA	1606	C	O4'-C1'-N1	7.81	114.45	108.20
53	BA	715	A	N1-C6-N6	-7.81	113.92	118.60
53	BA	1475	G	O4'-C1'-N9	7.81	114.45	108.20
21	AA	600	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	890	G	O4'-C1'-N9	7.80	114.44	108.20
53	BA	2497	A	N1-C6-N6	-7.80	113.92	118.60
54	BB	109	A	C5-C6-N1	7.80	121.60	117.70
53	BA	678	C	N3-C2-O2	-7.80	116.44	121.90
53	BA	1566	A	N1-C6-N6	-7.80	113.92	118.60
53	BA	722	A	N1-C6-N6	-7.80	113.92	118.60
53	BA	2651	C	N3-C2-O2	-7.80	116.44	121.90
53	BA	1900	A	C4-C5-C6	-7.80	113.10	117.00
53	BA	1785	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	1219	A	C5-C6-N1	7.80	121.60	117.70
53	BA	1522	A	C5-C6-N1	7.80	121.60	117.70
53	BA	1899	A	C4-C5-C6	-7.80	113.10	117.00
21	AA	1349	A	N1-C6-N6	-7.79	113.92	118.60
53	BA	2634	A	C4-C5-C6	-7.79	113.10	117.00
21	AA	315	A	C5-C6-N1	7.79	121.60	117.70
53	BA	119	A	C5-C6-N1	7.79	121.60	117.70
53	BA	1558	C	N3-C2-O2	-7.79	116.45	121.90
53	BA	216	A	C5-C6-N1	7.79	121.59	117.70
21	AA	973	G	O4'-C1'-N9	7.79	114.43	108.20
24	BC	237	ARG	NE-CZ-NH2	-7.79	116.41	120.30
53	BA	2761	A	C5-C6-N1	7.79	121.59	117.70
53	BA	1027	A	C5-C6-N1	7.79	121.59	117.70
53	BA	1098	A	N1-C6-N6	-7.79	113.93	118.60
53	BA	1749	A	C5-C6-N1	7.79	121.59	117.70
53	BA	196	A	O4'-C1'-N9	7.78	114.43	108.20
53	BA	925	A	C4-C5-C6	-7.78	113.11	117.00
53	BA	1000	A	C4-C5-C6	-7.78	113.11	117.00
53	BA	1690	A	C5-C6-N1	7.78	121.59	117.70
53	BA	507	A	C4-C5-C6	-7.78	113.11	117.00
53	BA	1433	A	C5-C6-N1	7.78	121.59	117.70
53	BA	2037	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	1338	G	N3-C2-N2	-7.78	114.46	119.90
53	BA	104	A	C5-C6-N1	7.78	121.59	117.70
53	BA	2734	A	C5-C6-N1	7.78	121.59	117.70
53	BA	1454	C	N1-C2-O2	7.78	123.57	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1144	A	N1-C6-N6	-7.77	113.94	118.60
53	BA	1597	A	C5-C6-N1	7.77	121.59	117.70
53	BA	1237	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	1157	A	C4-C5-C6	-7.77	113.11	117.00
29	BH	97	ARG	NE-CZ-NH1	7.77	124.18	120.30
53	BA	1347	A	C5-C6-N1	7.77	121.58	117.70
53	BA	2313	C	N3-C2-O2	-7.77	116.46	121.90
53	BA	2577	A	C5-C6-N1	7.77	121.58	117.70
21	AA	1285	A	C5-C6-N1	7.76	121.58	117.70
21	AA	994	A	C4-C5-C6	-7.76	113.12	117.00
53	BA	1298	C	N3-C2-O2	-7.76	116.47	121.90
21	AA	523	A	N1-C6-N6	-7.76	113.94	118.60
53	BA	324	A	C4-C5-C6	-7.76	113.12	117.00
53	BA	556	A	C5-C6-N1	7.76	121.58	117.70
53	BA	673	C	O4'-C1'-N1	7.76	114.41	108.20
53	BA	2434	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	841	C	N3-C2-O2	-7.76	116.47	121.90
21	AA	1117	A	C5-C6-N1	7.76	121.58	117.70
53	BA	1365	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	767	A	C4-C5-C6	-7.76	113.12	117.00
21	AA	1339	A	C5-C6-N1	7.76	121.58	117.70
21	AA	1501	C	N3-C2-O2	-7.76	116.47	121.90
53	BA	63	A	C5-C6-N1	7.76	121.58	117.70
53	BA	2088	A	C4-C5-C6	-7.76	113.12	117.00
53	BA	384	A	C5-C6-N1	7.75	121.58	117.70
53	BA	1638	C	N3-C2-O2	-7.75	116.47	121.90
21	AA	1111	A	C4-C5-C6	-7.75	113.12	117.00
53	BA	2020	A	N1-C6-N6	-7.75	113.95	118.60
53	BA	2232	C	O4'-C1'-N1	7.75	114.40	108.20
21	AA	1038	C	N3-C2-O2	-7.75	116.47	121.90
53	BA	191	A	C5-C6-N1	7.75	121.58	117.70
53	BA	1705	A	N1-C6-N6	-7.75	113.95	118.60
53	BA	750	A	C5-C6-N1	7.75	121.57	117.70
53	BA	1168	G	N1-C6-O6	-7.75	115.25	119.90
53	BA	2339	C	O4'-C1'-N1	7.75	114.40	108.20
53	BA	160	A	C4-C5-C6	-7.75	113.13	117.00
53	BA	2634	A	C5-C6-N1	7.75	121.57	117.70
53	BA	205	G	O4'-C1'-N9	7.74	114.39	108.20
53	BA	2426	A	C4-C5-C6	-7.74	113.13	117.00
40	BS	18	ARG	NE-CZ-NH1	7.74	124.17	120.30
53	BA	965	C	N3-C2-O2	-7.74	116.48	121.90
21	AA	695	A	C4-C5-C6	-7.74	113.13	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	44	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	1374	A	C5-C6-N1	7.74	121.57	117.70
53	BA	1607	C	N3-C2-O2	-7.74	116.48	121.90
22	A1	41	A	C5-C6-N1	7.74	121.57	117.70
53	BA	165	A	C5-C6-N1	7.74	121.57	117.70
53	BA	590	A	N1-C6-N6	-7.74	113.96	118.60
53	BA	1117	C	N3-C2-O2	-7.74	116.48	121.90
22	A1	76	A	C4-C5-C6	-7.73	113.13	117.00
53	BA	592	A	C5-C6-N1	7.73	121.57	117.70
21	AA	878	A	C5-C6-N1	7.73	121.57	117.70
53	BA	2711	A	C5-C6-N1	7.73	121.57	117.70
21	AA	1430	A	C4-C5-C6	-7.73	113.14	117.00
53	BA	2134	A	C5-C6-N1	7.73	121.56	117.70
53	BA	2147	A	C4-C5-C6	-7.73	113.13	117.00
53	BA	990	A	N1-C6-N6	-7.73	113.96	118.60
53	BA	1262	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	1227	A	O4'-C1'-N9	7.73	114.38	108.20
22	A1	58	A	C5-C6-N1	7.73	121.56	117.70
53	BA	2183	A	C4-C5-C6	-7.73	113.14	117.00
53	BA	706	A	C4-C5-C6	-7.72	113.14	117.00
21	AA	1252	A	N1-C6-N6	-7.72	113.97	118.60
53	BA	382	A	C5-C6-N1	7.72	121.56	117.70
53	BA	2378	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	353	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	883	C	N3-C2-O2	-7.72	116.50	121.90
21	AA	967	C	N3-C2-O2	-7.72	116.50	121.90
53	BA	863	A	N1-C6-N6	-7.72	113.97	118.60
53	BA	19	A	N1-C6-N6	-7.72	113.97	118.60
53	BA	529	A	N1-C6-N6	-7.72	113.97	118.60
53	BA	2176	A	C4-C5-C6	-7.72	113.14	117.00
53	BA	1129	A	C5-C6-N1	7.71	121.56	117.70
53	BA	1803	A	N1-C6-N6	-7.71	113.97	118.60
53	BA	947	A	C5-C6-N1	7.71	121.56	117.70
53	BA	218	A	N1-C6-N6	-7.71	113.97	118.60
20	AU	16	ARG	NE-CZ-NH1	7.71	124.15	120.30
21	AA	1179	A	N1-C6-N6	-7.71	113.97	118.60
53	BA	1977	A	C5-C6-N1	7.71	121.55	117.70
21	AA	608	A	C5-C6-N1	7.71	121.55	117.70
53	BA	1342	A	C5-C6-N1	7.71	121.55	117.70
53	BA	294	A	C5-C6-N1	7.71	121.55	117.70
24	BC	216	ARG	NE-CZ-NH1	7.70	124.15	120.30
53	BA	1156	A	C4-C5-C6	-7.70	113.15	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2377	A	C5-C6-N1	7.70	121.55	117.70
21	AA	532	A	C5-C6-N1	7.70	121.55	117.70
53	BA	654	A	C5-C6-N1	7.70	121.55	117.70
21	AA	675	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	949	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	1000	A	N1-C6-N6	-7.70	113.98	118.60
20	AU	46	ARG	NE-CZ-NH1	7.70	124.15	120.30
21	AA	1111	A	C5-C6-N1	7.70	121.55	117.70
40	BS	95	ARG	NE-CZ-NH1	7.70	124.15	120.30
53	BA	1711	A	C4-C5-C6	-7.70	113.15	117.00
53	BA	2173	A	C5-C6-N1	7.70	121.55	117.70
53	BA	2453	A	C5-C6-N1	7.70	121.55	117.70
35	BN	30	ARG	NE-CZ-NH1	7.69	124.15	120.30
53	BA	10	A	C4-C5-C6	-7.69	113.15	117.00
53	BA	1708	C	N3-C2-O2	-7.69	116.52	121.90
21	AA	1502	A	O4'-C1'-N9	7.69	114.35	108.20
22	A1	69	A	N1-C6-N6	-7.69	113.98	118.60
53	BA	161	A	N1-C6-N6	-7.69	113.99	118.60
12	AM	112	ARG	NE-CZ-NH1	7.69	124.14	120.30
53	BA	863	A	C5-C6-N1	7.69	121.54	117.70
53	BA	2054	A	N1-C6-N6	-7.69	113.99	118.60
21	AA	1130	A	N1-C6-N6	-7.68	113.99	118.60
53	BA	1050	A	C5-C6-N1	7.68	121.54	117.70
53	BA	1810	A	C5-C6-N1	7.68	121.54	117.70
53	BA	2450	A	N1-C6-N6	-7.68	113.99	118.60
53	BA	449	A	C4-C5-C6	-7.68	113.16	117.00
53	BA	2359	C	N3-C2-O2	-7.68	116.52	121.90
21	AA	263	A	N1-C6-N6	-7.68	113.99	118.60
53	BA	2589	A	C5-C6-N1	7.68	121.54	117.70
21	AA	768	A	C4-C5-C6	-7.68	113.16	117.00
53	BA	2792	A	C5-C6-N1	7.68	121.54	117.70
53	BA	152	A	C5-C6-N1	7.68	121.54	117.70
21	AA	546	A	C4-C5-C6	-7.67	113.16	117.00
21	AA	878	A	C4-C5-C6	-7.67	113.16	117.00
53	BA	1327	A	C5-C6-N1	7.67	121.54	117.70
53	BA	1953	A	C5-C6-N1	7.67	121.54	117.70
21	AA	83	C	N3-C2-O2	-7.67	116.53	121.90
53	BA	876	C	N3-C2-O2	-7.67	116.53	121.90
53	BA	1103	A	C5-C6-N1	7.67	121.53	117.70
21	AA	309	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1319	A	N1-C6-N6	-7.67	114.00	118.60
53	BA	2670	A	C5-C6-N1	7.67	121.53	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1871	A	C5-C6-N1	7.67	121.53	117.70
53	BA	2771	C	N3-C2-O2	-7.67	116.53	121.90
21	AA	67	C	N1-C2-O2	7.66	123.50	118.90
21	AA	1456	A	N1-C6-N6	-7.66	114.00	118.60
21	AA	915	A	C5-C6-N1	7.66	121.53	117.70
21	AA	363	A	C5-C6-N1	7.66	121.53	117.70
53	BA	547	A	C5-C6-N1	7.66	121.53	117.70
53	BA	1570	A	C4-C5-C6	-7.66	113.17	117.00
53	BA	1728	C	N1-C2-O2	7.66	123.50	118.90
53	BA	1872	A	N1-C6-N6	-7.66	114.00	118.60
53	BA	2536	G	O4'-C1'-N9	7.66	114.33	108.20
53	BA	1009	A	N1-C6-N6	-7.66	114.01	118.60
53	BA	2478	A	C5-C6-N1	7.66	121.53	117.70
53	BA	2062	A	O4'-C1'-N9	7.66	114.32	108.20
53	BA	2314	A	C5-C6-N1	7.66	121.53	117.70
21	AA	162	A	N1-C6-N6	-7.65	114.01	118.60
53	BA	257	C	O4'-C1'-N1	7.65	114.32	108.20
21	AA	918	A	N1-C6-N6	-7.65	114.01	118.60
53	BA	1952	A	C5-C6-N1	7.65	121.53	117.70
53	BA	149	A	N1-C6-N6	-7.65	114.01	118.60
53	BA	1090	A	N1-C6-N6	-7.65	114.01	118.60
53	BA	1236	G	O4'-C1'-N9	7.65	114.32	108.20
21	AA	306	A	C5-C6-N1	7.65	121.52	117.70
33	BL	60	ARG	NE-CZ-NH1	7.65	124.12	120.30
53	BA	644	A	C5-C6-N1	7.65	121.52	117.70
53	BA	988	A	C5-C6-N1	7.64	121.52	117.70
21	AA	694	A	N1-C6-N6	-7.64	114.02	118.60
53	BA	126	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	412	A	C5-C6-N1	7.64	121.52	117.70
21	AA	640	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	1306	A	C5-C6-N1	7.64	121.52	117.70
53	BA	118	A	C5-C6-N1	7.64	121.52	117.70
53	BA	722	A	C5-C6-N1	7.64	121.52	117.70
53	BA	2860	A	C5-C6-N1	7.64	121.52	117.70
53	BA	2326	C	N3-C2-O2	-7.64	116.55	121.90
53	BA	346	A	C5-C6-N1	7.64	121.52	117.70
53	BA	1274	A	C5-C6-N1	7.64	121.52	117.70
21	AA	918	A	C5-C6-N1	7.63	121.52	117.70
48	B0	9	ARG	NE-CZ-NH2	7.63	124.12	120.30
53	BA	515	A	C5-C6-N1	7.63	121.52	117.70
53	BA	2498	C	O4'-C1'-N1	7.63	114.31	108.20
53	BA	1879	C	N3-C2-O2	-7.63	116.56	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	586	A	C5-C6-N1	7.63	121.52	117.70
53	BA	960	A	C5-C6-N1	7.63	121.52	117.70
53	BA	1403	A	N1-C6-N6	-7.63	114.02	118.60
53	BA	1745	A	N1-C6-N6	-7.63	114.02	118.60
53	BA	2476	A	C5-C6-N1	7.63	121.51	117.70
21	AA	825	A	C5-C6-N1	7.63	121.51	117.70
54	BB	46	A	C5-C6-N1	7.63	121.51	117.70
21	AA	629	A	C5-C6-N1	7.62	121.51	117.70
21	AA	816	A	C5-C6-N1	7.62	121.51	117.70
53	BA	1213	A	C4-C5-C6	-7.62	113.19	117.00
53	BA	1656	C	N3-C2-O2	-7.62	116.56	121.90
21	AA	1054	C	O4'-C1'-N1	7.62	114.30	108.20
53	BA	1143	A	C5-C6-N1	7.62	121.51	117.70
21	AA	432	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	1031	C	N1-C2-O2	7.62	123.47	118.90
53	BA	897	C	N3-C2-O2	-7.62	116.57	121.90
53	BA	2755	C	N3-C2-O2	-7.62	116.57	121.90
21	AA	28	A	C5-C6-N1	7.62	121.51	117.70
21	AA	468	A	C5-C6-N1	7.62	121.51	117.70
53	BA	888	C	N3-C2-O2	-7.62	116.57	121.90
21	AA	182	A	C5-C6-N1	7.62	121.51	117.70
53	BA	1434	A	C5-C6-N1	7.62	121.51	117.70
53	BA	2205	A	C5-C6-N1	7.62	121.51	117.70
21	AA	502	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	1510	C	N3-C2-O2	-7.61	116.57	121.90
53	BA	454	A	N1-C6-N6	-7.61	114.03	118.60
53	BA	2565	A	N1-C6-N6	-7.61	114.03	118.60
53	BA	1953	A	C4-C5-C6	-7.61	113.19	117.00
21	AA	1433	A	C5-C6-N1	7.61	121.51	117.70
53	BA	563	A	C5-C6-N1	7.61	121.50	117.70
53	BA	626	A	C5-C6-N1	7.61	121.50	117.70
34	BM	50	ARG	NE-CZ-NH1	7.61	124.10	120.30
53	BA	2287	A	N1-C6-N6	-7.61	114.03	118.60
50	B2	14	ARG	NE-CZ-NH1	7.61	124.10	120.30
53	BA	1315	C	N3-C2-O2	-7.61	116.57	121.90
53	BA	2248	C	N3-C2-O2	-7.61	116.58	121.90
21	AA	1327	C	N3-C2-O2	-7.61	116.58	121.90
53	BA	1233	C	N3-C2-O2	-7.61	116.58	121.90
53	BA	1287	A	C4-C5-C6	-7.61	113.20	117.00
53	BA	2430	A	C5-C6-N1	7.60	121.50	117.70
21	AA	188	C	N3-C2-O2	-7.60	116.58	121.90
21	AA	496	A	C5-C6-N1	7.60	121.50	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1876	A	N1-C6-N6	-7.60	114.04	118.60
25	BD	83	ARG	NE-CZ-NH1	7.60	124.10	120.30
53	BA	517	C	O4'-C1'-N1	7.60	114.28	108.20
21	AA	1336	C	N1-C2-O2	7.60	123.46	118.90
54	BB	57	A	C5-C6-N1	7.60	121.50	117.70
53	BA	1090	A	C4-C5-C6	-7.60	113.20	117.00
53	BA	1701	A	C5-C6-N1	7.60	121.50	117.70
21	AA	547	A	C4-C5-C6	-7.59	113.20	117.00
53	BA	634	C	N3-C2-O2	-7.59	116.58	121.90
53	BA	1916	A	C5-C6-N1	7.59	121.50	117.70
21	AA	171	A	C4-C5-C6	-7.59	113.20	117.00
21	AA	1145	A	C5-C6-N1	7.59	121.50	117.70
31	BJ	96	ARG	NE-CZ-NH2	7.59	124.09	120.30
53	BA	2900	A	N1-C6-N6	-7.59	114.05	118.60
21	AA	334	C	N3-C2-O2	-7.59	116.59	121.90
35	BN	86	ARG	NE-CZ-NH1	7.59	124.09	120.30
5	AF	44	ARG	NE-CZ-NH1	7.58	124.09	120.30
21	AA	1096	C	N3-C2-O2	-7.58	116.59	121.90
53	BA	2497	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1000	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1132	C	N3-C2-O2	-7.58	116.59	121.90
21	AA	547	A	C5-C6-N1	7.58	121.49	117.70
40	BS	110	ARG	NE-CZ-NH2	7.58	124.09	120.30
21	AA	1245	C	N3-C2-O2	-7.58	116.60	121.90
53	BA	1566	A	C5-C6-N1	7.58	121.49	117.70
25	BD	124	ARG	NE-CZ-NH1	7.57	124.09	120.30
53	BA	793	A	C5-C6-N1	7.57	121.49	117.70
53	BA	1264	A	C5-C6-N1	7.57	121.49	117.70
53	BA	788	A	N1-C6-N6	-7.57	114.06	118.60
53	BA	791	C	N3-C2-O2	-7.57	116.60	121.90
6	AG	118	ARG	NE-CZ-NH1	7.57	124.08	120.30
21	AA	195	A	C4-C5-C6	-7.57	113.22	117.00
21	AA	478	A	C5-C6-N1	7.57	121.48	117.70
53	BA	1384	A	C4-C5-C6	-7.57	113.22	117.00
53	BA	2015	A	C5-C6-N1	7.57	121.48	117.70
53	BA	182	A	N1-C6-N6	-7.56	114.06	118.60
21	AA	1283	U	N3-C2-O2	-7.56	116.91	122.20
53	BA	161	A	C5-C6-N1	7.56	121.48	117.70
21	AA	8	A	C5-C6-N1	7.56	121.48	117.70
21	AA	414	A	N1-C6-N6	-7.56	114.06	118.60
21	AA	1534	A	C5-C6-N1	7.56	121.48	117.70
53	BA	925	A	C5-C6-N1	7.56	121.48	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1802	A	C5-C6-N1	7.56	121.48	117.70
53	BA	2425	A	C4-C5-C6	-7.56	113.22	117.00
21	AA	1151	A	N1-C6-N6	-7.56	114.06	118.60
53	BA	1260	A	N1-C6-N6	-7.56	114.06	118.60
21	AA	1374	A	C4-C5-C6	-7.55	113.22	117.00
53	BA	10	A	C5-C6-N1	7.55	121.47	117.70
53	BA	1140	C	O4'-C1'-N1	7.55	114.24	108.20
21	AA	1274	A	C5-C6-N1	7.55	121.47	117.70
53	BA	2666	C	N3-C2-O2	-7.55	116.61	121.90
53	BA	61	C	N3-C2-O2	-7.55	116.62	121.90
53	BA	2590	A	C4-C5-C6	-7.55	113.23	117.00
53	BA	505	A	C5-C6-N1	7.54	121.47	117.70
21	AA	431	A	N1-C6-N6	-7.54	114.07	118.60
22	A1	66	A	C5-C6-N1	7.54	121.47	117.70
53	BA	2606	C	N3-C2-O2	-7.54	116.62	121.90
21	AA	321	A	C5-C6-N1	7.54	121.47	117.70
53	BA	1109	C	N3-C2-O2	-7.54	116.62	121.90
53	BA	2374	C	N3-C2-O2	-7.54	116.62	121.90
53	BA	2577	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	802	A	C5-C6-N1	7.54	121.47	117.70
53	BA	1761	C	N1-C2-O2	7.54	123.42	118.90
53	BA	105	C	O4'-C1'-N1	7.54	114.23	108.20
53	BA	1152	C	N3-C2-O2	-7.54	116.62	121.90
53	BA	735	A	N1-C6-N6	-7.54	114.08	118.60
53	BA	1096	A	C5-C6-N1	7.54	121.47	117.70
21	AA	129	A	C5-C6-N1	7.54	121.47	117.70
53	BA	415	A	C5-C6-N1	7.54	121.47	117.70
21	AA	309	A	C5-C6-N1	7.53	121.47	117.70
53	BA	2082	A	C5-C6-N1	7.53	121.47	117.70
53	BA	672	C	N3-C2-O2	-7.53	116.63	121.90
53	BA	1378	A	C4-C5-C6	-7.53	113.23	117.00
3	AD	103	ARG	NE-CZ-NH2	-7.53	116.53	120.30
21	AA	1408	A	C5-C6-N1	7.53	121.47	117.70
53	BA	2792	A	N1-C6-N6	-7.53	114.08	118.60
21	AA	1499	A	C5-C6-N1	7.53	121.47	117.70
54	BB	12	C	N3-C2-O2	-7.53	116.63	121.90
53	BA	2469	A	C5-C6-N1	7.53	121.46	117.70
53	BA	1791	A	C5-C6-N1	7.52	121.46	117.70
53	BA	515	A	C4-C5-C6	-7.52	113.24	117.00
53	BA	1010	A	C5-C6-N1	7.52	121.46	117.70
53	BA	1894	C	N1-C2-O2	7.52	123.41	118.90
21	AA	749	A	C5-C6-N1	7.52	121.46	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	227	A	C5-C6-N1	7.52	121.46	117.70
53	BA	1264	A	N1-C6-N6	-7.52	114.09	118.60
53	BA	1677	A	C5-C6-N1	7.52	121.46	117.70
53	BA	2103	C	O4'-C1'-N1	7.52	114.21	108.20
53	BA	643	A	N1-C6-N6	-7.52	114.09	118.60
53	BA	892	A	C5-C6-N1	7.52	121.46	117.70
53	BA	401	A	C5-C6-N1	7.51	121.46	117.70
53	BA	1762	A	C5-C6-N1	7.51	121.46	117.70
53	BA	655	A	C5-C6-N1	7.51	121.46	117.70
53	BA	936	A	N1-C6-N6	-7.51	114.09	118.60
53	BA	1603	A	C4-C5-C6	-7.51	113.24	117.00
53	BA	2369	A	C4-C5-C6	-7.51	113.24	117.00
21	AA	167	A	C5-C6-N1	7.51	121.45	117.70
53	BA	435	C	N3-C2-O2	-7.51	116.64	121.90
21	AA	16	A	C5-C6-N1	7.51	121.45	117.70
21	AA	1230	C	N3-C2-O2	-7.51	116.65	121.90
53	BA	2031	A	N1-C6-N6	-7.51	114.10	118.60
53	BA	2184	A	N1-C6-N6	-7.51	114.10	118.60
21	AA	873	A	C4-C5-C6	-7.50	113.25	117.00
21	AA	1289	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1376	U	O4'-C1'-N1	7.50	114.20	108.20
53	BA	671	C	N3-C2-O2	-7.50	116.65	121.90
54	BB	36	C	O4'-C1'-N1	7.50	114.20	108.20
21	AA	807	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1105	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	286	C	N3-C2-O2	-7.50	116.65	121.90
21	AA	155	A	C5-C6-N1	7.50	121.45	117.70
21	AA	499	A	C4-C5-C6	-7.50	113.25	117.00
21	AA	1344	C	N3-C2-O2	-7.50	116.65	121.90
53	BA	121	G	O4'-C1'-N9	7.50	114.20	108.20
21	AA	1044	A	C4-C5-C6	-7.50	113.25	117.00
34	BM	59	ARG	NE-CZ-NH1	7.50	124.05	120.30
53	BA	423	A	C4-C5-C6	-7.49	113.25	117.00
53	BA	430	A	N1-C6-N6	-7.49	114.10	118.60
21	AA	819	A	C4-C5-C6	-7.49	113.25	117.00
53	BA	2005	A	C4-C5-C6	-7.49	113.25	117.00
21	AA	546	A	N1-C6-N6	-7.49	114.11	118.60
53	BA	801	G	N3-C2-N2	-7.49	114.66	119.90
53	BA	2741	A	C5-C6-N1	7.49	121.44	117.70
53	BA	1311	G	N3-C2-N2	-7.49	114.66	119.90
21	AA	583	A	N1-C6-N6	-7.49	114.11	118.60
53	BA	804	A	C5-C6-N1	7.49	121.44	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1987	A	N1-C6-N6	-7.49	114.11	118.60
53	BA	57	C	N3-C2-O2	-7.48	116.66	121.90
53	BA	607	U	O4'-C1'-N1	7.48	114.18	108.20
53	BA	2835	A	C4-C5-C6	-7.48	113.26	117.00
8	AI	48	ARG	NE-CZ-NH1	7.48	124.04	120.30
53	BA	2888	C	N3-C2-O2	-7.48	116.67	121.90
21	AA	1136	C	N3-C2-O2	-7.48	116.67	121.90
53	BA	2667	C	N3-C2-O2	-7.48	116.67	121.90
21	AA	336	A	N1-C6-N6	-7.48	114.11	118.60
21	AA	974	A	C4-C5-C6	-7.48	113.26	117.00
53	BA	56	A	C5-C6-N1	7.48	121.44	117.70
21	AA	1167	A	N1-C6-N6	-7.47	114.12	118.60
35	BN	63	ARG	NE-CZ-NH1	7.47	124.04	120.30
53	BA	2468	A	C4-C5-C6	-7.47	113.26	117.00
21	AA	1349	A	C5-C6-N1	7.47	121.44	117.70
53	BA	1244	A	C4-C5-C6	-7.47	113.26	117.00
53	BA	2585	U	O4'-C1'-N1	7.47	114.18	108.20
54	BB	97	C	N3-C2-O2	-7.47	116.67	121.90
53	BA	992	C	O4'-C1'-N1	7.47	114.18	108.20
53	BA	2628	C	N1-C2-O2	7.47	123.38	118.90
21	AA	80	A	C5-C6-N1	7.47	121.44	117.70
53	BA	1993	U	O4'-C1'-N1	7.47	114.17	108.20
53	BA	2275	C	N3-C2-O2	-7.47	116.67	121.90
53	BA	2291	U	O4'-C1'-N1	7.47	114.17	108.20
21	AA	649	A	C4-C5-C6	-7.47	113.27	117.00
41	BT	12	ARG	NE-CZ-NH1	7.47	124.03	120.30
21	AA	193	C	N3-C2-O2	-7.46	116.67	121.90
21	AA	998	C	N3-C2-O2	-7.46	116.67	121.90
53	BA	1591	A	C4-C5-C6	-7.46	113.27	117.00
21	AA	906	A	C5-C6-N1	7.46	121.43	117.70
21	AA	647	C	N3-C2-O2	-7.46	116.68	121.90
53	BA	2600	A	C5-C6-N1	7.46	121.43	117.70
21	AA	696	A	N1-C6-N6	-7.46	114.13	118.60
53	BA	1630	A	C4-C5-C6	-7.46	113.27	117.00
53	BA	2142	A	N1-C6-N6	-7.46	114.13	118.60
54	BB	88	C	N3-C2-O2	-7.46	116.68	121.90
53	BA	1610	A	N1-C6-N6	-7.45	114.13	118.60
53	BA	1679	A	C4-C5-C6	-7.45	113.27	117.00
53	BA	89	A	C4-C5-C6	-7.45	113.28	117.00
53	BA	1095	A	C4-C5-C6	-7.45	113.27	117.00
53	BA	788	A	O4'-C1'-N9	7.45	114.16	108.20
53	BA	1787	A	C4-C5-C6	-7.45	113.28	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	756	A	C4-C5-C6	-7.45	113.28	117.00
21	AA	320	A	C5-C6-N1	7.45	121.42	117.70
22	A1	16	C	N1-C2-O2	7.45	123.37	118.90
53	BA	699	A	C5-C6-N1	7.45	121.42	117.70
53	BA	1118	C	N3-C2-O2	-7.45	116.69	121.90
53	BA	2736	A	N1-C6-N6	-7.45	114.13	118.60
53	BA	2142	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	995	C	N1-C2-O2	7.44	123.36	118.90
21	AA	1451	U	O4'-C1'-N1	7.44	114.15	108.20
53	BA	374	A	N1-C6-N6	-7.44	114.13	118.60
53	BA	1787	A	C5-C6-N1	7.44	121.42	117.70
3	AD	55	ARG	NE-CZ-NH1	7.44	124.02	120.30
53	BA	262	A	C5-C6-N1	7.44	121.42	117.70
53	BA	2639	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	196	A	C4-C5-C6	-7.44	113.28	117.00
53	BA	2566	A	C5-C6-N1	7.43	121.42	117.70
21	AA	463	U	O4'-C1'-N1	7.43	114.15	108.20
53	BA	1304	A	C5-C6-N1	7.43	121.42	117.70
53	BA	2654	A	C5-C6-N1	7.43	121.42	117.70
21	AA	397	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	855	U	O4'-C1'-N1	7.43	114.14	108.20
21	AA	1468	A	N1-C6-N6	-7.43	114.14	118.60
39	BR	68	ARG	NE-CZ-NH1	7.43	124.01	120.30
21	AA	931	C	O4'-C1'-N1	7.42	114.14	108.20
21	AA	959	A	C4-C5-C6	-7.42	113.29	117.00
53	BA	1795	C	N3-C2-O2	-7.42	116.71	121.90
1	AB	138	ARG	NE-CZ-NH1	7.42	124.01	120.30
21	AA	116	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	270	A	C5-C6-N1	7.42	121.41	117.70
21	AA	812	G	O4'-C1'-N9	7.42	114.13	108.20
53	BA	1774	C	N3-C2-O2	-7.42	116.71	121.90
53	BA	2039	U	O4'-C1'-N1	7.42	114.13	108.20
53	BA	2080	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	1346	A	O4'-C1'-N9	7.41	114.13	108.20
53	BA	1286	A	C5-C6-N1	7.41	121.41	117.70
53	BA	2761	A	C4-C5-C6	-7.41	113.29	117.00
53	BA	89	A	C5-C6-N1	7.41	121.41	117.70
53	BA	1694	C	N3-C2-O2	-7.41	116.71	121.90
53	BA	2720	U	O4'-C1'-N1	7.41	114.13	108.20
21	AA	937	A	C4-C5-C6	-7.41	113.30	117.00
53	BA	523	C	N3-C2-O2	-7.41	116.71	121.90
53	BA	627	A	C4-C5-C6	-7.41	113.30	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	675	A	C5-C6-N1	7.41	121.40	117.70
53	BA	730	A	N1-C6-N6	-7.41	114.16	118.60
53	BA	2886	A	C4-C5-C6	-7.41	113.30	117.00
21	AA	329	A	C4-C5-C6	-7.41	113.30	117.00
53	BA	131	A	C5-C6-N1	7.41	121.40	117.70
21	AA	718	A	C5-C6-N1	7.41	121.40	117.70
53	BA	2471	A	N1-C6-N6	-7.41	114.16	118.60
53	BA	2031	A	C4-C5-C6	-7.40	113.30	117.00
21	AA	1225	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	1418	A	N1-C6-N6	-7.40	114.16	118.60
29	BH	27	ARG	NE-CZ-NH1	7.40	124.00	120.30
53	BA	2462	C	N3-C2-O2	-7.40	116.72	121.90
4	AE	53	ARG	NE-CZ-NH2	7.40	124.00	120.30
21	AA	1363	A	C5-C6-N1	7.40	121.40	117.70
35	BN	90	ARG	NE-CZ-NH1	7.40	124.00	120.30
53	BA	1847	A	N1-C6-N6	-7.40	114.16	118.60
53	BA	2809	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	55	A	N1-C6-N6	-7.40	114.16	118.60
53	BA	231	A	C5-C6-N1	7.40	121.40	117.70
53	BA	384	A	C4-C5-C6	-7.40	113.30	117.00
53	BA	2806	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	631	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	1151	A	C5-C6-N1	7.40	121.40	117.70
53	BA	402	A	C4-C5-C6	-7.40	113.30	117.00
53	BA	743	A	C5-C6-N1	7.40	121.40	117.70
53	BA	1551	A	C5-C6-N1	7.40	121.40	117.70
53	BA	2800	A	C4-C5-C6	-7.40	113.30	117.00
53	BA	2835	A	C5-C6-N1	7.40	121.40	117.70
21	AA	738	C	N3-C2-O2	-7.40	116.72	121.90
20	AU	20	ARG	NE-CZ-NH1	7.39	124.00	120.30
33	BL	69	ARG	NE-CZ-NH1	7.39	124.00	120.30
53	BA	91	A	C5-C6-N1	7.39	121.40	117.70
21	AA	1055	A	C5-C6-N1	7.39	121.40	117.70
53	BA	1396	U	O4'-C1'-N1	7.39	114.11	108.20
53	BA	1586	A	C5-C6-N1	7.39	121.40	117.70
53	BA	1650	A	N1-C6-N6	-7.39	114.16	118.60
53	BA	517	C	N3-C2-O2	-7.39	116.73	121.90
53	BA	1582	C	N3-C2-O2	-7.39	116.73	121.90
21	AA	1274	A	C4-C5-C6	-7.39	113.31	117.00
53	BA	244	A	C4-C5-C6	-7.39	113.31	117.00
53	BA	1151	A	N1-C6-N6	-7.39	114.17	118.60
22	A1	25	C	N3-C2-O2	-7.39	116.73	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	735	A	C5-C6-N1	7.39	121.39	117.70
53	BA	1090	A	C5-C6-N1	7.39	121.39	117.70
53	BA	1508	A	O4'-C1'-N9	7.39	114.11	108.20
53	BA	1387	A	C5-C6-N1	7.39	121.39	117.70
53	BA	1676	A	N1-C6-N6	-7.39	114.17	118.60
53	BA	2014	A	N1-C6-N6	-7.39	114.17	118.60
21	AA	919	A	C5-C6-N1	7.38	121.39	117.70
50	B2	39	ARG	NE-CZ-NH1	7.38	123.99	120.30
53	BA	718	A	N1-C6-N6	-7.38	114.17	118.60
53	BA	1096	A	C4-C5-C6	-7.38	113.31	117.00
53	BA	2632	A	C5-C6-N1	7.38	121.39	117.70
21	AA	10	A	C4-C5-C6	-7.38	113.31	117.00
21	AA	649	A	C5-C6-N1	7.38	121.39	117.70
53	BA	480	A	C5-C6-N1	7.38	121.39	117.70
53	BA	749	A	C5-C6-N1	7.38	121.39	117.70
53	BA	1196	C	N3-C2-O2	-7.38	116.73	121.90
21	AA	1267	C	N1-C2-O2	7.38	123.33	118.90
53	BA	734	A	C5-C6-N1	7.38	121.39	117.70
53	BA	62	U	O4'-C1'-N1	7.38	114.10	108.20
53	BA	71	A	O4'-C1'-N9	7.38	114.10	108.20
53	BA	1413	A	C4-C5-C6	-7.38	113.31	117.00
54	BB	34	A	C5-C6-N1	7.38	121.39	117.70
8	AI	122	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	622	A	C4-C5-C6	-7.38	113.31	117.00
53	BA	1705	A	C4-C5-C6	-7.38	113.31	117.00
21	AA	728	A	C5-C6-N1	7.37	121.39	117.70
53	BA	404	A	C4-C5-C6	-7.37	113.31	117.00
53	BA	666	A	C5-C6-N1	7.37	121.39	117.70
53	BA	1871	A	N1-C6-N6	-7.37	114.18	118.60
53	BA	2628	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	663	A	C4-C5-C6	-7.37	113.32	117.00
21	AA	814	A	C5-C6-N1	7.37	121.38	117.70
21	AA	1059	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	1369	C	N3-C2-O2	-7.37	116.74	121.90
53	BA	908	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	67	C	N3-C2-O2	-7.37	116.74	121.90
53	BA	1962	C	N3-C2-O2	-7.37	116.74	121.90
14	AO	52	ARG	NE-CZ-NH1	7.36	123.98	120.30
21	AA	969	A	C5-C6-N1	7.36	121.38	117.70
53	BA	323	C	N1-C2-O2	7.36	123.32	118.90
53	BA	1978	A	C4-C5-C6	-7.36	113.32	117.00
53	BA	2261	C	N3-C2-O2	-7.36	116.75	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1434	A	C5-C6-N1	7.36	121.38	117.70
53	BA	2706	A	N1-C6-N6	-7.36	114.18	118.60
22	A1	38	A	N1-C6-N6	-7.36	114.18	118.60
53	BA	1321	A	C5-C6-N1	7.36	121.38	117.70
53	BA	1591	A	C5-C6-N1	7.36	121.38	117.70
21	AA	77	A	N1-C6-N6	-7.36	114.19	118.60
21	AA	393	A	N1-C6-N6	-7.36	114.19	118.60
21	AA	1234	C	N3-C2-O2	-7.36	116.75	121.90
53	BA	889	C	N3-C2-O2	-7.36	116.75	121.90
53	BA	1029	A	C4-C5-C6	-7.36	113.32	117.00
53	BA	2161	C	N3-C2-O2	-7.35	116.75	121.90
53	BA	816	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	1519	A	N1-C6-N6	-7.35	114.19	118.60
53	BA	1836	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	5	U	O4'-C1'-N1	7.35	114.08	108.20
21	AA	381	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	792	A	N1-C6-N6	-7.35	114.19	118.60
53	BA	1158	C	N3-C2-O2	-7.35	116.76	121.90
53	BA	1689	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	1302	C	N3-C2-O2	-7.35	116.76	121.90
53	BA	1764	C	N3-C2-O2	-7.35	116.76	121.90
53	BA	2169	A	O4'-C1'-N9	7.35	114.08	108.20
54	BB	78	A	C5-C6-N1	7.35	121.37	117.70
53	BA	1040	A	C5-C6-N1	7.35	121.37	117.70
53	BA	2381	A	C5-C6-N1	7.35	121.37	117.70
6	AG	108	ARG	NE-CZ-NH1	7.34	123.97	120.30
53	BA	354	A	N1-C6-N6	-7.34	114.19	118.60
21	AA	415	A	C5-C6-N1	7.34	121.37	117.70
21	AA	680	C	N3-C2-O2	-7.34	116.76	121.90
53	BA	1672	A	C4-C5-C6	-7.34	113.33	117.00
12	AM	2	ARG	NE-CZ-NH1	7.34	123.97	120.30
21	AA	279	A	C5-C6-N1	7.34	121.37	117.70
21	AA	971	G	O4'-C1'-N9	7.34	114.07	108.20
21	AA	1465	A	C4-C5-C6	-7.34	113.33	117.00
53	BA	268	C	N3-C2-O2	-7.34	116.76	121.90
53	BA	1799	G	C8-N9-C4	-7.34	103.46	106.40
21	AA	177	G	O4'-C1'-N9	7.34	114.07	108.20
53	BA	737	C	O4'-C1'-N1	7.34	114.07	108.20
53	BA	1027	A	C4-C5-C6	-7.34	113.33	117.00
53	BA	270	A	C4-C5-C6	-7.33	113.33	117.00
53	BA	2199	A	N1-C6-N6	-7.33	114.20	118.60
53	BA	2750	A	C5-C6-N1	7.33	121.37	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1272	A	O4'-C1'-N9	7.33	114.07	108.20
53	BA	1505	A	C5-C6-N1	7.33	121.37	117.70
53	BA	509	C	N3-C2-O2	-7.33	116.77	121.90
53	BA	2426	A	C5-C6-N1	7.33	121.36	117.70
21	AA	124	C	N3-C2-O2	-7.33	116.77	121.90
53	BA	1092	C	O4'-C1'-N1	7.33	114.06	108.20
53	BA	2705	A	C5-C6-N1	7.33	121.36	117.70
53	BA	843	G	O4'-C1'-N9	7.33	114.06	108.20
21	AA	271	C	O4'-C1'-N1	7.32	114.06	108.20
53	BA	83	A	C5-C6-N1	7.32	121.36	117.70
53	BA	927	A	N1-C6-N6	-7.32	114.21	118.60
54	BB	73	A	C5-C6-N1	7.32	121.36	117.70
53	BA	213	A	C5-C6-N1	7.32	121.36	117.70
53	BA	391	A	C4-C5-C6	-7.32	113.34	117.00
53	BA	1706	C	N3-C2-O2	-7.32	116.78	121.90
53	BA	1905	C	N3-C2-O2	-7.32	116.78	121.90
53	BA	2126	A	C5-C6-N1	7.32	121.36	117.70
53	BA	125	A	C4-C5-C6	-7.32	113.34	117.00
21	AA	262	A	C5-C6-N1	7.32	121.36	117.70
53	BA	2392	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	1350	A	N7-C8-N9	7.31	117.46	113.80
53	BA	2072	C	N3-C2-O2	-7.31	116.78	121.90
53	BA	2840	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	780	A	C5-C6-N1	7.31	121.36	117.70
23	A2	91	A	C5-C6-N1	7.31	121.36	117.70
53	BA	1237	A	C5-C6-N1	7.31	121.36	117.70
21	AA	658	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	1130	A	C5-C6-N1	7.31	121.36	117.70
53	BA	2000	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	108	G	O4'-C1'-N9	7.31	114.05	108.20
21	AA	825	A	C4-C5-C6	-7.31	113.34	117.00
53	BA	689	A	C5-C6-N1	7.31	121.36	117.70
53	BA	1932	A	C4-C5-C6	-7.31	113.34	117.00
53	BA	2467	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	1453	G	O4'-C1'-N9	7.31	114.05	108.20
22	A1	60	C	N1-C2-O2	7.31	123.28	118.90
53	BA	479	A	C5-C6-N1	7.31	121.35	117.70
53	BA	1535	A	C4-C5-C6	-7.31	113.35	117.00
53	BA	1669	A	C4-C5-C6	-7.31	113.35	117.00
53	BA	1786	A	N1-C6-N6	-7.31	114.22	118.60
53	BA	2601	C	N3-C2-O2	-7.31	116.78	121.90
21	AA	1430	A	C5-C6-N1	7.30	121.35	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1134	A	C4-C5-C6	-7.30	113.35	117.00
53	BA	172	A	N1-C6-N6	-7.30	114.22	118.60
53	BA	2727	A	C5-C6-N1	7.30	121.35	117.70
3	AD	2	ARG	NE-CZ-NH1	7.30	123.95	120.30
21	AA	579	A	C5-C6-N1	7.30	121.35	117.70
53	BA	896	A	C5-C6-N1	7.30	121.35	117.70
54	BB	36	C	N1-C2-O2	7.30	123.28	118.90
21	AA	596	A	N1-C6-N6	-7.30	114.22	118.60
53	BA	635	C	N3-C2-O2	-7.30	116.79	121.90
54	BB	62	C	N3-C2-O2	-7.30	116.79	121.90
21	AA	554	A	C5-C6-N1	7.29	121.35	117.70
21	AA	787	A	C4-C5-C6	-7.29	113.35	117.00
53	BA	236	C	N3-C2-O2	-7.29	116.80	121.90
53	BA	1918	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	71	A	C5-C6-N1	7.29	121.35	117.70
21	AA	253	A	C5-C6-N1	7.29	121.35	117.70
53	BA	2019	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	1169	A	C5-C6-N1	7.29	121.34	117.70
21	AA	98	A	C4-C5-C6	-7.29	113.36	117.00
21	AA	243	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1000	A	C4-C5-C6	-7.29	113.36	117.00
53	BA	1393	A	N1-C6-N6	-7.29	114.23	118.60
53	BA	1020	A	N1-C6-N6	-7.29	114.23	118.60
53	BA	1802	A	C4-C5-C6	-7.29	113.36	117.00
53	BA	2117	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	1431	A	C5-C6-N1	7.28	121.34	117.70
53	BA	718	A	C5-C6-N1	7.28	121.34	117.70
53	BA	722	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	460	A	C5-C6-N1	7.28	121.34	117.70
53	BA	1632	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	712	A	C4-C5-C6	-7.28	113.36	117.00
53	BA	433	C	N3-C2-O2	-7.28	116.81	121.90
53	BA	2733	A	C5-C6-N1	7.28	121.34	117.70
53	BA	1574	C	N3-C2-O2	-7.27	116.81	121.90
53	BA	2322	A	N1-C6-N6	-7.27	114.24	118.60
53	BA	730	A	C5-C6-N1	7.27	121.33	117.70
53	BA	823	C	N3-C2-O2	-7.27	116.81	121.90
4	AE	92	ARG	NE-CZ-NH1	7.27	123.94	120.30
21	AA	1201	A	P-O3'-C3'	7.27	128.42	119.70
53	BA	936	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	236	A	C5-C6-N1	7.27	121.33	117.70
21	AA	871	U	O4'-C1'-N1	7.27	114.01	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1961	C	N3-C2-O2	-7.27	116.81	121.90
53	BA	2456	C	N3-C2-O2	-7.27	116.81	121.90
21	AA	729	A	C5-C6-N1	7.26	121.33	117.70
30	BI	126	ARG	NE-CZ-NH1	7.26	123.93	120.30
53	BA	63	A	C4-C5-C6	-7.26	113.37	117.00
53	BA	1121	C	N3-C2-O2	-7.26	116.81	121.90
53	BA	1387	A	O4'-C1'-N9	7.26	114.01	108.20
53	BA	2721	A	C5-C6-N1	7.26	121.33	117.70
21	AA	325	A	C5-C6-N1	7.26	121.33	117.70
53	BA	802	A	C5-C6-N1	7.26	121.33	117.70
53	BA	849	A	C4-C5-C6	-7.26	113.37	117.00
15	AP	28	ARG	NE-CZ-NH1	7.26	123.93	120.30
21	AA	602	A	C5-C6-N1	7.26	121.33	117.70
52	B4	24	ARG	NE-CZ-NH1	7.25	123.93	120.30
53	BA	1731	G	O4'-C1'-N9	7.25	114.00	108.20
21	AA	938	A	C5-C6-N1	7.25	121.33	117.70
23	A2	91	A	C4-C5-C6	-7.25	113.37	117.00
53	BA	1127	A	C5-C6-N1	7.25	121.33	117.70
53	BA	2853	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	1520	C	N3-C2-O2	-7.25	116.82	121.90
53	BA	1293	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	502	A	C5-C6-N1	7.25	121.33	117.70
21	AA	1447	A	C4-C5-C6	-7.25	113.38	117.00
53	BA	899	A	N1-C6-N6	-7.25	114.25	118.60
53	BA	1487	U	O4'-C1'-N1	7.25	114.00	108.20
53	BA	2078	C	N3-C4-C5	7.25	124.80	121.90
21	AA	530	G	O4'-C1'-N9	7.25	114.00	108.20
22	A1	72	C	O4'-C1'-N1	7.25	114.00	108.20
53	BA	2530	A	C5-C6-N1	7.25	121.32	117.70
5	AF	24	ARG	NE-CZ-NH1	7.24	123.92	120.30
6	AG	3	ARG	NE-CZ-NH1	7.24	123.92	120.30
21	AA	706	A	C5-C6-N1	7.24	121.32	117.70
53	BA	2009	A	C4-C5-C6	-7.24	113.38	117.00
9	AJ	45	ARG	NE-CZ-NH1	7.24	123.92	120.30
53	BA	1612	C	N3-C2-O2	-7.24	116.83	121.90
53	BA	1877	A	C5-C6-N1	7.24	121.32	117.70
21	AA	1502	A	C4-C5-C6	-7.24	113.38	117.00
53	BA	804	A	N1-C6-N6	-7.24	114.26	118.60
53	BA	2267	A	C5-C6-N1	7.24	121.32	117.70
21	AA	148	G	N3-C2-N2	-7.24	114.83	119.90
53	BA	1553	A	C5-C6-N1	7.24	121.32	117.70
21	AA	878	A	N1-C6-N6	-7.24	114.26	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	206	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	1524	C	N3-C2-O2	-7.23	116.84	121.90
53	BA	677	A	C5-C6-N1	7.23	121.32	117.70
53	BA	1070	A	C4-C5-C6	-7.23	113.38	117.00
53	BA	1515	A	C5-C6-N1	7.23	121.32	117.70
53	BA	1548	A	N1-C6-N6	-7.23	114.26	118.60
53	BA	1801	A	C5-C6-N1	7.23	121.32	117.70
53	BA	2205	A	N1-C6-N6	-7.23	114.26	118.60
53	BA	1027	A	N1-C6-N6	-7.23	114.26	118.60
53	BA	1609	A	C4-C5-C6	-7.23	113.39	117.00
53	BA	853	C	N3-C2-O2	-7.23	116.84	121.90
53	BA	1746	A	N1-C6-N6	-7.23	114.26	118.60
21	AA	784	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1518	A	N1-C6-N6	-7.22	114.27	118.60
33	BL	132	ARG	NE-CZ-NH1	7.22	123.91	120.30
53	BA	1032	A	C5-C6-N1	7.22	121.31	117.70
53	BA	1314	C	N3-C2-O2	-7.22	116.84	121.90
53	BA	1420	A	N1-C6-N6	-7.22	114.27	118.60
53	BA	103	A	C4-C5-C6	-7.22	113.39	117.00
53	BA	522	A	N1-C6-N6	-7.22	114.27	118.60
36	BO	15	ARG	NE-CZ-NH1	7.22	123.91	120.30
53	BA	1005	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	495	A	C5-C6-N1	7.22	121.31	117.70
53	BA	472	A	C5-C6-N1	7.22	121.31	117.70
44	BW	19	ARG	NE-CZ-NH1	7.22	123.91	120.30
21	AA	624	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	675	A	C5-C6-N1	7.21	121.31	117.70
53	BA	320	A	C5-C6-N1	7.21	121.31	117.70
53	BA	911	A	C4-C5-C6	-7.21	113.39	117.00
53	BA	1040	A	C4-C5-C6	-7.21	113.39	117.00
53	BA	1155	A	C4-C5-C6	-7.21	113.39	117.00
53	BA	2094	A	N1-C6-N6	-7.21	114.27	118.60
53	BA	2723	C	N3-C2-O2	-7.21	116.85	121.90
43	BV	79	ARG	NE-CZ-NH1	7.21	123.91	120.30
53	BA	1603	A	C5-C6-N1	7.21	121.31	117.70
54	BB	11	C	N3-C2-O2	-7.21	116.85	121.90
53	BA	540	C	N3-C2-O2	-7.21	116.85	121.90
54	BB	116	G	O4'-C1'-N9	7.21	113.97	108.20
21	AA	643	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	1080	A	C5-C6-N1	7.21	121.30	117.70
21	AA	1188	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1500	A	C4-C5-C6	-7.21	113.40	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	330	A	C5-C6-N1	7.21	121.30	117.70
53	BA	1847	A	C5-C6-N1	7.21	121.30	117.70
3	AD	13	ARG	NE-CZ-NH1	7.21	123.90	120.30
53	BA	1204	A	C5-C6-N1	7.21	121.30	117.70
53	BA	2837	A	N1-C6-N6	-7.21	114.28	118.60
21	AA	1163	A	C4-C5-C6	-7.21	113.40	117.00
21	AA	1447	A	N1-C6-N6	-7.21	114.28	118.60
53	BA	278	A	C5-C6-N1	7.21	121.30	117.70
53	BA	394	C	N3-C2-O2	-7.21	116.86	121.90
2	AC	106	ARG	NE-CZ-NH1	7.20	123.90	120.30
21	AA	1054	C	N3-C2-O2	-7.20	116.86	121.90
53	BA	1578	U	O4'-C1'-N1	7.20	113.96	108.20
53	BA	1843	C	N3-C2-O2	-7.20	116.86	121.90
10	AK	126	ARG	NE-CZ-NH2	7.20	123.90	120.30
21	AA	349	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	790	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1396	A	C4-C5-C6	-7.20	113.40	117.00
53	BA	1647	U	N3-C2-O2	-7.20	117.16	122.20
21	AA	712	A	C5-C6-N1	7.20	121.30	117.70
21	AA	787	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	1032	G	O4'-C1'-N9	7.20	113.96	108.20
21	AA	1200	C	C3'-C2'-C1'	7.20	107.26	101.50
21	AA	1329	A	C4-C5-C6	-7.20	113.40	117.00
53	BA	228	C	N3-C2-O2	-7.20	116.86	121.90
53	BA	2760	C	O4'-C1'-N1	7.20	113.96	108.20
21	AA	653	U	O4'-C1'-N1	7.20	113.96	108.20
53	BA	270	A	C5-C6-N1	7.20	121.30	117.70
53	BA	432	A	N1-C6-N6	-7.20	114.28	118.60
53	BA	693	A	C5-C6-N1	7.20	121.30	117.70
53	BA	2078	C	N3-C2-O2	-7.20	116.86	121.90
53	BA	2706	A	C5-C6-N1	7.20	121.30	117.70
53	BA	878	A	C4-C5-C6	-7.19	113.40	117.00
21	AA	1229	A	C5-C6-N1	7.19	121.30	117.70
21	AA	1349	A	C4-C5-C6	-7.19	113.40	117.00
53	BA	1913	A	C5-C6-N1	7.19	121.30	117.70
21	AA	1046	A	C5-C6-N1	7.19	121.29	117.70
53	BA	1265	A	C4-C5-C6	-7.19	113.41	117.00
21	AA	143	A	N1-C6-N6	-7.19	114.29	118.60
21	AA	513	C	O4'-C1'-N1	7.19	113.95	108.20
21	AA	1281	C	N3-C2-O2	-7.19	116.87	121.90
53	BA	602	A	C5-C6-N1	7.19	121.29	117.70
53	BA	1040	A	N1-C6-N6	-7.19	114.29	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2767	C	N3-C2-O2	-7.19	116.87	121.90
53	BA	2826	A	C5-C6-N1	7.19	121.29	117.70
21	AA	430	A	C5-C6-N1	7.19	121.29	117.70
21	AA	451	A	N1-C6-N6	-7.19	114.29	118.60
20	AU	17	ARG	NE-CZ-NH1	7.18	123.89	120.30
53	BA	101	A	C5-C6-N1	7.18	121.29	117.70
53	BA	789	A	C5-C6-N1	7.18	121.29	117.70
53	BA	1352	U	O4'-C1'-N1	7.18	113.95	108.20
21	AA	465	A	C5-C6-N1	7.18	121.29	117.70
21	AA	687	A	N1-C6-N6	-7.18	114.29	118.60
53	BA	10	A	N1-C6-N6	-7.18	114.29	118.60
53	BA	503	A	O4'-C1'-N9	7.18	113.94	108.20
21	AA	167	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	123	U	O4'-C1'-N1	7.18	113.94	108.20
21	AA	1219	A	C4-C5-C6	-7.18	113.41	117.00
53	BA	2176	A	C5-C6-N1	7.18	121.29	117.70
21	AA	309	A	C4-C5-C6	-7.17	113.41	117.00
35	BN	64	ARG	NE-CZ-NH1	7.17	123.89	120.30
53	BA	234	U	O4'-C1'-N1	7.17	113.94	108.20
24	BC	261	ARG	NE-CZ-NH1	7.17	123.89	120.30
45	BX	73	ARG	NE-CZ-NH1	7.17	123.89	120.30
53	BA	79	C	N3-C2-O2	-7.17	116.88	121.90
53	BA	183	C	N3-C2-O2	-7.17	116.88	121.90
22	A1	26	A	C5-C6-N1	7.17	121.28	117.70
23	A2	82	A	C4-C5-C6	-7.17	113.42	117.00
53	BA	2830	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	314	C	N3-C2-O2	-7.17	116.88	121.90
53	BA	219	A	C4-C5-C6	-7.17	113.42	117.00
53	BA	2309	A	C4-C5-C6	-7.17	113.42	117.00
21	AA	1170	A	C5-C6-N1	7.17	121.28	117.70
22	A1	16	C	C6-N1-C2	-7.17	117.43	120.30
53	BA	1153	C	N3-C2-O2	-7.17	116.89	121.90
21	AA	282	A	C4-C5-C6	-7.16	113.42	117.00
32	BK	98	ARG	NE-CZ-NH1	7.16	123.88	120.30
53	BA	157	C	N3-C2-O2	-7.16	116.89	121.90
53	BA	208	C	N3-C2-O2	-7.16	116.89	121.90
53	BA	650	C	N3-C2-O2	-7.16	116.89	121.90
53	BA	1664	A	N1-C6-N6	-7.16	114.30	118.60
53	BA	2450	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	1429	A	C4-C5-C6	-7.16	113.42	117.00
53	BA	1427	A	C4-C5-C6	-7.16	113.42	117.00
53	BA	1678	A	C5-C6-N1	7.16	121.28	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	116	A	C4-C5-C6	-7.16	113.42	117.00
53	BA	2263	C	N3-C2-O2	-7.16	116.89	121.90
53	BA	2902	C	N3-C2-O2	-7.16	116.89	121.90
54	BB	28	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	618	C	N3-C2-O2	-7.16	116.89	121.90
53	BA	529	A	C5-C6-N1	7.16	121.28	117.70
53	BA	197	A	C4-C5-C6	-7.16	113.42	117.00
53	BA	460	A	N1-C6-N6	-7.16	114.31	118.60
53	BA	2288	A	C4-C5-C6	-7.16	113.42	117.00
53	BA	2461	A	C5-C6-N1	7.16	121.28	117.70
53	BA	244	A	C5-C6-N1	7.15	121.28	117.70
53	BA	1490	A	C5-C6-N1	7.15	121.28	117.70
53	BA	2424	C	N3-C2-O2	-7.15	116.89	121.90
21	AA	316	C	O4'-C1'-N1	7.15	113.92	108.20
21	AA	949	A	C5-C6-N1	7.15	121.27	117.70
34	BM	81	ARG	NE-CZ-NH2	7.15	123.87	120.30
53	BA	371	A	C4-C5-C6	-7.15	113.43	117.00
53	BA	2284	A	C5-C6-N1	7.15	121.27	117.70
21	AA	81	A	C5-C6-N1	7.15	121.27	117.70
53	BA	1098	A	C5-C6-N1	7.15	121.27	117.70
2	AC	135	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	AC	142	ARG	NE-CZ-NH1	7.14	123.87	120.30
3	AD	96	ARG	NE-CZ-NH1	7.14	123.87	120.30
21	AA	101	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	586	C	N3-C2-O2	-7.14	116.90	121.90
53	BA	265	A	O4'-C1'-N9	7.14	113.92	108.20
21	AA	120	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	482	A	C5-C6-N1	7.14	121.27	117.70
53	BA	878	A	N1-C6-N6	-7.14	114.31	118.60
53	BA	1404	C	O4'-C1'-N1	7.14	113.92	108.20
53	BA	2841	C	N3-C2-O2	-7.14	116.90	121.90
53	BA	639	U	O4'-C1'-N1	7.14	113.91	108.20
53	BA	2527	C	N3-C2-O2	-7.14	116.90	121.90
53	BA	911	A	C5-C6-N1	7.14	121.27	117.70
53	BA	2064	C	N3-C2-O2	-7.14	116.91	121.90
21	AA	253	A	C4-C5-C6	-7.13	113.43	117.00
21	AA	263	A	C5-C6-N1	7.13	121.27	117.70
53	BA	1866	A	C5-C6-N1	7.13	121.27	117.70
53	BA	1654	A	N1-C6-N6	-7.13	114.32	118.60
3	AD	153	ARG	NE-CZ-NH1	7.13	123.87	120.30
21	AA	642	A	C5-C6-N1	7.13	121.27	117.70
53	BA	2799	A	N1-C6-N6	-7.13	114.32	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	330	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	611	C	N3-C2-O2	-7.13	116.91	121.90
21	AA	1219	A	N1-C6-N6	-7.13	114.32	118.60
53	BA	2055	C	N3-C2-O2	-7.13	116.91	121.90
53	BA	2883	A	C5-C6-N1	7.13	121.26	117.70
22	A1	21	A	N1-C6-N6	-7.13	114.32	118.60
53	BA	1297	C	N3-C2-O2	-7.13	116.91	121.90
53	BA	1938	A	C5-C6-N1	7.13	121.26	117.70
53	BA	201	C	N3-C2-O2	-7.12	116.91	121.90
53	BA	1322	A	C4-C5-C6	-7.12	113.44	117.00
53	BA	1504	A	N1-C6-N6	-7.12	114.33	118.60
21	AA	102	G	C8-N9-C4	-7.12	103.55	106.40
21	AA	295	C	N3-C2-O2	-7.12	116.91	121.90
53	BA	2665	A	C5-C6-N1	7.12	121.26	117.70
21	AA	26	A	C5-C6-N1	7.12	121.26	117.70
53	BA	1413	A	C5-C6-N1	7.12	121.26	117.70
53	BA	1614	A	N1-C6-N6	-7.12	114.33	118.60
53	BA	2047	C	N3-C2-O2	-7.12	116.92	121.90
53	BA	1552	A	C5-C6-N1	7.12	121.26	117.70
53	BA	422	A	C5-C6-N1	7.12	121.26	117.70
53	BA	482	A	N1-C6-N6	-7.12	114.33	118.60
53	BA	1650	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	1429	A	C5-C6-N1	7.12	121.26	117.70
53	BA	2115	G	O4'-C1'-N9	7.12	113.89	108.20
21	AA	171	A	C5-C6-N1	7.11	121.26	117.70
53	BA	2156	G	N1-C6-O6	-7.11	115.63	119.90
21	AA	303	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	1467	C	N3-C2-O2	-7.11	116.92	121.90
53	BA	1477	A	C5-C6-N1	7.11	121.26	117.70
53	BA	1608	A	C5-C6-N1	7.11	121.26	117.70
21	AA	621	A	C4-C5-C6	-7.11	113.44	117.00
53	BA	460	A	C4-C5-C6	-7.11	113.44	117.00
21	AA	712	A	N1-C6-N6	-7.11	114.33	118.60
53	BA	2225	A	C5-C6-N1	7.11	121.25	117.70
21	AA	189	A	C5-C6-N1	7.11	121.25	117.70
53	BA	2851	A	C5-C6-N1	7.11	121.25	117.70
53	BA	278	A	N1-C6-N6	-7.10	114.34	118.60
16	AQ	64	ARG	NE-CZ-NH2	7.10	123.85	120.30
21	AA	908	A	C5-C6-N1	7.10	121.25	117.70
23	A2	80	C	N3-C2-O2	-7.10	116.93	121.90
53	BA	2029	G	N3-C2-N2	-7.10	114.93	119.90
53	BA	2042	A	C4-C5-C6	-7.10	113.45	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BB	35	C	N1-C2-O2	7.10	123.16	118.90
21	AA	1411	C	O4'-C1'-N1	7.10	113.88	108.20
53	BA	538	A	N1-C6-N6	-7.10	114.34	118.60
21	AA	1314	C	O4'-C1'-N1	7.10	113.88	108.20
21	AA	411	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1251	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1518	A	C5-C6-N1	7.10	121.25	117.70
53	BA	251	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1067	A	C4-C5-C6	-7.10	113.45	117.00
53	BA	2036	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	681	A	C4-C5-C6	-7.09	113.45	117.00
53	BA	331	C	N3-C2-O2	-7.09	116.94	121.90
53	BA	685	A	C4-C5-C6	-7.09	113.45	117.00
21	AA	320	A	C4-C5-C6	-7.09	113.45	117.00
53	BA	2386	A	C5-C6-N1	7.09	121.25	117.70
2	AC	178	ARG	NE-CZ-NH1	7.09	123.85	120.30
14	AO	83	ARG	NE-CZ-NH1	7.09	123.85	120.30
21	AA	490	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	969	A	C4-C5-C6	-7.09	113.45	117.00
53	BA	452	G	C8-N9-C4	-7.09	103.56	106.40
53	BA	1936	A	N1-C6-N6	-7.09	114.35	118.60
53	BA	1254	A	N1-C6-N6	-7.09	114.35	118.60
21	AA	448	A	C5-C6-N1	7.09	121.24	117.70
36	BO	102	ARG	NE-CZ-NH1	7.08	123.84	120.30
16	AQ	61	ARG	NE-CZ-NH1	7.08	123.84	120.30
21	AA	344	A	C5-C6-N1	7.08	121.24	117.70
53	BA	853	C	O4'-C1'-N1	7.08	113.87	108.20
53	BA	1392	A	C1'-O4'-C4'	-7.08	104.23	109.90
53	BA	2059	A	N1-C6-N6	-7.08	114.35	118.60
53	BA	1914	C	N3-C2-O2	-7.08	116.94	121.90
53	BA	2033	A	C4-C5-C6	-7.08	113.46	117.00
53	BA	2566	A	N1-C6-N6	-7.08	114.35	118.60
53	BA	2078	C	N1-C2-O2	7.08	123.15	118.90
21	AA	155	A	C4-C5-C6	-7.08	113.46	117.00
51	B3	44	ARG	NE-CZ-NH2	-7.08	116.76	120.30
53	BA	1999	C	N3-C2-O2	-7.08	116.95	121.90
53	BA	2829	A	C5-C6-N1	7.08	121.24	117.70
21	AA	872	A	C5-C6-N1	7.07	121.24	117.70
21	AA	876	C	N3-C2-O2	-7.07	116.95	121.90
53	BA	2826	A	N1-C6-N6	-7.07	114.36	118.60
54	BB	59	A	C5-C6-N1	7.07	121.24	117.70
21	AA	397	A	C4-C5-C6	-7.07	113.46	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BF	177	ARG	NE-CZ-NH1	7.07	123.84	120.30
53	BA	599	A	C5-C6-N1	7.07	121.24	117.70
53	BA	959	A	N1-C6-N6	-7.07	114.36	118.60
53	BA	2810	A	N1-C6-N6	-7.07	114.36	118.60
53	BA	2814	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	1503	A	N1-C6-N6	-7.07	114.36	118.60
53	BA	1593	A	C5-C6-N1	7.07	121.24	117.70
53	BA	13	A	C5-C6-N1	7.07	121.23	117.70
21	AA	162	A	C4-C5-C6	-7.07	113.47	117.00
45	BX	26	ARG	NE-CZ-NH1	7.07	123.83	120.30
53	BA	1308	A	C5-C6-N1	7.07	121.23	117.70
53	BA	2741	A	N1-C6-N6	-7.07	114.36	118.60
53	BA	144	A	C5-C6-N1	7.07	121.23	117.70
53	BA	752	A	C1'-O4'-C4'	-7.07	104.25	109.90
53	BA	1165	A	C5-C6-N1	7.07	121.23	117.70
53	BA	2310	C	N3-C2-O2	-7.07	116.95	121.90
54	BB	63	C	N3-C2-O2	-7.06	116.95	121.90
21	AA	816	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	959	A	C5-C6-N1	7.06	121.23	117.70
53	BA	1901	A	C5-C6-N1	7.06	121.23	117.70
53	BA	2757	A	N1-C6-N6	-7.06	114.36	118.60
54	BB	115	A	N1-C6-N6	-7.06	114.36	118.60
29	BH	123	ARG	NE-CZ-NH1	7.06	123.83	120.30
53	BA	526	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	352	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	1063	C	N3-C2-O2	-7.06	116.96	121.90
53	BA	507	A	N1-C6-N6	-7.06	114.37	118.60
53	BA	602	A	C4-C5-C6	-7.06	113.47	117.00
53	BA	1480	C	N3-C2-O2	-7.06	116.96	121.90
18	AS	36	ARG	NE-CZ-NH1	7.06	123.83	120.30
21	AA	1275	A	C5-C6-N1	7.06	121.23	117.70
55	B5	134	ARG	NE-CZ-NH1	7.06	123.83	120.30
21	AA	908	A	C4-C5-C6	-7.05	113.47	117.00
21	AA	948	C	N3-C2-O2	-7.05	116.96	121.90
21	AA	1092	A	C5-C6-N1	7.05	121.23	117.70
53	BA	1312	U	O4'-C1'-N1	7.05	113.84	108.20
53	BA	1966	A	C4-C5-C6	-7.05	113.47	117.00
53	BA	2506	U	O4'-C1'-N1	7.05	113.84	108.20
53	BA	2554	U	C1'-O4'-C4'	-7.05	104.26	109.90
21	AA	1280	A	C5-C6-N1	7.05	121.23	117.70
53	BA	2748	A	C5-C6-N1	7.05	121.23	117.70
21	AA	1483	A	N1-C6-N6	-7.05	114.37	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	146	A	C5-C6-N1	7.05	121.23	117.70
21	AA	353	A	C5-C6-N1	7.05	121.22	117.70
21	AA	1167	A	C5-C6-N1	7.05	121.22	117.70
53	BA	1213	A	N1-C6-N6	-7.05	114.37	118.60
21	AA	1117	A	C4-C5-C6	-7.05	113.48	117.00
53	BA	1111	A	C5-C6-N1	7.05	121.22	117.70
53	BA	666	A	C4-C5-C6	-7.05	113.48	117.00
53	BA	812	C	N3-C2-O2	-7.05	116.97	121.90
53	BA	1918	A	C5-C6-N1	7.05	121.22	117.70
53	BA	2439	A	C5-C6-N1	7.05	121.22	117.70
53	BA	2658	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	408	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	825	A	N1-C6-N6	-7.04	114.37	118.60
53	BA	352	A	N1-C6-N6	-7.04	114.37	118.60
53	BA	1378	A	O4'-C1'-N9	7.04	113.83	108.20
53	BA	1606	C	N1-C2-O2	7.04	123.13	118.90
53	BA	2030	A	C5-C6-N1	7.04	121.22	117.70
53	BA	789	A	C4-C5-C6	-7.04	113.48	117.00
53	BA	1706	C	N1-C2-O2	7.04	123.12	118.90
21	AA	8	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	26	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	876	C	O4'-C1'-N1	7.04	113.83	108.20
53	BA	218	A	C5-C6-N1	7.04	121.22	117.70
53	BA	592	A	C4-C5-C6	-7.04	113.48	117.00
53	BA	1353	A	C5-C6-N1	7.04	121.22	117.70
54	BB	114	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	163	C	N3-C2-O2	-7.04	116.97	121.90
53	BA	217	A	C5-C6-N1	7.04	121.22	117.70
53	BA	1088	A	N1-C6-N6	-7.04	114.38	118.60
53	BA	1572	A	C5-C6-N1	7.04	121.22	117.70
9	AJ	62	ARG	NE-CZ-NH1	7.04	123.82	120.30
21	AA	1129	C	N3-C2-O2	-7.04	116.97	121.90
53	BA	1717	A	C5-C6-N1	7.04	121.22	117.70
53	BA	2119	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	841	C	C1'-O4'-C4'	-7.03	104.27	109.90
21	AA	1274	A	N1-C6-N6	-7.03	114.38	118.60
53	BA	1746	A	C5-C6-N1	7.03	121.22	117.70
53	BA	951	C	O4'-C1'-N1	7.03	113.83	108.20
53	BA	541	A	N1-C6-N6	-7.03	114.38	118.60
21	AA	909	A	C5-C6-N1	7.03	121.21	117.70
53	BA	1928	A	C5-C6-N1	7.03	121.21	117.70
53	BA	2805	C	N3-C2-O2	-7.03	116.98	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	BO	25	ARG	NE-CZ-NH1	7.02	123.81	120.30
53	BA	2765	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1330	U	O4'-C1'-N1	7.02	113.82	108.20
53	BA	454	A	C5-C6-N1	7.02	121.21	117.70
53	BA	2534	A	C5-C6-N1	7.02	121.21	117.70
53	BA	1590	A	C5-C6-N1	7.02	121.21	117.70
21	AA	129	A	C4-C5-C6	-7.02	113.49	117.00
21	AA	181	A	C4-C5-C6	-7.02	113.49	117.00
53	BA	348	A	C5-C6-N1	7.02	121.21	117.70
53	BA	1754	A	C5-C6-N1	7.02	121.21	117.70
40	BS	95	ARG	NE-CZ-NH2	-7.02	116.79	120.30
10	AK	121	ARG	NE-CZ-NH1	7.01	123.81	120.30
21	AA	743	A	C5-C6-N1	7.01	121.21	117.70
53	BA	985	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	1350	A	C5-N7-C8	-7.01	100.39	103.90
53	BA	935	C	N3-C2-O2	-7.01	116.99	121.90
53	BA	1731	G	C8-N9-C4	-7.01	103.59	106.40
53	BA	2893	A	C4-C5-C6	-7.01	113.49	117.00
21	AA	1055	A	C4-C5-C6	-7.01	113.50	117.00
53	BA	14	A	N1-C6-N6	-7.01	114.39	118.60
53	BA	344	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	1217	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	1324	A	N1-C6-N6	-7.01	114.40	118.60
53	BA	56	A	C4-C5-C6	-7.01	113.50	117.00
53	BA	2766	A	C5-C6-N1	7.01	121.20	117.70
53	BA	2740	A	C5-C6-N1	7.00	121.20	117.70
21	AA	882	C	N3-C2-O2	-7.00	117.00	121.90
54	BB	38	C	O4'-C1'-N1	7.00	113.80	108.20
21	AA	190	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	912	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	1216	A	C4-C5-C6	-7.00	113.50	117.00
53	BA	1298	C	N1-C2-O2	7.00	123.10	118.90
53	BA	1565	C	N3-C2-O2	-7.00	117.00	121.90
53	BA	1759	A	C5-C6-N1	7.00	121.20	117.70
53	BA	2088	A	N1-C6-N6	-7.00	114.40	118.60
53	BA	2806	C	N1-C2-O2	7.00	123.10	118.90
13	AN	41	ARG	NE-CZ-NH1	7.00	123.80	120.30
21	AA	469	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	1428	A	C5-C6-N1	7.00	121.20	117.70
21	AA	110	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	796	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	895	G	C5-C6-N1	7.00	115.00	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1082	A	C5-C6-N1	7.00	121.20	117.70
53	BA	2111	U	O4'-C1'-N1	7.00	113.80	108.20
21	AA	460	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	1411	C	N3-C2-O2	-7.00	117.00	121.90
22	A1	13	C	O4'-C1'-N1	7.00	113.80	108.20
53	BA	739	A	N1-C6-N6	-7.00	114.40	118.60
53	BA	928	A	C5-C6-N1	7.00	121.20	117.70
53	BA	1008	A	N1-C6-N6	-7.00	114.40	118.60
53	BA	1889	A	C5-C6-N1	7.00	121.20	117.70
53	BA	2058	A	C4-C5-C6	-7.00	113.50	117.00
53	BA	2851	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	496	A	N1-C6-N6	-7.00	114.40	118.60
13	AN	61	ARG	NE-CZ-NH1	6.99	123.80	120.30
34	BM	16	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	AB	62	ARG	NE-CZ-NH1	6.99	123.80	120.30
53	BA	716	A	C5-C6-N1	6.99	121.19	117.70
53	BA	2377	A	C4-C5-C6	-6.99	113.51	117.00
53	BA	2463	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	1214	C	N3-C4-C5	6.99	124.69	121.90
53	BA	1888	G	O4'-C1'-N9	6.99	113.79	108.20
53	BA	2635	A	N1-C6-N6	-6.99	114.41	118.60
21	AA	1236	A	C5-C6-N1	6.99	121.19	117.70
53	BA	2758	A	C5-C6-N1	6.99	121.19	117.70
53	BA	571	U	O4'-C1'-N1	6.98	113.79	108.20
53	BA	756	A	C5-C6-N1	6.98	121.19	117.70
21	AA	501	C	N3-C2-O2	-6.98	117.01	121.90
53	BA	2101	A	C4-C5-C6	-6.98	113.51	117.00
53	BA	2745	C	N3-C2-O2	-6.98	117.01	121.90
53	BA	2868	A	N1-C6-N6	-6.98	114.41	118.60
37	BP	71	ARG	NE-CZ-NH1	6.98	123.79	120.30
53	BA	22	C	N3-C2-O2	-6.98	117.01	121.90
53	BA	246	C	N3-C2-O2	-6.98	117.01	121.90
21	AA	489	C	N3-C2-O2	-6.98	117.02	121.90
53	BA	503	A	N1-C6-N6	-6.98	114.41	118.60
53	BA	1942	C	N3-C2-O2	-6.98	117.02	121.90
54	BB	49	C	N3-C2-O2	-6.98	117.02	121.90
21	AA	787	A	C5-C6-N1	6.98	121.19	117.70
53	BA	104	A	N1-C6-N6	-6.98	114.41	118.60
53	BA	368	A	C5-C6-N1	6.98	121.19	117.70
53	BA	1278	C	O4'-C1'-N1	6.98	113.78	108.20
53	BA	1847	A	O4'-C1'-N9	6.98	113.78	108.20
53	BA	2845	U	O4'-C1'-N1	6.98	113.78	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	78	A	N1-C6-N6	-6.98	114.42	118.60
21	AA	694	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	1336	C	N3-C2-O2	-6.98	117.02	121.90
53	BA	316	C	N3-C2-O2	-6.98	117.02	121.90
53	BA	2043	C	N3-C2-O2	-6.98	117.02	121.90
21	AA	250	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	1035	A	C5-C6-N1	6.97	121.19	117.70
53	BA	364	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	1684	G	N1-C6-O6	-6.97	115.72	119.90
21	AA	238	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	1005	A	C4-C5-C6	-6.97	113.51	117.00
53	BA	106	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	1276	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	719	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	631	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	389	A	C4-C5-C6	-6.97	113.52	117.00
21	AA	1277	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	1072	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	1085	A	N1-C6-N6	-6.97	114.42	118.60
53	BA	1477	A	C4-C5-C6	-6.97	113.52	117.00
21	AA	559	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	1308	U	O4'-C1'-N1	6.97	113.77	108.20
53	BA	560	C	N3-C2-O2	-6.97	117.02	121.90
53	BA	2459	A	C5-C6-N1	6.97	121.18	117.70
53	BA	2515	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	274	A	O4'-C1'-N9	6.96	113.77	108.20
21	AA	739	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	1213	A	C4-C5-C6	-6.96	113.52	117.00
53	BA	1746	A	C4-C5-C6	-6.96	113.52	117.00
54	BB	58	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	831	A	C4-C5-C6	-6.96	113.52	117.00
53	BA	19	A	C4-C5-C6	-6.96	113.52	117.00
53	BA	38	A	C4-C5-C6	-6.96	113.52	117.00
53	BA	288	U	O4'-C1'-N1	6.96	113.77	108.20
53	BA	2314	A	C4-C5-C6	-6.96	113.52	117.00
53	BA	2594	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	1409	C	N3-C2-O2	-6.95	117.03	121.90
53	BA	131	A	N1-C6-N6	-6.95	114.43	118.60
53	BA	730	A	C4-C5-C6	-6.95	113.52	117.00
53	BA	814	C	N3-C2-O2	-6.95	117.03	121.90
53	BA	1723	G	N1-C6-O6	-6.95	115.73	119.90
53	BA	2813	A	C4-C5-C6	-6.95	113.52	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AL	113	ARG	NE-CZ-NH1	6.95	123.78	120.30
21	AA	782	A	C5-C6-N1	6.95	121.17	117.70
21	AA	797	C	N3-C2-O2	-6.95	117.03	121.90
26	BE	21	ARG	NE-CZ-NH1	6.95	123.78	120.30
53	BA	239	C	N3-C2-O2	-6.95	117.03	121.90
53	BA	1194	A	C4-C5-C6	-6.95	113.53	117.00
53	BA	2598	A	C5-C6-N1	6.95	121.17	117.70
53	BA	2868	A	C4-C5-C6	-6.95	113.52	117.00
2	AC	131	ARG	NE-CZ-NH1	6.95	123.77	120.30
21	AA	58	C	O4'-C1'-N1	6.95	113.76	108.20
22	A1	48	C	N3-C2-O2	-6.95	117.04	121.90
53	BA	1167	C	N3-C2-O2	-6.95	117.04	121.90
21	AA	676	A	C5-C6-N1	6.95	121.17	117.70
21	AA	1131	G	N3-C2-N2	-6.95	115.04	119.90
53	BA	992	C	N3-C2-O2	-6.95	117.04	121.90
53	BA	1373	A	N1-C6-N6	-6.95	114.43	118.60
53	BA	1348	C	O4'-C1'-N1	6.94	113.75	108.20
53	BA	2809	A	C5-C6-N1	6.94	121.17	117.70
21	AA	135	C	O4'-C1'-N1	6.94	113.75	108.20
21	AA	460	A	O4'-C1'-N9	6.94	113.75	108.20
21	AA	915	A	C4-C5-C6	-6.94	113.53	117.00
53	BA	627	A	N1-C6-N6	-6.94	114.43	118.60
53	BA	2366	A	C5-C6-N1	6.94	121.17	117.70
21	AA	120	A	N1-C6-N6	-6.94	114.44	118.60
53	BA	1128	G	C1'-O4'-C4'	-6.94	104.35	109.90
21	AA	672	U	O4'-C1'-N1	6.94	113.75	108.20
3	AD	110	ARG	NE-CZ-NH1	6.94	123.77	120.30
21	AA	1476	A	C5-C6-N1	6.94	121.17	117.70
53	BA	900	A	N1-C6-N6	-6.94	114.44	118.60
53	BA	1888	G	C5'-C4'-O4'	6.94	117.42	109.10
53	BA	800	A	C5-C6-N1	6.94	121.17	117.70
53	BA	909	A	C5-C6-N1	6.93	121.17	117.70
53	BA	1382	G	O4'-C1'-N9	6.93	113.75	108.20
21	AA	120	A	C5-C6-N1	6.93	121.17	117.70
21	AA	131	A	C4-C5-C6	-6.93	113.53	117.00
53	BA	479	A	C4-C5-C6	-6.93	113.53	117.00
53	BA	2750	A	C4-C5-C6	-6.93	113.53	117.00
54	BB	104	A	C5-C6-N1	6.93	121.17	117.70
21	AA	452	A	C5-C6-N1	6.93	121.17	117.70
21	AA	364	A	C5-C6-N1	6.93	121.17	117.70
21	AA	999	C	N3-C2-O2	-6.93	117.05	121.90
53	BA	996	A	N1-C6-N6	-6.93	114.44	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1625	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	756	C	N1-C2-O2	6.93	123.06	118.90
53	BA	2268	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	435	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	1329	A	N1-C6-N6	-6.92	114.45	118.60
53	BA	6	A	C5-C6-N1	6.92	121.16	117.70
21	AA	89	U	O4'-C1'-N1	6.92	113.74	108.20
21	AA	483	C	O4'-C1'-N1	6.92	113.74	108.20
53	BA	1161	C	O4'-C1'-N1	6.92	113.74	108.20
21	AA	151	A	C5-C6-N1	6.92	121.16	117.70
21	AA	889	A	C5-C6-N1	6.92	121.16	117.70
53	BA	2732	G	N3-C2-N2	-6.92	115.06	119.90
53	BA	2882	A	C5-C6-N1	6.92	121.16	117.70
21	AA	77	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	217	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	452	A	C4-C5-C6	-6.92	113.54	117.00
53	BA	2516	A	C5-C6-N1	6.92	121.16	117.70
53	BA	2738	A	C4-C5-C6	-6.92	113.54	117.00
53	BA	513	A	N1-C6-N6	-6.92	114.45	118.60
53	BA	1502	A	C5-C6-N1	6.92	121.16	117.70
37	BP	112	ARG	NE-CZ-NH1	6.92	123.76	120.30
53	BA	149	A	C4-C5-C6	-6.92	113.54	117.00
53	BA	1759	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	872	A	O4'-C1'-N9	6.91	113.73	108.20
53	BA	526	A	N1-C6-N6	-6.91	114.45	118.60
53	BA	1399	C	N3-C2-O2	-6.91	117.06	121.90
53	BA	2587	A	C5-C6-N1	6.91	121.16	117.70
53	BA	623	C	N3-C2-O2	-6.91	117.06	121.90
53	BA	2023	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	660	C	O4'-C1'-N1	6.91	113.73	108.20
22	A1	30	C	N3-C2-O2	-6.91	117.06	121.90
53	BA	865	C	N3-C2-O2	-6.91	117.06	121.90
5	AF	45	ARG	NE-CZ-NH1	6.91	123.75	120.30
21	AA	93	U	O4'-C1'-N1	6.91	113.73	108.20
21	AA	401	C	N3-C2-O2	-6.91	117.06	121.90
53	BA	2635	A	C4-C5-C6	-6.91	113.55	117.00
53	BA	440	C	N3-C2-O2	-6.91	117.06	121.90
53	BA	751	A	C5-C6-N1	6.91	121.15	117.70
53	BA	2699	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	539	A	N1-C6-N6	-6.90	114.46	118.60
54	BB	15	A	O4'-C1'-N9	6.90	113.72	108.20
21	AA	1287	A	C4-C5-C6	-6.90	113.55	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1492	A	O4'-C1'-N9	6.90	113.72	108.20
53	BA	482	A	C5-C6-N1	6.90	121.15	117.70
53	BA	2362	C	N3-C2-O2	-6.90	117.07	121.90
2	AC	64	ARG	NE-CZ-NH1	6.89	123.75	120.30
53	BA	2498	C	C3'-C2'-C1'	6.89	107.02	101.50
53	BA	2232	C	N3-C2-O2	-6.89	117.08	121.90
53	BA	2037	A	C4-C5-C6	-6.89	113.56	117.00
21	AA	200	G	O4'-C1'-N9	6.89	113.71	108.20
53	BA	1084	A	C5-C6-N1	6.89	121.14	117.70
53	BA	1549	A	C4-C5-C6	-6.89	113.56	117.00
53	BA	1569	A	C4-C5-C6	-6.89	113.56	117.00
53	BA	309	A	C5-C6-N1	6.89	121.14	117.70
53	BA	140	C	N3-C2-O2	-6.89	117.08	121.90
53	BA	274	C	N3-C2-O2	-6.89	117.08	121.90
54	BB	94	A	C4-C5-C6	-6.89	113.56	117.00
53	BA	352	A	C4-C5-C6	-6.88	113.56	117.00
53	BA	668	A	C5-C6-N1	6.88	121.14	117.70
53	BA	676	A	C4-C5-C6	-6.88	113.56	117.00
53	BA	2332	C	N3-C4-N4	-6.88	113.18	118.00
21	AA	95	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	495	A	C4-C5-C6	-6.88	113.56	117.00
53	BA	1872	A	C5-C6-N1	6.88	121.14	117.70
53	BA	2151	U	O4'-C1'-N1	6.88	113.71	108.20
21	AA	228	A	C5-C6-N1	6.88	121.14	117.70
21	AA	722	G	C3'-C2'-C1'	6.88	107.00	101.50
21	AA	32	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	689	C	O4'-C1'-N1	6.88	113.70	108.20
21	AA	1380	U	O4'-C1'-N1	6.88	113.70	108.20
14	AO	57	ARG	NE-CZ-NH1	6.88	123.74	120.30
53	BA	1614	A	C5-C6-N1	6.88	121.14	117.70
53	BA	1960	A	C4-C5-C6	-6.88	113.56	117.00
53	BA	2626	C	N3-C2-O2	-6.88	117.08	121.90
53	BA	457	A	C5-C6-N1	6.88	121.14	117.70
53	BA	531	C	N3-C2-O2	-6.88	117.09	121.90
53	BA	1494	A	N1-C6-N6	-6.88	114.47	118.60
53	BA	2531	A	N1-C6-N6	-6.88	114.47	118.60
53	BA	1571	A	C5-C6-N1	6.88	121.14	117.70
53	BA	2071	A	C4-C5-C6	-6.88	113.56	117.00
24	BC	86	ARG	NE-CZ-NH1	6.87	123.74	120.30
30	BI	133	ARG	NE-CZ-NH1	6.87	123.74	120.30
53	BA	897	C	N1-C2-O2	6.87	123.02	118.90
21	AA	330	C	N1-C2-O2	6.87	123.02	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	489	C	O4'-C1'-N1	6.87	113.70	108.20
21	AA	533	A	C5-C6-N1	6.87	121.14	117.70
21	AA	630	A	C4-C5-C6	-6.87	113.56	117.00
53	BA	1711	A	C5-C6-N1	6.87	121.14	117.70
21	AA	715	A	N1-C6-N6	-6.87	114.48	118.60
53	BA	532	A	N1-C6-N6	-6.87	114.48	118.60
53	BA	582	A	C4-C5-C6	-6.87	113.56	117.00
53	BA	590	A	C5-C6-N1	6.87	121.14	117.70
7	AH	14	ARG	NE-CZ-NH1	6.87	123.73	120.30
21	AA	873	A	N1-C6-N6	-6.87	114.48	118.60
35	BN	4	ARG	NE-CZ-NH1	6.87	123.73	120.30
53	BA	1229	C	N3-C2-O2	-6.87	117.09	121.90
53	BA	2815	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	181	A	C5-C6-N1	6.87	121.13	117.70
21	AA	1350	A	C8-N9-C4	-6.87	103.05	105.80
53	BA	345	A	C5-C6-N1	6.87	121.13	117.70
53	BA	1075	C	O4'-C1'-N1	6.87	113.69	108.20
54	BB	78	A	C4-C5-C6	-6.87	113.57	117.00
53	BA	890	C	N3-C2-O2	-6.86	117.09	121.90
53	BA	896	A	N1-C6-N6	-6.86	114.48	118.60
53	BA	661	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	80	A	N1-C6-N6	-6.86	114.48	118.60
53	BA	2381	A	N1-C6-N6	-6.86	114.48	118.60
53	BA	2589	A	C4-C5-C6	-6.86	113.57	117.00
53	BA	910	A	C4-C5-C6	-6.86	113.57	117.00
53	BA	1351	C	O4'-C1'-N1	6.86	113.69	108.20
53	BA	2198	A	N1-C6-N6	-6.86	114.48	118.60
21	AA	974	A	O4'-C1'-N9	6.86	113.68	108.20
53	BA	125	A	C5-C6-N1	6.86	121.13	117.70
53	BA	2135	A	C4-C5-C6	-6.86	113.57	117.00
53	BA	1967	C	N3-C2-O2	-6.85	117.10	121.90
53	BA	504	A	C5-C6-N1	6.85	121.13	117.70
53	BA	2077	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	1370	G	N3-C4-C5	-6.85	125.17	128.60
21	AA	1100	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	1340	A	C5-C6-N1	6.85	121.12	117.70
53	BA	490	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	465	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	914	A	C5-C6-N1	6.85	121.12	117.70
21	AA	1412	C	N3-C2-O2	-6.85	117.11	121.90
53	BA	2019	A	C5-C6-N1	6.85	121.12	117.70
21	AA	298	A	C4-C5-C6	-6.84	113.58	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	724	U	O4'-C1'-N1	6.84	113.67	108.20
53	BA	835	C	N3-C2-O2	-6.84	117.11	121.90
53	BA	1354	A	N1-C6-N6	-6.84	114.49	118.60
53	BA	1635	A	C4-C5-C6	-6.84	113.58	117.00
54	BB	45	A	C5-C6-N1	6.84	121.12	117.70
53	BA	2395	C	N1-C2-O2	6.84	123.00	118.90
21	AA	379	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	1150	A	C4-C5-C6	-6.84	113.58	117.00
53	BA	1313	U	N3-C2-O2	-6.84	117.41	122.20
53	BA	1557	C	N3-C2-O2	-6.84	117.11	121.90
53	BA	1912	A	C4-C5-C6	-6.84	113.58	117.00
53	BA	2037	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1462	C	N3-C2-O2	-6.84	117.11	121.90
22	A1	56	C	N3-C2-O2	-6.84	117.11	121.90
53	BA	1202	G	N1-C6-O6	-6.84	115.80	119.90
53	BA	1768	C	N3-C2-O2	-6.84	117.11	121.90
55	B5	53	ARG	NE-CZ-NH1	6.84	123.72	120.30
53	BA	1453	A	C4-C5-C6	-6.83	113.58	117.00
53	BA	877	A	N1-C6-N6	-6.83	114.50	118.60
53	BA	946	C	N3-C2-O2	-6.83	117.12	121.90
53	BA	2035	G	O4'-C1'-N9	6.83	113.67	108.20
21	AA	580	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1397	C	N3-C2-O2	-6.83	117.12	121.90
53	BA	1685	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	790	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	1238	A	C5-C6-N1	6.83	121.11	117.70
53	BA	991	C	N3-C2-O2	-6.83	117.12	121.90
53	BA	1057	A	N1-C6-N6	-6.83	114.50	118.60
53	BA	1829	A	C5-C6-N1	6.83	121.11	117.70
2	AC	163	ARG	NE-CZ-NH1	6.83	123.71	120.30
21	AA	466	A	C5-C6-N1	6.83	121.11	117.70
53	BA	2163	A	C4-C5-C6	-6.83	113.59	117.00
21	AA	923	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1293	C	N3-C2-O2	-6.82	117.12	121.90
53	BA	680	C	N3-C2-O2	-6.82	117.12	121.90
53	BA	1123	C	N3-C2-O2	-6.82	117.12	121.90
54	BB	46	A	C4-C5-C6	-6.82	113.59	117.00
53	BA	332	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1403	C	N3-C2-O2	-6.82	117.13	121.90
53	BA	1664	A	C4-C5-C6	-6.82	113.59	117.00
53	BA	1689	A	C5-C6-N1	6.82	121.11	117.70
21	AA	1256	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(^{o})	Ideal(^{o})
14	AO	87	ARG	NE-CZ-NH1	6.82	123.71	120.30
21	AA	808	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	910	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	1110	A	C4-C5-C6	-6.82	113.59	117.00
53	BA	1549	A	C5-C6-N1	6.82	121.11	117.70
53	BA	1284	A	C5-C6-N1	6.82	121.11	117.70
53	BA	1512	C	N3-C2-O2	-6.82	117.13	121.90
5	AF	2	ARG	NE-CZ-NH1	6.81	123.71	120.30
53	BA	1129	A	C4-C5-C6	-6.81	113.59	117.00
53	BA	1393	A	C4-C5-C6	-6.81	113.59	117.00
24	BC	220	ARG	NE-CZ-NH1	6.81	123.70	120.30
53	BA	670	A	C5-C6-N1	6.81	121.11	117.70
53	BA	1175	A	C4-C5-C6	-6.81	113.59	117.00
53	BA	1306	C	O4'-C1'-N1	6.81	113.65	108.20
21	AA	1152	A	N1-C6-N6	-6.81	114.51	118.60
53	BA	640	C	N3-C2-O2	-6.81	117.13	121.90
53	BA	1139	G	N7-C8-N9	6.81	116.50	113.10
53	BA	1241	A	C5-C6-N1	6.81	121.11	117.70
53	BA	2713	U	O4'-C1'-N1	6.81	113.65	108.20
22	A1	69	A	C5-C6-N1	6.81	121.10	117.70
53	BA	2183	A	C5-C6-N1	6.81	121.10	117.70
53	BA	728	G	C5-C6-N1	6.81	114.90	111.50
21	AA	395	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	1192	C	N3-C2-O2	-6.80	117.14	121.90
53	BA	1291	C	N3-C2-O2	-6.80	117.14	121.90
53	BA	2154	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	1357	A	C5-C6-N1	6.80	121.10	117.70
21	AA	857	C	N3-C2-O2	-6.80	117.14	121.90
50	B2	19	ARG	NE-CZ-NH2	6.80	123.70	120.30
53	BA	255	A	C5-C6-N1	6.80	121.10	117.70
53	BA	513	A	C5-C6-N1	6.80	121.10	117.70
21	AA	923	A	C5-C6-N1	6.80	121.10	117.70
53	BA	1128	G	N1-C6-O6	-6.80	115.82	119.90
18	AS	31	ARG	NE-CZ-NH1	6.80	123.70	120.30
24	BC	132	ARG	NE-CZ-NH1	6.80	123.70	120.30
36	BO	9	ARG	NE-CZ-NH1	6.80	123.70	120.30
53	BA	860	U	O4'-C1'-N1	6.80	113.64	108.20
53	BA	2778	A	C5-C6-N1	6.80	121.10	117.70
54	BB	17	C	N3-C2-O2	-6.80	117.14	121.90
53	BA	2369	A	O4'-C1'-N9	6.79	113.64	108.20
53	BA	310	A	C4-C5-C6	-6.79	113.60	117.00
53	BA	661	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(^{o})	Ideal(^{o})
53	BA	2459	A	C4-C5-C6	-6.79	113.60	117.00
21	AA	101	A	C5-C6-N1	6.79	121.10	117.70
53	BA	1969	A	C5-C6-N1	6.79	121.09	117.70
53	BA	2899	A	C4-C5-C6	-6.79	113.61	117.00
53	BA	335	C	N3-C2-O2	-6.79	117.15	121.90
53	BA	1009	A	C5-C6-N1	6.79	121.09	117.70
21	AA	869	G	N1-C6-O6	-6.79	115.83	119.90
21	AA	1045	C	N3-C2-O2	-6.79	117.15	121.90
53	BA	125	A	N1-C6-N6	-6.79	114.53	118.60
53	BA	693	A	C4-C5-C6	-6.79	113.61	117.00
53	BA	821	A	C4-C5-C6	-6.79	113.61	117.00
53	BA	1497	U	O4'-C1'-N1	6.79	113.63	108.20
21	AA	1146	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	1301	U	O4'-C1'-N1	6.79	113.63	108.20
21	AA	1410	A	C5-C6-N1	6.79	121.09	117.70
53	BA	1837	C	N3-C2-O2	-6.79	117.15	121.90
53	BA	2115	G	N3-C4-C5	-6.79	125.21	128.60
21	AA	681	A	C5-C6-N1	6.78	121.09	117.70
53	BA	233	A	C4-C5-C6	-6.78	113.61	117.00
53	BA	1292	G	N1-C6-O6	-6.78	115.83	119.90
53	BA	1982	U	O4'-C1'-N1	6.78	113.63	108.20
21	AA	873	A	C5-C6-N1	6.78	121.09	117.70
53	BA	1181	U	O4'-C1'-N1	6.78	113.62	108.20
21	AA	935	A	C5-C6-N1	6.78	121.09	117.70
53	BA	2691	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	856	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	1469	C	N3-C2-O2	-6.78	117.16	121.90
53	BA	614	A	C5-C6-N1	6.78	121.09	117.70
53	BA	1678	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	325	A	C4-C5-C6	-6.78	113.61	117.00
53	BA	1253	A	C5-C6-N1	6.78	121.09	117.70
53	BA	2799	A	C5-C6-N1	6.78	121.09	117.70
21	AA	1146	A	C5-C6-N1	6.77	121.09	117.70
53	BA	2247	A	O4'-C1'-N9	6.77	113.62	108.20
53	BA	347	A	C5-C6-N1	6.77	121.09	117.70
21	AA	1531	A	C5-C6-N1	6.77	121.09	117.70
11	AL	35	ARG	NE-CZ-NH1	6.77	123.68	120.30
22	A1	73	A	C4-C5-C6	-6.77	113.61	117.00
53	BA	217	A	N1-C6-N6	-6.77	114.54	118.60
53	BA	1075	C	N3-C2-O2	-6.77	117.16	121.90
53	BA	786	C	N3-C2-O2	-6.77	117.16	121.90
53	BA	1503	A	C5-C6-N1	6.77	121.08	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	53	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	1239	A	N1-C6-N6	-6.77	114.54	118.60
21	AA	51	A	C4-C5-C6	-6.76	113.62	117.00
53	BA	616	A	N1-C6-N6	-6.76	114.54	118.60
2	AC	58	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	418	C	N3-C2-O2	-6.76	117.17	121.90
53	BA	432	A	C5-C6-N1	6.76	121.08	117.70
54	BB	58	A	N1-C6-N6	-6.76	114.54	118.60
16	AQ	76	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	1037	C	N3-C4-N4	-6.76	113.27	118.00
53	BA	1028	A	C4-C5-C6	-6.76	113.62	117.00
53	BA	1417	C	O4'-C1'-N1	6.76	113.61	108.20
53	BA	2785	C	N3-C2-O2	-6.76	117.17	121.90
54	BB	66	A	N1-C6-N6	-6.76	114.54	118.60
21	AA	977	A	C5-C6-N1	6.76	121.08	117.70
53	BA	42	A	N1-C6-N6	-6.76	114.54	118.60
53	BA	241	A	O4'-C1'-N9	6.76	113.61	108.20
53	BA	1760	C	N3-C2-O2	-6.76	117.17	121.90
53	BA	505	A	C4-C5-C6	-6.76	113.62	117.00
53	BA	1278	C	N3-C2-O2	-6.76	117.17	121.90
53	BA	149	A	C5-C6-N1	6.75	121.08	117.70
53	BA	2513	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	545	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	1262	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	1452	C	N3-C2-O2	-6.75	117.17	121.90
53	BA	348	A	C4-C5-C6	-6.75	113.62	117.00
53	BA	2306	C	N3-C2-O2	-6.75	117.17	121.90
53	BA	2858	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	393	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1228	C	N3-C2-O2	-6.75	117.17	121.90
53	BA	503	A	C5-C6-N1	6.75	121.08	117.70
53	BA	1536	C	N3-C2-O2	-6.75	117.17	121.90
53	BA	1870	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	178	C	N3-C2-O2	-6.75	117.17	121.90
6	AG	77	ARG	NE-CZ-NH1	6.75	123.67	120.30
53	BA	1367	A	N1-C6-N6	-6.75	114.55	118.60
53	BA	2154	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1434	A	C4-C5-C6	-6.75	113.63	117.00
53	BA	1161	C	N3-C2-O2	-6.75	117.18	121.90
53	BA	2823	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	19	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	371	A	C4-C5-C6	-6.75	113.63	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	422	A	C4-C5-C6	-6.75	113.63	117.00
53	BA	1373	A	C5-C6-N1	6.75	121.07	117.70
53	BA	2765	A	N1-C6-N6	-6.75	114.55	118.60
21	AA	300	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1317	C	N3-C2-O2	-6.74	117.18	121.90
53	BA	661	A	N1-C6-N6	-6.74	114.55	118.60
53	BA	1254	A	C5-C6-N1	6.74	121.07	117.70
53	BA	1919	A	N1-C6-N6	-6.74	114.55	118.60
53	BA	352	A	C5-C6-N1	6.74	121.07	117.70
53	BA	2809	A	C4-C5-C6	-6.74	113.63	117.00
11	AL	11	ARG	NE-CZ-NH1	6.74	123.67	120.30
21	AA	192	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1466	C	N3-C2-O2	-6.74	117.18	121.90
44	BW	76	ARG	NE-CZ-NH1	6.74	123.67	120.30
53	BA	454	A	C4-C5-C6	-6.74	113.63	117.00
53	BA	892	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	912	C	N1-C2-O2	6.74	122.94	118.90
53	BA	726	G	O4'-C1'-N9	6.74	113.59	108.20
53	BA	1417	C	N3-C2-O2	-6.74	117.18	121.90
53	BA	2020	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	923	A	N1-C6-N6	-6.74	114.56	118.60
21	AA	101	A	N1-C6-N6	-6.74	114.56	118.60
21	AA	1036	A	C4-C5-C6	-6.74	113.63	117.00
53	BA	524	G	N1-C6-O6	-6.74	115.86	119.90
53	BA	2717	C	N3-C2-O2	-6.74	117.19	121.90
21	AA	32	A	C4-C5-C6	-6.73	113.63	117.00
51	B3	12	ARG	NE-CZ-NH1	6.73	123.67	120.30
53	BA	199	A	C4-C5-C6	-6.73	113.63	117.00
53	BA	1165	A	C4-C5-C6	-6.73	113.63	117.00
53	BA	2451	A	C4-C5-C6	-6.73	113.63	117.00
35	BN	46	ARG	NE-CZ-NH1	6.73	123.67	120.30
53	BA	1981	A	C5-C6-N1	6.73	121.07	117.70
53	BA	2700	A	C5-C6-N1	6.73	121.06	117.70
26	BE	117	ARG	NE-CZ-NH1	6.73	123.66	120.30
53	BA	2676	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	958	A	C1'-O4'-C4'	-6.73	104.52	109.90
53	BA	973	A	C5-C6-N1	6.73	121.06	117.70
53	BA	2394	C	N3-C2-O2	-6.73	117.19	121.90
53	BA	2765	A	C4-C5-C6	-6.73	113.64	117.00
4	AE	137	ARG	NE-CZ-NH1	6.73	123.66	120.30
53	BA	533	G	N9-C4-C5	6.73	108.09	105.40
21	AA	824	G	N1-C6-O6	-6.72	115.87	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	983	A	C5-C6-N1	6.72	121.06	117.70
53	BA	1908	C	O4'-C1'-N1	6.72	113.58	108.20
21	AA	65	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	250	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	559	A	C5-C6-N1	6.72	121.06	117.70
53	BA	73	A	C4-C5-C6	-6.72	113.64	117.00
53	BA	239	C	O4'-C1'-N1	6.72	113.58	108.20
21	AA	1234	C	O4'-C1'-N1	6.72	113.58	108.20
53	BA	95	A	C4-C5-C6	-6.72	113.64	117.00
53	BA	387	U	N3-C2-O2	-6.72	117.50	122.20
21	AA	295	C	O4'-C1'-N1	6.72	113.58	108.20
53	BA	483	A	C5-C6-N1	6.72	121.06	117.70
53	BA	1016	G	N1-C6-O6	-6.72	115.87	119.90
53	BA	1089	A	C4-C5-C6	-6.72	113.64	117.00
53	BA	1784	A	N1-C6-N6	-6.72	114.57	118.60
53	BA	1866	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	139	A	C5-C6-N1	6.72	121.06	117.70
21	AA	386	C	N3-C2-O2	-6.72	117.20	121.90
21	AA	334	C	N1-C2-O2	6.72	122.93	118.90
21	AA	742	G	N3-C2-N2	-6.72	115.20	119.90
47	BZ	29	ARG	NE-CZ-NH1	6.72	123.66	120.30
53	BA	1289	C	N3-C2-O2	-6.72	117.20	121.90
21	AA	792	A	C5-C6-N1	6.71	121.06	117.70
53	BA	336	C	N3-C2-O2	-6.71	117.20	121.90
53	BA	398	C	C6-N1-C2	-6.71	117.61	120.30
21	AA	498	A	N1-C6-N6	-6.71	114.57	118.60
21	AA	790	A	C4-C5-C6	-6.71	113.64	117.00
53	BA	2513	A	N1-C6-N6	-6.71	114.57	118.60
21	AA	396	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	1043	G	N1-C6-O6	-6.71	115.87	119.90
21	AA	1362	A	C4-C5-C6	-6.71	113.64	117.00
21	AA	1449	C	N3-C2-O2	-6.71	117.20	121.90
53	BA	289	G	N1-C6-O6	-6.71	115.87	119.90
53	BA	691	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	1176	A	C5-C6-N1	6.71	121.05	117.70
21	AA	1339	A	C4-C5-C6	-6.71	113.65	117.00
53	BA	782	A	N1-C6-N6	-6.71	114.58	118.60
53	BA	2376	A	C4-C5-C6	-6.71	113.64	117.00
21	AA	263	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	607	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	1171	A	C5-C6-N1	6.71	121.05	117.70
41	BT	6	ARG	NE-CZ-NH2	6.71	123.65	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	984	A	C5-C6-N1	6.71	121.05	117.70
53	BA	1713	A	C5-C6-N1	6.71	121.05	117.70
53	BA	2635	A	C5-C6-N1	6.71	121.05	117.70
53	BA	1780	A	C5-C6-N1	6.70	121.05	117.70
54	BB	110	C	N3-C2-O2	-6.70	117.21	121.90
53	BA	1599	U	O4'-C1'-N1	6.70	113.56	108.20
21	AA	1483	A	C5-C6-N1	6.70	121.05	117.70
22	A1	68	C	N3-C2-O2	-6.70	117.21	121.90
53	BA	2695	U	O4'-C1'-N1	6.70	113.56	108.20
14	AO	76	ARG	NE-CZ-NH1	6.70	123.65	120.30
21	AA	567	G	N3-C4-C5	-6.70	125.25	128.60
21	AA	1397	C	N1-C2-O2	6.70	122.92	118.90
21	AA	751	U	O4'-C1'-N1	6.70	113.56	108.20
53	BA	902	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	1012	A	C5-C6-N1	6.70	121.05	117.70
40	BS	92	ARG	NE-CZ-NH2	6.70	123.65	120.30
53	BA	2347	C	N3-C2-O2	-6.70	117.21	121.90
48	B0	49	ARG	NE-CZ-NH2	6.69	123.65	120.30
53	BA	182	A	C5-C6-N1	6.69	121.05	117.70
49	B1	43	ARG	NE-CZ-NH1	6.69	123.65	120.30
53	BA	223	A	C5-C6-N1	6.69	121.05	117.70
53	BA	669	G	O4'-C1'-N9	6.69	113.55	108.20
53	BA	1076	C	O4'-C1'-N1	6.69	113.55	108.20
53	BA	1142	A	C5-C6-N1	6.69	121.05	117.70
53	BA	2333	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	1149	C	O4'-C1'-N1	6.69	113.55	108.20
22	A1	11	C	N3-C2-O2	-6.69	117.22	121.90
53	BA	1470	A	N1-C6-N6	-6.69	114.59	118.60
53	BA	2710	C	N3-C2-O2	-6.69	117.22	121.90
53	BA	1958	C	N3-C2-O2	-6.69	117.22	121.90
53	BA	2434	A	C5-C6-N1	6.69	121.04	117.70
53	BA	2566	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	143	A	C5-C6-N1	6.68	121.04	117.70
21	AA	569	C	N3-C4-C5	6.68	124.57	121.90
21	AA	1196	A	C4-C5-C6	-6.68	113.66	117.00
53	BA	556	A	C4-C5-C6	-6.68	113.66	117.00
53	BA	2496	C	N3-C2-O2	-6.68	117.22	121.90
53	BA	2670	A	C4-C5-C6	-6.68	113.66	117.00
53	BA	98	G	N1-C6-O6	-6.68	115.89	119.90
53	BA	528	A	N1-C6-N6	-6.68	114.59	118.60
53	BA	2560	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1331	G	N1-C6-O6	-6.68	115.89	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1288	G	N3-C4-C5	-6.68	125.26	128.60
53	BA	2499	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	936	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	1128	C	N3-C2-O2	-6.68	117.22	121.90
53	BA	1505	A	C4-C5-C6	-6.68	113.66	117.00
53	BA	1874	C	O4'-C1'-N1	6.68	113.54	108.20
53	BA	2679	A	C5-C6-N1	6.68	121.04	117.70
53	BA	1742	U	O4'-C1'-N1	6.68	113.54	108.20
53	BA	2013	A	C5-C6-N1	6.68	121.04	117.70
53	BA	1215	G	N3-C2-N2	-6.68	115.23	119.90
53	BA	2097	A	C5-C6-N1	6.68	121.04	117.70
53	BA	231	A	O4'-C1'-N9	6.67	113.54	108.20
53	BA	1076	C	N3-C2-O2	-6.67	117.23	121.90
53	BA	1262	A	C5-C6-N1	6.67	121.04	117.70
53	BA	428	A	C4-C5-C6	-6.67	113.66	117.00
53	BA	14	A	C5-C6-N1	6.67	121.04	117.70
53	BA	421	C	N3-C2-O2	-6.67	117.23	121.90
53	BA	2097	A	C4-C5-C6	-6.67	113.67	117.00
22	A1	66	A	N1-C6-N6	-6.67	114.60	118.60
53	BA	47	C	N3-C2-O2	-6.67	117.23	121.90
53	BA	2169	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	1288	A	C5-C6-N1	6.67	121.03	117.70
53	BA	737	C	N3-C2-O2	-6.67	117.23	121.90
53	BA	2725	A	C5-C6-N1	6.67	121.03	117.70
54	BB	15	A	C5-C6-N1	6.67	121.03	117.70
21	AA	66	A	C4-C5-C6	-6.67	113.67	117.00
53	BA	2660	A	C5-C6-N1	6.67	121.03	117.70
21	AA	1180	A	C5-C6-N1	6.67	121.03	117.70
27	BF	109	ARG	NE-CZ-NH1	6.67	123.63	120.30
21	AA	687	A	C4-C5-C6	-6.66	113.67	117.00
22	A1	75	C	N3-C2-O2	-6.66	117.23	121.90
21	AA	52	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	520	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	777	A	C4-C5-C6	-6.66	113.67	117.00
53	BA	1366	A	C5-C6-N1	6.66	121.03	117.70
53	BA	1780	A	O4'-C1'-N9	6.66	113.53	108.20
53	BA	1919	A	C5-C6-N1	6.66	121.03	117.70
53	BA	1140	C	N3-C2-O2	-6.66	117.24	121.90
53	BA	2515	C	O4'-C1'-N1	6.66	113.53	108.20
21	AA	812	G	N3-C4-C5	-6.66	125.27	128.60
21	AA	469	C	O4'-C1'-N1	6.66	113.53	108.20
21	AA	1418	A	C5-C6-N1	6.66	121.03	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1487	G	N3-C2-N2	-6.66	115.24	119.90
22	A1	41	A	C4-C5-C6	-6.66	113.67	117.00
53	BA	2654	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	87	C	N3-C2-O2	-6.65	117.24	121.90
53	BA	323	C	C1'-O4'-C4'	-6.65	104.58	109.90
53	BA	1967	C	O4'-C1'-N1	6.65	113.52	108.20
53	BA	2612	C	N3-C2-O2	-6.65	117.24	121.90
53	BA	959	A	C5-C6-N1	6.65	121.03	117.70
53	BA	1844	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	673	A	C5-C6-N1	6.65	121.02	117.70
21	AA	1322	C	N3-C2-O2	-6.65	117.25	121.90
53	BA	2225	A	N1-C6-N6	-6.65	114.61	118.60
21	AA	744	C	N3-C2-O2	-6.65	117.25	121.90
44	BW	10	ARG	NE-CZ-NH2	6.65	123.62	120.30
53	BA	84	A	C5-C6-N1	6.65	121.02	117.70
53	BA	1133	A	C4-C5-C6	-6.65	113.68	117.00
53	BA	1229	C	O4'-C1'-N1	6.65	113.52	108.20
53	BA	1803	A	C4-C5-C6	-6.65	113.68	117.00
53	BA	2746	U	O4'-C1'-N1	6.65	113.52	108.20
21	AA	665	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	823	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	1114	C	N3-C2-O2	-6.65	117.25	121.90
53	BA	1252	G	P-O3'-C3'	6.65	127.67	119.70
21	AA	1069	C	N3-C2-O2	-6.64	117.25	121.90
53	BA	2260	C	N3-C2-O2	-6.64	117.25	121.90
19	AT	9	ARG	NE-CZ-NH1	6.64	123.62	120.30
21	AA	306	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	1080	A	C4-C5-C6	-6.64	113.68	117.00
53	BA	104	A	C4-C5-C6	-6.64	113.68	117.00
53	BA	660	C	N3-C2-O2	-6.64	117.25	121.90
53	BA	1469	A	C6-C5-N7	6.64	136.95	132.30
53	BA	1881	C	O4'-C1'-N1	6.64	113.51	108.20
21	AA	1394	A	C4-C5-C6	-6.64	113.68	117.00
53	BA	1732	C	N3-C2-O2	-6.64	117.25	121.90
3	AD	80	ARG	NE-CZ-NH2	-6.64	116.98	120.30
21	AA	23	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	805	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	906	A	N1-C6-N6	-6.64	114.62	118.60
21	AA	1092	A	C4-C5-C6	-6.64	113.68	117.00
21	AA	1162	C	N3-C2-O2	-6.64	117.25	121.90
54	BB	113	C	N3-C2-O2	-6.64	117.25	121.90
53	BA	1053	C	O4'-C1'-N1	6.64	113.51	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	AK	105	ARG	NE-CZ-NH1	6.64	123.62	120.30
21	AA	156	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	223	A	C5-C6-N1	6.64	121.02	117.70
21	AA	732	C	N3-C2-O2	-6.64	117.25	121.90
53	BA	2873	A	N1-C6-N6	-6.64	114.62	118.60
21	AA	370	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	665	A	C5-C6-N1	6.63	121.02	117.70
21	AA	695	A	N1-C6-N6	-6.63	114.62	118.60
54	BB	53	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	1004	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	60	A	N1-C6-N6	-6.63	114.62	118.60
21	AA	511	C	N3-C2-O2	-6.63	117.26	121.90
32	BK	108	ARG	NE-CZ-NH1	6.63	123.61	120.30
53	BA	192	C	N1-C2-O2	6.63	122.88	118.90
53	BA	1641	A	C5-C6-N1	6.63	121.01	117.70
53	BA	1969	A	O4'-C1'-N9	6.63	113.50	108.20
53	BA	2241	A	C4-C5-C6	-6.63	113.69	117.00
53	BA	2429	G	C8-N9-C4	-6.63	103.75	106.40
53	BA	2587	A	C4-C5-C6	-6.63	113.69	117.00
53	BA	1691	C	N3-C2-O2	-6.62	117.26	121.90
53	BA	2008	C	N3-C2-O2	-6.62	117.26	121.90
53	BA	2133	G	C5-C6-N1	6.62	114.81	111.50
53	BA	581	C	N3-C2-O2	-6.62	117.26	121.90
53	BA	911	A	N1-C6-N6	-6.62	114.63	118.60
53	BA	1279	G	C5-C6-N1	6.62	114.81	111.50
53	BA	1634	A	C5-C6-N1	6.62	121.01	117.70
53	BA	2270	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	1192	C	O4'-C1'-N1	6.62	113.50	108.20
53	BA	1279	G	N1-C6-O6	-6.62	115.93	119.90
53	BA	1385	A	C4-C5-C6	-6.62	113.69	117.00
53	BA	2206	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	940	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	1508	A	C4-C5-C6	-6.62	113.69	117.00
43	BV	18	ARG	NE-CZ-NH1	6.62	123.61	120.30
53	BA	2759	G	N1-C6-O6	-6.62	115.93	119.90
21	AA	1252	A	C4-C5-C6	-6.62	113.69	117.00
53	BA	974	G	N9-C1'-C2'	6.62	122.60	114.00
53	BA	1615	C	N3-C2-O2	-6.62	117.27	121.90
53	BA	1918	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	285	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	910	C	O4'-C1'-N1	6.61	113.49	108.20
53	BA	575	A	N1-C6-N6	-6.61	114.63	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	998	C	N3-C2-O2	-6.61	117.27	121.90
3	AD	164	ARG	NE-CZ-NH1	6.61	123.61	120.30
21	AA	288	A	N1-C6-N6	-6.61	114.63	118.60
21	AA	1437	A	C5-C6-N1	6.61	121.00	117.70
53	BA	2285	C	N3-C2-O2	-6.61	117.27	121.90
53	BA	1787	A	N1-C6-N6	-6.61	114.64	118.60
53	BA	2749	A	C5-C6-N1	6.61	121.00	117.70
26	BE	49	ARG	NE-CZ-NH1	6.61	123.60	120.30
53	BA	2243	U	O4'-C1'-N1	6.61	113.49	108.20
21	AA	510	A	C4-C5-C6	-6.61	113.70	117.00
28	BG	2	ARG	NE-CZ-NH2	6.61	123.60	120.30
53	BA	2760	C	N3-C2-O2	-6.61	117.28	121.90
53	BA	1231	U	O4'-C1'-N1	6.60	113.48	108.20
53	BA	1664	A	C5-C6-N1	6.60	121.00	117.70
53	BA	2837	A	C5-C6-N1	6.60	121.00	117.70
53	BA	398	C	O4'-C1'-N1	6.60	113.48	108.20
53	BA	758	C	N3-C2-O2	-6.60	117.28	121.90
53	BA	1431	A	C5-C6-N1	6.60	121.00	117.70
53	BA	2070	A	C5-C6-N1	6.60	121.00	117.70
53	BA	1641	A	N1-C6-N6	-6.60	114.64	118.60
53	BA	2753	A	C4-C5-C6	-6.60	113.70	117.00
53	BA	1427	A	C5-C6-N1	6.60	121.00	117.70
21	AA	1115	U	O4'-C1'-N1	6.60	113.48	108.20
21	AA	1317	C	N1-C2-O2	6.60	122.86	118.90
53	BA	915	C	N3-C2-O2	-6.60	117.28	121.90
53	BA	951	C	N3-C2-O2	-6.60	117.28	121.90
53	BA	1470	A	C4-C5-C6	-6.60	113.70	117.00
53	BA	1001	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	746	A	C5-C6-N1	6.59	121.00	117.70
53	BA	1701	A	C4-C5-C6	-6.59	113.70	117.00
53	BA	1908	C	N3-C2-O2	-6.59	117.28	121.90
53	BA	143	C	N3-C2-O2	-6.59	117.28	121.90
21	AA	746	A	C4-C5-C6	-6.59	113.70	117.00
53	BA	415	A	C4-C5-C6	-6.59	113.70	117.00
53	BA	597	G	N1-C6-O6	-6.59	115.95	119.90
53	BA	829	A	C4-C5-C6	-6.59	113.70	117.00
53	BA	599	A	C4-C5-C6	-6.59	113.70	117.00
53	BA	1196	C	O4'-C1'-N1	6.59	113.47	108.20
53	BA	2896	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	816	A	N1-C6-N6	-6.59	114.65	118.60
53	BA	249	C	P-O3'-C3'	6.58	127.60	119.70
53	BA	1396	U	N3-C2-O2	-6.58	117.59	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1508	A	N1-C6-N6	-6.58	114.65	118.60
53	BA	2025	C	N3-C2-O2	-6.58	117.29	121.90
53	BA	733	G	N1-C6-O6	-6.58	115.95	119.90
53	BA	1685	C	O4'-C1'-N1	6.58	113.47	108.20
53	BA	1882	U	O4'-C1'-N1	6.58	113.47	108.20
21	AA	1284	C	O4'-C1'-N1	6.58	113.46	108.20
36	BO	33	ARG	NE-CZ-NH2	6.58	123.59	120.30
53	BA	245	G	C8-N9-C4	-6.58	103.77	106.40
53	BA	1611	C	N3-C2-O2	-6.58	117.29	121.90
14	AO	88	ARG	NE-CZ-NH1	6.58	123.59	120.30
21	AA	1479	C	N3-C2-O2	-6.58	117.30	121.90
53	BA	152	A	C4-C5-C6	-6.58	113.71	117.00
53	BA	516	C	N3-C2-O2	-6.58	117.29	121.90
53	BA	845	A	C5-C6-N1	6.58	120.99	117.70
54	BB	94	A	C5-C6-N1	6.58	120.99	117.70
21	AA	1521	C	N3-C4-C5	6.58	124.53	121.90
53	BA	1301	A	C2-N3-C4	6.58	113.89	110.60
21	AA	533	A	C3'-C2'-C1'	6.58	106.76	101.50
53	BA	1169	A	C5-C6-N1	6.58	120.99	117.70
53	BA	1180	U	O4'-C1'-N1	6.58	113.46	108.20
53	BA	1207	C	N3-C2-O2	-6.58	117.30	121.90
53	BA	1552	A	O4'-C1'-N9	6.58	113.46	108.20
53	BA	1652	A	C5-C6-N1	6.58	120.99	117.70
53	BA	2043	C	N1-C2-O2	6.58	122.84	118.90
53	BA	2171	A	C5-C6-N1	6.58	120.99	117.70
53	BA	776	G	O4'-C1'-N9	6.57	113.46	108.20
53	BA	828	U	N3-C2-O2	-6.57	117.60	122.20
53	BA	1415	U	O4'-C1'-N1	6.57	113.46	108.20
53	BA	2675	A	C4-C5-C6	-6.57	113.71	117.00
53	BA	558	U	O4'-C1'-N1	6.57	113.46	108.20
53	BA	477	A	C5-C6-N1	6.57	120.98	117.70
53	BA	743	A	C4-C5-C6	-6.57	113.72	117.00
53	BA	847	U	N3-C2-O2	-6.57	117.60	122.20
53	BA	111	A	C5-C6-N1	6.57	120.98	117.70
53	BA	1525	A	C5-C6-N1	6.57	120.98	117.70
53	BA	1545	A	C4-C5-C6	-6.57	113.72	117.00
53	BA	2405	G	N1-C6-O6	-6.57	115.96	119.90
19	AT	17	ARG	NE-CZ-NH1	6.57	123.58	120.30
21	AA	117	G	N1-C6-O6	-6.57	115.96	119.90
21	AA	448	A	C4-C5-C6	-6.57	113.72	117.00
53	BA	130	C	O4'-C1'-N1	6.57	113.45	108.20
53	BA	838	C	N1-C2-O2	6.57	122.84	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1275	A	C5-C6-N1	6.57	120.98	117.70
53	BA	1786	A	C5-C6-N1	6.57	120.98	117.70
53	BA	1990	C	N3-C2-O2	-6.57	117.31	121.90
53	BA	2142	A	C5-C6-N1	6.57	120.98	117.70
53	BA	2614	A	C5-C6-N1	6.57	120.98	117.70
21	AA	143	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	906	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	1448	C	N3-C2-O2	-6.56	117.31	121.90
53	BA	164	C	N3-C2-O2	-6.56	117.31	121.90
53	BA	300	A	C5-C6-N1	6.56	120.98	117.70
53	BA	2358	A	C5-C6-N1	6.56	120.98	117.70
53	BA	71	A	C5-C6-N1	6.56	120.98	117.70
21	AA	1492	A	C4-C5-C6	-6.56	113.72	117.00
50	B2	34	ARG	NE-CZ-NH2	-6.56	117.02	120.30
53	BA	145	C	O4'-C1'-N1	6.56	113.45	108.20
53	BA	2212	A	C5-C6-N1	6.56	120.98	117.70
53	BA	2650	U	O4'-C1'-N1	6.56	113.45	108.20
53	BA	2054	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	400	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	900	A	C5-C6-N1	6.56	120.98	117.70
53	BA	429	A	C4-C5-C6	-6.56	113.72	117.00
53	BA	1287	A	C3'-C2'-C1'	6.56	106.75	101.50
53	BA	2590	A	C5-C6-N1	6.56	120.98	117.70
21	AA	136	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	903	G	C8-N9-C4	-6.55	103.78	106.40
53	BA	126	A	C4-C5-C6	-6.55	113.72	117.00
53	BA	1909	C	N3-C2-O2	-6.55	117.31	121.90
53	BA	2352	A	C5-C6-N1	6.55	120.98	117.70
21	AA	587	G	N1-C6-O6	-6.55	115.97	119.90
21	AA	78	A	C5-C6-N1	6.55	120.97	117.70
33	BL	33	ARG	NE-CZ-NH1	6.55	123.57	120.30
53	BA	126	A	C5-C6-N1	6.55	120.97	117.70
53	BA	2263	C	N1-C2-O2	6.55	122.83	118.90
53	BA	2065	C	N3-C2-O2	-6.55	117.32	121.90
53	BA	2342	C	N3-C2-O2	-6.55	117.32	121.90
21	AA	461	A	C4-C5-C6	-6.55	113.73	117.00
53	BA	1920	C	N3-C2-O2	-6.55	117.32	121.90
21	AA	48	C	N1-C2-O2	6.54	122.83	118.90
21	AA	988	G	N1-C6-O6	-6.54	115.97	119.90
53	BA	759	G	N1-C6-O6	-6.54	115.97	119.90
53	BA	2448	A	C5-C6-N1	6.54	120.97	117.70
37	BP	52	ARG	NE-CZ-NH1	6.54	123.57	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	624	C	N3-C2-O2	-6.54	117.32	121.90
53	BA	1347	A	C4-C5-C6	-6.54	113.73	117.00
53	BA	1893	C	N3-C2-O2	-6.54	117.32	121.90
53	BA	2824	C	N3-C2-O2	-6.54	117.32	121.90
53	BA	919	U	O4'-C1'-N1	6.54	113.43	108.20
54	BB	104	A	C4-C5-C6	-6.54	113.73	117.00
53	BA	284	U	O4'-C1'-N1	6.54	113.43	108.20
21	AA	980	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	1521	C	N3-C2-O2	-6.54	117.32	121.90
53	BA	280	U	N3-C2-O2	-6.54	117.62	122.20
53	BA	541	A	C5-C6-N1	6.54	120.97	117.70
53	BA	2157	G	N3-C4-C5	-6.54	125.33	128.60
53	BA	2284	A	N1-C6-N6	-6.54	114.68	118.60
53	BA	83	A	C4-C5-C6	-6.54	113.73	117.00
53	BA	301	G	O4'-C1'-N9	6.54	113.43	108.20
53	BA	430	A	C5-C6-N1	6.54	120.97	117.70
53	BA	1023	U	O4'-C1'-N1	6.54	113.43	108.20
21	AA	1021	A	C5-C6-N1	6.53	120.97	117.70
53	BA	16	C	N3-C2-O2	-6.53	117.33	121.90
53	BA	627	A	C5-C6-N1	6.53	120.97	117.70
53	BA	2798	U	O4'-C1'-N1	6.53	113.43	108.20
54	BB	3	C	O4'-C1'-N1	6.53	113.43	108.20
53	BA	385	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	865	A	C6-C5-N7	6.53	136.87	132.30
21	AA	1063	C	C6-N1-C2	-6.53	117.69	120.30
22	A1	9	A	N1-C6-N6	-6.53	114.68	118.60
53	BA	2381	A	C4-C5-C6	-6.53	113.73	117.00
53	BA	2591	C	N3-C2-O2	-6.53	117.33	121.90
53	BA	761	A	C5-C6-N1	6.53	120.97	117.70
6	AG	108	ARG	NE-CZ-NH2	-6.53	117.04	120.30
21	AA	72	A	C4-C5-C6	-6.53	113.74	117.00
21	AA	493	A	C5-C6-N1	6.53	120.96	117.70
53	BA	1089	A	N1-C6-N6	-6.53	114.68	118.60
53	BA	1806	C	N3-C2-O2	-6.53	117.33	121.90
53	BA	2359	C	O4'-C1'-N1	6.53	113.42	108.20
21	AA	36	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	366	A	C5-C6-N1	6.53	120.96	117.70
21	AA	441	A	C5-C6-N1	6.53	120.96	117.70
21	AA	931	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1103	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1358	U	C5-C6-N1	-6.53	119.44	122.70
53	BA	1350	C	N3-C2-O2	-6.53	117.33	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1803	A	C5-C6-N1	6.53	120.96	117.70
21	AA	608	A	C4-C5-C6	-6.52	113.74	117.00
53	BA	1268	A	C5-C6-N1	6.52	120.96	117.70
53	BA	2250	G	N1-C6-O6	-6.52	115.99	119.90
21	AA	556	C	N3-C2-O2	-6.52	117.33	121.90
53	BA	226	A	C5-C6-N1	6.52	120.96	117.70
53	BA	2090	A	C4-C5-C6	-6.52	113.74	117.00
4	AE	44	ARG	NE-CZ-NH1	6.52	123.56	120.30
53	BA	95	A	C5-C6-N1	6.52	120.96	117.70
54	BB	101	A	C5-C6-N1	6.52	120.96	117.70
21	AA	356	A	C5-C6-N1	6.52	120.96	117.70
21	AA	383	A	C5-C6-N1	6.52	120.96	117.70
53	BA	1739	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	99	C	N3-C2-O2	-6.52	117.34	121.90
53	BA	1509	A	C5-C6-N1	6.52	120.96	117.70
21	AA	689	C	N3-C2-O2	-6.51	117.34	121.90
53	BA	753	A	C5-C6-N1	6.51	120.96	117.70
53	BA	1020	A	C5-C6-N1	6.51	120.96	117.70
53	BA	1941	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	1097	C	N3-C2-O2	-6.51	117.34	121.90
53	BA	1885	A	C4-C5-C6	-6.51	113.75	117.00
53	BA	2416	C	N3-C2-O2	-6.51	117.34	121.90
53	BA	2516	A	C4-C5-C6	-6.51	113.75	117.00
53	BA	2748	A	C4-C5-C6	-6.51	113.74	117.00
53	BA	74	A	C5-C6-N1	6.51	120.95	117.70
53	BA	2014	A	C5-C6-N1	6.51	120.95	117.70
53	BA	2477	U	O4'-C1'-N1	6.51	113.41	108.20
21	AA	532	A	C4-C5-C6	-6.51	113.75	117.00
53	BA	119	A	C4-C5-C6	-6.51	113.75	117.00
53	BA	1191	G	N3-C4-C5	-6.51	125.35	128.60
11	AL	8	ARG	NE-CZ-NH2	6.50	123.55	120.30
53	BA	933	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1172	C	N3-C2-O2	-6.50	117.35	121.90
54	BB	35	C	N3-C4-C5	6.50	124.50	121.90
21	AA	305	G	O4'-C1'-N9	6.50	113.40	108.20
21	AA	421	U	N3-C2-O2	-6.50	117.65	122.20
53	BA	492	A	C5-C6-N1	6.50	120.95	117.70
53	BA	2164	C	N1-C2-O2	6.50	122.80	118.90
53	BA	32	C	N3-C2-O2	-6.50	117.35	121.90
53	BA	1727	C	N3-C2-O2	-6.50	117.35	121.90
53	BA	2435	A	N1-C6-N6	-6.50	114.70	118.60
21	AA	374	A	N1-C6-N6	-6.50	114.70	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1269	A	C4-C5-C6	-6.50	113.75	117.00
53	BA	2449	U	O4'-C1'-N1	6.50	113.40	108.20
53	BA	2899	A	C5-C6-N1	6.50	120.95	117.70
21	AA	78	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	374	A	C5-C6-N1	6.50	120.95	117.70
21	AA	432	A	C5-C6-N1	6.50	120.95	117.70
53	BA	2177	C	N3-C2-O2	-6.50	117.35	121.90
22	A1	73	A	C5-C6-N1	6.50	120.95	117.70
21	AA	74	A	C5-C6-N1	6.49	120.95	117.70
53	BA	979	A	C5-C6-N1	6.49	120.95	117.70
53	BA	2741	A	C4-C5-C6	-6.49	113.75	117.00
53	BA	1937	A	O4'-C1'-N9	6.49	113.39	108.20
53	BA	2407	A	C5-C6-N1	6.49	120.95	117.70
21	AA	579	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	1225	A	C4-C5-C6	-6.49	113.75	117.00
31	BJ	95	ARG	NE-CZ-NH1	6.49	123.55	120.30
53	BA	405	U	O4'-C1'-N1	6.49	113.39	108.20
53	BA	2620	C	N3-C2-O2	-6.49	117.36	121.90
53	BA	721	A	C4-C5-C6	-6.49	113.75	117.00
53	BA	1354	A	C5-C6-N1	6.49	120.94	117.70
53	BA	1548	A	C5-C6-N1	6.49	120.94	117.70
22	A1	26	A	C4-C5-C6	-6.49	113.76	117.00
53	BA	328	U	O4'-C1'-N1	6.49	113.39	108.20
53	BA	1404	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	264	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	275	G	C5-C6-N1	6.48	114.74	111.50
21	AA	420	U	O4'-C1'-N1	6.48	113.39	108.20
21	AA	574	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	637	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	1107	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	1269	A	C4-C5-C6	-6.48	113.76	117.00
24	BC	213	ARG	NE-CZ-NH2	-6.48	117.06	120.30
53	BA	515	A	N1-C6-N6	-6.48	114.71	118.60
53	BA	1398	C	N3-C2-O2	-6.48	117.36	121.90
53	BA	2358	A	C4-C5-C6	-6.48	113.76	117.00
53	BA	764	A	N1-C6-N6	-6.48	114.71	118.60
53	BA	981	A	C5-C6-N1	6.48	120.94	117.70
53	BA	1079	C	N3-C2-O2	-6.48	117.36	121.90
53	BA	1564	C	N3-C2-O2	-6.48	117.37	121.90
21	AA	1328	C	N3-C2-O2	-6.47	117.37	121.90
53	BA	1558	C	N1-C2-O2	6.47	122.78	118.90
53	BA	2160	C	N3-C2-O2	-6.47	117.37	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2393	U	O4'-C1'-N1	6.47	113.38	108.20
53	BA	2578	G	N1-C6-O6	-6.47	116.02	119.90
21	AA	1501	C	N1-C2-O2	6.47	122.78	118.90
53	BA	2652	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	403	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	510	A	C5-C6-N1	6.47	120.94	117.70
21	AA	1529	G	C1'-O4'-C4'	-6.47	104.72	109.90
25	BD	128	ARG	NE-CZ-NH2	6.47	123.53	120.30
53	BA	372	G	C8-N9-C4	-6.47	103.81	106.40
53	BA	380	G	N1-C6-O6	-6.47	116.02	119.90
53	BA	1607	C	N1-C2-O2	6.47	122.78	118.90
21	AA	338	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	930	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1413	A	C5-C6-N1	6.47	120.93	117.70
53	BA	395	U	O4'-C1'-N1	6.47	113.37	108.20
53	BA	1144	A	C5-C6-N1	6.47	120.93	117.70
53	BA	1211	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	414	A	C4-C5-C6	-6.47	113.77	117.00
53	BA	147	C	N3-C2-O2	-6.46	117.37	121.90
53	BA	1832	C	N3-C2-O2	-6.46	117.37	121.90
53	BA	2616	C	N3-C2-O2	-6.46	117.38	121.90
53	BA	2822	G	N1-C6-O6	-6.46	116.02	119.90
53	BA	2681	C	N3-C4-C5	6.46	124.48	121.90
21	AA	502	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	728	A	N1-C6-N6	-6.46	114.72	118.60
53	BA	423	A	C5-C6-N1	6.46	120.93	117.70
21	AA	366	A	N1-C6-N6	-6.46	114.72	118.60
13	AN	90	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	223	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	976	G	C5-C6-N1	6.46	114.73	111.50
21	AA	1484	C	O4'-C1'-N1	6.46	113.37	108.20
53	BA	812	C	N1-C2-O2	6.46	122.78	118.90
53	BA	1357	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	1160	G	N3-C2-N2	-6.46	115.38	119.90
24	BC	166	ARG	NE-CZ-NH2	-6.46	117.07	120.30
53	BA	2318	G	N1-C6-O6	-6.46	116.03	119.90
21	AA	63	C	N3-C2-O2	-6.45	117.38	121.90
53	BA	735	A	C4-C5-C6	-6.45	113.77	117.00
53	BA	972	A	C4-C5-C6	-6.45	113.77	117.00
53	BA	1367	A	C5-C6-N1	6.45	120.93	117.70
53	BA	2736	A	C5-C6-N1	6.45	120.93	117.70
22	A1	64	U	O4'-C1'-N1	6.45	113.36	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	BF	149	ARG	NE-CZ-NH1	6.45	123.53	120.30
21	AA	869	G	C5-C6-N1	6.45	114.72	111.50
6	AG	142	ARG	NE-CZ-NH1	6.45	123.53	120.30
21	AA	602	A	C4-C5-C6	-6.45	113.78	117.00
53	BA	945	A	C5-C6-N1	6.45	120.92	117.70
53	BA	1528	A	C4-C5-C6	-6.45	113.78	117.00
53	BA	2404	U	O4'-C1'-N1	6.45	113.36	108.20
53	BA	658	U	O4'-C1'-N1	6.45	113.36	108.20
14	AO	71	ARG	NE-CZ-NH1	6.45	123.52	120.30
53	BA	332	A	N1-C6-N6	-6.45	114.73	118.60
53	BA	635	C	N1-C2-O2	6.44	122.77	118.90
53	BA	786	C	N1-C2-O2	6.44	122.77	118.90
53	BA	1269	A	N1-C6-N6	-6.44	114.73	118.60
53	BA	1610	A	C4-C5-C6	-6.44	113.78	117.00
53	BA	2225	A	O4'-C1'-N9	6.44	113.36	108.20
53	BA	2227	A	C5-C6-N1	6.44	120.92	117.70
16	AQ	10	ARG	NE-CZ-NH1	6.44	123.52	120.30
47	BZ	15	ARG	NE-CZ-NH2	-6.44	117.08	120.30
53	BA	1641	A	C4-C5-C6	-6.44	113.78	117.00
53	BA	204	A	C4-C5-C6	-6.44	113.78	117.00
53	BA	1699	G	N3-C2-N2	-6.44	115.39	119.90
53	BA	1893	C	O4'-C1'-N1	6.44	113.35	108.20
53	BA	941	A	C5'-C4'-O4'	6.44	116.83	109.10
53	BA	1821	A	C4-C5-C6	-6.44	113.78	117.00
53	BA	2814	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1433	A	C4-C5-C6	-6.44	113.78	117.00
53	BA	1943	U	O4'-C1'-N1	6.44	113.35	108.20
53	BA	2776	A	C5-C6-N1	6.44	120.92	117.70
53	BA	52	A	C5-C6-N1	6.44	120.92	117.70
53	BA	1518	C	N3-C2-O2	-6.44	117.39	121.90
53	BA	62	U	N3-C2-O2	-6.43	117.70	122.20
53	BA	1165	A	N1-C6-N6	-6.43	114.74	118.60
2	AC	125	ARG	NE-CZ-NH1	6.43	123.52	120.30
53	BA	1260	A	C4-C5-C6	-6.43	113.78	117.00
53	BA	2469	A	C4-C5-C6	-6.43	113.78	117.00
53	BA	1290	C	N3-C2-O2	-6.43	117.40	121.90
53	BA	1434	A	N1-C6-N6	-6.43	114.74	118.60
53	BA	1794	A	C4-C5-C6	-6.43	113.78	117.00
53	BA	1985	C	N3-C2-O2	-6.43	117.40	121.90
6	AG	91	ARG	NE-CZ-NH1	6.43	123.52	120.30
21	AA	1458	G	N1-C6-O6	-6.43	116.04	119.90
21	AA	1493	A	C4-C5-C6	-6.43	113.78	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	715	A	C5-C6-N1	6.43	120.92	117.70
53	BA	1051	G	C5-C6-N1	6.43	114.71	111.50
28	BG	162	ARG	NE-CZ-NH1	6.43	123.51	120.30
21	AA	69	G	C8-N9-C4	-6.43	103.83	106.40
53	BA	533	G	C8-N9-C4	-6.43	103.83	106.40
21	AA	301	G	O4'-C1'-N9	6.42	113.34	108.20
21	AA	336	A	C5-C6-N1	6.42	120.91	117.70
21	AA	1238	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1301	U	N3-C2-O2	-6.42	117.70	122.20
53	BA	196	A	C5-C6-N1	6.42	120.91	117.70
53	BA	1049	C	N3-C2-O2	-6.42	117.40	121.90
53	BA	1775	U	O4'-C1'-N1	6.42	113.34	108.20
53	BA	2556	C	N3-C2-O2	-6.42	117.40	121.90
13	AN	65	ARG	NE-CZ-NH1	6.42	123.51	120.30
21	AA	960	U	N3-C2-O2	-6.42	117.70	122.20
53	BA	66	C	N3-C2-O2	-6.42	117.40	121.90
53	BA	346	A	O4'-C1'-N9	6.42	113.34	108.20
53	BA	778	G	N3-C4-C5	-6.42	125.39	128.60
21	AA	719	C	N1-C2-O2	6.42	122.75	118.90
53	BA	825	A	C5-C6-N1	6.42	120.91	117.70
53	BA	1005	C	C6-N1-C2	-6.42	117.73	120.30
53	BA	2466	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	631	C	N1-C2-O2	6.42	122.75	118.90
53	BA	228	C	O4'-C1'-N1	6.42	113.34	108.20
53	BA	372	G	O4'-C1'-N9	6.42	113.33	108.20
53	BA	435	C	O4'-C1'-N1	6.42	113.33	108.20
53	BA	564	C	N3-C2-O2	-6.42	117.41	121.90
53	BA	1843	C	N1-C2-O2	6.42	122.75	118.90
53	BA	179	C	N3-C2-O2	-6.42	117.41	121.90
53	BA	433	C	O4'-C1'-N1	6.42	113.33	108.20
53	BA	633	A	C4-C5-C6	-6.42	113.79	117.00
53	BA	897	C	N3-C4-C5	6.42	124.47	121.90
53	BA	2482	A	C5-C6-N1	6.42	120.91	117.70
53	BA	2108	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	492	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	909	A	N1-C6-N6	-6.41	114.75	118.60
21	AA	1443	C	N3-C2-O2	-6.41	117.41	121.90
53	BA	226	A	N1-C6-N6	-6.41	114.75	118.60
53	BA	255	A	C4-C5-C6	-6.41	113.79	117.00
53	BA	13	A	C4-C5-C6	-6.41	113.79	117.00
53	BA	1162	G	N1-C6-O6	-6.41	116.05	119.90
21	AA	73	C	N3-C2-O2	-6.41	117.41	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1037	C	N1-C2-O2	6.41	122.75	118.90
21	AA	1298	U	N3-C2-O2	-6.41	117.71	122.20
53	BA	318	C	N3-C2-O2	-6.41	117.41	121.90
53	BA	1656	C	N1-C2-O2	6.41	122.75	118.90
53	BA	2825	G	N3-C2-N2	-6.41	115.41	119.90
7	AH	116	ARG	NE-CZ-NH1	6.41	123.50	120.30
53	BA	1490	A	O4'-C1'-N9	6.41	113.33	108.20
53	BA	2347	C	O4'-C1'-N1	6.41	113.33	108.20
53	BA	2887	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	36	C	N1-C2-O2	6.41	122.74	118.90
53	BA	632	A	C5-C6-N1	6.41	120.90	117.70
21	AA	614	C	O4'-C1'-N1	6.40	113.32	108.20
22	A1	18	G	O4'-C1'-N9	6.40	113.32	108.20
53	BA	808	G	O4'-C1'-N9	6.40	113.32	108.20
53	BA	1007	C	N3-C2-O2	-6.40	117.42	121.90
53	BA	1515	A	C4-C5-C6	-6.40	113.80	117.00
53	BA	219	A	C6-C5-N7	6.40	136.78	132.30
53	BA	1006	C	N3-C2-O2	-6.40	117.42	121.90
53	BA	1752	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	518	C	N3-C2-O2	-6.40	117.42	121.90
53	BA	820	A	C4-C5-C6	-6.40	113.80	117.00
53	BA	944	C	N3-C2-O2	-6.40	117.42	121.90
53	BA	43	G	C8-N9-C4	-6.40	103.84	106.40
53	BA	240	C	N1-C2-O2	6.40	122.74	118.90
53	BA	772	C	O4'-C1'-N1	6.40	113.32	108.20
53	BA	964	C	N3-C2-O2	-6.40	117.42	121.90
53	BA	1922	G	N1-C6-O6	-6.40	116.06	119.90
21	AA	693	G	N3-C4-C5	-6.40	125.40	128.60
21	AA	519	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	770	C	O4'-C1'-N1	6.39	113.31	108.20
53	BA	1128	G	O4'-C1'-N9	6.39	113.31	108.20
53	BA	2140	G	N1-C6-O6	-6.39	116.06	119.90
53	BA	1318	U	O4'-C1'-N1	6.39	113.31	108.20
21	AA	307	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	978	A	C5-C6-N1	6.39	120.89	117.70
21	AA	1456	A	C4-C5-C6	-6.39	113.81	117.00
21	AA	1254	A	C4-C5-C6	-6.39	113.81	117.00
22	A1	65	C	N3-C2-O2	-6.39	117.43	121.90
45	BX	27	ARG	NE-CZ-NH1	6.39	123.50	120.30
53	BA	892	A	N1-C6-N6	-6.39	114.77	118.60
53	BA	1703	G	N1-C6-O6	-6.39	116.07	119.90
53	BA	2887	A	C5-C6-N1	6.39	120.89	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1161	C	O4'-C1'-N1	6.39	113.31	108.20
53	BA	1257	C	N3-C2-O2	-6.39	117.43	121.90
53	BA	2602	A	C5-C6-N1	6.39	120.89	117.70
21	AA	993	G	O4'-C1'-N9	6.38	113.31	108.20
53	BA	621	A	C5-C6-N1	6.38	120.89	117.70
53	BA	895	U	O4'-C1'-N1	6.38	113.31	108.20
53	BA	1795	C	O4'-C1'-N1	6.38	113.31	108.20
53	BA	783	A	C5'-C4'-O4'	6.38	116.76	109.10
53	BA	1644	C	N3-C2-O2	-6.38	117.43	121.90
53	BA	2261	C	O4'-C1'-N1	6.38	113.31	108.20
53	BA	97	C	N3-C2-O2	-6.38	117.43	121.90
54	BB	52	A	N1-C6-N6	-6.38	114.77	118.60
21	AA	197	A	N1-C6-N6	-6.38	114.77	118.60
21	AA	225	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	256	U	O4'-C1'-N1	6.38	113.30	108.20
21	AA	934	C	N1-C2-O2	6.38	122.73	118.90
26	BE	79	ARG	NE-CZ-NH1	6.38	123.49	120.30
53	BA	906	U	O4'-C1'-N1	6.38	113.30	108.20
53	BA	2579	C	N3-C2-O2	-6.38	117.44	121.90
53	BA	2757	A	C5-C6-N1	6.38	120.89	117.70
28	BG	68	ARG	NE-CZ-NH1	6.38	123.49	120.30
53	BA	1987	A	C5-C6-N1	6.38	120.89	117.70
53	BA	1548	A	C4-C5-C6	-6.38	113.81	117.00
53	BA	1574	C	N1-C2-O2	6.38	122.72	118.90
53	BA	1686	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	25	C	N3-C2-O2	-6.37	117.44	121.90
53	BA	161	A	C4-C5-C6	-6.37	113.81	117.00
53	BA	584	C	N3-C2-O2	-6.37	117.44	121.90
53	BA	632	A	N1-C6-N6	-6.37	114.78	118.60
53	BA	2059	A	C5-C6-N1	6.37	120.89	117.70
53	BA	2791	G	N1-C6-O6	-6.37	116.08	119.90
55	B5	60	ARG	NE-CZ-NH2	6.37	123.49	120.30
21	AA	271	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	889	A	C4-C5-C6	-6.37	113.81	117.00
53	BA	1127	A	C4-C5-C6	-6.37	113.81	117.00
53	BA	2430	A	C4-C5-C6	-6.37	113.81	117.00
53	BA	2526	G	N1-C6-O6	-6.37	116.08	119.90
21	AA	216	U	O4'-C1'-N1	6.37	113.30	108.20
21	AA	539	A	C5-C6-N1	6.37	120.89	117.70
53	BA	885	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	205	A	C5-C6-N1	6.37	120.89	117.70
21	AA	335	C	N3-C2-O2	-6.37	117.44	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1368	A	C4-C5-C6	-6.37	113.81	117.00
53	BA	582	A	C5-C6-N1	6.37	120.88	117.70
53	BA	2193	G	O4'-C1'-N9	6.37	113.30	108.20
53	BA	1600	C	N3-C2-O2	-6.37	117.44	121.90
53	BA	90	U	O4'-C1'-N1	6.37	113.29	108.20
53	BA	2339	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1250	A	C5-C6-N1	6.36	120.88	117.70
53	BA	2879	A	O4'-C1'-N9	6.36	113.29	108.20
54	BB	60	C	N3-C2-O2	-6.36	117.44	121.90
14	AO	76	ARG	NE-CZ-NH2	-6.36	117.12	120.30
53	BA	772	C	N3-C2-O2	-6.36	117.45	121.90
53	BA	1592	C	N3-C2-O2	-6.36	117.45	121.90
53	BA	1733	G	C5-C6-N1	6.36	114.68	111.50
53	BA	2054	A	C5-C6-N1	6.36	120.88	117.70
53	BA	2199	A	C5-C6-N1	6.36	120.88	117.70
21	AA	84	U	O4'-C1'-N1	6.36	113.29	108.20
21	AA	1407	C	N3-C2-O2	-6.36	117.45	121.90
53	BA	282	A	C5-C6-N1	6.36	120.88	117.70
53	BA	732	C	O4'-C1'-N1	6.36	113.29	108.20
53	BA	1104	C	N3-C2-O2	-6.36	117.45	121.90
53	BA	2087	G	C5-C6-N1	6.36	114.68	111.50
53	BA	2101	A	C5-C6-N1	6.36	120.88	117.70
21	AA	274	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	1513	A	C5-C6-N1	6.36	120.88	117.70
53	BA	1974	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	119	A	C4-C5-C6	-6.36	113.82	117.00
53	BA	1698	A	C5-C6-N1	6.36	120.88	117.70
53	BA	267	C	N3-C2-O2	-6.36	117.45	121.90
53	BA	650	C	N1-C2-O2	6.36	122.71	118.90
21	AA	1521	C	N1-C2-O2	6.35	122.71	118.90
34	BM	38	ARG	NE-CZ-NH1	6.35	123.48	120.30
53	BA	1744	A	C5-C6-N1	6.35	120.88	117.70
21	AA	417	G	N1-C6-O6	-6.35	116.09	119.90
21	AA	1171	A	C4-C5-C6	-6.35	113.82	117.00
53	BA	626	A	C4-C5-C6	-6.35	113.82	117.00
53	BA	2029	G	C8-N9-C4	-6.35	103.86	106.40
53	BA	2152	G	C5-C6-N1	6.35	114.68	111.50
21	AA	1237	C	N3-C2-O2	-6.35	117.45	121.90
53	BA	25	U	O4'-C1'-N1	6.35	113.28	108.20
53	BA	181	A	C5-C6-N1	6.35	120.88	117.70
53	BA	2006	C	C6-N1-C2	-6.35	117.76	120.30
21	AA	328	C	N3-C2-O2	-6.35	117.46	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	575	G	P-O3'-C3'	6.35	127.32	119.70
21	AA	733	G	N1-C6-O6	-6.35	116.09	119.90
39	BR	79	ARG	NE-CZ-NH2	6.35	123.47	120.30
53	BA	231	A	C4-C5-C6	-6.35	113.83	117.00
53	BA	644	A	C4-C5-C6	-6.35	113.83	117.00
53	BA	1640	A	C4-C5-C6	-6.35	113.83	117.00
54	BB	8	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	640	A	C5-C6-N1	6.35	120.87	117.70
53	BA	1386	C	N3-C2-O2	-6.35	117.46	121.90
53	BA	1389	G	O4'-C1'-N9	6.35	113.28	108.20
53	BA	1591	A	C6-C5-N7	6.35	136.74	132.30
53	BA	1749	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	188	C	N1-C2-O2	6.34	122.71	118.90
21	AA	716	A	C5-C6-N1	6.34	120.87	117.70
21	AA	733	G	O4'-C1'-N9	6.34	113.28	108.20
22	A1	31	C	N3-C2-O2	-6.34	117.46	121.90
53	BA	49	A	C5-C6-N1	6.34	120.87	117.70
53	BA	201	C	N3-C4-C5	6.34	124.44	121.90
53	BA	1032	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	2027	G	N1-C6-O6	-6.34	116.09	119.90
53	BA	622	G	N3-C4-C5	-6.34	125.43	128.60
53	BA	819	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	971	G	N1-C6-O6	-6.34	116.10	119.90
53	BA	1351	C	N3-C2-O2	-6.34	117.46	121.90
53	BA	1711	A	N1-C6-N6	-6.34	114.80	118.60
53	BA	1801	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	2277	G	C8-N9-C4	-6.34	103.86	106.40
53	BA	2455	G	C8-N9-C4	-6.34	103.86	106.40
21	AA	178	C	O4'-C1'-N1	6.34	113.27	108.20
45	BX	56	ARG	NE-CZ-NH2	-6.34	117.13	120.30
53	BA	1269	A	C5-C6-N1	6.34	120.87	117.70
53	BA	2721	A	C4-C5-C6	-6.34	113.83	117.00
25	BD	46	ARG	NE-CZ-NH1	6.34	123.47	120.30
53	BA	510	C	N3-C2-O2	-6.34	117.46	121.90
53	BA	679	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	635	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	190	A	N1-C6-N6	-6.34	114.80	118.60
53	BA	1496	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	2725	A	C4-C5-C6	-6.34	113.83	117.00
53	BA	2753	A	C5-C6-N1	6.34	120.87	117.70
53	BA	2825	G	C8-N9-C4	-6.34	103.86	106.40
54	BB	71	C	N3-C2-O2	-6.34	117.46	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	241	G	C5-C6-N1	6.33	114.67	111.50
53	BA	749	A	C4-C5-C6	-6.33	113.83	117.00
53	BA	995	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	560	A	C4-C5-C6	-6.33	113.83	117.00
21	AA	1263	C	N3-C2-O2	-6.33	117.47	121.90
53	BA	1508	A	C4-C5-C6	-6.33	113.83	117.00
53	BA	2041	U	O4'-C1'-N1	6.33	113.27	108.20
21	AA	568	G	N1-C6-O6	-6.33	116.10	119.90
53	BA	504	A	O4'-C1'-N9	6.33	113.27	108.20
53	BA	2582	G	C8-N9-C4	-6.33	103.87	106.40
54	BB	19	C	N3-C2-O2	-6.33	117.47	121.90
53	BA	2585	U	N1-C1'-C2'	-6.33	105.04	112.00
21	AA	207	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	251	G	C5-C6-N1	6.33	114.66	111.50
21	AA	1254	A	N1-C6-N6	-6.33	114.80	118.60
53	BA	256	A	C5-C6-N1	6.33	120.86	117.70
53	BA	984	A	C4-C5-C6	-6.33	113.83	117.00
53	BA	1762	A	C4-C5-C6	-6.33	113.84	117.00
53	BA	2205	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	381	C	N1-C2-O2	6.33	122.70	118.90
21	AA	1044	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	1480	A	C4-C5-C6	-6.33	113.84	117.00
53	BA	501	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	519	C	C3'-C2'-C1'	6.33	106.56	101.50
21	AA	1176	A	C4-C5-C6	-6.33	113.84	117.00
53	BA	787	C	N3-C4-C5	6.33	124.43	121.90
53	BA	899	A	C5-C6-N1	6.33	120.86	117.70
53	BA	1158	C	N1-C2-O2	6.33	122.69	118.90
53	BA	1936	A	C4-C5-C6	-6.33	113.84	117.00
53	BA	343	C	N3-C2-O2	-6.32	117.47	121.90
53	BA	753	A	C4-C5-C6	-6.32	113.84	117.00
53	BA	1140	C	C3'-C2'-C1'	6.32	106.56	101.50
53	BA	2095	A	C4-C5-C6	-6.32	113.84	117.00
53	BA	514	A	C4-C5-C6	-6.32	113.84	117.00
53	BA	727	A	C5-C6-N1	6.32	120.86	117.70
53	BA	2288	A	C5-C6-N1	6.32	120.86	117.70
53	BA	2534	A	C4-C5-C6	-6.32	113.84	117.00
23	A2	79	A	C4-C5-C6	-6.32	113.84	117.00
53	BA	1414	C	O4'-C1'-N1	6.32	113.25	108.20
53	BA	1552	A	N1-C6-N6	-6.32	114.81	118.60
3	AD	183	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	523	A	C5-C6-N1	6.32	120.86	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1665	A	N1-C6-N6	-6.32	114.81	118.60
21	AA	49	U	O4'-C1'-N1	6.32	113.25	108.20
21	AA	844	G	C5-C6-N1	6.32	114.66	111.50
54	BB	118	C	O4'-C1'-N1	6.32	113.25	108.20
53	BA	739	A	C5-C6-N1	6.31	120.86	117.70
53	BA	1088	A	C5-C6-N1	6.31	120.86	117.70
40	BS	25	ARG	NE-CZ-NH1	6.31	123.46	120.30
53	BA	2901	C	N3-C2-O2	-6.31	117.48	121.90
54	BB	31	C	C6-N1-C2	-6.31	117.78	120.30
21	AA	498	A	C5-C6-N1	6.31	120.86	117.70
21	AA	750	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	1352	C	N1-C2-O2	6.31	122.69	118.90
50	B2	12	ARG	NE-CZ-NH2	6.31	123.46	120.30
53	BA	2383	G	C5-C6-N1	6.31	114.66	111.50
38	BQ	47	ARG	NE-CZ-NH1	6.31	123.45	120.30
53	BA	115	C	N3-C2-O2	-6.31	117.48	121.90
53	BA	484	C	N3-C2-O2	-6.31	117.48	121.90
53	BA	2332	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	321	A	C4-C5-C6	-6.31	113.85	117.00
53	BA	559	G	O4'-C1'-N9	6.31	113.25	108.20
21	AA	338	A	N1-C6-N6	-6.30	114.82	118.60
44	BW	40	ARG	NE-CZ-NH1	6.30	123.45	120.30
53	BA	1934	C	N3-C2-O2	-6.30	117.49	121.90
53	BA	2029	G	N7-C8-N9	6.30	116.25	113.10
21	AA	1398	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	285	C	O4'-C1'-N1	6.30	113.24	108.20
21	AA	411	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	807	A	C4-C5-C6	-6.30	113.85	117.00
53	BA	922	C	N3-C2-O2	-6.30	117.49	121.90
53	BA	957	C	N3-C4-C5	6.30	124.42	121.90
34	BM	44	ARG	NE-CZ-NH1	6.30	123.45	120.30
53	BA	296	U	O4'-C1'-N1	6.30	113.24	108.20
53	BA	848	C	N3-C2-O2	-6.30	117.49	121.90
53	BA	1544	A	C4-C5-C6	-6.30	113.85	117.00
53	BA	1783	A	C4-C5-C6	-6.30	113.85	117.00
53	BA	1848	A	C5-C6-N1	6.30	120.85	117.70
53	BA	2298	A	C5-C6-N1	6.30	120.85	117.70
21	AA	836	G	N1-C6-O6	-6.30	116.12	119.90
53	BA	398	C	N3-C2-O2	-6.30	117.49	121.90
53	BA	1064	C	N3-C2-O2	-6.30	117.49	121.90
53	BA	1070	A	C5-C6-N1	6.30	120.85	117.70
21	AA	861	G	C5-C6-N1	6.29	114.65	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1983	G	N3-C4-C5	-6.29	125.45	128.60
26	BE	40	ARG	NE-CZ-NH1	6.29	123.45	120.30
53	BA	715	A	C4-C5-C6	-6.29	113.85	117.00
53	BA	1243	C	N1-C2-O2	6.29	122.68	118.90
53	BA	1461	C	N3-C2-O2	-6.29	117.50	121.90
53	BA	1618	A	C5-C6-N1	6.29	120.85	117.70
53	BA	2521	C	N3-C2-O2	-6.29	117.49	121.90
53	BA	1539	U	C1'-O4'-C4'	-6.29	104.87	109.90
53	BA	1735	A	C4-C5-C6	-6.29	113.85	117.00
53	BA	2033	A	C6-C5-N7	6.29	136.70	132.30
53	BA	2758	A	C4-C5-C6	-6.29	113.85	117.00
53	BA	2764	A	C5-C6-N1	6.29	120.85	117.70
53	BA	1677	A	C4-C5-C6	-6.29	113.86	117.00
53	BA	1879	C	N1-C2-O2	6.29	122.67	118.90
53	BA	633	A	C5-C6-N1	6.29	120.84	117.70
53	BA	2270	A	N1-C6-N6	-6.29	114.83	118.60
53	BA	2551	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	1303	C	N3-C2-O2	-6.29	117.50	121.90
53	BA	975	A	C4-C5-C6	-6.29	113.86	117.00
32	BK	49	ARG	NE-CZ-NH1	6.29	123.44	120.30
53	BA	817	C	N1-C2-O2	6.29	122.67	118.90
53	BA	1142	A	C4-C5-C6	-6.29	113.86	117.00
53	BA	1868	C	N3-C2-O2	-6.29	117.50	121.90
53	BA	2626	C	O4'-C1'-N1	6.29	113.23	108.20
23	A2	88	U	C5-C6-N1	-6.28	119.56	122.70
53	BA	334	C	N3-C2-O2	-6.28	117.50	121.90
53	BA	870	U	O4'-C1'-N1	6.28	113.23	108.20
53	BA	1146	C	N3-C2-O2	-6.28	117.50	121.90
53	BA	1172	C	O4'-C1'-N1	6.28	113.23	108.20
21	AA	563	A	C4-C5-C6	-6.28	113.86	117.00
53	BA	1216	G	N1-C6-O6	-6.28	116.13	119.90
21	AA	434	U	O4'-C1'-N1	6.28	113.22	108.20
53	BA	508	A	C4-C5-C6	-6.28	113.86	117.00
53	BA	1429	G	N1-C6-O6	-6.28	116.13	119.90
53	BA	2146	C	N1-C2-O2	6.28	122.67	118.90
21	AA	40	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	10	A	C5-C6-N1	6.28	120.84	117.70
21	AA	430	A	N1-C6-N6	-6.28	114.83	118.60
21	AA	1325	C	N3-C2-O2	-6.28	117.51	121.90
21	AA	1255	G	O4'-C1'-N9	6.28	113.22	108.20
21	AA	1300	G	O4'-C1'-N9	6.28	113.22	108.20
21	AA	1331	G	N9-C4-C5	6.28	107.91	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	322	A	C5-C6-N1	6.28	120.84	117.70
53	BA	459	U	O4'-C1'-N1	6.28	113.22	108.20
53	BA	1536	C	N1-C2-O2	6.28	122.67	118.90
53	BA	2215	C	N3-C2-O2	-6.28	117.51	121.90
53	BA	2856	A	N1-C6-N6	-6.28	114.83	118.60
54	BB	61	G	N3-C2-N2	-6.28	115.51	119.90
21	AA	195	A	C6-C5-N7	6.27	136.69	132.30
21	AA	82	G	N1-C6-O6	-6.27	116.14	119.90
53	BA	19	A	C5-C6-N1	6.27	120.84	117.70
53	BA	788	A	C5-C6-N1	6.27	120.84	117.70
53	BA	1244	A	N1-C6-N6	-6.27	114.84	118.60
53	BA	2432	A	C5-C6-N1	6.27	120.84	117.70
53	BA	601	C	N3-C2-O2	-6.27	117.51	121.90
53	BA	2095	A	C5-C6-N1	6.27	120.83	117.70
53	BA	2146	C	N3-C2-O2	-6.27	117.51	121.90
53	BA	2495	G	C5-C6-N1	6.27	114.64	111.50
53	BA	901	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	430	A	C4-C5-C6	-6.27	113.87	117.00
21	AA	1404	C	N3-C2-O2	-6.27	117.51	121.90
22	A1	20	G	O4'-C1'-N9	6.27	113.21	108.20
53	BA	150	U	O4'-C1'-N1	6.27	113.21	108.20
53	BA	203	A	C5-C6-N1	6.27	120.83	117.70
53	BA	1561	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	667	G	N9-C4-C5	6.27	107.91	105.40
53	BA	908	C	N1-C2-O2	6.27	122.66	118.90
21	AA	1362	A	C5-C6-N1	6.26	120.83	117.70
53	BA	575	A	C4-C5-C6	-6.26	113.87	117.00
53	BA	1320	C	C6-N1-C2	-6.26	117.79	120.30
21	AA	18	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	996	A	C5-C6-N1	6.26	120.83	117.70
21	AA	1296	C	N3-C2-O2	-6.26	117.52	121.90
53	BA	322	A	C4-C5-C6	-6.26	113.87	117.00
53	BA	1431	A	C4-C5-C6	-6.26	113.87	117.00
53	BA	2556	C	O4'-C1'-N1	6.26	113.21	108.20
21	AA	308	C	N3-C2-O2	-6.26	117.52	121.90
53	BA	1730	C	N1-C2-O2	6.26	122.66	118.90
53	BA	2000	C	N1-C2-O2	6.26	122.66	118.90
53	BA	2738	A	C5-C6-N1	6.26	120.83	117.70
53	BA	2322	A	C5-C6-N1	6.26	120.83	117.70
53	BA	497	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	311	C	N1-C2-O2	6.26	122.65	118.90
21	AA	590	U	O4'-C1'-N1	6.26	113.20	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1038	C	N1-C2-O2	6.26	122.65	118.90
22	A1	69	A	C4-C5-C6	-6.26	113.87	117.00
53	BA	397	U	O4'-C1'-N1	6.26	113.20	108.20
53	BA	1647	U	N1-C2-N3	6.26	118.65	114.90
21	AA	435	A	C5-C6-N1	6.25	120.83	117.70
53	BA	1614	A	O4'-C1'-N9	6.25	113.20	108.20
53	BA	2214	C	N1-C2-O2	6.25	122.65	118.90
53	BA	2258	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	28	A	C4-C5-C6	-6.25	113.87	117.00
53	BA	236	C	N1-C2-O2	6.25	122.65	118.90
53	BA	1272	A	C5-C6-N1	6.25	120.83	117.70
53	BA	1757	A	C5-C6-N1	6.25	120.83	117.70
53	BA	1993	U	C5-C6-N1	-6.25	119.57	122.70
21	AA	1105	A	C5-C6-N1	6.25	120.83	117.70
35	BN	71	ARG	NE-CZ-NH2	6.25	123.43	120.30
53	BA	739	A	C4-C5-C6	-6.25	113.88	117.00
53	BA	2879	A	C4-C5-C6	-6.25	113.87	117.00
7	AH	87	ARG	NE-CZ-NH1	6.25	123.42	120.30
53	BA	177	G	N3-C4-C5	-6.25	125.47	128.60
53	BA	570	G	C1'-O4'-C4'	-6.25	104.90	109.90
53	BA	732	C	N3-C2-O2	-6.25	117.53	121.90
53	BA	1965	C	N3-C2-O2	-6.25	117.53	121.90
53	BA	2346	A	C5-C6-N1	6.25	120.82	117.70
21	AA	277	C	O4'-C1'-N1	6.25	113.20	108.20
53	BA	524	G	O4'-C1'-N9	6.25	113.20	108.20
53	BA	2646	C	N1-C2-O2	6.25	122.65	118.90
54	BB	42	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	1331	G	O4'-C1'-N9	6.24	113.19	108.20
53	BA	426	C	N3-C2-O2	-6.24	117.53	121.90
53	BA	610	C	N3-C2-O2	-6.24	117.53	121.90
53	BA	1743	G	C5-C6-N1	6.24	114.62	111.50
21	AA	850	U	C5-C6-N1	-6.24	119.58	122.70
53	BA	1353	A	C4-C5-C6	-6.24	113.88	117.00
53	BA	2086	U	O4'-C1'-N1	6.24	113.19	108.20
53	BA	2350	C	O4'-C1'-N1	6.24	113.19	108.20
21	AA	272	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	1480	A	C5-C6-N1	6.24	120.82	117.70
53	BA	1551	A	C4-C5-C6	-6.24	113.88	117.00
53	BA	2866	U	O4'-C1'-N1	6.24	113.19	108.20
53	BA	1059	G	O4'-C1'-N9	6.24	113.19	108.20
53	BA	1270	C	O4'-C1'-N1	6.24	113.19	108.20
53	BA	2119	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(^{o})	Ideal(^{o})
21	AA	1369	C	O4'-C1'-N1	6.24	113.19	108.20
43	BV	19	ARG	NH1-CZ-NH2	-6.24	112.54	119.40
21	AA	784	A	N1-C6-N6	-6.23	114.86	118.60
21	AA	1094	G	O4'-C1'-N9	6.23	113.19	108.20
53	BA	1526	C	N3-C2-O2	-6.23	117.54	121.90
11	AL	109	ARG	NE-CZ-NH1	6.23	123.42	120.30
21	AA	1310	G	N1-C6-O6	-6.23	116.16	119.90
21	AA	1428	A	C4-C5-C6	-6.23	113.88	117.00
53	BA	429	A	C5-C6-N1	6.23	120.82	117.70
53	BA	1336	A	C5-C6-N1	6.23	120.82	117.70
53	BA	1936	A	C5-C6-N1	6.23	120.82	117.70
54	BB	68	C	N3-C2-O2	-6.23	117.54	121.90
53	BA	1732	C	N1-C2-O2	6.23	122.64	118.90
53	BA	2657	A	C5-C6-N1	6.23	120.81	117.70
21	AA	708	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1379	G	N1-C6-O6	-6.23	116.16	119.90
22	A1	59	U	N3-C2-O2	-6.23	117.84	122.20
53	BA	1142	A	P-O3'-C3'	6.23	127.17	119.70
21	AA	962	C	N3-C2-O2	-6.23	117.54	121.90
53	BA	1472	C	N3-C2-O2	-6.23	117.54	121.90
12	AM	56	ARG	NE-CZ-NH1	6.22	123.41	120.30
21	AA	16	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	336	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1150	A	C5-C6-N1	6.22	120.81	117.70
53	BA	314	C	N3-C2-O2	-6.22	117.54	121.90
53	BA	608	A	C4-C5-C6	-6.22	113.89	117.00
53	BA	2341	G	C5-C6-N1	6.22	114.61	111.50
53	BA	2589	A	O4'-C1'-N9	6.22	113.18	108.20
53	BA	2781	A	C4-C5-C6	-6.22	113.89	117.00
53	BA	1103	A	C4-C5-C6	-6.22	113.89	117.00
53	BA	2777	G	C5-C6-N1	6.22	114.61	111.50
53	BA	402	A	N1-C6-N6	-6.22	114.87	118.60
53	BA	483	A	N1-C6-N6	-6.22	114.87	118.60
53	BA	840	C	N3-C2-O2	-6.22	117.55	121.90
53	BA	1028	A	N1-C6-N6	-6.22	114.87	118.60
21	AA	1517	G	C5-C6-N1	6.22	114.61	111.50
53	BA	1363	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	422	C	N3-C2-O2	-6.22	117.55	121.90
53	BA	125	A	O4'-C1'-N9	6.22	113.17	108.20
53	BA	1679	A	C5-C6-N1	6.22	120.81	117.70
53	BA	1854	A	C5-C6-N1	6.22	120.81	117.70
53	BA	1998	A	C5-C6-N1	6.22	120.81	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2446	G	C5-C6-N1	6.22	114.61	111.50
3	AD	43	ARG	NE-CZ-NH1	6.21	123.41	120.30
53	BA	800	A	C4-C5-C6	-6.21	113.89	117.00
54	BB	44	G	C5-C6-N1	6.21	114.61	111.50
21	AA	739	C	N1-C2-O2	6.21	122.63	118.90
53	BA	1945	G	N1-C6-O6	-6.21	116.17	119.90
21	AA	251	G	N1-C6-O6	-6.21	116.17	119.90
53	BA	2681	C	N3-C2-O2	-6.21	117.55	121.90
53	BA	1830	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1141	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	1483	A	C4-C5-C6	-6.21	113.90	117.00
53	BA	2072	C	O4'-C1'-N1	6.21	113.17	108.20
21	AA	932	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1350	A	O4'-C1'-N9	6.21	113.17	108.20
53	BA	66	C	O4'-C1'-N1	6.21	113.17	108.20
53	BA	820	A	C5-C6-N1	6.21	120.80	117.70
53	BA	1938	A	C4-C5-C6	-6.21	113.90	117.00
53	BA	918	A	C5-C6-N1	6.21	120.80	117.70
53	BA	1116	G	N9-C4-C5	6.21	107.88	105.40
53	BA	1960	A	C5-C6-N1	6.21	120.80	117.70
21	AA	373	A	N1-C6-N6	-6.20	114.88	118.60
53	BA	1136	G	N3-C4-C5	-6.20	125.50	128.60
21	AA	109	A	C4-C5-C6	-6.20	113.90	117.00
22	A1	71	C	N3-C2-O2	-6.20	117.56	121.90
53	BA	49	A	P-O3'-C3'	6.20	127.14	119.70
53	BA	709	U	O4'-C1'-N1	6.20	113.16	108.20
27	BF	166	ARG	NE-CZ-NH1	6.20	123.40	120.30
53	BA	1233	C	O4'-C1'-N1	6.20	113.16	108.20
53	BA	1802	A	N1-C6-N6	-6.20	114.88	118.60
53	BA	2518	A	C4-C5-C6	-6.20	113.90	117.00
9	AJ	5	ARG	NE-CZ-NH2	-6.20	117.20	120.30
21	AA	1261	A	C5-C6-N1	6.20	120.80	117.70
53	BA	1293	C	N1-C2-O2	6.20	122.62	118.90
53	BA	1791	A	C4-C5-C6	-6.20	113.90	117.00
53	BA	2872	A	C5-C6-N1	6.20	120.80	117.70
22	A1	20	G	C5-C6-N1	6.20	114.60	111.50
33	BL	123	ARG	NE-CZ-NH1	6.20	123.40	120.30
53	BA	559	G	N1-C6-O6	-6.20	116.18	119.90
53	BA	670	A	P-O3'-C3'	6.20	127.13	119.70
21	AA	759	A	C5-C6-N1	6.19	120.80	117.70
53	BA	2517	C	N1-C2-O2	6.19	122.62	118.90
53	BA	276	U	O4'-C1'-N1	6.19	113.15	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1144	A	C4-C5-C6	-6.19	113.90	117.00
53	BA	1902	C	O4'-C1'-N1	6.19	113.16	108.20
53	BA	2198	A	C4-C5-C6	-6.19	113.90	117.00
21	AA	58	C	N3-C2-O2	-6.19	117.57	121.90
24	BC	268	ARG	NE-CZ-NH1	6.19	123.39	120.30
53	BA	349	U	O4'-C1'-N1	6.19	113.15	108.20
53	BA	1607	C	O4'-C1'-N1	6.19	113.15	108.20
53	BA	1796	U	O4'-C1'-N1	6.19	113.15	108.20
53	BA	2030	A	C4-C5-C6	-6.19	113.91	117.00
53	BA	2261	C	P-O3'-C3'	6.19	127.13	119.70
53	BA	1615	C	C5'-C4'-O4'	6.19	116.53	109.10
53	BA	2171	A	O4'-C1'-N9	6.19	113.15	108.20
21	AA	52	C	O4'-C1'-N1	6.19	113.15	108.20
21	AA	419	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	487	A	C5-C6-N1	6.19	120.79	117.70
21	AA	1155	A	C5-C6-N1	6.19	120.79	117.70
28	BG	94	ARG	NE-CZ-NH1	6.19	123.39	120.30
21	AA	1431	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	1509	C	N3-C2-O2	-6.18	117.57	121.90
53	BA	629	G	N3-C4-C5	-6.18	125.51	128.60
53	BA	793	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	55	A	C5-C6-N1	6.18	120.79	117.70
21	AA	284	C	N3-C2-O2	-6.18	117.58	121.90
53	BA	905	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	389	A	C5-C6-N1	6.18	120.79	117.70
21	AA	553	A	C5-C6-N1	6.18	120.79	117.70
53	BA	404	A	N1-C6-N6	-6.18	114.89	118.60
53	BA	915	C	N1-C2-O2	6.18	122.61	118.90
53	BA	2447	G	O4'-C1'-N9	6.18	113.14	108.20
4	AE	156	ARG	NE-CZ-NH2	6.18	123.39	120.30
53	BA	434	U	O4'-C1'-N1	6.18	113.14	108.20
53	BA	668	A	C4-C5-C6	-6.18	113.91	117.00
53	BA	1247	A	C5-C6-N1	6.18	120.79	117.70
54	BB	99	A	C5-C6-N1	6.18	120.79	117.70
21	AA	924	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	177	G	O4'-C1'-N9	6.17	113.14	108.20
53	BA	762	U	P-O3'-C3'	6.17	127.11	119.70
53	BA	1297	C	O4'-C1'-N1	6.17	113.14	108.20
21	AA	679	C	N3-C2-O2	-6.17	117.58	121.90
36	BO	16	ARG	NE-CZ-NH1	6.17	123.39	120.30
53	BA	2268	A	C5-C6-N1	6.17	120.79	117.70
53	BA	2450	A	C5-C6-N1	6.17	120.79	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	468	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	918	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	1311	A	C6-C5-N7	6.17	136.62	132.30
53	BA	611	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	782	A	C5-C6-N1	6.17	120.79	117.70
53	BA	1528	A	C5-C6-N1	6.17	120.79	117.70
53	BA	2156	G	C5-C6-N1	6.17	114.58	111.50
21	AA	1202	U	O4'-C1'-N1	6.17	113.14	108.20
54	BB	91	C	C1'-O4'-C4'	-6.17	104.96	109.90
54	BB	91	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	85	U	O4'-C1'-N1	6.17	113.13	108.20
21	AA	206	C	N1-C2-O2	6.17	122.60	118.90
21	AA	265	G	N1-C6-O6	-6.17	116.20	119.90
21	AA	1282	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	1646	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	2184	A	C4-C5-C6	-6.17	113.92	117.00
54	BB	39	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	311	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	956	G	N3-C4-C5	-6.17	125.52	128.60
53	BA	2019	A	C4-C5-C6	-6.17	113.92	117.00
53	BA	2496	C	N1-C2-O2	6.17	122.60	118.90
21	AA	51	A	C5-C6-N1	6.17	120.78	117.70
53	BA	181	A	C4'-C3'-C2'	-6.17	96.44	102.60
53	BA	257	C	N3-C2-O2	-6.17	117.58	121.90
53	BA	414	C	N3-C2-O2	-6.16	117.58	121.90
53	BA	738	G	N1-C6-O6	-6.16	116.20	119.90
53	BA	1507	C	N3-C2-O2	-6.16	117.58	121.90
53	BA	903	C	N3-C2-O2	-6.16	117.59	121.90
53	BA	1395	A	C4-C5-C6	-6.16	113.92	117.00
53	BA	535	G	C5-C6-N1	6.16	114.58	111.50
53	BA	686	U	O4'-C1'-N1	6.16	113.13	108.20
21	AA	210	C	O4'-C1'-N1	6.16	113.13	108.20
21	AA	603	U	C5-C6-N1	-6.16	119.62	122.70
21	AA	1346	A	C5-C6-N1	6.16	120.78	117.70
21	AA	1384	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	1385	G	N1-C6-O6	-6.16	116.21	119.90
53	BA	238	C	N3-C2-O2	-6.16	117.59	121.90
53	BA	1371	G	N3-C2-N2	-6.16	115.59	119.90
21	AA	47	C	N3-C4-C5	6.16	124.36	121.90
21	AA	576	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	729	A	C4-C5-C6	-6.16	113.92	117.00
33	BL	126	ARG	NE-CZ-NH1	6.16	123.38	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	816	C	O4'-C1'-N1	6.16	113.12	108.20
53	BA	1940	U	N3-C2-O2	-6.16	117.89	122.20
53	BA	2503	A	P-O3'-C3'	6.16	127.09	119.70
54	BB	93	C	N3-C2-O2	-6.16	117.59	121.90
53	BA	458	G	C5-C6-N1	6.15	114.58	111.50
53	BA	2666	C	N1-C2-O2	6.15	122.59	118.90
6	AG	137	ARG	NE-CZ-NH2	-6.15	117.22	120.30
53	BA	112	U	C5-C6-N1	-6.15	119.62	122.70
53	BA	1926	U	N1-C2-N3	6.15	118.59	114.90
21	AA	76	G	N1-C6-O6	-6.15	116.21	119.90
21	AA	342	C	N3-C2-O2	-6.15	117.59	121.90
22	A1	36	C	O4'-C1'-N1	6.15	113.12	108.20
27	BF	70	ARG	NE-CZ-NH2	6.15	123.38	120.30
53	BA	518	G	N1-C6-O6	-6.15	116.21	119.90
53	BA	2425	A	C5'-C4'-C3'	-6.15	106.16	116.00
54	BB	89	U	C5-C6-N1	-6.15	119.62	122.70
2	AC	126	ARG	NE-CZ-NH1	6.15	123.37	120.30
21	AA	1388	C	O4'-C1'-N1	6.15	113.12	108.20
21	AA	477	C	N3-C2-O2	-6.15	117.60	121.90
53	BA	2611	C	N3-C2-O2	-6.15	117.60	121.90
53	BA	2856	A	C5-C6-N1	6.15	120.77	117.70
21	AA	612	C	N3-C2-O2	-6.14	117.60	121.90
53	BA	2184	A	C5-C6-N1	6.14	120.77	117.70
53	BA	2411	A	C5-C6-N1	6.14	120.77	117.70
21	AA	896	C	N1-C2-O2	6.14	122.58	118.90
21	AA	1292	G	N1-C6-O6	-6.14	116.21	119.90
21	AA	1298	U	C1'-O4'-C4'	-6.14	104.99	109.90
53	BA	1262	A	C4-C5-C6	-6.14	113.93	117.00
53	BA	1507	C	N3-C4-C5	6.14	124.36	121.90
53	BA	1583	A	C4-C5-C6	-6.14	113.93	117.00
53	BA	1833	C	N3-C2-O2	-6.14	117.60	121.90
53	BA	2364	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	1448	C	N1-C2-O2	6.14	122.58	118.90
53	BA	885	C	O4'-C1'-N1	6.14	113.11	108.20
21	AA	269	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	735	C	N3-C2-O2	-6.14	117.60	121.90
22	A1	6	A	C5-C6-N1	6.14	120.77	117.70
53	BA	1086	A	C5-C6-N1	6.14	120.77	117.70
53	BA	2841	C	N1-C2-O2	6.14	122.58	118.90
53	BA	443	A	N1-C6-N6	-6.14	114.92	118.60
53	BA	1332	G	O4'-C1'-N9	6.14	113.11	108.20
53	BA	1338	G	C5-C6-N1	6.14	114.57	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	163	C	O4'-C1'-N1	6.14	113.11	108.20
21	AA	536	C	N3-C2-O2	-6.14	117.61	121.90
21	AA	630	A	C6-C5-N7	6.14	136.60	132.30
21	AA	855	U	C5-C6-N1	-6.14	119.63	122.70
53	BA	174	U	O4'-C1'-N1	6.14	113.11	108.20
53	BA	512	G	O4'-C1'-N9	6.14	113.11	108.20
21	AA	53	A	O4'-C1'-N9	6.13	113.11	108.20
21	AA	67	C	N3-C4-C5	6.13	124.35	121.90
21	AA	1019	A	C5-C6-N1	6.13	120.77	117.70
53	BA	1695	G	N3-C4-C5	-6.13	125.53	128.60
53	BA	2362	C	C5'-C4'-O4'	6.13	116.46	109.10
53	BA	2439	A	C4-C5-C6	-6.13	113.93	117.00
21	AA	573	A	C5-C6-N1	6.13	120.77	117.70
1	AB	73	ARG	NE-CZ-NH1	6.13	123.37	120.30
21	AA	752	G	C8-N9-C4	-6.13	103.95	106.40
53	BA	847	U	O4'-C1'-N1	6.13	113.11	108.20
53	BA	1397	U	O4'-C1'-N1	6.13	113.11	108.20
53	BA	2314	A	N1-C6-N6	-6.13	114.92	118.60
53	BA	436	C	N3-C2-O2	-6.13	117.61	121.90
53	BA	456	C	N3-C4-C5	6.13	124.35	121.90
1	AB	112	ARG	NE-CZ-NH1	6.13	123.36	120.30
14	AO	53	ARG	NE-CZ-NH2	-6.13	117.24	120.30
21	AA	687	A	C5-C6-N1	6.13	120.76	117.70
21	AA	892	A	C5-C6-N1	6.13	120.77	117.70
53	BA	181	A	C4-C5-C6	-6.13	113.94	117.00
53	BA	565	C	O4'-C1'-N1	6.13	113.10	108.20
53	BA	1034	G	C5-C6-N1	6.13	114.56	111.50
53	BA	1237	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	456	A	N1-C6-N6	-6.13	114.92	118.60
21	AA	864	A	C5-C6-N1	6.13	120.76	117.70
53	BA	2094	A	C5-C6-N1	6.13	120.76	117.70
53	BA	2662	A	N1-C6-N6	-6.13	114.92	118.60
53	BA	2839	G	C8-N9-C4	-6.13	103.95	106.40
21	AA	526	C	N3-C2-O2	-6.12	117.61	121.90
22	A1	3	G	O4'-C1'-N9	6.12	113.10	108.20
53	BA	2021	C	N3-C2-O2	-6.12	117.61	121.90
53	BA	2129	C	N3-C2-O2	-6.12	117.61	121.90
53	BA	2425	A	O4'-C1'-N9	6.12	113.10	108.20
21	AA	200	G	C5-C6-N1	6.12	114.56	111.50
21	AA	1468	A	C5-C6-N1	6.12	120.76	117.70
53	BA	1270	C	N3-C2-O2	-6.12	117.61	121.90
53	BA	2612	C	N1-C2-O2	6.12	122.57	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1259	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	1413	A	C4-C5-C6	-6.12	113.94	117.00
53	BA	1608	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	131	A	C5-C6-N1	6.12	120.76	117.70
21	AA	866	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	1177	G	N3-C2-N2	-6.12	115.62	119.90
53	BA	141	G	N1-C6-O6	-6.12	116.23	119.90
53	BA	573	U	P-O3'-C3'	6.12	127.04	119.70
53	BA	1735	A	C5-C6-N1	6.12	120.76	117.70
21	AA	525	C	N3-C2-O2	-6.12	117.62	121.90
53	BA	1916	A	C4-C5-C6	-6.12	113.94	117.00
12	AM	78	ARG	NE-CZ-NH2	6.12	123.36	120.30
21	AA	1095	U	C5-C6-N1	-6.12	119.64	122.70
53	BA	118	A	O4'-C1'-N9	6.12	113.09	108.20
53	BA	900	A	C5-C6-N1	6.12	120.76	117.70
53	BA	980	A	C5-C6-N1	6.12	120.76	117.70
53	BA	1181	U	C5-C6-N1	-6.12	119.64	122.70
53	BA	2684	U	O4'-C1'-N1	6.12	113.09	108.20
21	AA	50	A	C4-C5-C6	-6.11	113.94	117.00
21	AA	621	A	C6-C5-N7	6.11	136.58	132.30
21	AA	1149	C	N3-C2-O2	-6.11	117.62	121.90
53	BA	479	A	C6-C5-N7	6.11	136.58	132.30
53	BA	1504	A	C5-C6-N1	6.11	120.76	117.70
53	BA	2440	C	N1-C2-O2	6.11	122.57	118.90
21	AA	20	U	O4'-C1'-N1	6.11	113.09	108.20
21	AA	1179	A	C5-C6-N1	6.11	120.75	117.70
21	AA	1217	C	N1-C2-O2	6.11	122.57	118.90
53	BA	1302	A	C5-C6-N1	6.11	120.75	117.70
29	BH	51	ARG	NE-CZ-NH1	6.11	123.35	120.30
53	BA	1292	G	C5-C6-N1	6.11	114.55	111.50
21	AA	144	G	N3-C4-C5	-6.11	125.55	128.60
21	AA	267	C	N3-C2-O2	-6.11	117.63	121.90
21	AA	895	G	N1-C6-O6	-6.11	116.24	119.90
21	AA	896	C	N3-C2-O2	-6.11	117.63	121.90
21	AA	1508	A	C5-C6-N1	6.11	120.75	117.70
13	AN	13	ARG	NE-CZ-NH1	6.10	123.35	120.30
21	AA	678	U	O4'-C1'-N1	6.10	113.08	108.20
21	AA	1109	C	N1-C2-O2	6.10	122.56	118.90
53	BA	109	C	N3-C2-O2	-6.10	117.63	121.90
53	BA	562	U	N3-C2-O2	-6.10	117.93	122.20
53	BA	1676	A	C5-C6-N1	6.10	120.75	117.70
54	BB	10	G	O4'-C1'-N9	6.10	113.08	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	36	C	N3-C2-O2	-6.10	117.63	121.90
52	B4	19	ARG	NE-CZ-NH1	6.10	123.35	120.30
53	BA	1126	A	C4-C5-C6	-6.10	113.95	117.00
53	BA	1970	A	C5-C6-N1	6.10	120.75	117.70
53	BA	2382	G	O4'-C1'-N9	6.10	113.08	108.20
53	BA	2392	A	C5-C6-N1	6.10	120.75	117.70
53	BA	2565	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	475	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1399	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1484	C	N3-C2-O2	-6.10	117.63	121.90
38	BQ	54	ARG	NE-CZ-NH1	6.10	123.35	120.30
53	BA	787	C	N1-C2-O2	6.10	122.56	118.90
53	BA	1359	A	C5-C6-N1	6.10	120.75	117.70
53	BA	2380	C	O4'-C1'-N1	6.10	113.08	108.20
53	BA	2799	A	C4-C5-C6	-6.10	113.95	117.00
53	BA	1834	U	O4'-C1'-N1	6.10	113.08	108.20
53	BA	2354	C	N3-C2-O2	-6.10	117.63	121.90
27	BF	124	ARG	NE-CZ-NH1	-6.09	117.25	120.30
53	BA	821	A	C5-C6-N1	6.09	120.75	117.70
53	BA	972	A	C5-C6-N1	6.09	120.75	117.70
53	BA	1030	C	N3-C2-O2	-6.09	117.63	121.90
53	BA	1158	C	N3-C4-C5	6.09	124.34	121.90
21	AA	832	G	N1-C6-O6	-6.09	116.24	119.90
21	AA	978	A	C4-C5-C6	-6.09	113.95	117.00
53	BA	603	A	N1-C6-N6	-6.09	114.94	118.60
53	BA	2378	A	C5-C6-N1	6.09	120.75	117.70
21	AA	1329	A	C5-C6-N1	6.09	120.75	117.70
21	AA	1529	G	O4'-C1'-N9	6.09	113.07	108.20
53	BA	1419	A	N1-C6-N6	-6.09	114.94	118.60
53	BA	2633	G	N1-C6-O6	-6.09	116.25	119.90
21	AA	451	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	562	U	O4'-C1'-N1	6.09	113.07	108.20
22	A1	11	C	N3-C4-C5	6.09	124.34	121.90
27	BF	132	ARG	NE-CZ-NH1	6.09	123.34	120.30
31	BJ	35	ARG	NE-CZ-NH1	6.09	123.34	120.30
53	BA	1466	U	O4'-C1'-N1	6.09	113.07	108.20
54	BB	68	C	O4'-C1'-N1	6.09	113.07	108.20
53	BA	1	G	N3-C4-C5	-6.09	125.56	128.60
53	BA	985	C	N1-C2-O2	6.09	122.55	118.90
53	BA	2712	C	N3-C2-O2	-6.09	117.64	121.90
53	BA	2735	G	C5-C6-N1	6.09	114.54	111.50
21	AA	901	A	C4-C5-C6	-6.08	113.96	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1237	C	N1-C2-O2	6.08	122.55	118.90
53	BA	1670	C	N3-C2-O2	-6.08	117.64	121.90
53	BA	2496	C	N3-C4-C5	6.08	124.33	121.90
21	AA	382	A	C5-C6-N1	6.08	120.74	117.70
21	AA	652	U	O4'-C1'-N1	6.08	113.07	108.20
48	B0	39	ARG	NE-CZ-NH1	6.08	123.34	120.30
53	BA	227	A	C4-C5-C6	-6.08	113.96	117.00
53	BA	2834	G	C5-C6-N1	6.08	114.54	111.50
21	AA	266	G	N3-C2-N2	-6.08	115.64	119.90
21	AA	946	A	C5-C6-N1	6.08	120.74	117.70
21	AA	1437	A	N1-C6-N6	-6.08	114.95	118.60
53	BA	629	G	N1-C6-O6	-6.08	116.25	119.90
21	AA	53	A	C5-C6-N1	6.08	120.74	117.70
53	BA	391	A	N1-C6-N6	-6.08	114.95	118.60
53	BA	2795	C	N3-C2-O2	-6.08	117.65	121.90
3	AD	12	ARG	NE-CZ-NH1	6.08	123.34	120.30
21	AA	409	U	O4'-C1'-N1	6.08	113.06	108.20
21	AA	602	A	C6-C5-N7	6.08	136.55	132.30
21	AA	1305	G	C5-C6-N1	6.08	114.54	111.50
21	AA	1389	C	N3-C2-O2	-6.08	117.65	121.90
53	BA	105	C	N3-C2-O2	-6.08	117.65	121.90
53	BA	144	A	C4-C5-C6	-6.08	113.96	117.00
53	BA	223	A	C4-C5-C6	-6.08	113.96	117.00
53	BA	743	A	C6-C5-N7	6.08	136.55	132.30
53	BA	929	U	O4'-C1'-N1	6.08	113.06	108.20
53	BA	1682	G	O4'-C1'-N9	6.08	113.06	108.20
53	BA	2153	C	N3-C2-O2	-6.08	117.65	121.90
53	BA	2527	C	O4'-C1'-N1	6.08	113.06	108.20
21	AA	1042	A	O4'-C1'-N9	6.07	113.06	108.20
32	BK	17	ARG	NE-CZ-NH1	6.07	123.34	120.30
46	BY	48	ARG	NE-CZ-NH1	6.07	123.34	120.30
53	BA	151	C	N3-C2-O2	-6.07	117.65	121.90
53	BA	165	A	C6-C5-N7	6.07	136.55	132.30
53	BA	609	A	C5-C6-N1	6.07	120.74	117.70
53	BA	2406	A	C1'-O4'-C4'	-6.07	105.04	109.90
10	AK	105	ARG	NE-CZ-NH2	-6.07	117.26	120.30
21	AA	403	C	O4'-C1'-N1	6.07	113.06	108.20
21	AA	916	U	O4'-C1'-N1	6.07	113.06	108.20
37	BP	50	ARG	NE-CZ-NH1	6.07	123.33	120.30
53	BA	787	C	N3-C2-O2	-6.07	117.65	121.90
53	BA	1411	U	C5-C6-N1	-6.07	119.67	122.70
53	BA	1741	C	N3-C2-O2	-6.07	117.65	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	272	A	C5-C6-N1	6.07	120.73	117.70
53	BA	2598	A	C4-C5-C6	-6.07	113.97	117.00
54	BB	32	U	O4'-C1'-N1	6.07	113.06	108.20
21	AA	150	U	O4'-C1'-N1	6.07	113.05	108.20
53	BA	488	G	N1-C6-O6	-6.07	116.26	119.90
53	BA	634	C	O4'-C1'-N1	6.07	113.06	108.20
53	BA	1111	A	N1-C6-N6	-6.07	114.96	118.60
53	BA	1287	A	C1'-O4'-C4'	-6.07	105.05	109.90
21	AA	759	A	C4-C5-C6	-6.07	113.97	117.00
22	A1	62	C	N3-C2-O2	-6.07	117.65	121.90
53	BA	225	C	N3-C2-O2	-6.07	117.66	121.90
53	BA	269	C	N3-C2-O2	-6.07	117.65	121.90
53	BA	2893	A	N1-C6-N6	-6.07	114.96	118.60
54	BB	61	G	N9-C4-C5	6.07	107.83	105.40
38	BQ	29	ARG	NE-CZ-NH1	6.06	123.33	120.30
21	AA	1102	A	C5-C6-N1	6.06	120.73	117.70
53	BA	412	A	C6-C5-N7	6.06	136.54	132.30
53	BA	1337	G	N1-C6-O6	-6.06	116.26	119.90
53	BA	2055	C	N1-C2-O2	6.06	122.54	118.90
53	BA	118	A	C4-C5-C6	-6.06	113.97	117.00
53	BA	128	C	N3-C2-O2	-6.06	117.66	121.90
54	BB	41	G	C5-C6-N1	6.06	114.53	111.50
37	BP	100	ARG	NE-CZ-NH2	-6.06	117.27	120.30
53	BA	603	A	C5-C6-N1	6.06	120.73	117.70
53	BA	2617	U	O4'-C1'-N1	6.06	113.05	108.20
21	AA	1067	A	C6-C5-N7	6.06	136.54	132.30
21	AA	1218	C	N3-C2-O2	-6.06	117.66	121.90
53	BA	1365	A	C4-C5-C6	-6.06	113.97	117.00
53	BA	1480	C	N1-C2-O2	6.06	122.53	118.90
53	BA	2446	G	N1-C6-O6	-6.06	116.27	119.90
21	AA	1120	C	N3-C2-O2	-6.06	117.66	121.90
53	BA	835	C	N1-C2-O2	6.06	122.53	118.90
53	BA	1370	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	770	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	940	C	O4'-C1'-N1	6.05	113.04	108.20
21	AA	1210	C	N3-C2-O2	-6.05	117.66	121.90
53	BA	963	U	C1'-O4'-C4'	-6.05	105.06	109.90
53	BA	2336	A	C5-C6-N1	6.05	120.73	117.70
53	BA	2503	A	O4'-C1'-N9	6.05	113.04	108.20
54	BB	52	A	C5-C6-N1	6.05	120.73	117.70
54	BB	71	C	O4'-C1'-N1	6.05	113.04	108.20
21	AA	1211	U	C5-C6-N1	-6.05	119.67	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1318	A	C5-C6-N1	6.05	120.73	117.70
53	BA	2574	G	N7-C8-N9	6.05	116.13	113.10
53	BA	2133	G	N1-C6-O6	-6.05	116.27	119.90
53	BA	347	A	C4-C5-C6	-6.05	113.98	117.00
53	BA	2546	U	O4'-C1'-N1	6.05	113.04	108.20
19	AT	59	ARG	NE-CZ-NH1	6.05	123.32	120.30
21	AA	383	A	C4-C5-C6	-6.05	113.98	117.00
21	AA	545	C	N1-C2-O2	6.05	122.53	118.90
21	AA	611	C	N1-C2-O2	6.05	122.53	118.90
21	AA	1237	C	C3'-C2'-C1'	6.05	106.34	101.50
53	BA	408	G	C5-C6-N1	6.05	114.52	111.50
53	BA	947	A	C4-C5-C6	-6.05	113.98	117.00
53	BA	2572	A	C4-C5-C6	-6.05	113.98	117.00
21	AA	667	G	C8-N9-C4	-6.04	103.98	106.40
21	AA	1501	C	N3-C4-C5	6.04	124.32	121.90
22	A1	10	G	N3-C4-C5	-6.04	125.58	128.60
53	BA	1007	C	N3-C4-C5	6.04	124.32	121.90
53	BA	2679	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	967	C	N1-C2-O2	6.04	122.53	118.90
53	BA	253	C	N3-C2-O2	-6.04	117.67	121.90
53	BA	752	A	N1-C6-N6	-6.04	114.97	118.60
54	BB	109	A	C4-C5-C6	-6.04	113.98	117.00
54	BB	111	U	O4'-C1'-N1	6.04	113.03	108.20
21	AA	139	A	C4-C5-C6	-6.04	113.98	117.00
53	BA	351	C	N3-C2-O2	-6.04	117.67	121.90
53	BA	943	A	C5-C6-N1	6.04	120.72	117.70
53	BA	968	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	192	A	C4-C5-C6	-6.04	113.98	117.00
53	BA	246	C	O4'-C1'-N1	6.04	113.03	108.20
53	BA	1230	A	C4-C5-C6	-6.04	113.98	117.00
53	BA	1547	C	N3-C2-O2	-6.04	117.67	121.90
53	BA	2706	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	121	U	O4'-C1'-N1	6.04	113.03	108.20
53	BA	53	A	C4-C5-C6	-6.04	113.98	117.00
53	BA	2564	A	C4-C5-C6	-6.04	113.98	117.00
53	BA	767	U	O4'-C1'-N1	6.04	113.03	108.20
53	BA	1115	G	C8-N9-C4	-6.04	103.99	106.40
53	BA	2265	U	O4'-C1'-N1	6.04	113.03	108.20
22	A1	72	C	N3-C2-O2	-6.03	117.68	121.90
53	BA	357	C	N3-C2-O2	-6.03	117.68	121.90
53	BA	692	C	N3-C2-O2	-6.03	117.68	121.90
53	BA	2435	A	C5-C6-N1	6.03	120.72	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	243	A	N1-C6-N6	-6.03	114.98	118.60
23	A2	88	U	O4'-C1'-N1	6.03	113.03	108.20
21	AA	886	G	N1-C6-O6	-6.03	116.28	119.90
53	BA	1675	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	555	U	C5-C6-N1	-6.03	119.69	122.70
21	AA	737	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	729	A	O4'-C1'-N9	6.03	113.02	108.20
21	AA	1365	G	N1-C6-O6	-6.03	116.28	119.90
22	A1	36	C	C6-N1-C2	-6.03	117.89	120.30
53	BA	338	G	C4'-C3'-C2'	-6.03	96.57	102.60
53	BA	2157	G	C5-C6-N1	6.03	114.51	111.50
53	BA	2619	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	1397	C	O4'-C1'-N1	6.02	113.02	108.20
53	BA	1142	A	O4'-C1'-N9	6.02	113.02	108.20
53	BA	2081	U	N1-C2-N3	6.02	118.51	114.90
53	BA	2413	G	C5-C6-N1	6.02	114.51	111.50
53	BA	927	A	C5-C6-N1	6.02	120.71	117.70
53	BA	2374	C	N1-C2-O2	6.02	122.51	118.90
54	BB	87	U	C5-C6-N1	-6.02	119.69	122.70
21	AA	749	A	C6-C5-N7	6.02	136.51	132.30
21	AA	862	C	N3-C2-O2	-6.02	117.69	121.90
53	BA	167	A	C5-C6-N1	6.02	120.71	117.70
53	BA	2870	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	193	C	C3'-C2'-C1'	6.02	106.31	101.50
21	AA	431	A	C5-C6-N1	6.02	120.71	117.70
21	AA	1487	G	O4'-C1'-N9	6.02	113.02	108.20
53	BA	127	A	C5-C6-N1	6.02	120.71	117.70
53	BA	447	A	C5-C6-N1	6.02	120.71	117.70
21	AA	183	C	N1-C2-O2	6.02	122.51	118.90
21	AA	702	A	C5-C6-N1	6.02	120.71	117.70
22	A1	6	A	C4-C5-C6	-6.02	113.99	117.00
53	BA	309	A	N1-C6-N6	-6.02	114.99	118.60
53	BA	394	C	O4'-C1'-N1	6.02	113.01	108.20
53	BA	2364	C	O4'-C1'-N1	6.02	113.01	108.20
53	BA	2600	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	261	U	N3-C2-O2	-6.02	117.99	122.20
53	BA	752	A	C5-C6-N1	6.02	120.71	117.70
53	BA	1590	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	1525	G	N1-C6-O6	-6.01	116.29	119.90
53	BA	69	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	565	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	1324	G	O4'-C1'-N9	6.01	113.01	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1354	A	C4-C5-C6	-6.01	113.99	117.00
53	BA	1575	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	1718	G	C5-C6-N1	6.01	114.51	111.50
53	BA	2467	C	O4'-C1'-N1	6.01	113.01	108.20
21	AA	1236	A	N1-C6-N6	-6.01	114.99	118.60
53	BA	1700	A	C5-C6-N1	6.01	120.71	117.70
21	AA	1113	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	1362	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	2416	C	C6-N1-C2	-6.01	117.89	120.30
21	AA	145	G	C5-C6-N1	6.01	114.50	111.50
21	AA	437	U	O4'-C1'-N1	6.01	113.01	108.20
53	BA	1173	U	O4'-C1'-N1	6.01	113.01	108.20
21	AA	1226	C	N3-C2-O2	-6.01	117.69	121.90
53	BA	1846	G	O4'-C1'-N9	6.01	113.01	108.20
53	BA	1876	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	1031	C	O4'-C1'-N1	6.01	113.01	108.20
26	BE	88	ARG	NE-CZ-NH2	6.01	123.30	120.30
53	BA	533	G	N1-C6-O6	-6.01	116.30	119.90
53	BA	613	A	C3'-C2'-C1'	6.01	106.31	101.50
53	BA	1098	A	O4'-C1'-N9	6.01	113.01	108.20
53	BA	1477	A	N1-C6-N6	-6.01	115.00	118.60
53	BA	1757	A	C4-C5-C6	-6.01	114.00	117.00
53	BA	2066	C	O4'-C1'-N1	6.01	113.00	108.20
53	BA	2170	A	C5-C6-N1	6.01	120.70	117.70
53	BA	1799	G	N9-C4-C5	6.00	107.80	105.40
53	BA	2	G	C5-C6-N1	6.00	114.50	111.50
53	BA	103	A	C6-C5-N7	6.00	136.50	132.30
21	AA	385	C	N3-C2-O2	-6.00	117.70	121.90
53	BA	253	C	N1-C2-O2	6.00	122.50	118.90
53	BA	570	G	C5'-C4'-O4'	6.00	116.30	109.10
53	BA	1054	A	N1-C6-N6	-6.00	115.00	118.60
53	BA	1056	G	P-O3'-C3'	6.00	126.90	119.70
53	BA	1153	C	N1-C2-O2	6.00	122.50	118.90
42	BU	85	ARG	NE-CZ-NH2	6.00	123.30	120.30
53	BA	443	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	903	G	N7-C8-N9	6.00	116.10	113.10
21	AA	1152	A	C5-C6-N1	6.00	120.70	117.70
53	BA	1459	G	O4'-C1'-N9	6.00	113.00	108.20
21	AA	443	C	N3-C2-O2	-6.00	117.70	121.90
53	BA	663	G	N3-C2-N2	-6.00	115.70	119.90
21	AA	849	G	N1-C6-O6	-6.00	116.30	119.90
21	AA	1328	C	N3-C4-C5	6.00	124.30	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	57	C	N1-C2-O2	6.00	122.50	118.90
21	AA	150	U	C5-C6-N1	-5.99	119.70	122.70
24	BC	213	ARG	NE-CZ-NH1	5.99	123.30	120.30
21	AA	251	G	N3-C4-C5	-5.99	125.60	128.60
53	BA	14	A	C4-C5-C6	-5.99	114.00	117.00
4	AE	111	ARG	NE-CZ-NH1	5.99	123.30	120.30
21	AA	1370	G	C5-C6-N1	5.99	114.50	111.50
53	BA	76	C	N1-C2-O2	5.99	122.50	118.90
53	BA	580	U	O4'-C1'-N1	5.99	112.99	108.20
53	BA	1141	U	O4'-C1'-N1	5.99	112.99	108.20
53	BA	2342	C	N1-C2-O2	5.99	122.49	118.90
53	BA	2814	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	1042	A	C4-C5-C6	-5.99	114.01	117.00
53	BA	616	A	C5-C6-N1	5.99	120.69	117.70
53	BA	723	C	N3-C2-O2	-5.99	117.71	121.90
53	BA	2880	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	523	A	C4-C5-C6	-5.99	114.01	117.00
53	BA	1052	C	N1-C2-O2	5.99	122.49	118.90
53	BA	2266	A	C4-C5-C6	-5.99	114.01	117.00
1	AB	34	ARG	NE-CZ-NH1	5.99	123.29	120.30
21	AA	636	U	C5-C6-N1	-5.99	119.71	122.70
21	AA	211	G	N1-C6-O6	-5.98	116.31	119.90
21	AA	1081	A	C5-C6-N1	5.98	120.69	117.70
21	AA	824	G	C5-C6-N1	5.98	114.49	111.50
53	BA	1772	A	C4-C5-C6	-5.98	114.01	117.00
53	BA	1829	A	C4-C5-C6	-5.98	114.01	117.00
53	BA	1940	U	C1'-O4'-C4'	-5.98	105.11	109.90
53	BA	2283	C	O4'-C1'-N1	5.98	112.99	108.20
21	AA	82	G	O4'-C1'-N9	5.98	112.98	108.20
21	AA	228	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	296	U	C5-C6-N1	-5.98	119.71	122.70
21	AA	322	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	578	C	N3-C2-O2	-5.98	117.71	121.90
21	AA	753	A	C5-C6-N1	5.98	120.69	117.70
21	AA	754	C	N1-C2-O2	5.98	122.49	118.90
21	AA	961	U	O4'-C1'-N1	5.98	112.98	108.20
53	BA	64	A	C5-C6-N1	5.98	120.69	117.70
53	BA	401	A	C4-C5-C6	-5.98	114.01	117.00
53	BA	704	G	O4'-C1'-N9	5.98	112.98	108.20
53	BA	1340	U	N3-C2-O2	-5.98	118.01	122.20
53	BA	1494	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	905	U	C5-C6-N1	-5.98	119.71	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BM	6	ARG	NE-CZ-NH1	5.98	123.29	120.30
53	BA	756	A	N1-C6-N6	-5.98	115.01	118.60
53	BA	1197	G	C5-C6-N1	5.98	114.49	111.50
21	AA	32	A	C5-C6-N1	5.98	120.69	117.70
21	AA	614	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	1043	G	C5-C6-N1	5.98	114.49	111.50
21	AA	79	G	N3-C2-N2	-5.97	115.72	119.90
21	AA	296	U	N3-C2-O2	-5.97	118.02	122.20
21	AA	352	C	N1-C2-O2	5.97	122.48	118.90
53	BA	1383	A	C5-C6-N1	5.97	120.69	117.70
53	BA	2816	G	N1-C6-O6	-5.97	116.31	119.90
54	BB	115	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	35	G	C5-C6-N1	5.97	114.49	111.50
21	AA	172	A	C5-C6-N1	5.97	120.69	117.70
21	AA	1191	A	C5-C6-N1	5.97	120.69	117.70
53	BA	105	C	C3'-C2'-C1'	5.97	106.28	101.50
21	AA	1145	A	N1-C6-N6	-5.97	115.02	118.60
53	BA	167	A	N1-C6-N6	-5.97	115.02	118.60
53	BA	1084	A	C4-C5-C6	-5.97	114.01	117.00
53	BA	1227	G	O4'-C1'-N9	5.97	112.98	108.20
53	BA	1994	C	N3-C2-O2	-5.97	117.72	121.90
53	BA	901	C	O4'-C1'-N1	5.97	112.97	108.20
53	BA	1493	C	N3-C2-O2	-5.97	117.72	121.90
53	BA	1606	C	C6-N1-C2	-5.97	117.91	120.30
53	BA	2451	A	C5-C6-N1	5.97	120.69	117.70
53	BA	2771	C	N1-C2-O2	5.97	122.48	118.90
53	BA	2900	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	28	A	C6-C5-N7	5.97	136.48	132.30
22	A1	10	G	N1-C6-O6	-5.97	116.32	119.90
24	BC	174	ARG	NE-CZ-NH1	5.97	123.28	120.30
53	BA	234	U	N1-C2-N3	5.97	118.48	114.90
53	BA	918	A	N1-C6-N6	-5.97	115.02	118.60
53	BA	1221	C	N3-C2-O2	-5.97	117.72	121.90
53	BA	2531	A	C5-C6-N1	5.97	120.68	117.70
21	AA	378	G	C5'-C4'-O4'	5.96	116.26	109.10
21	AA	573	A	O4'-C4'-C3'	5.96	110.87	106.10
21	AA	715	A	C5-C6-N1	5.96	120.68	117.70
53	BA	184	C	N3-C2-O2	-5.96	117.72	121.90
53	BA	870	U	C5-C6-N1	-5.96	119.72	122.70
53	BA	2178	C	N3-C2-O2	-5.96	117.72	121.90
53	BA	2503	A	C5-C6-N1	5.96	120.68	117.70
54	BB	31	C	N3-C2-O2	-5.96	117.72	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	867	C	N3-C2-O2	-5.96	117.73	121.90
53	BA	2087	G	N3-C4-C5	-5.96	125.62	128.60
21	AA	324	G	C8-N9-C4	-5.96	104.02	106.40
53	BA	1912	A	C1'-O4'-C4'	-5.96	105.13	109.90
21	AA	1503	A	C4-C5-C6	-5.96	114.02	117.00
53	BA	191	A	N1-C6-N6	-5.96	115.02	118.60
21	AA	569	C	N3-C2-O2	-5.96	117.73	121.90
53	BA	2303	G	N1-C6-O6	-5.96	116.33	119.90
21	AA	190	A	C6-C5-N7	5.96	136.47	132.30
21	AA	831	A	C6-C5-N7	5.96	136.47	132.30
21	AA	1032	G	C3'-C2'-C1'	5.96	106.27	101.50
53	BA	1080	A	C5-C6-N1	5.96	120.68	117.70
53	BA	1272	A	C4-C5-C6	-5.96	114.02	117.00
53	BA	2191	A	C4-C5-C6	-5.96	114.02	117.00
53	BA	2502	G	N1-C6-O6	-5.96	116.33	119.90
53	BA	2518	A	C2-N3-C4	5.96	113.58	110.60
21	AA	1273	C	N3-C2-O2	-5.96	117.73	121.90
53	BA	806	C	N3-C2-O2	-5.96	117.73	121.90
53	BA	1874	C	N3-C2-O2	-5.96	117.73	121.90
53	BA	2179	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	408	A	C5-C6-N1	5.95	120.68	117.70
21	AA	1223	C	N3-C2-O2	-5.95	117.73	121.90
53	BA	2086	U	N1-C2-N3	5.95	118.47	114.90
53	BA	2208	C	N3-C2-O2	-5.95	117.73	121.90
53	BA	2581	G	N1-C6-O6	-5.95	116.33	119.90
53	BA	2764	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	160	A	C5-C6-N1	5.95	120.68	117.70
53	BA	145	C	N3-C2-O2	-5.95	117.73	121.90
53	BA	1233	C	N3-C4-C5	5.95	124.28	121.90
53	BA	1285	A	C5-C6-N1	5.95	120.67	117.70
53	BA	2676	C	N1-C2-O2	5.95	122.47	118.90
54	BB	108	A	C5-C6-N1	5.95	120.67	117.70
21	AA	507	C	N3-C2-O2	-5.95	117.73	121.90
22	A1	10	G	C5-C6-N1	5.95	114.47	111.50
53	BA	586	A	C4-C5-C6	-5.95	114.03	117.00
53	BA	1453	A	C2-N3-C4	5.95	113.57	110.60
53	BA	2539	C	N3-C2-O2	-5.95	117.74	121.90
54	BB	26	C	N3-C2-O2	-5.95	117.74	121.90
21	AA	830	G	N1-C6-O6	-5.95	116.33	119.90
53	BA	725	G	N3-C4-C5	-5.95	125.63	128.60
53	BA	1914	C	N1-C2-O2	5.95	122.47	118.90
53	BA	2212	A	N9-C4-C5	5.95	108.18	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2516	A	C6-C5-N7	5.95	136.46	132.30
21	AA	117	G	C8-N9-C4	-5.95	104.02	106.40
21	AA	1100	C	N1-C2-O2	5.95	122.47	118.90
21	AA	1179	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	1287	A	C5-C6-N1	5.95	120.67	117.70
21	AA	1326	U	O4'-C1'-N1	5.95	112.96	108.20
21	AA	1519	A	C5-C6-N1	5.95	120.67	117.70
53	BA	8	C	N3-C2-O2	-5.95	117.74	121.90
53	BA	1218	G	C5-C6-N1	5.95	114.47	111.50
53	BA	2087	G	N1-C6-O6	-5.95	116.33	119.90
21	AA	597	G	N9-C4-C5	5.94	107.78	105.40
53	BA	1323	C	N1-C2-O2	5.94	122.47	118.90
53	BA	1457	U	O4'-C1'-N1	5.94	112.95	108.20
21	AA	661	G	N1-C6-O6	-5.94	116.33	119.90
53	BA	1089	A	C5-C6-N1	5.94	120.67	117.70
53	BA	1462	C	N3-C2-O2	-5.94	117.74	121.90
53	BA	2244	U	C5-C6-N1	-5.94	119.73	122.70
21	AA	1280	A	C4-C5-C6	-5.94	114.03	117.00
53	BA	613	A	C4-C5-C6	-5.94	114.03	117.00
53	BA	624	C	N1-C2-O2	5.94	122.46	118.90
53	BA	1275	A	C4-C5-C6	-5.94	114.03	117.00
53	BA	1299	G	O4'-C1'-N9	5.94	112.95	108.20
53	BA	2053	G	C5'-C4'-O4'	5.94	116.23	109.10
53	BA	2308	G	O4'-C1'-N9	5.94	112.95	108.20
53	BA	2399	G	O4'-C1'-N9	5.94	112.95	108.20
53	BA	2433	A	C5-C6-N1	5.94	120.67	117.70
21	AA	1511	G	C5-C6-N1	5.94	114.47	111.50
53	BA	471	A	C5-C6-N1	5.94	120.67	117.70
53	BA	640	C	N1-C2-O2	5.94	122.46	118.90
53	BA	1411	U	O4'-C1'-N1	5.94	112.95	108.20
53	BA	2418	A	C6-C5-N7	5.94	136.46	132.30
53	BA	2494	G	C5-C6-N1	5.94	114.47	111.50
54	BB	73	A	C4-C5-C6	-5.94	114.03	117.00
53	BA	974	G	N7-C8-N9	5.94	116.07	113.10
53	BA	1699	G	O4'-C1'-N9	5.94	112.95	108.20
53	BA	1872	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	200	G	N1-C6-O6	-5.93	116.34	119.90
21	AA	1267	C	O4'-C1'-N1	5.93	112.95	108.20
53	BA	1156	A	P-O3'-C3'	5.93	126.82	119.70
53	BA	1503	A	C4-C5-C6	-5.93	114.03	117.00
53	BA	1919	A	C4-C5-C6	-5.93	114.03	117.00
11	AL	98	ARG	NE-CZ-NH1	5.93	123.27	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	74	A	N1-C6-N6	-5.93	115.04	118.60
21	AA	1468	A	O4'-C1'-N9	5.93	112.94	108.20
53	BA	2153	C	N3-C4-C5	5.93	124.27	121.90
21	AA	372	C	O4'-C1'-N1	5.93	112.94	108.20
21	AA	914	A	C4-C5-C6	-5.93	114.04	117.00
53	BA	241	A	N1-C6-N6	-5.93	115.04	118.60
53	BA	421	C	N1-C2-O2	5.93	122.46	118.90
53	BA	2577	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	760	G	N1-C6-O6	-5.93	116.34	119.90
48	B0	51	ARG	NE-CZ-NH1	5.93	123.26	120.30
21	AA	1402	C	N1-C2-O2	5.93	122.46	118.90
53	BA	271	G	O4'-C1'-N9	5.93	112.94	108.20
53	BA	710	U	C5-C6-N1	-5.93	119.74	122.70
53	BA	2305	U	O4'-C1'-N1	5.93	112.94	108.20
53	BA	2366	A	N1-C6-N6	-5.93	115.04	118.60
53	BA	2537	U	N3-C2-O2	-5.93	118.05	122.20
53	BA	2680	U	O4'-C1'-N1	5.93	112.94	108.20
21	AA	808	C	N1-C2-O2	5.92	122.45	118.90
53	BA	1819	A	N1-C6-N6	-5.92	115.05	118.60
53	BA	1877	A	C4-C5-C6	-5.92	114.04	117.00
24	BC	211	ARG	NE-CZ-NH1	5.92	123.26	120.30
53	BA	2180	U	O4'-C1'-N1	5.92	112.94	108.20
21	AA	673	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	812	G	C4'-C3'-C2'	-5.92	96.68	102.60
53	BA	214	G	N1-C6-O6	-5.92	116.35	119.90
53	BA	1197	G	N1-C6-O6	-5.92	116.35	119.90
53	BA	2621	G	N1-C6-O6	-5.92	116.35	119.90
54	BB	60	C	C6-N1-C2	-5.92	117.93	120.30
21	AA	211	G	N3-C4-C5	-5.92	125.64	128.60
21	AA	520	A	C5-C6-N1	5.92	120.66	117.70
21	AA	740	U	O4'-C1'-N1	5.92	112.94	108.20
21	AA	1272	G	N9-C4-C5	5.92	107.77	105.40
21	AA	1319	A	C5-C6-N1	5.92	120.66	117.70
53	BA	60	G	O4'-C1'-N9	5.92	112.93	108.20
53	BA	216	A	C4-C5-C6	-5.92	114.04	117.00
53	BA	452	G	N1-C6-O6	-5.92	116.35	119.90
53	BA	1076	C	N1-C2-O2	5.92	122.45	118.90
53	BA	1809	A	C5-C6-N1	5.92	120.66	117.70
21	AA	911	U	C5-C6-N1	-5.92	119.74	122.70
21	AA	1107	C	O4'-C1'-N1	5.92	112.93	108.20
53	BA	664	G	N1-C6-O6	-5.92	116.35	119.90
21	AA	29	U	O4'-C1'-N1	5.92	112.93	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	488	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	509	A	C5-C6-N1	5.92	120.66	117.70
53	BA	1260	A	C5-C6-N1	5.92	120.66	117.70
53	BA	2206	C	N1-C2-O2	5.92	122.45	118.90
21	AA	1089	G	N9-C4-C5	5.91	107.77	105.40
21	AA	1466	C	O4'-C1'-N1	5.91	112.93	108.20
53	BA	742	A	C5-C6-N1	5.91	120.66	117.70
53	BA	1754	A	C4-C5-C6	-5.91	114.04	117.00
53	BA	1890	A	C4-C5-C6	-5.91	114.04	117.00
53	BA	236	C	N3-C4-C5	5.91	124.27	121.90
53	BA	934	U	O4'-C1'-N1	5.91	112.93	108.20
53	BA	1139	G	N3-C2-N2	-5.91	115.76	119.90
53	BA	2430	A	C1'-O4'-C4'	-5.91	105.17	109.90
21	AA	620	C	O4'-C1'-N1	5.91	112.93	108.20
21	AA	651	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	811	C	O4'-C1'-N1	5.91	112.93	108.20
21	AA	1167	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	1169	A	C4-C5-C6	-5.91	114.05	117.00
53	BA	553	G	N1-C6-O6	-5.91	116.36	119.90
53	BA	1836	C	C5'-C4'-O4'	5.91	116.19	109.10
53	BA	2237	G	N1-C6-O6	-5.91	116.36	119.90
53	BA	854	C	N1-C2-O2	5.91	122.44	118.90
21	AA	964	A	C5-C6-N1	5.91	120.65	117.70
53	BA	451	U	C4'-C3'-C2'	-5.91	96.69	102.60
53	BA	1577	C	N3-C2-O2	-5.91	117.77	121.90
53	BA	2385	C	N3-C2-O2	-5.91	117.77	121.90
53	BA	2815	C	O4'-C1'-N1	5.91	112.92	108.20
53	BA	2821	A	C4-C5-C6	-5.91	114.05	117.00
54	BB	15	A	C3'-C2'-C1'	5.91	106.22	101.50
21	AA	234	C	N3-C2-O2	-5.90	117.77	121.90
39	BR	90	ARG	NE-CZ-NH2	5.90	123.25	120.30
53	BA	1062	G	N3-C4-C5	-5.90	125.65	128.60
53	BA	2594	C	N1-C2-O2	5.90	122.44	118.90
35	BN	90	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
53	BA	534	U	O4'-C1'-N1	5.90	112.92	108.20
53	BA	683	U	O4'-C1'-N1	5.90	112.92	108.20
53	BA	941	A	C4-C5-C6	-5.90	114.05	117.00
53	BA	1021	A	C5-C6-N1	5.90	120.65	117.70
53	BA	2228	G	C5-C6-N1	5.90	114.45	111.50
21	AA	356	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	364	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	718	A	C4-C5-C6	-5.90	114.05	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1533	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	684	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	1360	A	C4-C5-C6	-5.90	114.05	117.00
53	BA	470	A	C5-C6-N1	5.90	120.65	117.70
53	BA	2112	G	C5-C6-N1	5.90	114.45	111.50
53	BA	966	G	N1-C6-O6	-5.90	116.36	119.90
53	BA	2236	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	90	C	N3-C2-O2	-5.89	117.77	121.90
21	AA	136	C	O4'-C1'-N1	5.89	112.92	108.20
21	AA	837	U	N3-C2-O2	-5.89	118.07	122.20
53	BA	504	A	C4-C5-C6	-5.89	114.05	117.00
53	BA	575	A	C5-C6-N1	5.89	120.65	117.70
53	BA	1052	C	N3-C2-O2	-5.89	117.77	121.90
53	BA	2045	C	N3-C2-O2	-5.89	117.77	121.90
53	BA	2651	C	N1-C2-O2	5.89	122.44	118.90
21	AA	1366	C	N3-C2-O2	-5.89	117.78	121.90
53	BA	606	U	O4'-C1'-N1	5.89	112.91	108.20
53	BA	2573	C	N1-C2-O2	5.89	122.44	118.90
53	BA	2578	G	N3-C4-C5	-5.89	125.65	128.60
53	BA	2522	U	C5-C6-N1	-5.89	119.75	122.70
21	AA	563	A	C2-N3-C4	5.89	113.54	110.60
21	AA	977	A	O4'-C1'-N9	5.89	112.91	108.20
53	BA	1179	G	C8-N9-C4	-5.89	104.04	106.40
53	BA	1704	C	N3-C2-O2	-5.89	117.78	121.90
53	BA	2001	C	N3-C4-C5	5.89	124.26	121.90
53	BA	2052	A	C2-N3-C4	5.89	113.55	110.60
53	BA	2275	C	N1-C2-O2	5.89	122.43	118.90
53	BA	2562	U	O4'-C1'-N1	5.89	112.91	108.20
21	AA	1507	A	C5-C6-N1	5.89	120.64	117.70
53	BA	2147	A	C6-C5-N7	5.89	136.42	132.30
21	AA	1122	U	O4'-C1'-N1	5.89	112.91	108.20
53	BA	993	G	C5-C6-N1	5.89	114.44	111.50
53	BA	1345	C	N3-C2-O2	-5.89	117.78	121.90
53	BA	1887	C	N3-C2-O2	-5.89	117.78	121.90
17	AR	69	TYR	CB-CG-CD1	-5.88	117.47	121.00
21	AA	1025	U	O4'-C1'-N1	5.88	112.91	108.20
53	BA	1487	U	C5'-C4'-O4'	5.88	116.16	109.10
53	BA	1616	A	C5-C6-N1	5.88	120.64	117.70
53	BA	80	G	C5-C6-N1	5.88	114.44	111.50
53	BA	2236	U	N1-C2-N3	5.88	118.43	114.90
53	BA	2320	U	O4'-C1'-N1	5.88	112.91	108.20
21	AA	1035	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(^{o})	Ideal(^{o})
53	BA	119	A	C5'-C4'-C3'	-5.88	106.59	116.00
53	BA	569	U	N3-C2-O2	-5.88	118.08	122.20
53	BA	990	A	C4-C5-C6	-5.88	114.06	117.00
53	BA	1145	C	N3-C2-O2	-5.88	117.78	121.90
53	BA	2727	A	C4-C5-C6	-5.88	114.06	117.00
53	BA	2755	C	O4'-C1'-N1	5.88	112.91	108.20
53	BA	337	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	456	A	C5-C6-N1	5.88	120.64	117.70
53	BA	461	C	O4'-C1'-N1	5.88	112.90	108.20
53	BA	1233	C	N1-C2-O2	5.88	122.43	118.90
53	BA	1789	A	C5-C6-N1	5.88	120.64	117.70
21	AA	655	A	C5-C6-N1	5.88	120.64	117.70
21	AA	810	C	N3-C2-O2	-5.88	117.79	121.90
44	BW	54	ARG	NE-CZ-NH1	5.88	123.24	120.30
53	BA	2543	G	N3-C4-C5	-5.88	125.66	128.60
54	BB	11	C	N1-C2-O2	5.88	122.43	118.90
21	AA	996	A	C4-C5-C6	-5.88	114.06	117.00
53	BA	275	C	N3-C2-O2	-5.87	117.79	121.90
53	BA	1328	A	C4-C5-C6	-5.87	114.06	117.00
53	BA	2501	C	N3-C4-N4	-5.87	113.89	118.00
53	BA	2617	U	N1-C2-N3	5.87	118.42	114.90
21	AA	660	C	N3-C2-O2	-5.87	117.79	121.90
53	BA	433	C	C3'-C2'-C1'	5.87	106.20	101.50
53	BA	1185	G	C3'-C2'-C1'	5.87	106.20	101.50
53	BA	1522	A	C4-C5-C6	-5.87	114.06	117.00
53	BA	1446	C	N3-C2-O2	-5.87	117.79	121.90
53	BA	1900	A	C5-C6-N1	5.87	120.64	117.70
53	BA	2882	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	236	A	N1-C6-N6	-5.87	115.08	118.60
21	AA	926	G	C3'-C2'-C1'	5.87	106.19	101.50
23	A2	83	U	C5-C6-N1	-5.87	119.77	122.70
53	BA	935	C	N3-C4-N4	-5.87	113.89	118.00
53	BA	1243	C	O4'-C1'-N1	5.87	112.89	108.20
21	AA	233	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1507	A	N1-C6-N6	-5.87	115.08	118.60
53	BA	2222	C	N3-C2-O2	-5.87	117.79	121.90
53	BA	2380	C	N3-C2-O2	-5.87	117.79	121.90
46	BY	47	ARG	NE-CZ-NH1	5.87	123.23	120.30
53	BA	886	A	C4-C5-C6	-5.87	114.07	117.00
53	BA	2427	C	N3-C2-O2	-5.87	117.80	121.90
53	BA	2774	C	O4'-C1'-N1	5.87	112.89	108.20
1	AB	207	ARG	NE-CZ-NH1	5.86	123.23	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	38	A	C6-C5-N7	5.86	136.40	132.30
53	BA	1691	C	N3-C4-C5	5.86	124.25	121.90
53	BA	2332	C	N1-C2-O2	5.86	122.42	118.90
21	AA	637	C	N1-C2-O2	5.86	122.42	118.90
22	A1	8	U	N3-C2-O2	-5.86	118.10	122.20
53	BA	690	G	N1-C6-O6	-5.86	116.38	119.90
21	AA	747	A	C5-C6-N1	5.86	120.63	117.70
53	BA	354	A	C4-C5-C6	-5.86	114.07	117.00
53	BA	419	U	O4'-C1'-N1	5.86	112.89	108.20
53	BA	2108	A	C5-C6-N1	5.86	120.63	117.70
21	AA	37	U	C4'-C3'-C2'	-5.86	96.74	102.60
53	BA	2055	C	N3-C4-C5	5.86	124.24	121.90
21	AA	533	A	O4'-C4'-C3'	5.86	110.79	106.10
21	AA	1050	G	N3-C2-N2	-5.86	115.80	119.90
21	AA	1248	A	C5-C6-N1	5.86	120.63	117.70
42	BU	21	ARG	NE-CZ-NH1	5.86	123.23	120.30
53	BA	522	A	C5-C6-N1	5.86	120.63	117.70
53	BA	940	G	C5'-C4'-O4'	5.86	116.13	109.10
53	BA	2430	A	N1-C6-N6	-5.86	115.09	118.60
21	AA	1161	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	1400	C	N3-C2-O2	-5.86	117.80	121.90
53	BA	441	U	C5-C6-N1	-5.86	119.77	122.70
53	BA	1229	C	N1-C2-O2	5.86	122.41	118.90
53	BA	2797	U	N3-C2-O2	-5.86	118.10	122.20
21	AA	1022	A	C4-C5-C6	-5.85	114.07	117.00
53	BA	172	A	C4-C5-C6	-5.85	114.07	117.00
53	BA	816	C	C5'-C4'-O4'	5.85	116.12	109.10
53	BA	1569	A	C6-C5-N7	5.85	136.40	132.30
53	BA	2207	C	O4'-C1'-N1	5.85	112.88	108.20
53	BA	2433	A	C4-C5-C6	-5.85	114.07	117.00
53	BA	2727	A	C6-C5-N7	5.85	136.40	132.30
21	AA	1102	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	1136	C	N1-C2-O2	5.85	122.41	118.90
53	BA	1537	G	O4'-C1'-N9	5.85	112.88	108.20
53	BA	1822	C	N3-C2-O2	-5.85	117.80	121.90
53	BA	2060	A	C5-C6-N1	5.85	120.63	117.70
53	BA	2174	C	N3-C2-O2	-5.85	117.80	121.90
30	BI	7	TYR	CB-CG-CD1	-5.85	117.49	121.00
53	BA	109	C	N1-C2-O2	5.85	122.41	118.90
53	BA	1728	C	O4'-C1'-N1	5.85	112.88	108.20
53	BA	384	A	N1-C6-N6	-5.85	115.09	118.60
53	BA	1152	C	O4'-C1'-N1	5.85	112.88	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	478	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	768	A	N1-C6-N6	-5.84	115.09	118.60
22	A1	29	U	O4'-C1'-N1	5.84	112.88	108.20
53	BA	112	U	O4'-C1'-N1	5.84	112.88	108.20
21	AA	26	A	C4-C5-C6	-5.84	114.08	117.00
53	BA	1399	C	O4'-C1'-N1	5.84	112.87	108.20
53	BA	1467	U	O4'-C1'-N1	5.84	112.87	108.20
53	BA	1947	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	597	G	N1-C6-O6	-5.84	116.40	119.90
21	AA	1155	A	C4-C5-C6	-5.84	114.08	117.00
53	BA	1023	U	N1-C2-N3	5.84	118.40	114.90
53	BA	2609	U	C5-C6-N1	-5.84	119.78	122.70
21	AA	515	G	O4'-C1'-N9	5.84	112.87	108.20
21	AA	90	C	N1-C2-O2	5.84	122.40	118.90
21	AA	1206	G	N3-C4-C5	-5.84	125.68	128.60
53	BA	998	C	O4'-C1'-N1	5.84	112.87	108.20
53	BA	1074	G	N7-C8-N9	5.84	116.02	113.10
53	BA	1571	A	C4-C5-C6	-5.84	114.08	117.00
53	BA	1618	A	C4-C5-C6	-5.84	114.08	117.00
53	BA	1630	A	C5-C6-N1	5.84	120.62	117.70
53	BA	1887	C	O4'-C1'-N1	5.84	112.87	108.20
53	BA	2690	U	N3-C2-O2	-5.84	118.11	122.20
54	BB	66	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	648	A	C6-C5-N7	5.83	136.38	132.30
53	BA	778	G	C8-N9-C4	-5.83	104.07	106.40
53	BA	2638	G	C5-C6-N1	5.83	114.42	111.50
54	BB	50	A	C6-C5-N7	5.83	136.38	132.30
21	AA	429	U	N1-C1'-C2'	5.83	121.58	114.00
53	BA	443	A	C5-C6-N1	5.83	120.62	117.70
53	BA	485	C	N3-C2-O2	-5.83	117.82	121.90
53	BA	1913	A	C4-C5-C6	-5.83	114.08	117.00
53	BA	2510	C	N1-C2-O2	5.83	122.40	118.90
21	AA	300	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	658	C	N1-C2-O2	5.83	122.40	118.90
53	BA	269	C	N3-C4-C5	5.83	124.23	121.90
21	AA	1534	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	328	C	N1-C2-O2	5.83	122.40	118.90
21	AA	569	C	N1-C2-O2	5.83	122.40	118.90
21	AA	1093	A	C6-C5-N7	5.83	136.38	132.30
21	AA	1284	C	N3-C2-O2	-5.83	117.82	121.90
23	A2	92	U	N3-C2-O2	-5.83	118.12	122.20
53	BA	2076	U	O4'-C1'-N1	5.83	112.86	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2283	C	N3-C2-O2	-5.83	117.82	121.90
54	BB	97	C	N1-C2-O2	5.83	122.40	118.90
21	AA	872	A	C4-C5-C6	-5.83	114.09	117.00
53	BA	1611	C	C5'-C4'-O4'	5.83	116.09	109.10
53	BA	1962	C	N1-C2-O2	5.83	122.40	118.90
53	BA	156	A	C5-C6-N1	5.83	120.61	117.70
53	BA	686	U	N3-C2-O2	-5.83	118.12	122.20
53	BA	1026	G	C5-C6-N1	5.83	114.41	111.50
53	BA	1691	C	O4'-C1'-N1	5.83	112.86	108.20
53	BA	2132	U	O4'-C1'-N1	5.83	112.86	108.20
21	AA	503	C	N3-C2-O2	-5.82	117.82	121.90
53	BA	671	C	N1-C2-O2	5.82	122.39	118.90
53	BA	675	A	C4-C5-C6	-5.82	114.09	117.00
53	BA	1315	C	N3-C4-N4	-5.82	113.92	118.00
54	BB	38	C	N3-C2-O2	-5.82	117.82	121.90
21	AA	54	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	764	C	N3-C2-O2	-5.82	117.82	121.90
21	AA	853	C	O4'-C1'-N1	5.82	112.86	108.20
21	AA	866	C	N3-C4-C5	5.82	124.23	121.90
53	BA	888	C	N1-C2-O2	5.82	122.39	118.90
53	BA	1178	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	576	C	O4'-C1'-N1	5.82	112.86	108.20
53	BA	1088	A	C4-C5-C6	-5.82	114.09	117.00
53	BA	2566	A	P-O3'-C3'	5.82	126.68	119.70
22	A1	11	C	N1-C2-O2	5.82	122.39	118.90
53	BA	1544	A	N1-C6-N6	-5.82	115.11	118.60
53	BA	2617	U	N3-C2-O2	-5.82	118.13	122.20
53	BA	195	A	C6-C5-N7	5.82	136.37	132.30
53	BA	281	C	N3-C2-O2	-5.82	117.83	121.90
53	BA	2369	A	C5-C6-N1	5.82	120.61	117.70
53	BA	2554	U	C5'-C4'-O4'	5.82	116.08	109.10
54	BB	56	G	N1-C6-O6	-5.82	116.41	119.90
21	AA	568	G	C5-C6-N1	5.81	114.41	111.50
53	BA	991	C	O4'-C1'-N1	5.81	112.85	108.20
53	BA	2052	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	239	U	O4'-C1'-N1	5.81	112.85	108.20
21	AA	1275	A	C4-C5-C6	-5.81	114.09	117.00
53	BA	779	U	C5-C6-N1	-5.81	119.79	122.70
53	BA	919	U	N1-C2-N3	5.81	118.39	114.90
53	BA	1366	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	528	C	N3-C2-O2	-5.81	117.83	121.90
53	BA	704	G	N1-C6-O6	-5.81	116.41	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	740	C	N3-C2-O2	-5.81	117.83	121.90
53	BA	1173	U	C5-C6-N1	-5.81	119.79	122.70
21	AA	482	A	N1-C6-N6	-5.81	115.11	118.60
21	AA	793	U	C1'-O4'-C4'	-5.81	105.25	109.90
21	AA	857	C	N1-C2-O2	5.81	122.39	118.90
53	BA	39	G	N1-C6-O6	-5.81	116.42	119.90
53	BA	79	C	O4'-C1'-N1	5.81	112.85	108.20
53	BA	587	C	N3-C2-O2	-5.81	117.83	121.90
53	BA	1510	G	N3-C2-N2	-5.81	115.83	119.90
53	BA	2368	C	N3-C2-O2	-5.81	117.83	121.90
53	BA	2736	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	498	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	892	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	943	U	O4'-C1'-N1	5.81	112.85	108.20
53	BA	615	U	C5-C6-N1	-5.81	119.80	122.70
53	BA	2725	A	N1-C6-N6	-5.81	115.12	118.60
22	A1	59	U	C3'-C2'-C1'	5.81	106.14	101.50
53	BA	808	G	C5-C6-N1	5.81	114.40	111.50
21	AA	116	A	C5-C6-N1	5.80	120.60	117.70
21	AA	189	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1353	G	C5-C6-N1	5.80	114.40	111.50
53	BA	155	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	1060	U	C5-C6-N1	-5.80	119.80	122.70
53	BA	1385	A	C5-C6-N1	5.80	120.60	117.70
53	BA	1494	A	C5-C6-N1	5.80	120.60	117.70
54	BB	65	U	O4'-C1'-N1	5.80	112.84	108.20
53	BA	642	U	O4'-C1'-N1	5.80	112.84	108.20
53	BA	943	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	2144	G	N1-C6-O6	-5.80	116.42	119.90
53	BA	2303	G	O4'-C1'-N9	5.80	112.84	108.20
21	AA	135	C	N3-C2-O2	-5.80	117.84	121.90
50	B2	35	ARG	NE-CZ-NH1	5.80	123.20	120.30
53	BA	563	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	747	U	O4'-C1'-N1	5.80	112.84	108.20
21	AA	328	C	N3-C4-C5	5.80	124.22	121.90
21	AA	399	G	C8-N9-C4	-5.80	104.08	106.40
21	AA	1250	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	1597	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	1840	G	N3-C2-N2	-5.80	115.84	119.90
53	BA	1969	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	2506	U	N3-C2-O2	-5.80	118.14	122.20
21	AA	1007	U	N3-C2-O2	-5.80	118.14	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1378	A	C6-C5-N7	5.80	136.36	132.30
21	AA	34	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	975	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1297	G	C5-C6-N1	5.80	114.40	111.50
21	AA	1468	A	C4-C5-C6	-5.80	114.10	117.00
53	BA	107	G	C5-C6-N1	5.80	114.40	111.50
53	BA	527	C	N3-C2-O2	-5.80	117.84	121.90
53	BA	815	C	C5'-C4'-C3'	-5.80	106.72	116.00
53	BA	1139	G	C8-N9-C4	-5.80	104.08	106.40
53	BA	1584	U	C5-C6-N1	-5.80	119.80	122.70
53	BA	2700	A	C4-C5-C6	-5.80	114.10	117.00
22	A1	23	A	C5-C6-N1	5.79	120.60	117.70
53	BA	49	A	C4-C5-C6	-5.79	114.10	117.00
53	BA	2034	U	O4'-C1'-N1	5.79	112.84	108.20
53	BA	2638	G	N3-C4-C5	-5.79	125.70	128.60
21	AA	1145	A	C4-C5-C6	-5.79	114.10	117.00
21	AA	1273	C	O4'-C1'-N1	5.79	112.83	108.20
53	BA	310	A	C5-C6-N1	5.79	120.60	117.70
53	BA	452	G	N9-C4-C5	5.79	107.72	105.40
53	BA	2085	U	O4'-C1'-N1	5.79	112.83	108.20
53	BA	2116	G	C8-N9-C4	-5.79	104.08	106.40
53	BA	2885	G	O4'-C1'-N9	5.79	112.83	108.20
21	AA	990	C	N3-C2-O2	-5.79	117.85	121.90
53	BA	1208	C	O4'-C1'-N1	5.79	112.83	108.20
53	BA	1373	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	59	A	C4-C5-C6	-5.79	114.11	117.00
38	BQ	91	ARG	NE-CZ-NH2	-5.79	117.41	120.30
53	BA	444	C	N3-C2-O2	-5.79	117.85	121.90
53	BA	643	A	C5-C6-N1	5.79	120.59	117.70
53	BA	807	U	O4'-C1'-N1	5.79	112.83	108.20
53	BA	1550	C	N3-C2-O2	-5.79	117.85	121.90
54	BB	70	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	103	U	O4'-C1'-N1	5.79	112.83	108.20
53	BA	896	A	C4-C5-C6	-5.79	114.11	117.00
53	BA	2022	U	O4'-C1'-N1	5.79	112.83	108.20
21	AA	366	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	968	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	1525	G	C5-C6-N1	5.79	114.39	111.50
53	BA	96	C	O4'-C1'-N1	5.79	112.83	108.20
53	BA	796	C	N3-C2-O2	-5.79	117.85	121.90
53	BA	952	G	C5-C6-N1	5.79	114.39	111.50
53	BA	2352	A	C4-C5-C6	-5.79	114.11	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	766	A	C5-C6-N1	5.78	120.59	117.70
21	AA	1366	C	N1-C2-O2	5.78	122.37	118.90
53	BA	146	A	C4-C5-C6	-5.78	114.11	117.00
53	BA	840	C	N1-C2-O2	5.78	122.37	118.90
53	BA	924	G	N1-C6-O6	-5.78	116.43	119.90
53	BA	1268	A	C4-C5-C6	-5.78	114.11	117.00
53	BA	1937	A	C6-C5-N7	5.78	136.35	132.30
53	BA	2023	C	N1-C2-O2	5.78	122.37	118.90
53	BA	2766	A	C4-C5-C6	-5.78	114.11	117.00
53	BA	2841	C	N3-C4-C5	5.78	124.21	121.90
21	AA	339	C	N3-C2-O2	-5.78	117.85	121.90
53	BA	2272	U	C4-C5-C6	5.78	123.17	119.70
21	AA	398	U	O4'-C1'-N1	5.78	112.83	108.20
21	AA	1530	G	N1-C6-O6	-5.78	116.43	119.90
42	BU	5	ARG	NE-CZ-NH1	5.78	123.19	120.30
53	BA	820	A	N1-C6-N6	-5.78	115.13	118.60
53	BA	835	C	N3-C4-C5	5.78	124.21	121.90
53	BA	1064	C	N1-C2-O2	5.78	122.37	118.90
53	BA	2498	C	C6-N1-C2	-5.78	117.99	120.30
53	BA	2562	U	C5-C6-N1	-5.78	119.81	122.70
53	BA	2731	G	O4'-C1'-N9	5.78	112.82	108.20
53	BA	2787	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	483	C	N3-C2-O2	-5.78	117.86	121.90
53	BA	1599	U	N1-C2-N3	5.78	118.37	114.90
53	BA	2871	U	N3-C2-O2	-5.78	118.15	122.20
53	BA	727	A	O4'-C1'-N9	5.78	112.82	108.20
53	BA	1572	A	N1-C6-N6	-5.78	115.13	118.60
21	AA	429	U	C3'-C2'-C1'	-5.78	96.88	101.50
21	AA	1005	A	N1-C6-N6	-5.78	115.14	118.60
21	AA	1203	C	N3-C2-O2	-5.78	117.86	121.90
53	BA	220	G	C5-C6-N1	5.78	114.39	111.50
53	BA	1775	U	C5-C6-N1	-5.78	119.81	122.70
53	BA	2614	A	C4-C5-C6	-5.78	114.11	117.00
53	BA	879	G	C8-N9-C4	-5.77	104.09	106.40
53	BA	635	C	N3-C4-C5	5.77	124.21	121.90
53	BA	660	C	N1-C2-O2	5.77	122.36	118.90
53	BA	2007	U	O4'-C1'-N1	5.77	112.82	108.20
53	BA	2498	C	N3-C2-O2	-5.77	117.86	121.90
53	BA	2610	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	573	A	C3'-C2'-C1'	5.77	106.12	101.50
21	AA	802	A	C4-C5-C6	-5.77	114.11	117.00
53	BA	1903	G	O4'-C1'-N9	5.77	112.82	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	487	A	C4-C5-C6	-5.77	114.11	117.00
21	AA	1200	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	1474	U	O4'-C1'-N1	5.77	112.82	108.20
24	BC	202	ARG	NE-CZ-NH1	5.77	123.19	120.30
53	BA	621	A	C4-C5-C6	-5.77	114.11	117.00
53	BA	734	A	C4-C5-C6	-5.77	114.11	117.00
53	BA	1117	C	N3-C4-N4	-5.77	113.96	118.00
53	BA	1207	C	N1-C2-O2	5.77	122.36	118.90
53	BA	2272	U	C5-C6-N1	-5.77	119.81	122.70
53	BA	2435	A	C4-C5-C6	-5.77	114.11	117.00
53	BA	2660	A	O4'-C1'-N9	5.77	112.82	108.20
7	AH	113	ARG	NE-CZ-NH1	5.77	123.18	120.30
17	AR	47	ARG	NE-CZ-NH1	5.77	123.18	120.30
21	AA	1350	A	C5-C6-N1	5.77	120.58	117.70
53	BA	164	C	O4'-C1'-N1	5.77	112.81	108.20
53	BA	327	G	N1-C6-O6	-5.77	116.44	119.90
53	BA	330	A	O4'-C1'-N9	5.77	112.81	108.20
53	BA	795	C	N1-C2-O2	5.77	122.36	118.90
53	BA	1681	G	O4'-C1'-N9	5.77	112.81	108.20
53	BA	1685	C	N3-C4-C5	5.77	124.21	121.90
53	BA	2173	A	C4-C5-C6	-5.77	114.12	117.00
53	BA	2324	U	O4'-C1'-N1	5.77	112.81	108.20
53	BA	2412	A	C5-C6-N1	5.77	120.58	117.70
53	BA	2444	G	N1-C6-O6	-5.77	116.44	119.90
53	BA	2792	A	C4-C5-C6	-5.77	114.12	117.00
53	BA	226	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	1525	G	N3-C4-C5	-5.76	125.72	128.60
53	BA	725	G	N1-C6-O6	-5.76	116.44	119.90
53	BA	1083	U	N3-C2-O2	-5.76	118.17	122.20
53	BA	1706	C	N3-C4-C5	5.76	124.21	121.90
53	BA	1793	C	N3-C2-O2	-5.76	117.86	121.90
54	BB	41	G	N3-C4-C5	-5.76	125.72	128.60
21	AA	1151	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	617	G	C5-C6-N1	5.76	114.38	111.50
21	AA	1015	G	N3-C2-N2	-5.76	115.87	119.90
53	BA	432	A	C4-C5-C6	-5.76	114.12	117.00
53	BA	1191	G	C5-C6-N1	5.76	114.38	111.50
53	BA	1731	G	N3-C4-C5	-5.76	125.72	128.60
53	BA	1821	A	C5-C6-N1	5.76	120.58	117.70
21	AA	790	A	O4'-C4'-C3'	5.76	110.71	106.10
21	AA	1198	G	N1-C6-O6	-5.76	116.44	119.90
53	BA	484	C	N1-C2-O2	5.76	122.36	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1424	G	N1-C6-O6	-5.76	116.44	119.90
54	BB	34	A	C6-C5-N7	5.76	136.33	132.30
21	AA	536	C	N1-C2-O2	5.76	122.36	118.90
21	AA	1377	A	C4-C5-C6	-5.76	114.12	117.00
53	BA	415	A	C6-C5-N7	5.76	136.33	132.30
53	BA	1568	G	N1-C6-O6	-5.76	116.44	119.90
53	BA	2000	C	O4'-C1'-N1	5.76	112.81	108.20
12	AM	69	ARG	NE-CZ-NH1	5.76	123.18	120.30
21	AA	770	C	C4'-C3'-C2'	-5.76	96.84	102.60
21	AA	860	A	C5-C6-N1	5.76	120.58	117.70
21	AA	1064	G	C5-C6-N1	5.76	114.38	111.50
53	BA	2561	U	O4'-C1'-N1	5.76	112.81	108.20
53	BA	96	C	N3-C2-O2	-5.75	117.87	121.90
53	BA	179	C	N1-C2-O2	5.75	122.35	118.90
53	BA	208	C	N1-C2-O2	5.75	122.35	118.90
53	BA	1534	U	N1-C2-N3	5.75	118.35	114.90
21	AA	186	C	N3-C2-O2	-5.75	117.87	121.90
27	BF	29	ARG	NE-CZ-NH1	5.75	123.18	120.30
53	BA	158	U	C5-C6-N1	-5.75	119.82	122.70
53	BA	1541	C	N3-C2-O2	-5.75	117.87	121.90
53	BA	1800	C	N3-C2-O2	-5.75	117.87	121.90
53	BA	2215	C	C5'-C4'-O4'	5.75	116.00	109.10
53	BA	2511	U	C5-C4-O4	-5.75	122.45	125.90
53	BA	2731	G	C3'-C2'-C1'	5.75	106.10	101.50
53	BA	2825	G	N3-C4-C5	-5.75	125.72	128.60
21	AA	531	U	O4'-C1'-N1	5.75	112.80	108.20
53	BA	345	A	C3'-C2'-C1'	5.75	106.10	101.50
53	BA	407	G	N1-C6-O6	-5.75	116.45	119.90
53	BA	1378	A	P-O3'-C3'	5.75	126.60	119.70
53	BA	1999	C	O4'-C1'-N1	5.75	112.80	108.20
21	AA	106	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	830	G	N3-C4-C5	-5.75	125.72	128.60
21	AA	854	U	N1-C2-N3	5.75	118.35	114.90
21	AA	1101	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	1301	U	C5-C6-N1	-5.75	119.83	122.70
53	BA	1420	A	C3'-C2'-C1'	5.75	106.10	101.50
53	BA	1553	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	462	G	O4'-C1'-N9	5.75	112.80	108.20
53	BA	449	A	C6-C5-N7	5.75	136.32	132.30
53	BA	792	A	C5-C6-N1	5.75	120.57	117.70
53	BA	1410	G	N1-C6-O6	-5.75	116.45	119.90
53	BA	1461	C	O4'-C1'-N1	5.75	112.80	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2214	C	O4'-C1'-N1	5.75	112.80	108.20
21	AA	1287	A	C6-C5-N7	5.75	136.32	132.30
32	BK	64	ARG	NE-CZ-NH1	5.75	123.17	120.30
53	BA	311	A	C4-C5-C6	-5.75	114.13	117.00
53	BA	914	G	N3-C2-N2	-5.75	115.88	119.90
53	BA	1214	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	203	G	C4'-C3'-C2'	-5.74	96.86	102.60
53	BA	249	C	N1-C2-O2	5.74	122.35	118.90
53	BA	524	G	C5-C6-N1	5.74	114.37	111.50
53	BA	1141	U	N1-C2-N3	5.74	118.35	114.90
53	BA	1793	C	O4'-C1'-N1	5.74	112.80	108.20
53	BA	2431	U	O4'-C1'-N1	5.74	112.80	108.20
54	BB	101	A	C4-C5-C6	-5.74	114.13	117.00
53	BA	8	C	N3-C4-C5	5.74	124.20	121.90
53	BA	774	G	C5-C6-N1	5.74	114.37	111.50
53	BA	913	U	C5-C6-N1	-5.74	119.83	122.70
53	BA	2891	U	O4'-C1'-N1	5.74	112.79	108.20
15	AP	25	ARG	NE-CZ-NH1	-5.74	117.43	120.30
21	AA	100	G	N1-C6-O6	-5.74	116.45	119.90
21	AA	343	U	N1-C2-N3	5.74	118.34	114.90
53	BA	1795	C	N1-C2-O2	5.74	122.34	118.90
21	AA	519	C	O4'-C1'-N1	5.74	112.79	108.20
21	AA	1096	C	N1-C2-O2	5.74	122.34	118.90
21	AA	1318	A	C4-C5-C6	-5.74	114.13	117.00
53	BA	76	C	N3-C2-O2	-5.74	117.88	121.90
53	BA	509	C	N1-C2-O2	5.74	122.34	118.90
53	BA	1526	C	N1-C2-O2	5.74	122.34	118.90
53	BA	2674	G	N1-C6-O6	-5.74	116.46	119.90
53	BA	2705	A	C4-C5-C6	-5.74	114.13	117.00
53	BA	118	A	C5'-C4'-O4'	5.74	115.98	109.10
17	AR	60	ARG	NE-CZ-NH1	5.74	123.17	120.30
21	AA	1070	U	O4'-C1'-N1	5.74	112.79	108.20
53	BA	64	A	C4-C5-C6	-5.74	114.13	117.00
53	BA	1179	G	N3-C2-N2	-5.74	115.89	119.90
53	BA	1189	A	N1-C6-N6	-5.74	115.16	118.60
53	BA	761	A	C4-C5-C6	-5.73	114.13	117.00
53	BA	1173	U	N1-C2-N3	5.73	118.34	114.90
53	BA	1574	C	C5'-C4'-O4'	5.73	115.98	109.10
21	AA	1472	U	O4'-C1'-N1	5.73	112.79	108.20
53	BA	532	A	C5-C6-N1	5.73	120.57	117.70
53	BA	2278	A	C5-C6-N1	5.73	120.57	117.70
54	BB	3	C	N3-C2-O2	-5.73	117.89	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	899	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	1037	C	O4'-C1'-N1	5.73	112.78	108.20
53	BA	245	G	N7-C8-N9	5.73	115.97	113.10
53	BA	688	U	O4'-C1'-N1	5.73	112.78	108.20
53	BA	1473	G	N1-C6-O6	-5.73	116.46	119.90
21	AA	1200	C	O4'-C1'-N1	5.73	112.78	108.20
53	BA	1748	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	179	A	C6-C5-N7	5.73	136.31	132.30
21	AA	393	A	C4-C5-C6	-5.73	114.14	117.00
21	AA	470	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	612	C	N1-C2-O2	5.73	122.34	118.90
53	BA	1016	G	O4'-C1'-N9	5.73	112.78	108.20
53	BA	1111	A	C4-C5-C6	-5.73	114.14	117.00
53	BA	1499	C	O4'-C1'-N1	5.73	112.78	108.20
21	AA	991	U	O4'-C1'-N1	5.73	112.78	108.20
21	AA	1206	G	C5-C6-N1	5.73	114.36	111.50
53	BA	205	G	N3-C4-C5	-5.73	125.74	128.60
53	BA	1323	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	617	G	N1-C6-O6	-5.72	116.47	119.90
21	AA	1476	A	C4-C5-C6	-5.72	114.14	117.00
53	BA	304	U	O4'-C1'-N1	5.72	112.78	108.20
53	BA	320	A	C4-C5-C6	-5.72	114.14	117.00
53	BA	399	U	O4'-C1'-N1	5.72	112.78	108.20
53	BA	1639	C	N1-C2-O2	5.72	122.33	118.90
53	BA	1990	C	N1-C2-O2	5.72	122.33	118.90
53	BA	2440	C	C2-N3-C4	-5.72	117.04	119.90
8	AI	10	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
21	AA	564	C	N3-C2-O2	-5.72	117.89	121.90
40	BS	84	ARG	NE-CZ-NH1	5.72	123.16	120.30
53	BA	298	G	N3-C4-C5	-5.72	125.74	128.60
53	BA	478	A	C5-C6-N1	5.72	120.56	117.70
53	BA	675	A	N1-C6-N6	-5.72	115.17	118.60
53	BA	775	G	N3-C4-C5	-5.72	125.74	128.60
21	AA	296	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	1390	U	O4'-C1'-N1	5.72	112.78	108.20
38	BQ	27	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
53	BA	1325	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	769	G	N7-C8-N9	5.72	115.96	113.10
53	BA	375	G	C5-C6-N1	5.72	114.36	111.50
53	BA	1092	C	N3-C2-O2	-5.72	117.90	121.90
53	BA	1319	C	N3-C2-O2	-5.72	117.90	121.90
54	BB	43	C	N3-C2-O2	-5.72	117.90	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	215	C	N3-C2-O2	-5.72	117.90	121.90
53	BA	1127	A	N1-C6-N6	-5.72	115.17	118.60
53	BA	1208	C	N3-C2-O2	-5.72	117.90	121.90
53	BA	1578	U	N1-C2-N3	5.72	118.33	114.90
53	BA	2606	C	N3-C4-C5	5.72	124.19	121.90
53	BA	2865	U	N3-C2-O2	-5.72	118.20	122.20
21	AA	971	G	C3'-C2'-C1'	-5.71	96.93	101.50
53	BA	916	G	C8-N9-C4	-5.71	104.11	106.40
53	BA	1087	G	N3-C2-N2	-5.71	115.90	119.90
53	BA	1122	G	N3-C2-N2	-5.71	115.90	119.90
53	BA	1773	A	N1-C6-N6	-5.71	115.17	118.60
21	AA	726	C	N1-C2-O2	5.71	122.33	118.90
21	AA	742	G	C8-N9-C4	-5.71	104.11	106.40
21	AA	1243	C	N3-C2-O2	-5.71	117.90	121.90
53	BA	229	C	N3-C2-O2	-5.71	117.90	121.90
53	BA	502	A	C5-C6-N1	5.71	120.56	117.70
21	AA	1140	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	492	C	N1-C2-O2	5.71	122.33	118.90
51	B3	39	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	AC	87	ARG	NE-CZ-NH1	5.71	123.15	120.30
53	BA	511	U	O4'-C4'-C3'	5.71	110.67	106.10
53	BA	1414	C	N3-C2-O2	-5.71	117.90	121.90
53	BA	1805	A	C5-C6-N1	5.71	120.55	117.70
53	BA	264	C	N3-C2-O2	-5.71	117.91	121.90
53	BA	470	A	C4-C5-C6	-5.71	114.15	117.00
53	BA	539	G	C5'-C4'-O4'	5.71	115.95	109.10
53	BA	2059	A	C4-C5-C6	-5.71	114.15	117.00
53	BA	2609	U	O4'-C1'-N1	5.71	112.77	108.20
21	AA	1430	A	C6-C5-N7	5.71	136.29	132.30
53	BA	2848	G	N1-C6-O6	-5.71	116.48	119.90
53	BA	190	A	C5-C6-N1	5.70	120.55	117.70
53	BA	465	G	N1-C6-O6	-5.70	116.48	119.90
53	BA	1283	G	N3-C4-C5	-5.70	125.75	128.60
53	BA	2829	A	C4-C5-C6	-5.70	114.15	117.00
3	AD	164	ARG	NE-CZ-NH2	5.70	123.15	120.30
21	AA	379	C	N1-C2-O2	5.70	122.32	118.90
21	AA	962	C	N1-C2-O2	5.70	122.32	118.90
21	AA	1291	U	O4'-C1'-N1	5.70	112.76	108.20
53	BA	1059	G	N9-C4-C5	5.70	107.68	105.40
53	BA	1556	C	N3-C2-O2	-5.70	117.91	121.90
53	BA	956	G	N1-C6-O6	-5.70	116.48	119.90
53	BA	1074	G	C8-N9-C4	-5.70	104.12	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2443	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	883	C	N1-C2-O2	5.70	122.32	118.90
53	BA	767	U	C5-C6-N1	-5.70	119.85	122.70
53	BA	1406	U	C5-C6-N1	-5.70	119.85	122.70
53	BA	2150	C	N3-C2-O2	-5.70	117.91	121.90
53	BA	1788	C	N3-C2-O2	-5.70	117.91	121.90
53	BA	2442	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	86	G	N9-C4-C5	5.70	107.68	105.40
21	AA	1288	A	C4-C5-C6	-5.70	114.15	117.00
53	BA	766	U	O4'-C1'-N1	5.70	112.76	108.20
53	BA	1545	A	C5-C6-N1	5.70	120.55	117.70
53	BA	1704	C	O4'-C1'-N1	5.70	112.76	108.20
53	BA	2243	U	C5-C6-N1	-5.70	119.85	122.70
53	BA	2304	G	N1-C6-O6	-5.69	116.48	119.90
21	AA	44	A	C4-C5-C6	-5.69	114.15	117.00
21	AA	95	C	N3-C4-C5	5.69	124.18	121.90
53	BA	540	C	N1-C2-O2	5.69	122.32	118.90
53	BA	630	G	C5-C6-N1	5.69	114.35	111.50
53	BA	1240	U	O4'-C1'-N1	5.69	112.75	108.20
53	BA	1488	C	N1-C2-O2	5.69	122.31	118.90
21	AA	220	G	N3-C2-N2	-5.69	115.92	119.90
21	AA	1007	U	C5-C6-N1	-5.69	119.86	122.70
53	BA	1598	A	C5-C6-N1	5.69	120.55	117.70
53	BA	1932	A	C6-C5-N7	5.69	136.28	132.30
53	BA	2490	G	N3-C2-N2	-5.69	115.92	119.90
21	AA	554	A	C4-C5-C6	-5.69	114.16	117.00
21	AA	1054	C	N1-C2-O2	5.69	122.31	118.90
22	A1	23	A	N1-C6-N6	-5.69	115.19	118.60
53	BA	360	U	O4'-C1'-N1	5.69	112.75	108.20
53	BA	676	A	C5-C6-N1	5.69	120.55	117.70
53	BA	750	A	C4-C5-C6	-5.69	114.16	117.00
53	BA	2589	A	C6-C5-N7	5.69	136.28	132.30
53	BA	2649	C	C6-N1-C2	-5.69	118.02	120.30
53	BA	2698	U	O4'-C1'-N1	5.69	112.75	108.20
53	BA	876	C	N1-C2-O2	5.69	122.31	118.90
53	BA	1590	A	C6-C5-N7	5.69	136.28	132.30
21	AA	806	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	868	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	908	A	N1-C6-N6	-5.68	115.19	118.60
53	BA	362	A	C5-C6-N1	5.68	120.54	117.70
53	BA	937	C	N3-C2-O2	-5.68	117.92	121.90
53	BA	1394	U	C5-C6-N1	-5.68	119.86	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1637	A	C5-C6-N1	5.68	120.54	117.70
53	BA	2112	G	N3-C4-C5	-5.68	125.76	128.60
53	BA	2806	C	N3-C4-C5	5.68	124.17	121.90
21	AA	267	C	N1-C2-O2	5.68	122.31	118.90
21	AA	426	U	O4'-C1'-N1	5.68	112.75	108.20
21	AA	511	C	O4'-C1'-N1	5.68	112.75	108.20
21	AA	866	C	N1-C2-O2	5.68	122.31	118.90
21	AA	1178	G	C8-N9-C4	-5.68	104.13	106.40
53	BA	1308	A	O4'-C1'-N9	5.68	112.75	108.20
53	BA	1410	G	C8-N9-C4	-5.68	104.13	106.40
53	BA	1686	C	N1-C2-O2	5.68	122.31	118.90
53	BA	2096	C	N3-C2-O2	-5.68	117.92	121.90
53	BA	2602	A	O4'-C1'-N9	5.68	112.75	108.20
22	A1	25	C	O4'-C1'-N1	5.68	112.74	108.20
53	BA	129	C	N3-C2-O2	-5.68	117.92	121.90
53	BA	1057	A	C5-C6-N1	5.68	120.54	117.70
53	BA	1384	A	C6-C5-N7	5.68	136.28	132.30
21	AA	1188	A	C4-C5-C6	-5.68	114.16	117.00
53	BA	782	A	O4'-C1'-N9	5.68	112.74	108.20
53	BA	1234	U	O4'-C1'-N1	5.68	112.74	108.20
53	BA	1838	C	N3-C2-O2	-5.68	117.93	121.90
53	BA	2488	G	O4'-C1'-N9	5.68	112.74	108.20
53	BA	361	G	N1-C6-O6	-5.68	116.49	119.90
53	BA	1031	G	N9-C4-C5	5.68	107.67	105.40
21	AA	853	C	N3-C2-O2	-5.67	117.93	121.90
53	BA	852	U	O4'-C1'-N1	5.67	112.74	108.20
53	BA	1109	C	N1-C2-O2	5.67	122.31	118.90
53	BA	2407	A	C4-C5-C6	-5.67	114.16	117.00
53	BA	1810	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	970	C	N1-C2-O2	5.67	122.30	118.90
21	AA	1019	A	C4-C5-C6	-5.67	114.16	117.00
53	BA	1012	U	C5-C6-N1	-5.67	119.86	122.70
53	BA	1104	C	O4'-C1'-N1	5.67	112.74	108.20
53	BA	1412	U	C5-C6-N1	-5.67	119.86	122.70
53	BA	1812	U	O4'-C1'-N1	5.67	112.74	108.20
21	AA	288	A	C5-C6-N1	5.67	120.53	117.70
21	AA	1451	U	N3-C2-O2	-5.67	118.23	122.20
53	BA	1214	A	C5-C6-N1	5.67	120.53	117.70
53	BA	2357	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	595	A	O4'-C1'-N9	5.67	112.73	108.20
21	AA	1016	A	C5-C6-N1	5.67	120.53	117.70
53	BA	984	A	C6-C5-N7	5.67	136.27	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1155	A	C5-C6-N1	5.67	120.53	117.70
53	BA	2513	A	C5-C6-N1	5.67	120.53	117.70
53	BA	2825	G	N7-C8-N9	5.67	115.93	113.10
21	AA	83	C	N1-C2-O2	5.67	122.30	118.90
21	AA	688	G	C8-N9-C4	-5.67	104.13	106.40
21	AA	1346	A	C4-C5-C6	-5.67	114.17	117.00
29	BH	50	ARG	NE-CZ-NH1	5.67	123.13	120.30
53	BA	2755	C	N1-C2-O2	5.67	122.30	118.90
8	AI	32	ARG	NE-CZ-NH1	5.66	123.13	120.30
53	BA	1970	A	C4-C5-C6	-5.66	114.17	117.00
53	BA	2058	A	O4'-C1'-N9	5.66	112.73	108.20
53	BA	2578	G	C5-C6-N1	5.66	114.33	111.50
21	AA	319	G	O4'-C1'-N9	5.66	112.73	108.20
53	BA	2248	C	O4'-C1'-N1	5.66	112.73	108.20
53	BA	2561	U	N3-C2-O2	-5.66	118.24	122.20
21	AA	144	G	C5-C6-N1	5.66	114.33	111.50
21	AA	940	C	N1-C2-O2	5.66	122.30	118.90
53	BA	1284	A	N1-C6-N6	-5.66	115.20	118.60
53	BA	2350	C	N3-C2-O2	-5.66	117.94	121.90
53	BA	2763	G	N3-C2-N2	-5.66	115.94	119.90
21	AA	199	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	235	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	265	G	N3-C4-C5	-5.66	125.77	128.60
22	A1	25	C	N1-C2-O2	5.66	122.30	118.90
51	B3	7	ARG	NE-CZ-NH1	5.66	123.13	120.30
53	BA	28	A	C4-C5-C6	-5.66	114.17	117.00
53	BA	903	C	N1-C2-O2	5.66	122.30	118.90
53	BA	1168	G	C5-C6-N1	5.66	114.33	111.50
53	BA	1518	C	O4'-C1'-N1	5.66	112.73	108.20
21	AA	968	A	C2-N3-C4	5.66	113.43	110.60
21	AA	1066	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1519	A	C4-C5-C6	-5.66	114.17	117.00
53	BA	66	C	N1-C2-O2	5.66	122.29	118.90
53	BA	267	C	O4'-C1'-N1	5.66	112.72	108.20
53	BA	1141	U	C3'-C2'-C1'	5.66	106.02	101.50
53	BA	1996	C	N3-C2-O2	-5.66	117.94	121.90
53	BA	2723	C	O4'-C1'-N1	5.66	112.72	108.20
53	BA	8	C	N1-C2-O2	5.65	122.29	118.90
53	BA	528	A	C5-C6-N1	5.65	120.53	117.70
53	BA	2515	C	C4'-C3'-C2'	-5.65	96.95	102.60
3	AD	164	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
21	AA	911	U	O4'-C1'-N1	5.65	112.72	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	935	A	C4-C5-C6	-5.65	114.17	117.00
53	BA	757	G	C8-N9-C4	-5.65	104.14	106.40
53	BA	1083	U	N1-C2-N3	5.65	118.29	114.90
21	AA	765	G	N3-C2-N2	-5.65	115.94	119.90
21	AA	883	C	N3-C4-C5	5.65	124.16	121.90
21	AA	1082	A	C4-C5-C6	-5.65	114.17	117.00
53	BA	453	A	C4-C5-C6	-5.65	114.17	117.00
53	BA	1186	G	N1-C6-O6	-5.65	116.51	119.90
54	BB	29	A	C6-C5-N7	5.65	136.25	132.30
21	AA	1518	A	O4'-C1'-N9	5.65	112.72	108.20
53	BA	919	U	C5-C6-N1	-5.65	119.88	122.70
53	BA	1181	U	N1-C2-N3	5.65	118.29	114.90
21	AA	1404	C	N3-C4-C5	5.65	124.16	121.90
53	BA	2072	C	N1-C2-O2	5.65	122.29	118.90
53	BA	2386	A	C4-C5-C6	-5.65	114.18	117.00
53	BA	2581	G	C8-N9-C4	-5.65	104.14	106.40
21	AA	633	G	N3-C2-N2	-5.65	115.95	119.90
53	BA	299	A	C5-C6-N1	5.64	120.52	117.70
53	BA	2874	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	549	C	N1-C2-O2	5.64	122.28	118.90
21	AA	1201	A	C5-C6-N1	5.64	120.52	117.70
21	AA	1327	C	N1-C2-O2	5.64	122.28	118.90
21	AA	1493	A	C1'-O4'-C4'	-5.64	105.39	109.90
53	BA	44	A	C6-C5-N7	5.64	136.25	132.30
53	BA	510	C	N1-C2-O2	5.64	122.29	118.90
53	BA	990	A	C5-C6-N1	5.64	120.52	117.70
53	BA	2642	G	O4'-C1'-N9	5.64	112.71	108.20
53	BA	2882	A	C6-C5-N7	5.64	136.25	132.30
53	BA	436	C	N1-C2-O2	5.64	122.28	118.90
53	BA	1824	G	N1-C6-O6	-5.64	116.52	119.90
53	BA	2415	G	C4'-C3'-C2'	-5.64	96.96	102.60
53	BA	2425	A	C6-C5-N7	5.64	136.25	132.30
21	AA	889	A	N1-C6-N6	-5.64	115.22	118.60
53	BA	466	A	C4-C5-C6	-5.64	114.18	117.00
53	BA	574	A	C4-C5-C6	-5.64	114.18	117.00
53	BA	614	A	N1-C6-N6	-5.64	115.22	118.60
53	BA	1164	C	N3-C2-O2	-5.64	117.95	121.90
53	BA	1501	G	C5-C6-N1	5.64	114.32	111.50
53	BA	2860	A	C4-C5-C6	-5.64	114.18	117.00
53	BA	21	A	C5-C6-N1	5.64	120.52	117.70
53	BA	192	C	O4'-C1'-N1	5.64	112.71	108.20
53	BA	927	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(^{o})	Ideal(^{o})
53	BA	1359	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	642	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	1013	G	N1-C6-O6	-5.64	116.52	119.90
53	BA	538	A	C5-C6-N1	5.64	120.52	117.70
53	BA	1215	G	C8-N9-C4	-5.64	104.15	106.40
53	BA	1677	A	O4'-C1'-N9	5.64	112.71	108.20
53	BA	2573	C	O4'-C1'-N1	5.64	112.71	108.20
21	AA	530	G	N3-C4-C5	-5.63	125.78	128.60
53	BA	160	A	C6-C5-N7	5.63	136.24	132.30
53	BA	1157	G	C5-C6-N1	5.63	114.32	111.50
53	BA	1459	G	N3-C4-C5	-5.63	125.78	128.60
53	BA	1898	U	C5-C6-N1	-5.63	119.88	122.70
53	BA	2473	U	O4'-C1'-N1	5.63	112.71	108.20
21	AA	439	U	O4'-C1'-N1	5.63	112.71	108.20
53	BA	1521	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	100	G	C5-C6-N1	5.63	114.32	111.50
21	AA	1130	A	C4-C5-C6	-5.63	114.18	117.00
53	BA	173	A	C5-C6-N1	5.63	120.52	117.70
53	BA	1495	A	C5-C6-N1	5.63	120.52	117.70
53	BA	2153	C	N1-C2-O2	5.63	122.28	118.90
54	BB	54	G	C4'-C3'-C2'	-5.63	96.97	102.60
21	AA	9	G	N3-C2-N2	-5.63	115.96	119.90
21	AA	616	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	1117	A	C1'-O4'-C4'	-5.63	105.40	109.90
53	BA	1390	U	C5'-C4'-C3'	-5.63	106.99	116.00
53	BA	1858	A	C5-C6-N1	5.63	120.52	117.70
21	AA	392	C	N3-C2-O2	-5.63	117.96	121.90
53	BA	205	G	N1-C6-O6	-5.63	116.52	119.90
53	BA	979	A	C4-C5-C6	-5.63	114.19	117.00
53	BA	1412	U	N3-C2-O2	-5.63	118.26	122.20
53	BA	1971	U	C5-C6-N1	-5.63	119.89	122.70
53	BA	2388	A	C5'-C4'-O4'	5.63	115.85	109.10
53	BA	2873	A	C5-C6-N1	5.63	120.51	117.70
54	BB	12	C	N1-C2-O2	5.63	122.28	118.90
21	AA	184	G	O4'-C1'-N9	5.63	112.70	108.20
21	AA	676	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	877	G	C5-C6-N1	5.63	114.31	111.50
22	A1	3	G	N1-C6-O6	-5.63	116.52	119.90
22	A1	17	U	N3-C2-O2	-5.63	118.26	122.20
53	BA	509	C	N3-C4-N4	-5.63	114.06	118.00
53	BA	1116	G	N3-C2-N2	-5.63	115.96	119.90
53	BA	1417	C	N1-C2-O2	5.63	122.28	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1632	A	C5-C6-N1	5.63	120.51	117.70
53	BA	1871	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1075	U	O4'-C1'-N1	5.62	112.70	108.20
21	AA	1376	U	N1-C2-N3	5.62	118.28	114.90
53	BA	2854	G	C5-C6-N1	5.62	114.31	111.50
11	AL	49	ARG	NE-CZ-NH1	5.62	123.11	120.30
21	AA	326	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	636	U	O4'-C1'-N1	5.62	112.70	108.20
53	BA	970	U	O4'-C1'-N1	5.62	112.70	108.20
53	BA	1226	A	C4-C5-C6	-5.62	114.19	117.00
53	BA	1512	C	O4'-C1'-N1	5.62	112.70	108.20
21	AA	844	G	N1-C6-O6	-5.62	116.53	119.90
53	BA	519	U	O4'-C1'-N1	5.62	112.70	108.20
53	BA	1305	C	N3-C2-O2	-5.62	117.97	121.90
9	AJ	16	ARG	NE-CZ-NH1	5.62	123.11	120.30
21	AA	360	G	O4'-C1'-N9	5.62	112.70	108.20
53	BA	1392	A	C5'-C4'-O4'	5.62	115.84	109.10
53	BA	1633	G	C8-N9-C4	-5.62	104.15	106.40
53	BA	2028	U	O4'-C1'-N1	5.62	112.70	108.20
53	BA	2307	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	290	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	337	G	N3-C4-C5	-5.62	125.79	128.60
21	AA	1098	C	N3-C2-O2	-5.62	117.97	121.90
22	A1	2	G	O4'-C1'-N9	5.62	112.69	108.20
53	BA	1151	A	C5-C6-N1	5.62	120.51	117.70
53	BA	1300	G	N3-C4-C5	-5.62	125.79	128.60
53	BA	1493	C	O4'-C1'-N1	5.62	112.69	108.20
53	BA	1535	A	C6-C5-N7	5.62	136.23	132.30
53	BA	1977	A	C4-C5-C6	-5.62	114.19	117.00
53	BA	2512	C	N1-C2-O2	5.62	122.27	118.90
21	AA	92	U	N1-C2-N3	5.62	118.27	114.90
21	AA	205	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	947	G	C5-C6-N1	5.62	114.31	111.50
53	BA	557	C	C4'-C3'-C2'	-5.62	96.98	102.60
53	BA	1007	C	N1-C2-O2	5.62	122.27	118.90
53	BA	2003	A	C4-C5-C6	-5.62	114.19	117.00
53	BA	2726	A	C5-C6-N1	5.62	120.51	117.70
21	AA	736	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	1053	G	N3-C2-N2	-5.62	115.97	119.90
21	AA	1059	C	N1-C2-O2	5.62	122.27	118.90
21	AA	1513	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1531	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(^{o})	Ideal(^{o})
53	BA	1382	G	N3-C4-C5	-5.62	125.79	128.60
21	AA	555	U	N3-C2-O2	-5.61	118.27	122.20
21	AA	1327	C	N3-C4-C5	5.61	124.15	121.90
53	BA	757	G	N3-C2-N2	-5.61	115.97	119.90
53	BA	859	G	C5-C6-N1	5.61	114.31	111.50
21	AA	1328	C	N1-C2-O2	5.61	122.27	118.90
53	BA	7	G	C5-C6-N1	5.61	114.31	111.50
53	BA	309	A	C4-C5-C6	-5.61	114.19	117.00
53	BA	330	A	C4-C5-C6	-5.61	114.19	117.00
53	BA	2091	C	O4'-C1'-N1	5.61	112.69	108.20
53	BA	2831	G	N1-C6-O6	-5.61	116.53	119.90
21	AA	313	A	C5-C6-N1	5.61	120.50	117.70
53	BA	336	C	N1-C2-O2	5.61	122.27	118.90
21	AA	161	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	316	C	N1-C2-O2	5.61	122.27	118.90
53	BA	1459	G	C8-N9-C4	-5.61	104.16	106.40
53	BA	1853	A	C5-C6-N1	5.61	120.50	117.70
21	AA	811	C	C3'-C2'-C1'	5.61	105.98	101.50
21	AA	1089	G	C8-N9-C4	-5.61	104.16	106.40
53	BA	545	U	N1-C2-N3	5.61	118.26	114.90
53	BA	736	C	N3-C2-O2	-5.61	117.98	121.90
53	BA	2022	U	N3-C2-O2	-5.61	118.28	122.20
21	AA	132	C	N3-C2-O2	-5.60	117.98	121.90
10	AK	97	ARG	NE-CZ-NH1	5.60	123.10	120.30
21	AA	35	G	N1-C6-O6	-5.60	116.54	119.90
21	AA	387	U	O4'-C1'-N1	5.60	112.68	108.20
53	BA	1113	U	O4'-C1'-N1	5.60	112.68	108.20
53	BA	1406	U	O4'-C1'-N1	5.60	112.68	108.20
53	BA	1419	A	O4'-C1'-N9	5.60	112.68	108.20
53	BA	1453	A	C1'-O4'-C4'	-5.60	105.42	109.90
53	BA	1742	U	N1-C2-N3	5.60	118.26	114.90
53	BA	2000	C	N3-C4-C5	5.60	124.14	121.90
21	AA	157	U	O4'-C1'-N1	5.60	112.68	108.20
21	AA	948	C	N1-C2-O2	5.60	122.26	118.90
21	AA	1333	A	C4-C5-C6	-5.60	114.20	117.00
53	BA	1610	A	C2-N3-C4	5.60	113.40	110.60
53	BA	1673	G	N3-C2-N2	-5.60	115.98	119.90
53	BA	1814	G	C8-N9-C4	-5.60	104.16	106.40
53	BA	1856	U	O4'-C1'-N1	5.60	112.68	108.20
53	BA	2482	A	C4-C5-C6	-5.60	114.20	117.00
54	BB	97	C	C5'-C4'-O4'	5.60	115.82	109.10
5	AF	79	ARG	NE-CZ-NH1	5.60	123.10	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	826	U	O4'-C1'-N1	5.60	112.68	108.20
53	BA	900	A	C4-C5-C6	-5.60	114.20	117.00
53	BA	1002	G	N3-C4-C5	-5.60	125.80	128.60
53	BA	1100	C	N3-C2-O2	-5.60	117.98	121.90
53	BA	1318	U	C3'-C2'-C1'	5.60	105.98	101.50
53	BA	1727	C	O4'-C1'-N1	5.60	112.68	108.20
53	BA	2077	A	C4-C5-C6	-5.60	114.20	117.00
53	BA	2111	U	C5-C6-N1	-5.60	119.90	122.70
53	BA	2243	U	N1-C2-N3	5.60	118.26	114.90
53	BA	2356	U	C5'-C4'-O4'	5.60	115.82	109.10
21	AA	88	U	C5-C6-N1	-5.60	119.90	122.70
21	AA	301	G	N1-C6-O6	-5.60	116.54	119.90
53	BA	1891	G	C5-C6-N1	5.60	114.30	111.50
21	AA	47	C	N3-C2-O2	-5.59	117.98	121.90
21	AA	1047	G	C5-C6-N1	5.59	114.30	111.50
53	BA	550	C	N3-C2-O2	-5.59	117.98	121.90
53	BA	2649	C	N3-C2-O2	-5.59	117.98	121.90
21	AA	1293	C	N1-C2-O2	5.59	122.26	118.90
53	BA	1281	G	N3-C2-N2	-5.59	115.98	119.90
21	AA	80	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	1029	U	C5-C6-N1	-5.59	119.90	122.70
21	AA	1128	C	N1-C2-O2	5.59	122.25	118.90
21	AA	1350	A	C4-C5-C6	-5.59	114.20	117.00
53	BA	2200	C	N3-C2-O2	-5.59	117.99	121.90
53	BA	2606	C	O4'-C1'-N1	5.59	112.67	108.20
21	AA	419	C	O4'-C1'-N1	5.59	112.67	108.20
21	AA	1410	A	C4-C5-C6	-5.59	114.21	117.00
53	BA	1405	U	N3-C2-O2	-5.59	118.29	122.20
53	BA	2399	G	N1-C6-O6	-5.59	116.55	119.90
53	BA	2512	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	846	G	C4'-C3'-C2'	-5.59	97.01	102.60
53	BA	973	A	O4'-C1'-N9	5.59	112.67	108.20
53	BA	2453	A	C4-C5-C6	-5.59	114.21	117.00
53	BA	2540	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1352	C	N3-C4-C5	5.59	124.13	121.90
53	BA	1069	A	C5-C6-N1	5.59	120.49	117.70
53	BA	1139	G	C5-N7-C8	-5.59	101.51	104.30
21	AA	940	C	N3-C4-C5	5.58	124.13	121.90
21	AA	1449	C	N1-C2-O2	5.58	122.25	118.90
53	BA	729	G	C5-C6-N1	5.58	114.29	111.50
21	AA	355	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	909	A	C4-C5-C6	-5.58	114.21	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1190	G	P-O3'-C3'	5.58	126.40	119.70
53	BA	61	C	N3-C4-N4	-5.58	114.09	118.00
53	BA	815	C	N3-C2-O2	-5.58	117.99	121.90
53	BA	1326	U	O4'-C1'-N1	5.58	112.67	108.20
53	BA	2731	G	N1-C6-O6	-5.58	116.55	119.90
54	BB	52	A	C4-C5-C6	-5.58	114.21	117.00
3	AD	103	ARG	NE-CZ-NH1	5.58	123.09	120.30
21	AA	129	A	O4'-C1'-N9	5.58	112.67	108.20
35	BN	96	ARG	NE-CZ-NH1	5.58	123.09	120.30
53	BA	46	G	C5'-C4'-O4'	5.58	115.80	109.10
53	BA	211	C	N3-C2-O2	-5.58	117.99	121.90
53	BA	2313	C	N1-C2-O2	5.58	122.25	118.90
53	BA	2463	C	N1-C2-O2	5.58	122.25	118.90
53	BA	2554	U	O4'-C1'-N1	5.58	112.67	108.20
53	BA	850	U	C5-C6-N1	-5.58	119.91	122.70
53	BA	2561	U	C5-C6-N1	-5.58	119.91	122.70
21	AA	64	G	N3-C4-C5	-5.58	125.81	128.60
21	AA	1257	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	1324	A	C4-C5-C6	-5.58	114.21	117.00
35	BN	90	ARG	NE-CZ-NH2	5.58	123.09	120.30
53	BA	1918	A	O4'-C1'-N9	5.58	112.66	108.20
53	BA	2015	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	752	G	N9-C4-C5	5.58	107.63	105.40
21	AA	1359	C	N3-C2-O2	-5.58	118.00	121.90
53	BA	1467	U	N3-C2-O2	-5.58	118.30	122.20
53	BA	1628	G	N1-C6-O6	-5.58	116.55	119.90
53	BA	1925	C	C6-N1-C2	-5.58	118.07	120.30
21	AA	1310	G	N9-C4-C5	5.58	107.63	105.40
33	BL	60	ARG	NE-CZ-NH2	-5.58	117.51	120.30
53	BA	879	G	N7-C8-N9	5.58	115.89	113.10
53	BA	988	A	C4-C5-C6	-5.58	114.21	117.00
53	BA	1348	C	N3-C2-O2	-5.58	118.00	121.90
53	BA	2013	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	1028	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	1493	A	O4'-C1'-N9	5.57	112.66	108.20
53	BA	1246	A	N1-C6-N6	-5.57	115.26	118.60
53	BA	1647	U	C6-N1-C2	-5.57	117.66	121.00
53	BA	1892	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	556	C	N1-C2-O2	5.57	122.24	118.90
53	BA	243	U	C5-C6-N1	-5.57	119.91	122.70
21	AA	733	G	N3-C4-C5	-5.57	125.81	128.60
21	AA	1432	G	O4'-C1'-N9	5.57	112.66	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	540	C	N3-C4-C5	5.57	124.13	121.90
53	BA	838	C	O4'-C1'-N1	5.57	112.66	108.20
53	BA	902	C	N1-C2-O2	5.57	122.24	118.90
53	BA	1633	G	N9-C4-C5	5.57	107.63	105.40
53	BA	1952	A	C4-C5-C6	-5.57	114.22	117.00
53	BA	2538	C	N3-C2-O2	-5.57	118.00	121.90
53	BA	2776	A	O4'-C1'-N9	5.57	112.66	108.20
53	BA	334	C	N1-C2-O2	5.57	122.24	118.90
53	BA	1012	U	N3-C2-O2	-5.57	118.30	122.20
21	AA	98	A	C6-C5-N7	5.57	136.20	132.30
21	AA	893	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	1378	C	N1-C2-O2	5.57	122.24	118.90
53	BA	1505	A	C6-C5-N7	5.57	136.20	132.30
53	BA	2455	G	N7-C8-N9	5.57	115.88	113.10
54	BB	92	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	99	C	N1-C2-O2	5.57	122.24	118.90
53	BA	227	A	O4'-C1'-N9	5.57	112.65	108.20
53	BA	994	C	N1-C2-O2	5.57	122.24	118.90
53	BA	1057	A	C4-C5-C6	-5.57	114.22	117.00
53	BA	1974	C	C4'-C3'-C2'	-5.57	97.03	102.60
21	AA	232	G	C8-N9-C4	-5.56	104.17	106.40
21	AA	320	A	C6-C5-N7	5.56	136.19	132.30
21	AA	1052	U	C5-C6-N1	-5.56	119.92	122.70
53	BA	94	A	C6-C5-N7	5.56	136.19	132.30
53	BA	255	A	N1-C6-N6	-5.56	115.26	118.60
53	BA	393	C	N3-C2-O2	-5.56	118.01	121.90
53	BA	458	G	N1-C6-O6	-5.56	116.56	119.90
53	BA	487	C	N3-C2-O2	-5.56	118.01	121.90
53	BA	2062	A	C1'-O4'-C4'	-5.56	105.45	109.90
11	AL	88	ASP	CB-CG-OD1	5.56	123.31	118.30
21	AA	596	A	C5-C6-N1	5.56	120.48	117.70
21	AA	868	C	O4'-C1'-N1	5.56	112.65	108.20
53	BA	1447	C	N3-C2-O2	-5.56	118.01	121.90
53	BA	1573	G	O4'-C1'-N9	5.56	112.65	108.20
19	AT	73	ARG	NE-CZ-NH1	5.56	123.08	120.30
21	AA	40	C	O4'-C1'-N1	5.56	112.65	108.20
21	AA	104	G	C5-C6-N1	5.56	114.28	111.50
53	BA	623	C	N1-C2-O2	5.56	122.24	118.90
53	BA	640	C	N3-C4-C5	5.56	124.12	121.90
54	BB	25	U	C5-C6-N1	-5.56	119.92	122.70
21	AA	249	U	O4'-C1'-N1	5.56	112.65	108.20
53	BA	314	C	O4'-C1'-N1	5.56	112.64	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1279	G	N3-C4-C5	-5.56	125.82	128.60
21	AA	837	U	C5-C6-N1	-5.56	119.92	122.70
53	BA	1194	A	C5-C6-N1	5.56	120.48	117.70
21	AA	47	C	N1-C2-O2	5.55	122.23	118.90
22	A1	74	C	C1'-O4'-C4'	-5.55	105.46	109.90
23	A2	80	C	N1-C2-O2	5.55	122.23	118.90
53	BA	773	U	C5-C6-N1	-5.55	119.92	122.70
53	BA	777	G	C8-N9-C4	-5.55	104.18	106.40
53	BA	1403	A	C5-C6-N1	5.55	120.48	117.70
53	BA	2899	A	N1-C6-N6	-5.55	115.27	118.60
21	AA	302	G	C5-C6-N1	5.55	114.28	111.50
30	BI	87	SER	C-N-CA	5.55	133.96	122.30
21	AA	33	A	C4-C5-C6	-5.55	114.22	117.00
21	AA	42	G	C5-C6-N1	5.55	114.28	111.50
21	AA	737	C	C4'-C3'-C2'	-5.55	97.05	102.60
21	AA	1038	C	N3-C4-C5	5.55	124.12	121.90
53	BA	1172	C	N3-C2-O2	-5.55	118.01	121.90
53	BA	2497	A	C4-C5-C6	-5.55	114.22	117.00
53	BA	2509	G	C4'-C3'-C2'	-5.55	97.05	102.60
53	BA	2767	C	N1-C2-O2	5.55	122.23	118.90
21	AA	291	U	O4'-C1'-N1	5.55	112.64	108.20
53	BA	817	C	N3-C4-C5	5.55	124.12	121.90
53	BA	1308	A	C4-C5-C6	-5.55	114.22	117.00
53	BA	1333	G	N1-C6-O6	-5.55	116.57	119.90
53	BA	1654	A	C5-C6-N1	5.55	120.47	117.70
53	BA	1709	U	O4'-C1'-N1	5.55	112.64	108.20
53	BA	1889	A	C4-C5-C6	-5.55	114.23	117.00
21	AA	1325	C	O4'-C1'-N1	5.55	112.64	108.20
53	BA	311	A	O4'-C1'-N9	5.55	112.64	108.20
53	BA	518	G	N3-C4-C5	-5.55	125.83	128.60
53	BA	748	G	O4'-C1'-N9	5.55	112.64	108.20
53	BA	1722	A	C5-C6-N1	5.55	120.47	117.70
21	AA	504	C	N1-C2-O2	5.55	122.23	118.90
21	AA	894	G	C5-C6-N1	5.55	114.27	111.50
21	AA	1261	A	N1-C6-N6	-5.55	115.27	118.60
53	BA	339	U	N1-C2-N3	5.55	118.23	114.90
53	BA	1855	U	O4'-C1'-N1	5.55	112.64	108.20
53	BA	634	C	N1-C2-O2	5.54	122.23	118.90
21	AA	301	G	C8-N9-C4	-5.54	104.18	106.40
21	AA	742	G	O4'-C1'-N9	5.54	112.64	108.20
28	BG	93	TYR	CB-CG-CD2	-5.54	117.67	121.00
38	BQ	23	TYR	CB-CG-CD2	-5.54	117.67	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	713	G	N1-C6-O6	-5.54	116.57	119.90
53	BA	1275	A	O4'-C4'-C3'	5.54	110.53	106.10
53	BA	1288	G	N1-C6-O6	-5.54	116.57	119.90
53	BA	1471	G	N7-C8-N9	5.54	115.87	113.10
54	BB	27	C	N3-C4-C5	5.54	124.12	121.90
8	AI	123	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	514	C	N3-C2-O2	-5.54	118.02	121.90
53	BA	849	A	C6-C5-N7	5.54	136.18	132.30
53	BA	924	G	N3-C4-C5	-5.54	125.83	128.60
53	BA	2127	G	O4'-C1'-N9	5.54	112.63	108.20
54	BB	30	C	O4'-C1'-N1	5.54	112.63	108.20
21	AA	177	G	N3-C4-C5	-5.54	125.83	128.60
21	AA	1248	A	C4-C5-C6	-5.54	114.23	117.00
53	BA	84	A	C4-C5-C6	-5.54	114.23	117.00
53	BA	380	G	C5-C6-N1	5.54	114.27	111.50
53	BA	620	G	O4'-C1'-N9	5.54	112.63	108.20
21	AA	381	C	O4'-C1'-N1	5.54	112.63	108.20
21	AA	609	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	1398	A	C2'-C3'-O3'	5.54	122.56	113.70
21	AA	1504	G	N1-C6-O6	-5.54	116.58	119.90
53	BA	516	C	C4'-C3'-C2'	-5.54	97.06	102.60
53	BA	764	A	C5-C6-N1	5.54	120.47	117.70
53	BA	2730	C	O4'-C1'-N1	5.54	112.63	108.20
53	BA	2787	C	N1-C2-O2	5.54	122.22	118.90
21	AA	1348	U	C5-C6-N1	-5.54	119.93	122.70
53	BA	1894	C	N3-C4-C5	5.54	124.11	121.90
53	BA	2071	A	C6-C5-N7	5.54	136.18	132.30
21	AA	772	U	C5-C6-N1	-5.54	119.93	122.70
53	BA	252	G	C5-C6-N1	5.54	114.27	111.50
53	BA	1542	U	O4'-C1'-N1	5.54	112.63	108.20
53	BA	1616	A	C4-C5-C6	-5.54	114.23	117.00
53	BA	1750	G	C5-C6-N1	5.54	114.27	111.50
21	AA	395	C	N1-C2-O2	5.53	122.22	118.90
29	BH	116	ARG	NE-CZ-NH1	5.53	123.07	120.30
53	BA	2029	G	O4'-C1'-N9	5.53	112.63	108.20
53	BA	2525	G	O4'-C1'-N9	5.53	112.63	108.20
53	BA	1235	G	N7-C8-N9	5.53	115.87	113.10
21	AA	211	G	C5-C6-N1	5.53	114.27	111.50
21	AA	459	A	C5-C6-N1	5.53	120.47	117.70
21	AA	1320	C	N3-C2-O2	-5.53	118.03	121.90
53	BA	1021	A	C4-C5-C6	-5.53	114.23	117.00
53	BA	1039	A	C6-C5-N7	5.53	136.17	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1246	A	C5-C6-N1	5.53	120.47	117.70
53	BA	1661	G	C5-C6-N1	5.53	114.27	111.50
53	BA	1857	G	O4'-C1'-N9	5.53	112.62	108.20
53	BA	2305	U	C4-C5-C6	5.53	123.02	119.70
21	AA	412	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	767	A	C6-C5-N7	5.53	136.17	132.30
53	BA	691	C	N1-C2-O2	5.53	122.22	118.90
53	BA	2264	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	153	C	O4'-C1'-N1	5.53	112.62	108.20
21	AA	879	C	N3-C2-O2	-5.53	118.03	121.90
53	BA	944	C	O4'-C1'-N1	5.53	112.62	108.20
53	BA	1392	A	C4-C5-C6	-5.53	114.24	117.00
53	BA	2226	C	N3-C2-O2	-5.53	118.03	121.90
53	BA	2636	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	300	A	N1-C6-N6	-5.53	115.28	118.60
53	BA	1819	A	C5-C6-N1	5.53	120.46	117.70
53	BA	1880	U	O4'-C1'-N1	5.53	112.62	108.20
54	BB	30	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	720	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	1123	U	O4'-C1'-N1	5.52	112.62	108.20
53	BA	85	G	C5-C6-N1	5.52	114.26	111.50
53	BA	1420	A	C5-C6-N1	5.52	120.46	117.70
53	BA	1463	C	N3-C2-O2	-5.52	118.03	121.90
53	BA	1531	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	1486	G	O4'-C1'-N9	5.52	112.62	108.20
53	BA	869	G	N3-C4-C5	-5.52	125.84	128.60
53	BA	1488	C	O4'-C1'-N1	5.52	112.62	108.20
53	BA	1895	C	N3-C2-O2	-5.52	118.03	121.90
53	BA	2848	G	O4'-C1'-N9	5.52	112.62	108.20
21	AA	623	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	1342	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	757	U	O4'-C1'-N1	5.52	112.61	108.20
22	A1	51	C	N3-C2-O2	-5.52	118.04	121.90
53	BA	1176	U	C5-C6-N1	-5.52	119.94	122.70
53	BA	338	G	C8-N9-C4	-5.52	104.19	106.40
53	BA	553	G	N9-C4-C5	5.52	107.61	105.40
53	BA	1932	A	O4'-C1'-N9	5.52	112.61	108.20
53	BA	2175	C	N3-C2-O2	-5.52	118.04	121.90
53	BA	2244	U	O4'-C1'-N1	5.52	112.61	108.20
53	BA	2451	A	C4'-C3'-C2'	-5.52	97.08	102.60
53	BA	2834	G	N3-C4-C5	-5.52	125.84	128.60
53	BA	1284	A	C4-C5-C6	-5.52	114.24	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2826	A	C4-C5-C6	-5.52	114.24	117.00
54	BB	46	A	C6-C5-N7	5.52	136.16	132.30
53	BA	142	A	C4-C5-C6	-5.51	114.24	117.00
53	BA	407	G	O4'-C1'-N9	5.51	112.61	108.20
53	BA	1309	G	C5-C6-N1	5.51	114.26	111.50
53	BA	1639	C	O4'-C1'-N1	5.51	112.61	108.20
53	BA	1708	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	779	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	944	G	N1-C6-O6	-5.51	116.59	119.90
53	BA	48	G	C5-C6-N1	5.51	114.26	111.50
53	BA	500	G	N1-C6-O6	-5.51	116.59	119.90
53	BA	699	A	C4-C5-C6	-5.51	114.24	117.00
53	BA	2116	G	N3-C2-N2	-5.51	116.04	119.90
53	BA	2796	U	O4'-C1'-N1	5.51	112.61	108.20
21	AA	456	A	C4-C5-C6	-5.51	114.24	117.00
21	AA	496	A	C4-C5-C6	-5.51	114.24	117.00
21	AA	756	C	N3-C4-C5	5.51	124.11	121.90
21	AA	972	C	N3-C2-O2	-5.51	118.04	121.90
53	BA	274	C	O4'-C1'-N1	5.51	112.61	108.20
53	BA	971	G	C5-C6-N1	5.51	114.26	111.50
53	BA	1140	C	P-O3'-C3'	5.51	126.31	119.70
53	BA	2196	C	N3-C2-O2	-5.51	118.04	121.90
53	BA	2403	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	214	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	1371	G	C5-C6-N1	5.51	114.25	111.50
53	BA	952	G	N1-C6-O6	-5.51	116.59	119.90
53	BA	1690	A	C4-C5-C6	-5.51	114.25	117.00
53	BA	2237	G	C5-C6-N1	5.51	114.25	111.50
21	AA	634	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	641	U	C5-C6-N1	-5.51	119.95	122.70
21	AA	848	C	N3-C2-O2	-5.51	118.04	121.90
53	BA	616	A	C4-C5-C6	-5.51	114.25	117.00
21	AA	522	C	N3-C2-O2	-5.51	118.05	121.90
21	AA	823	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	854	U	O4'-C1'-N1	5.51	112.61	108.20
21	AA	1473	G	N1-C6-O6	-5.51	116.60	119.90
53	BA	1010	A	C4-C5-C6	-5.51	114.25	117.00
53	BA	1346	G	N1-C6-O6	-5.51	116.60	119.90
53	BA	2239	G	C5-C6-N1	5.51	114.25	111.50
53	BA	2311	A	C4-C5-C6	-5.51	114.25	117.00
53	BA	2645	G	O4'-C1'-N9	5.51	112.61	108.20
21	AA	1072	G	N1-C6-O6	-5.50	116.60	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	501	A	C5-C6-N1	5.50	120.45	117.70
53	BA	632	A	C4-C5-C6	-5.50	114.25	117.00
53	BA	645	C	N3-C2-O2	-5.50	118.05	121.90
8	AI	17	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	AA	534	U	O4'-C1'-N1	5.50	112.60	108.20
53	BA	201	C	N1-C2-O2	5.50	122.20	118.90
53	BA	362	A	O4'-C1'-N9	5.50	112.60	108.20
53	BA	1210	G	N1-C6-O6	-5.50	116.60	119.90
53	BA	2478	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	1309	G	C8-N9-C4	-5.50	104.20	106.40
21	AA	1488	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	1493	A	C2-N3-C4	5.50	113.35	110.60
53	BA	2270	A	C5-N7-C8	-5.50	101.15	103.90
21	AA	175	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	1081	A	C4-C5-C6	-5.50	114.25	117.00
53	BA	155	A	C4'-C3'-C2'	-5.50	97.10	102.60
53	BA	930	G	C5-C6-N1	5.50	114.25	111.50
53	BA	1025	G	C8-N9-C4	-5.50	104.20	106.40
53	BA	2525	G	C8-N9-C4	-5.50	104.20	106.40
21	AA	1204	A	C5-C6-N1	5.50	120.45	117.70
53	BA	62	U	C1'-O4'-C4'	-5.50	105.50	109.90
53	BA	2827	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	333	U	O4'-C1'-N1	5.50	112.60	108.20
53	BA	224	U	C5-C6-N1	-5.50	119.95	122.70
53	BA	1280	G	C5-C6-N1	5.50	114.25	111.50
53	BA	2895	G	C8-N9-C4	-5.50	104.20	106.40
21	AA	879	C	N1-C2-O2	5.50	122.20	118.90
21	AA	1114	C	O4'-C1'-N1	5.50	112.60	108.20
21	AA	732	C	N1-C2-O2	5.49	122.20	118.90
21	AA	919	A	N1-C6-N6	-5.49	115.30	118.60
21	AA	1190	G	C5-C6-N1	5.49	114.25	111.50
21	AA	1308	U	C1'-O4'-C4'	-5.49	105.50	109.90
21	AA	1399	C	N3-C4-C5	5.49	124.10	121.90
53	BA	1327	A	C4-C5-C6	-5.49	114.25	117.00
53	BA	1836	C	O4'-C1'-N1	5.49	112.60	108.20
53	BA	1910	G	C5-C6-N1	5.49	114.25	111.50
53	BA	2243	U	N3-C2-O2	-5.49	118.36	122.20
53	BA	2832	U	C5-C6-N1	-5.49	119.95	122.70
54	BB	56	G	C5-C6-N1	5.49	114.25	111.50
21	AA	282	A	C6-C5-N7	5.49	136.14	132.30
53	BA	12	U	C5-C6-N1	-5.49	119.95	122.70
53	BA	1121	C	N1-C2-O2	5.49	122.19	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1939	U	N1-C2-N3	5.49	118.19	114.90
21	AA	353	A	O4'-C1'-N9	5.49	112.59	108.20
21	AA	501	C	N1-C2-O2	5.49	122.19	118.90
53	BA	1559	U	N1-C2-N3	5.49	118.19	114.90
53	BA	1691	C	N1-C2-O2	5.49	122.19	118.90
21	AA	1203	C	O4'-C1'-N1	5.49	112.59	108.20
53	BA	407	G	N3-C4-C5	-5.49	125.86	128.60
53	BA	1439	A	C4-C5-C6	-5.49	114.25	117.00
53	BA	1738	G	C5-C6-N1	5.49	114.24	111.50
53	BA	1871	A	C2-N3-C4	5.49	113.34	110.60
53	BA	2733	A	C4-C5-C6	-5.49	114.25	117.00
54	BB	90	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	961	U	N3-C2-O2	-5.49	118.36	122.20
22	A1	30	C	O4'-C1'-N1	5.49	112.59	108.20
22	A1	35	A	C5-C6-N1	5.49	120.44	117.70
49	B1	27	ARG	NE-CZ-NH2	5.49	123.04	120.30
53	BA	779	U	N3-C2-O2	-5.49	118.36	122.20
53	BA	1179	G	N7-C8-N9	5.49	115.84	113.10
53	BA	2001	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	504	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	970	C	N3-C4-C5	5.49	124.09	121.90
53	BA	1603	A	C6-C5-N7	5.49	136.14	132.30
53	BA	2098	U	O4'-C1'-N1	5.49	112.59	108.20
53	BA	2536	G	N9-C4-C5	5.49	107.59	105.40
53	BA	2752	C	O4'-C1'-N1	5.49	112.59	108.20
53	BA	905	A	C5-C6-N1	5.48	120.44	117.70
53	BA	1231	U	N3-C2-O2	-5.48	118.36	122.20
53	BA	2481	G	N3-C4-C5	-5.48	125.86	128.60
21	AA	867	G	O4'-C1'-N9	5.48	112.58	108.20
32	BK	30	ARG	NE-CZ-NH2	-5.48	117.56	120.30
53	BA	2212	A	C8-N9-C4	-5.48	103.61	105.80
53	BA	2457	U	C5-C6-N1	-5.48	119.96	122.70
21	AA	74	A	C4-C5-C6	-5.48	114.26	117.00
53	BA	130	C	N3-C2-O2	-5.48	118.06	121.90
53	BA	2629	U	N3-C2-O2	-5.48	118.36	122.20
53	BA	2726	A	C4-C5-C6	-5.48	114.26	117.00
53	BA	2900	A	C5-C6-N1	5.48	120.44	117.70
21	AA	1170	A	C4-C5-C6	-5.48	114.26	117.00
53	BA	1883	U	O4'-C1'-N1	5.48	112.58	108.20
48	B0	15	ARG	NE-CZ-NH1	5.48	123.04	120.30
53	BA	99	U	N3-C2-O2	-5.48	118.36	122.20
53	BA	502	A	C4-C5-C6	-5.48	114.26	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1008	A	C5-C6-N1	5.48	120.44	117.70
53	BA	1167	C	O4'-C1'-N1	5.48	112.58	108.20
53	BA	1294	U	O4'-C1'-N1	5.48	112.58	108.20
53	BA	1769	U	C4'-C3'-C2'	-5.48	97.12	102.60
53	BA	1842	G	N9-C4-C5	5.48	107.59	105.40
53	BA	2073	C	N3-C2-O2	-5.48	118.07	121.90
53	BA	2505	G	C5-C6-N1	5.48	114.24	111.50
53	BA	2643	G	N1-C6-O6	-5.48	116.61	119.90
54	BB	55	U	O4'-C1'-N1	5.48	112.58	108.20
53	BA	748	G	N3-C2-N2	-5.48	116.07	119.90
53	BA	2063	C	N3-C2-O2	-5.48	118.07	121.90
21	AA	1045	C	C6-N1-C2	-5.47	118.11	120.30
28	BG	148	ARG	NE-CZ-NH1	5.47	123.04	120.30
53	BA	33	C	N3-C2-O2	-5.47	118.07	121.90
53	BA	620	G	N3-C2-N2	-5.47	116.07	119.90
53	BA	1542	U	C5-C6-N1	-5.47	119.96	122.70
53	BA	1904	G	N1-C6-O6	-5.47	116.61	119.90
53	BA	1924	C	N3-C2-O2	-5.47	118.07	121.90
53	BA	2009	A	C6-C5-N7	5.47	136.13	132.30
53	BA	2629	U	O4'-C1'-N1	5.47	112.58	108.20
54	BB	4	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	117	G	N9-C4-C5	5.47	107.59	105.40
21	AA	1326	U	N3-C2-O2	-5.47	118.37	122.20
53	BA	990	A	C5'-C4'-O4'	5.47	115.67	109.10
53	BA	1532	A	C4-C5-C6	-5.47	114.26	117.00
53	BA	1655	A	C5-C6-N1	5.47	120.44	117.70
53	BA	2115	G	N1-C6-O6	-5.47	116.62	119.90
14	AO	62	ARG	NE-CZ-NH1	5.47	123.04	120.30
53	BA	1944	U	O4'-C1'-N1	5.47	112.58	108.20
21	AA	261	U	N1-C2-N3	5.47	118.18	114.90
21	AA	1180	A	C4-C5-C6	-5.47	114.27	117.00
45	BX	56	ARG	NE-CZ-NH1	5.47	123.03	120.30
48	B0	49	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
53	BA	353	C	N1-C2-O2	5.47	122.18	118.90
53	BA	870	U	N3-C2-O2	-5.47	118.37	122.20
53	BA	1153	C	O4'-C1'-N1	5.47	112.58	108.20
53	BA	1461	C	N1-C2-O2	5.47	122.18	118.90
53	BA	2863	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	415	A	C4-C5-C6	-5.47	114.27	117.00
53	BA	1376	C	N3-C2-O2	-5.47	118.07	121.90
53	BA	1566	A	C4-C5-C6	-5.47	114.27	117.00
53	BA	2704	C	O4'-C1'-N1	5.47	112.57	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2787	C	N3-C4-C5	5.47	124.09	121.90
53	BA	2788	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	585	G	C8-N9-C4	-5.47	104.21	106.40
21	AA	772	U	O4'-C1'-N1	5.47	112.57	108.20
33	BL	59	ARG	NE-CZ-NH1	5.47	123.03	120.30
53	BA	167	A	C4-C5-C6	-5.47	114.27	117.00
53	BA	401	A	O4'-C1'-N9	5.47	112.57	108.20
53	BA	480	A	C4-C5-C6	-5.47	114.27	117.00
53	BA	1620	G	C5-C6-N1	5.47	114.23	111.50
53	BA	1918	A	C3'-C2'-C1'	5.47	105.87	101.50
53	BA	2351	G	O4'-C1'-N9	5.47	112.57	108.20
53	BA	2714	G	C5-C6-N1	5.47	114.23	111.50
21	AA	339	C	N1-C2-O2	5.46	122.18	118.90
21	AA	747	A	C4-C5-C6	-5.46	114.27	117.00
23	A2	82	A	C6-C5-N7	5.46	136.12	132.30
53	BA	356	G	N1-C6-O6	-5.46	116.62	119.90
53	BA	2392	A	C4-C5-C6	-5.46	114.27	117.00
21	AA	620	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	663	A	C6-C5-N7	5.46	136.12	132.30
53	BA	894	U	O4'-C1'-N1	5.46	112.57	108.20
53	BA	1296	G	N1-C6-O6	-5.46	116.62	119.90
53	BA	1408	G	N7-C8-N9	5.46	115.83	113.10
54	BB	88	C	N3-C4-C5	5.46	124.08	121.90
21	AA	1204	A	C4-C5-C6	-5.46	114.27	117.00
35	BN	8	ARG	NE-CZ-NH1	5.46	123.03	120.30
53	BA	682	G	O4'-C1'-N9	5.46	112.57	108.20
53	BA	2058	A	C6-C5-N7	5.46	136.12	132.30
53	BA	2409	G	C5-C6-N1	5.46	114.23	111.50
53	BA	2834	G	N1-C6-O6	-5.46	116.62	119.90
53	BA	907	G	N3-C4-C5	-5.46	125.87	128.60
22	A1	35	A	C4-C5-C6	-5.46	114.27	117.00
51	B3	41	ARG	NE-CZ-NH1	5.46	123.03	120.30
53	BA	39	G	C5-C6-N1	5.46	114.23	111.50
53	BA	198	C	N3-C2-O2	-5.46	118.08	121.90
53	BA	1102	C	N3-C2-O2	-5.46	118.08	121.90
53	BA	2322	A	C4-C5-C6	-5.46	114.27	117.00
53	BA	2655	G	C3'-C2'-C1'	-5.46	97.13	101.50
21	AA	506	G	N3-C2-N2	-5.46	116.08	119.90
21	AA	662	U	O4'-C1'-N1	5.46	112.56	108.20
53	BA	106	C	O4'-C1'-N1	5.46	112.56	108.20
53	BA	305	C	N3-C2-O2	-5.46	118.08	121.90
53	BA	381	G	C5-C6-N1	5.46	114.23	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	717	C	C1'-O4'-C4'	-5.46	105.53	109.90
53	BA	1212	G	C5-C6-N1	5.46	114.23	111.50
53	BA	1697	G	C5-C6-N1	5.46	114.23	111.50
53	BA	2715	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	609	A	O4'-C1'-N9	5.45	112.56	108.20
21	AA	1003	G	O4'-C1'-N9	5.45	112.56	108.20
53	BA	57	C	N3-C4-C5	5.45	124.08	121.90
53	BA	75	G	C5-C6-N1	5.45	114.23	111.50
53	BA	127	A	C4-C5-C6	-5.45	114.27	117.00
53	BA	2001	C	N1-C2-O2	5.45	122.17	118.90
53	BA	2502	G	N3-C4-C5	-5.45	125.87	128.60
53	BA	2535	G	C8-N9-C4	-5.45	104.22	106.40
53	BA	2867	G	N3-C4-C5	-5.45	125.87	128.60
21	AA	207	C	N1-C2-O2	5.45	122.17	118.90
21	AA	350	G	C8-N9-C4	-5.45	104.22	106.40
36	BO	7	ARG	NE-CZ-NH1	5.45	123.03	120.30
53	BA	17	G	C5-C6-N1	5.45	114.23	111.50
53	BA	1578	U	C4-C5-C6	5.45	122.97	119.70
53	BA	2888	C	N1-C2-O2	5.45	122.17	118.90
21	AA	382	A	C4-C5-C6	-5.45	114.27	117.00
53	BA	534	U	C5-C6-N1	-5.45	119.97	122.70
53	BA	860	U	C5-C6-N1	-5.45	119.97	122.70
53	BA	1696	G	N1-C6-O6	-5.45	116.63	119.90
54	BB	118	C	N3-C2-O2	-5.45	118.08	121.90
21	AA	286	C	N1-C2-O2	5.45	122.17	118.90
21	AA	454	G	C5-C6-N1	5.45	114.22	111.50
53	BA	264	C	N3-C4-C5	5.45	124.08	121.90
53	BA	1276	A	C4-C5-C6	-5.45	114.28	117.00
53	BA	1605	C	N3-C2-O2	-5.45	118.09	121.90
53	BA	2675	A	C6-C5-N7	5.45	136.11	132.30
53	BA	2794	C	N3-C2-O2	-5.45	118.09	121.90
21	AA	1233	G	N1-C6-O6	-5.45	116.63	119.90
21	AA	1499	A	C4-C5-C6	-5.45	114.28	117.00
53	BA	1342	A	N1-C6-N6	-5.45	115.33	118.60
21	AA	241	G	N3-C4-C5	-5.45	125.88	128.60
21	AA	349	A	C4-C5-C6	-5.45	114.28	117.00
53	BA	970	U	N3-C2-O2	-5.45	118.39	122.20
53	BA	1735	A	N1-C6-N6	-5.45	115.33	118.60
53	BA	1794	A	C6-C5-N7	5.45	136.11	132.30
53	BA	2582	G	N3-C4-C5	-5.45	125.88	128.60
21	AA	832	G	C5-C6-N1	5.44	114.22	111.50
53	BA	250	G	N3-C2-N2	-5.44	116.09	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2272	U	N1-C2-N3	5.44	118.17	114.90
53	BA	2838	G	N7-C8-N9	5.44	115.82	113.10
21	AA	996	A	N1-C6-N6	-5.44	115.33	118.60
21	AA	1360	A	O4'-C1'-N9	5.44	112.55	108.20
21	AA	1380	U	C5-C6-N1	-5.44	119.98	122.70
53	BA	7	G	N1-C6-O6	-5.44	116.63	119.90
53	BA	174	U	C5-C6-N1	-5.44	119.98	122.70
53	BA	388	G	N3-C2-N2	-5.44	116.09	119.90
53	BA	582	A	C6-C5-N7	5.44	136.11	132.30
53	BA	834	G	N3-C4-C5	-5.44	125.88	128.60
53	BA	1153	C	N3-C4-C5	5.44	124.08	121.90
53	BA	2738	A	C6-C5-N7	5.44	136.11	132.30
21	AA	835	U	O4'-C1'-N1	5.44	112.55	108.20
53	BA	556	A	C6-C5-N7	5.44	136.11	132.30
53	BA	1102	C	O4'-C1'-N1	5.44	112.55	108.20
53	BA	1934	C	O4'-C1'-N1	5.44	112.55	108.20
53	BA	2743	U	N1-C2-N3	5.44	118.17	114.90
22	A1	40	G	N9-C4-C5	5.44	107.58	105.40
53	BA	187	G	C8-N9-C4	-5.44	104.22	106.40
53	BA	492	A	C4-C5-C6	-5.44	114.28	117.00
53	BA	777	G	C4'-C3'-C2'	-5.44	97.16	102.60
53	BA	1749	A	C6-C5-N7	5.44	136.11	132.30
53	BA	1837	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	1178	G	N7-C8-N9	5.44	115.82	113.10
21	AA	1293	C	N3-C4-C5	5.44	124.08	121.90
53	BA	1	G	C5-C6-N1	5.44	114.22	111.50
53	BA	551	G	N7-C8-N9	5.44	115.82	113.10
53	BA	1122	G	C5-C6-N1	5.44	114.22	111.50
53	BA	2032	G	N3-C4-C5	-5.44	125.88	128.60
53	BA	2333	A	C6-C5-N7	5.44	136.11	132.30
53	BA	2378	A	C4-C5-C6	-5.44	114.28	117.00
53	BA	2756	U	N1-C1'-C2'	5.44	121.07	114.00
21	AA	912	C	N3-C4-C5	5.44	124.08	121.90
21	AA	957	U	C5-C6-N1	-5.44	119.98	122.70
53	BA	2114	A	C6-C5-N7	5.44	136.10	132.30
53	BA	2238	G	O4'-C1'-N9	5.44	112.55	108.20
21	AA	207	C	N3-C4-C5	5.43	124.07	121.90
21	AA	327	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	897	C	N3-C2-O2	-5.43	118.10	121.90
53	BA	634	C	N3-C4-C5	5.43	124.07	121.90
53	BA	744	U	C5-C6-N1	-5.43	119.98	122.70
53	BA	972	A	N1-C6-N6	-5.43	115.34	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1816	C	P-O3'-C3'	5.43	126.22	119.70
53	BA	2593	U	O4'-C1'-N1	5.43	112.55	108.20
53	BA	2820	A	C4-C5-C6	-5.43	114.28	117.00
54	BB	8	C	O4'-C1'-N1	5.43	112.55	108.20
21	AA	776	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	1268	G	C5-C6-N1	5.43	114.22	111.50
21	AA	1465	A	C6-C5-N7	5.43	136.10	132.30
27	BF	147	ARG	NE-CZ-NH1	5.43	123.02	120.30
53	BA	968	C	C4'-C3'-C2'	-5.43	97.17	102.60
53	BA	1986	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	635	A	C6-C5-N7	5.43	136.10	132.30
21	AA	1032	G	P-O3'-C3'	5.43	126.22	119.70
21	AA	1183	U	N3-C2-O2	-5.43	118.40	122.20
53	BA	2282	G	C1'-O4'-C4'	-5.43	105.56	109.90
53	BA	2282	G	O4'-C1'-N9	5.43	112.55	108.20
21	AA	44	A	C5-C6-N1	5.43	120.42	117.70
21	AA	582	C	O4'-C1'-N1	5.43	112.54	108.20
21	AA	1333	A	O4'-C1'-N9	5.43	112.54	108.20
53	BA	914	G	C8-N9-C4	-5.43	104.23	106.40
53	BA	1145	C	O4'-C1'-N1	5.43	112.54	108.20
53	BA	1785	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	585	G	N7-C8-N9	5.43	115.81	113.10
21	AA	921	U	O4'-C1'-N1	5.43	112.54	108.20
27	BF	114	ARG	NE-CZ-NH2	5.43	123.01	120.30
53	BA	723	C	N1-C2-O2	5.43	122.16	118.90
53	BA	2221	G	N3-C2-N2	-5.43	116.10	119.90
13	AN	85	ARG	NE-CZ-NH2	-5.43	117.59	120.30
21	AA	278	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	502	A	O4'-C1'-N9	5.43	112.54	108.20
21	AA	1341	U	O4'-C1'-N1	5.43	112.54	108.20
30	BI	87	SER	CA-C-N	5.43	127.06	116.20
53	BA	302	C	N3-C2-O2	-5.43	118.10	121.90
53	BA	1051	G	N1-C6-O6	-5.43	116.64	119.90
53	BA	1186	G	C5-C6-N1	5.43	114.21	111.50
53	BA	1271	G	N3-C4-C5	-5.43	125.89	128.60
53	BA	1300	G	N1-C6-O6	-5.43	116.64	119.90
53	BA	1774	C	O4'-C1'-N1	5.43	112.54	108.20
53	BA	2734	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	1347	G	N1-C6-O6	-5.42	116.64	119.90
53	BA	301	G	N3-C4-C5	-5.42	125.89	128.60
53	BA	2143	C	N3-C2-O2	-5.42	118.10	121.90
53	BA	2646	C	N3-C4-C5	5.42	124.07	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	268	C	N1-C2-O2	5.42	122.15	118.90
53	BA	880	G	C8-N9-C4	-5.42	104.23	106.40
53	BA	1683	U	N3-C2-O2	-5.42	118.40	122.20
21	AA	696	A	O4'-C1'-N9	5.42	112.54	108.20
21	AA	1281	C	N3-C4-C5	5.42	124.07	121.90
22	A1	9	A	C5-C6-N1	5.42	120.41	117.70
38	BQ	10	ARG	NE-CZ-NH1	5.42	123.01	120.30
53	BA	729	G	N1-C6-O6	-5.42	116.65	119.90
53	BA	898	C	N3-C2-O2	-5.42	118.11	121.90
53	BA	1654	A	C4-C5-C6	-5.42	114.29	117.00
53	BA	2348	U	O4'-C1'-N1	5.42	112.54	108.20
53	BA	2793	C	N3-C2-O2	-5.42	118.11	121.90
53	BA	1236	G	N9-C4-C5	5.42	107.57	105.40
53	BA	2203	U	N3-C2-O2	-5.42	118.41	122.20
53	BA	2328	A	C6-C5-N7	5.42	136.09	132.30
21	AA	176	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	882	C	O4'-C1'-N1	5.42	112.53	108.20
21	AA	1112	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	1195	C	N3-C2-O2	-5.42	118.11	121.90
53	BA	119	A	C6-C5-N7	5.42	136.09	132.30
53	BA	282	A	C4-C5-C6	-5.42	114.29	117.00
53	BA	1064	C	N3-C4-C5	5.42	124.07	121.90
53	BA	2689	U	N3-C2-O2	-5.42	118.41	122.20
21	AA	613	C	N3-C2-O2	-5.42	118.11	121.90
21	AA	883	C	C2-N3-C4	-5.42	117.19	119.90
21	AA	1033	G	C5-C6-N1	5.42	114.21	111.50
21	AA	1213	A	C6-C5-N7	5.42	136.09	132.30
21	AA	1332	A	C5-C6-N1	5.42	120.41	117.70
21	AA	1348	U	N3-C2-O2	-5.42	118.41	122.20
21	AA	1403	C	N3-C4-C5	5.42	124.07	121.90
53	BA	112	U	N1-C2-N3	5.42	118.15	114.90
53	BA	2198	A	C5-C6-N1	5.42	120.41	117.70
21	AA	1262	C	O4'-C1'-N1	5.42	112.53	108.20
21	AA	1310	G	O4'-C1'-N9	5.42	112.53	108.20
53	BA	350	G	N1-C6-O6	-5.42	116.65	119.90
53	BA	1295	C	N3-C2-O2	-5.42	118.11	121.90
53	BA	2514	U	O4'-C1'-N1	5.42	112.53	108.20
21	AA	246	A	C5-C6-N1	5.41	120.41	117.70
21	AA	255	G	N1-C6-O6	-5.41	116.65	119.90
21	AA	608	A	N1-C6-N6	-5.41	115.35	118.60
21	AA	1239	A	C5-C6-N1	5.41	120.41	117.70
53	BA	225	C	N1-C2-O2	5.41	122.15	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	759	G	C5-C6-N1	5.41	114.21	111.50
53	BA	1030	C	C6-N1-C2	-5.41	118.13	120.30
53	BA	2420	C	N3-C2-O2	-5.41	118.11	121.90
21	AA	499	A	C6-C5-N7	5.41	136.09	132.30
21	AA	841	C	N3-C4-N4	-5.41	114.21	118.00
21	AA	1510	C	N1-C2-O2	5.41	122.15	118.90
53	BA	1115	G	O4'-C1'-N9	5.41	112.53	108.20
53	BA	2888	C	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	893	C	O4'-C1'-N1	5.41	112.53	108.20
21	AA	1033	G	N1-C6-O6	-5.41	116.65	119.90
21	AA	1322	C	O4'-C1'-N1	5.41	112.53	108.20
53	BA	128	C	N1-C2-O2	5.41	122.15	118.90
53	BA	306	U	N1-C2-N3	5.41	118.15	114.90
53	BA	482	A	C4-C5-C6	-5.41	114.30	117.00
53	BA	1288	G	C5-C6-N1	5.41	114.20	111.50
53	BA	1402	U	O4'-C1'-N1	5.41	112.53	108.20
53	BA	2155	U	N1-C2-N3	5.41	118.15	114.90
53	BA	2517	C	N3-C4-C5	5.41	124.06	121.90
21	AA	24	U	O4'-C1'-N1	5.41	112.53	108.20
21	AA	416	G	N3-C2-N2	-5.41	116.11	119.90
21	AA	467	U	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	616	G	C5-C6-N1	5.41	114.20	111.50
21	AA	978	A	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	1254	A	C5-C6-N1	5.41	120.40	117.70
21	AA	1408	A	C4-C5-C6	-5.41	114.30	117.00
22	A1	73	A	O4'-C1'-N9	5.41	112.53	108.20
53	BA	232	G	C5-C6-N1	5.41	114.20	111.50
53	BA	1352	U	N1-C2-N3	5.41	118.14	114.90
53	BA	1529	G	N3-C4-C5	-5.41	125.90	128.60
53	BA	2060	A	C4-C5-C6	-5.41	114.30	117.00
53	BA	1881	C	N3-C2-O2	-5.41	118.11	121.90
21	AA	311	C	N3-C4-C5	5.41	124.06	121.90
21	AA	1388	C	N3-C2-O2	-5.41	118.11	121.90
53	BA	446	G	O4'-C1'-N9	5.41	112.53	108.20
53	BA	480	A	C5'-C4'-O4'	5.41	115.59	109.10
53	BA	704	G	C8-N9-C4	-5.41	104.24	106.40
53	BA	1108	U	N3-C2-O2	-5.41	118.42	122.20
53	BA	2134	A	C4-C5-C6	-5.41	114.30	117.00
53	BA	2444	G	C8-N9-C4	-5.41	104.24	106.40
53	BA	670	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	7	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	62	U	C3'-C2'-C1'	5.40	105.82	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	343	U	C5-C6-N1	-5.40	120.00	122.70
21	AA	704	A	C6-C5-N7	5.40	136.08	132.30
25	BD	184	ARG	NE-CZ-NH2	5.40	123.00	120.30
53	BA	709	U	C5-C6-N1	-5.40	120.00	122.70
53	BA	995	C	N1-C2-O2	5.40	122.14	118.90
53	BA	1242	U	O4'-C1'-N1	5.40	112.52	108.20
53	BA	1741	C	O4'-C1'-N1	5.40	112.52	108.20
53	BA	1985	C	N1-C2-O2	5.40	122.14	118.90
53	BA	2515	C	C6-N1-C2	-5.40	118.14	120.30
53	BA	2606	C	N1-C2-O2	5.40	122.14	118.90
21	AA	1051	C	N3-C2-O2	-5.40	118.12	121.90
53	BA	785	G	C5'-C4'-C3'	-5.40	107.36	116.00
53	BA	786	C	N3-C4-C5	5.40	124.06	121.90
53	BA	873	C	N3-C2-O2	-5.40	118.12	121.90
53	BA	1388	G	N3-C4-C5	-5.40	125.90	128.60
53	BA	1575	C	N1-C2-O2	5.40	122.14	118.90
53	BA	2628	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	431	A	C4-C5-C6	-5.40	114.30	117.00
53	BA	2080	A	C5-C6-N1	5.40	120.40	117.70
53	BA	2650	U	C5-C6-N1	-5.40	120.00	122.70
21	AA	314	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	609	A	C5-C6-N1	5.40	120.40	117.70
21	AA	1008	U	N3-C2-O2	-5.40	118.42	122.20
21	AA	1303	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	1424	U	O4'-C1'-N1	5.40	112.52	108.20
53	BA	225	C	N3-C4-C5	5.40	124.06	121.90
53	BA	351	C	O4'-C1'-N1	5.40	112.52	108.20
53	BA	425	G	C5-C6-N1	5.40	114.20	111.50
53	BA	717	C	N3-C2-O2	-5.40	118.12	121.90
53	BA	999	U	N3-C2-O2	-5.40	118.42	122.20
53	BA	1303	G	C5-C6-N1	5.40	114.20	111.50
53	BA	1957	C	N1-C2-O2	5.40	122.14	118.90
21	AA	1201	A	C4-C5-C6	-5.40	114.30	117.00
53	BA	401	A	C6-C5-N7	5.40	136.08	132.30
53	BA	833	A	C5-C6-N1	5.40	120.40	117.70
21	AA	1243	C	C6-N1-C2	-5.39	118.14	120.30
22	A1	61	C	N3-C2-O2	-5.39	118.12	121.90
53	BA	156	A	C4-C5-C6	-5.39	114.30	117.00
53	BA	659	G	N1-C6-O6	-5.39	116.66	119.90
53	BA	1649	G	C5-C6-N1	5.39	114.20	111.50
53	BA	1924	C	N1-C2-O2	5.39	122.14	118.90
53	BA	2225	A	C4-C5-C6	-5.39	114.30	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2502	G	O4'-C1'-N9	5.39	112.52	108.20
53	BA	175	G	C5-C6-N1	5.39	114.20	111.50
53	BA	721	A	C6-C5-N7	5.39	136.07	132.30
53	BA	1253	A	C4-C5-C6	-5.39	114.30	117.00
53	BA	2089	C	N3-C2-O2	-5.39	118.12	121.90
53	BA	2277	G	N7-C8-N9	5.39	115.80	113.10
53	BA	2683	C	N3-C2-O2	-5.39	118.12	121.90
21	AA	99	C	N3-C4-C5	5.39	124.06	121.90
21	AA	699	C	N3-C2-O2	-5.39	118.13	121.90
21	AA	934	C	P-O3'-C3'	5.39	126.17	119.70
53	BA	1419	A	C5-C6-N1	5.39	120.40	117.70
53	BA	2902	C	O4'-C1'-N1	5.39	112.51	108.20
21	AA	939	G	C5-C6-N1	5.39	114.19	111.50
22	A1	67	U	C5'-C4'-O4'	5.39	115.57	109.10
53	BA	110	G	C8-N9-C4	-5.39	104.24	106.40
53	BA	462	C	N3-C2-O2	-5.39	118.13	121.90
53	BA	1314	C	C6-N1-C2	-5.39	118.14	120.30
53	BA	1349	C	N3-C2-O2	-5.39	118.13	121.90
53	BA	2632	A	C4-C5-C6	-5.39	114.31	117.00
21	AA	558	G	C8-N9-C4	-5.39	104.25	106.40
21	AA	575	G	N7-C8-N9	5.39	115.79	113.10
21	AA	716	A	C4-C5-C6	-5.39	114.31	117.00
21	AA	851	G	C5-C6-N1	5.39	114.19	111.50
53	BA	209	C	N3-C2-O2	-5.39	118.13	121.90
53	BA	584	C	N1-C2-O2	5.39	122.13	118.90
53	BA	1536	C	N3-C4-C5	5.39	124.06	121.90
53	BA	2027	G	C5-C6-N1	5.39	114.19	111.50
53	BA	2131	U	C5-C6-N1	-5.39	120.01	122.70
21	AA	628	G	C8-N9-C4	-5.39	104.25	106.40
21	AA	1315	U	O4'-C1'-N1	5.39	112.51	108.20
53	BA	294	A	C4-C5-C6	-5.39	114.31	117.00
53	BA	822	G	N3-C4-C5	-5.39	125.91	128.60
53	BA	1498	C	N3-C2-O2	-5.39	118.13	121.90
53	BA	2050	C	N3-C2-O2	-5.39	118.13	121.90
9	AJ	31	ARG	NE-CZ-NH1	5.38	122.99	120.30
21	AA	223	A	C6-C5-N7	5.38	136.07	132.30
21	AA	1006	G	N3-C2-N2	-5.38	116.13	119.90
21	AA	1534	A	O4'-C1'-N9	5.38	112.51	108.20
22	A1	28	C	N3-C2-O2	-5.38	118.13	121.90
53	BA	683	U	C5-C6-N1	-5.38	120.01	122.70
53	BA	1506	U	C5-C6-N1	-5.38	120.01	122.70
53	BA	1986	C	C4'-C3'-C2'	-5.38	97.22	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2416	C	O4'-C1'-N1	5.38	112.51	108.20
53	BA	2639	A	C6-C5-N7	5.38	136.07	132.30
21	AA	750	C	N1-C2-O2	5.38	122.13	118.90
21	AA	841	C	N1-C2-O2	5.38	122.13	118.90
21	AA	1218	C	N1-C2-O2	5.38	122.13	118.90
53	BA	672	C	N1-C2-O2	5.38	122.13	118.90
53	BA	1141	U	N3-C2-O2	-5.38	118.43	122.20
53	BA	1668	A	O4'-C1'-N9	5.38	112.51	108.20
53	BA	2803	G	N1-C6-O6	-5.38	116.67	119.90
21	AA	676	A	N1-C6-N6	-5.38	115.37	118.60
53	BA	78	U	N1-C2-N3	5.38	118.13	114.90
53	BA	508	A	C6-C5-N7	5.38	136.07	132.30
53	BA	891	G	C5-C6-N1	5.38	114.19	111.50
53	BA	922	C	C4'-C3'-C2'	-5.38	97.22	102.60
53	BA	1507	C	N1-C2-O2	5.38	122.13	118.90
53	BA	2467	C	N3-C4-N4	-5.38	114.23	118.00
53	BA	2715	C	N1-C2-O2	5.38	122.13	118.90
21	AA	312	C	N3-C2-O2	-5.38	118.13	121.90
22	A1	75	C	N1-C2-O2	5.38	122.13	118.90
53	BA	928	A	C4-C5-C6	-5.38	114.31	117.00
53	BA	1112	G	C5-C6-N1	5.38	114.19	111.50
53	BA	2457	U	N3-C2-O2	-5.38	118.43	122.20
21	AA	1027	C	N3-C2-O2	-5.38	118.14	121.90
22	A1	32	C	N3-C2-O2	-5.38	118.14	121.90
53	BA	88	G	C5-C6-N1	5.38	114.19	111.50
53	BA	864	G	C5-C6-N1	5.38	114.19	111.50
53	BA	1226	A	C5-C6-N1	5.38	120.39	117.70
53	BA	1633	G	N1-C6-O6	-5.38	116.67	119.90
53	BA	2886	A	C2-N3-C4	5.38	113.29	110.60
54	BB	59	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	758	C	N3-C2-O2	-5.38	118.14	121.90
53	BA	655	A	C4-C5-C6	-5.38	114.31	117.00
53	BA	976	G	C3'-C2'-C1'	5.38	105.80	101.50
53	BA	1215	G	N9-C4-C5	5.38	107.55	105.40
53	BA	1772	A	C5-C6-N1	5.38	120.39	117.70
21	AA	1347	G	O4'-C1'-N9	5.38	112.50	108.20
53	BA	2006	C	N3-C2-O2	-5.38	118.14	121.90
53	BA	2164	C	N3-C4-C5	5.38	124.05	121.90
53	BA	2484	G	C5-C6-N1	5.38	114.19	111.50
21	AA	277	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	1390	U	N3-C2-O2	-5.37	118.44	122.20
53	BA	609	A	C4-C5-C6	-5.37	114.31	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	876	C	O4'-C1'-N1	5.37	112.50	108.20
53	BA	1335	C	N3-C2-O2	-5.37	118.14	121.90
53	BA	2559	C	C4'-C3'-C2'	-5.37	97.23	102.60
53	BA	2611	C	N1-C2-O2	5.37	122.12	118.90
53	BA	2772	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	1351	U	N3-C2-O2	-5.37	118.44	122.20
53	BA	1981	A	C4-C5-C6	-5.37	114.31	117.00
53	BA	2544	G	C5-C6-N1	5.37	114.19	111.50
53	BA	2028	U	C5-C6-N1	-5.37	120.02	122.70
21	AA	1105	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	1326	U	C5-C6-N1	-5.37	120.02	122.70
21	AA	1471	U	O4'-C1'-N1	5.37	112.50	108.20
22	A1	21	A	C5-C6-N1	5.37	120.38	117.70
53	BA	121	G	C3'-C2'-C1'	5.37	105.80	101.50
53	BA	362	A	C4-C5-C6	-5.37	114.31	117.00
53	BA	2583	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	1460	C	N3-C2-O2	-5.37	118.14	121.90
53	BA	416	U	O4'-C1'-N1	5.37	112.49	108.20
53	BA	1068	G	N3-C4-C5	-5.37	125.92	128.60
53	BA	1591	A	O4'-C1'-N9	5.37	112.49	108.20
21	AA	578	C	N1-C2-O2	5.37	122.12	118.90
21	AA	624	C	O4'-C1'-N1	5.37	112.49	108.20
21	AA	667	G	N3-C2-N2	-5.37	116.14	119.90
21	AA	969	A	O4'-C1'-N9	5.37	112.49	108.20
53	BA	247	G	N1-C6-O6	-5.37	116.68	119.90
53	BA	344	A	C6-C5-N7	5.37	136.06	132.30
53	BA	451	U	O4'-C1'-N1	5.37	112.49	108.20
53	BA	803	U	O4'-C1'-N1	5.37	112.49	108.20
53	BA	1006	C	O4'-C1'-N1	5.37	112.49	108.20
53	BA	1859	U	C5-C6-N1	-5.37	120.02	122.70
53	BA	1983	G	C5-C6-N1	5.37	114.18	111.50
53	BA	2846	G	C5-C6-N1	5.37	114.18	111.50
21	AA	177	G	C8-N9-C4	-5.36	104.25	106.40
21	AA	699	C	N1-C2-O2	5.36	122.12	118.90
53	BA	23	G	C5-C6-N1	5.36	114.18	111.50
53	BA	671	C	O4'-C1'-N1	5.36	112.49	108.20
53	BA	1920	C	O4'-C1'-N1	5.36	112.49	108.20
53	BA	2575	C	N3-C2-O2	-5.36	118.14	121.90
53	BA	2690	U	C5-C6-N1	-5.36	120.02	122.70
53	BA	2749	A	C4-C5-C6	-5.36	114.32	117.00
53	BA	2897	U	C5-C6-N1	-5.36	120.02	122.70
21	AA	598	U	C5'-C4'-O4'	5.36	115.53	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	5	A	C5-C6-N1	5.36	120.38	117.70
53	BA	1054	A	C5-C6-N1	5.36	120.38	117.70
53	BA	2275	C	O4'-C4'-C3'	5.36	110.39	106.10
53	BA	2403	C	O4'-C1'-N1	5.36	112.49	108.20
21	AA	81	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	155	A	C6-C5-N7	5.36	136.05	132.30
21	AA	582	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	600	A	C4-C5-C6	-5.36	114.32	117.00
53	BA	518	G	C5-C6-N1	5.36	114.18	111.50
53	BA	765	C	N3-C2-O2	-5.36	118.15	121.90
53	BA	921	C	N3-C2-O2	-5.36	118.15	121.90
53	BA	1710	G	N1-C6-O6	-5.36	116.68	119.90
53	BA	1732	C	O4'-C1'-N1	5.36	112.49	108.20
53	BA	2441	U	N3-C2-O2	-5.36	118.45	122.20
21	AA	1129	C	N1-C2-O2	5.36	122.11	118.90
37	BP	108	ARG	NE-CZ-NH1	5.36	122.98	120.30
53	BA	1108	U	N1-C2-N3	5.36	118.11	114.90
53	BA	1370	C	O4'-C1'-N1	5.36	112.49	108.20
54	BB	62	C	N1-C2-O2	5.36	122.12	118.90
21	AA	1373	G	C8-N9-C4	-5.36	104.26	106.40
21	AA	1493	A	C3'-C2'-C1'	5.36	105.79	101.50
22	A1	58	A	C4-C5-C6	-5.36	114.32	117.00
24	BC	13	ARG	NE-CZ-NH1	5.36	122.98	120.30
53	BA	366	C	O4'-C1'-N1	5.36	112.49	108.20
53	BA	1195	G	C8-N9-C4	-5.36	104.26	106.40
53	BA	1392	A	C5-C6-N1	5.36	120.38	117.70
11	AL	94	TYR	CB-CG-CD2	-5.36	117.79	121.00
33	BL	48	ARG	NE-CZ-NH2	-5.36	117.62	120.30
53	BA	546	U	N3-C2-O2	-5.36	118.45	122.20
53	BA	1599	U	C5-C6-N1	-5.36	120.02	122.70
53	BA	1920	C	C6-N1-C2	-5.36	118.16	120.30
53	BA	2704	C	N3-C2-O2	-5.36	118.15	121.90
54	BB	27	C	N3-C2-O2	-5.36	118.15	121.90
53	BA	814	C	O4'-C1'-N1	5.35	112.48	108.20
21	AA	1055	A	C6-C5-N7	5.35	136.05	132.30
53	BA	851	C	N3-C2-O2	-5.35	118.15	121.90
53	BA	1476	U	O4'-C1'-N1	5.35	112.48	108.20
53	BA	1637	A	O4'-C1'-N9	5.35	112.48	108.20
53	BA	2254	C	N3-C2-O2	-5.35	118.15	121.90
21	AA	739	C	N3-C4-C5	5.35	124.04	121.90
53	BA	2278	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	38	G	C5'-C4'-O4'	5.35	115.52	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	705	A	C4-C5-C6	-5.35	114.33	117.00
53	BA	2015	A	N1-C6-N6	-5.35	115.39	118.60
53	BA	2139	U	O4'-C1'-N1	5.35	112.48	108.20
53	BA	2280	G	C5-C6-N1	5.35	114.17	111.50
53	BA	2310	C	C3'-C2'-C1'	5.35	105.78	101.50
53	BA	2601	C	N1-C2-O2	5.35	122.11	118.90
21	AA	554	A	C6-C5-N7	5.35	136.04	132.30
21	AA	1282	C	N1-C2-O2	5.35	122.11	118.90
21	AA	1391	U	N3-C2-O2	-5.35	118.46	122.20
53	BA	369	U	C5-C6-N1	-5.35	120.03	122.70
53	BA	1023	U	O4'-C1'-C2'	-5.35	100.45	105.80
53	BA	1357	C	O4'-C1'-N1	5.35	112.48	108.20
53	BA	1882	U	N1-C2-N3	5.35	118.11	114.90
53	BA	2438	U	N3-C2-O2	-5.35	118.46	122.20
53	BA	2813	A	C6-C5-N7	5.35	136.04	132.30
53	BA	2849	U	N1-C2-N3	5.35	118.11	114.90
21	AA	1148	U	N3-C2-O2	-5.35	118.46	122.20
53	BA	258	G	C5-C6-N1	5.35	114.17	111.50
53	BA	1382	G	N1-C6-O6	-5.35	116.69	119.90
53	BA	1667	G	C5-C6-N1	5.35	114.17	111.50
53	BA	2292	U	C5-C6-N1	-5.35	120.03	122.70
53	BA	2521	C	O4'-C1'-N1	5.35	112.48	108.20
53	BA	2659	G	C5-C6-N1	5.35	114.17	111.50
4	AE	68	ARG	NE-CZ-NH2	-5.34	117.63	120.30
21	AA	93	U	N3-C2-O2	-5.34	118.46	122.20
21	AA	887	G	N1-C6-O6	-5.34	116.69	119.90
53	BA	1235	G	C8-N9-C4	-5.34	104.26	106.40
53	BA	1630	A	C6-C5-N7	5.34	136.04	132.30
53	BA	2113	U	O4'-C1'-N1	5.34	112.48	108.20
53	BA	2755	C	N3-C4-C5	5.34	124.04	121.90
54	BB	14	U	O4'-C1'-N1	5.34	112.47	108.20
52	B4	24	ARG	NE-CZ-NH2	-5.34	117.63	120.30
53	BA	2850	A	C6-C5-N7	5.34	136.04	132.30
53	BA	2864	G	O4'-C1'-N9	5.34	112.47	108.20
54	BB	67	G	C5-C6-N1	5.34	114.17	111.50
21	AA	343	U	N3-C2-O2	-5.34	118.46	122.20
21	AA	1463	U	O4'-C1'-N1	5.34	112.47	108.20
53	BA	473	G	C5-C6-N1	5.34	114.17	111.50
53	BA	923	G	N3-C4-C5	-5.34	125.93	128.60
53	BA	2538	C	O4'-C1'-N1	5.34	112.47	108.20
21	AA	429	U	C5-C6-N1	-5.34	120.03	122.70
21	AA	890	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(^{o})	Ideal(^{o})
21	AA	1312	G	C5-C6-N1	5.34	114.17	111.50
21	AA	1382	C	N3-C2-O2	-5.34	118.16	121.90
53	BA	859	G	N3-C4-C5	-5.34	125.93	128.60
53	BA	1024	G	C5-C6-N1	5.34	114.17	111.50
53	BA	1574	C	N3-C4-C5	5.34	124.04	121.90
53	BA	1634	A	C4-C5-C6	-5.34	114.33	117.00
53	BA	2404	U	C5-C6-N1	-5.34	120.03	122.70
21	AA	467	U	N1-C2-N3	5.34	118.10	114.90
53	BA	1227	G	C5-C6-N1	5.34	114.17	111.50
54	BB	57	A	C4-C5-C6	-5.34	114.33	117.00
22	A1	70	C	O4'-C1'-N1	5.34	112.47	108.20
53	BA	834	G	N1-C6-O6	-5.34	116.70	119.90
53	BA	1242	U	N3-C2-O2	-5.34	118.46	122.20
53	BA	2092	U	N3-C2-O2	-5.34	118.47	122.20
53	BA	1147	A	C6-C5-N7	5.33	136.03	132.30
53	BA	2131	U	N3-C2-O2	-5.33	118.47	122.20
53	BA	2805	C	O4'-C1'-N1	5.33	112.47	108.20
21	AA	18	C	O4'-C1'-N1	5.33	112.47	108.20
21	AA	260	G	O4'-C1'-N9	5.33	112.47	108.20
53	BA	1055	G	C8-N9-C4	-5.33	104.27	106.40
53	BA	1182	G	N1-C6-O6	-5.33	116.70	119.90
53	BA	1301	A	C4-C5-C6	-5.33	114.33	117.00
53	BA	1964	G	O4'-C1'-N9	5.33	112.47	108.20
53	BA	2073	C	C4'-C3'-C2'	-5.33	97.27	102.60
53	BA	2728	U	C5-C6-N1	-5.33	120.03	122.70
21	AA	1358	U	N3-C2-O2	-5.33	118.47	122.20
53	BA	51	G	N1-C6-O6	-5.33	116.70	119.90
53	BA	451	U	N3-C2-O2	-5.33	118.47	122.20
53	BA	620	G	N3-C4-C5	-5.33	125.94	128.60
53	BA	1135	C	N1-C2-O2	5.33	122.10	118.90
53	BA	2016	U	O4'-C1'-N1	5.33	112.47	108.20
53	BA	2454	G	N7-C8-N9	5.33	115.77	113.10
53	BA	895	U	C5-C6-N1	-5.33	120.03	122.70
53	BA	1176	U	O4'-C1'-N1	5.33	112.46	108.20
53	BA	2476	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	408	A	C6-C5-N7	5.33	136.03	132.30
21	AA	1007	U	O4'-C1'-N1	5.33	112.46	108.20
21	AA	1053	G	C5-C6-N1	5.33	114.16	111.50
21	AA	1096	C	N3-C4-N4	-5.33	114.27	118.00
22	A1	30	C	N3-C4-C5	5.33	124.03	121.90
53	BA	379	G	N1-C6-O6	-5.33	116.70	119.90
53	BA	799	G	N3-C4-C5	-5.33	125.94	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1053	C	N3-C2-O2	-5.33	118.17	121.90
53	BA	1627	G	N3-C4-C5	-5.33	125.94	128.60
53	BA	1681	G	N3-C2-N2	-5.33	116.17	119.90
53	BA	1715	G	C8-N9-C4	-5.33	104.27	106.40
53	BA	2162	G	N3-C2-N2	-5.33	116.17	119.90
53	BA	2707	U	O4'-C1'-N1	5.33	112.46	108.20
54	BB	63	C	N1-C2-O2	5.33	122.10	118.90
53	BA	346	A	C4-C5-C6	-5.33	114.34	117.00
53	BA	1044	C	N1-C2-O2	5.33	122.10	118.90
53	BA	1205	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	102	G	N7-C8-N9	5.33	115.76	113.10
21	AA	490	C	N1-C2-O2	5.33	122.09	118.90
21	AA	1121	U	O4'-C1'-N1	5.33	112.46	108.20
53	BA	66	C	N3-C4-C5	5.33	124.03	121.90
53	BA	293	U	N3-C2-O2	-5.33	118.47	122.20
53	BA	1299	G	N7-C8-N9	5.33	115.76	113.10
53	BA	1471	G	C8-N9-C4	-5.33	104.27	106.40
53	BA	2652	C	N1-C2-O2	5.33	122.10	118.90
53	BA	2832	U	O4'-C1'-N1	5.33	112.46	108.20
21	AA	46	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	93	U	C5-C6-N1	-5.32	120.04	122.70
21	AA	576	C	N1-C2-O2	5.32	122.09	118.90
21	AA	738	C	O4'-C1'-N1	5.32	112.46	108.20
21	AA	859	G	C8-N9-C4	-5.32	104.27	106.40
21	AA	1497	G	N9-C4-C5	5.32	107.53	105.40
53	BA	935	C	O4'-C1'-N1	5.32	112.46	108.20
53	BA	1410	G	N9-C4-C5	5.32	107.53	105.40
53	BA	2568	U	C5-C6-N1	-5.32	120.04	122.70
53	BA	2685	G	N1-C6-O6	-5.32	116.71	119.90
53	BA	2865	U	C5-C6-N1	-5.32	120.04	122.70
54	BB	88	C	N1-C2-O2	5.32	122.09	118.90
54	BB	54	G	C8-N9-C4	-5.32	104.27	106.40
48	B0	49	ARG	NE-CZ-NH1	5.32	122.96	120.30
53	BA	248	G	N7-C8-N9	5.32	115.76	113.10
53	BA	2138	G	N3-C2-N2	-5.32	116.18	119.90
53	BA	2462	C	N1-C2-O2	5.32	122.09	118.90
53	BA	2629	U	C5-C6-N1	-5.32	120.04	122.70
53	BA	2690	U	N1-C2-N3	5.32	118.09	114.90
53	BA	2030	A	O4'-C1'-N9	5.32	112.45	108.20
21	AA	48	C	N3-C4-C5	5.32	124.03	121.90
21	AA	1211	U	N1-C2-N3	5.32	118.09	114.90
21	AA	1427	C	N3-C2-O2	-5.32	118.18	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1708	C	C4'-C3'-C2'	-5.32	97.28	102.60
53	BA	2004	G	N1-C6-O6	-5.32	116.71	119.90
53	BA	2494	G	N3-C4-C5	-5.32	125.94	128.60
21	AA	1278	G	C5-C6-N1	5.32	114.16	111.50
21	AA	1351	U	C5-C6-N1	-5.32	120.04	122.70
53	BA	531	C	N1-C2-O2	5.32	122.09	118.90
53	BA	683	U	N1-C2-N3	5.32	118.09	114.90
53	BA	970	U	N1-C2-N3	5.32	118.09	114.90
53	BA	1480	C	N3-C4-C5	5.32	124.03	121.90
53	BA	1773	A	C5-C6-N1	5.32	120.36	117.70
53	BA	2209	G	C8-N9-C4	-5.32	104.27	106.40
53	BA	2658	C	O4'-C1'-N1	5.32	112.45	108.20
21	AA	647	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	1229	A	C4-C5-C6	-5.31	114.34	117.00
34	BM	66	ARG	NE-CZ-NH1	5.31	122.96	120.30
21	AA	222	C	N3-C2-O2	-5.31	118.18	121.90
21	AA	1381	U	N3-C2-O2	-5.31	118.48	122.20
53	BA	342	A	O4'-C1'-N9	5.31	112.45	108.20
53	BA	364	C	N1-C2-O2	5.31	122.09	118.90
53	BA	1518	C	N1-C2-O2	5.31	122.09	118.90
53	BA	1988	G	O4'-C1'-N9	5.31	112.45	108.20
53	BA	2043	C	N3-C4-C5	5.31	124.03	121.90
54	BB	30	C	N1-C2-O2	5.31	122.09	118.90
21	AA	1038	C	O4'-C1'-N1	5.31	112.45	108.20
53	BA	331	C	O4'-C1'-N1	5.31	112.45	108.20
53	BA	964	C	C6-N1-C2	-5.31	118.18	120.30
53	BA	2581	G	N3-C4-C5	-5.31	125.94	128.60
54	BB	87	U	O4'-C1'-N1	5.31	112.45	108.20
21	AA	696	A	C5-C6-N1	5.31	120.36	117.70
21	AA	1281	C	N1-C2-O2	5.31	122.09	118.90
53	BA	596	U	O4'-C1'-N1	5.31	112.45	108.20
53	BA	1637	A	C4'-C3'-C2'	-5.31	97.29	102.60
21	AA	726	C	N3-C4-C5	5.31	124.02	121.90
21	AA	1343	G	N1-C6-O6	-5.31	116.72	119.90
21	AA	1453	G	N3-C4-C5	-5.31	125.95	128.60
53	BA	1934	C	N1-C2-O2	5.31	122.08	118.90
53	BA	2141	G	C5-C6-N1	5.31	114.15	111.50
21	AA	1296	C	C3'-C2'-C1'	5.31	105.75	101.50
53	BA	215	G	N1-C6-O6	-5.31	116.72	119.90
53	BA	744	U	O4'-C1'-N1	5.31	112.44	108.20
2	AC	131	ARG	NE-CZ-NH2	-5.30	117.65	120.30
21	AA	711	G	N1-C6-O6	-5.30	116.72	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	33	U	C5-C6-N1	-5.30	120.05	122.70
22	A1	70	C	N3-C2-O2	-5.30	118.19	121.90
53	BA	838	C	C5'-C4'-O4'	5.30	115.47	109.10
53	BA	875	G	N1-C6-O6	-5.30	116.72	119.90
53	BA	996	A	C4-C5-C6	-5.30	114.35	117.00
53	BA	2399	G	C5-C6-N1	5.30	114.15	111.50
53	BA	2756	U	N3-C2-O2	-5.30	118.49	122.20
53	BA	2844	G	N3-C4-C5	-5.30	125.95	128.60
53	BA	678	C	N1-C2-O2	5.30	122.08	118.90
53	BA	1403	A	O4'-C1'-N9	5.30	112.44	108.20
53	BA	1917	U	O4'-C1'-N1	5.30	112.44	108.20
53	BA	2183	A	C6-C5-N7	5.30	136.01	132.30
54	BB	89	U	N3-C2-O2	-5.30	118.49	122.20
21	AA	289	G	N7-C8-N9	5.30	115.75	113.10
53	BA	147	C	N1-C2-O2	5.30	122.08	118.90
53	BA	375	G	N3-C4-C5	-5.30	125.95	128.60
53	BA	2408	U	O4'-C1'-N1	5.30	112.44	108.20
53	BA	2452	C	N1-C2-O2	5.30	122.08	118.90
53	BA	2500	U	N3-C2-O2	-5.30	118.49	122.20
53	BA	208	C	N3-C4-C5	5.30	124.02	121.90
53	BA	886	A	C6-C5-N7	5.30	136.01	132.30
53	BA	1924	C	O4'-C1'-N1	5.30	112.44	108.20
53	BA	2456	C	O4'-C1'-N1	5.30	112.44	108.20
54	BB	43	C	N3-C4-C5	5.30	124.02	121.90
53	BA	283	G	N1-C6-O6	-5.30	116.72	119.90
53	BA	917	A	N1-C6-N6	-5.30	115.42	118.60
53	BA	2417	C	N1-C2-O2	5.30	122.08	118.90
21	AA	144	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	1322	C	N1-C2-O2	5.30	122.08	118.90
21	AA	1401	G	C8-N9-C4	-5.30	104.28	106.40
21	AA	1446	A	C5-C6-N1	5.30	120.35	117.70
21	AA	1508	A	C4'-C3'-C2'	-5.30	97.30	102.60
53	BA	491	G	C5-C6-N1	5.30	114.15	111.50
53	BA	639	U	N3-C2-O2	-5.30	118.49	122.20
53	BA	882	G	C5-C6-N1	5.30	114.15	111.50
53	BA	929	U	C5-C6-N1	-5.30	120.05	122.70
53	BA	996	A	C5-C6-N1	5.30	120.35	117.70
53	BA	1258	U	O4'-C1'-N1	5.30	112.44	108.20
53	BA	1737	G	C5-C6-N1	5.30	114.15	111.50
53	BA	2159	G	C5'-C4'-O4'	5.30	115.46	109.10
53	BA	2318	G	C5-C6-N1	5.30	114.15	111.50
53	BA	2362	C	N1-C2-O2	5.30	122.08	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2599	G	N1-C6-O6	-5.30	116.72	119.90
53	BA	2634	A	C6-C5-N7	5.30	136.01	132.30
53	BA	2777	G	O4'-C1'-N9	5.30	112.44	108.20
53	BA	1350	C	N1-C2-O2	5.29	122.08	118.90
53	BA	1832	C	N1-C2-O2	5.29	122.08	118.90
53	BA	2258	C	N1-C2-O2	5.29	122.08	118.90
53	BA	2569	G	C5-C6-N1	5.29	114.15	111.50
21	AA	647	C	N1-C2-O2	5.29	122.08	118.90
37	BP	88	ARG	NE-CZ-NH1	5.29	122.95	120.30
53	BA	232	G	N1-C6-O6	-5.29	116.72	119.90
53	BA	1316	U	C5-C6-N1	-5.29	120.05	122.70
53	BA	1472	C	O4'-C1'-N1	5.29	112.44	108.20
53	BA	1682	G	N1-C6-O6	-5.29	116.72	119.90
53	BA	1773	A	C4-C5-C6	-5.29	114.35	117.00
53	BA	2300	C	N3-C2-O2	-5.29	118.19	121.90
53	BA	2428	G	N1-C6-O6	-5.29	116.72	119.90
53	BA	2567	G	N9-C4-C5	5.29	107.52	105.40
54	BB	56	G	N3-C4-C5	-5.29	125.95	128.60
11	AL	113	ARG	NE-CZ-NH2	-5.29	117.65	120.30
21	AA	174	A	C6-C5-N7	5.29	136.00	132.30
21	AA	895	G	N3-C4-C5	-5.29	125.95	128.60
53	BA	353	C	N3-C2-O2	-5.29	118.20	121.90
53	BA	1261	C	N3-C2-O2	-5.29	118.20	121.90
53	BA	1672	A	C6-C5-N7	5.29	136.00	132.30
53	BA	1922	G	C5-C6-N1	5.29	114.15	111.50
53	BA	2222	C	O4'-C1'-N1	5.29	112.43	108.20
53	BA	2366	A	C4-C5-C6	-5.29	114.35	117.00
53	BA	2463	C	N3-C4-C5	5.29	124.02	121.90
53	BA	2575	C	O4'-C1'-N1	5.29	112.43	108.20
53	BA	1897	G	N3-C4-C5	-5.29	125.95	128.60
53	BA	2494	G	N1-C6-O6	-5.29	116.73	119.90
21	AA	738	C	N3-C4-C5	5.29	124.02	121.90
21	AA	1288	A	C6-C5-N7	5.29	136.00	132.30
53	BA	25	U	C3'-C2'-C1'	5.29	105.73	101.50
53	BA	601	C	O4'-C1'-N1	5.29	112.43	108.20
53	BA	1073	A	O4'-C1'-N9	5.29	112.43	108.20
53	BA	2331	G	N3-C4-C5	-5.29	125.95	128.60
21	AA	1071	C	N3-C2-O2	-5.29	118.20	121.90
21	AA	231	U	O4'-C1'-N1	5.29	112.43	108.20
21	AA	922	G	N3-C4-C5	-5.29	125.96	128.60
53	BA	233	A	C5-C6-N1	5.29	120.34	117.70
53	BA	441	U	N3-C2-O2	-5.29	118.50	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	713	G	O4'-C1'-N9	5.29	112.43	108.20
53	BA	1095	A	C6-C5-N7	5.29	136.00	132.30
53	BA	1118	C	N1-C2-O2	5.29	122.07	118.90
53	BA	1311	G	O4'-C1'-N9	5.29	112.43	108.20
53	BA	2497	A	O4'-C1'-N9	5.29	112.43	108.20
14	AO	63	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	AA	513	C	N3-C2-O2	-5.28	118.20	121.90
21	AA	735	C	C4'-C3'-C2'	-5.28	97.32	102.60
53	BA	91	A	C4-C5-C6	-5.28	114.36	117.00
53	BA	268	C	N3-C4-N4	-5.28	114.30	118.00
53	BA	1083	U	C4-C5-C6	5.28	122.87	119.70
53	BA	1329	U	N1-C2-N3	5.28	118.07	114.90
53	BA	1533	C	N3-C2-O2	-5.28	118.20	121.90
53	BA	2033	A	C1'-O4'-C4'	-5.28	105.67	109.90
21	AA	252	U	N3-C2-O2	-5.28	118.50	122.20
21	AA	370	C	N1-C2-O2	5.28	122.07	118.90
21	AA	1532	U	N3-C2-O2	-5.28	118.50	122.20
53	BA	1614	A	C4-C5-C6	-5.28	114.36	117.00
53	BA	1816	C	N3-C2-O2	-5.28	118.20	121.90
21	AA	183	C	C6-N1-C2	-5.28	118.19	120.30
21	AA	532	A	O4'-C1'-N9	5.28	112.42	108.20
21	AA	904	U	O4'-C1'-N1	5.28	112.42	108.20
21	AA	1520	C	O4'-C1'-N1	5.28	112.42	108.20
53	BA	666	A	C6-C5-N7	5.28	136.00	132.30
53	BA	2021	C	O4'-C1'-N1	5.28	112.42	108.20
53	BA	2261	C	N1-C2-O2	5.28	122.07	118.90
21	AA	255	G	O4'-C1'-N9	5.28	112.42	108.20
21	AA	674	G	N1-C6-O6	-5.28	116.73	119.90
21	AA	1345	U	N3-C2-O2	-5.28	118.50	122.20
53	BA	88	G	N3-C4-C5	-5.28	125.96	128.60
53	BA	1322	A	C6-C5-N7	5.28	136.00	132.30
53	BA	1460	U	O4'-C1'-N1	5.28	112.42	108.20
53	BA	1682	G	N9-C4-C5	5.28	107.51	105.40
53	BA	1898	U	N3-C2-O2	-5.28	118.50	122.20
21	AA	71	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	236	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1437	A	C4-C5-C6	-5.28	114.36	117.00
32	BK	78	ARG	NE-CZ-NH1	5.28	122.94	120.30
53	BA	1016	G	C5-C6-N1	5.28	114.14	111.50
53	BA	2858	C	N1-C2-O2	5.28	122.07	118.90
21	AA	221	C	N3-C2-O2	-5.28	118.21	121.90
21	AA	1360	A	C6-C5-N7	5.28	135.99	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	37	C	C4'-C3'-C2'	-5.28	97.32	102.60
53	BA	55	G	N1-C6-O6	-5.28	116.73	119.90
53	BA	1003	G	N1-C6-O6	-5.28	116.73	119.90
53	BA	1484	U	N3-C2-O2	-5.28	118.51	122.20
53	BA	1905	C	N3-C4-C5	5.28	124.01	121.90
53	BA	2250	G	N9-C4-C5	5.28	107.51	105.40
53	BA	2301	C	N3-C2-O2	-5.28	118.21	121.90
53	BA	560	C	N1-C2-O2	5.27	122.06	118.90
53	BA	2645	G	C3'-C2'-C1'	5.27	105.72	101.50
21	AA	149	A	C5-C6-N1	5.27	120.34	117.70
21	AA	1011	C	N3-C2-O2	-5.27	118.21	121.90
53	BA	69	C	O4'-C1'-N1	5.27	112.42	108.20
53	BA	731	C	N3-C2-O2	-5.27	118.21	121.90
53	BA	1093	G	C5-C6-N1	5.27	114.14	111.50
53	BA	1236	G	N3-C2-N2	-5.27	116.21	119.90
53	BA	1564	C	N1-C2-O2	5.27	122.06	118.90
53	BA	2014	A	C4-C5-C6	-5.27	114.36	117.00
53	BA	2445	G	N1-C6-O6	-5.27	116.74	119.90
20	AU	33	ARG	NE-CZ-NH1	5.27	122.94	120.30
53	BA	80	G	N1-C6-O6	-5.27	116.74	119.90
53	BA	289	G	C5-C6-N1	5.27	114.14	111.50
53	BA	2033	A	C2-N3-C4	5.27	113.24	110.60
21	AA	108	G	C5-C6-N1	5.27	114.13	111.50
21	AA	229	U	O4'-C1'-N1	5.27	112.42	108.20
21	AA	1336	C	N3-C4-C5	5.27	124.01	121.90
21	AA	1377	A	C2-N3-C4	5.27	113.23	110.60
53	BA	314	C	C6-N1-C2	-5.27	118.19	120.30
53	BA	486	C	N3-C2-O2	-5.27	118.21	121.90
53	BA	2282	G	C5-C6-N1	5.27	114.14	111.50
53	BA	2767	C	N3-C4-C5	5.27	124.01	121.90
53	BA	2778	A	O4'-C1'-N9	5.27	112.42	108.20
54	BB	114	C	N1-C2-O2	5.27	122.06	118.90
21	AA	1205	U	C5-C6-N1	-5.27	120.07	122.70
34	BM	51	ARG	NE-CZ-NH1	5.27	122.93	120.30
53	BA	178	G	C5-C6-N1	5.27	114.13	111.50
53	BA	439	A	C4-C5-C6	-5.27	114.37	117.00
53	BA	861	A	C6-C5-N7	5.27	135.99	132.30
53	BA	2206	C	O4'-C1'-N1	5.27	112.42	108.20
21	AA	559	A	C4-C5-C6	-5.27	114.37	117.00
21	AA	335	C	N1-C2-O2	5.26	122.06	118.90
52	B4	19	ARG	NE-CZ-NH2	-5.26	117.67	120.30
53	BA	996	A	C5'-C4'-C3'	-5.26	107.58	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1504	A	C4-C5-C6	-5.26	114.37	117.00
53	BA	2590	A	C6-C5-N7	5.26	135.99	132.30
53	BA	2658	C	C5'-C4'-O4'	5.26	115.42	109.10
53	BA	2740	A	C4-C5-C6	-5.26	114.37	117.00
54	BB	74	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	55	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	637	C	N3-C4-C5	5.26	124.00	121.90
21	AA	1363	A	C4-C5-C6	-5.26	114.37	117.00
53	BA	1421	G	C5-C6-N1	5.26	114.13	111.50
53	BA	1902	C	N3-C2-O2	-5.26	118.22	121.90
53	BA	2272	U	N3-C2-O2	-5.26	118.52	122.20
21	AA	603	U	N3-C2-O2	-5.26	118.52	122.20
21	AA	944	G	O4'-C1'-N9	5.26	112.41	108.20
53	BA	1294	U	C4'-C3'-C2'	-5.26	97.34	102.60
53	BA	1416	G	C5-C6-N1	5.26	114.13	111.50
53	BA	1592	C	O4'-C1'-N1	5.26	112.41	108.20
53	BA	1669	A	C2-N3-C4	5.26	113.23	110.60
53	BA	2033	A	C5'-C4'-O4'	5.26	115.41	109.10
21	AA	556	C	N3-C4-C5	5.26	124.00	121.90
21	AA	771	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	1497	G	O4'-C1'-N9	5.26	112.41	108.20
53	BA	63	A	C6-C5-N7	5.26	135.98	132.30
53	BA	1116	G	C8-N9-C4	-5.26	104.30	106.40
21	AA	218	U	O4'-C1'-N1	5.26	112.41	108.20
53	BA	242	G	N3-C4-C5	-5.26	125.97	128.60
53	BA	592	A	C6-C5-N7	5.26	135.98	132.30
53	BA	1507	C	O4'-C1'-N1	5.26	112.41	108.20
53	BA	2797	U	C5-C6-N1	-5.26	120.07	122.70
21	AA	372	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	737	C	O4'-C1'-N1	5.26	112.41	108.20
21	AA	782	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1379	G	N3-C4-C5	-5.26	125.97	128.60
22	A1	39	G	C8-N9-C4	-5.26	104.30	106.40
53	BA	2593	U	C5-C6-N1	-5.26	120.07	122.70
54	BB	11	C	N3-C4-C5	5.26	124.00	121.90
21	AA	886	G	N9-C4-C5	5.25	107.50	105.40
22	A1	66	A	C4-C5-C6	-5.25	114.37	117.00
53	BA	419	U	N3-C2-O2	-5.25	118.52	122.20
53	BA	528	A	C4-C5-C6	-5.25	114.37	117.00
53	BA	614	A	N9-C1'-C2'	-5.25	106.22	112.00
53	BA	2489	U	N3-C2-O2	-5.25	118.52	122.20
21	AA	697	U	C4-C5-C6	5.25	122.85	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	776	G	N3-C2-N2	-5.25	116.22	119.90
53	BA	785	G	N3-C4-C5	-5.25	125.97	128.60
53	BA	930	G	N1-C6-O6	-5.25	116.75	119.90
53	BA	1081	U	O4'-C1'-N1	5.25	112.40	108.20
53	BA	1933	G	C5-C6-N1	5.25	114.13	111.50
53	BA	2378	A	O4'-C1'-N9	5.25	112.40	108.20
53	BA	2817	U	C5-C6-N1	-5.25	120.07	122.70
21	AA	36	C	N3-C4-C5	5.25	124.00	121.90
21	AA	373	A	C4-C5-C6	-5.25	114.37	117.00
21	AA	1158	C	N3-C4-N4	-5.25	114.32	118.00
53	BA	379	G	O4'-C1'-N9	5.25	112.40	108.20
53	BA	424	G	C5'-C4'-O4'	5.25	115.40	109.10
53	BA	486	C	O4'-C1'-N1	5.25	112.40	108.20
53	BA	914	G	O4'-C1'-N9	5.25	112.40	108.20
53	BA	917	A	C5-C6-N1	5.25	120.33	117.70
28	BG	169	ARG	NE-CZ-NH2	5.25	122.92	120.30
53	BA	1224	U	O4'-C1'-N1	5.25	112.40	108.20
21	AA	911	U	N3-C2-O2	-5.25	118.53	122.20
21	AA	1147	C	O4'-C1'-N1	5.25	112.40	108.20
53	BA	243	U	O4'-C1'-N1	5.25	112.40	108.20
53	BA	539	G	N3-C4-C5	-5.25	125.98	128.60
53	BA	898	C	N3-C4-C5	5.25	124.00	121.90
53	BA	1104	C	N1-C2-O2	5.25	122.05	118.90
53	BA	1197	G	O4'-C1'-N9	5.25	112.40	108.20
53	BA	1797	G	N7-C8-N9	5.25	115.72	113.10
53	BA	2094	A	C4-C5-C6	-5.25	114.38	117.00
53	BA	2103	C	N3-C2-O2	-5.25	118.23	121.90
53	BA	2403	C	C4'-C3'-C2'	-5.25	97.35	102.60
54	BB	66	A	O4'-C1'-N9	5.25	112.40	108.20
21	AA	83	C	N3-C4-C5	5.25	124.00	121.90
21	AA	512	U	C5'-C4'-O4'	5.25	115.40	109.10
21	AA	1045	C	O4'-C1'-N1	5.25	112.40	108.20
53	BA	316	C	O4'-C1'-N1	5.25	112.40	108.20
53	BA	424	G	N1-C6-O6	-5.25	116.75	119.90
53	BA	457	A	C4-C5-C6	-5.25	114.38	117.00
53	BA	1400	U	C5-C6-N1	-5.25	120.08	122.70
53	BA	2424	C	N1-C2-O2	5.25	122.05	118.90
24	BC	86	ARG	CD-NE-CZ	5.25	130.94	123.60
53	BA	1204	A	C4-C5-C6	-5.25	114.38	117.00
53	BA	1778	U	N3-C2-O2	-5.25	118.53	122.20
53	BA	2784	U	O4'-C1'-N1	5.25	112.40	108.20
21	AA	595	A	C5-C6-N1	5.24	120.32	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	269	C	N1-C2-O2	5.24	122.05	118.90
53	BA	694	U	N3-C2-O2	-5.24	118.53	122.20
53	BA	1034	G	N1-C6-O6	-5.24	116.75	119.90
53	BA	1637	A	C4-C5-C6	-5.24	114.38	117.00
53	BA	1820	U	N3-C2-O2	-5.24	118.53	122.20
53	BA	2723	C	N1-C2-O2	5.24	122.05	118.90
53	BA	2853	C	C2-N3-C4	-5.24	117.28	119.90
21	AA	1400	C	N1-C2-O2	5.24	122.05	118.90
53	BA	382	A	N1-C6-N6	-5.24	115.45	118.60
53	BA	1905	C	N1-C2-O2	5.24	122.05	118.90
21	AA	89	U	N1-C2-N3	5.24	118.05	114.90
21	AA	376	G	C5-C6-N1	5.24	114.12	111.50
21	AA	1235	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	1344	C	N1-C2-O2	5.24	122.04	118.90
38	BQ	63	ARG	NE-CZ-NH1	5.24	122.92	120.30
50	B2	28	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
53	BA	268	C	N3-C4-C5	5.24	124.00	121.90
53	BA	1840	G	N7-C8-N9	5.24	115.72	113.10
21	AA	571	U	C5-C6-N1	-5.24	120.08	122.70
21	AA	769	G	C8-N9-C4	-5.24	104.31	106.40
53	BA	516	C	O4'-C1'-N1	5.24	112.39	108.20
53	BA	980	A	C4-C5-C6	-5.24	114.38	117.00
53	BA	1795	C	N3-C4-C5	5.24	124.00	121.90
53	BA	2473	U	N3-C2-O2	-5.24	118.53	122.20
54	BB	17	C	O4'-C1'-N1	5.24	112.39	108.20
54	BB	32	U	N3-C2-O2	-5.24	118.53	122.20
3	AD	134	TYR	CB-CG-CD2	-5.24	117.86	121.00
21	AA	82	G	C5-C6-N1	5.24	114.12	111.50
53	BA	379	G	N9-C4-C5	5.24	107.50	105.40
53	BA	900	A	C4'-C3'-C2'	-5.24	97.36	102.60
53	BA	1067	A	C4-C5-C6	-5.24	114.38	117.00
53	BA	1655	A	N1-C6-N6	-5.24	115.46	118.60
53	BA	2155	U	C5-C6-N1	-5.24	120.08	122.70
53	BA	2627	G	C5-C6-N1	5.24	114.12	111.50
21	AA	1263	C	N3-C4-C5	5.24	124.00	121.90
21	AA	1506	U	O4'-C1'-N1	5.24	112.39	108.20
44	BW	24	ARG	NE-CZ-NH2	5.24	122.92	120.30
53	BA	1	G	N1-C6-O6	-5.24	116.76	119.90
53	BA	407	G	C5-C6-N1	5.24	114.12	111.50
53	BA	428	A	N1-C6-N6	-5.24	115.46	118.60
53	BA	1126	A	P-O3'-C3'	5.24	125.98	119.70
53	BA	1129	A	C6-C5-N7	5.24	135.97	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1158	C	C4'-C3'-C2'	-5.24	97.36	102.60
53	BA	1251	C	N3-C2-O2	-5.24	118.23	121.90
53	BA	1660	G	N3-C4-C5	-5.24	125.98	128.60
53	BA	1666	G	N9-C4-C5	5.24	107.49	105.40
53	BA	1799	G	N7-C8-N9	5.24	115.72	113.10
53	BA	91	A	O4'-C1'-N9	5.23	112.39	108.20
53	BA	435	C	C2-N3-C4	-5.23	117.28	119.90
53	BA	1443	U	O4'-C1'-N1	5.23	112.39	108.20
53	BA	1469	A	C2-N3-C4	5.23	113.22	110.60
53	BA	1859	U	O4'-C1'-N1	5.23	112.39	108.20
53	BA	1960	A	O4'-C1'-N9	5.23	112.39	108.20
53	BA	2617	U	C4'-C3'-C2'	-5.23	97.37	102.60
53	BA	2674	G	N3-C4-C5	-5.23	125.98	128.60
21	AA	1197	A	C5-C6-N1	5.23	120.32	117.70
53	BA	228	C	N1-C2-O2	5.23	122.04	118.90
53	BA	1302	A	C4-C5-C6	-5.23	114.38	117.00
53	BA	1454	C	O4'-C1'-N1	5.23	112.39	108.20
53	BA	1676	A	O4'-C1'-N9	5.23	112.39	108.20
53	BA	2149	U	O4'-C1'-N1	5.23	112.39	108.20
21	AA	550	G	C5-C6-N1	5.23	114.12	111.50
21	AA	1090	U	N3-C2-O2	-5.23	118.54	122.20
53	BA	138	U	O4'-C1'-N1	5.23	112.38	108.20
53	BA	195	A	C5'-C4'-O4'	5.23	115.38	109.10
53	BA	459	U	C5-C6-N1	-5.23	120.08	122.70
53	BA	1236	G	C8-N9-C4	-5.23	104.31	106.40
53	BA	2047	C	N1-C2-O2	5.23	122.04	118.90
53	BA	2172	U	C5-C6-N1	-5.23	120.08	122.70
54	BB	77	U	O4'-C1'-N1	5.23	112.39	108.20
21	AA	699	C	N3-C4-C5	5.23	123.99	121.90
21	AA	1360	A	C4'-C3'-C2'	-5.23	97.37	102.60
53	BA	325	G	O4'-C1'-N9	5.23	112.38	108.20
53	BA	616	A	O4'-C1'-N9	5.23	112.38	108.20
53	BA	966	G	C5-C6-N1	5.23	114.11	111.50
53	BA	1403	A	C4-C5-C6	-5.23	114.39	117.00
53	BA	1804	C	N3-C2-O2	-5.23	118.24	121.90
53	BA	2472	G	N3-C4-C5	-5.23	125.98	128.60
21	AA	466	A	O4'-C1'-N9	5.23	112.38	108.20
21	AA	1436	U	O4'-C1'-N1	5.23	112.38	108.20
53	BA	855	G	C5-C6-N1	5.23	114.11	111.50
53	BA	871	U	C5-C6-N1	-5.23	120.09	122.70
53	BA	1995	U	O4'-C1'-N1	5.23	112.38	108.20
53	BA	2072	C	N3-C4-C5	5.23	123.99	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	302	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	1407	C	O4'-C1'-N1	5.23	112.38	108.20
53	BA	944	C	C1'-O4'-C4'	-5.23	105.72	109.90
53	BA	1612	C	N1-C2-O2	5.23	122.03	118.90
53	BA	1808	A	C4-C5-C6	-5.23	114.39	117.00
53	BA	2682	A	C6-C5-N7	5.23	135.96	132.30
21	AA	381	C	N3-C4-C5	5.22	123.99	121.90
21	AA	930	C	O4'-C1'-N1	5.22	112.38	108.20
53	BA	98	G	N3-C4-C5	-5.22	125.99	128.60
53	BA	395	U	N3-C2-O2	-5.22	118.54	122.20
53	BA	442	G	C5-C6-N1	5.22	114.11	111.50
53	BA	783	A	C5-C6-N1	5.22	120.31	117.70
53	BA	1315	C	N3-C4-C5	5.22	123.99	121.90
53	BA	1791	A	C6-C5-N7	5.22	135.96	132.30
53	BA	2438	U	C5-C6-N1	-5.22	120.09	122.70
53	BA	2510	C	O4'-C1'-N1	5.22	112.38	108.20
53	BA	2843	G	O4'-C1'-N9	5.22	112.38	108.20
21	AA	217	C	O4'-C1'-N1	5.22	112.38	108.20
53	BA	355	U	O4'-C1'-N1	5.22	112.38	108.20
53	BA	1844	C	N1-C2-O2	5.22	122.03	118.90
53	BA	2447	G	N3-C4-C5	-5.22	125.99	128.60
53	BA	2551	C	C6-N1-C2	-5.22	118.21	120.30
53	BA	2785	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	206	C	N3-C4-C5	5.22	123.99	121.90
53	BA	2812	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	73	C	N1-C2-O2	5.22	122.03	118.90
21	AA	494	G	C5-C6-N1	5.22	114.11	111.50
21	AA	722	G	N3-C4-C5	-5.22	125.99	128.60
21	AA	858	G	C8-N9-C4	-5.22	104.31	106.40
21	AA	1200	C	N1-C2-O2	5.22	122.03	118.90
53	BA	837	C	N3-C2-O2	-5.22	118.25	121.90
53	BA	1332	G	N7-C8-N9	5.22	115.71	113.10
53	BA	2069	G	N3-C2-N2	-5.22	116.25	119.90
53	BA	1798	U	O4'-C1'-N1	5.22	112.37	108.20
53	BA	2567	G	N3-C2-N2	-5.22	116.25	119.90
53	BA	2859	G	N1-C6-O6	-5.22	116.77	119.90
53	BA	1839	G	C5-C6-N1	5.22	114.11	111.50
53	BA	1864	U	O4'-C1'-N1	5.22	112.37	108.20
53	BA	1868	C	C5'-C4'-O4'	5.22	115.36	109.10
53	BA	2227	A	C4'-C3'-C2'	-5.22	97.38	102.60
21	AA	298	A	C6-C5-N7	5.21	135.95	132.30
53	BA	939	G	N3-C4-C5	-5.21	125.99	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1640	A	C2-N3-C4	5.21	113.21	110.60
53	BA	2286	G	C5-C6-N1	5.21	114.11	111.50
21	AA	938	A	C4-C5-C6	-5.21	114.39	117.00
21	AA	199	A	C6-C5-N7	5.21	135.95	132.30
21	AA	1324	A	C5-C6-N1	5.21	120.31	117.70
53	BA	713	G	N9-C4-C5	5.21	107.48	105.40
53	BA	2524	G	N7-C8-N9	5.21	115.71	113.10
53	BA	2633	G	C5-C6-N1	5.21	114.11	111.50
21	AA	280	C	N3-C2-O2	-5.21	118.25	121.90
53	BA	1203	U	N3-C2-O2	-5.21	118.55	122.20
21	AA	570	G	C8-N9-C4	-5.21	104.32	106.40
21	AA	629	A	C4-C5-C6	-5.21	114.40	117.00
21	AA	1069	C	O4'-C1'-N1	5.21	112.37	108.20
21	AA	1500	A	C6-C5-N7	5.21	135.95	132.30
25	BD	59	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
53	BA	221	A	C4-C5-C6	-5.21	114.40	117.00
53	BA	1783	A	C5-C6-N1	5.21	120.31	117.70
53	BA	2752	C	N3-C2-O2	-5.21	118.25	121.90
21	AA	867	G	C4'-C3'-C2'	-5.21	97.39	102.60
21	AA	919	A	C4-C5-C6	-5.21	114.40	117.00
53	BA	104	A	C4'-C3'-C2'	-5.21	97.39	102.60
53	BA	595	C	N3-C2-O2	-5.21	118.26	121.90
53	BA	740	C	C5'-C4'-O4'	5.21	115.35	109.10
39	BR	84	ARG	NE-CZ-NH1	5.21	122.90	120.30
53	BA	590	A	C4-C5-C6	-5.21	114.40	117.00
21	AA	10	A	O4'-C1'-N9	5.20	112.36	108.20
21	AA	153	C	N3-C2-O2	-5.20	118.26	121.90
21	AA	175	C	N1-C2-O2	5.20	122.02	118.90
21	AA	472	U	O4'-C1'-N1	5.20	112.36	108.20
21	AA	521	G	N3-C2-N2	-5.20	116.26	119.90
21	AA	781	A	C5-C6-N1	5.20	120.30	117.70
53	BA	315	G	N1-C6-O6	-5.20	116.78	119.90
53	BA	713	G	N3-C2-N2	-5.20	116.26	119.90
53	BA	1069	A	C8-N9-C4	-5.20	103.72	105.80
53	BA	1658	C	N3-C2-O2	-5.20	118.26	121.90
53	BA	2167	U	O4'-C1'-N1	5.20	112.36	108.20
53	BA	2207	C	N3-C2-O2	-5.20	118.26	121.90
53	BA	2326	C	N1-C2-O2	5.20	122.02	118.90
53	BA	2600	A	C6-C5-N7	5.20	135.94	132.30
53	BA	2870	C	O4'-C1'-N1	5.20	112.36	108.20
54	BB	42	C	N1-C2-O2	5.20	122.02	118.90
17	AR	42	ARG	NE-CZ-NH1	5.20	122.90	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	562	U	C5-C6-N1	-5.20	120.10	122.70
53	BA	1688	U	N1-C2-N3	5.20	118.02	114.90
21	AA	646	G	C8-N9-C4	-5.20	104.32	106.40
21	AA	697	U	N1-C2-N3	5.20	118.02	114.90
21	AA	956	U	C5-C6-N1	-5.20	120.10	122.70
21	AA	1416	G	N9-C4-C5	5.20	107.48	105.40
31	BJ	116	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
53	BA	11	C	N3-C2-O2	-5.20	118.26	121.90
53	BA	519	U	C5-C6-N1	-5.20	120.10	122.70
53	BA	801	G	O4'-C4'-C3'	5.20	110.26	106.10
53	BA	1289	C	C6-N1-C2	-5.20	118.22	120.30
53	BA	1453	A	C6-C5-N7	5.20	135.94	132.30
53	BA	2155	U	N3-C2-O2	-5.20	118.56	122.20
54	BB	44	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	60	A	C5-C6-N1	5.20	120.30	117.70
21	AA	108	G	N3-C4-C5	-5.20	126.00	128.60
53	BA	78	U	C4-C5-C6	5.20	122.82	119.70
53	BA	654	A	C4-C5-C6	-5.20	114.40	117.00
53	BA	695	G	C5-C6-N1	5.20	114.10	111.50
53	BA	1660	G	C5'-C4'-C3'	-5.20	107.68	116.00
53	BA	1825	U	C5-C6-N1	-5.20	120.10	122.70
53	BA	2045	C	O4'-C1'-N1	5.20	112.36	108.20
53	BA	2090	A	C5-C6-N1	5.20	120.30	117.70
53	BA	2718	G	C8-N9-C4	-5.20	104.32	106.40
21	AA	715	A	C4-C5-C6	-5.20	114.40	117.00
53	BA	375	G	N1-C6-O6	-5.20	116.78	119.90
53	BA	2203	U	N1-C2-N3	5.20	118.02	114.90
21	AA	549	C	N3-C4-C5	5.20	123.98	121.90
21	AA	549	C	O4'-C1'-N1	5.20	112.36	108.20
53	BA	70	G	N3-C4-C5	-5.20	126.00	128.60
53	BA	262	A	C4-C5-C6	-5.20	114.40	117.00
53	BA	1091	G	C8-N9-C4	-5.20	104.32	106.40
53	BA	1556	C	O4'-C1'-N1	5.20	112.36	108.20
53	BA	1992	G	N3-C4-C5	-5.20	126.00	128.60
53	BA	2305	U	N3-C2-O2	-5.20	118.56	122.20
53	BA	2840	C	O4'-C1'-N1	5.20	112.36	108.20
21	AA	1281	C	C2-N3-C4	-5.19	117.30	119.90
53	BA	426	C	N3-C4-C5	5.19	123.98	121.90
53	BA	1638	C	C4'-C3'-C2'	-5.19	97.41	102.60
53	BA	1842	G	N1-C6-O6	-5.19	116.78	119.90
21	AA	350	G	N9-C4-C5	5.19	107.48	105.40
21	AA	1396	A	C6-C5-N7	5.19	135.94	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	800	A	C6-C5-N7	5.19	135.94	132.30
53	BA	1500	G	N3-C4-C5	-5.19	126.00	128.60
53	BA	2167	U	N1-C2-N3	5.19	118.02	114.90
53	BA	2305	U	N1-C2-N3	5.19	118.02	114.90
53	BA	2817	U	N3-C2-O2	-5.19	118.57	122.20
21	AA	216	U	N1-C2-N3	5.19	118.01	114.90
21	AA	534	U	C3'-C2'-C1'	5.19	105.65	101.50
21	AA	770	C	C6-N1-C2	-5.19	118.22	120.30
53	BA	56	A	C6-C5-N7	5.19	135.93	132.30
53	BA	674	G	C5-C6-N1	5.19	114.10	111.50
53	BA	753	A	C6-C5-N7	5.19	135.93	132.30
53	BA	1328	A	C6-C5-N7	5.19	135.93	132.30
53	BA	1423	G	C8-N9-C4	-5.19	104.32	106.40
53	BA	1863	G	N1-C6-O6	-5.19	116.79	119.90
53	BA	2211	A	C6-C5-N7	5.19	135.93	132.30
53	BA	2468	A	C2-N3-C4	5.19	113.20	110.60
54	BB	107	G	N3-C4-C5	-5.19	126.00	128.60
21	AA	1200	C	N3-C4-C5	5.19	123.98	121.90
53	BA	1817	G	N3-C2-N2	-5.19	116.27	119.90
53	BA	2056	G	N3-C4-C5	-5.19	126.00	128.60
53	BA	2718	G	N1-C6-O6	-5.19	116.79	119.90
21	AA	251	G	C2-N3-C4	5.19	114.49	111.90
21	AA	654	G	N1-C6-O6	-5.19	116.79	119.90
21	AA	852	G	N3-C2-N2	-5.19	116.27	119.90
21	AA	985	C	N3-C2-O2	-5.19	118.27	121.90
21	AA	1036	A	C5-C6-N1	5.19	120.29	117.70
22	A1	74	C	N3-C4-C5	5.19	123.97	121.90
53	BA	42	A	C5-C6-N1	5.19	120.29	117.70
53	BA	188	G	N1-C6-O6	-5.19	116.79	119.90
53	BA	215	G	C5-C6-N1	5.19	114.09	111.50
53	BA	606	U	N3-C2-O2	-5.19	118.57	122.20
53	BA	767	U	N3-C2-O2	-5.19	118.57	122.20
53	BA	1010	A	C6-C5-N7	5.19	135.93	132.30
53	BA	1473	G	N9-C4-C5	5.19	107.47	105.40
53	BA	1695	G	C5-C6-N1	5.19	114.09	111.50
53	BA	2869	G	N3-C2-N2	-5.19	116.27	119.90
21	AA	562	U	C5-C6-N1	-5.18	120.11	122.70
53	BA	673	C	N1-C2-O2	5.18	122.01	118.90
53	BA	940	G	N3-C4-C5	-5.18	126.01	128.60
53	BA	948	C	N3-C2-O2	-5.18	118.27	121.90
53	BA	962	G	N3-C2-N2	-5.18	116.27	119.90
53	BA	1031	G	N1-C6-O6	-5.18	116.79	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1331	G	C8-N9-C4	-5.18	104.33	106.40
53	BA	1502	A	C6-C5-N7	5.18	135.93	132.30
53	BA	2578	G	P-O3'-C3'	5.18	125.92	119.70
21	AA	160	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	344	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	421	U	O4'-C1'-N1	5.18	112.35	108.20
53	BA	889	C	C6-N1-C2	-5.18	118.23	120.30
53	BA	1718	G	C5'-C4'-O4'	5.18	115.32	109.10
53	BA	2369	A	C6-C5-N7	5.18	135.93	132.30
53	BA	2730	C	N3-C2-O2	-5.18	118.27	121.90
54	BB	108	A	C4-C5-C6	-5.18	114.41	117.00
22	A1	48	C	N3-C4-C5	5.18	123.97	121.90
53	BA	418	C	N3-C2-O2	-5.18	118.27	121.90
21	AA	148	G	C1'-O4'-C4'	-5.18	105.76	109.90
21	AA	862	C	N1-C2-O2	5.18	122.01	118.90
53	BA	78	U	O4'-C1'-N1	5.18	112.34	108.20
53	BA	726	G	C5-C6-N1	5.18	114.09	111.50
53	BA	1192	G	N1-C6-O6	-5.18	116.79	119.90
53	BA	1825	U	N3-C2-O2	-5.18	118.57	122.20
53	BA	2117	A	C2-N3-C4	5.18	113.19	110.60
21	AA	945	G	N3-C2-N2	-5.18	116.28	119.90
53	BA	37	C	N3-C2-O2	-5.18	118.28	121.90
53	BA	718	A	C4-C5-C6	-5.18	114.41	117.00
6	AG	78	ARG	NE-CZ-NH1	5.18	122.89	120.30
21	AA	826	C	N3-C2-O2	-5.18	118.28	121.90
21	AA	939	G	N1-C6-O6	-5.18	116.79	119.90
53	BA	613	A	C2-N3-C4	5.18	113.19	110.60
53	BA	827	U	C5-C6-N1	-5.18	120.11	122.70
53	BA	2297	A	C5-C6-N1	5.18	120.29	117.70
53	BA	2840	C	N1-C2-O2	5.18	122.01	118.90
21	AA	301	G	N3-C4-C5	-5.17	126.01	128.60
53	BA	361	G	C5-C6-N1	5.17	114.09	111.50
53	BA	1784	A	O4'-C1'-N9	5.17	112.34	108.20
53	BA	2168	G	N3-C4-C5	-5.17	126.01	128.60
53	BA	2195	U	O4'-C1'-N1	5.17	112.34	108.20
53	BA	2540	C	O4'-C1'-N1	5.17	112.34	108.20
28	BG	34	ARG	NE-CZ-NH1	5.17	122.89	120.30
53	BA	1232	G	N3-C4-C5	-5.17	126.01	128.60
53	BA	1340	U	C5-C6-N1	-5.17	120.11	122.70
53	BA	1640	A	C6-C5-N7	5.17	135.92	132.30
21	AA	396	C	O4'-C1'-N1	5.17	112.34	108.20
21	AA	744	C	N3-C4-C5	5.17	123.97	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1172	C	N1-C2-O2	5.17	122.00	118.90
21	AA	1347	G	C5-C6-N1	5.17	114.09	111.50
21	AA	1438	G	N1-C6-O6	-5.17	116.80	119.90
32	BK	31	ARG	NE-CZ-NH1	5.17	122.89	120.30
53	BA	62	U	C5-C6-N1	-5.17	120.11	122.70
53	BA	80	G	N3-C4-C5	-5.17	126.02	128.60
53	BA	1929	G	N3-C2-N2	-5.17	116.28	119.90
53	BA	1965	C	O4'-C1'-N1	5.17	112.34	108.20
53	BA	2265	U	N1-C2-N3	5.17	118.00	114.90
53	BA	2711	A	C6-C5-N7	5.17	135.92	132.30
53	BA	673	C	C2-N3-C4	-5.17	117.31	119.90
53	BA	1189	A	C5-C6-N1	5.17	120.28	117.70
21	AA	342	C	O4'-C1'-N1	5.17	112.33	108.20
21	AA	867	G	C8-N9-C4	-5.17	104.33	106.40
53	BA	622	G	C5-C6-N1	5.17	114.08	111.50
53	BA	1003	G	C5-C6-N1	5.17	114.08	111.50
53	BA	1428	C	O4'-C1'-N1	5.17	112.33	108.20
53	BA	2287	A	C5-C6-N1	5.17	120.28	117.70
53	BA	2532	G	N3-C4-C5	-5.17	126.02	128.60
53	BA	2567	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	124	C	N3-C4-N4	-5.17	114.38	118.00
21	AA	266	G	C5-C6-N1	5.17	114.08	111.50
21	AA	1059	C	N3-C4-C5	5.17	123.97	121.90
21	AA	1185	G	N3-C4-C5	-5.17	126.02	128.60
53	BA	45	G	C5-C6-N1	5.17	114.08	111.50
53	BA	650	C	N3-C4-C5	5.17	123.97	121.90
53	BA	680	C	N1-C2-O2	5.17	122.00	118.90
53	BA	893	C	N3-C2-O2	-5.17	118.28	121.90
53	BA	1271	G	N1-C6-O6	-5.17	116.80	119.90
53	BA	1350	C	O4'-C1'-N1	5.17	112.33	108.20
53	BA	2415	G	N3-C2-N2	-5.17	116.28	119.90
21	AA	242	G	O4'-C1'-N9	5.17	112.33	108.20
21	AA	586	C	O4'-C1'-N1	5.17	112.33	108.20
29	BH	68	ARG	NE-CZ-NH1	5.17	122.88	120.30
53	BA	2137	U	O4'-C1'-C2'	-5.17	100.64	105.80
53	BA	2261	C	N3-C4-C5	5.17	123.97	121.90
53	BA	2607	G	C5-C6-N1	5.17	114.08	111.50
20	AU	32	ARG	NE-CZ-NH2	5.16	122.88	120.30
21	AA	535	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	820	U	N3-C2-O2	-5.16	118.59	122.20
21	AA	1299	A	C5-C6-N1	5.16	120.28	117.70
53	BA	1203	U	C5-C6-N1	-5.16	120.12	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1939	U	C4-C5-C6	5.16	122.80	119.70
53	BA	1984	G	C5-C6-N1	5.16	114.08	111.50
53	BA	2873	A	C4-C5-C6	-5.16	114.42	117.00
53	BA	2877	G	N3-C4-C5	-5.16	126.02	128.60
21	AA	63	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1331	G	C4-C5-N7	-5.16	108.73	110.80
53	BA	810	U	N3-C2-O2	-5.16	118.59	122.20
21	AA	566	G	N3-C2-N2	-5.16	116.29	119.90
21	AA	1192	C	N3-C4-C5	5.16	123.96	121.90
21	AA	1339	A	C6-C5-N7	5.16	135.91	132.30
53	BA	583	G	N1-C6-O6	-5.16	116.80	119.90
53	BA	764	A	C4-C5-C6	-5.16	114.42	117.00
53	BA	791	C	N1-C2-O2	5.16	122.00	118.90
53	BA	1292	G	N3-C4-C5	-5.16	126.02	128.60
53	BA	1653	G	N3-C4-C5	-5.16	126.02	128.60
53	BA	2023	C	N3-C4-C5	5.16	123.97	121.90
53	BA	2465	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	1365	G	C5-C6-N1	5.16	114.08	111.50
53	BA	339	U	O4'-C1'-N1	5.16	112.33	108.20
53	BA	2237	G	N3-C4-C5	-5.16	126.02	128.60
53	BA	2471	A	C4-C5-C6	-5.16	114.42	117.00
53	BA	2832	U	N3-C2-O2	-5.16	118.59	122.20
53	BA	2871	U	C5-C6-N1	-5.16	120.12	122.70
21	AA	315	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	1209	C	N3-C2-O2	-5.16	118.29	121.90
53	BA	395	U	C5-C6-N1	-5.16	120.12	122.70
53	BA	881	G	N3-C4-C5	-5.16	126.02	128.60
53	BA	2689	U	O4'-C1'-N1	5.16	112.33	108.20
2	AC	130	ARG	NE-CZ-NH2	5.16	122.88	120.30
21	AA	84	U	C5-C6-N1	-5.16	120.12	122.70
21	AA	459	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	970	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1041	G	N1-C6-O6	-5.16	116.81	119.90
21	AA	1446	A	C1'-O4'-C4'	-5.16	105.78	109.90
53	BA	665	U	O4'-C1'-N1	5.16	112.33	108.20
53	BA	844	A	C6-C5-N7	5.16	135.91	132.30
53	BA	1150	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	764	C	O4'-C1'-N1	5.15	112.32	108.20
22	A1	5	G	N1-C6-O6	-5.15	116.81	119.90
53	BA	444	C	N1-C2-O2	5.15	121.99	118.90
53	BA	723	C	O4'-C1'-N1	5.15	112.32	108.20
53	BA	2076	U	N1-C2-N3	5.15	117.99	114.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2145	C	N1-C2-O2	5.15	121.99	118.90
21	AA	597	G	C4-C5-N7	-5.15	108.74	110.80
21	AA	1025	U	O4'-C4'-C3'	5.15	110.22	106.10
21	AA	1290	G	C5-N7-C8	-5.15	101.72	104.30
22	A1	8	U	N1-C2-N3	5.15	117.99	114.90
53	BA	2	G	N1-C6-O6	-5.15	116.81	119.90
53	BA	117	G	N3-C4-C5	-5.15	126.02	128.60
53	BA	1773	A	C4'-C3'-C2'	-5.15	97.45	102.60
53	BA	2760	C	N1-C2-O2	5.15	121.99	118.90
53	BA	2886	A	C6-C5-N7	5.15	135.91	132.30
55	B5	164	ARG	NE-CZ-NH1	5.15	122.88	120.30
21	AA	435	A	C6-C5-N7	5.15	135.91	132.30
21	AA	610	U	N3-C2-O2	-5.15	118.59	122.20
21	AA	964	A	C4-C5-C6	-5.15	114.42	117.00
21	AA	1248	A	N1-C6-N6	-5.15	115.51	118.60
21	AA	1284	C	C6-N1-C2	-5.15	118.24	120.30
53	BA	43	G	N9-C4-C5	5.15	107.46	105.40
53	BA	1367	A	C4-C5-C6	-5.15	114.42	117.00
53	BA	1415	U	N1-C2-N3	5.15	117.99	114.90
53	BA	1867	G	O4'-C1'-N9	5.15	112.32	108.20
53	BA	2871	U	N1-C2-N3	5.15	117.99	114.90
21	AA	1108	G	N1-C6-O6	-5.15	116.81	119.90
21	AA	1411	C	N1-C2-O2	5.15	121.99	118.90
53	BA	2279	G	N1-C6-O6	-5.15	116.81	119.90
21	AA	402	G	N3-C4-C5	-5.15	126.03	128.60
21	AA	748	G	O4'-C1'-N9	5.15	112.32	108.20
21	AA	1249	C	O4'-C1'-N1	5.15	112.32	108.20
53	BA	1308	A	C6-C5-N7	5.15	135.90	132.30
53	BA	2247	A	C5-C6-N1	5.15	120.27	117.70
53	BA	89	A	C6-C5-N7	5.15	135.90	132.30
53	BA	691	C	N3-C4-C5	5.15	123.96	121.90
53	BA	1085	A	C5-C6-N1	5.15	120.27	117.70
53	BA	1108	U	C4-C5-C6	5.15	122.79	119.70
21	AA	520	A	C6-C5-N7	5.14	135.90	132.30
21	AA	1263	C	O4'-C1'-N1	5.14	112.31	108.20
23	A2	79	A	C2-N3-C4	5.14	113.17	110.60
53	BA	112	U	N3-C2-O2	-5.14	118.60	122.20
53	BA	271	G	N7-C8-N9	5.14	115.67	113.10
53	BA	334	C	O4'-C1'-N1	5.14	112.31	108.20
53	BA	895	U	N3-C2-O2	-5.14	118.60	122.20
53	BA	1178	C	N1-C2-O2	5.14	121.99	118.90
53	BA	1335	C	C6-N1-C2	-5.14	118.24	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1531	C	N1-C2-O2	5.14	121.99	118.90
53	BA	1694	C	N1-C2-O2	5.14	121.99	118.90
53	BA	2072	C	C4'-C3'-C2'	-5.14	97.46	102.60
53	BA	2204	G	C5-C6-N1	5.14	114.07	111.50
53	BA	2686	G	N3-C4-C5	-5.14	126.03	128.60
53	BA	2795	C	O4'-C1'-N1	5.14	112.32	108.20
53	BA	2813	A	O4'-C1'-N9	5.14	112.31	108.20
54	BB	34	A	O4'-C1'-N9	5.14	112.32	108.20
22	A1	42	G	C5-C6-N1	5.14	114.07	111.50
53	BA	1628	G	C5-C6-N1	5.14	114.07	111.50
53	BA	1941	C	O4'-C1'-N1	5.14	112.31	108.20
53	BA	2728	U	N3-C2-O2	-5.14	118.60	122.20
27	BF	91	ARG	NE-CZ-NH1	5.14	122.87	120.30
53	BA	1078	U	O4'-C1'-N1	5.14	112.31	108.20
21	AA	68	G	N3-C2-N2	-5.14	116.30	119.90
21	AA	95	C	N1-C2-O2	5.14	121.98	118.90
21	AA	98	A	O4'-C1'-N9	5.14	112.31	108.20
21	AA	266	G	N3-C4-C5	-5.14	126.03	128.60
21	AA	639	G	N7-C8-N9	5.14	115.67	113.10
21	AA	1498	U	C5-C6-N1	-5.14	120.13	122.70
53	BA	45	G	P-O3'-C3'	5.14	125.87	119.70
53	BA	785	G	N1-C6-O6	-5.14	116.82	119.90
53	BA	1190	G	N3-C4-C5	-5.14	126.03	128.60
53	BA	1554	U	N3-C2-O2	-5.14	118.60	122.20
53	BA	1697	G	N3-C4-C5	-5.14	126.03	128.60
53	BA	1772	A	C4'-C3'-C2'	-5.14	97.46	102.60
53	BA	2065	C	N3-C4-C5	5.14	123.96	121.90
53	BA	2085	U	N1-C2-N3	5.14	117.98	114.90
53	BA	2278	A	C6-C5-N7	5.14	135.90	132.30
53	BA	2576	G	C5-C6-N1	5.14	114.07	111.50
53	BA	2853	C	N3-C4-C5	5.14	123.96	121.90
54	BB	95	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	1260	G	N3-C4-C5	-5.14	126.03	128.60
53	BA	1638	C	O4'-C1'-N1	5.14	112.31	108.20
53	BA	2520	C	N3-C2-O2	-5.14	118.30	121.90
21	AA	69	G	N3-C4-C5	-5.14	126.03	128.60
21	AA	365	U	N3-C2-O2	-5.14	118.61	122.20
21	AA	971	G	C5-C6-N1	5.14	114.07	111.50
21	AA	1395	C	N1-C2-O2	5.14	121.98	118.90
53	BA	430	A	C4-C5-C6	-5.14	114.43	117.00
53	BA	491	G	N3-C4-C5	-5.14	126.03	128.60
53	BA	1401	G	N3-C2-N2	-5.14	116.30	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2189	U	C5-C6-N1	-5.14	120.13	122.70
53	BA	2291	U	N1-C2-N3	5.14	117.98	114.90
21	AA	10	A	C6-C5-N7	5.13	135.89	132.30
21	AA	1462	C	O4'-C1'-N1	5.13	112.31	108.20
53	BA	222	A	C4-C5-C6	-5.13	114.43	117.00
53	BA	527	C	O4'-C1'-N1	5.13	112.31	108.20
53	BA	1138	G	C5-C6-N1	5.13	114.07	111.50
53	BA	1540	G	C8-N9-C4	-5.13	104.35	106.40
53	BA	2317	A	O4'-C1'-N9	5.13	112.31	108.20
53	BA	2429	G	N7-C8-N9	5.13	115.67	113.10
53	BA	762	U	C5-C6-N1	-5.13	120.13	122.70
53	BA	788	A	C4-C5-C6	-5.13	114.43	117.00
53	BA	2347	C	N1-C2-O2	5.13	121.98	118.90
21	AA	102	G	N3-C4-C5	-5.13	126.03	128.60
21	AA	130	A	C6-C5-N7	5.13	135.89	132.30
21	AA	1173	U	O4'-C1'-N1	5.13	112.31	108.20
21	AA	1266	G	C8-N9-C4	-5.13	104.35	106.40
53	BA	283	G	O4'-C1'-N9	5.13	112.31	108.20
53	BA	1117	C	N1-C2-O2	5.13	121.98	118.90
53	BA	1310	G	C4'-C3'-C2'	-5.13	97.47	102.60
53	BA	1769	U	C5-C6-N1	-5.13	120.13	122.70
53	BA	1972	G	C5-C6-N1	5.13	114.07	111.50
54	BB	28	C	N1-C2-O2	5.13	121.98	118.90
21	AA	545	C	N3-C4-C5	5.13	123.95	121.90
21	AA	977	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	1401	G	N3-C4-C5	-5.13	126.03	128.60
53	BA	150	U	C4'-C3'-C2'	-5.13	97.47	102.60
53	BA	192	C	N3-C4-C5	5.13	123.95	121.90
53	BA	217	A	C4-C5-C6	-5.13	114.44	117.00
53	BA	1189	A	C4-C5-C6	-5.13	114.44	117.00
54	BB	28	C	C2-N3-C4	-5.13	117.33	119.90
21	AA	907	A	C4-C5-C6	-5.13	114.44	117.00
22	A1	13	C	C4'-C3'-C2'	-5.13	97.47	102.60
53	BA	137	U	N3-C2-O2	-5.13	118.61	122.20
53	BA	1405	U	N1-C2-N3	5.13	117.98	114.90
53	BA	1898	U	O4'-C1'-N1	5.13	112.30	108.20
21	AA	213	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	374	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	794	A	C6-C5-N7	5.13	135.89	132.30
21	AA	1160	G	C8-N9-C4	-5.13	104.35	106.40
21	AA	1356	G	C8-N9-C4	-5.13	104.35	106.40
53	BA	370	G	C8-N9-C4	-5.13	104.35	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	968	C	N1-C2-O2	5.13	121.98	118.90
53	BA	1356	G	O4'-C1'-N9	5.13	112.30	108.20
53	BA	1501	G	N1-C6-O6	-5.13	116.82	119.90
53	BA	2185	U	O4'-C1'-N1	5.13	112.30	108.20
54	BB	63	C	O4'-C1'-N1	5.13	112.30	108.20
22	A1	22	G	O4'-C1'-N9	5.12	112.30	108.20
43	BV	19	ARG	NE-CZ-NH2	5.12	122.86	120.30
53	BA	197	A	C6-C5-N7	5.12	135.89	132.30
53	BA	800	A	C5-C6-N6	5.12	127.80	123.70
53	BA	1320	C	N1-C2-O2	5.12	121.97	118.90
53	BA	2267	A	C4-C5-C6	-5.12	114.44	117.00
53	BA	2509	G	C5'-C4'-O4'	5.12	115.25	109.10
53	BA	2703	C	N3-C2-O2	-5.12	118.31	121.90
53	BA	2845	U	N3-C2-O2	-5.12	118.61	122.20
21	AA	262	A	N1-C2-N3	-5.12	126.74	129.30
21	AA	603	U	O4'-C1'-N1	5.12	112.30	108.20
21	AA	1124	G	N1-C6-O6	-5.12	116.83	119.90
53	BA	133	U	C5-C6-N1	-5.12	120.14	122.70
53	BA	1443	U	N3-C2-O2	-5.12	118.61	122.20
53	BA	1668	A	C4-C5-C6	-5.12	114.44	117.00
53	BA	1939	U	C5-C6-N1	-5.12	120.14	122.70
53	BA	2231	U	O4'-C1'-N1	5.12	112.30	108.20
53	BA	2333	A	C3'-C2'-C1'	5.12	105.60	101.50
53	BA	2665	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	728	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	856	C	N1-C2-O2	5.12	121.97	118.90
21	AA	1303	C	N1-C2-O2	5.12	121.97	118.90
53	BA	349	U	N3-C2-O2	-5.12	118.61	122.20
53	BA	1584	U	C4-C5-C6	5.12	122.77	119.70
53	BA	2086	U	C4-C5-C6	5.12	122.77	119.70
53	BA	2469	A	C6-C5-N7	5.12	135.88	132.30
53	BA	2687	U	N3-C2-O2	-5.12	118.61	122.20
21	AA	669	G	C5-C6-N1	5.12	114.06	111.50
53	BA	825	A	C6-C5-N7	5.12	135.88	132.30
21	AA	423	G	O4'-C1'-N9	5.12	112.30	108.20
21	AA	829	G	O4'-C1'-N9	5.12	112.30	108.20
21	AA	887	G	C5-C6-N1	5.12	114.06	111.50
21	AA	969	A	C6-C5-N7	5.12	135.88	132.30
21	AA	988	G	O4'-C1'-N9	5.12	112.29	108.20
21	AA	1191	A	C5'-C4'-O4'	5.12	115.24	109.10
53	BA	1319	C	C6-N1-C2	-5.12	118.25	120.30
53	BA	1448	G	O4'-C1'-N9	5.12	112.30	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2122	U	O4'-C1'-N1	5.12	112.30	108.20
53	BA	2411	A	C4-C5-C6	-5.12	114.44	117.00
53	BA	2864	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	69	G	N9-C4-C5	5.12	107.45	105.40
21	AA	406	G	C5-C6-N1	5.12	114.06	111.50
53	BA	2509	G	C8-N9-C4	-5.12	104.35	106.40
21	AA	679	C	O4'-C1'-N1	5.12	112.29	108.20
21	AA	849	G	N9-C4-C5	5.12	107.45	105.40
21	AA	1117	A	C5'-C4'-O4'	5.12	115.24	109.10
21	AA	1338	G	N9-C4-C5	5.12	107.45	105.40
53	BA	458	G	N3-C4-C5	-5.12	126.04	128.60
53	BA	2323	G	N3-C4-C5	-5.12	126.04	128.60
21	AA	835	U	N1-C2-N3	5.11	117.97	114.90
21	AA	1157	A	C6-C5-N7	5.11	135.88	132.30
21	AA	1340	A	C6-C5-N7	5.11	135.88	132.30
53	BA	813	U	O4'-C1'-N1	5.11	112.29	108.20
53	BA	1200	C	N3-C2-O2	-5.11	118.32	121.90
53	BA	1561	C	N1-C2-O2	5.11	121.97	118.90
53	BA	2583	G	N3-C2-N2	-5.11	116.32	119.90
53	BA	84	A	O4'-C1'-N9	5.11	112.29	108.20
53	BA	533	G	N3-C4-C5	-5.11	126.04	128.60
53	BA	987	C	N3-C2-O2	-5.11	118.32	121.90
53	BA	2618	G	N3-C2-N2	-5.11	116.32	119.90
21	AA	288	A	C4-C5-C6	-5.11	114.44	117.00
21	AA	319	G	N3-C4-C5	-5.11	126.05	128.60
21	AA	717	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	1404	C	O4'-C1'-N1	5.11	112.29	108.20
53	BA	461	C	N3-C2-O2	-5.11	118.32	121.90
53	BA	692	C	N1-C2-O2	5.11	121.97	118.90
53	BA	977	G	N7-C8-N9	5.11	115.66	113.10
53	BA	1542	U	C4-C5-C6	5.11	122.77	119.70
53	BA	1649	G	N1-C6-O6	-5.11	116.83	119.90
53	BA	1731	G	N7-C8-N9	5.11	115.66	113.10
53	BA	2209	G	N7-C8-N9	5.11	115.66	113.10
53	BA	2533	U	C5-C6-N1	-5.11	120.14	122.70
53	BA	2573	C	N3-C4-C5	5.11	123.94	121.90
53	BA	2719	G	N1-C6-O6	-5.11	116.83	119.90
21	AA	73	C	N3-C4-C5	5.11	123.94	121.90
21	AA	575	G	C8-N9-C4	-5.11	104.36	106.40
21	AA	578	C	C4'-C3'-C2'	-5.11	97.49	102.60
53	BA	607	U	C5-C6-N1	-5.11	120.14	122.70
53	BA	913	U	N3-C2-O2	-5.11	118.62	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BB	28	C	N3-C4-C5	5.11	123.94	121.90
21	AA	66	A	C2-N3-C4	5.11	113.15	110.60
21	AA	965	U	C5-C6-N1	-5.11	120.15	122.70
53	BA	234	U	C4-C5-C6	5.11	122.76	119.70
53	BA	567	U	O4'-C1'-N1	5.11	112.29	108.20
53	BA	656	G	C5-C6-N1	5.11	114.05	111.50
53	BA	1478	G	N3-C4-C5	-5.11	126.05	128.60
53	BA	1605	C	C6-N1-C2	-5.11	118.26	120.30
53	BA	1685	C	N1-C2-O2	5.11	121.97	118.90
53	BA	2480	C	N3-C2-O2	-5.11	118.33	121.90
21	AA	351	G	N1-C6-O6	-5.11	116.84	119.90
21	AA	1190	G	N1-C6-O6	-5.11	116.84	119.90
21	AA	1376	U	C4-C5-C6	5.11	122.76	119.70
21	AA	1514	G	C8-N9-C4	-5.11	104.36	106.40
53	BA	1741	C	C4'-C3'-C2'	-5.11	97.49	102.60
53	BA	2032	G	C5-C6-N1	5.11	114.05	111.50
53	BA	2524	G	C8-N9-C4	-5.11	104.36	106.40
21	AA	266	G	N9-C4-C5	5.10	107.44	105.40
53	BA	231	A	C6-C5-N7	5.10	135.87	132.30
53	BA	2133	G	N3-C4-C5	-5.10	126.05	128.60
53	BA	2617	U	C5-C6-N1	-5.10	120.15	122.70
53	BA	2865	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	390	U	N1-C2-N3	5.10	117.96	114.90
21	AA	956	U	N1-C2-N3	5.10	117.96	114.90
53	BA	752	A	C4-C5-C6	-5.10	114.45	117.00
53	BA	757	G	N7-C8-N9	5.10	115.65	113.10
53	BA	1202	G	N9-C4-C5	5.10	107.44	105.40
53	BA	2172	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	974	A	C6-C5-N7	5.10	135.87	132.30
21	AA	1053	G	C4'-C3'-O3'	5.10	123.20	113.00
21	AA	1245	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1325	C	C4'-C3'-C2'	-5.10	97.50	102.60
53	BA	488	G	N9-C4-C5	5.10	107.44	105.40
53	BA	1999	C	N1-C2-O2	5.10	121.96	118.90
53	BA	2662	A	C8-N9-C4	-5.10	103.76	105.80
21	AA	43	C	N3-C2-O2	-5.10	118.33	121.90
21	AA	297	G	C5-C6-N1	5.10	114.05	111.50
21	AA	776	G	C5-C6-N1	5.10	114.05	111.50
21	AA	1438	G	C5-C6-N1	5.10	114.05	111.50
53	BA	290	U	C5-C6-N1	-5.10	120.15	122.70
53	BA	698	C	N3-C2-O2	-5.10	118.33	121.90
53	BA	2181	U	O4'-C1'-N1	5.10	112.28	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2483	C	N1-C2-O2	5.10	121.96	118.90
21	AA	618	C	N3-C4-C5	5.10	123.94	121.90
21	AA	777	A	C6-C5-N7	5.10	135.87	132.30
21	AA	1507	A	C4-C5-C6	-5.10	114.45	117.00
53	BA	139	U	N3-C2-O2	-5.10	118.63	122.20
53	BA	378	C	N3-C2-O2	-5.10	118.33	121.90
53	BA	560	C	N3-C4-C5	5.10	123.94	121.90
53	BA	1299	G	N3-C2-N2	-5.10	116.33	119.90
53	BA	1526	C	N3-C4-C5	5.10	123.94	121.90
53	BA	1726	C	C4'-C3'-C2'	-5.10	97.50	102.60
53	BA	1730	C	C2-N3-C4	-5.10	117.35	119.90
53	BA	2881	U	O4'-C1'-N1	5.10	112.28	108.20
54	BB	13	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	939	G	N3-C4-C5	-5.10	126.05	128.60
21	AA	1296	C	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1314	C	N3-C2-O2	-5.10	118.33	121.90
53	BA	1682	G	C8-N9-C4	-5.10	104.36	106.40
53	BA	2507	C	N3-C2-O2	-5.10	118.33	121.90
53	BA	2901	C	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1102	A	C5'-C4'-C3'	-5.09	107.85	116.00
21	AA	1400	C	N3-C4-C5	5.09	123.94	121.90
45	BX	10	ARG	NE-CZ-NH1	5.09	122.85	120.30
53	BA	704	G	N9-C4-C5	5.09	107.44	105.40
53	BA	1015	U	O4'-C1'-N1	5.09	112.28	108.20
53	BA	1768	C	O4'-C1'-N1	5.09	112.28	108.20
53	BA	1822	C	C6-N1-C2	-5.09	118.26	120.30
53	BA	2296	U	O3'-P-O5'	-5.09	94.32	104.00
53	BA	2489	U	C5-C6-N1	-5.09	120.15	122.70
21	AA	469	C	N1-C2-O2	5.09	121.96	118.90
21	AA	1001	C	N3-C2-O2	-5.09	118.33	121.90
53	BA	355	U	N1-C2-N3	5.09	117.96	114.90
53	BA	472	A	C4-C5-C6	-5.09	114.45	117.00
11	AL	82	ARG	NE-CZ-NH2	-5.09	117.75	120.30
21	AA	1211	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	1485	U	O4'-C1'-N1	5.09	112.27	108.20
53	BA	1585	C	N3-C2-O2	-5.09	118.33	121.90
53	BA	2287	A	C8-N9-C4	-5.09	103.76	105.80
53	BA	2346	A	C4-C5-C6	-5.09	114.45	117.00
15	AP	14	ARG	NE-CZ-NH1	5.09	122.84	120.30
21	AA	103	U	N1-C2-N3	5.09	117.95	114.90
21	AA	214	C	C4'-C3'-C2'	-5.09	97.51	102.60
21	AA	443	C	O4'-C1'-N1	5.09	112.27	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	999	C	C2-N3-C4	-5.09	117.36	119.90
53	BA	27	G	C5-C6-N1	5.09	114.05	111.50
53	BA	337	C	N1-C2-O2	5.09	121.95	118.90
53	BA	1026	G	O4'-C1'-N9	5.09	112.27	108.20
53	BA	1406	U	N3-C2-O2	-5.09	118.64	122.20
53	BA	1535	A	C2-N3-C4	5.09	113.14	110.60
53	BA	2592	G	C8-N9-C4	-5.09	104.36	106.40
39	BR	21	ARG	NE-CZ-NH1	5.09	122.84	120.30
53	BA	157	C	O4'-C1'-N1	5.09	112.27	108.20
53	BA	471	A	N1-C6-N6	-5.09	115.55	118.60
53	BA	1435	G	N1-C6-O6	-5.09	116.85	119.90
53	BA	1760	C	N3-C4-C5	5.09	123.94	121.90
53	BA	2472	G	C5-C6-N1	5.09	114.04	111.50
53	BA	2839	G	N7-C8-N9	5.09	115.64	113.10
21	AA	545	C	O4'-C1'-N1	5.09	112.27	108.20
21	AA	856	C	N3-C4-C5	5.09	123.93	121.90
21	AA	928	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	1472	U	C5'-C4'-O4'	5.09	115.20	109.10
24	BC	270	ARG	NE-CZ-NH2	5.09	122.84	120.30
53	BA	2581	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	1366	C	N3-C4-C5	5.08	123.93	121.90
53	BA	334	C	N3-C4-C5	5.08	123.93	121.90
53	BA	399	U	N3-C2-O2	-5.08	118.64	122.20
53	BA	827	U	C3'-C2'-C1'	5.08	105.57	101.50
53	BA	881	G	C5-C6-N1	5.08	114.04	111.50
53	BA	970	U	C5-C6-N1	-5.08	120.16	122.70
53	BA	1379	U	O4'-C1'-N1	5.08	112.27	108.20
53	BA	2365	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	585	G	N3-C4-C5	-5.08	126.06	128.60
21	AA	616	G	O4'-C1'-N9	5.08	112.27	108.20
21	AA	1042	A	C6-C5-N7	5.08	135.86	132.30
21	AA	1279	G	N3-C4-C5	-5.08	126.06	128.60
21	AA	1460	C	O4'-C1'-N1	5.08	112.27	108.20
53	BA	142	A	O4'-C1'-N9	5.08	112.27	108.20
53	BA	727	A	C4-C5-C6	-5.08	114.46	117.00
53	BA	922	C	C6-N1-C2	-5.08	118.27	120.30
21	AA	5	U	N3-C2-O2	-5.08	118.64	122.20
21	AA	811	C	N3-C2-O2	-5.08	118.34	121.90
21	AA	1352	C	C2-N3-C4	-5.08	117.36	119.90
53	BA	1101	U	N1-C2-N3	5.08	117.95	114.90
53	BA	1761	C	N3-C4-C5	5.08	123.93	121.90
53	BA	1972	G	C3'-C2'-C1'	5.08	105.56	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2051	A	C4-C5-C6	-5.08	114.46	117.00
53	BA	2436	G	C8-N9-C4	-5.08	104.37	106.40
54	BB	94	A	C6-C5-N7	5.08	135.86	132.30
21	AA	574	A	C6-C5-N7	5.08	135.86	132.30
22	A1	24	G	N3-C4-C5	-5.08	126.06	128.60
53	BA	2146	C	N3-C4-C5	5.08	123.93	121.90
53	BA	2501	C	N1-C2-O2	5.08	121.95	118.90
53	BA	2879	A	C2-N3-C4	5.08	113.14	110.60
21	AA	427	U	O4'-C1'-N1	5.08	112.26	108.20
21	AA	1210	C	C6-N1-C2	-5.08	118.27	120.30
53	BA	637	A	C6-C5-N7	5.08	135.85	132.30
53	BA	1313	U	N1-C2-N3	5.08	117.95	114.90
53	BA	1683	U	O4'-C1'-N1	5.08	112.26	108.20
53	BA	1868	C	O4'-C1'-N1	5.08	112.26	108.20
53	BA	2147	A	O4'-C1'-N9	5.08	112.26	108.20
53	BA	2405	G	C5-C6-N1	5.08	114.04	111.50
53	BA	2564	A	C5'-C4'-O4'	5.08	115.19	109.10
22	A1	14	A	N1-C6-N6	-5.08	115.55	118.60
53	BA	273	G	N1-C6-O6	-5.08	116.85	119.90
53	BA	1043	C	N3-C2-O2	-5.08	118.35	121.90
53	BA	1135	C	C5'-C4'-C3'	-5.08	107.88	116.00
53	BA	1586	A	C4-C5-C6	-5.08	114.46	117.00
1	AB	221	ARG	NE-CZ-NH1	5.08	122.84	120.30
21	AA	570	G	N9-C4-C5	5.08	107.43	105.40
21	AA	756	C	O4'-C1'-N1	5.08	112.26	108.20
25	BD	179	ARG	NE-CZ-NH1	5.08	122.84	120.30
53	BA	629	G	C5-C6-N1	5.08	114.04	111.50
53	BA	719	C	N3-C2-O2	-5.08	118.35	121.90
53	BA	1002	G	O4'-C1'-N9	5.08	112.26	108.20
53	BA	1721	G	C8-N9-C4	-5.08	104.37	106.40
53	BA	1732	C	N3-C4-C5	5.08	123.93	121.90
53	BA	2408	U	C5-C6-N1	-5.08	120.16	122.70
53	BA	2574	G	C8-N9-C4	-5.08	104.37	106.40
21	AA	152	A	C6-C5-N7	5.07	135.85	132.30
21	AA	204	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	1401	G	N7-C8-N9	5.07	115.64	113.10
53	BA	720	U	O4'-C1'-N1	5.07	112.26	108.20
53	BA	919	U	N3-C2-O2	-5.07	118.65	122.20
53	BA	1076	C	N3-C4-C5	5.07	123.93	121.90
53	BA	2126	A	C4-C5-C6	-5.07	114.46	117.00
53	BA	2579	C	N1-C2-O2	5.07	121.94	118.90
54	BB	12	C	O4'-C1'-N1	5.07	112.26	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	238	C	C3'-C2'-C1'	5.07	105.56	101.50
53	BA	1254	A	C4-C5-C6	-5.07	114.46	117.00
21	AA	467	U	N3-C2-O2	-5.07	118.65	122.20
21	AA	1353	G	N3-C4-C5	-5.07	126.06	128.60
53	BA	387	U	N1-C2-N3	5.07	117.94	114.90
53	BA	490	C	N3-C4-C5	5.07	123.93	121.90
53	BA	1222	U	O4'-C1'-N1	5.07	112.26	108.20
53	BA	1707	G	N7-C8-N9	5.07	115.64	113.10
53	BA	2695	U	N1-C2-N3	5.07	117.94	114.90
21	AA	473	U	O4'-C1'-N1	5.07	112.25	108.20
53	BA	695	G	N1-C6-O6	-5.07	116.86	119.90
53	BA	1893	C	C6-N1-C2	-5.07	118.27	120.30
21	AA	89	U	C4-C5-C6	5.07	122.74	119.70
21	AA	1136	C	N3-C4-C5	5.07	123.93	121.90
53	BA	6	A	O4'-C1'-N9	5.07	112.25	108.20
53	BA	43	G	N3-C4-C5	-5.07	126.07	128.60
53	BA	60	G	C1'-O4'-C4'	-5.07	105.84	109.90
53	BA	446	G	N1-C6-O6	-5.07	116.86	119.90
53	BA	446	G	O4'-C4'-C3'	5.07	110.15	106.10
53	BA	693	A	C4'-C3'-C2'	-5.07	97.53	102.60
53	BA	1037	G	C5'-C4'-O4'	5.07	115.18	109.10
53	BA	1055	G	N9-C4-C5	5.07	107.43	105.40
53	BA	1775	U	N3-C2-O2	-5.07	118.65	122.20
53	BA	2317	A	C5-C6-N1	5.07	120.23	117.70
53	BA	2869	G	C8-N9-C4	-5.07	104.37	106.40
54	BB	29	A	O4'-C1'-N9	5.07	112.25	108.20
53	BA	279	A	C6-C5-N7	5.07	135.84	132.30
53	BA	344	A	O4'-C1'-N9	5.07	112.25	108.20
53	BA	1331	G	N7-C8-N9	5.07	115.63	113.10
53	BA	1551	A	C5'-C4'-O4'	5.07	115.18	109.10
53	BA	1598	A	N1-C6-N6	-5.07	115.56	118.60
53	BA	2383	G	N1-C6-O6	-5.07	116.86	119.90
53	BA	2441	U	O4'-C1'-N1	5.07	112.25	108.20
53	BA	2588	G	N1-C6-O6	-5.07	116.86	119.90
53	BA	2689	U	C5-C6-N1	-5.07	120.17	122.70
27	BF	94	ARG	NE-CZ-NH1	5.06	122.83	120.30
53	BA	1784	A	C5-C6-N1	5.06	120.23	117.70
53	BA	2475	C	C6-N1-C2	-5.06	118.27	120.30
21	AA	700	G	C5'-C4'-O4'	5.06	115.18	109.10
21	AA	1143	G	C5-C6-N1	5.06	114.03	111.50
53	BA	132	G	O4'-C1'-N9	5.06	112.25	108.20
53	BA	287	G	C8-N9-C4	-5.06	104.38	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1013	C	N3-C2-O2	-5.06	118.36	121.90
53	BA	1786	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	1091	U	C5'-C4'-O4'	5.06	115.17	109.10
21	AA	1119	C	N3-C2-O2	-5.06	118.36	121.90
26	BE	102	ARG	NE-CZ-NH1	5.06	122.83	120.30
53	BA	550	C	N3-C4-C5	5.06	123.92	121.90
53	BA	743	A	O4'-C1'-N9	5.06	112.25	108.20
21	AA	738	C	N1-C2-O2	5.06	121.94	118.90
21	AA	922	G	C5-C6-N1	5.06	114.03	111.50
21	AA	1025	U	N1-C2-N3	5.06	117.94	114.90
53	BA	138	U	N3-C2-O2	-5.06	118.66	122.20
53	BA	773	U	N3-C2-O2	-5.06	118.66	122.20
53	BA	1768	C	C4'-C3'-C2'	-5.06	97.54	102.60
53	BA	1852	U	N1-C2-N3	5.06	117.94	114.90
53	BA	2040	G	N3-C4-C5	-5.06	126.07	128.60
53	BA	2471	A	C5-C6-N1	5.06	120.23	117.70
21	AA	308	C	N3-C4-C5	5.06	123.92	121.90
21	AA	898	G	O4'-C1'-N9	5.06	112.25	108.20
21	AA	905	U	N3-C2-O2	-5.06	118.66	122.20
53	BA	97	C	O4'-C1'-N1	5.06	112.25	108.20
53	BA	512	G	N9-C4-C5	5.06	107.42	105.40
53	BA	1136	G	C8-N9-C4	-5.06	104.38	106.40
53	BA	1500	G	N1-C6-O6	-5.06	116.86	119.90
53	BA	1524	G	N3-C2-N2	-5.06	116.36	119.90
53	BA	1643	G	N3-C4-C5	-5.06	126.07	128.60
53	BA	1674	G	N7-C8-N9	5.06	115.63	113.10
53	BA	2063	C	N3-C4-C5	5.06	123.92	121.90
53	BA	2473	U	C5-C6-N1	-5.06	120.17	122.70
21	AA	1212	U	O4'-C1'-N1	5.06	112.25	108.20
22	A1	48	C	C2-N3-C4	-5.06	117.37	119.90
53	BA	1808	A	C5-C6-N1	5.06	120.23	117.70
21	AA	242	G	C5-C6-N1	5.05	114.03	111.50
21	AA	1113	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1348	U	N1-C2-N3	5.05	117.93	114.90
21	AA	1498	U	N1-C2-N3	5.05	117.93	114.90
53	BA	277	G	O4'-C1'-N9	5.05	112.24	108.20
53	BA	537	G	O4'-C1'-N9	5.05	112.24	108.20
53	BA	593	U	O4'-C1'-N1	5.05	112.24	108.20
53	BA	1183	U	C5-C6-N1	-5.05	120.17	122.70
53	BA	1323	C	N3-C4-C5	5.05	123.92	121.90
53	BA	1907	G	C8-N9-C4	-5.05	104.38	106.40
54	BB	36	C	N3-C4-C5	5.05	123.92	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	793	U	C3'-C2'-C1'	5.05	105.54	101.50
21	AA	1004	A	C6-C5-N7	5.05	135.84	132.30
21	AA	1316	G	N3-C4-C5	-5.05	126.07	128.60
41	BT	76	ARG	NE-CZ-NH1	5.05	122.83	120.30
53	BA	1083	U	C5-C6-N1	-5.05	120.17	122.70
53	BA	1086	A	O4'-C1'-N9	5.05	112.24	108.20
53	BA	2316	G	N7-C8-N9	5.05	115.63	113.10
53	BA	295	G	O4'-C1'-N9	5.05	112.24	108.20
53	BA	317	G	N3-C4-C5	-5.05	126.07	128.60
53	BA	1072	C	O4'-C4'-C3'	5.05	110.14	106.10
53	BA	1832	C	C3'-C2'-C1'	5.05	105.54	101.50
21	AA	411	A	O4'-C1'-N9	5.05	112.24	108.20
21	AA	802	A	O4'-C1'-N9	5.05	112.24	108.20
21	AA	900	A	C4-C5-C6	-5.05	114.47	117.00
21	AA	1395	C	O4'-C1'-N1	5.05	112.24	108.20
53	BA	69	C	C6-N1-C2	-5.05	118.28	120.30
53	BA	131	A	C4-C5-C6	-5.05	114.47	117.00
53	BA	158	U	O4'-C1'-N1	5.05	112.24	108.20
53	BA	1267	U	O4'-C1'-N1	5.05	112.24	108.20
53	BA	2165	C	N3-C2-O2	-5.05	118.36	121.90
53	BA	2226	C	O4'-C1'-N1	5.05	112.24	108.20
53	BA	2277	G	N9-C4-C5	5.05	107.42	105.40
53	BA	2338	C	N3-C2-O2	-5.05	118.36	121.90
53	BA	2448	A	C4-C5-C6	-5.05	114.47	117.00
53	BA	2582	G	N7-C8-N9	5.05	115.62	113.10
53	BA	2688	G	C4'-C3'-C2'	-5.05	97.55	102.60
53	BA	2747	G	O4'-C1'-N9	5.05	112.24	108.20
21	AA	980	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1069	C	N1-C2-O2	5.05	121.93	118.90
53	BA	116	C	N3-C2-O2	-5.05	118.37	121.90
53	BA	1542	U	N1-C2-N3	5.05	117.93	114.90
53	BA	2680	U	C5-C6-N1	-5.05	120.18	122.70
21	AA	184	G	C5-C6-N1	5.05	114.02	111.50
21	AA	272	C	N1-C2-O2	5.05	121.93	118.90
21	AA	489	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1152	A	C4-C5-C6	-5.05	114.48	117.00
53	BA	544	C	N1-C2-O2	5.05	121.93	118.90
53	BA	1987	A	C4-C5-C6	-5.05	114.48	117.00
53	BA	2495	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	681	A	C6-C5-N7	5.04	135.83	132.30
53	BA	677	A	C5'-C4'-O4'	5.04	115.15	109.10
53	BA	1116	G	N1-C6-O6	-5.04	116.87	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	1539	U	O4'-C1'-N1	5.04	112.24	108.20
21	AA	786	G	C5-C6-N1	5.04	114.02	111.50
47	BZ	15	ARG	CD-NE-CZ	5.04	130.66	123.60
53	BA	500	G	C5-C6-N1	5.04	114.02	111.50
53	BA	983	A	C4-C5-C6	-5.04	114.48	117.00
53	BA	1117	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	1425	G	C5-C6-N1	5.04	114.02	111.50
53	BA	1599	U	N3-C2-O2	-5.04	118.67	122.20
53	BA	2043	C	C5'-C4'-C3'	-5.04	107.93	116.00
53	BA	2356	U	O4'-C1'-N1	5.04	112.23	108.20
53	BA	2664	G	C5-C6-N1	5.04	114.02	111.50
53	BA	2811	G	O4'-C1'-N9	5.04	112.23	108.20
53	BA	2857	G	N3-C4-C5	-5.04	126.08	128.60
53	BA	2863	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	218	U	C5-C6-N1	-5.04	120.18	122.70
21	AA	561	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	655	A	N1-C6-N6	-5.04	115.58	118.60
21	AA	1131	G	N9-C4-C5	5.04	107.42	105.40
53	BA	143	C	N1-C2-O2	5.04	121.92	118.90
53	BA	451	U	C5-C6-N1	-5.04	120.18	122.70
53	BA	888	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	1206	G	C5-C6-N1	5.04	114.02	111.50
53	BA	1724	G	C5-C6-N1	5.04	114.02	111.50
53	BA	1971	U	N3-C2-O2	-5.04	118.67	122.20
53	BA	455	C	N3-C2-O2	-5.04	118.37	121.90
53	BA	799	G	C5'-C4'-O4'	5.04	115.15	109.10
53	BA	1216	G	N3-C4-C5	-5.04	126.08	128.60
53	BA	1764	C	N1-C2-O2	5.04	121.92	118.90
53	BA	1945	G	C5-C6-N1	5.04	114.02	111.50
53	BA	2208	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	2535	G	N7-C8-N9	5.04	115.62	113.10
21	AA	999	C	N3-C4-C5	5.04	123.92	121.90
21	AA	1112	C	N1-C2-O2	5.04	121.92	118.90
53	BA	12	U	N3-C2-O2	-5.04	118.67	122.20
53	BA	400	G	C5-C6-N1	5.04	114.02	111.50
53	BA	1306	C	N3-C2-O2	-5.04	118.37	121.90
53	BA	2150	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	2426	A	C6-C5-N7	5.04	135.83	132.30
53	BA	2444	G	O4'-C1'-N9	5.04	112.23	108.20
53	BA	2558	C	N3-C2-O2	-5.04	118.37	121.90
53	BA	2588	G	C5-C6-N1	5.04	114.02	111.50
21	AA	278	G	N3-C4-C5	-5.04	126.08	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1251	A	C4-C5-C6	-5.04	114.48	117.00
53	BA	210	C	N3-C2-O2	-5.04	118.37	121.90
53	BA	221	A	C2-N3-C4	5.04	113.12	110.60
53	BA	751	A	C4-C5-C6	-5.04	114.48	117.00
53	BA	940	G	C5-C6-N1	5.04	114.02	111.50
53	BA	2245	U	C5-C6-N1	-5.04	120.18	122.70
21	AA	313	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	1245	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	1407	C	C6-N1-C2	-5.04	118.29	120.30
53	BA	177	G	N1-C6-O6	-5.04	116.88	119.90
53	BA	289	G	O4'-C1'-N9	5.04	112.23	108.20
53	BA	343	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	726	G	N1-C6-O6	-5.04	116.88	119.90
53	BA	1411	U	N3-C2-O2	-5.04	118.67	122.20
53	BA	1644	C	O4'-C1'-N1	5.04	112.23	108.20
53	BA	2440	C	N3-C4-C5	5.04	123.91	121.90
53	BA	2643	G	N3-C4-C5	-5.04	126.08	128.60
53	BA	2697	G	N1-C6-O6	-5.04	116.88	119.90
53	BA	2716	C	N3-C2-O2	-5.04	118.38	121.90
21	AA	97	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	562	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	829	G	C8-N9-C4	-5.03	104.39	106.40
21	AA	1131	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	1230	C	N1-C2-O2	5.03	121.92	118.90
21	AA	1272	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	1348	U	C4'-C3'-C2'	-5.03	97.57	102.60
53	BA	846	U	N3-C2-O2	-5.03	118.68	122.20
53	BA	1044	C	N3-C4-N4	-5.03	114.48	118.00
53	BA	1169	A	C6-C5-N7	5.03	135.82	132.30
53	BA	2508	G	O4'-C1'-N9	5.03	112.23	108.20
21	AA	721	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	1290	G	N3-C2-N2	-5.03	116.38	119.90
53	BA	1782	U	N3-C2-O2	-5.03	118.68	122.20
54	BB	33	G	C5-C6-N1	5.03	114.02	111.50
21	AA	329	A	C6-C5-N7	5.03	135.82	132.30
21	AA	1013	G	C5-C6-N1	5.03	114.02	111.50
21	AA	1013	G	N3-C4-C5	-5.03	126.08	128.60
21	AA	1272	G	C8-N9-C4	-5.03	104.39	106.40
22	A1	27	C	N3-C2-O2	-5.03	118.38	121.90
53	BA	425	G	N1-C6-O6	-5.03	116.88	119.90
53	BA	572	A	C4-C5-C6	-5.03	114.48	117.00
53	BA	1840	G	C8-N9-C4	-5.03	104.39	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	BA	2889	C	C6-N1-C2	-5.03	118.29	120.30
21	AA	305	G	N1-C6-O6	-5.03	116.88	119.90
54	BB	56	G	O4'-C4'-C3'	5.03	110.12	106.10
22	A1	76	A	O4'-C1'-N9	5.03	112.22	108.20
53	BA	1737	G	N3-C4-C5	-5.03	126.09	128.60
53	BA	1755	A	C6-C5-N7	5.03	135.82	132.30
53	BA	2199	A	C4-C5-C6	-5.03	114.49	117.00
53	BA	2434	A	C4-C5-C6	-5.03	114.49	117.00
21	AA	688	G	N7-C8-N9	5.03	115.61	113.10
53	BA	1194	A	C4'-C3'-C2'	-5.03	97.58	102.60
53	BA	1467	U	C5-C6-N1	-5.03	120.19	122.70
53	BA	2003	A	C5-C6-N1	5.03	120.21	117.70
53	BA	2298	A	O4'-C1'-N9	5.03	112.22	108.20
53	BA	2427	C	O4'-C4'-C3'	5.03	110.12	106.10
53	BA	2773	C	N3-C2-O2	-5.03	118.38	121.90
21	AA	958	A	C6-C5-N7	5.02	135.82	132.30
53	BA	1191	G	O4'-C1'-N9	5.02	112.22	108.20
53	BA	1723	G	O4'-C1'-N9	5.02	112.22	108.20
21	AA	169	C	N3-C2-O2	-5.02	118.38	121.90
21	AA	849	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	861	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	944	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	988	G	C5-C6-N1	5.02	114.01	111.50
22	A1	15	G	N9-C4-C5	5.02	107.41	105.40
53	BA	364	C	O4'-C1'-N1	5.02	112.22	108.20
53	BA	1524	G	O4'-C1'-N9	5.02	112.22	108.20
53	BA	1648	U	O4'-C1'-N1	5.02	112.22	108.20
53	BA	1755	A	C4-C5-C6	-5.02	114.49	117.00
53	BA	2342	C	O4'-C1'-N1	5.02	112.22	108.20
53	BA	2796	U	C5-C6-N1	-5.02	120.19	122.70
21	AA	110	C	O4'-C1'-N1	5.02	112.22	108.20
53	BA	790	U	N3-C2-O2	-5.02	118.69	122.20
21	AA	15	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	97	G	O4'-C1'-N9	5.02	112.22	108.20
21	AA	279	A	C3'-C2'-C1'	5.02	105.52	101.50
21	AA	791	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	991	U	C5-C6-N1	-5.02	120.19	122.70
53	BA	514	A	C6-C5-N7	5.02	135.81	132.30
53	BA	1063	G	C5-C6-N1	5.02	114.01	111.50
53	BA	1482	G	N3-C4-C5	-5.02	126.09	128.60
53	BA	2069	G	C8-N9-C4	-5.02	104.39	106.40
54	BB	87	U	N3-C2-O2	-5.02	118.69	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	275	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	993	G	N3-C4-N9	5.02	129.01	126.00
21	AA	1009	U	N3-C2-O2	-5.02	118.69	122.20
21	AA	1028	C	O4'-C1'-N1	5.02	112.21	108.20
21	AA	1492	A	C3'-C2'-C1'	-5.02	97.49	101.50
27	BF	6	TYR	CB-CG-CD2	-5.02	117.99	121.00
53	BA	1770	G	C5-C6-N1	5.02	114.01	111.50
53	BA	2359	C	N1-C2-O2	5.02	121.91	118.90
53	BA	2831	G	C5-C6-N1	5.02	114.01	111.50
21	AA	1379	G	O4'-C1'-N9	5.02	112.21	108.20
53	BA	182	A	C4-C5-C6	-5.02	114.49	117.00
21	AA	166	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	418	C	N1-C2-O2	5.01	121.91	118.90
21	AA	1425	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	1513	A	N1-C6-N6	-5.01	115.59	118.60
53	BA	562	U	C4-C5-C6	5.01	122.71	119.70
53	BA	962	G	N7-C8-N9	5.01	115.61	113.10
53	BA	1125	G	C8-N9-C4	-5.01	104.39	106.40
53	BA	1741	C	C6-N1-C2	-5.01	118.29	120.30
53	BA	2212	A	C5-C6-N6	5.01	127.71	123.70
53	BA	2266	A	C6-C5-N7	5.01	135.81	132.30
53	BA	2713	U	C4-C5-C6	5.01	122.71	119.70
21	AA	6	G	C5-C6-N1	5.01	114.01	111.50
21	AA	618	C	O4'-C1'-N1	5.01	112.21	108.20
53	BA	989	G	N9-C4-C5	5.01	107.41	105.40
53	BA	1522	A	O4'-C1'-N9	5.01	112.21	108.20
53	BA	2707	U	C4'-C3'-C2'	-5.01	97.59	102.60
21	AA	107	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	368	U	N3-C2-O2	-5.01	118.69	122.20
21	AA	1516	G	N1-C6-O6	-5.01	116.89	119.90
53	BA	148	U	C5-C6-N1	-5.01	120.19	122.70
53	BA	642	U	N3-C2-O2	-5.01	118.69	122.20
53	BA	802	A	C4-C5-C6	-5.01	114.49	117.00
53	BA	864	G	N3-C4-C5	-5.01	126.09	128.60
53	BA	1698	A	N1-C6-N6	-5.01	115.59	118.60
53	BA	1879	C	N3-C4-C5	5.01	123.90	121.90
53	BA	1982	U	N1-C2-N3	5.01	117.91	114.90
53	BA	2327	A	C4-C5-C6	-5.01	114.49	117.00
53	BA	2539	C	N1-C2-O2	5.01	121.91	118.90
53	BA	2548	U	C5-C6-N1	-5.01	120.19	122.70
53	BA	2663	G	O4'-C1'-N9	5.01	112.21	108.20
21	AA	292	G	C5-C6-N1	5.01	114.00	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	449	G	C8-N9-C4	-5.01	104.40	106.40
21	AA	468	A	O4'-C1'-N9	5.01	112.21	108.20
21	AA	836	G	N3-C4-C5	-5.01	126.09	128.60
21	AA	1283	U	C4-C5-C6	5.01	122.71	119.70
21	AA	1469	C	N1-C2-O2	5.01	121.91	118.90
53	BA	406	G	N1-C6-O6	-5.01	116.89	119.90
53	BA	470	A	N1-C6-N6	-5.01	115.59	118.60
53	BA	790	U	N1-C2-N3	5.01	117.91	114.90
53	BA	817	C	C4'-C3'-C2'	-5.01	97.59	102.60
53	BA	1748	C	O4'-C1'-N1	5.01	112.21	108.20
53	BA	1752	C	N3-C4-C5	5.01	123.90	121.90
53	BA	1768	C	C5'-C4'-O4'	5.01	115.11	109.10
53	BA	1062	G	C3'-C2'-C1'	5.01	105.51	101.50
4	AE	92	ARG	CD-NE-CZ	5.01	130.61	123.60
21	AA	421	U	C5-C6-N1	-5.01	120.20	122.70
21	AA	775	G	N3-C2-N2	-5.01	116.40	119.90
21	AA	1215	G	N1-C6-O6	-5.01	116.90	119.90
53	BA	1433	A	C4-C5-C6	-5.01	114.50	117.00
53	BA	1497	U	C1'-O4'-C4'	-5.01	105.89	109.90
53	BA	1675	C	O4'-C1'-N1	5.01	112.21	108.20
53	BA	2046	G	N3-C4-C5	-5.01	126.10	128.60
21	AA	975	A	C4'-C3'-C2'	-5.00	97.59	102.60
21	AA	675	A	C6-C5-N7	5.00	135.80	132.30
53	BA	287	G	C4'-C3'-C2'	-5.00	97.60	102.60
53	BA	390	U	O4'-C1'-C2'	-5.00	100.80	105.80
53	BA	612	G	N1-C6-O6	-5.00	116.90	119.90
53	BA	912	C	N1-C2-O2	5.00	121.90	118.90
53	BA	1834	U	N3-C2-O2	-5.00	118.70	122.20
53	BA	2057	G	N1-C6-O6	-5.00	116.90	119.90
53	BA	2127	G	C5'-C4'-O4'	5.00	115.10	109.10
53	BA	2404	U	N1-C2-N3	5.00	117.90	114.90
21	AA	666	G	N3-C2-N2	-5.00	116.40	119.90
21	AA	1244	G	N3-C4-C5	-5.00	126.10	128.60
53	BA	199	A	C6-C5-N7	5.00	135.80	132.30
53	BA	493	G	N1-C6-O6	-5.00	116.90	119.90
53	BA	2344	U	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (1028) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	11	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
22	A1	17	U	Sidechain
22	A1	18	G	Sidechain
22	A1	19	G	Sidechain
22	A1	20	G	Sidechain
22	A1	27	C	Sidechain
22	A1	31	C	Sidechain
22	A1	41	A	Sidechain
22	A1	44	G	Sidechain
22	A1	50	G	Sidechain
22	A1	52	G	Sidechain
22	A1	56	C	Sidechain
22	A1	6	A	Sidechain
22	A1	63	G	Sidechain
22	A1	68	C	Sidechain
22	A1	74	C	Sidechain
22	A1	75	C	Sidechain
22	A1	76	A	Sidechain
23	A2	84	G	Sidechain
23	A2	88	U	Sidechain
21	AA	100	G	Sidechain
21	AA	1010	U	Sidechain
21	AA	1019	A	Sidechain
21	AA	1025	U	Sidechain
21	AA	1026	G	Sidechain
21	AA	1038	C	Sidechain
21	AA	1040	U	Sidechain
21	AA	1044	A	Sidechain
21	AA	1049	U	Sidechain
21	AA	1051	C	Sidechain
21	AA	1054	C	Sidechain
21	AA	1055	A	Sidechain
21	AA	1056	U	Sidechain
21	AA	1060	U	Sidechain
21	AA	1064	G	Sidechain
21	AA	1071	C	Sidechain
21	AA	1072	G	Sidechain
21	AA	1077	G	Sidechain
21	AA	1078	U	Sidechain
21	AA	108	G	Sidechain
21	AA	1085	U	Sidechain
21	AA	1086	U	Sidechain
21	AA	1087	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	AA	1089	G	Sidechain
21	AA	109	A	Sidechain
21	AA	1091	U	Sidechain
21	AA	1092	A	Sidechain
21	AA	1094	G	Sidechain
21	AA	1095	U	Sidechain
21	AA	1100	C	Sidechain
21	AA	1118	U	Sidechain
21	AA	1119	C	Sidechain
21	AA	112	G	Sidechain
21	AA	1124	G	Sidechain
21	AA	1125	U	Sidechain
21	AA	1126	U	Sidechain
21	AA	1128	C	Sidechain
21	AA	1133	G	Sidechain
21	AA	1137	C	Sidechain
21	AA	1139	G	Sidechain
21	AA	1141	C	Sidechain
21	AA	1145	A	Sidechain
21	AA	1147	C	Sidechain
21	AA	1149	C	Sidechain
21	AA	116	A	Sidechain
21	AA	1160	G	Sidechain
21	AA	1162	C	Sidechain
21	AA	1166	G	Sidechain
21	AA	1168	U	Sidechain
21	AA	1169	A	Sidechain
21	AA	1170	A	Sidechain
21	AA	1172	C	Sidechain
21	AA	1176	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1179	A	Sidechain
21	AA	1189	U	Sidechain
21	AA	1190	G	Sidechain
21	AA	1191	A	Sidechain
21	AA	120	A	Sidechain
21	AA	1218	C	Sidechain
21	AA	122	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1226	C	Sidechain
21	AA	123	U	Sidechain
21	AA	1231	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	AA	1233	G	Sidechain
21	AA	1237	C	Sidechain
21	AA	1244	G	Sidechain
21	AA	1258	G	Sidechain
21	AA	1266	G	Sidechain
21	AA	1270	G	Sidechain
21	AA	1275	A	Sidechain
21	AA	1279	G	Sidechain
21	AA	128	G	Sidechain
21	AA	1282	C	Sidechain
21	AA	1285	A	Sidechain
21	AA	1295	U	Sidechain
21	AA	1298	U	Sidechain
21	AA	130	A	Sidechain
21	AA	1300	G	Sidechain
21	AA	1308	U	Sidechain
21	AA	1311	A	Sidechain
21	AA	1316	G	Sidechain
21	AA	1317	C	Sidechain
21	AA	1326	U	Sidechain
21	AA	1327	C	Sidechain
21	AA	1328	C	Sidechain
21	AA	1335	U	Sidechain
21	AA	1336	C	Sidechain
21	AA	1337	G	Sidechain
21	AA	1345	U	Sidechain
21	AA	1351	U	Sidechain
21	AA	1352	C	Sidechain
21	AA	1353	G	Sidechain
21	AA	1357	A	Sidechain
21	AA	1358	U	Sidechain
21	AA	136	C	Sidechain
21	AA	1360	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	1367	C	Sidechain
21	AA	1368	A	Sidechain
21	AA	1380	U	Sidechain
21	AA	1387	G	Sidechain
21	AA	1396	A	Sidechain
21	AA	1405	G	Sidechain
21	AA	1417	G	Sidechain
21	AA	1435	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	AA	1436	U	Sidechain
21	AA	1438	G	Sidechain
21	AA	1442	G	Sidechain
21	AA	1444	U	Sidechain
21	AA	1452	C	Sidechain
21	AA	1461	G	Sidechain
21	AA	1471	U	Sidechain
21	AA	1473	G	Sidechain
21	AA	1477	U	Sidechain
21	AA	1482	G	Sidechain
21	AA	149	A	Sidechain
21	AA	1492	A	Sidechain
21	AA	1494	G	Sidechain
21	AA	1495	U	Sidechain
21	AA	1502	A	Sidechain
21	AA	151	A	Sidechain
21	AA	1510	C	Sidechain
21	AA	1519	A	Sidechain
21	AA	1521	C	Sidechain
21	AA	1525	G	Sidechain
21	AA	1527	U	Sidechain
21	AA	1528	U	Sidechain
21	AA	1529	G	Sidechain
21	AA	153	C	Sidechain
21	AA	1532	U	Sidechain
21	AA	159	G	Sidechain
21	AA	163	C	Sidechain
21	AA	165	G	Sidechain
21	AA	167	A	Sidechain
21	AA	173	U	Sidechain
21	AA	175	C	Sidechain
21	AA	179	A	Sidechain
21	AA	183	C	Sidechain
21	AA	187	G	Sidechain
21	AA	193	C	Sidechain
21	AA	194	C	Sidechain
21	AA	21	G	Sidechain
21	AA	217	C	Sidechain
21	AA	218	U	Sidechain
21	AA	223	A	Sidechain
21	AA	227	G	Sidechain
21	AA	229	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	AA	242	G	Sidechain
21	AA	243	A	Sidechain
21	AA	250	A	Sidechain
21	AA	251	G	Sidechain
21	AA	260	G	Sidechain
21	AA	265	G	Sidechain
21	AA	274	A	Sidechain
21	AA	277	C	Sidechain
21	AA	286	C	Sidechain
21	AA	297	G	Sidechain
21	AA	300	A	Sidechain
21	AA	302	G	Sidechain
21	AA	308	C	Sidechain
21	AA	309	A	Sidechain
21	AA	310	G	Sidechain
21	AA	318	G	Sidechain
21	AA	323	U	Sidechain
21	AA	324	G	Sidechain
21	AA	326	G	Sidechain
21	AA	330	C	Sidechain
21	AA	334	C	Sidechain
21	AA	349	A	Sidechain
21	AA	35	G	Sidechain
21	AA	36	C	Sidechain
21	AA	362	G	Sidechain
21	AA	363	A	Sidechain
21	AA	368	U	Sidechain
21	AA	369	G	Sidechain
21	AA	37	U	Sidechain
21	AA	372	C	Sidechain
21	AA	378	G	Sidechain
21	AA	380	G	Sidechain
21	AA	382	A	Sidechain
21	AA	383	A	Sidechain
21	AA	388	G	Sidechain
21	AA	390	U	Sidechain
21	AA	391	G	Sidechain
21	AA	394	G	Sidechain
21	AA	399	G	Sidechain
21	AA	400	C	Sidechain
21	AA	401	C	Sidechain
21	AA	403	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	AA	404	G	Sidechain
21	AA	406	G	Sidechain
21	AA	410	G	Sidechain
21	AA	42	G	Sidechain
21	AA	428	G	Sidechain
21	AA	429	U	Sidechain
21	AA	435	A	Sidechain
21	AA	442	G	Sidechain
21	AA	444	G	Sidechain
21	AA	452	A	Sidechain
21	AA	455	G	Sidechain
21	AA	464	U	Sidechain
21	AA	475	C	Sidechain
21	AA	478	A	Sidechain
21	AA	487	A	Sidechain
21	AA	490	C	Sidechain
21	AA	491	G	Sidechain
21	AA	494	G	Sidechain
21	AA	496	A	Sidechain
21	AA	505	G	Sidechain
21	AA	506	G	Sidechain
21	AA	509	A	Sidechain
21	AA	512	U	Sidechain
21	AA	515	G	Sidechain
21	AA	516	U	Sidechain
21	AA	517	G	Sidechain
21	AA	518	C	Sidechain
21	AA	519	C	Sidechain
21	AA	523	A	Sidechain
21	AA	526	C	Sidechain
21	AA	532	A	Sidechain
21	AA	534	U	Sidechain
21	AA	536	C	Sidechain
21	AA	538	G	Sidechain
21	AA	539	A	Sidechain
21	AA	542	G	Sidechain
21	AA	544	G	Sidechain
21	AA	547	A	Sidechain
21	AA	558	G	Sidechain
21	AA	561	U	Sidechain
21	AA	562	U	Sidechain
21	AA	564	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	AA	579	A	Sidechain
21	AA	59	A	Sidechain
21	AA	598	U	Sidechain
21	AA	6	G	Sidechain
21	AA	606	G	Sidechain
21	AA	608	A	Sidechain
21	AA	611	C	Sidechain
21	AA	624	C	Sidechain
21	AA	63	C	Sidechain
21	AA	635	A	Sidechain
21	AA	637	C	Sidechain
21	AA	641	U	Sidechain
21	AA	642	A	Sidechain
21	AA	643	C	Sidechain
21	AA	646	G	Sidechain
21	AA	647	C	Sidechain
21	AA	652	U	Sidechain
21	AA	657	U	Sidechain
21	AA	664	G	Sidechain
21	AA	665	A	Sidechain
21	AA	666	G	Sidechain
21	AA	67	C	Sidechain
21	AA	671	G	Sidechain
21	AA	676	A	Sidechain
21	AA	68	G	Sidechain
21	AA	690	G	Sidechain
21	AA	691	G	Sidechain
21	AA	698	G	Sidechain
21	AA	703	G	Sidechain
21	AA	716	A	Sidechain
21	AA	720	C	Sidechain
21	AA	722	G	Sidechain
21	AA	729	A	Sidechain
21	AA	734	G	Sidechain
21	AA	74	A	Sidechain
21	AA	741	G	Sidechain
21	AA	752	G	Sidechain
21	AA	754	C	Sidechain
21	AA	765	G	Sidechain
21	AA	772	U	Sidechain
21	AA	774	G	Sidechain
21	AA	777	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	AA	792	A	Sidechain
21	AA	793	U	Sidechain
21	AA	797	C	Sidechain
21	AA	808	C	Sidechain
21	AA	81	A	Sidechain
21	AA	811	C	Sidechain
21	AA	812	G	Sidechain
21	AA	815	A	Sidechain
21	AA	82	G	Sidechain
21	AA	825	A	Sidechain
21	AA	826	C	Sidechain
21	AA	836	G	Sidechain
21	AA	838	G	Sidechain
21	AA	842	U	Sidechain
21	AA	847	G	Sidechain
21	AA	849	G	Sidechain
21	AA	850	U	Sidechain
21	AA	856	C	Sidechain
21	AA	857	C	Sidechain
21	AA	858	G	Sidechain
21	AA	863	U	Sidechain
21	AA	867	G	Sidechain
21	AA	871	U	Sidechain
21	AA	874	G	Sidechain
21	AA	883	C	Sidechain
21	AA	891	U	Sidechain
21	AA	892	A	Sidechain
21	AA	894	G	Sidechain
21	AA	895	G	Sidechain
21	AA	896	C	Sidechain
21	AA	898	G	Sidechain
21	AA	901	A	Sidechain
21	AA	918	A	Sidechain
21	AA	92	U	Sidechain
21	AA	922	G	Sidechain
21	AA	926	G	Sidechain
21	AA	928	G	Sidechain
21	AA	93	U	Sidechain
21	AA	934	C	Sidechain
21	AA	946	A	Sidechain
21	AA	949	A	Sidechain
21	AA	95	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	AA	953	G	Sidechain
21	AA	965	U	Sidechain
21	AA	972	C	Sidechain
21	AA	975	A	Sidechain
21	AA	978	A	Sidechain
21	AA	98	A	Sidechain
21	AA	984	C	Sidechain
21	AA	987	G	Sidechain
21	AA	99	C	Sidechain
21	AA	997	U	Sidechain
21	AA	999	C	Sidechain
18	AS	74	ALA	Peptide
53	BA	1001	A	Sidechain
53	BA	1013	C	Sidechain
53	BA	1014	A	Sidechain
53	BA	1016	G	Sidechain
53	BA	102	U	Sidechain
53	BA	1022	G	Sidechain
53	BA	1025	G	Sidechain
53	BA	1036	G	Sidechain
53	BA	1038	G	Sidechain
53	BA	1044	C	Sidechain
53	BA	1051	G	Sidechain
53	BA	1060	U	Sidechain
53	BA	1062	G	Sidechain
53	BA	1066	U	Sidechain
53	BA	1069	A	Sidechain
53	BA	1075	C	Sidechain
53	BA	108	G	Sidechain
53	BA	1087	G	Sidechain
53	BA	1088	A	Sidechain
53	BA	1091	G	Sidechain
53	BA	1094	U	Sidechain
53	BA	1106	G	Sidechain
53	BA	1109	C	Sidechain
53	BA	1118	C	Sidechain
53	BA	1126	A	Sidechain
53	BA	1127	A	Sidechain
53	BA	1139	G	Sidechain
53	BA	1147	A	Sidechain
53	BA	1149	G	Sidechain
53	BA	1151	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	1154	G	Sidechain
53	BA	1162	G	Sidechain
53	BA	1182	G	Sidechain
53	BA	1183	U	Sidechain
53	BA	1187	G	Sidechain
53	BA	1188	U	Sidechain
53	BA	1190	G	Sidechain
53	BA	1191	G	Sidechain
53	BA	1195	G	Sidechain
53	BA	1196	C	Sidechain
53	BA	1199	U	Sidechain
53	BA	1201	U	Sidechain
53	BA	1215	G	Sidechain
53	BA	1220	G	Sidechain
53	BA	1223	G	Sidechain
53	BA	1224	U	Sidechain
53	BA	1227	G	Sidechain
53	BA	1231	U	Sidechain
53	BA	1234	U	Sidechain
53	BA	1235	G	Sidechain
53	BA	1236	G	Sidechain
53	BA	1243	C	Sidechain
53	BA	1244	A	Sidechain
53	BA	125	A	Sidechain
53	BA	126	A	Sidechain
53	BA	1266	G	Sidechain
53	BA	1268	A	Sidechain
53	BA	1270	C	Sidechain
53	BA	1271	G	Sidechain
53	BA	1272	A	Sidechain
53	BA	1274	A	Sidechain
53	BA	1276	A	Sidechain
53	BA	1279	G	Sidechain
53	BA	1283	G	Sidechain
53	BA	1286	A	Sidechain
53	BA	1291	C	Sidechain
53	BA	1292	G	Sidechain
53	BA	1308	A	Sidechain
53	BA	1310	G	Sidechain
53	BA	1311	G	Sidechain
53	BA	1317	G	Sidechain
53	BA	1320	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	1322	A	Sidechain
53	BA	1324	G	Sidechain
53	BA	1325	U	Sidechain
53	BA	1330	C	Sidechain
53	BA	1339	G	Sidechain
53	BA	1343	G	Sidechain
53	BA	1344	U	Sidechain
53	BA	1359	A	Sidechain
53	BA	1360	G	Sidechain
53	BA	1366	A	Sidechain
53	BA	137	U	Sidechain
53	BA	1370	C	Sidechain
53	BA	1376	C	Sidechain
53	BA	1378	A	Sidechain
53	BA	1392	A	Sidechain
53	BA	1394	U	Sidechain
53	BA	1395	A	Sidechain
53	BA	1396	U	Sidechain
53	BA	1399	C	Sidechain
53	BA	1410	G	Sidechain
53	BA	1425	G	Sidechain
53	BA	1426	G	Sidechain
53	BA	1429	G	Sidechain
53	BA	143	C	Sidechain
53	BA	1439	A	Sidechain
53	BA	1441	G	Sidechain
53	BA	1444	G	Sidechain
53	BA	1445	G	Sidechain
53	BA	1459	G	Sidechain
53	BA	1460	U	Sidechain
53	BA	1469	A	Sidechain
53	BA	147	C	Sidechain
53	BA	1472	C	Sidechain
53	BA	1476	U	Sidechain
53	BA	1478	G	Sidechain
53	BA	1490	A	Sidechain
53	BA	1492	G	Sidechain
53	BA	1494	A	Sidechain
53	BA	1514	G	Sidechain
53	BA	1519	G	Sidechain
53	BA	1522	A	Sidechain
53	BA	1523	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	1526	C	Sidechain
53	BA	1536	C	Sidechain
53	BA	1540	G	Sidechain
53	BA	1543	G	Sidechain
53	BA	1546	G	Sidechain
53	BA	1551	A	Sidechain
53	BA	1552	A	Sidechain
53	BA	1555	G	Sidechain
53	BA	1560	G	Sidechain
53	BA	1561	C	Sidechain
53	BA	1562	U	Sidechain
53	BA	1563	U	Sidechain
53	BA	1564	C	Sidechain
53	BA	1565	C	Sidechain
53	BA	1567	G	Sidechain
53	BA	1570	A	Sidechain
53	BA	1573	G	Sidechain
53	BA	1585	C	Sidechain
53	BA	159	G	Sidechain
53	BA	1595	C	Sidechain
53	BA	1599	U	Sidechain
53	BA	160	A	Sidechain
53	BA	1600	C	Sidechain
53	BA	1601	G	Sidechain
53	BA	1602	U	Sidechain
53	BA	1604	C	Sidechain
53	BA	1605	C	Sidechain
53	BA	1606	C	Sidechain
53	BA	1614	A	Sidechain
53	BA	1619	G	Sidechain
53	BA	1624	U	Sidechain
53	BA	163	C	Sidechain
53	BA	1631	G	Sidechain
53	BA	1632	A	Sidechain
53	BA	1641	A	Sidechain
53	BA	1642	G	Sidechain
53	BA	1653	G	Sidechain
53	BA	1655	A	Sidechain
53	BA	1656	C	Sidechain
53	BA	1658	C	Sidechain
53	BA	1671	U	Sidechain
53	BA	1673	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	1695	G	Sidechain
53	BA	1700	A	Sidechain
53	BA	1703	G	Sidechain
53	BA	1707	G	Sidechain
53	BA	1709	U	Sidechain
53	BA	1710	G	Sidechain
53	BA	1713	A	Sidechain
53	BA	1715	G	Sidechain
53	BA	1718	G	Sidechain
53	BA	1721	G	Sidechain
53	BA	1734	G	Sidechain
53	BA	1735	A	Sidechain
53	BA	1740	G	Sidechain
53	BA	1745	A	Sidechain
53	BA	1747	U	Sidechain
53	BA	1748	C	Sidechain
53	BA	1750	G	Sidechain
53	BA	1753	G	Sidechain
53	BA	1757	A	Sidechain
53	BA	1766	G	Sidechain
53	BA	177	G	Sidechain
53	BA	1773	A	Sidechain
53	BA	1777	U	Sidechain
53	BA	1779	U	Sidechain
53	BA	178	G	Sidechain
53	BA	1784	A	Sidechain
53	BA	179	C	Sidechain
53	BA	1794	A	Sidechain
53	BA	1797	G	Sidechain
53	BA	18	U	Sidechain
53	BA	1802	A	Sidechain
53	BA	1805	A	Sidechain
53	BA	181	A	Sidechain
53	BA	1810	A	Sidechain
53	BA	1811	G	Sidechain
53	BA	1816	C	Sidechain
53	BA	1817	G	Sidechain
53	BA	182	A	Sidechain
53	BA	1820	U	Sidechain
53	BA	1826	G	Sidechain
53	BA	1827	U	Sidechain
53	BA	183	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	1830	C	Sidechain
53	BA	1831	G	Sidechain
53	BA	1834	U	Sidechain
53	BA	1841	U	Sidechain
53	BA	1845	G	Sidechain
53	BA	1846	G	Sidechain
53	BA	1847	A	Sidechain
53	BA	1849	G	Sidechain
53	BA	1857	G	Sidechain
53	BA	1858	A	Sidechain
53	BA	186	G	Sidechain
53	BA	1861	G	Sidechain
53	BA	1867	G	Sidechain
53	BA	1869	G	Sidechain
53	BA	187	G	Sidechain
53	BA	1877	A	Sidechain
53	BA	1883	U	Sidechain
53	BA	1885	A	Sidechain
53	BA	1886	U	Sidechain
53	BA	19	A	Sidechain
53	BA	1901	A	Sidechain
53	BA	1910	G	Sidechain
53	BA	1918	A	Sidechain
53	BA	1920	C	Sidechain
53	BA	1925	C	Sidechain
53	BA	1927	A	Sidechain
53	BA	1932	A	Sidechain
53	BA	1937	A	Sidechain
53	BA	1938	A	Sidechain
53	BA	194	G	Sidechain
53	BA	1951	U	Sidechain
53	BA	1954	G	Sidechain
53	BA	1955	U	Sidechain
53	BA	1964	G	Sidechain
53	BA	1971	U	Sidechain
53	BA	1982	U	Sidechain
53	BA	1987	A	Sidechain
53	BA	199	A	Sidechain
53	BA	1993	U	Sidechain
53	BA	1996	C	Sidechain
53	BA	2002	G	Sidechain
53	BA	2005	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	2006	C	Sidechain
53	BA	2009	A	Sidechain
53	BA	201	C	Sidechain
53	BA	2016	U	Sidechain
53	BA	202	U	Sidechain
53	BA	2029	G	Sidechain
53	BA	2034	U	Sidechain
53	BA	2035	G	Sidechain
53	BA	2048	G	Sidechain
53	BA	205	G	Sidechain
53	BA	2052	A	Sidechain
53	BA	2057	G	Sidechain
53	BA	2061	G	Sidechain
53	BA	2062	A	Sidechain
53	BA	2064	C	Sidechain
53	BA	207	A	Sidechain
53	BA	2078	C	Sidechain
53	BA	208	C	Sidechain
53	BA	2080	A	Sidechain
53	BA	2093	G	Sidechain
53	BA	2094	A	Sidechain
53	BA	2101	A	Sidechain
53	BA	2103	C	Sidechain
53	BA	2109	U	Sidechain
53	BA	2126	A	Sidechain
53	BA	2132	U	Sidechain
53	BA	2133	G	Sidechain
53	BA	2136	G	Sidechain
53	BA	2137	U	Sidechain
53	BA	214	G	Sidechain
53	BA	2147	A	Sidechain
53	BA	215	G	Sidechain
53	BA	2154	A	Sidechain
53	BA	2157	G	Sidechain
53	BA	2158	A	Sidechain
53	BA	2159	G	Sidechain
53	BA	2160	C	Sidechain
53	BA	2163	A	Sidechain
53	BA	2165	C	Sidechain
53	BA	2168	G	Sidechain
53	BA	2178	C	Sidechain
53	BA	2181	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	2196	C	Sidechain
53	BA	2197	U	Sidechain
53	BA	220	G	Sidechain
53	BA	2206	C	Sidechain
53	BA	2207	C	Sidechain
53	BA	2218	G	Sidechain
53	BA	2219	U	Sidechain
53	BA	223	A	Sidechain
53	BA	2234	G	Sidechain
53	BA	2238	G	Sidechain
53	BA	2246	G	Sidechain
53	BA	2259	U	Sidechain
53	BA	2260	C	Sidechain
53	BA	2266	A	Sidechain
53	BA	2267	A	Sidechain
53	BA	227	A	Sidechain
53	BA	2279	G	Sidechain
53	BA	2280	G	Sidechain
53	BA	2282	G	Sidechain
53	BA	2286	G	Sidechain
53	BA	2288	A	Sidechain
53	BA	2292	U	Sidechain
53	BA	2296	U	Sidechain
53	BA	2299	U	Sidechain
53	BA	2303	G	Sidechain
53	BA	2310	C	Sidechain
53	BA	2314	A	Sidechain
53	BA	2321	U	Sidechain
53	BA	2324	U	Sidechain
53	BA	2338	C	Sidechain
53	BA	2345	G	Sidechain
53	BA	2349	G	Sidechain
53	BA	235	U	Sidechain
53	BA	2357	G	Sidechain
53	BA	2361	G	Sidechain
53	BA	2375	G	Sidechain
53	BA	2379	G	Sidechain
53	BA	2380	C	Sidechain
53	BA	2385	C	Sidechain
53	BA	2387	U	Sidechain
53	BA	239	C	Sidechain
53	BA	2391	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	2393	U	Sidechain
53	BA	24	G	Sidechain
53	BA	2401	U	Sidechain
53	BA	2402	U	Sidechain
53	BA	2406	A	Sidechain
53	BA	241	A	Sidechain
53	BA	2410	G	Sidechain
53	BA	2413	G	Sidechain
53	BA	2416	C	Sidechain
53	BA	2421	G	Sidechain
53	BA	2425	A	Sidechain
53	BA	2428	G	Sidechain
53	BA	2429	G	Sidechain
53	BA	243	U	Sidechain
53	BA	2433	A	Sidechain
53	BA	2434	A	Sidechain
53	BA	2439	A	Sidechain
53	BA	244	A	Sidechain
53	BA	2444	G	Sidechain
53	BA	2448	A	Sidechain
53	BA	2452	C	Sidechain
53	BA	2453	A	Sidechain
53	BA	2455	G	Sidechain
53	BA	2456	C	Sidechain
53	BA	2458	G	Sidechain
53	BA	246	C	Sidechain
53	BA	2460	U	Sidechain
53	BA	2464	G	Sidechain
53	BA	2465	C	Sidechain
53	BA	2469	A	Sidechain
53	BA	2470	G	Sidechain
53	BA	2475	C	Sidechain
53	BA	2476	A	Sidechain
53	BA	2478	A	Sidechain
53	BA	2481	G	Sidechain
53	BA	2485	G	Sidechain
53	BA	2489	U	Sidechain
53	BA	2498	C	Sidechain
53	BA	250	G	Sidechain
53	BA	2502	G	Sidechain
53	BA	2506	U	Sidechain
53	BA	2507	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	2516	A	Sidechain
53	BA	2517	C	Sidechain
53	BA	252	G	Sidechain
53	BA	2523	G	Sidechain
53	BA	2537	U	Sidechain
53	BA	2540	C	Sidechain
53	BA	2552	U	Sidechain
53	BA	256	A	Sidechain
53	BA	2560	A	Sidechain
53	BA	2564	A	Sidechain
53	BA	2566	A	Sidechain
53	BA	2567	G	Sidechain
53	BA	2576	G	Sidechain
53	BA	2582	G	Sidechain
53	BA	2583	G	Sidechain
53	BA	2585	U	Sidechain
53	BA	2586	U	Sidechain
53	BA	2587	A	Sidechain
53	BA	2595	G	Sidechain
53	BA	26	G	Sidechain
53	BA	2603	G	Sidechain
53	BA	2606	C	Sidechain
53	BA	2607	G	Sidechain
53	BA	2608	G	Sidechain
53	BA	2613	U	Sidechain
53	BA	2618	G	Sidechain
53	BA	2636	C	Sidechain
53	BA	2638	G	Sidechain
53	BA	264	C	Sidechain
53	BA	2642	G	Sidechain
53	BA	2645	G	Sidechain
53	BA	265	A	Sidechain
53	BA	2659	G	Sidechain
53	BA	2661	G	Sidechain
53	BA	2666	C	Sidechain
53	BA	2668	G	Sidechain
53	BA	268	C	Sidechain
53	BA	2680	U	Sidechain
53	BA	2685	G	Sidechain
53	BA	2688	G	Sidechain
53	BA	27	G	Sidechain
53	BA	2700	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	2709	G	Sidechain
53	BA	2715	C	Sidechain
53	BA	272	A	Sidechain
53	BA	2726	A	Sidechain
53	BA	273	G	Sidechain
53	BA	2733	A	Sidechain
53	BA	2747	G	Sidechain
53	BA	275	C	Sidechain
53	BA	2753	A	Sidechain
53	BA	2755	C	Sidechain
53	BA	2756	U	Sidechain
53	BA	2757	A	Sidechain
53	BA	2763	G	Sidechain
53	BA	2765	A	Sidechain
53	BA	2767	C	Sidechain
53	BA	2771	C	Sidechain
53	BA	2773	C	Sidechain
53	BA	2797	U	Sidechain
53	BA	2798	U	Sidechain
53	BA	28	A	Sidechain
53	BA	2804	U	Sidechain
53	BA	2807	U	Sidechain
53	BA	2812	G	Sidechain
53	BA	2813	A	Sidechain
53	BA	2816	G	Sidechain
53	BA	2822	G	Sidechain
53	BA	2824	C	Sidechain
53	BA	2825	G	Sidechain
53	BA	2832	U	Sidechain
53	BA	2835	A	Sidechain
53	BA	2836	U	Sidechain
53	BA	2838	G	Sidechain
53	BA	2839	G	Sidechain
53	BA	2843	G	Sidechain
53	BA	2846	G	Sidechain
53	BA	2847	U	Sidechain
53	BA	285	G	Sidechain
53	BA	2853	C	Sidechain
53	BA	2857	G	Sidechain
53	BA	2858	C	Sidechain
53	BA	2859	G	Sidechain
53	BA	2871	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	2872	A	Sidechain
53	BA	2873	A	Sidechain
53	BA	2874	C	Sidechain
53	BA	2875	C	Sidechain
53	BA	2879	A	Sidechain
53	BA	2883	A	Sidechain
53	BA	2884	U	Sidechain
53	BA	2885	G	Sidechain
53	BA	2887	A	Sidechain
53	BA	2892	G	Sidechain
53	BA	2893	A	Sidechain
53	BA	2895	G	Sidechain
53	BA	2897	U	Sidechain
53	BA	293	U	Sidechain
53	BA	298	G	Sidechain
53	BA	301	G	Sidechain
53	BA	307	G	Sidechain
53	BA	308	G	Sidechain
53	BA	310	A	Sidechain
53	BA	313	G	Sidechain
53	BA	327	G	Sidechain
53	BA	330	A	Sidechain
53	BA	332	A	Sidechain
53	BA	333	G	Sidechain
53	BA	339	U	Sidechain
53	BA	345	A	Sidechain
53	BA	350	G	Sidechain
53	BA	352	A	Sidechain
53	BA	356	G	Sidechain
53	BA	357	C	Sidechain
53	BA	359	G	Sidechain
53	BA	360	U	Sidechain
53	BA	361	G	Sidechain
53	BA	362	A	Sidechain
53	BA	370	G	Sidechain
53	BA	372	G	Sidechain
53	BA	373	U	Sidechain
53	BA	374	A	Sidechain
53	BA	376	G	Sidechain
53	BA	379	G	Sidechain
53	BA	389	G	Sidechain
53	BA	390	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	394	C	Sidechain
53	BA	395	U	Sidechain
53	BA	397	U	Sidechain
53	BA	405	U	Sidechain
53	BA	407	G	Sidechain
53	BA	418	C	Sidechain
53	BA	422	A	Sidechain
53	BA	426	C	Sidechain
53	BA	428	A	Sidechain
53	BA	43	G	Sidechain
53	BA	432	A	Sidechain
53	BA	446	G	Sidechain
53	BA	454	A	Sidechain
53	BA	458	G	Sidechain
53	BA	461	C	Sidechain
53	BA	463	G	Sidechain
53	BA	464	U	Sidechain
53	BA	469	G	Sidechain
53	BA	474	G	Sidechain
53	BA	475	C	Sidechain
53	BA	477	A	Sidechain
53	BA	481	G	Sidechain
53	BA	484	C	Sidechain
53	BA	49	A	Sidechain
53	BA	498	G	Sidechain
53	BA	500	G	Sidechain
53	BA	501	A	Sidechain
53	BA	502	A	Sidechain
53	BA	503	A	Sidechain
53	BA	505	A	Sidechain
53	BA	506	G	Sidechain
53	BA	512	G	Sidechain
53	BA	517	C	Sidechain
53	BA	520	G	Sidechain
53	BA	521	U	Sidechain
53	BA	527	C	Sidechain
53	BA	530	G	Sidechain
53	BA	533	G	Sidechain
53	BA	536	G	Sidechain
53	BA	539	G	Sidechain
53	BA	545	U	Sidechain
53	BA	547	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	548	G	Sidechain
53	BA	549	G	Sidechain
53	BA	559	G	Sidechain
53	BA	56	A	Sidechain
53	BA	570	G	Sidechain
53	BA	571	U	Sidechain
53	BA	575	A	Sidechain
53	BA	576	U	Sidechain
53	BA	577	G	Sidechain
53	BA	578	G	Sidechain
53	BA	58	G	Sidechain
53	BA	587	C	Sidechain
53	BA	597	G	Sidechain
53	BA	599	A	Sidechain
53	BA	603	A	Sidechain
53	BA	606	U	Sidechain
53	BA	607	U	Sidechain
53	BA	608	A	Sidechain
53	BA	610	C	Sidechain
53	BA	611	C	Sidechain
53	BA	614	A	Sidechain
53	BA	62	U	Sidechain
53	BA	620	G	Sidechain
53	BA	621	A	Sidechain
53	BA	629	G	Sidechain
53	BA	630	G	Sidechain
53	BA	632	A	Sidechain
53	BA	633	A	Sidechain
53	BA	643	A	Sidechain
53	BA	651	G	Sidechain
53	BA	652	U	Sidechain
53	BA	654	A	Sidechain
53	BA	661	A	Sidechain
53	BA	665	U	Sidechain
53	BA	669	G	Sidechain
53	BA	672	C	Sidechain
53	BA	673	C	Sidechain
53	BA	674	G	Sidechain
53	BA	675	A	Sidechain
53	BA	68	G	Sidechain
53	BA	683	U	Sidechain
53	BA	697	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	699	A	Sidechain
53	BA	70	G	Sidechain
53	BA	700	G	Sidechain
53	BA	701	G	Sidechain
53	BA	704	G	Sidechain
53	BA	712	G	Sidechain
53	BA	714	U	Sidechain
53	BA	716	A	Sidechain
53	BA	718	A	Sidechain
53	BA	726	G	Sidechain
53	BA	736	C	Sidechain
53	BA	738	G	Sidechain
53	BA	749	A	Sidechain
53	BA	75	G	Sidechain
53	BA	750	A	Sidechain
53	BA	752	A	Sidechain
53	BA	753	A	Sidechain
53	BA	76	C	Sidechain
53	BA	763	G	Sidechain
53	BA	765	C	Sidechain
53	BA	772	C	Sidechain
53	BA	775	G	Sidechain
53	BA	780	G	Sidechain
53	BA	783	A	Sidechain
53	BA	784	G	Sidechain
53	BA	785	G	Sidechain
53	BA	789	A	Sidechain
53	BA	797	G	Sidechain
53	BA	798	G	Sidechain
53	BA	800	A	Sidechain
53	BA	801	G	Sidechain
53	BA	805	G	Sidechain
53	BA	806	C	Sidechain
53	BA	810	U	Sidechain
53	BA	818	G	Sidechain
53	BA	828	U	Sidechain
53	BA	831	G	Sidechain
53	BA	834	G	Sidechain
53	BA	835	C	Sidechain
53	BA	841	G	Sidechain
53	BA	848	C	Sidechain
53	BA	851	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
53	BA	852	U	Sidechain
53	BA	856	G	Sidechain
53	BA	857	G	Sidechain
53	BA	858	G	Sidechain
53	BA	86	G	Sidechain
53	BA	861	A	Sidechain
53	BA	862	G	Sidechain
53	BA	863	A	Sidechain
53	BA	882	G	Sidechain
53	BA	883	G	Sidechain
53	BA	892	A	Sidechain
53	BA	896	A	Sidechain
53	BA	897	C	Sidechain
53	BA	900	A	Sidechain
53	BA	907	G	Sidechain
53	BA	912	C	Sidechain
53	BA	916	G	Sidechain
53	BA	920	A	Sidechain
53	BA	923	G	Sidechain
53	BA	932	U	Sidechain
53	BA	934	U	Sidechain
53	BA	948	C	Sidechain
53	BA	956	G	Sidechain
53	BA	959	A	Sidechain
53	BA	964	C	Sidechain
53	BA	969	G	Sidechain
53	BA	971	G	Sidechain
53	BA	972	A	Sidechain
53	BA	976	G	Sidechain
53	BA	979	A	Sidechain
53	BA	982	C	Sidechain
53	BA	988	A	Sidechain
53	BA	989	G	Sidechain
53	BA	999	U	Sidechain
54	BB	10	G	Sidechain
54	BB	105	G	Sidechain
54	BB	107	G	Sidechain
54	BB	112	G	Sidechain
54	BB	117	G	Sidechain
54	BB	13	G	Sidechain
54	BB	14	U	Sidechain
54	BB	2	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
54	BB	21	G	Sidechain
54	BB	25	U	Sidechain
54	BB	27	C	Sidechain
54	BB	35	C	Sidechain
54	BB	4	C	Sidechain
54	BB	40	U	Sidechain
54	BB	50	A	Sidechain
54	BB	56	G	Sidechain
54	BB	60	C	Sidechain
54	BB	61	G	Sidechain
54	BB	64	G	Sidechain
54	BB	73	A	Sidechain
54	BB	75	G	Sidechain
54	BB	80	U	Sidechain
54	BB	81	G	Sidechain
54	BB	83	G	Sidechain
54	BB	85	G	Sidechain
54	BB	89	U	Sidechain
54	BB	93	C	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	1	0
2	AC	1625	0	1699	2	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	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	AP	639	0	656	0	0
16	AQ	652	0	695	1	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16108	7	0
22	A1	1627	0	808	0	0
23	A2	309	0	158	0	0
24	BC	2083	0	2157	0	0
25	BD	1565	0	1616	0	0
26	BE	1552	0	1619	0	0
27	BF	1420	0	1460	1	0
28	BG	1323	0	1374	0	0
29	BH	1111	0	1148	0	0
30	BI	1032	0	1088	0	0
31	BJ	1129	0	1162	1	0
32	BK	939	0	1012	1	0
33	BL	1045	0	1117	2	0
34	BM	1074	0	1157	1	0
35	BN	961	0	1000	0	0
36	BO	892	0	923	0	0
37	BP	917	0	965	0	0
38	BQ	947	0	1022	0	0
39	BR	816	0	839	1	0
40	BS	857	0	922	0	0
41	BT	739	0	807	0	0
42	BU	780	0	834	0	0
43	BV	753	0	780	0	0
44	BW	599	0	614	0	0
45	BX	625	0	655	0	0
46	BY	509	0	543	0	0
47	BZ	449	0	491	1	0
48	B0	444	0	461	0	0
49	B1	413	0	444	1	0
50	B2	377	0	418	0	0
51	B3	504	0	574	1	0
52	B4	302	0	343	0	0
53	BA	62317	0	30428	10	0
54	BB	2504	0	1247	0	0
55	B5	1658	0	1751	0	0
56	A1	7	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	BA	10	0	10	1	0
All	All	146011	0	97443	27	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 (27) 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)
53:BA:2644:G:H2'	53:BA:2645:G:C8	2.46	0.51
53:BA:1287:A:H2'	53:BA:1288:G:C2	2.47	0.50
49:B1:9:LYS:HE3	49:B1:19:PHE:CD2	2.49	0.48
21:AA:292:G:C5	21:AA:293:G:H1'	2.48	0.47
33:BL:54:GLN:HE21	53:BA:2428:G:N2	2.11	0.47
53:BA:2506:U:C4'	57:BA:3001:FME:HE3	2.45	0.46
31:BJ:47:HIS:CG	53:BA:536:G:H21	2.34	0.45
32:BK:107:LEU:H	32:BK:107:LEU:HD23	1.82	0.45
53:BA:752:A:H2'	53:BA:1781:U:C5	2.52	0.44
21:AA:35:G:H2'	21:AA:36:C:C6	2.53	0.44
53:BA:1646:C:H3'	53:BA:1647:U:C5'	2.48	0.44
53:BA:1570:A:H2'	53:BA:1571:A:C8	2.52	0.44
27:BF:107:VAL:H	27:BF:108:PRO:CD	2.30	0.44
21:AA:235:C:H2'	21:AA:236:A:C8	2.54	0.43
34:BM:14:LYS:HE3	53:BA:956:G:C8	2.54	0.43
47:BZ:28:LEU:H	47:BZ:28:LEU:HD23	1.84	0.43
16:AQ:67:SER:HB2	16:AQ:70:LYS:HE2	2.01	0.42
1:AB:185:ILE:HD12	1:AB:185:ILE:N	2.34	0.42
2:AC:149:LYS:HE3	2:AC:200:TRP:CZ3	2.55	0.42
2:AC:149:LYS:HE3	2:AC:200:TRP:CE3	2.54	0.42
21:AA:989:U:H2'	21:AA:990:C:C6	2.55	0.42
21:AA:420:U:H2'	21:AA:422:C:C5	2.55	0.42
39:BR:24:LYS:HE2	39:BR:66:HIS:CG	2.55	0.42
33:BL:2:ARG:HA	33:BL:3:LEU:O	2.18	0.42
21:AA:920:U:H2'	21:AA:921:U:C6	2.55	0.41
21:AA:1053:G:H2'	21:AA:1199:U:C5	2.55	0.41
51:B3:51:LYS:HE3	53:BA:938:G:OP1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	218/220 (99%)	193 (88%)	24 (11%)	1 (0%)	29	69
2	AC	205/208 (99%)	186 (91%)	11 (5%)	8 (4%)	3	23
3	AD	203/206 (98%)	192 (95%)	9 (4%)	2 (1%)	15	55
4	AE	150/152 (99%)	141 (94%)	5 (3%)	4 (3%)	5	31
5	AF	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	15	55
6	AG	150/152 (99%)	138 (92%)	8 (5%)	4 (3%)	5	31
7	AH	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	19	60
8	AI	126/128 (98%)	115 (91%)	9 (7%)	2 (2%)	9	44
9	AJ	98/100 (98%)	87 (89%)	8 (8%)	3 (3%)	4	27
10	AK	116/118 (98%)	108 (93%)	6 (5%)	2 (2%)	9	42
11	AL	121/124 (98%)	111 (92%)	6 (5%)	4 (3%)	4	26
12	AM	112/115 (97%)	94 (84%)	15 (13%)	3 (3%)	5	31
13	AN	98/101 (97%)	89 (91%)	7 (7%)	2 (2%)	7	38
14	AO	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
15	AP	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	12	48
17	AR	55/57 (96%)	51 (93%)	2 (4%)	2 (4%)	3	25
18	AS	79/81 (98%)	73 (92%)	3 (4%)	3 (4%)	3	24
19	AT	84/86 (98%)	74 (88%)	7 (8%)	3 (4%)	3	25
20	AU	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
24	BC	270/273 (99%)	245 (91%)	17 (6%)	8 (3%)	4	28
25	BD	207/209 (99%)	174 (84%)	21 (10%)	12 (6%)	1	18
26	BE	199/201 (99%)	182 (92%)	13 (6%)	4 (2%)	7	38
27	BF	176/179 (98%)	143 (81%)	26 (15%)	7 (4%)	3	23
28	BG	174/177 (98%)	152 (87%)	18 (10%)	4 (2%)	6	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	BH	147/149 (99%)	131 (89%)	15 (10%)	1 (1%)	22 63
30	BI	139/142 (98%)	128 (92%)	11 (8%)	0	100 100
31	BJ	140/142 (99%)	129 (92%)	6 (4%)	5 (4%)	3 25
32	BK	121/123 (98%)	105 (87%)	11 (9%)	5 (4%)	3 23
33	BL	141/144 (98%)	117 (83%)	14 (10%)	10 (7%)	1 14
34	BM	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	10 46
35	BN	119/121 (98%)	103 (87%)	13 (11%)	3 (2%)	5 32
36	BO	114/117 (97%)	108 (95%)	6 (5%)	0	100 100
37	BP	112/115 (97%)	99 (88%)	10 (9%)	3 (3%)	5 31
38	BQ	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	9 42
39	BR	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	7 38
40	BS	108/110 (98%)	97 (90%)	10 (9%)	1 (1%)	17 57
41	BT	92/94 (98%)	73 (79%)	11 (12%)	8 (9%)	1 11
42	BU	101/104 (97%)	86 (85%)	10 (10%)	5 (5%)	2 20
43	BV	92/94 (98%)	82 (89%)	8 (9%)	2 (2%)	6 35
44	BW	78/80 (98%)	62 (80%)	8 (10%)	8 (10%)	0 8
45	BX	75/79 (95%)	64 (85%)	8 (11%)	3 (4%)	3 23
46	BY	61/63 (97%)	55 (90%)	4 (7%)	2 (3%)	4 26
47	BZ	56/59 (95%)	50 (89%)	5 (9%)	1 (2%)	8 40
48	B0	54/57 (95%)	50 (93%)	3 (6%)	1 (2%)	8 38
49	B1	50/52 (96%)	45 (90%)	4 (8%)	1 (2%)	7 38
50	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6 34
51	B3	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
52	B4	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2 19
55	B5	221/234 (94%)	211 (96%)	8 (4%)	2 (1%)	17 57
All	All	5876/6008 (98%)	5278 (90%)	447 (8%)	151 (3%)	8 31

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	105	ILE
24	BC	206	LYS
25	BD	9	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	BD	150	GLN
25	BD	188	LEU
27	BF	12	VAL
33	BL	57	LEU
38	BQ	87	VAL
41	BT	81	LYS
42	BU	43	LYS
44	BW	37	VAL
46	BY	2	LYS
48	B0	24	VAL
49	B1	50	GLU
50	B2	15	SER
2	AC	4	VAL
2	AC	163	ARG
2	AC	189	HIS
3	AD	35	GLN
3	AD	84	ASN
4	AE	89	THR
6	AG	113	LYS
7	AH	105	THR
8	AI	120	ALA
10	AK	126	ARG
12	AM	85	TYR
13	AN	100	SER
16	AQ	39	ARG
18	AS	77	ARG
19	AT	84	LYS
25	BD	2	ILE
25	BD	22	ILE
25	BD	51	THR
25	BD	114	LYS
25	BD	170	VAL
27	BF	107	VAL
27	BF	135	ILE
27	BF	136	ILE
28	BG	22	VAL
28	BG	57	TYR
31	BJ	47	HIS
31	BJ	112	GLY
33	BL	4	ASN
33	BL	29	LYS
33	BL	30	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	BN	11	ASN
37	BP	74	GLN
39	BR	44	GLY
41	BT	63	VAL
42	BU	51	LEU
45	BX	17	ARG
46	BY	7	ARG
47	BZ	31	ILE
52	B4	4	ARG
52	B4	16	ILE
1	AB	128	LEU
6	AG	56	SER
9	AJ	75	ASP
11	AL	78	VAL
12	AM	23	GLY
12	AM	42	VAL
17	AR	20	ILE
17	AR	47	ARG
24	BC	19	VAL
24	BC	153	LEU
24	BC	228	ASP
25	BD	106	LYS
25	BD	119	ALA
26	BE	90	GLN
26	BE	165	HIS
27	BF	72	SER
31	BJ	81	ILE
32	BK	32	TYR
33	BL	55	MET
33	BL	75	ALA
35	BN	10	LEU
35	BN	103	ARG
39	BR	53	PHE
41	BT	28	ASN
41	BT	68	LYS
41	BT	88	LYS
43	BV	71	LYS
44	BW	10	ARG
44	BW	11	ASN
44	BW	14	ASP
44	BW	51	GLY
45	BX	21	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AC	180	ASP
2	AC	195	ILE
6	AG	129	ASN
8	AI	55	ASP
9	AJ	33	GLY
11	AL	33	CYS
11	AL	117	GLY
18	AS	6	LYS
19	AT	43	LYS
24	BC	47	ARG
24	BC	196	ASN
24	BC	197	ALA
24	BC	204	LEU
25	BD	27	ILE
29	BH	10	ALA
37	BP	31	VAL
40	BS	41	LYS
41	BT	15	HIS
41	BT	36	LYS
42	BU	5	ARG
44	BW	23	LYS
44	BW	41	GLY
44	BW	78	PHE
45	BX	27	ARG
2	AC	167	TYR
4	AE	121	ASN
6	AG	114	SER
9	AJ	41	PRO
18	AS	79	TYR
26	BE	94	GLN
27	BF	148	VAL
28	BG	9	VAL
31	BJ	79	GLY
32	BK	47	ILE
33	BL	3	LEU
33	BL	7	SER
34	BM	134	THR
37	BP	85	VAL
42	BU	12	VAL
42	BU	45	GLN
43	BV	54	ALA
55	B5	207	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AC	144	GLY
4	AE	43	GLY
5	AF	6	ILE
13	AN	63	ARG
31	BJ	78	THR
32	BK	46	ALA
38	BQ	90	ASP
41	BT	11	LEU
10	AK	73	VAL
11	AL	43	LYS
25	BD	73	VAL
33	BL	101	ILE
55	B5	91	GLY
26	BE	59	PRO
27	BF	103	ILE
33	BL	88	GLY
19	AT	3	ILE
28	BG	116	LEU
32	BK	93	GLN
2	AC	13	ILE
32	BK	26	GLY
34	BM	36	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	180/180 (100%)	177 (98%)	3 (2%)	60	78
2	AC	170/171 (99%)	169 (99%)	1 (1%)	86	92
3	AD	172/173 (99%)	171 (99%)	1 (1%)	86	92
4	AE	113/113 (100%)	112 (99%)	1 (1%)	78	87
5	AF	87/87 (100%)	85 (98%)	2 (2%)	50	70
6	AG	123/123 (100%)	122 (99%)	1 (1%)	81	89
7	AH	104/105 (99%)	103 (99%)	1 (1%)	76	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AI	105/105 (100%)	102 (97%)	3 (3%)	42	64
9	AJ	86/86 (100%)	84 (98%)	2 (2%)	50	70
10	AK	90/90 (100%)	88 (98%)	2 (2%)	52	71
11	AL	103/104 (99%)	101 (98%)	2 (2%)	57	75
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	80 (96%)	3 (4%)	35	59
14	AO	76/77 (99%)	74 (97%)	2 (3%)	46	66
15	AP	65/65 (100%)	64 (98%)	1 (2%)	65	80
16	AQ	74/74 (100%)	73 (99%)	1 (1%)	67	80
17	AR	48/48 (100%)	47 (98%)	1 (2%)	53	72
18	AS	70/70 (100%)	67 (96%)	3 (4%)	29	53
19	AT	65/65 (100%)	64 (98%)	1 (2%)	65	80
20	AU	44/44 (100%)	43 (98%)	1 (2%)	50	70
24	BC	216/217 (100%)	214 (99%)	2 (1%)	78	87
25	BD	164/164 (100%)	162 (99%)	2 (1%)	71	83
26	BE	165/165 (100%)	161 (98%)	4 (2%)	49	69
27	BF	149/150 (99%)	144 (97%)	5 (3%)	37	60
28	BG	137/138 (99%)	134 (98%)	3 (2%)	52	71
29	BH	114/114 (100%)	113 (99%)	1 (1%)	78	87
30	BI	109/110 (99%)	108 (99%)	1 (1%)	78	87
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	78	87
32	BK	103/103 (100%)	98 (95%)	5 (5%)	25	50
33	BL	102/103 (99%)	100 (98%)	2 (2%)	55	74
34	BM	109/109 (100%)	106 (97%)	3 (3%)	43	65
35	BN	100/100 (100%)	98 (98%)	2 (2%)	55	74
36	BO	86/87 (99%)	85 (99%)	1 (1%)	71	83
37	BP	99/100 (99%)	98 (99%)	1 (1%)	76	86
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	82 (98%)	2 (2%)	49	69
40	BS	93/93 (100%)	91 (98%)	2 (2%)	52	71
41	BT	80/80 (100%)	78 (98%)	2 (2%)	47	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BU	83/84 (99%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	76 (97%)	2 (3%)	46	66
44	BW	59/59 (100%)	55 (93%)	4 (7%)	16	41
45	BX	67/68 (98%)	65 (97%)	2 (3%)	41	63
46	BY	55/55 (100%)	55 (100%)	0	100	100
47	BZ	48/49 (98%)	45 (94%)	3 (6%)	18	43
48	B0	47/48 (98%)	46 (98%)	1 (2%)	53	72
49	B1	45/45 (100%)	44 (98%)	1 (2%)	52	71
50	B2	38/38 (100%)	37 (97%)	1 (3%)	46	66
51	B3	51/52 (98%)	48 (94%)	3 (6%)	19	45
52	B4	34/34 (100%)	34 (100%)	0	100	100
55	B5	173/181 (96%)	167 (96%)	6 (4%)	36	59
All	All	4842/4870 (99%)	4748 (98%)	94 (2%)	59	75

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	187	ASP
1	AB	204	ASP
1	AB	209	VAL
2	AC	35	ASP
3	AD	55	ARG
4	AE	105	ILE
5	AF	36	ILE
5	AF	41	ASP
6	AG	51	GLN
7	AH	105	THR
8	AI	3	ASN
8	AI	66	VAL
8	AI	98	ARG
9	AJ	48	ARG
9	AJ	50	THR
10	AK	55	ARG
10	AK	84	MET
11	AL	19	ASN
11	AL	34	THR
13	AN	6	MET
13	AN	40	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AN	41	ARG
14	AO	5	GLU
14	AO	45	HIS
15	AP	1	MET
16	AQ	41	THR
17	AR	69	TYR
18	AS	11	ASP
18	AS	30	LEU
18	AS	54	ARG
19	AT	27	MET
20	AU	20	ARG
24	BC	89	ASN
24	BC	263	ASP
25	BD	148	GLN
25	BD	164	GLN
26	BE	3	LEU
26	BE	60	TRP
26	BE	69	ARG
26	BE	120	VAL
27	BF	41	GLU
27	BF	46	LYS
27	BF	113	PHE
27	BF	122	ASP
27	BF	129	MET
28	BG	154	GLU
28	BG	162	ARG
28	BG	163	TYR
29	BH	104	THR
30	BI	16	MET
31	BJ	1	MET
32	BK	4	GLU
32	BK	29	HIS
32	BK	32	TYR
32	BK	80	ASP
32	BK	105	ARG
33	BL	21	ARG
33	BL	39	LYS
34	BM	81	ARG
34	BM	97	GLN
34	BM	126	ILE
35	BN	1	MET
35	BN	3	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	BO	36	TYR
37	BP	74	GLN
39	BR	2	TYR
39	BR	82	HIS
40	BS	15	GLN
40	BS	77	ASP
41	BT	60	THR
41	BT	86	THR
43	BV	12	GLN
43	BV	51	GLN
44	BW	31	LEU
44	BW	38	ARG
44	BW	39	GLN
44	BW	55	ASP
45	BX	26	ARG
45	BX	31	ASN
47	BZ	28	LEU
47	BZ	31	ILE
47	BZ	33	HIS
48	B0	41	HIS
49	B1	24	LYS
50	B2	1	MET
51	B3	23	HIS
51	B3	27	ASN
51	B3	48	MET
55	B5	40	GLU
55	B5	51	ASP
55	B5	97	MET
55	B5	109	MET
55	B5	126	GLN
55	B5	148	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
52	B4	37	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	195 (12%)	46 (3%)
22	A1	73/76 (96%)	7 (9%)	2 (2%)
23	A2	14/15 (93%)	4 (28%)	2 (14%)
53	BA	2902/2903 (99%)	455 (15%)	123 (4%)
54	BB	116/118 (98%)	19 (16%)	2 (1%)
All	All	4635/4645 (99%)	680 (14%)	175 (3%)

All (680) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	8	A
21	AA	9	G
21	AA	16	A
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	50	A
21	AA	51	A
21	AA	66	A
21	AA	80	A
21	AA	81	A
21	AA	83	C
21	AA	85	U
21	AA	86	G
21	AA	87	C
21	AA	109	A
21	AA	110	C
21	AA	112	G
21	AA	121	U
21	AA	144	G
21	AA	148	G
21	AA	188	C
21	AA	194	C
21	AA	198	G
21	AA	209	U
21	AA	225	C
21	AA	240	G
21	AA	245	U
21	AA	247	G
21	AA	251	G
21	AA	266	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	AA	275	G
21	AA	280	C
21	AA	289	G
21	AA	324	G
21	AA	329	A
21	AA	331	G
21	AA	332	G
21	AA	347	G
21	AA	352	C
21	AA	354	G
21	AA	367	U
21	AA	372	C
21	AA	373	A
21	AA	381	C
21	AA	389	A
21	AA	397	A
21	AA	398	U
21	AA	411	A
21	AA	412	A
21	AA	413	G
21	AA	414	A
21	AA	421	U
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	451	A
21	AA	463	U
21	AA	464	U
21	AA	465	A
21	AA	466	A
21	AA	468	A
21	AA	479	U
21	AA	481	G
21	AA	484	G
21	AA	511	C
21	AA	512	U
21	AA	518	C
21	AA	527	G
21	AA	530	G
21	AA	531	U
21	AA	532	A
21	AA	533	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	AA	534	U
21	AA	535	A
21	AA	547	A
21	AA	557	G
21	AA	559	A
21	AA	560	A
21	AA	563	A
21	AA	564	C
21	AA	567	G
21	AA	572	A
21	AA	574	A
21	AA	576	C
21	AA	633	G
21	AA	665	A
21	AA	673	A
21	AA	674	G
21	AA	687	A
21	AA	695	A
21	AA	700	G
21	AA	702	A
21	AA	704	A
21	AA	723	U
21	AA	733	G
21	AA	734	G
21	AA	755	G
21	AA	794	A
21	AA	812	G
21	AA	816	A
21	AA	817	C
21	AA	819	A
21	AA	821	G
21	AA	841	C
21	AA	843	U
21	AA	845	A
21	AA	864	A
21	AA	872	A
21	AA	873	A
21	AA	877	G
21	AA	890	G
21	AA	918	A
21	AA	927	G
21	AA	934	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	AA	935	A
21	AA	945	G
21	AA	960	U
21	AA	969	A
21	AA	971	G
21	AA	974	A
21	AA	975	A
21	AA	977	A
21	AA	978	A
21	AA	991	U
21	AA	993	G
21	AA	995	C
21	AA	1004	A
21	AA	1008	U
21	AA	1017	U
21	AA	1020	G
21	AA	1030	U
21	AA	1031	C
21	AA	1033	G
21	AA	1037	C
21	AA	1054	C
21	AA	1065	U
21	AA	1066	C
21	AA	1094	G
21	AA	1101	A
21	AA	1136	C
21	AA	1137	C
21	AA	1138	G
21	AA	1139	G
21	AA	1145	A
21	AA	1159	U
21	AA	1190	G
21	AA	1191	A
21	AA	1197	A
21	AA	1200	C
21	AA	1201	A
21	AA	1202	U
21	AA	1212	U
21	AA	1217	C
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	AA	1238	A
21	AA	1256	A
21	AA	1257	A
21	AA	1267	C
21	AA	1279	G
21	AA	1280	A
21	AA	1281	C
21	AA	1285	A
21	AA	1286	U
21	AA	1287	A
21	AA	1290	G
21	AA	1300	G
21	AA	1301	U
21	AA	1302	C
21	AA	1303	C
21	AA	1305	G
21	AA	1320	C
21	AA	1323	G
21	AA	1330	U
21	AA	1338	G
21	AA	1340	A
21	AA	1346	A
21	AA	1349	A
21	AA	1379	G
21	AA	1397	C
21	AA	1398	A
21	AA	1399	C
21	AA	1401	G
21	AA	1411	C
21	AA	1418	A
21	AA	1419	G
21	AA	1432	G
21	AA	1447	A
21	AA	1459	G
21	AA	1460	C
21	AA	1499	A
22	A1	10	G
22	A1	16	C
22	A1	17	U
22	A1	45	G
22	A1	49	G
22	A1	74	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	A1	75	C
23	A2	81	U
23	A2	82	A
23	A2	85	G
23	A2	92	U
53	BA	9	G
53	BA	10	A
53	BA	15	G
53	BA	20	C
53	BA	34	U
53	BA	46	G
53	BA	50	U
53	BA	62	U
53	BA	71	A
53	BA	74	A
53	BA	75	G
53	BA	77	G
53	BA	91	A
53	BA	101	A
53	BA	119	A
53	BA	120	U
53	BA	122	G
53	BA	126	A
53	BA	127	A
53	BA	142	A
53	BA	149	A
53	BA	181	A
53	BA	196	A
53	BA	197	A
53	BA	199	A
53	BA	200	U
53	BA	205	G
53	BA	216	A
53	BA	222	A
53	BA	224	U
53	BA	233	A
53	BA	242	G
53	BA	243	U
53	BA	248	G
53	BA	250	G
53	BA	265	A
53	BA	272	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	273	G
53	BA	277	G
53	BA	278	A
53	BA	299	A
53	BA	330	A
53	BA	331	C
53	BA	332	A
53	BA	345	A
53	BA	370	G
53	BA	373	U
53	BA	374	A
53	BA	386	G
53	BA	387	U
53	BA	388	G
53	BA	390	U
53	BA	391	A
53	BA	411	G
53	BA	430	A
53	BA	435	C
53	BA	447	A
53	BA	451	U
53	BA	452	G
53	BA	454	A
53	BA	455	C
53	BA	457	A
53	BA	472	A
53	BA	473	G
53	BA	474	G
53	BA	480	A
53	BA	481	G
53	BA	482	A
53	BA	505	A
53	BA	506	G
53	BA	508	A
53	BA	510	C
53	BA	511	U
53	BA	512	G
53	BA	526	A
53	BA	527	C
53	BA	528	A
53	BA	529	A
53	BA	530	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	531	C
53	BA	532	A
53	BA	533	G
53	BA	546	U
53	BA	547	A
53	BA	572	A
53	BA	574	A
53	BA	581	C
53	BA	587	C
53	BA	588	U
53	BA	590	A
53	BA	603	A
53	BA	607	U
53	BA	613	A
53	BA	614	A
53	BA	615	U
53	BA	616	A
53	BA	617	G
53	BA	627	A
53	BA	631	A
53	BA	637	A
53	BA	644	A
53	BA	645	C
53	BA	653	U
53	BA	655	A
53	BA	671	C
53	BA	672	C
53	BA	686	U
53	BA	717	C
53	BA	719	C
53	BA	730	A
53	BA	747	U
53	BA	752	A
53	BA	753	A
53	BA	763	G
53	BA	764	A
53	BA	765	C
53	BA	776	G
53	BA	782	A
53	BA	783	A
53	BA	784	G
53	BA	785	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	792	A
53	BA	793	A
53	BA	805	G
53	BA	811	U
53	BA	812	C
53	BA	827	U
53	BA	829	A
53	BA	830	G
53	BA	831	G
53	BA	846	U
53	BA	858	G
53	BA	888	C
53	BA	889	C
53	BA	896	A
53	BA	897	C
53	BA	910	A
53	BA	914	G
53	BA	915	C
53	BA	931	U
53	BA	932	U
53	BA	941	A
53	BA	946	C
53	BA	960	A
53	BA	961	C
53	BA	962	G
53	BA	974	G
53	BA	975	A
53	BA	976	G
53	BA	977	G
53	BA	982	C
53	BA	983	A
53	BA	984	A
53	BA	996	A
53	BA	1012	U
53	BA	1013	C
53	BA	1021	A
53	BA	1022	G
53	BA	1026	G
53	BA	1034	G
53	BA	1038	G
53	BA	1046	A
53	BA	1057	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	1060	U
53	BA	1063	G
53	BA	1070	A
53	BA	1071	G
53	BA	1073	A
53	BA	1076	C
53	BA	1078	U
53	BA	1079	C
53	BA	1088	A
53	BA	1089	A
53	BA	1091	G
53	BA	1112	G
53	BA	1124	G
53	BA	1127	A
53	BA	1128	G
53	BA	1129	A
53	BA	1132	U
53	BA	1133	A
53	BA	1134	A
53	BA	1135	C
53	BA	1141	U
53	BA	1142	A
53	BA	1143	A
53	BA	1149	G
53	BA	1150	C
53	BA	1156	A
53	BA	1176	U
53	BA	1186	G
53	BA	1204	A
53	BA	1213	A
53	BA	1230	A
53	BA	1231	U
53	BA	1236	G
53	BA	1237	A
53	BA	1241	A
53	BA	1244	A
53	BA	1247	A
53	BA	1250	G
53	BA	1253	A
53	BA	1256	G
53	BA	1261	C
53	BA	1266	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	1267	U
53	BA	1272	A
53	BA	1274	A
53	BA	1275	A
53	BA	1276	A
53	BA	1291	C
53	BA	1300	G
53	BA	1301	A
53	BA	1309	G
53	BA	1314	C
53	BA	1315	C
53	BA	1320	C
53	BA	1325	U
53	BA	1333	G
53	BA	1341	G
53	BA	1345	C
53	BA	1350	C
53	BA	1365	A
53	BA	1366	A
53	BA	1374	G
53	BA	1379	U
53	BA	1383	A
53	BA	1390	U
53	BA	1396	U
53	BA	1416	G
53	BA	1420	A
53	BA	1427	A
53	BA	1428	C
53	BA	1452	G
53	BA	1453	A
53	BA	1455	G
53	BA	1458	U
53	BA	1459	G
53	BA	1461	C
53	BA	1475	G
53	BA	1482	G
53	BA	1490	A
53	BA	1494	A
53	BA	1508	A
53	BA	1509	A
53	BA	1535	A
53	BA	1537	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	1538	G
53	BA	1539	U
53	BA	1554	U
53	BA	1555	G
53	BA	1560	G
53	BA	1566	A
53	BA	1569	A
53	BA	1584	U
53	BA	1585	C
53	BA	1597	A
53	BA	1600	C
53	BA	1607	C
53	BA	1608	A
53	BA	1609	A
53	BA	1610	A
53	BA	1615	C
53	BA	1626	A
53	BA	1636	U
53	BA	1646	C
53	BA	1647	U
53	BA	1648	U
53	BA	1654	A
53	BA	1655	A
53	BA	1670	C
53	BA	1674	G
53	BA	1683	U
53	BA	1684	G
53	BA	1728	C
53	BA	1731	G
53	BA	1739	A
53	BA	1758	U
53	BA	1764	C
53	BA	1773	A
53	BA	1780	A
53	BA	1782	U
53	BA	1800	C
53	BA	1808	A
53	BA	1810	A
53	BA	1816	C
53	BA	1821	A
53	BA	1847	A
53	BA	1876	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	1877	A
53	BA	1884	G
53	BA	1906	G
53	BA	1913	A
53	BA	1914	C
53	BA	1929	G
53	BA	1937	A
53	BA	1939	U
53	BA	1943	U
53	BA	1953	A
53	BA	1954	G
53	BA	1963	U
53	BA	1964	G
53	BA	1965	C
53	BA	1966	A
53	BA	1967	C
53	BA	1970	A
53	BA	1972	G
53	BA	1992	G
53	BA	1993	U
53	BA	1996	C
53	BA	1997	C
53	BA	2022	U
53	BA	2023	C
53	BA	2030	A
53	BA	2031	A
53	BA	2032	G
53	BA	2033	A
53	BA	2034	U
53	BA	2043	C
53	BA	2053	G
53	BA	2055	C
53	BA	2056	G
53	BA	2059	A
53	BA	2060	A
53	BA	2061	G
53	BA	2069	G
53	BA	2073	C
53	BA	2093	G
53	BA	2094	A
53	BA	2102	G
53	BA	2104	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	2112	G
53	BA	2113	U
53	BA	2115	G
53	BA	2116	G
53	BA	2130	U
53	BA	2131	U
53	BA	2133	G
53	BA	2134	A
53	BA	2136	G
53	BA	2137	U
53	BA	2155	U
53	BA	2159	G
53	BA	2169	A
53	BA	2172	U
53	BA	2173	A
53	BA	2174	C
53	BA	2204	G
53	BA	2207	C
53	BA	2212	A
53	BA	2213	U
53	BA	2225	A
53	BA	2238	G
53	BA	2239	G
53	BA	2262	U
53	BA	2266	A
53	BA	2267	A
53	BA	2269	G
53	BA	2283	C
53	BA	2297	A
53	BA	2304	G
53	BA	2305	U
53	BA	2308	G
53	BA	2313	C
53	BA	2320	U
53	BA	2321	U
53	BA	2322	A
53	BA	2325	G
53	BA	2333	A
53	BA	2334	U
53	BA	2335	A
53	BA	2339	C
53	BA	2347	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	2350	C
53	BA	2352	A
53	BA	2353	G
53	BA	2383	G
53	BA	2385	C
53	BA	2390	U
53	BA	2391	G
53	BA	2403	C
53	BA	2407	A
53	BA	2420	C
53	BA	2424	C
53	BA	2427	C
53	BA	2429	G
53	BA	2430	A
53	BA	2432	A
53	BA	2438	U
53	BA	2439	A
53	BA	2441	U
53	BA	2448	A
53	BA	2452	C
53	BA	2468	A
53	BA	2469	A
53	BA	2476	A
53	BA	2488	G
53	BA	2491	U
53	BA	2498	C
53	BA	2500	U
53	BA	2501	C
53	BA	2502	G
53	BA	2503	A
53	BA	2504	U
53	BA	2505	G
53	BA	2518	A
53	BA	2529	G
53	BA	2530	A
53	BA	2531	A
53	BA	2534	A
53	BA	2543	G
53	BA	2566	A
53	BA	2567	G
53	BA	2573	C
53	BA	2578	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	2582	G
53	BA	2584	U
53	BA	2588	G
53	BA	2599	G
53	BA	2613	U
53	BA	2614	A
53	BA	2615	U
53	BA	2616	C
53	BA	2629	U
53	BA	2639	A
53	BA	2640	G
53	BA	2646	C
53	BA	2660	A
53	BA	2669	G
53	BA	2689	U
53	BA	2690	U
53	BA	2712	C
53	BA	2755	C
53	BA	2757	A
53	BA	2765	A
53	BA	2777	G
53	BA	2778	A
53	BA	2780	G
53	BA	2790	U
53	BA	2791	G
53	BA	2797	U
53	BA	2798	U
53	BA	2799	A
53	BA	2800	A
53	BA	2809	A
53	BA	2817	U
53	BA	2820	A
53	BA	2823	A
53	BA	2835	A
53	BA	2836	U
53	BA	2868	A
53	BA	2880	C
53	BA	2886	A
53	BA	2894	G
53	BA	2895	G
54	BB	13	G
54	BB	14	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	BB	15	A
54	BB	16	G
54	BB	25	U
54	BB	35	C
54	BB	36	C
54	BB	42	C
54	BB	44	G
54	BB	45	A
54	BB	56	G
54	BB	57	A
54	BB	74	U
54	BB	81	G
54	BB	87	U
54	BB	90	C
54	BB	91	C
54	BB	109	A
54	BB	118	C

All (175) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	32	A
21	AA	80	A
21	AA	109	A
21	AA	173	U
21	AA	239	U
21	AA	279	A
21	AA	329	A
21	AA	372	C
21	AA	451	A
21	AA	461	A
21	AA	530	G
21	AA	532	A
21	AA	533	A
21	AA	559	A
21	AA	575	G
21	AA	618	C
21	AA	700	G
21	AA	723	U
21	AA	812	G
21	AA	841	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	AA	872	A
21	AA	934	C
21	AA	944	G
21	AA	958	A
21	AA	974	A
21	AA	978	A
21	AA	992	U
21	AA	1053	G
21	AA	1065	U
21	AA	1137	C
21	AA	1139	G
21	AA	1159	U
21	AA	1190	G
21	AA	1200	C
21	AA	1201	A
21	AA	1225	A
21	AA	1296	C
21	AA	1358	U
21	AA	1398	A
21	AA	1399	C
21	AA	1432	G
21	AA	1447	A
21	AA	1455	G
21	AA	1459	G
21	AA	1529	G
22	A1	10	G
22	A1	16	C
23	A2	81	U
23	A2	84	G
53	BA	9	G
53	BA	48	G
53	BA	49	A
53	BA	60	G
53	BA	142	A
53	BA	196	A
53	BA	215	G
53	BA	242	G
53	BA	249	C
53	BA	276	U
53	BA	278	A
53	BA	323	C
53	BA	386	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	387	U
53	BA	424	G
53	BA	446	G
53	BA	473	G
53	BA	479	A
53	BA	482	A
53	BA	505	A
53	BA	510	C
53	BA	511	U
53	BA	520	G
53	BA	571	U
53	BA	573	U
53	BA	587	C
53	BA	613	A
53	BA	627	A
53	BA	629	G
53	BA	643	A
53	BA	670	A
53	BA	686	U
53	BA	728	G
53	BA	752	A
53	BA	762	U
53	BA	764	A
53	BA	776	G
53	BA	792	A
53	BA	811	U
53	BA	816	C
53	BA	829	A
53	BA	888	C
53	BA	914	G
53	BA	941	A
53	BA	944	C
53	BA	957	C
53	BA	961	C
53	BA	962	G
53	BA	963	U
53	BA	975	A
53	BA	976	G
53	BA	1021	A
53	BA	1056	G
53	BA	1062	G
53	BA	1070	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	1072	C
53	BA	1078	U
53	BA	1087	G
53	BA	1088	A
53	BA	1126	A
53	BA	1128	G
53	BA	1134	A
53	BA	1204	A
53	BA	1236	G
53	BA	1252	G
53	BA	1266	G
53	BA	1272	A
53	BA	1275	A
53	BA	1288	G
53	BA	1289	C
53	BA	1300	G
53	BA	1325	U
53	BA	1365	A
53	BA	1451	C
53	BA	1458	U
53	BA	1508	A
53	BA	1539	U
53	BA	1554	U
53	BA	1608	A
53	BA	1610	A
53	BA	1625	C
53	BA	1637	A
53	BA	1655	A
53	BA	1668	A
53	BA	1780	A
53	BA	1929	G
53	BA	1936	A
53	BA	1952	A
53	BA	1953	A
53	BA	1966	A
53	BA	1972	G
53	BA	2033	A
53	BA	2060	A
53	BA	2062	A
53	BA	2115	G
53	BA	2130	U
53	BA	2225	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	BA	2261	C
53	BA	2266	A
53	BA	2275	C
53	BA	2288	A
53	BA	2321	U
53	BA	2335	A
53	BA	2438	U
53	BA	2451	A
53	BA	2468	A
53	BA	2487	G
53	BA	2503	A
53	BA	2518	A
53	BA	2531	A
53	BA	2566	A
53	BA	2581	G
53	BA	2602	A
53	BA	2665	A
53	BA	2666	C
53	BA	2712	C
53	BA	2756	U
53	BA	2777	G
53	BA	2778	A
53	BA	2790	U
53	BA	2799	A
53	BA	2832	U
53	BA	2884	U
54	BB	12	C
54	BB	56	G

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

6 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	7MG	A1	46	22	22,26,27	5.57	1 (4%)	29,39,42	1.41	1 (3%)
22	5MU	A1	54	22	19,22,23	0.77	0	28,32,35	1.41	3 (10%)
22	CM0	A1	34	23,22	22,26,27	1.30	2 (9%)	28,37,40	1.10	1 (3%)
22	6MZ	A1	37	22	18,25,26	1.10	1 (5%)	16,36,39	1.30	2 (12%)
22	PSU	A1	55	22	18,21,22	0.85	0	22,30,33	1.02	1 (4%)
22	4SU	A1	7	22	18,21,22	1.44	1 (5%)	26,30,33	0.87	1 (3%)

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	7MG	A1	46	22	-	0/7/37/38	0/3/3/3
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
22	CM0	A1	34	23,22	-	3/12/30/31	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	PSU	A1	55	22	-	1/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-25.87	1.31	1.46
22	A1	7	4SU	C5-C4	-5.02	1.36	1.42
22	A1	34	CM0	O5-C5	-4.69	1.25	1.36
22	A1	37	6MZ	C8-N7	-2.50	1.30	1.34
22	A1	34	CM0	O8-C8	-2.04	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	46	7MG	N9-C8-N7	5.65	111.47	103.38
22	A1	54	5MU	C5M-C5-C6	-3.75	117.84	122.85
22	A1	37	6MZ	C9-N6-C6	3.12	125.56	122.87
22	A1	54	5MU	C6-C5-C4	3.02	120.55	118.03
22	A1	37	6MZ	C2-N1-C6	2.90	119.08	116.59
22	A1	55	PSU	C6-C5-C4	2.81	120.17	118.20
22	A1	34	CM0	C7-O5-C5	2.78	121.22	117.58
22	A1	54	5MU	C5M-C5-C4	2.58	121.61	118.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	7	4SU	C6-C5-C4	2.06	121.74	119.95

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9
22	A1	55	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	C6-C5-O5-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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	FME	BA	3001	56	8,9,10	0.59	0	7,9,11	1.39	1 (14%)
56	VAL	A1	101	57,22	4,6,7	0.49	0	6,7,9	1.45	1 (16%)

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	FME	BA	3001	56	-	2/7/9/11	-
56	VAL	A1	101	57,22	-	0/5/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	A1	101	VAL	O-C-CA	-3.52	115.55	124.78
57	BA	3001	FME	C-CA-N	2.50	114.25	109.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	BA	3001	FME	O1-CN-N-CA
57	BA	3001	FME	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	3001	FME	1	0

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.

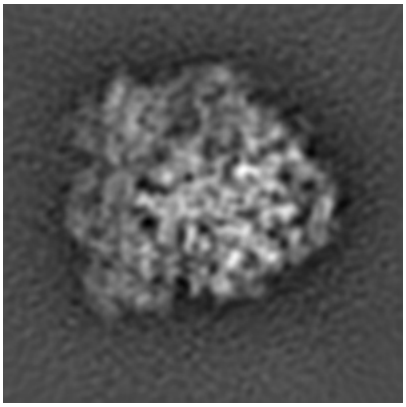
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1724. These allow visual inspection of the internal detail of the map and identification of artifacts.

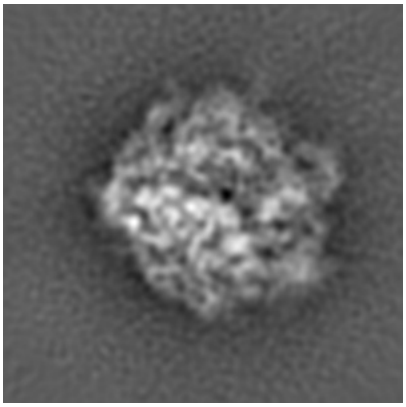
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

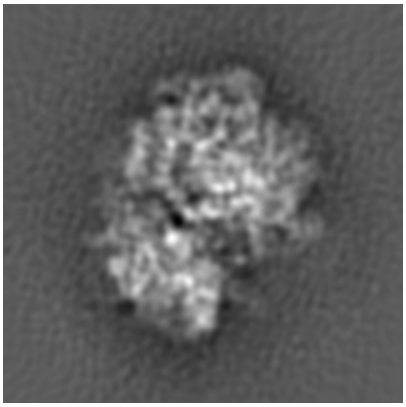
6.1.1 Primary map



X



Y

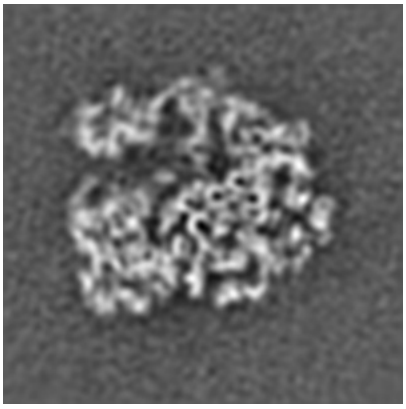


Z

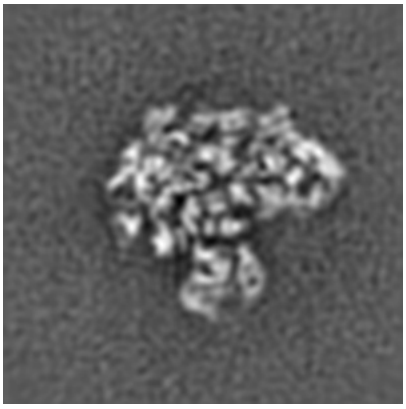
The images above show the map projected in three orthogonal directions.

6.2 Central slices

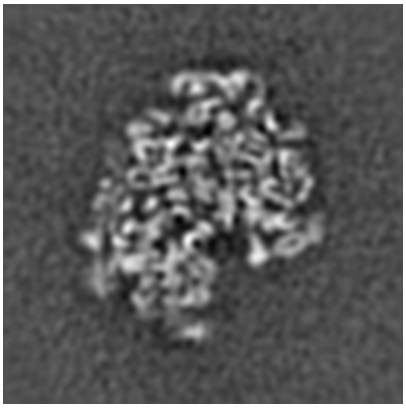
6.2.1 Primary map



X Index: 96



Y Index: 96

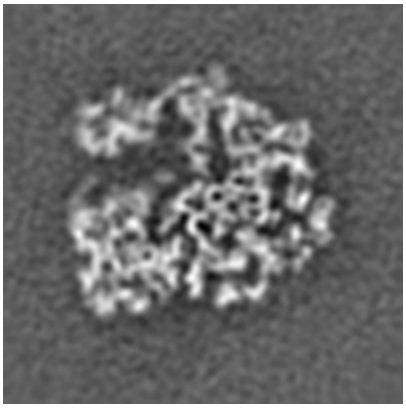


Z Index: 96

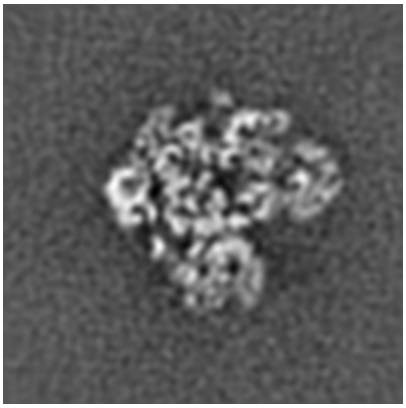
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

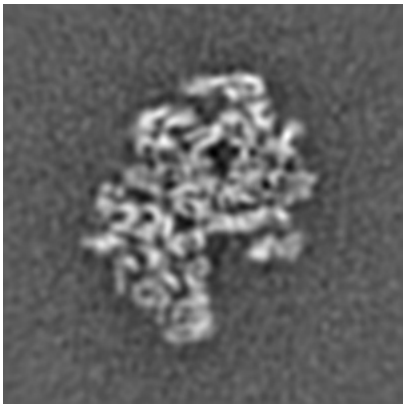
6.3.1 Primary map



X Index: 97



Y Index: 92

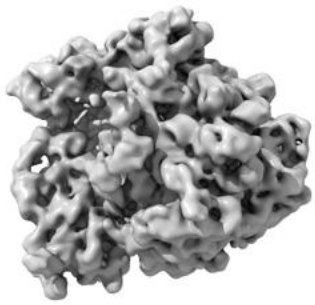


Z Index: 91

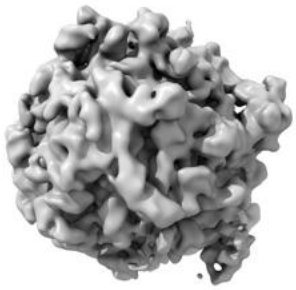
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

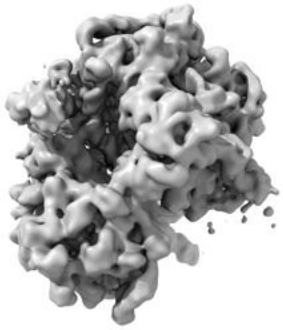
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 40.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

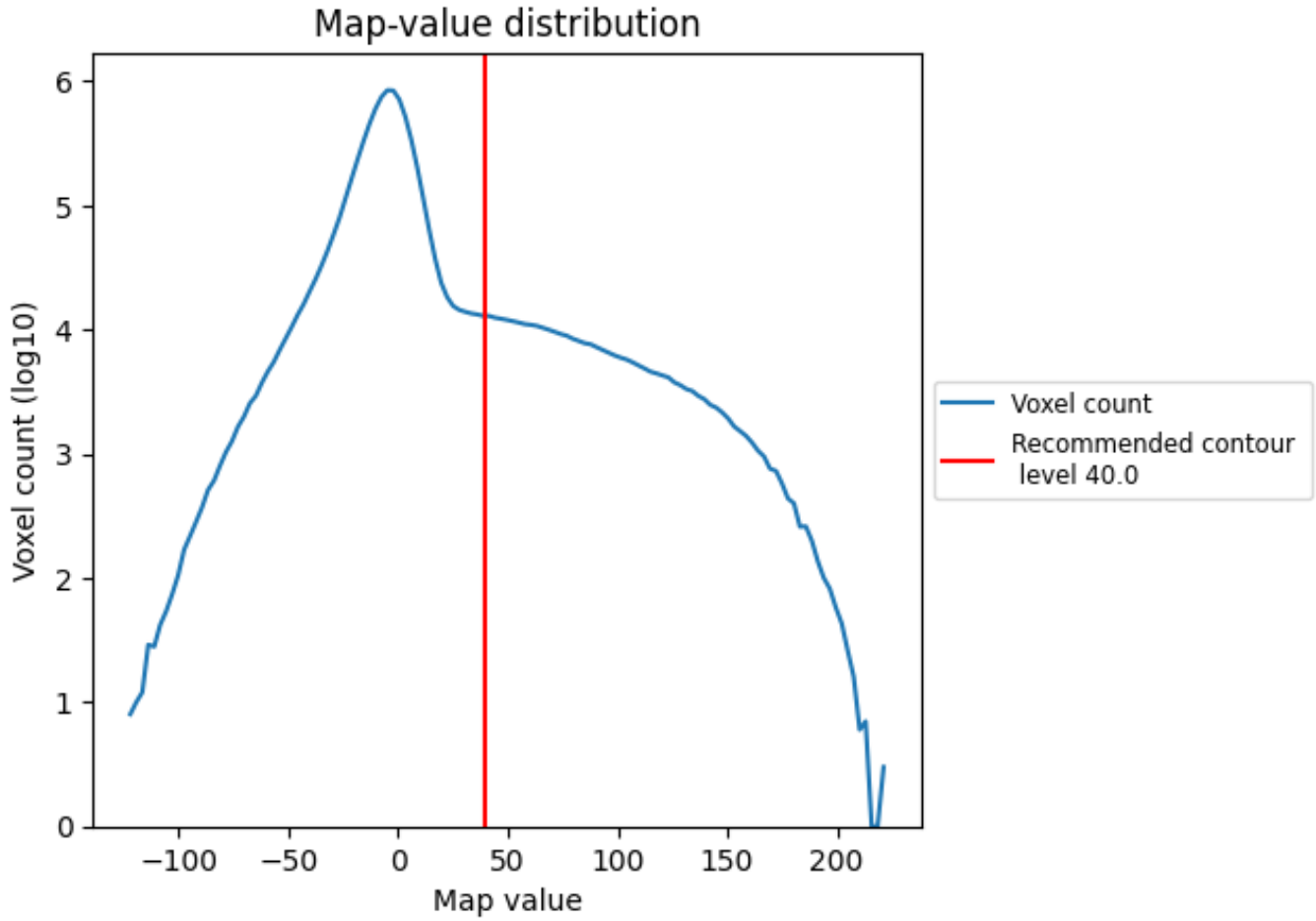
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

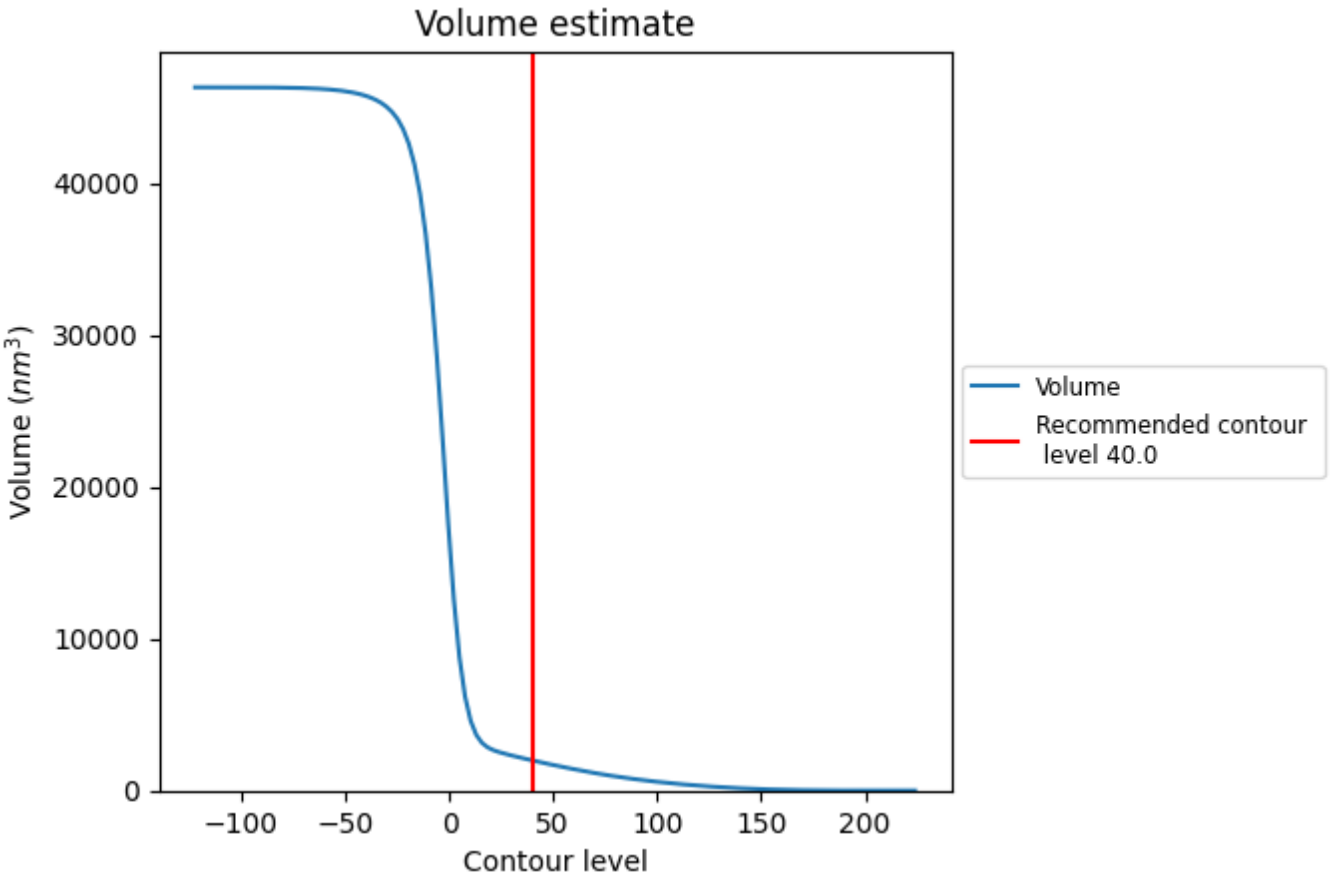
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

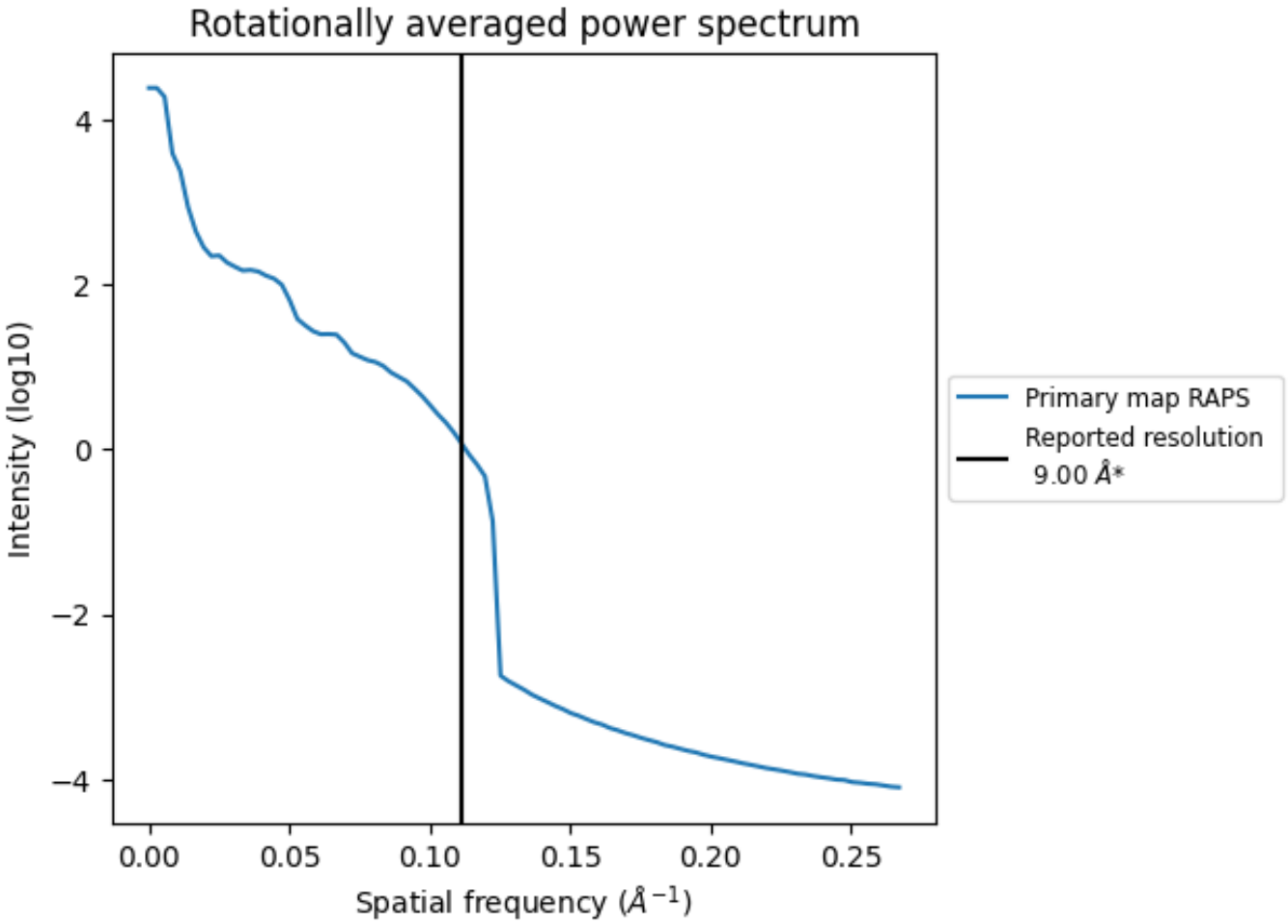
7.2 Volume estimate



The volume at the recommended contour level is 1986 nm^3; this corresponds to an approximate mass of 1794 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.111 Å^{-1}

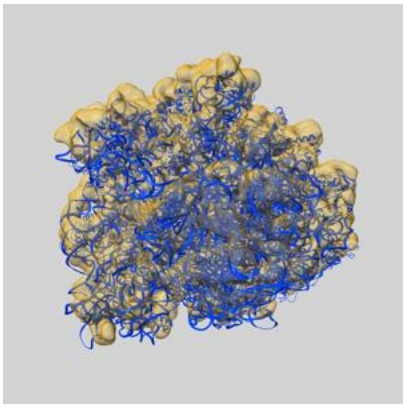
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

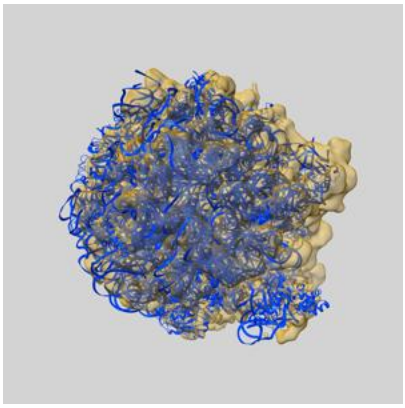
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1724 and PDB model 4V7A. Per-residue inclusion information can be found in section 3 on page 17.

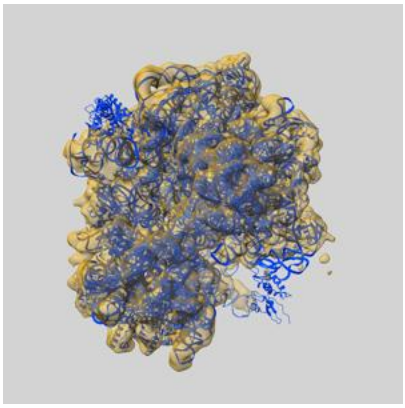
9.1 Map-model overlay



X



Y



Z

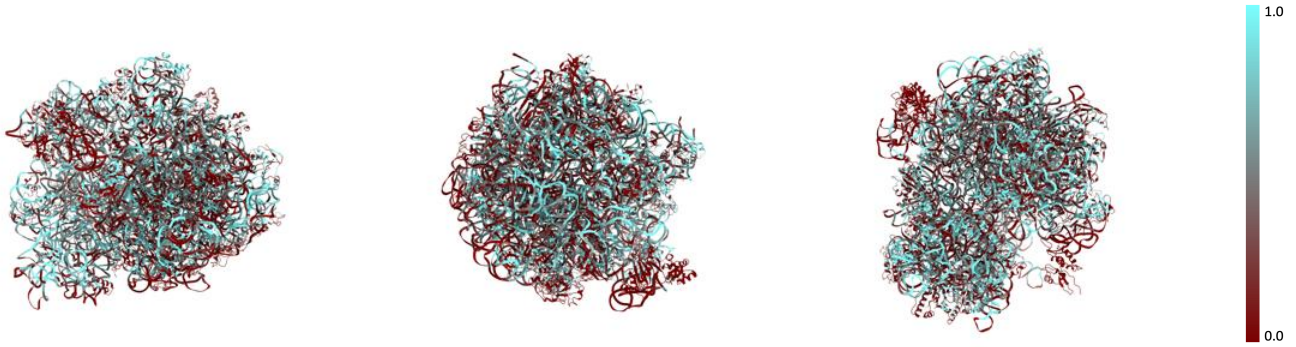
The images above show the 3D surface view of the map at the recommended contour level 40.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

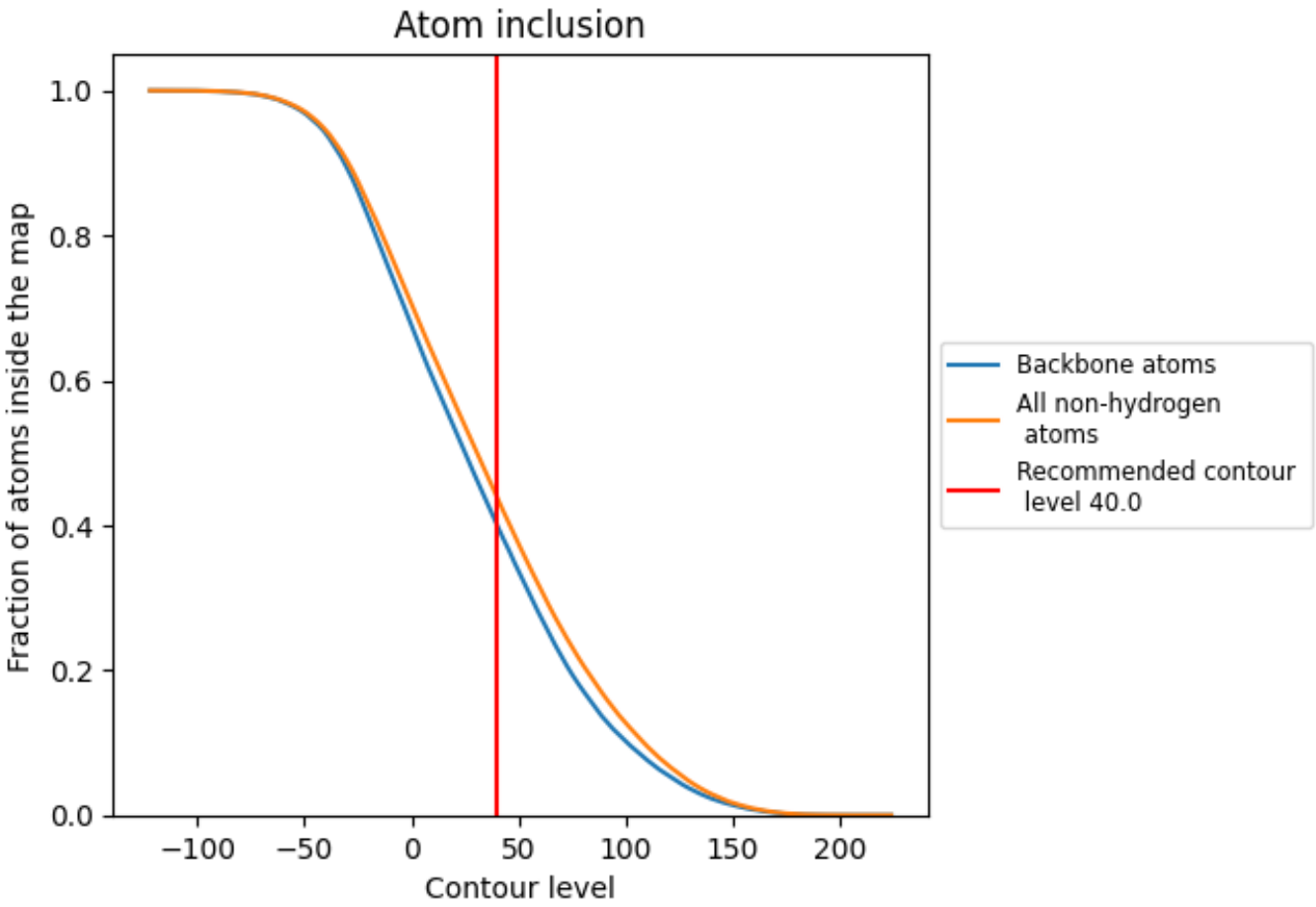
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (40.0).

9.4 Atom inclusion (i)



At the recommended contour level, 40% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (40.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4381	-0.0050
A1	0.4504	0.0020
A2	0.3236	-0.0520
AA	0.5085	-0.0040
AB	0.2664	-0.0000
AC	0.3559	-0.0030
AD	0.3421	-0.0160
AE	0.4300	0.0150
AF	0.2811	-0.0160
AG	0.4368	0.0260
AH	0.4792	-0.0000
AI	0.5392	0.0110
AJ	0.3010	0.0130
AK	0.3965	-0.0220
AL	0.3898	-0.0020
AM	0.5243	0.0280
AN	0.4625	0.0020
AO	0.3174	-0.0060
AP	0.4344	0.0060
AQ	0.3622	-0.0190
AR	0.4875	0.0390
AS	0.4375	0.0020
AT	0.3696	-0.0400
AU	0.2518	-0.0130
B0	0.3808	0.0110
B1	0.2005	-0.0140
B2	0.3634	-0.0360
B3	0.3401	-0.0240
B4	0.4418	-0.0230
B5	0.0337	0.0060
BA	0.4545	-0.0070
BB	0.4772	-0.0150
BC	0.4546	0.0110
BD	0.3836	-0.0090
BE	0.4579	-0.0020

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BF	0.4678	0.0020
BG	0.4025	0.0180
BH	0.0283	-0.0480
BI	0.0000	0.0060
BJ	0.4182	0.0070
BK	0.3753	-0.0060
BL	0.4409	-0.0070
BM	0.4376	-0.0040
BN	0.3218	-0.0170
BO	0.5423	-0.0110
BP	0.2455	-0.0350
BQ	0.4449	0.0000
BR	0.3087	-0.0060
BS	0.3840	0.0010
BT	0.3375	-0.0040
BU	0.2708	-0.0030
BV	0.4634	-0.0050
BW	0.3918	-0.0280
BX	0.3577	-0.0250
BY	0.2455	-0.0170
BZ	0.4783	0.0010