Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:49 AM EST

PDB ID	:	4V6Y
EMDB ID	:	EMD-1716
Title	:	E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in classic pre-translocation state (pre1a)
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	:	12.00 Å(reported)
Based on initial models	:	2HGP, 2WRI, 2K4C, 3I1O

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 ⓘ 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 ⓘ) were used in the production of this report:

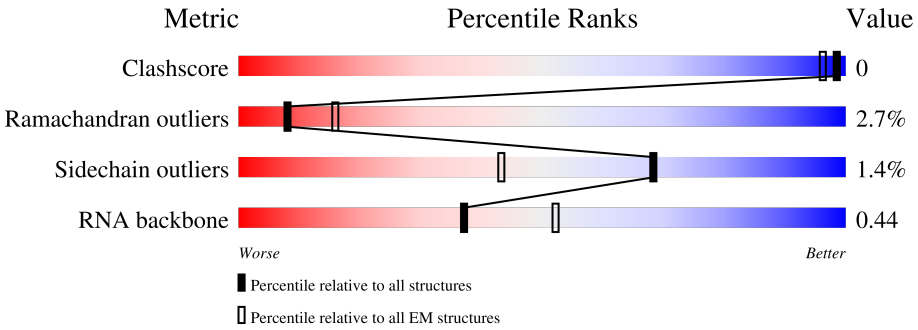
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 12.00 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	45% 93% 7%
2	AC	208	32% 92% 7%
3	AD	206	44% 87% 12%
4	AE	152	42% 89% 11%
5	AF	101	63% 87% 13%
6	AG	152	55% 88% 12%
7	AH	130	22% 91% 8%

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Mol	Chain	Length	Quality of chain
8	AI	128	47% 81% 18%
9	AJ	100	43% 84% 16%
10	AK	118	40% 89% 11%
11	AL	124	54% 85% 15%
12	AM	115	53% 85% 14%
13	AN	101	28% 86% 12%
14	AO	89	43% 87% 12%
15	AP	81	23% 84% 16%
16	AQ	82	46% 90% 9%
17	AR	57	53% 93% 7%
18	AS	81	42% 89% 11%
19	AT	86	37% 90% 10%
20	AU	53	34% 66% 26% 8%
21	AA	1533	30% 15% 56% 24% 5%
22	A1	76	53% 12% 61% 22% 5%
23	A2	15	60% 20% 40% 20% 20%
24	A3	77	39% 17% 55% 18% 10%
25	BC	273	51% 91% 8%
26	BD	209	35% 89% 11%
27	BE	201	45% 89% 10%
28	BF	179	37% 89% 11%
29	BG	177	50% 92% 7%
30	BH	149	87% 94% 5%
31	BI	142	95% 94% 5%
32	BJ	142	32% 91% 8%

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Mol	Chain	Length	Quality of chain
33	BK	123	53% 90% 10%
34	BL	144	51% 85% 14%
35	BM	136	39% 88% 12%
36	BN	121	49% 88% 12%
37	BO	117	30% 89% 10%
38	BP	115	37% 83% 16%
39	BQ	118	41% 84% 14%
40	BR	103	51% 89% 10%
41	BS	110	48% 92% 8%
42	BT	94	44% 91% 7%
43	BU	104	47% 90% 8%
44	BV	94	44% 95% 5%
45	BW	80	45% 88% 12%
46	BX	79	68% 84% 10%
47	BY	63	56% 90% 10%
48	BZ	59	29% 90% 7%
49	B0	57	58% 88% 11%
50	B1	52	40% 88% 12%
51	B2	46	57% 76% 22%
52	B3	65	58% 86% 12%
53	B4	38	39% 89% 8%
54	BA	2903	31% 16% 55% 24%
55	BB	118	27% 15% 59% 19% 5%
56	B5	234	89% 88% 6% 5%

2 Entry composition (i)

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	ACE	-	acetylation	UNP P0A7U3
AS	81	NH2	-	amidation	UNP P0A7U3

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AU	2	ACE	-	acetylation	UNP P68679
AU	54	NH2	-	amidation	UNP P68679

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

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

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

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

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

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

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

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

- Molecule 25 is a protein called 50S ribosomal protein L35.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 26 is a protein called 50S ribosomal protein L36.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

- Molecule 38 is a protein called 50S ribosomal protein L17.

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

- Molecule 39 is a protein called 50S ribosomal protein L18.

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

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

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

- Molecule 45 is a protein called 50S ribosomal protein L24.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	2	ACE	-	acetylation	UNP P0A7N9
B1	53	NH2	-	amidation	UNP P0A7N9

- Molecule 51 is a protein called 50S ribosomal protein L32.

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

- Molecule 52 is a protein called 50S ribosomal protein L33.

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

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

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

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

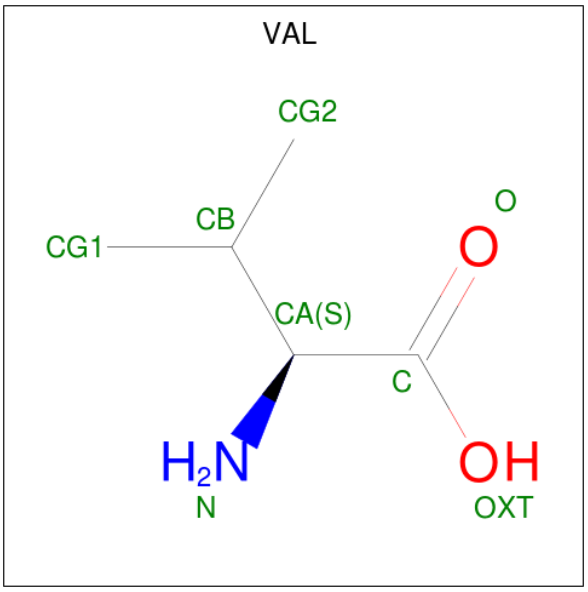
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

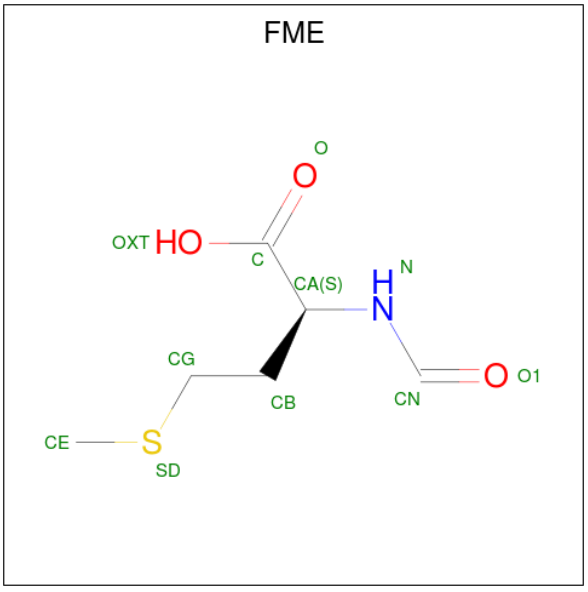
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



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

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



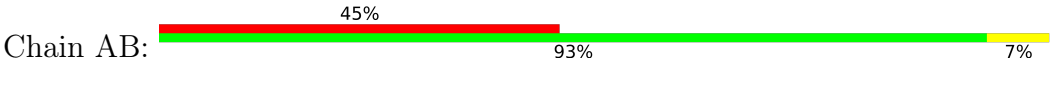
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
58	BA	1	10	6	1	2	1	0

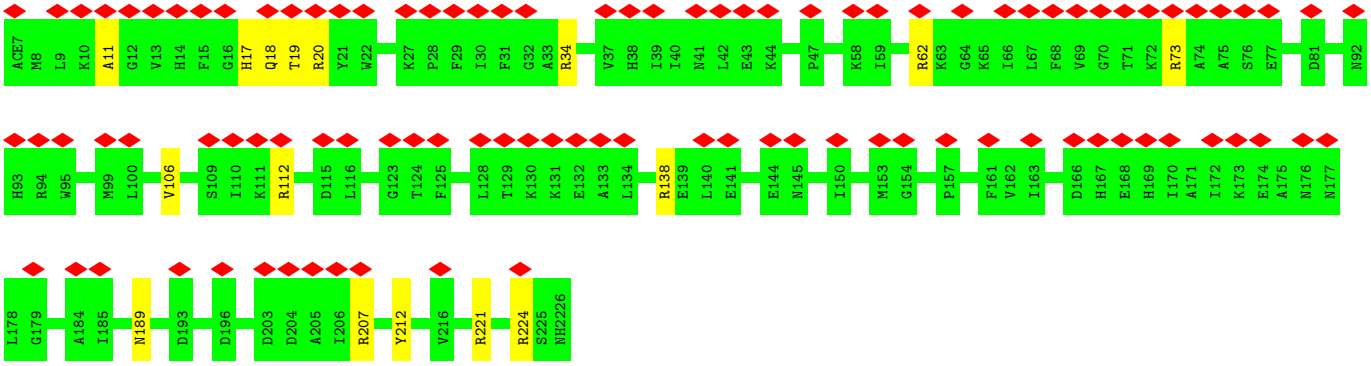
3 Residue-property plots (i)

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

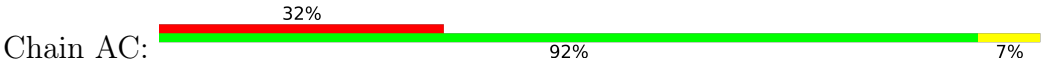
Chain AB:

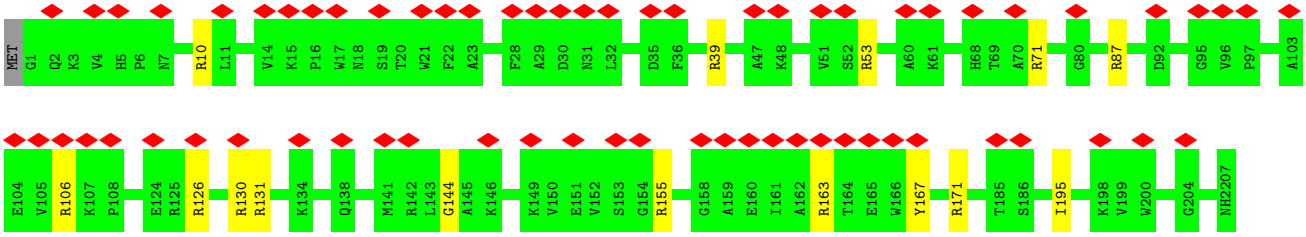




• Molecule 2: 30S ribosomal protein S3

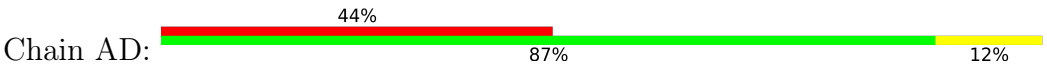
Chain AC:

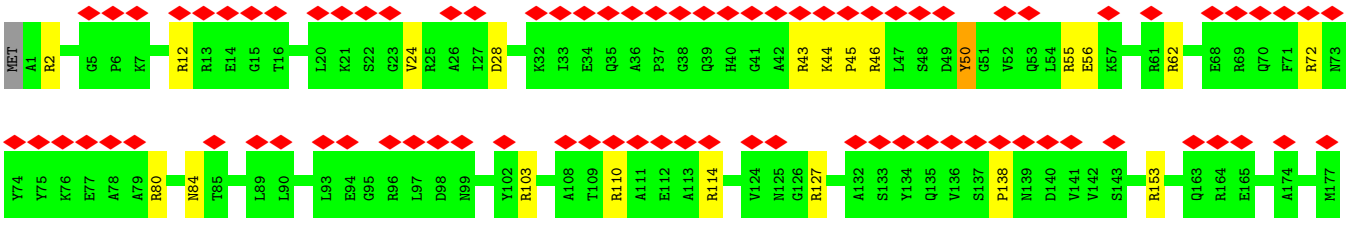


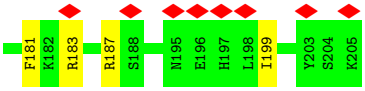


• Molecule 3: 30S ribosomal protein S4

Chain AD:

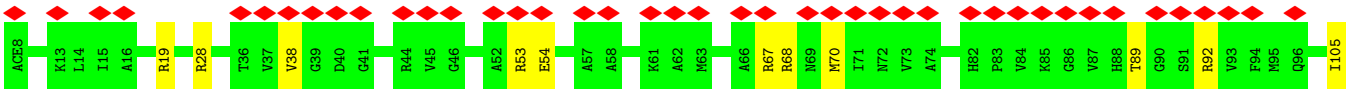


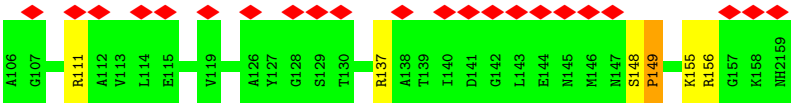




• Molecule 4: 30S ribosomal protein S5

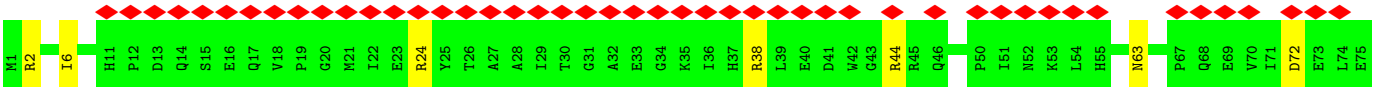
Chain AE:

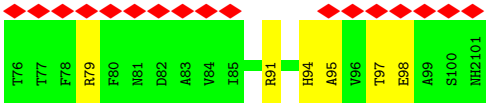




• Molecule 5: 30S ribosomal protein S6

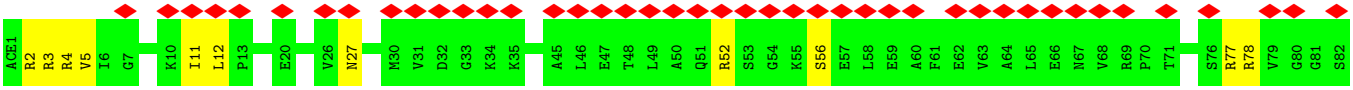
Chain AF:

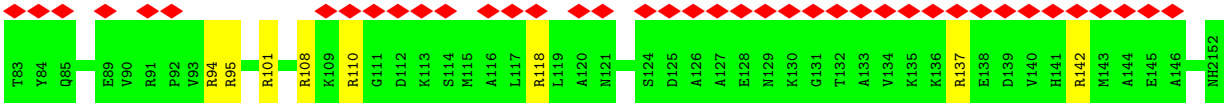




• Molecule 6: 30S ribosomal protein S7

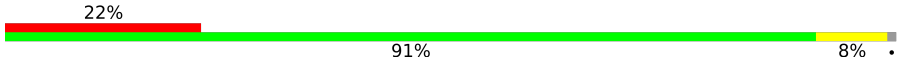
Chain AG:

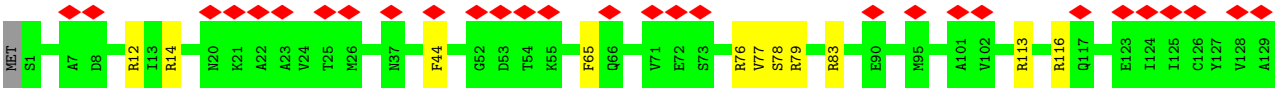




• Molecule 7: 30S ribosomal protein S8

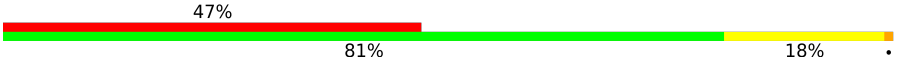
Chain AH:

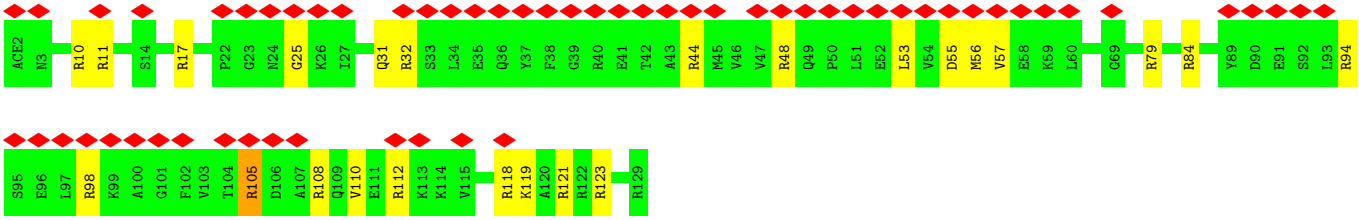




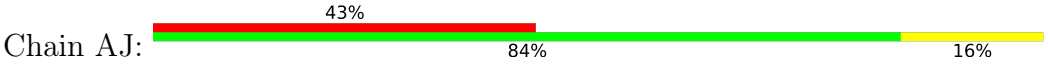
• Molecule 8: 30S ribosomal protein S9

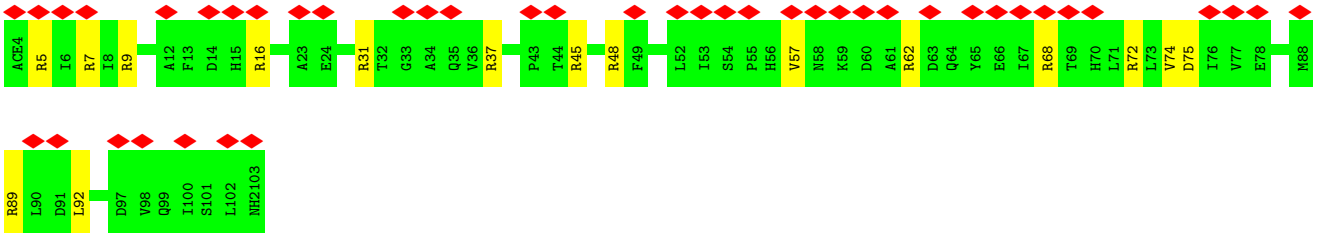
Chain AI:



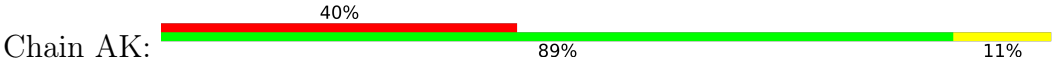


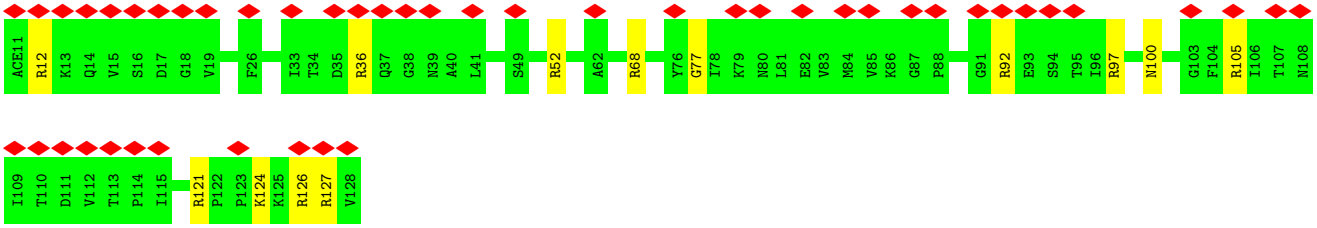
• Molecule 9: 30S ribosomal protein S10



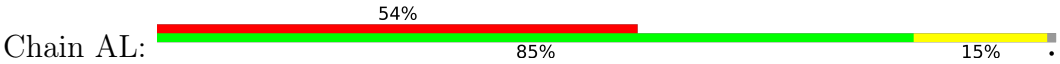


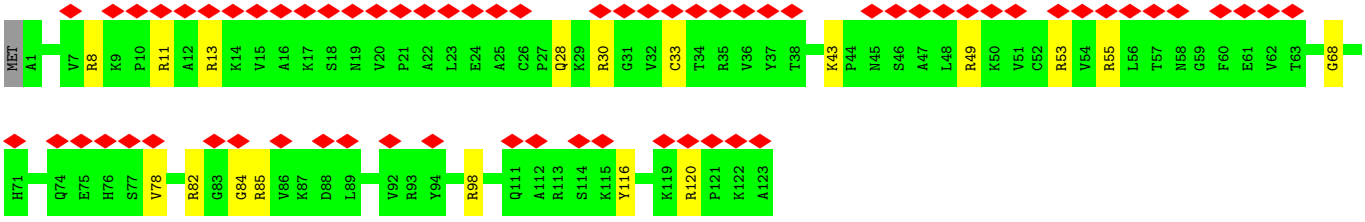
• Molecule 10: 30S ribosomal protein S11



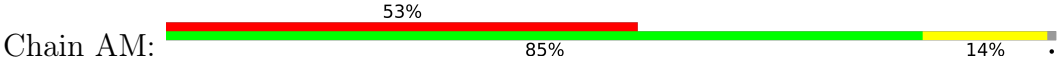


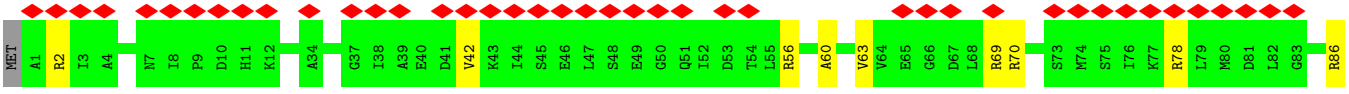
• Molecule 11: 30S ribosomal protein S12

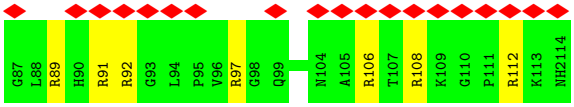




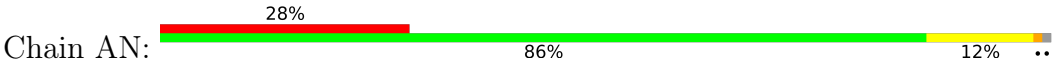
• Molecule 12: 30S ribosomal protein S13



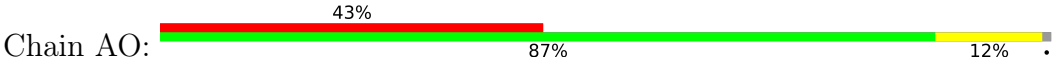




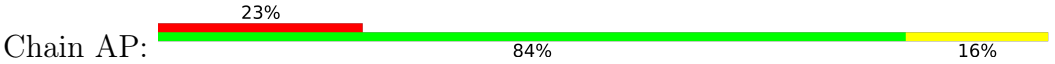
• Molecule 13: 30S ribosomal protein S14



• Molecule 14: 30S ribosomal protein S15



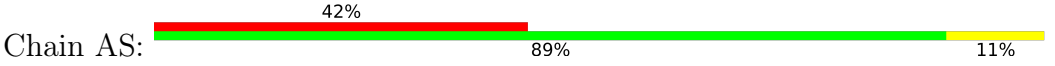
• Molecule 15: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S17

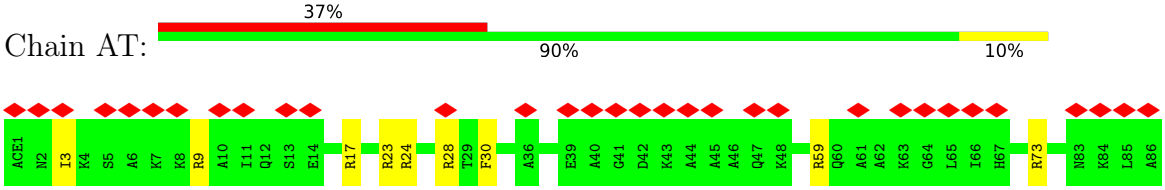
• Molecule 17: 30S ribosomal protein S18

• Molecule 18: 30S ribosomal protein S19



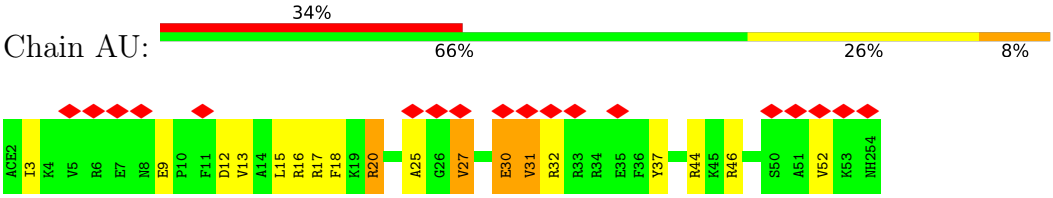
• Molecule 19: 30S ribosomal protein S20

Chain AT:



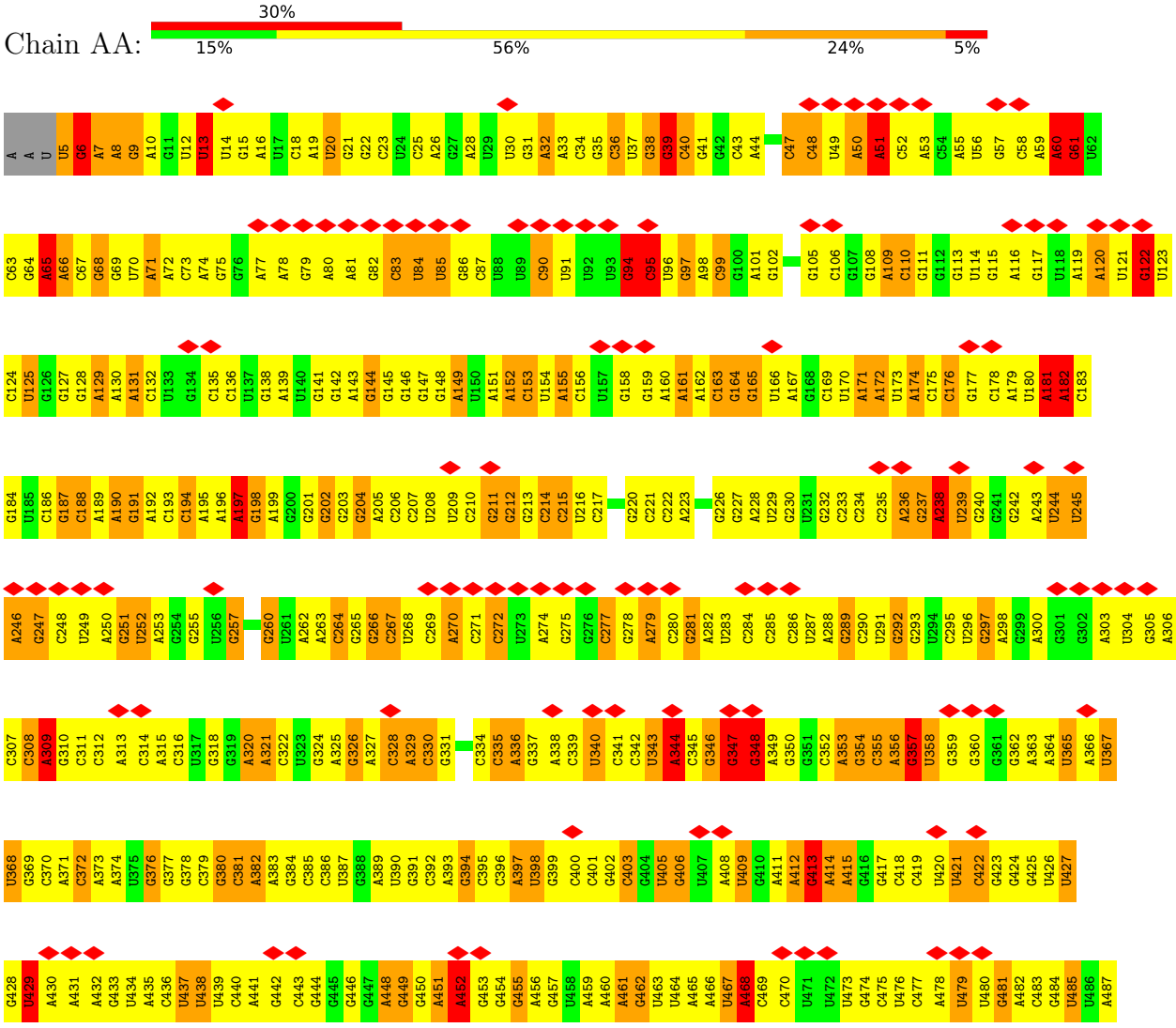
• Molecule 20: 30S ribosomal protein S21

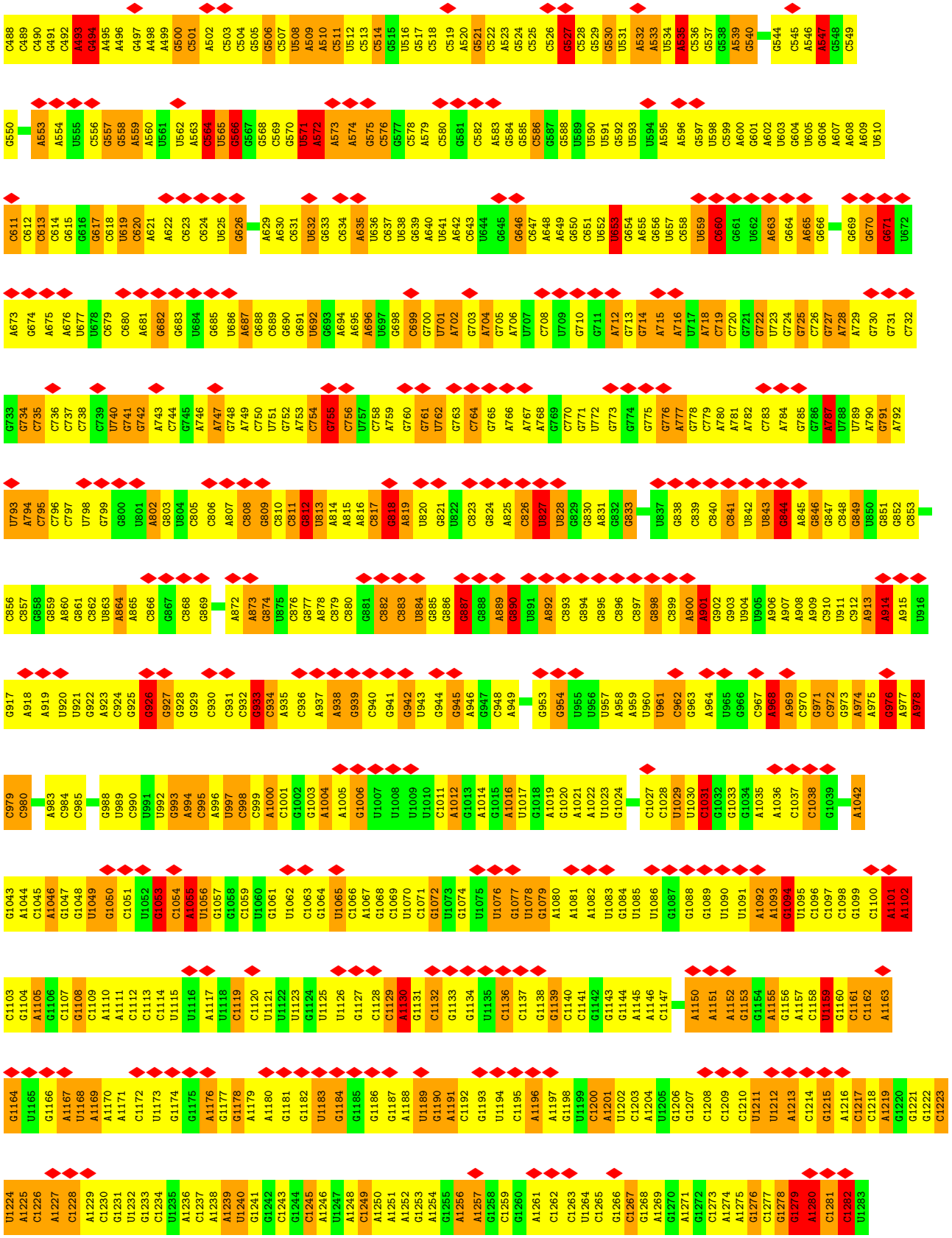
Chain AU:

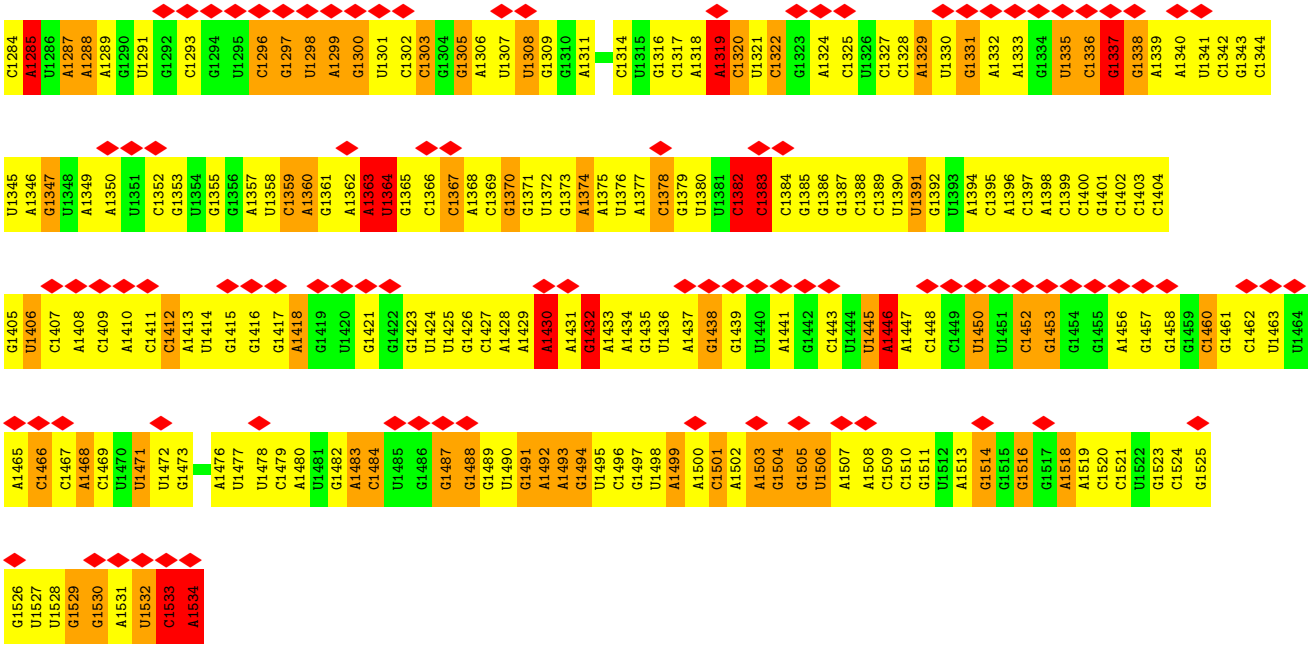


• Molecule 21: 16S ribosomal RNA

Chain AA:

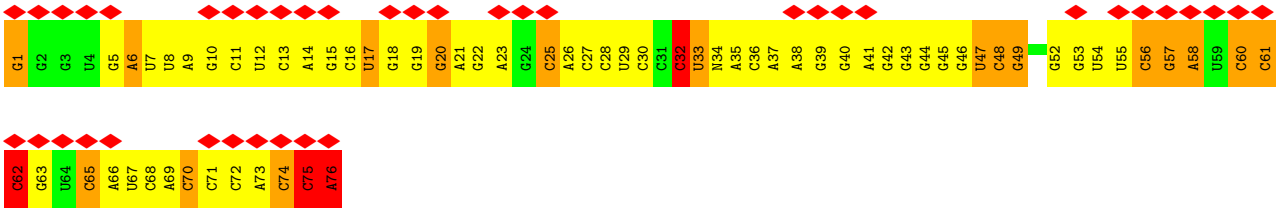






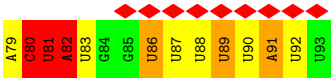
- Molecule 22: fMet-Val-tRNA-Val

Chain A1:



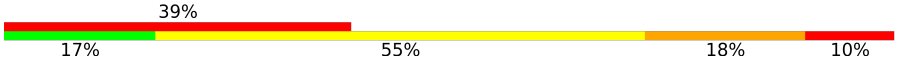
- Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

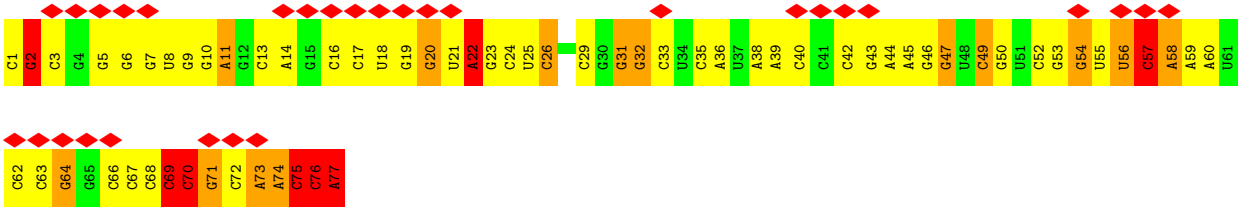
Chain A2:



- Molecule 24: tRNA-fMet

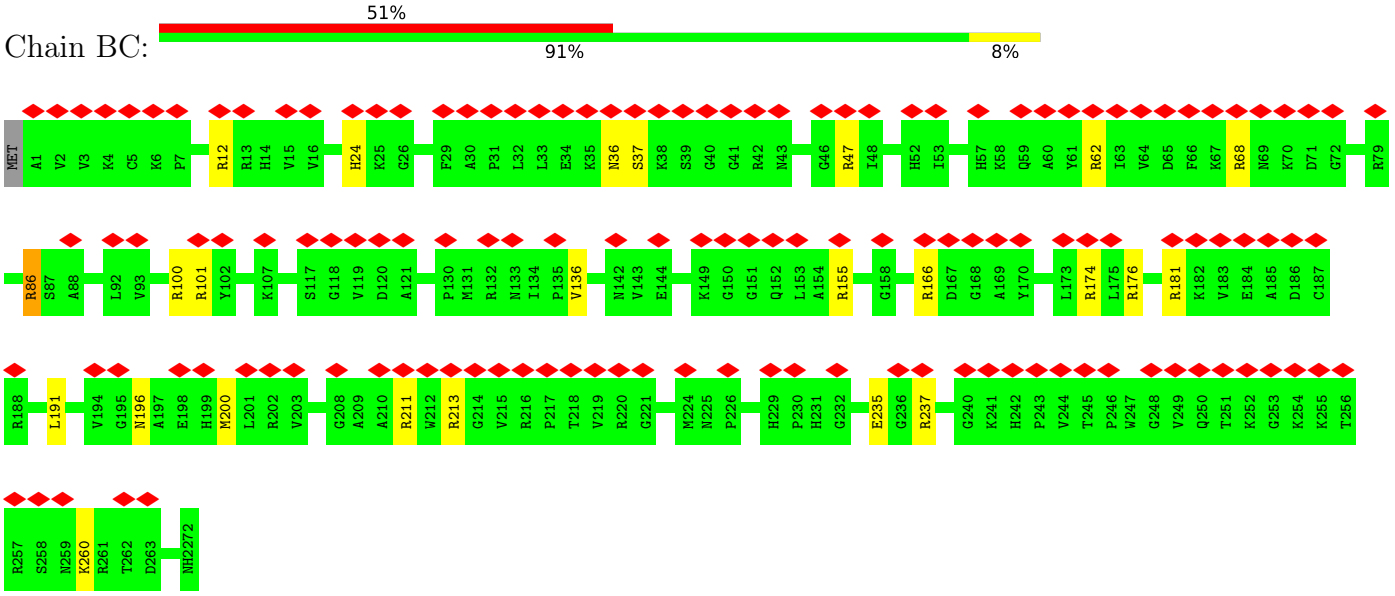
Chain A3:





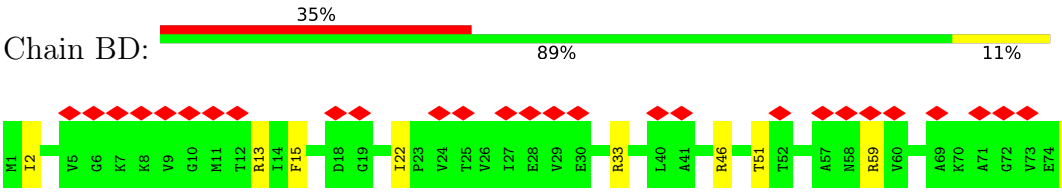
- Molecule 25: 50S ribosomal protein L35

Chain BC:



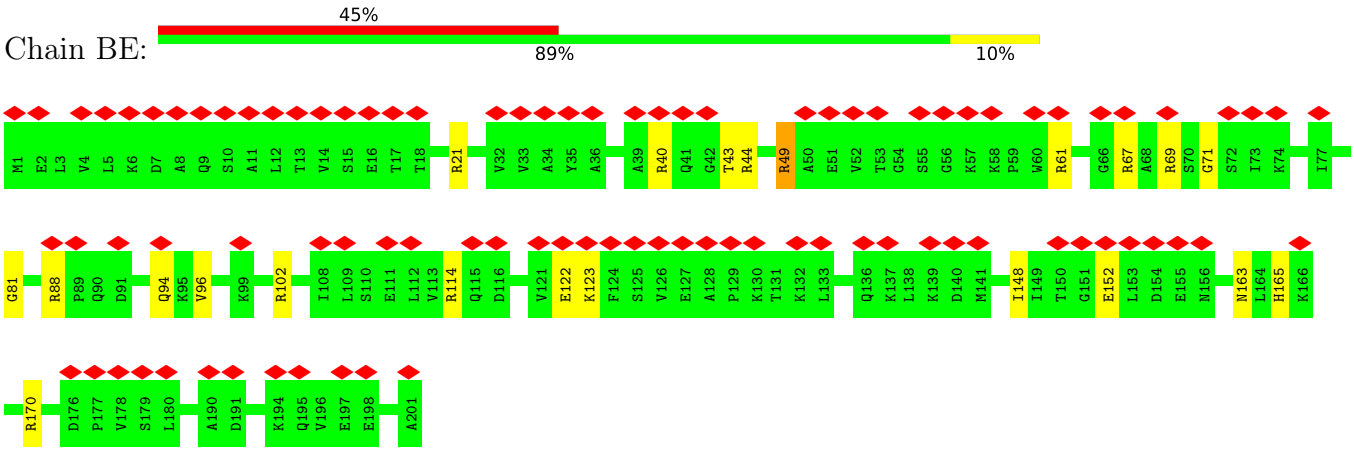
• Molecule 26: 50S ribosomal protein L36

Chain BD:



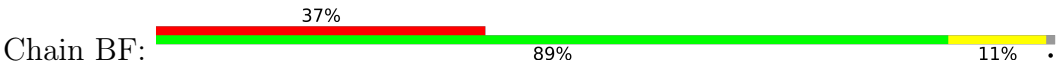
• Molecule 27: 50S ribosomal protein L2

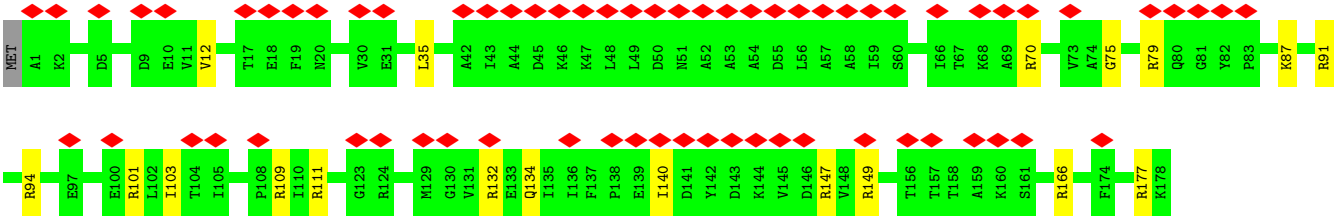
Chain BE:



• Molecule 28: 50S ribosomal protein L3

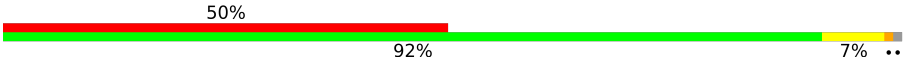
Chain BF:

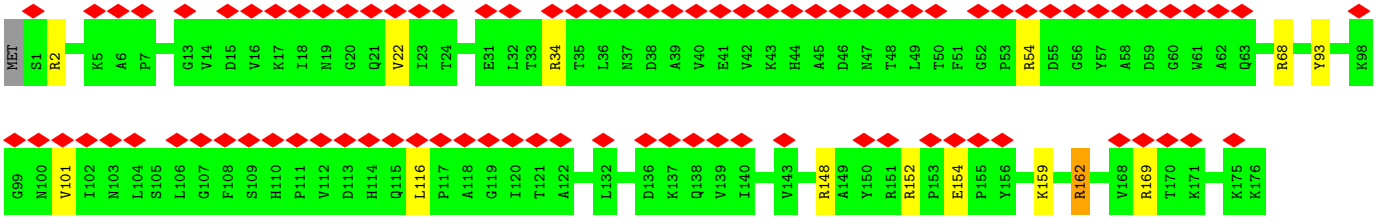




• Molecule 29: 50S ribosomal protein L4

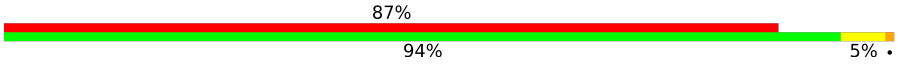
Chain BG:

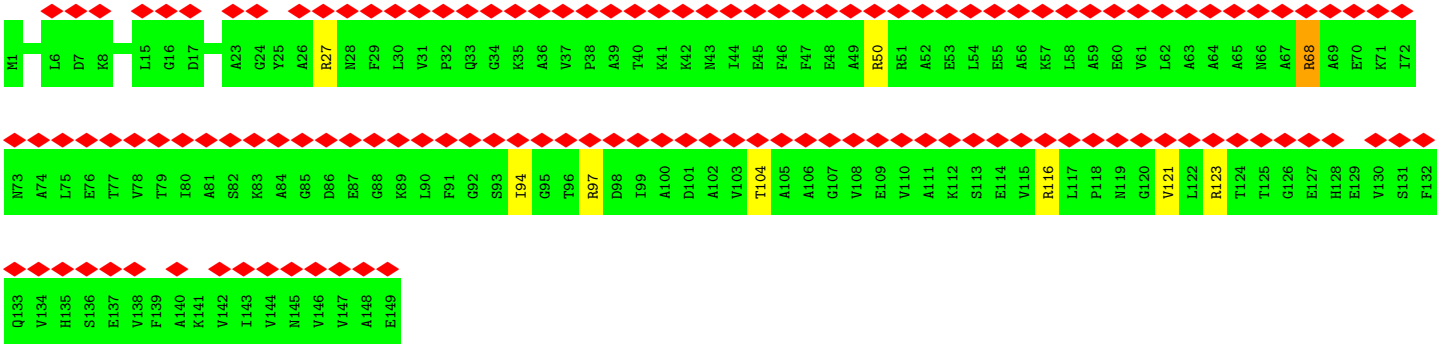




• Molecule 30: 50S ribosomal protein L5

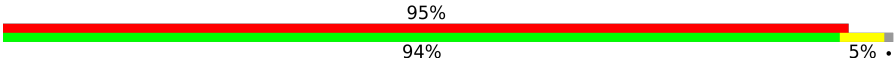
Chain BH:

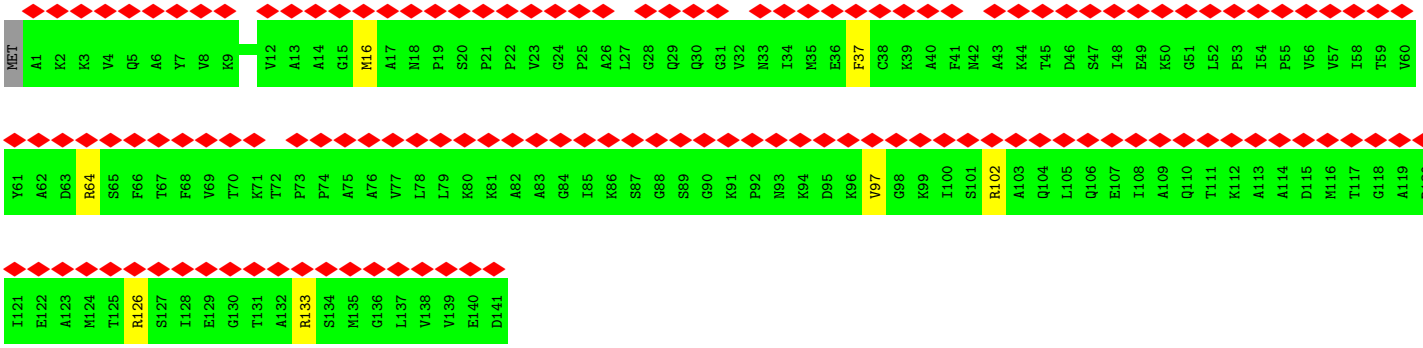




• Molecule 31: 50S ribosomal protein L6

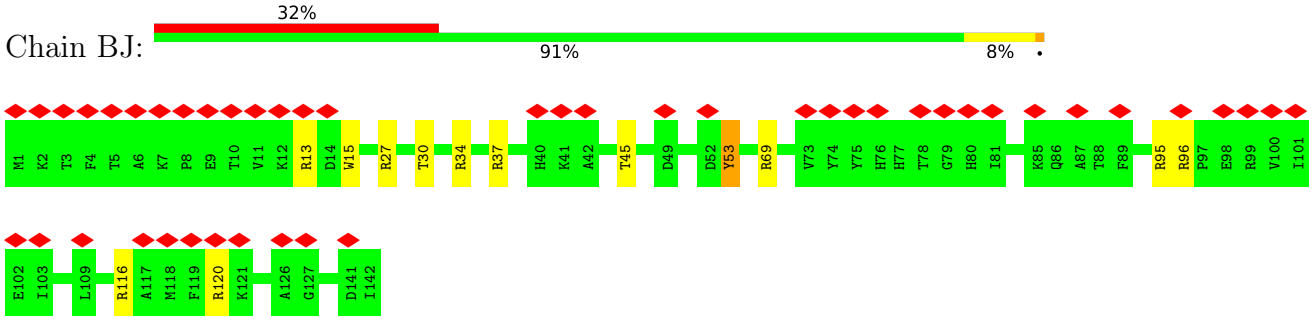
Chain BI:





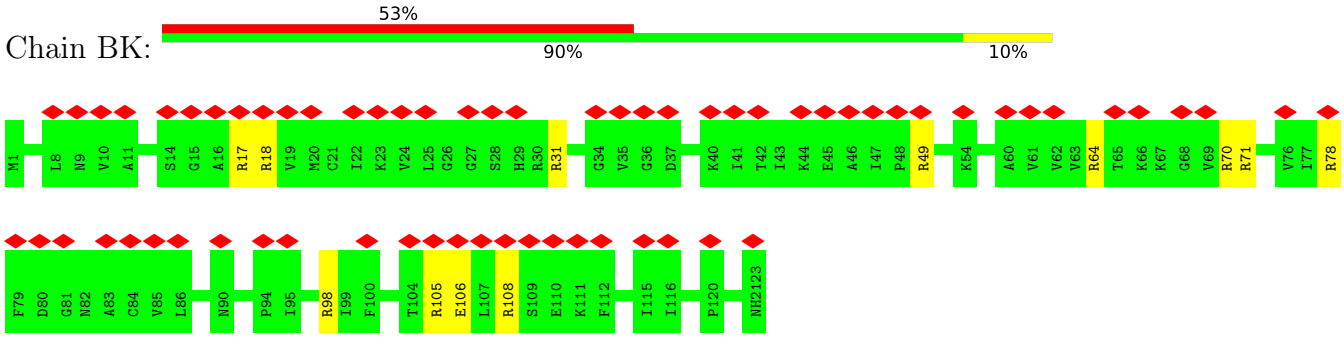
• Molecule 32: 50S ribosomal protein L9

Chain BJ:



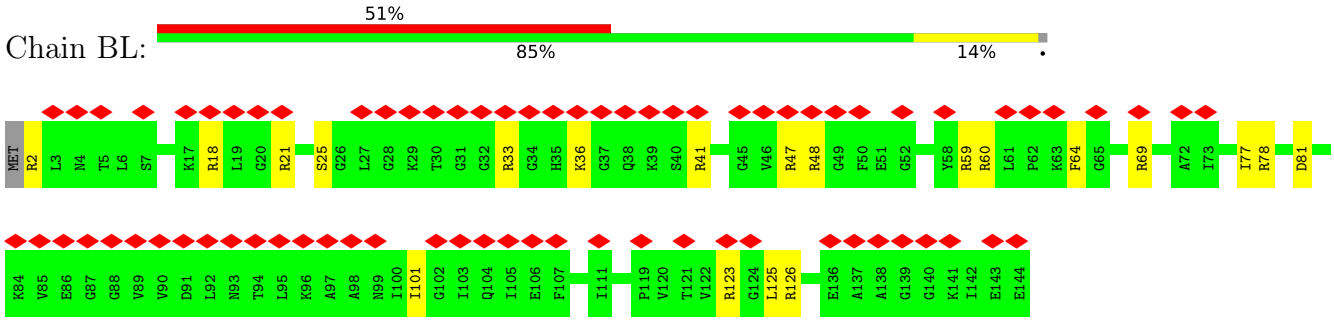
• Molecule 33: 50S ribosomal protein L11

Chain BK:



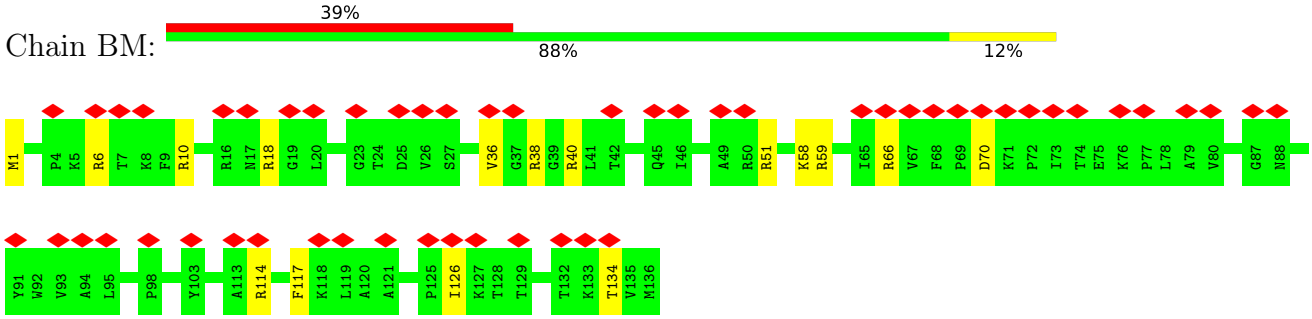
• Molecule 34: 50S ribosomal protein L13

Chain BL:



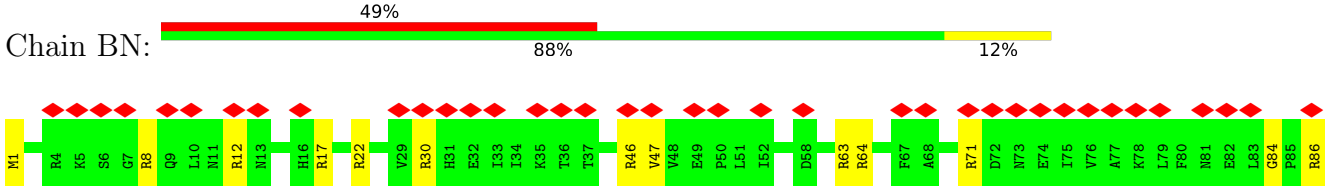
• Molecule 35: 50S ribosomal protein L14

Chain BM:



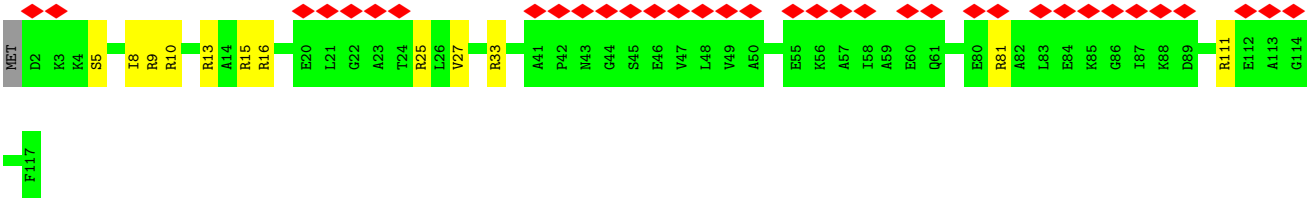
• Molecule 36: 50S ribosomal protein L15

Chain BN:



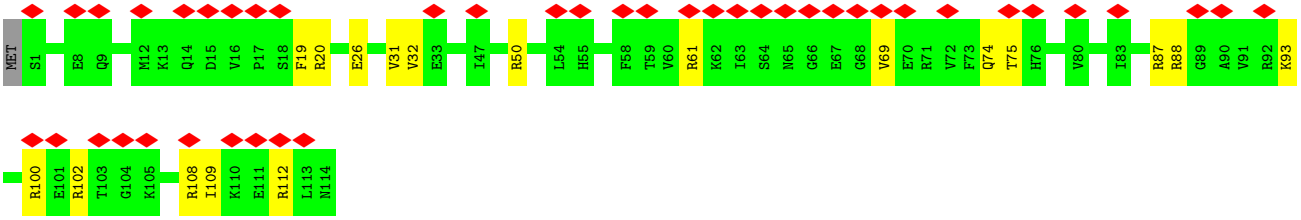
• Molecule 37: 50S ribosomal protein L16

Chain BO:



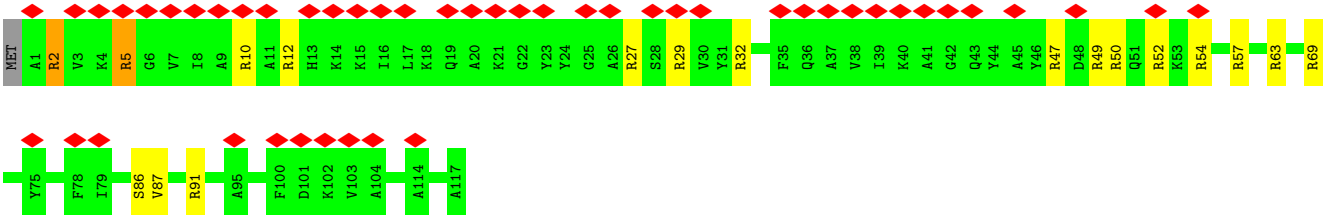
• Molecule 38: 50S ribosomal protein L17

Chain BP:



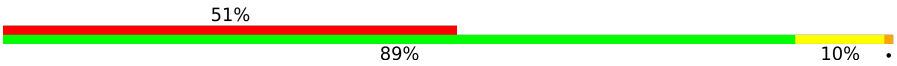
• Molecule 39: 50S ribosomal protein L18

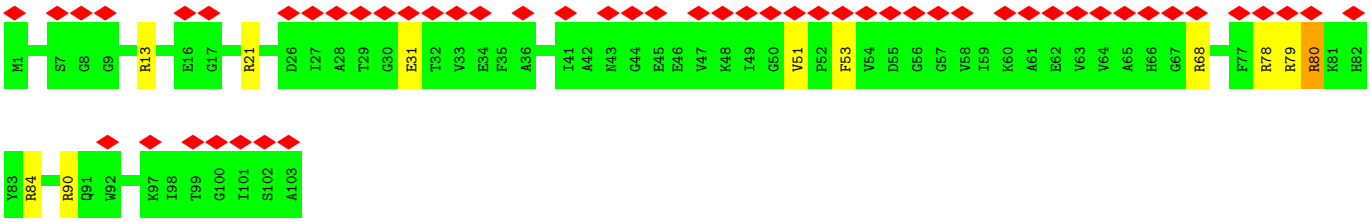
Chain BQ:



• Molecule 40: 50S ribosomal protein L19

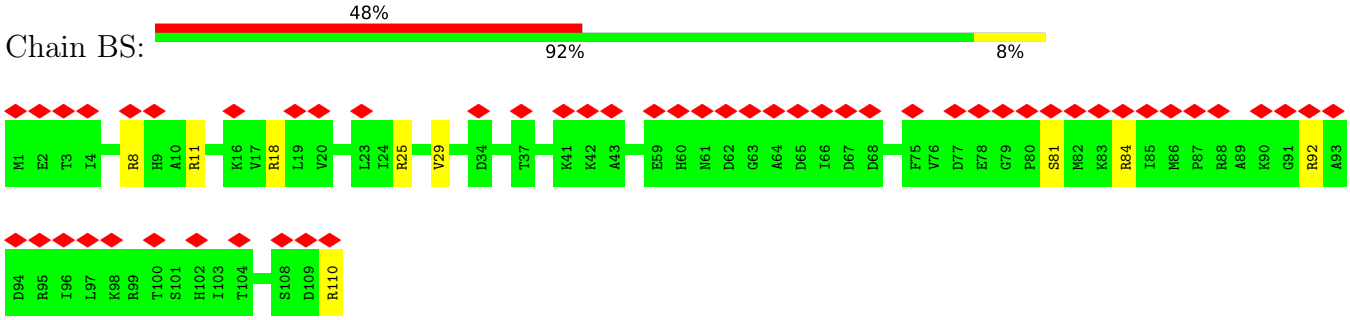
Chain BR:





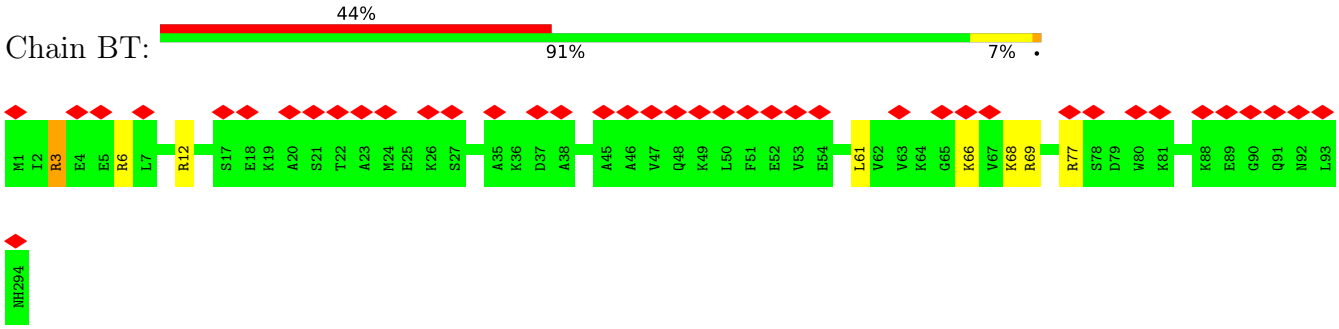
• Molecule 41: 50S ribosomal protein L20

Chain BS:



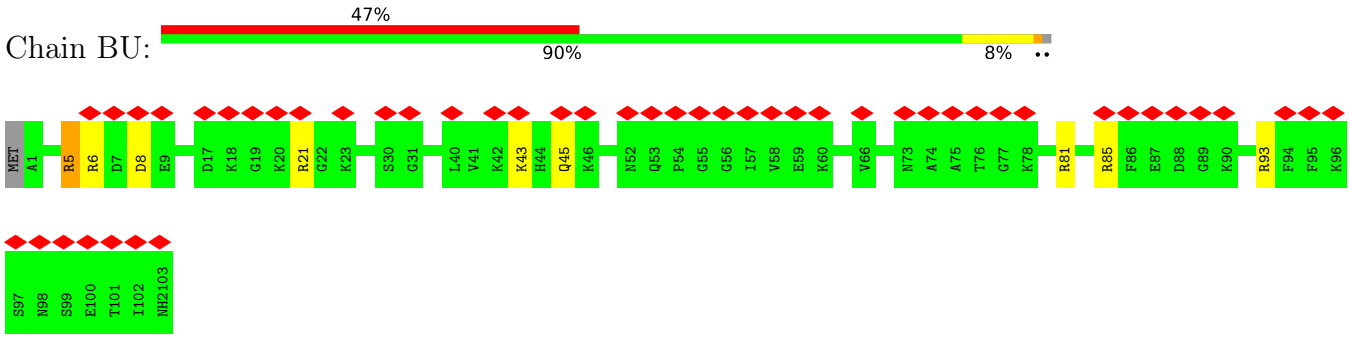
• Molecule 42: 50S ribosomal protein L21

Chain BT:



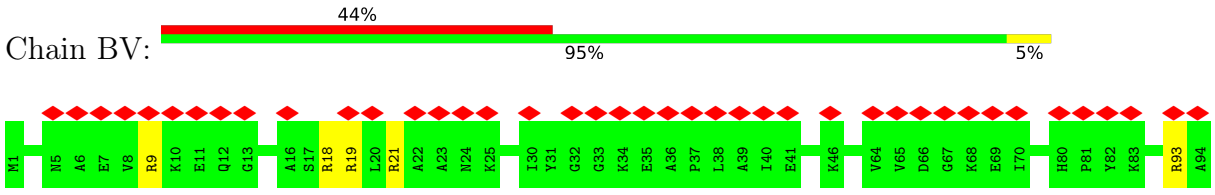
• Molecule 43: 50S ribosomal protein L22

Chain BU:



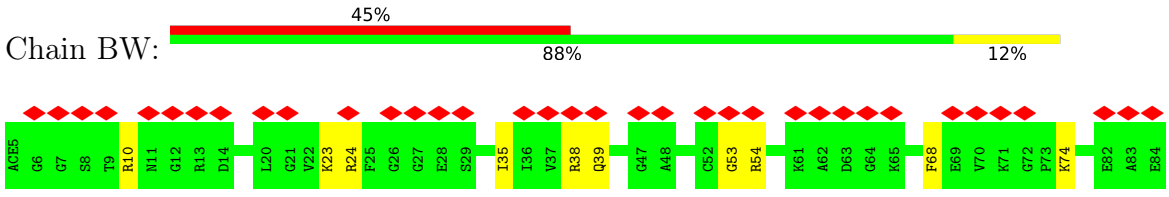
• Molecule 44: 50S ribosomal protein L23

Chain BV:



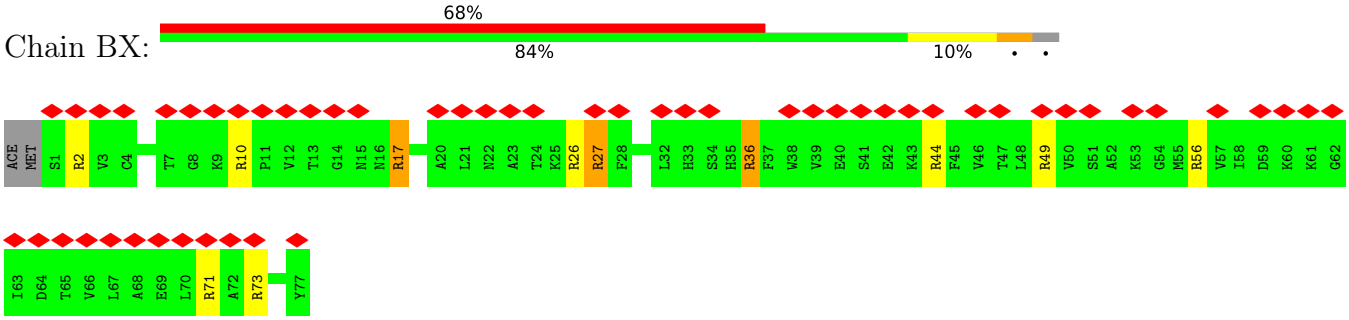
• Molecule 45: 50S ribosomal protein L24

Chain BW:



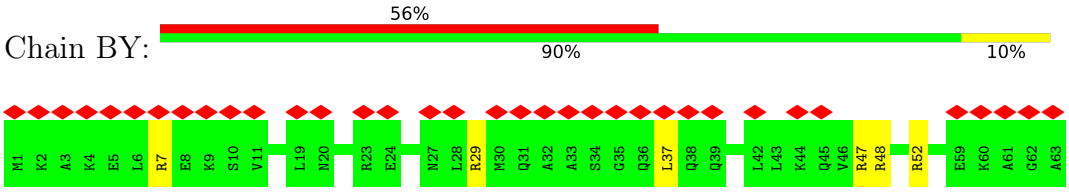
• Molecule 46: 50S ribosomal protein L25

Chain BX:



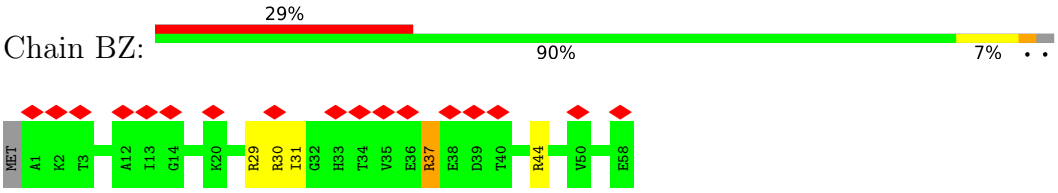
• Molecule 47: 50S ribosomal protein L27

Chain BY:



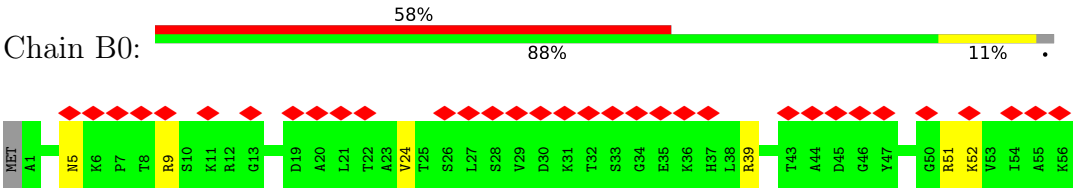
• Molecule 48: 50S ribosomal protein L28

Chain BZ:



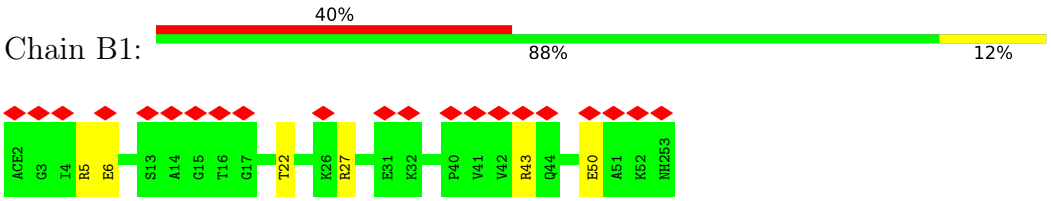
• Molecule 49: 50S ribosomal protein L29

Chain B0:



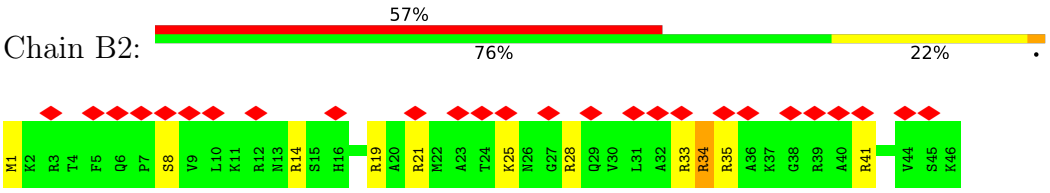
• Molecule 50: 50S ribosomal protein L30

Chain B1:



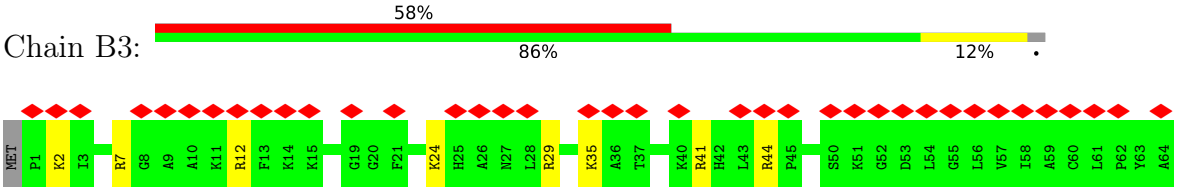
• Molecule 51: 50S ribosomal protein L32

Chain B2:



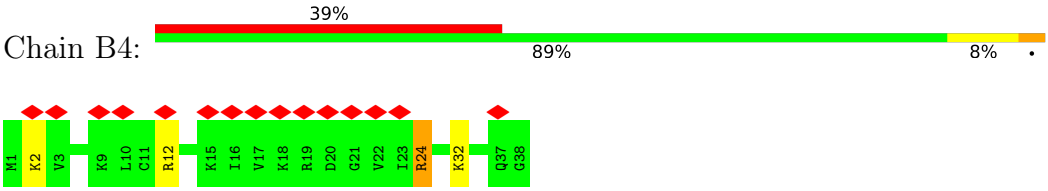
• Molecule 52: 50S ribosomal protein L33

Chain B3:



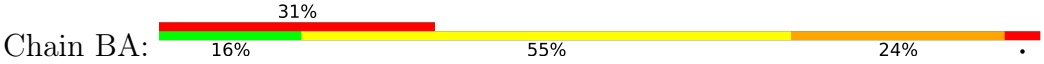
• Molecule 53: 50S ribosomal protein L34

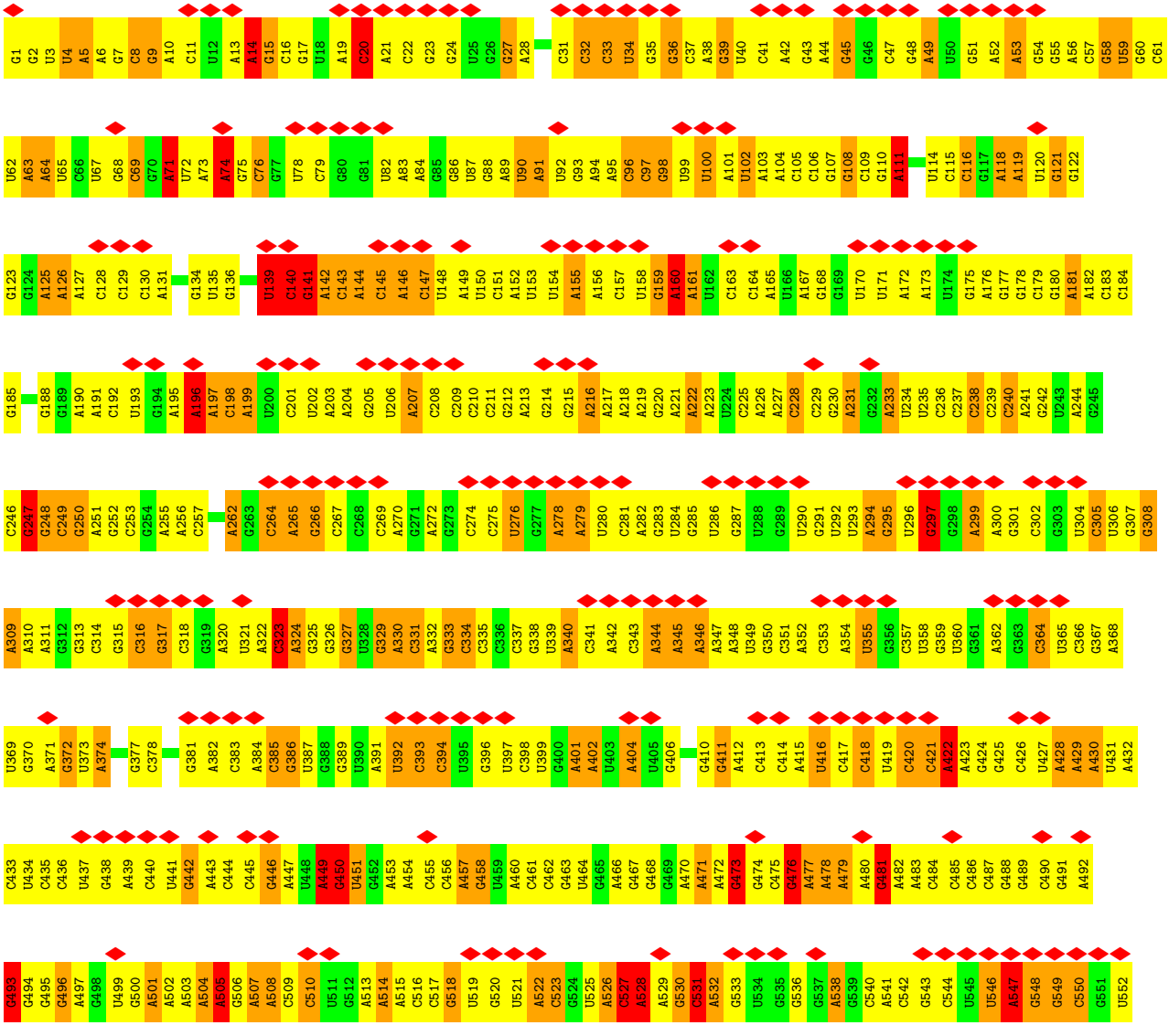
Chain B4:

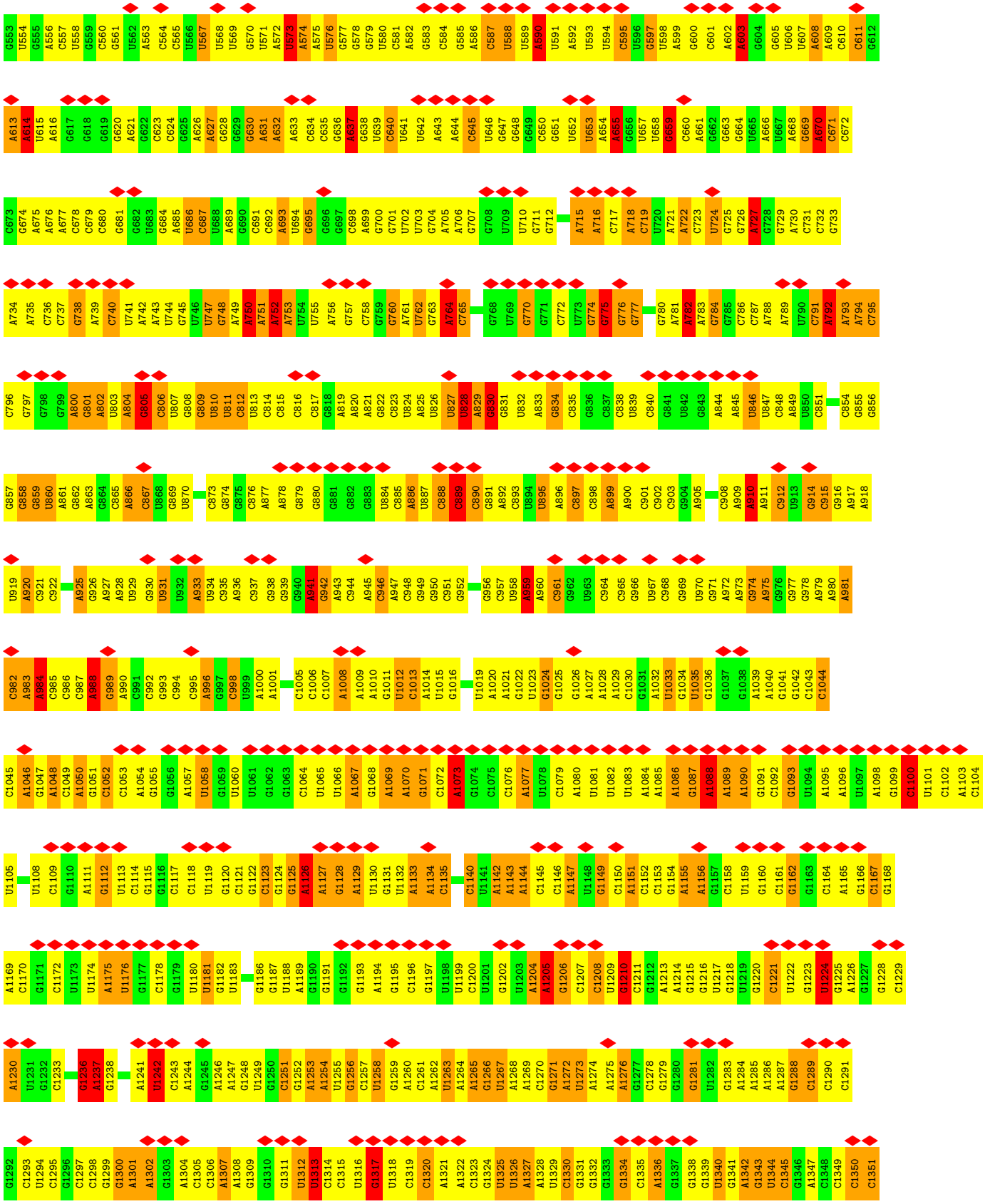


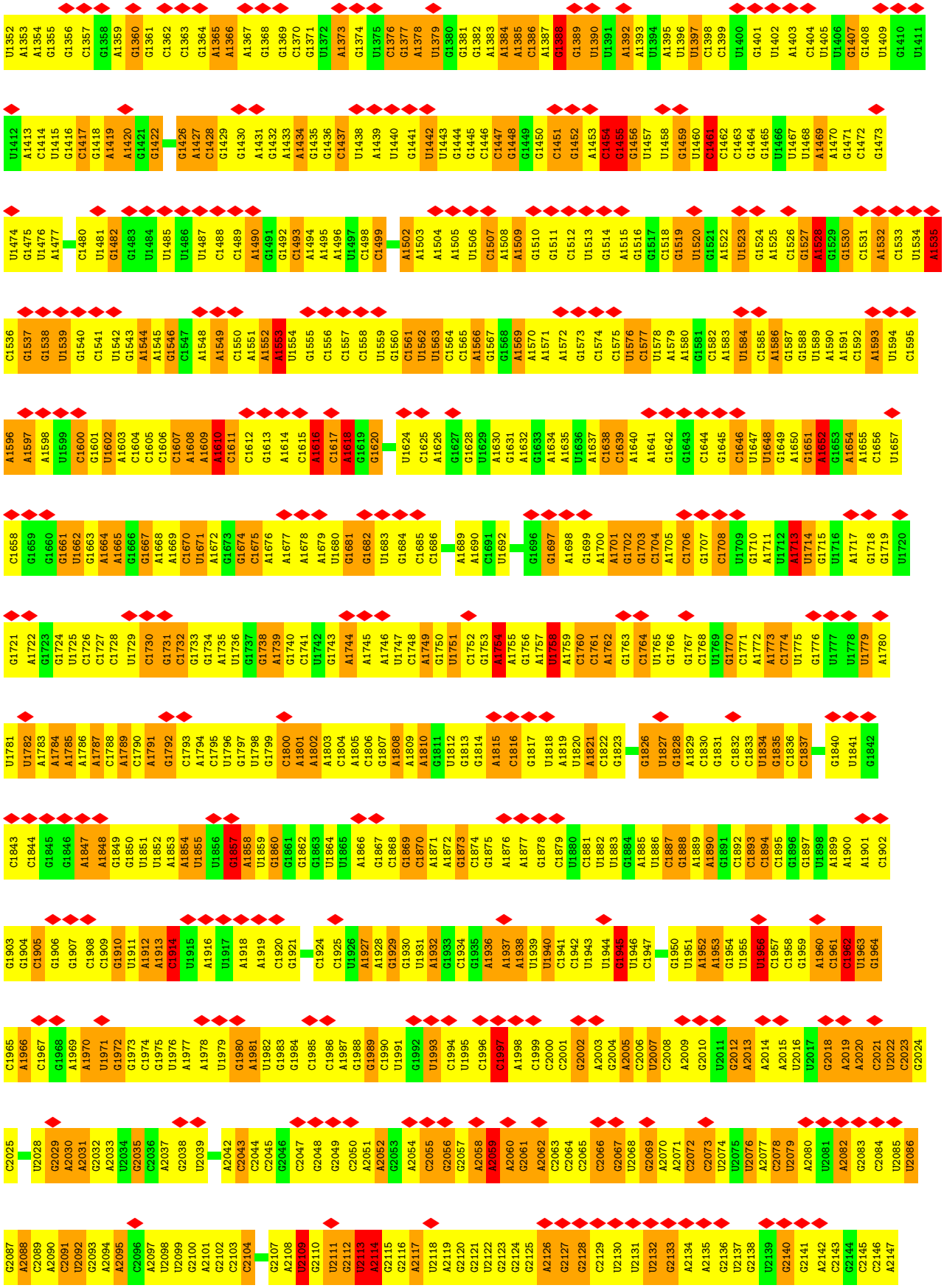
• Molecule 54: 23S ribosomal RNA

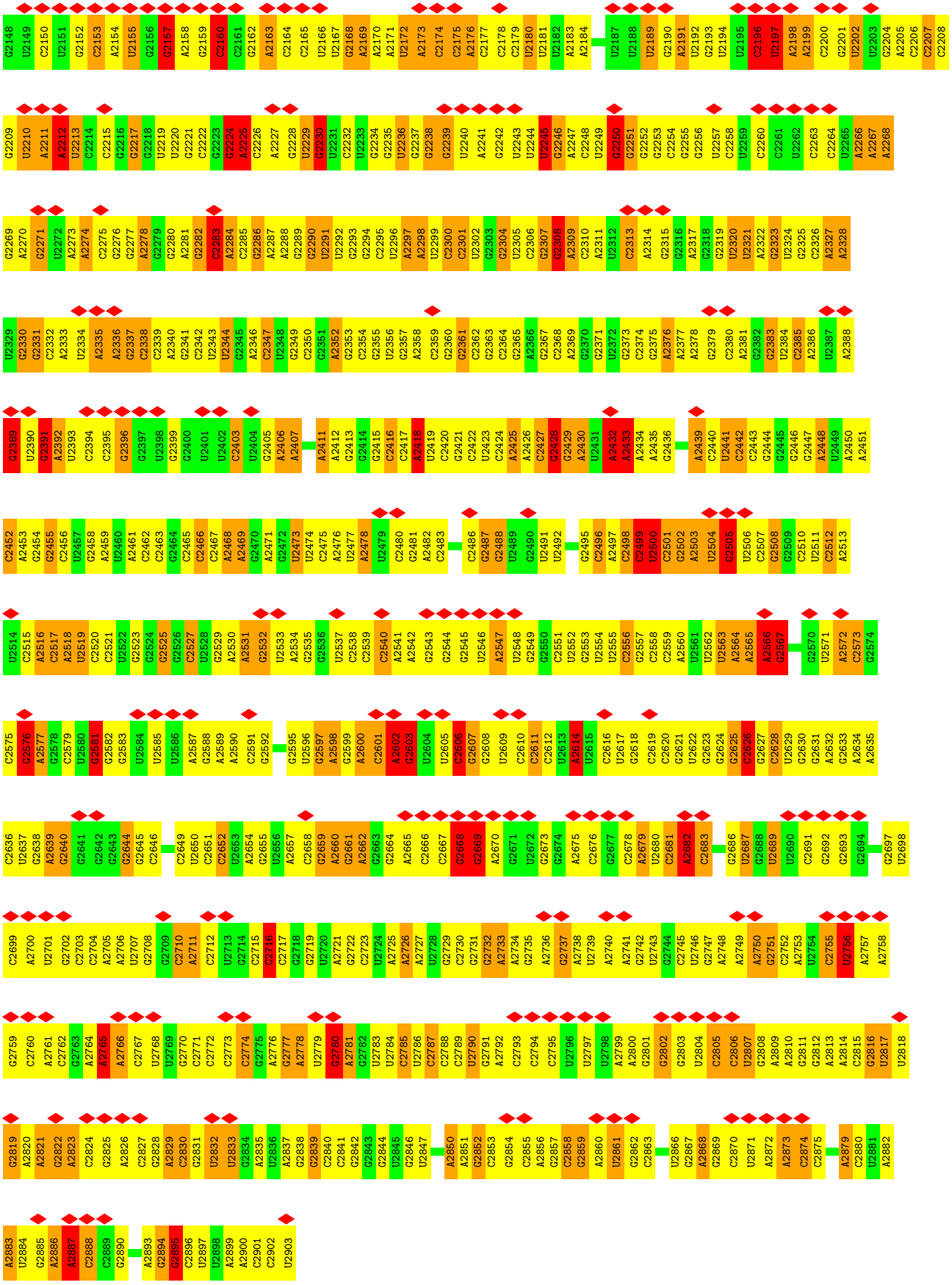
Chain BA:





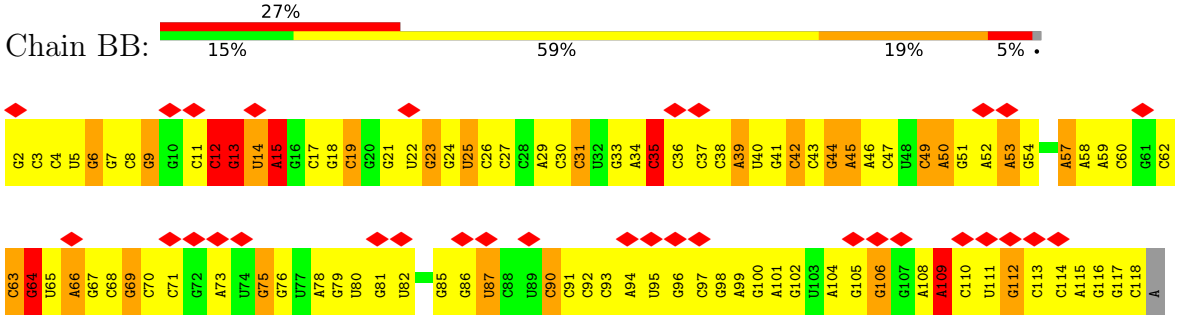






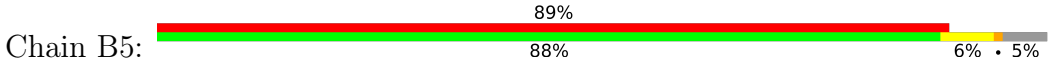
• Molecule 55: 5S ribosomal RNA

Chain BB:



• Molecule 56: 50S ribosomal protein L1

Chain B5:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14235	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	198.725	Depositor
Minimum map value	-116.714	Depositor
Average map value	-0.391	Depositor
Map value standard deviation	21.414	Depositor
Recommended contour level	30.0	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 (i)

5.1 Standard geometry (i)

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

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	0.72	0/1736	1.11	13/2340 (0.6%)
2	AC	0.76	0/1651	1.17	14/2225 (0.6%)
3	AD	0.76	0/1665	1.23	21/2227 (0.9%)
4	AE	0.70	0/1119	1.12	11/1506 (0.7%)
5	AF	0.79	0/835	1.15	7/1128 (0.6%)
6	AG	0.77	0/1188	1.24	16/1593 (1.0%)
7	AH	0.74	0/989	1.11	7/1326 (0.5%)
8	AI	0.85	0/1035	1.33	20/1377 (1.5%)
9	AJ	0.78	0/797	1.39	16/1079 (1.5%)
10	AK	0.80	0/894	1.27	12/1207 (1.0%)
11	AL	0.80	0/969	1.25	13/1300 (1.0%)
12	AM	0.82	0/884	1.29	13/1181 (1.1%)
13	AN	0.82	0/817	1.25	9/1088 (0.8%)
14	AO	0.77	0/722	1.18	6/964 (0.6%)
15	AP	0.82	0/648	1.42	14/870 (1.6%)
16	AQ	0.71	0/658	1.18	8/883 (0.9%)
17	AR	0.77	0/463	1.19	5/623 (0.8%)
18	AS	0.80	0/653	1.23	7/879 (0.8%)
19	AT	0.75	0/672	1.18	7/890 (0.8%)
20	AU	0.87	0/431	1.59	8/572 (1.4%)
21	AA	1.88	441/36759 (1.2%)	2.29	2411/57346 (4.2%)
22	A1	1.89	18/1668 (1.1%)	2.23	102/2595 (3.9%)
23	A2	1.67	1/343 (0.3%)	2.18	19/531 (3.6%)
24	A3	1.93	26/1722 (1.5%)	2.27	102/2685 (3.8%)
25	BC	0.79	0/2121	1.28	19/2852 (0.7%)
26	BD	0.72	0/1586	1.23	12/2134 (0.6%)
27	BE	0.71	0/1571	1.17	11/2113 (0.5%)
28	BF	0.77	0/1444	1.18	13/1937 (0.7%)
29	BG	0.72	0/1343	1.16	7/1816 (0.4%)
30	BH	0.67	0/1122	1.14	6/1515 (0.4%)
31	BI	0.69	0/1046	1.11	7/1410 (0.5%)
32	BJ	0.74	0/1152	1.23	9/1551 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BK	0.76	0/947	1.23	11/1268 (0.9%)
34	BL	0.76	0/1054	1.28	14/1403 (1.0%)
35	BM	0.79	0/1093	1.27	11/1460 (0.8%)
36	BN	0.80	0/973	1.26	12/1301 (0.9%)
37	BO	0.80	0/902	1.28	10/1209 (0.8%)
38	BP	0.77	0/929	1.26	9/1242 (0.7%)
39	BQ	0.80	0/960	1.37	17/1278 (1.3%)
40	BR	0.73	0/829	1.22	9/1107 (0.8%)
41	BS	0.71	0/864	1.18	7/1156 (0.6%)
42	BT	0.73	0/744	1.19	5/994 (0.5%)
43	BU	0.70	0/787	1.17	6/1051 (0.6%)
44	BV	0.72	0/766	1.12	5/1025 (0.5%)
45	BW	0.73	0/604	1.25	4/799 (0.5%)
46	BX	0.82	0/635	1.47	14/848 (1.7%)
47	BY	0.70	0/510	1.22	5/677 (0.7%)
48	BZ	0.73	0/453	1.27	4/605 (0.7%)
49	B0	0.78	0/450	1.25	4/599 (0.7%)
50	B1	0.75	0/417	1.10	3/556 (0.5%)
51	B2	0.91	0/380	1.45	8/498 (1.6%)
52	B3	0.73	0/513	1.24	6/676 (0.9%)
53	B4	0.72	0/303	1.25	3/397 (0.8%)
54	BA	1.74	667/69796 (1.0%)	2.28	4747/108888 (4.4%)
55	BB	1.83	58/2800 (2.1%)	2.30	198/4367 (4.5%)
56	B5	0.68	0/1673	1.14	10/2255 (0.4%)
All	All	1.56	1211/160085 (0.8%)	2.06	8067/239402 (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
3	AD	0	1
4	AE	0	1
13	AN	0	1
14	AO	0	1
21	AA	0	342
22	A1	0	13
23	A2	0	5
24	A3	0	19
46	BX	0	1
54	BA	0	646

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
55	BB	0	23
56	B5	0	1
All	All	0	1054

All (1211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2048	G	C2-N2	-6.80	1.27	1.34
24	A3	75	C	N3-C4	-6.76	1.29	1.33
21	AA	1063	C	C4-N4	-6.70	1.27	1.33
23	A2	80	C	C4-N4	-6.68	1.27	1.33
55	BB	113	C	C4-N4	-6.68	1.27	1.33
54	BA	2297	A	C6-N1	-6.65	1.30	1.35
54	BA	1646	C	C4-N4	-6.64	1.27	1.33
55	BB	34	A	C6-N1	-6.62	1.30	1.35
21	AA	658	C	C4-N4	-6.60	1.28	1.33
54	BA	2091	C	C4-N4	-6.58	1.28	1.33
21	AA	341	C	C4-N4	-6.57	1.28	1.33
21	AA	1113	C	C4-N4	-6.55	1.28	1.33
54	BA	32	C	C4-N4	-6.54	1.28	1.33
55	BB	90	C	C4-N4	-6.50	1.28	1.33
24	A3	63	C	C4-N4	-6.49	1.28	1.33
21	AA	1467	C	C4-N4	-6.48	1.28	1.33
24	A3	77	A	C6-N1	-6.46	1.31	1.35
54	BA	1556	C	C4-N4	-6.45	1.28	1.33
21	AA	183	C	C4-N4	-6.44	1.28	1.33
54	BA	565	C	C4-N4	-6.43	1.28	1.33
21	AA	422	C	C4-N4	-6.43	1.28	1.33
54	BA	343	C	C4-N4	-6.42	1.28	1.33
55	BB	27	C	C4-N4	-6.41	1.28	1.33
21	AA	197	A	C6-N1	-6.40	1.31	1.35
21	AA	490	C	C4-N4	-6.39	1.28	1.33
54	BA	1768	C	C4-N4	-6.38	1.28	1.33
54	BA	671	C	C4-N4	-6.38	1.28	1.33
21	AA	1257	A	C6-N1	-6.37	1.31	1.35
54	BA	1550	C	C4-N4	-6.37	1.28	1.33
54	BA	2282	G	C2-N2	-6.34	1.28	1.34
54	BA	2863	C	C4-N4	-6.34	1.28	1.33
54	BA	774	G	C2-N2	-6.32	1.28	1.34
54	BA	1389	G	C2-N2	-6.32	1.28	1.34
54	BA	51	G	C2-N2	-6.31	1.28	1.34
54	BA	1386	C	C4-N4	-6.30	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2326	C	C4-N4	-6.29	1.28	1.33
55	BB	4	C	C4-N4	-6.29	1.28	1.33
21	AA	342	C	C4-N4	-6.28	1.28	1.33
21	AA	1457	G	C2-N2	-6.28	1.28	1.34
54	BA	577	G	C6-N1	-6.25	1.35	1.39
54	BA	2427	C	C4-N4	-6.25	1.28	1.33
54	BA	1875	G	C2-N2	-6.25	1.28	1.34
21	AA	57	G	C2-N2	-6.24	1.28	1.34
21	AA	736	C	N3-C4	-6.23	1.29	1.33
21	AA	980	C	C4-N4	-6.23	1.28	1.33
21	AA	379	C	C4-N4	-6.22	1.28	1.33
54	BA	1370	C	C4-N4	-6.22	1.28	1.33
21	AA	52	C	C4-N4	-6.22	1.28	1.33
22	A1	72	C	C4-N4	-6.21	1.28	1.33
54	BA	37	C	C4-N4	-6.20	1.28	1.33
54	BA	2359	C	C4-N4	-6.20	1.28	1.33
21	AA	732	C	C4-N4	-6.20	1.28	1.33
54	BA	2064	C	C4-N4	-6.19	1.28	1.33
54	BA	2428	G	C2-N2	-6.19	1.28	1.34
54	BA	1724	G	C2-N2	-6.18	1.28	1.34
54	BA	2285	C	C4-N4	-6.17	1.28	1.33
54	BA	1950	G	C2-N2	-6.16	1.28	1.34
21	AA	186	C	C4-N4	-6.15	1.28	1.33
54	BA	2575	C	C4-N4	-6.15	1.28	1.33
54	BA	1043	C	C4-N4	-6.15	1.28	1.33
54	BA	806	C	C4-N4	-6.15	1.28	1.33
54	BA	1595	C	C4-N4	-6.15	1.28	1.33
24	A3	68	C	C4-N4	-6.15	1.28	1.33
54	BA	1793	C	C4-N4	-6.14	1.28	1.33
54	BA	433	C	C4-N4	-6.14	1.28	1.33
54	BA	2620	C	C4-N4	-6.14	1.28	1.33
21	AA	330	C	C4-N4	-6.13	1.28	1.33
54	BA	758	C	C4-N4	-6.13	1.28	1.33
22	A1	60	C	C4-N4	-6.12	1.28	1.33
54	BA	2420	C	C4-N4	-6.12	1.28	1.33
21	AA	176	C	C4-N4	-6.12	1.28	1.33
21	AA	1054	C	C4-N4	-6.12	1.28	1.33
54	BA	1833	C	C4-N4	-6.11	1.28	1.33
21	AA	1302	C	C4-N4	-6.10	1.28	1.33
54	BA	2045	C	C4-N4	-6.10	1.28	1.33
54	BA	1426	G	C2-N2	-6.09	1.28	1.34
21	AA	1407	C	C4-N4	-6.09	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1496	C	C4-N4	-6.09	1.28	1.33
55	BB	86	G	C2-N2	-6.09	1.28	1.34
54	BA	2025	C	C4-N4	-6.08	1.28	1.33
21	AA	1347	G	C2-N2	-6.08	1.28	1.34
21	AA	1228	C	C4-N4	-6.08	1.28	1.33
54	BA	781	A	C6-N1	-6.08	1.31	1.35
55	BB	91	C	C4-N4	-6.07	1.28	1.33
21	AA	675	A	C6-N1	-6.07	1.31	1.35
54	BA	1401	G	C2-N2	-6.07	1.28	1.34
54	BA	2595	G	C2-N2	-6.06	1.28	1.34
54	BA	1667	G	C2-N2	-6.06	1.28	1.34
54	BA	564	C	C4-N4	-6.06	1.28	1.33
24	A3	71	G	C2-N2	-6.05	1.28	1.34
54	BA	411	G	C2-N2	-6.05	1.28	1.34
21	AA	494	G	C2-N2	-6.05	1.28	1.34
21	AA	1192	C	C4-N4	-6.05	1.28	1.33
54	BA	2160	C	C4-N4	-6.04	1.28	1.33
24	A3	3	C	C4-N4	-6.04	1.28	1.33
54	BA	587	C	C4-N4	-6.04	1.28	1.33
21	AA	704	A	C6-N1	-6.04	1.31	1.35
54	BA	2222	C	C4-N4	-6.03	1.28	1.33
54	BA	2794	C	C4-N4	-6.03	1.28	1.33
21	AA	359	G	C2-N2	-6.03	1.28	1.34
21	AA	1182	G	C2-N2	-6.03	1.28	1.34
21	AA	674	G	C2-N2	-6.02	1.28	1.34
21	AA	418	C	C4-N4	-6.02	1.28	1.33
21	AA	369	G	C2-N2	-6.02	1.28	1.34
21	AA	1207	G	C2-N2	-6.02	1.28	1.34
21	AA	19	A	C6-N1	-6.01	1.31	1.35
54	BA	1362	C	N3-C4	-6.01	1.29	1.33
54	BA	1832	C	C4-N4	-6.01	1.28	1.33
22	A1	75	C	C4-N4	-6.01	1.28	1.33
54	BA	986	C	C4-N4	-6.00	1.28	1.33
21	AA	233	C	C4-N4	-6.00	1.28	1.33
21	AA	308	C	C4-N4	-6.00	1.28	1.33
21	AA	976	G	C2-N2	-6.00	1.28	1.34
21	AA	1112	C	N3-C4	-6.00	1.29	1.33
21	AA	1066	C	C4-N4	-6.00	1.28	1.33
54	BA	393	C	C4-N4	-5.99	1.28	1.33
21	AA	58	C	C4-N4	-5.99	1.28	1.33
54	BA	295	G	C6-N1	-5.99	1.35	1.39
54	BA	2104	C	C4-N4	-5.99	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	145	G	C2-N2	-5.99	1.28	1.34
21	AA	372	C	C4-N4	-5.98	1.28	1.33
54	BA	11	C	C4-N4	-5.98	1.28	1.33
54	BA	784	G	C2-N2	-5.98	1.28	1.34
54	BA	1870	C	C4-N4	-5.98	1.28	1.33
24	A3	69	C	C4-N4	-5.98	1.28	1.33
54	BA	1797	G	C2-N2	-5.97	1.28	1.34
54	BA	396	G	C2-N2	-5.97	1.28	1.34
54	BA	1710	G	C2-N2	-5.97	1.28	1.34
21	AA	475	C	C4-N4	-5.97	1.28	1.33
21	AA	1171	A	C6-N1	-5.97	1.31	1.35
21	AA	1479	C	C4-N4	-5.97	1.28	1.33
54	BA	285	G	C2-N2	-5.97	1.28	1.34
54	BA	2446	G	C2-N2	-5.96	1.28	1.34
24	A3	53	G	C6-N1	-5.96	1.35	1.39
54	BA	585	G	C2-N2	-5.96	1.28	1.34
24	A3	19	G	C2-N2	-5.96	1.28	1.34
54	BA	381	G	C2-N2	-5.96	1.28	1.34
54	BA	2636	C	C4-N4	-5.95	1.28	1.33
55	BB	3	C	C4-N4	-5.95	1.28	1.33
21	AA	931	C	N3-C4	-5.95	1.29	1.33
21	AA	1509	C	C4-N4	-5.95	1.28	1.33
55	BB	19	C	C4-N4	-5.95	1.28	1.33
54	BA	33	C	C4-N4	-5.94	1.28	1.33
54	BA	143	C	N3-C4	-5.94	1.29	1.33
54	BA	914	G	N1-C2	-5.94	1.32	1.37
55	BB	31	C	C4-N4	-5.94	1.28	1.33
21	AA	990	C	C4-N4	-5.94	1.28	1.33
54	BA	386	G	C2-N2	-5.94	1.28	1.34
21	AA	1469	C	C4-N4	-5.93	1.28	1.33
21	AA	1064	G	C2-N2	-5.93	1.28	1.34
54	BA	2049	G	C2-N2	-5.93	1.28	1.34
54	BA	444	C	N3-C4	-5.93	1.29	1.33
54	BA	1533	C	C4-N4	-5.93	1.28	1.33
54	BA	1558	C	C4-N4	-5.93	1.28	1.33
21	AA	520	A	C6-N1	-5.92	1.31	1.35
54	BA	2228	G	C2-N2	-5.92	1.28	1.34
21	AA	1051	C	C4-N4	-5.92	1.28	1.33
54	BA	1357	C	N3-C4	-5.92	1.29	1.33
21	AA	1344	C	C4-N4	-5.91	1.28	1.33
54	BA	389	G	C2-N2	-5.91	1.28	1.34
54	BA	584	C	C4-N4	-5.91	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1748	C	C4-N4	-5.91	1.28	1.33
21	AA	1061	G	C2-N2	-5.91	1.28	1.34
21	AA	453	G	C2-N2	-5.90	1.28	1.34
54	BA	2824	C	N3-C4	-5.90	1.29	1.33
54	BA	1345	C	C4-N4	-5.90	1.28	1.33
21	AA	234	C	C4-N4	-5.90	1.28	1.33
54	BA	454	A	C6-N1	-5.90	1.31	1.35
54	BA	2821	A	C6-N1	-5.90	1.31	1.35
54	BA	1398	C	C4-N4	-5.90	1.28	1.33
54	BA	1430	G	C2-N2	-5.90	1.28	1.34
55	BB	24	G	C2-N2	-5.89	1.28	1.34
21	AA	618	C	C4-N4	-5.89	1.28	1.33
21	AA	634	C	C4-N4	-5.89	1.28	1.33
21	AA	730	G	C2-N2	-5.88	1.28	1.34
21	AA	775	G	C2-N2	-5.88	1.28	1.34
54	BA	748	G	C2-N2	-5.88	1.28	1.34
54	BA	442	G	C2-N2	-5.88	1.28	1.34
21	AA	929	G	C2-N2	-5.88	1.28	1.34
21	AA	776	G	C2-N2	-5.88	1.28	1.34
21	AA	783	C	N3-C4	-5.88	1.29	1.33
54	BA	1121	C	C4-N4	-5.88	1.28	1.33
21	AA	726	C	N3-C4	-5.87	1.29	1.33
54	BA	1822	C	C4-N4	-5.87	1.28	1.33
21	AA	277	C	C4-N4	-5.87	1.28	1.33
21	AA	495	A	C6-N1	-5.87	1.31	1.35
54	BA	1272	A	C6-N1	-5.87	1.31	1.35
54	BA	2619	C	C4-N4	-5.87	1.28	1.33
54	BA	1211	C	C4-N4	-5.87	1.28	1.33
54	BA	2699	C	C4-N4	-5.86	1.28	1.33
54	BA	2165	C	C4-N4	-5.86	1.28	1.33
54	BA	1990	C	N3-C4	-5.86	1.29	1.33
54	BA	24	G	C2-N2	-5.86	1.28	1.34
55	BB	64	G	C6-N1	-5.86	1.35	1.39
21	AA	779	C	C4-N4	-5.86	1.28	1.33
54	BA	2396	G	C2-N2	-5.86	1.28	1.34
55	BB	116	G	C2-N2	-5.85	1.28	1.34
21	AA	1084	G	C2-N2	-5.85	1.28	1.34
54	BA	1741	C	C4-N4	-5.85	1.28	1.33
21	AA	1143	G	C2-N2	-5.84	1.28	1.34
54	BA	889	C	N3-C4	-5.84	1.29	1.33
54	BA	1361	G	C2-N2	-5.84	1.28	1.34
54	BA	2190	G	C2-N2	-5.84	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	34	C	C4'-C3'	-5.84	1.46	1.52
21	AA	136	C	C4-N4	-5.84	1.28	1.33
21	AA	824	G	C2-N2	-5.84	1.28	1.34
54	BA	1613	G	C2-N2	-5.84	1.28	1.34
54	BA	2037	A	C6-N1	-5.83	1.31	1.35
21	AA	1103	C	N3-C4	-5.83	1.29	1.33
54	BA	1959	G	C2-N2	-5.83	1.28	1.34
54	BA	637	A	C6-N1	-5.82	1.31	1.35
24	A3	76	C	N3-C4	-5.82	1.29	1.33
54	BA	1538	G	C2-N2	-5.82	1.28	1.34
55	BB	62	C	C4-N4	-5.82	1.28	1.33
54	BA	385	C	C4-N4	-5.82	1.28	1.33
54	BA	2443	C	C4-N4	-5.82	1.28	1.33
54	BA	134	G	C2-N2	-5.82	1.28	1.34
54	BA	1947	C	C4-N4	-5.82	1.28	1.33
21	AA	314	C	C4-N4	-5.82	1.28	1.33
54	BA	2442	C	C4-N4	-5.81	1.28	1.33
21	AA	481	G	C2-N2	-5.81	1.28	1.34
21	AA	579	A	C6-N1	-5.81	1.31	1.35
21	AA	1117	A	C6-N1	-5.81	1.31	1.35
21	AA	1412	C	C4-N4	-5.81	1.28	1.33
54	BA	2073	C	N3-C4	-5.81	1.29	1.33
21	AA	914	A	C6-N1	-5.81	1.31	1.35
21	AA	919	A	C6-N1	-5.81	1.31	1.35
54	BA	473	G	C2-N2	-5.81	1.28	1.34
54	BA	2338	C	C4-N4	-5.81	1.28	1.33
54	BA	2339	C	C4-N4	-5.81	1.28	1.33
54	BA	2374	C	C4-N4	-5.81	1.28	1.33
54	BA	69	C	C4-N4	-5.81	1.28	1.33
24	A3	62	C	C4-N4	-5.80	1.28	1.33
54	BA	2770	G	C2-N2	-5.80	1.28	1.34
21	AA	918	A	C6-N1	-5.80	1.31	1.35
54	BA	2012	G	C2-N2	-5.80	1.28	1.34
21	AA	1108	G	C2-N2	-5.80	1.28	1.34
54	BA	58	G	C2-N2	-5.80	1.28	1.34
54	BA	378	C	C4-N4	-5.80	1.28	1.33
54	BA	805	G	C2-N2	-5.80	1.28	1.34
54	BA	1429	G	C2-N2	-5.80	1.28	1.34
54	BA	1470	A	C6-N1	-5.80	1.31	1.35
21	AA	1098	C	N3-C4	-5.79	1.29	1.33
21	AA	57	G	C6-N1	-5.79	1.35	1.39
21	AA	673	A	C6-N1	-5.79	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1494	G	C2-N2	-5.79	1.28	1.34
54	BA	1697	G	C2-N2	-5.79	1.28	1.34
54	BA	2365	G	C2-N2	-5.79	1.28	1.34
21	AA	878	A	C6-N1	-5.79	1.31	1.35
54	BA	318	C	C4-N4	-5.79	1.28	1.33
55	BB	51	G	C2-N2	-5.79	1.28	1.34
24	A3	53	G	C2-N2	-5.79	1.28	1.34
21	AA	1146	A	C6-N1	-5.78	1.31	1.35
54	BA	1752	C	N3-C4	-5.78	1.29	1.33
21	AA	1447	A	C6-N1	-5.78	1.31	1.35
21	AA	1482	G	C2-N2	-5.78	1.28	1.34
21	AA	124	C	C4-N4	-5.78	1.28	1.33
21	AA	501	C	C4-N4	-5.78	1.28	1.33
21	AA	127	G	C2-N2	-5.78	1.28	1.34
54	BA	1961	C	C4-N4	-5.78	1.28	1.33
54	BA	2364	C	C4-N4	-5.78	1.28	1.33
21	AA	1231	G	C2-N2	-5.78	1.28	1.34
54	BA	2752	C	C4-N4	-5.78	1.28	1.33
54	BA	982	C	N3-C4	-5.77	1.29	1.33
54	BA	2795	C	C4-N4	-5.77	1.28	1.33
54	BA	2050	C	C4-N4	-5.77	1.28	1.33
54	BA	1541	C	C4-N4	-5.77	1.28	1.33
54	BA	2801	G	C2-N2	-5.77	1.28	1.34
21	AA	1226	C	N3-C4	-5.77	1.29	1.33
21	AA	1369	C	C4-N4	-5.76	1.28	1.33
21	AA	1502	A	C6-N1	-5.76	1.31	1.35
21	AA	1139	G	C2-N2	-5.76	1.28	1.34
54	BA	267	C	C4-N4	-5.76	1.28	1.33
54	BA	2353	G	C2-N2	-5.76	1.28	1.34
54	BA	729	G	C2-N2	-5.76	1.28	1.34
21	AA	235	C	C4-N4	-5.75	1.28	1.33
54	BA	1441	G	C2-N2	-5.75	1.28	1.34
21	AA	1209	C	C4-N4	-5.75	1.28	1.33
21	AA	1462	C	N3-C4	-5.75	1.29	1.33
54	BA	1382	G	C2-N2	-5.75	1.28	1.34
54	BA	1404	C	C4-N4	-5.75	1.28	1.33
54	BA	1985	C	N3-C4	-5.74	1.29	1.33
21	AA	676	A	C6-N1	-5.74	1.31	1.35
21	AA	1461	G	C2-N2	-5.74	1.28	1.34
21	AA	1433	A	C6-N1	-5.74	1.31	1.35
22	A1	61	C	C4-N4	-5.74	1.28	1.33
54	BA	1557	C	C4-N4	-5.74	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2850	A	C6-N1	-5.74	1.31	1.35
21	AA	848	C	C4-N4	-5.73	1.28	1.33
54	BA	1266	G	N1-C2	-5.73	1.33	1.37
54	BA	1093	G	C2-N2	-5.73	1.28	1.34
21	AA	880	C	C4-N4	-5.73	1.28	1.33
21	AA	1223	C	C4-N4	-5.73	1.28	1.33
54	BA	116	C	C4-N4	-5.73	1.28	1.33
54	BA	823	C	C4-N4	-5.73	1.28	1.33
55	BB	75	G	C2-N2	-5.73	1.28	1.34
21	AA	926	G	C6-N1	-5.72	1.35	1.39
54	BA	2717	C	C4-N4	-5.72	1.28	1.33
21	AA	1193	G	C2-N2	-5.72	1.28	1.34
54	BA	2067	G	C2-N2	-5.72	1.28	1.34
21	AA	868	C	C4-N4	-5.72	1.28	1.33
54	BA	2	G	C2-N2	-5.72	1.28	1.34
54	BA	2238	G	C2-N2	-5.72	1.28	1.34
55	BB	7	G	C2-N2	-5.72	1.28	1.34
54	BA	776	G	C2-N2	-5.72	1.28	1.34
54	BA	2033	A	C6-N1	-5.72	1.31	1.35
54	BA	1435	G	C2-N2	-5.71	1.28	1.34
54	BA	2228	G	C6-N1	-5.71	1.35	1.39
54	BA	2289	G	C2-N2	-5.71	1.28	1.34
54	BA	1701	A	C6-N1	-5.71	1.31	1.35
55	BB	75	G	C6-N1	-5.71	1.35	1.39
54	BA	2854	G	C2-N2	-5.71	1.28	1.34
54	BA	2083	G	C2-N2	-5.71	1.28	1.34
54	BA	2426	A	C6-N1	-5.70	1.31	1.35
54	BA	2521	C	C4-N4	-5.70	1.28	1.33
54	BA	1407	G	C2-N2	-5.70	1.28	1.34
54	BA	2361	G	C2-N2	-5.70	1.28	1.34
55	BB	105	G	C2-N2	-5.70	1.28	1.34
21	AA	370	C	C4-N4	-5.70	1.28	1.33
21	AA	128	G	C2-N2	-5.70	1.28	1.34
21	AA	1267	C	N3-C4	-5.69	1.29	1.33
54	BA	549	G	N1-C2	-5.69	1.33	1.37
55	BB	100	G	C2-N2	-5.69	1.28	1.34
21	AA	741	G	C2-N2	-5.69	1.28	1.34
21	AA	1482	G	C6-N1	-5.69	1.35	1.39
54	BA	719	C	N3-C4	-5.69	1.29	1.33
54	BA	1711	A	C5-C4	-5.69	1.34	1.38
21	AA	1516	G	C2-N2	-5.68	1.28	1.34
54	BA	845	A	C6-N1	-5.68	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	215	C	N3-C4	-5.68	1.29	1.33
54	BA	1080	A	C6-N1	-5.68	1.31	1.35
54	BA	1413	A	C6-N1	-5.68	1.31	1.35
55	BB	118	C	C4-N4	-5.68	1.28	1.33
54	BA	1472	C	C4-N4	-5.67	1.28	1.33
54	BA	2831	G	C2-N2	-5.67	1.28	1.34
54	BA	1984	G	C2-N2	-5.67	1.28	1.34
54	BA	1112	G	C2-N2	-5.67	1.28	1.34
54	BA	1114	C	C4-N4	-5.67	1.28	1.33
54	BA	176	A	C6-N1	-5.67	1.31	1.35
54	BA	1836	C	C4-N4	-5.67	1.28	1.33
54	BA	2200	C	N3-C4	-5.67	1.29	1.33
54	BA	2128	G	C2-N2	-5.66	1.28	1.34
21	AA	1195	C	C4-N4	-5.66	1.28	1.33
54	BA	164	C	C4-N4	-5.65	1.28	1.33
54	BA	295	G	C2-N2	-5.65	1.28	1.34
21	AA	385	C	N3-C4	-5.65	1.29	1.33
21	AA	1226	C	C4-N4	-5.65	1.28	1.33
54	BA	2607	G	C2-N2	-5.64	1.28	1.34
54	BA	2601	C	N3-C4	-5.64	1.30	1.33
21	AA	915	A	C6-N6	-5.64	1.29	1.33
21	AA	1438	G	C2-N2	-5.64	1.28	1.34
22	A1	30	C	C4-N4	-5.64	1.28	1.33
54	BA	145	C	C4-N4	-5.64	1.28	1.33
54	BA	445	C	C4-N4	-5.64	1.28	1.33
55	BB	60	C	C4-N4	-5.64	1.28	1.33
54	BA	1436	G	C2-N2	-5.64	1.28	1.34
54	BA	1710	G	C6-N1	-5.64	1.35	1.39
22	A1	52	G	C6-N1	-5.64	1.35	1.39
54	BA	531	C	N3-C4	-5.64	1.30	1.33
54	BA	1804	C	C4-N4	-5.64	1.28	1.33
21	AA	348	G	C2-N2	-5.63	1.28	1.34
54	BA	1314	C	C4-N4	-5.63	1.28	1.33
54	BA	2802	G	C6-N1	-5.63	1.35	1.39
21	AA	164	G	C2-N2	-5.63	1.28	1.34
21	AA	456	A	C6-N1	-5.63	1.31	1.35
21	AA	1215	G	C2-N2	-5.63	1.28	1.34
21	AA	1280	A	C6-N1	-5.63	1.31	1.35
54	BA	1601	G	C2-N2	-5.63	1.28	1.34
21	AA	144	G	C2-N2	-5.62	1.28	1.34
55	BB	98	G	C2-N2	-5.62	1.28	1.34
21	AA	271	C	C4-N4	-5.62	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2721	A	C6-N1	-5.62	1.31	1.35
21	AA	1234	C	C4-N4	-5.62	1.28	1.33
21	AA	1511	G	C2-N2	-5.62	1.28	1.34
21	AA	222	C	C4-N4	-5.62	1.28	1.33
21	AA	519	C	C4-N4	-5.61	1.28	1.33
21	AA	582	C	C4-N4	-5.61	1.28	1.33
54	BA	1679	A	C6-N1	-5.61	1.31	1.35
21	AA	1349	A	C6-N1	-5.61	1.31	1.35
21	AA	243	A	C6-N1	-5.61	1.31	1.35
21	AA	719	C	C4-N4	-5.61	1.28	1.33
21	AA	755	G	C2-N2	-5.61	1.28	1.34
21	AA	932	C	C4-N4	-5.61	1.28	1.33
54	BA	2805	C	C4-N4	-5.61	1.28	1.33
21	AA	191	G	C2-N2	-5.61	1.28	1.34
54	BA	1826	G	C2-N2	-5.61	1.28	1.34
54	BA	2383	G	C2-N2	-5.61	1.28	1.34
54	BA	2655	G	C2-N2	-5.61	1.28	1.34
55	BB	116	G	C6-N1	-5.61	1.35	1.39
54	BA	620	G	C2-N2	-5.61	1.28	1.34
55	BB	71	C	C4-N4	-5.61	1.28	1.33
21	AA	985	C	C4-N4	-5.60	1.28	1.33
54	BA	717	C	C4-N4	-5.60	1.28	1.33
54	BA	1045	C	C4-N4	-5.60	1.28	1.33
54	BA	1447	C	C4-N4	-5.60	1.28	1.33
21	AA	207	C	N3-C4	-5.60	1.30	1.33
21	AA	1210	C	C4-N4	-5.60	1.28	1.33
54	BA	54	G	C6-N1	-5.60	1.35	1.39
21	AA	192	A	C5-C4	-5.59	1.34	1.38
54	BA	2038	G	C6-N1	-5.59	1.35	1.39
21	AA	876	C	C4-N4	-5.59	1.28	1.33
21	AA	1361	G	C2-N2	-5.59	1.28	1.34
54	BA	1593	A	C6-N1	-5.59	1.31	1.35
54	BA	2263	C	N3-C4	-5.59	1.30	1.33
54	BA	2328	A	C6-N1	-5.59	1.31	1.35
21	AA	408	A	C6-N1	-5.58	1.31	1.35
54	BA	674	G	C2-N2	-5.58	1.28	1.34
21	AA	284	C	C4-N4	-5.58	1.28	1.33
54	BA	2520	C	C4-N4	-5.58	1.28	1.33
55	BB	64	G	C2-N2	-5.58	1.28	1.34
24	A3	1	C	N3-C4	-5.58	1.30	1.33
54	BA	2813	A	C6-N1	-5.58	1.31	1.35
54	BA	937	C	N3-C4	-5.58	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1356	G	C2-N2	-5.58	1.28	1.34
54	BA	1395	A	C6-N1	-5.58	1.31	1.35
54	BA	1802	A	C6-N1	-5.58	1.31	1.35
54	BA	1974	C	C4-N4	-5.58	1.28	1.33
21	AA	355	C	C4-N4	-5.58	1.28	1.33
54	BA	2815	C	C4-N4	-5.58	1.28	1.33
54	BA	2323	G	C2-N2	-5.57	1.28	1.34
54	BA	2499	C	C4-N4	-5.57	1.28	1.33
21	AA	1166	G	C2-N2	-5.57	1.28	1.34
54	BA	151	C	C4-N4	-5.57	1.28	1.33
54	BA	1376	C	C4-N4	-5.57	1.28	1.33
54	BA	2823	A	C6-N1	-5.57	1.31	1.35
54	BA	60	G	C2-N2	-5.57	1.28	1.34
54	BA	1538	G	C6-N1	-5.57	1.35	1.39
54	BA	2710	C	C4-N4	-5.57	1.28	1.33
54	BA	585	G	C6-N1	-5.56	1.35	1.39
21	AA	498	A	C5-C4	-5.56	1.34	1.38
54	BA	1954	G	C2-N2	-5.56	1.28	1.34
21	AA	1128	C	C4-N4	-5.56	1.28	1.33
54	BA	757	G	N1-C2	-5.56	1.33	1.37
54	BA	2175	C	C4-N4	-5.56	1.28	1.33
21	AA	1421	G	C2-N2	-5.56	1.28	1.34
21	AA	879	C	N3-C4	-5.55	1.30	1.33
54	BA	383	C	C4-N4	-5.55	1.28	1.33
21	AA	953	G	C2-N2	-5.55	1.28	1.34
54	BA	985	C	C4-N4	-5.55	1.28	1.33
54	BA	1772	A	C5-C4	-5.55	1.34	1.38
55	BB	29	A	C6-N1	-5.55	1.31	1.35
54	BA	2365	G	C6-N1	-5.55	1.35	1.39
54	BA	2452	C	C4-N4	-5.55	1.28	1.33
21	AA	347	G	C2-N2	-5.54	1.29	1.34
21	AA	376	G	C2-N2	-5.54	1.29	1.34
21	AA	568	G	C2-N2	-5.54	1.29	1.34
21	AA	1144	G	C2-N2	-5.54	1.29	1.34
54	BA	2723	C	C4-N4	-5.54	1.28	1.33
21	AA	725	G	C2-N2	-5.54	1.29	1.34
54	BA	128	C	N3-C4	-5.54	1.30	1.33
54	BA	2201	G	C2-N2	-5.54	1.29	1.34
21	AA	34	C	C4-N4	-5.54	1.28	1.33
54	BA	1290	C	C4-N4	-5.54	1.28	1.33
54	BA	1972	G	C2-N2	-5.54	1.29	1.34
54	BA	2626	C	C4-N4	-5.54	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	601	C	C4-N4	-5.54	1.28	1.33
54	BA	1490	A	C6-N1	-5.54	1.31	1.35
54	BA	1555	G	N1-C2	-5.54	1.33	1.37
54	BA	2591	C	N3-C4	-5.54	1.30	1.33
55	BB	8	C	N3-C4	-5.53	1.30	1.33
21	AA	384	G	C2-N2	-5.53	1.29	1.34
54	BA	809	G	C2-N2	-5.53	1.29	1.34
54	BA	2394	C	C4-N4	-5.53	1.28	1.33
21	AA	734	G	C2-N2	-5.53	1.29	1.34
54	BA	1092	C	C4-N4	-5.53	1.28	1.33
21	AA	217	C	C4-N4	-5.53	1.28	1.33
21	AA	354	G	C2-N2	-5.53	1.29	1.34
54	BA	1570	A	C6-N1	-5.53	1.31	1.35
21	AA	528	C	C4-N4	-5.53	1.28	1.33
21	AA	869	G	C6-N1	-5.53	1.35	1.39
21	AA	1418	A	C5-C4	-5.52	1.34	1.38
24	A3	5	G	C2-N2	-5.52	1.29	1.34
55	BB	94	A	C6-N1	-5.52	1.31	1.35
21	AA	727	G	N1-C2	-5.52	1.33	1.37
21	AA	1151	A	C6-N1	-5.52	1.31	1.35
54	BA	333	G	C2-N2	-5.52	1.29	1.34
24	A3	6	G	C2-N2	-5.51	1.29	1.34
21	AA	496	A	C6-N1	-5.51	1.31	1.35
21	AA	1388	C	C4-N4	-5.51	1.28	1.33
54	BA	936	A	C6-N1	-5.51	1.31	1.35
54	BA	2747	G	C2-N2	-5.51	1.29	1.34
54	BA	2162	G	C2-N2	-5.51	1.29	1.34
54	BA	2722	G	N1-C2	-5.51	1.33	1.37
21	AA	806	C	N3-C4	-5.50	1.30	1.33
55	BB	26	C	C4-N4	-5.50	1.28	1.33
21	AA	1421	G	C6-N1	-5.50	1.35	1.39
54	BA	1608	A	C6-N1	-5.50	1.31	1.35
21	AA	462	G	C2-N2	-5.50	1.29	1.34
21	AA	1342	C	C4-N4	-5.50	1.29	1.33
54	BA	2422	C	C4-N4	-5.50	1.29	1.33
54	BA	2901	C	C4-N4	-5.50	1.29	1.33
21	AA	1483	A	C6-N1	-5.49	1.31	1.35
54	BA	2301	C	C4-N4	-5.49	1.29	1.33
54	BA	2870	C	C4-N4	-5.49	1.29	1.33
21	AA	48	C	C4-N4	-5.49	1.29	1.33
54	BA	291	G	C2-N2	-5.49	1.29	1.34
21	AA	1217	C	C4-N4	-5.49	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1410	A	C6-N1	-5.49	1.31	1.35
54	BA	1044	C	C4-N4	-5.49	1.29	1.33
54	BA	1787	A	C6-N1	-5.49	1.31	1.35
54	BA	2747	G	C6-N1	-5.49	1.35	1.39
21	AA	77	A	C6-N1	-5.48	1.31	1.35
21	AA	444	G	C6-N1	-5.48	1.35	1.39
21	AA	525	C	C4-N4	-5.48	1.29	1.33
54	BA	130	C	C4-N4	-5.48	1.29	1.33
54	BA	291	G	C6-N1	-5.48	1.35	1.39
54	BA	2623	G	C2-N2	-5.48	1.29	1.34
54	BA	2712	C	C4-N4	-5.48	1.29	1.33
21	AA	392	C	C4-N4	-5.48	1.29	1.33
21	AA	419	C	C4-N4	-5.48	1.29	1.33
54	BA	1428	C	C4-N4	-5.48	1.29	1.33
21	AA	685	G	C6-N1	-5.47	1.35	1.39
21	AA	356	A	C5-C4	-5.47	1.34	1.38
54	BA	2875	C	C4-N4	-5.47	1.29	1.33
55	BB	52	A	C6-N1	-5.47	1.31	1.35
21	AA	178	C	C4-N4	-5.47	1.29	1.33
21	AA	266	G	C4'-O4'	-5.47	1.38	1.45
54	BA	2152	G	C2-N2	-5.47	1.29	1.34
54	BA	752	A	C6-N1	-5.47	1.31	1.35
55	BB	33	G	C2-N2	-5.47	1.29	1.34
21	AA	498	A	C6-N6	-5.47	1.29	1.33
54	BA	736	C	C4-N4	-5.46	1.29	1.33
54	BA	1401	G	C6-N1	-5.46	1.35	1.39
21	AA	1404	C	N3-C4	-5.46	1.30	1.33
54	BA	2024	G	C2-N2	-5.46	1.29	1.34
21	AA	685	G	C2-N2	-5.46	1.29	1.34
54	BA	1343	G	C2-N2	-5.46	1.29	1.34
54	BA	1464	G	C2-N2	-5.46	1.29	1.34
21	AA	206	C	N3-C4	-5.46	1.30	1.33
21	AA	1208	C	N3-C4	-5.46	1.30	1.33
54	BA	2258	C	N3-C4	-5.46	1.30	1.33
21	AA	1231	G	C6-N1	-5.46	1.35	1.39
22	A1	22	G	C2-N2	-5.46	1.29	1.34
54	BA	1077	A	C6-N1	-5.46	1.31	1.35
54	BA	1792	G	C2-N2	-5.46	1.29	1.34
54	BA	1879	C	C4-N4	-5.46	1.29	1.33
55	BB	6	G	C2-N2	-5.46	1.29	1.34
55	BB	49	C	C4-N4	-5.46	1.29	1.33
21	AA	164	G	C6-N1	-5.45	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2846	G	C2-N2	-5.45	1.29	1.34
21	AA	67	C	N3-C4	-5.45	1.30	1.33
21	AA	141	G	C2-N2	-5.45	1.29	1.34
54	BA	1986	C	C4-N4	-5.45	1.29	1.33
21	AA	425	G	C2-N2	-5.45	1.29	1.34
54	BA	910	A	C6-N1	-5.45	1.31	1.35
54	BA	2888	C	C4-N4	-5.45	1.29	1.33
54	BA	265	A	C6-N1	-5.44	1.31	1.35
21	AA	1109	C	C4-N4	-5.44	1.29	1.33
55	BB	2	G	C2-N2	-5.44	1.29	1.34
21	AA	281	G	C2-N2	-5.44	1.29	1.34
54	BA	334	C	N3-C4	-5.44	1.30	1.33
21	AA	21	G	N1-C2	-5.44	1.33	1.37
54	BA	2827	C	N3-C4	-5.44	1.30	1.33
21	AA	413	G	C2-N2	-5.44	1.29	1.34
21	AA	744	C	C4-N4	-5.44	1.29	1.33
54	BA	1339	G	C2-N2	-5.43	1.29	1.34
55	BB	117	G	C2-N2	-5.43	1.29	1.34
54	BA	942	G	C2-N2	-5.43	1.29	1.34
21	AA	227	G	C6-N1	-5.43	1.35	1.39
54	BA	1759	A	C6-N1	-5.43	1.31	1.35
54	BA	1034	G	C2-N2	-5.43	1.29	1.34
21	AA	708	C	N3-C4	-5.43	1.30	1.33
21	AA	1164	G	N1-C2	-5.43	1.33	1.37
54	BA	45	G	C2-N2	-5.43	1.29	1.34
54	BA	2038	G	C2-N2	-5.43	1.29	1.34
21	AA	382	A	C5-C4	-5.42	1.34	1.38
54	BA	384	A	C6-N1	-5.42	1.31	1.35
54	BA	1857	G	C2-N2	-5.42	1.29	1.34
21	AA	1405	G	C2-N2	-5.42	1.29	1.34
54	BA	396	G	C6-N1	-5.42	1.35	1.39
54	BA	2346	A	O3'-P	-5.42	1.54	1.61
21	AA	1193	G	C6-N1	-5.42	1.35	1.39
54	BA	1446	C	N3-C4	-5.42	1.30	1.33
21	AA	1225	A	C6-N1	-5.42	1.31	1.35
54	BA	2295	C	C4-N4	-5.42	1.29	1.33
54	BA	2802	G	C2-N2	-5.42	1.29	1.34
21	AA	586	C	C4-N4	-5.41	1.29	1.33
21	AA	803	G	C2-N2	-5.41	1.29	1.34
54	BA	7	G	C2-N2	-5.41	1.29	1.34
54	BA	885	C	C4-N4	-5.41	1.29	1.33
54	BA	2862	G	N1-C2	-5.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1047	G	C2-N2	-5.41	1.29	1.34
54	BA	1353	A	C6-N1	-5.41	1.31	1.35
54	BA	398	C	C4-N4	-5.41	1.29	1.33
54	BA	1718	G	C2-N2	-5.41	1.29	1.34
54	BA	1954	G	C6-N1	-5.41	1.35	1.39
54	BA	2396	G	C6-N1	-5.41	1.35	1.39
21	AA	1188	A	C6-N1	-5.41	1.31	1.35
54	BA	425	G	C2-N2	-5.41	1.29	1.34
55	BB	110	C	N3-C4	-5.41	1.30	1.33
54	BA	121	G	C2-N2	-5.40	1.29	1.34
21	AA	1426	G	C2-N2	-5.40	1.29	1.34
54	BA	54	G	C2-N2	-5.40	1.29	1.34
54	BA	1726	C	C4-N4	-5.40	1.29	1.33
54	BA	1564	C	C4-N4	-5.40	1.29	1.33
54	BA	2755	C	N3-C4	-5.40	1.30	1.33
21	AA	356	A	C6-N6	-5.39	1.29	1.33
21	AA	220	G	C2-N2	-5.39	1.29	1.34
54	BA	134	G	C6-N1	-5.39	1.35	1.39
54	BA	426	C	N3-C4	-5.39	1.30	1.33
54	BA	2304	G	C2-N2	-5.39	1.29	1.34
54	BA	1984	G	C6-N1	-5.39	1.35	1.39
54	BA	2043	C	N3-C4	-5.39	1.30	1.33
21	AA	750	C	C4-N4	-5.39	1.29	1.33
24	A3	43	G	C2-N2	-5.39	1.29	1.34
54	BA	516	C	C4-N4	-5.39	1.29	1.33
21	AA	95	C	N3-C4	-5.38	1.30	1.33
21	AA	394	G	C2-N2	-5.38	1.29	1.34
21	AA	455	G	C2-N2	-5.38	1.29	1.34
21	AA	403	C	C4-N4	-5.38	1.29	1.33
22	A1	13	C	C4-N4	-5.38	1.29	1.33
54	BA	651	G	C2-N2	-5.38	1.29	1.34
54	BA	1450	G	C2-N2	-5.38	1.29	1.34
54	BA	1960	A	C6-N1	-5.38	1.31	1.35
54	BA	2102	G	C2-N2	-5.37	1.29	1.34
24	A3	54	G	C2-N2	-5.37	1.29	1.34
54	BA	2140	G	C2-N2	-5.37	1.29	1.34
54	BA	175	G	C2-N2	-5.37	1.29	1.34
54	BA	1575	C	N3-C4	-5.37	1.30	1.33
24	A3	58	A	C5-C4	-5.37	1.34	1.38
54	BA	1526	C	N3-C4	-5.37	1.30	1.33
54	BA	2644	G	C2-N2	-5.37	1.29	1.34
54	BA	706	A	C6-N1	-5.36	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1353	G	C2-N2	-5.36	1.29	1.34
21	AA	1048	G	C2-N2	-5.36	1.29	1.34
54	BA	1368	G	C2-N2	-5.36	1.29	1.34
21	AA	939	G	C2-N2	-5.36	1.29	1.34
21	AA	1418	A	C6-N6	-5.36	1.29	1.33
54	BA	2856	A	C5-C4	-5.35	1.35	1.38
54	BA	160	A	C6-N1	-5.35	1.31	1.35
54	BA	1084	A	C6-N6	-5.35	1.29	1.33
54	BA	1872	A	C6-N1	-5.35	1.31	1.35
54	BA	2371	G	C2-N2	-5.35	1.29	1.34
21	AA	338	A	C6-N1	-5.35	1.31	1.35
21	AA	970	C	C4-N4	-5.35	1.29	1.33
21	AA	1524	C	C4-N4	-5.35	1.29	1.33
54	BA	1750	G	C2-N2	-5.35	1.29	1.34
54	BA	2127	G	C2-N2	-5.35	1.29	1.34
54	BA	2260	C	C4-N4	-5.35	1.29	1.33
54	BA	2603	G	N1-C2	-5.35	1.33	1.37
54	BA	217	A	C6-N1	-5.35	1.31	1.35
54	BA	1270	C	N3-C4	-5.35	1.30	1.33
54	BA	711	G	C2-N2	-5.35	1.29	1.34
21	AA	522	C	C4-N4	-5.34	1.29	1.33
21	AA	1147	C	C4-N4	-5.34	1.29	1.33
24	A3	40	C	C4-N4	-5.34	1.29	1.33
54	BA	9	G	C2-N2	-5.34	1.29	1.34
54	BA	624	C	C4-N4	-5.34	1.29	1.33
54	BA	668	A	C6-N1	-5.34	1.31	1.35
54	BA	2389	G	C2-N2	-5.34	1.29	1.34
21	AA	146	G	C2-N2	-5.34	1.29	1.34
54	BA	456	C	C4-N4	-5.34	1.29	1.33
54	BA	979	A	C6-N6	-5.34	1.29	1.33
54	BA	1256	G	C2-N2	-5.34	1.29	1.34
54	BA	2150	C	C4-N4	-5.34	1.29	1.33
21	AA	1416	G	C2-N2	-5.34	1.29	1.34
54	BA	2391	G	N1-C2	-5.34	1.33	1.37
54	BA	2686	G	C2-N2	-5.34	1.29	1.34
55	BB	51	G	C6-N1	-5.34	1.35	1.39
54	BA	391	A	C6-N1	-5.33	1.31	1.35
54	BA	672	C	C4-N4	-5.33	1.29	1.33
54	BA	1719	G	C2-N2	-5.33	1.29	1.34
21	AA	382	A	C6-N6	-5.33	1.29	1.33
21	AA	527	G	C2-N2	-5.33	1.29	1.34
21	AA	1468	A	C5-C4	-5.33	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1388	G	C2-N2	-5.33	1.29	1.34
54	BA	1681	G	C2-N2	-5.33	1.29	1.34
54	BA	1760	C	N3-C4	-5.33	1.30	1.33
54	BA	2842	G	C2-N2	-5.33	1.29	1.34
54	BA	287	G	N1-C2	-5.33	1.33	1.37
54	BA	627	A	C6-N1	-5.33	1.31	1.35
54	BA	1585	C	C4-N4	-5.33	1.29	1.33
54	BA	2899	A	C6-N1	-5.33	1.31	1.35
21	AA	359	G	C6-N1	-5.33	1.35	1.39
21	AA	468	A	C6-N1	-5.33	1.31	1.35
21	AA	511	C	N3-C4	-5.33	1.30	1.33
21	AA	877	G	C2-N2	-5.33	1.29	1.34
54	BA	536	G	C2-N2	-5.33	1.29	1.34
21	AA	205	A	C6-N1	-5.33	1.31	1.35
24	A3	19	G	C6-N1	-5.33	1.35	1.39
54	BA	49	A	C6-N6	-5.33	1.29	1.33
54	BA	669	G	N1-C2	-5.33	1.33	1.37
54	BA	1295	C	C4-N4	-5.33	1.29	1.33
54	BA	825	A	C6-N1	-5.32	1.31	1.35
21	AA	153	C	C4-N4	-5.32	1.29	1.33
54	BA	1615	C	C4-N4	-5.32	1.29	1.33
54	BA	2332	C	C4-N4	-5.32	1.29	1.33
21	AA	349	A	C5-C4	-5.32	1.35	1.38
21	AA	1366	C	N3-C4	-5.32	1.30	1.33
21	AA	1501	C	N3-C4	-5.32	1.30	1.33
54	BA	978	G	C2-N2	-5.32	1.29	1.34
54	BA	1980	G	N1-C2	-5.32	1.33	1.37
54	BA	2067	G	C6-N1	-5.32	1.35	1.39
54	BA	2896	C	C4-N4	-5.32	1.29	1.33
55	BB	114	C	C4-N4	-5.32	1.29	1.33
21	AA	930	C	N3-C4	-5.32	1.30	1.33
21	AA	15	G	C2-N2	-5.32	1.29	1.34
21	AA	1402	C	C4-N4	-5.32	1.29	1.33
54	BA	2624	G	N1-C2	-5.32	1.33	1.37
54	BA	1567	G	N1-C2	-5.31	1.33	1.37
21	AA	248	C	C4-N4	-5.31	1.29	1.33
21	AA	489	C	C4-N4	-5.31	1.29	1.33
21	AA	915	A	C5-C4	-5.31	1.35	1.38
21	AA	1305	G	C2-N2	-5.31	1.29	1.34
54	BA	518	G	C2-N2	-5.31	1.29	1.34
54	BA	2102	G	C6-N1	-5.31	1.35	1.39
54	BA	2762	C	N3-C4	-5.31	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	326	G	C2-N2	-5.31	1.29	1.34
54	BA	31	C	C4-N4	-5.31	1.29	1.33
54	BA	1436	G	C6-N1	-5.31	1.35	1.39
21	AA	844	G	C2-N2	-5.31	1.29	1.34
21	AA	236	A	C6-N1	-5.31	1.31	1.35
21	AA	191	G	C6-N1	-5.30	1.35	1.39
54	BA	1569	A	C6-N1	-5.30	1.31	1.35
21	AA	557	G	C2-N2	-5.30	1.29	1.34
21	AA	845	A	C6-N1	-5.30	1.31	1.35
21	AA	1172	C	N3-C4	-5.30	1.30	1.33
21	AA	497	G	N1-C2	-5.30	1.33	1.37
21	AA	941	G	C2-N2	-5.30	1.29	1.34
21	AA	1038	C	C4-N4	-5.30	1.29	1.33
54	BA	1036	G	C2-N2	-5.30	1.29	1.34
54	BA	2692	G	C6-N1	-5.30	1.35	1.39
55	BB	81	G	C2-N2	-5.30	1.29	1.34
22	A1	62	C	C4-C5	-5.30	1.38	1.43
21	AA	260	G	C2-N2	-5.30	1.29	1.34
21	AA	156	C	C4-N4	-5.29	1.29	1.33
21	AA	1503	A	C6-N1	-5.29	1.31	1.35
54	BA	1831	G	C2-N2	-5.29	1.29	1.34
21	AA	147	G	N1-C2	-5.29	1.33	1.37
21	AA	1497	G	N1-C2	-5.29	1.33	1.37
21	AA	31	G	N1-C2	-5.29	1.33	1.37
21	AA	1398	A	C6-N6	-5.29	1.29	1.33
24	A3	67	C	C4-N4	-5.29	1.29	1.33
54	BA	2405	G	C2-N2	-5.29	1.29	1.34
21	AA	1473	G	N1-C2	-5.29	1.33	1.37
54	BA	41	C	N3-C4	-5.29	1.30	1.33
54	BA	2123	G	C2-N2	-5.29	1.29	1.34
54	BA	2824	C	C4-N4	-5.29	1.29	1.33
54	BA	2080	A	C5-C4	-5.28	1.35	1.38
54	BA	700	G	C2-N2	-5.28	1.29	1.34
55	BB	23	G	C2-N2	-5.28	1.29	1.34
54	BA	1962	C	C4-N4	-5.28	1.29	1.33
54	BA	2084	C	N3-C4	-5.28	1.30	1.33
54	BA	1738	G	C2-N2	-5.28	1.29	1.34
21	AA	380	G	C2-N2	-5.28	1.29	1.34
54	BA	1708	C	C4-N4	-5.28	1.29	1.33
21	AA	459	A	C6-N1	-5.27	1.31	1.35
54	BA	1403	A	C5-C4	-5.27	1.35	1.38
21	AA	604	G	C2-N2	-5.27	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	315	G	C2-N2	-5.27	1.29	1.34
54	BA	418	C	C4-N4	-5.27	1.29	1.33
54	BA	1251	C	N3-C4	-5.27	1.30	1.33
54	BA	1704	C	C4-N4	-5.27	1.29	1.33
21	AA	728	A	C5-C4	-5.27	1.35	1.38
54	BA	352	A	C6-N1	-5.27	1.31	1.35
21	AA	737	C	C4-N4	-5.27	1.29	1.33
54	BA	2103	C	N3-C4	-5.27	1.30	1.33
21	AA	776	G	C6-N1	-5.26	1.35	1.39
54	BA	738	G	C2-N2	-5.26	1.29	1.34
54	BA	1703	G	N1-C2	-5.26	1.33	1.37
54	BA	1289	C	N3-C4	-5.26	1.30	1.33
54	BA	2337	G	C2-N2	-5.26	1.29	1.34
21	AA	188	C	C4-N4	-5.26	1.29	1.33
54	BA	2708	G	C2-N2	-5.26	1.29	1.34
21	AA	444	G	C2-N2	-5.26	1.29	1.34
54	BA	1102	C	C4-N4	-5.26	1.29	1.33
54	BA	2682	A	C6-N1	-5.26	1.31	1.35
54	BA	2777	G	C2-N2	-5.26	1.29	1.34
54	BA	281	C	C4-N4	-5.26	1.29	1.33
54	BA	342	A	C5-C4	-5.26	1.35	1.38
54	BA	979	A	C5-C4	-5.26	1.35	1.38
55	BB	37	C	N3-C4	-5.26	1.30	1.33
21	AA	363	A	C6-N1	-5.26	1.31	1.35
54	BA	1334	G	C2-N2	-5.26	1.29	1.34
21	AA	781	A	C5-C4	-5.25	1.35	1.38
54	BA	297	G	N1-C2	-5.25	1.33	1.37
54	BA	1934	C	C4-N4	-5.25	1.29	1.33
54	BA	2234	G	C2-N2	-5.25	1.29	1.34
54	BA	2350	C	C4-N4	-5.25	1.29	1.33
54	BA	2683	C	C4-N4	-5.25	1.29	1.33
55	BB	15	A	C6-N6	-5.25	1.29	1.33
21	AA	469	C	N3-C4	-5.25	1.30	1.33
54	BA	2177	C	C4-N4	-5.25	1.29	1.33
54	BA	2281	A	C6-N1	-5.25	1.31	1.35
54	BA	577	G	C2-N2	-5.25	1.29	1.34
54	BA	1069	A	C6-N1	-5.25	1.31	1.35
54	BA	1363	C	C4-N4	-5.25	1.29	1.33
21	AA	187	G	N1-C2	-5.25	1.33	1.37
21	AA	242	G	C2-N2	-5.25	1.29	1.34
21	AA	838	G	C2-N2	-5.25	1.29	1.34
54	BA	719	C	C4-N4	-5.25	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2600	A	C6-N1	-5.25	1.31	1.35
54	BA	1072	C	C4-N4	-5.25	1.29	1.33
54	BA	2692	G	C2-N2	-5.25	1.29	1.34
54	BA	1382	G	C6-N1	-5.25	1.35	1.39
55	BB	9	G	C2-N2	-5.25	1.29	1.34
24	A3	1	C	C4-N4	-5.24	1.29	1.33
54	BA	60	G	C6-N1	-5.24	1.35	1.39
21	AA	874	G	N1-C2	-5.24	1.33	1.37
54	BA	879	G	C2-N2	-5.24	1.29	1.34
54	BA	2314	A	C6-N1	-5.24	1.31	1.35
21	AA	680	C	N3-C4	-5.24	1.30	1.33
54	BA	167	A	C6-N1	-5.24	1.31	1.35
54	BA	1973	G	C2-N2	-5.24	1.29	1.34
54	BA	2029	G	C2-N2	-5.24	1.29	1.34
54	BA	2330	G	C2-N2	-5.24	1.29	1.34
21	AA	192	A	C6-N6	-5.24	1.29	1.33
21	AA	175	C	N3-C4	-5.24	1.30	1.33
54	BA	2611	C	N3-C4	-5.24	1.30	1.33
54	BA	2750	A	C6-N1	-5.24	1.31	1.35
21	AA	63	C	C4-N4	-5.23	1.29	1.33
21	AA	1322	C	C4-N4	-5.23	1.29	1.33
54	BA	2349	G	C2-N2	-5.23	1.29	1.34
54	BA	2683	C	N3-C4	-5.23	1.30	1.33
21	AA	357	G	C2-N2	-5.23	1.29	1.34
21	AA	1371	G	C2-N2	-5.23	1.29	1.34
54	BA	2042	A	C6-N1	-5.23	1.31	1.35
21	AA	1132	C	N3-C4	-5.23	1.30	1.33
54	BA	684	G	C2-N2	-5.23	1.29	1.34
21	AA	386	C	N3-C4	-5.23	1.30	1.33
21	AA	106	C	N3-C4	-5.22	1.30	1.33
21	AA	735	C	N3-C4	-5.22	1.30	1.33
54	BA	1355	G	C2-N2	-5.22	1.29	1.34
54	BA	2174	C	N3-C4	-5.22	1.30	1.33
21	AA	184	G	C2-N2	-5.22	1.29	1.34
21	AA	1159	U	C4'-O4'	-5.22	1.38	1.45
21	AA	1526	G	C2-N2	-5.22	1.29	1.34
54	BA	1514	G	C2-N2	-5.22	1.29	1.34
54	BA	1989	G	C2-N2	-5.22	1.29	1.34
21	AA	310	G	C2-N2	-5.22	1.29	1.34
54	BA	438	G	N1-C2	-5.22	1.33	1.37
54	BA	844	A	C6-N1	-5.22	1.31	1.35
54	BA	2196	C	N3-C4	-5.22	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2224	G	C2-N2	-5.22	1.29	1.34
54	BA	2294	G	C2-N2	-5.22	1.29	1.34
54	BA	2385	C	C4-N4	-5.22	1.29	1.33
21	AA	1156	G	C2-N2	-5.22	1.29	1.34
54	BA	68	G	N1-C2	-5.22	1.33	1.37
54	BA	347	A	C6-N1	-5.22	1.31	1.35
54	BA	1417	C	N3-C4	-5.22	1.30	1.33
54	BA	1753	G	C2-N2	-5.22	1.29	1.34
54	BA	1788	C	N3-C4	-5.22	1.30	1.33
22	A1	32	C	N3-C4	-5.21	1.30	1.33
54	BA	2078	C	N3-C4	-5.21	1.30	1.33
54	BA	1373	A	C6-N1	-5.21	1.31	1.35
54	BA	473	G	C6-N1	-5.21	1.35	1.39
54	BA	520	G	C2-N2	-5.21	1.29	1.34
54	BA	1543	G	C2-N2	-5.21	1.29	1.34
54	BA	1620	G	C2-N2	-5.21	1.29	1.34
54	BA	1800	C	C4-N4	-5.21	1.29	1.33
21	AA	457	G	C2-N2	-5.21	1.29	1.34
54	BA	35	G	C2-N2	-5.21	1.29	1.34
21	AA	364	A	C5-C4	-5.21	1.35	1.38
54	BA	2005	A	C6-N1	-5.21	1.31	1.35
54	BA	2093	G	N1-C2	-5.21	1.33	1.37
54	BA	2748	A	C6-N1	-5.21	1.31	1.35
55	BB	7	G	C6-N1	-5.21	1.35	1.39
24	A3	2	G	N1-C2	-5.21	1.33	1.37
54	BA	2616	C	C4-N4	-5.21	1.29	1.33
54	BA	544	C	C4-N4	-5.20	1.29	1.33
54	BA	2745	C	C4-N4	-5.20	1.29	1.33
21	AA	852	G	C2-N2	-5.20	1.29	1.34
21	AA	171	A	C6-N1	-5.20	1.31	1.35
21	AA	226	G	C2-N2	-5.20	1.29	1.34
21	AA	802	A	C6-N1	-5.20	1.31	1.35
21	AA	862	C	N3-C4	-5.20	1.30	1.33
21	AA	1428	A	C5-C4	-5.20	1.35	1.38
21	AA	1466	C	C4-N4	-5.20	1.29	1.33
54	BA	49	A	C5-C4	-5.20	1.35	1.38
54	BA	760	G	C2-N2	-5.20	1.29	1.34
21	AA	39	G	C2-N2	-5.20	1.29	1.34
21	AA	1249	C	C4-N4	-5.20	1.29	1.33
21	AA	1378	C	N3-C4	-5.20	1.30	1.33
54	BA	129	C	C4-N4	-5.20	1.29	1.33
54	BA	1544	A	C6-N1	-5.20	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1428	A	C6-N6	-5.19	1.29	1.33
21	AA	129	A	C5-C4	-5.19	1.35	1.38
54	BA	983	A	C6-N1	-5.19	1.31	1.35
54	BA	1740	G	C2-N2	-5.19	1.29	1.34
54	BA	2239	G	C2-N2	-5.19	1.29	1.34
54	BA	2893	A	C6-N1	-5.19	1.31	1.35
54	BA	1945	G	C2-N2	-5.19	1.29	1.34
21	AA	726	C	C4-N4	-5.19	1.29	1.33
54	BA	680	C	N3-C4	-5.18	1.30	1.33
54	BA	2221	G	C2-N2	-5.18	1.29	1.34
54	BA	1686	C	N3-C4	-5.18	1.30	1.33
54	BA	1788	C	C4-N4	-5.18	1.29	1.33
54	BA	2498	C	C4-N4	-5.18	1.29	1.33
21	AA	1102	A	C6-N1	-5.18	1.31	1.35
54	BA	449	A	C6-N1	-5.18	1.31	1.35
54	BA	2719	G	C2-N2	-5.18	1.29	1.34
21	AA	247	G	C2-N2	-5.18	1.29	1.34
21	AA	825	A	C6-N1	-5.18	1.31	1.35
54	BA	1766	G	C2-N2	-5.18	1.29	1.34
21	AA	35	G	C2-N2	-5.18	1.29	1.34
54	BA	2208	C	C4-N4	-5.18	1.29	1.33
54	BA	2789	C	C4-N4	-5.18	1.29	1.33
54	BA	447	A	C5-C4	-5.17	1.35	1.38
54	BA	2063	C	C4-N4	-5.17	1.29	1.33
54	BA	2230	G	N1-C2	-5.17	1.33	1.37
21	AA	16	A	C5-C4	-5.17	1.35	1.38
22	A1	1	G	C2-N2	-5.17	1.29	1.34
21	AA	97	G	N1-C2	-5.17	1.33	1.37
21	AA	470	C	C4-N4	-5.17	1.29	1.33
54	BA	2065	C	C4-N4	-5.17	1.29	1.33
55	BB	105	G	C6-N1	-5.17	1.35	1.39
21	AA	1100	C	C4-N4	-5.17	1.29	1.33
21	AA	349	A	C6-N6	-5.17	1.29	1.33
21	AA	518	C	N3-C4	-5.17	1.30	1.33
54	BA	1674	G	N1-C2	-5.17	1.33	1.37
21	AA	544	G	C2-N2	-5.17	1.29	1.34
21	AA	1409	C	N3-C4	-5.17	1.30	1.33
21	AA	1488	G	C2-N2	-5.17	1.29	1.34
54	BA	359	G	C2-N2	-5.17	1.29	1.34
54	BA	761	A	C6-N1	-5.17	1.31	1.35
21	AA	453	G	C6-N1	-5.16	1.35	1.39
24	A3	66	C	N3-C4	-5.16	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1127	A	C6-N1	-5.16	1.31	1.35
54	BA	2054	A	C6-N1	-5.16	1.31	1.35
21	AA	1493	A	C6-N6	-5.16	1.29	1.33
22	A1	18	G	C2-N2	-5.16	1.29	1.34
54	BA	1434	A	C5-C4	-5.16	1.35	1.38
54	BA	1512	C	C4-N4	-5.16	1.29	1.33
54	BA	2226	C	C4-N4	-5.16	1.29	1.33
54	BA	2428	G	C6-N1	-5.16	1.35	1.39
54	BA	1826	G	C6-N1	-5.16	1.35	1.39
21	AA	383	A	C6-N6	-5.16	1.29	1.33
54	BA	55	G	N1-C2	-5.16	1.33	1.37
54	BA	943	A	C6-N1	-5.16	1.31	1.35
21	AA	728	A	C6-N6	-5.16	1.29	1.33
54	BA	48	G	C2-N2	-5.16	1.29	1.34
54	BA	320	A	C6-N1	-5.16	1.31	1.35
54	BA	1972	G	C6-N1	-5.16	1.35	1.39
21	AA	959	A	C6-N1	-5.15	1.31	1.35
54	BA	496	G	C2-N2	-5.15	1.29	1.34
54	BA	192	C	C4-N4	-5.15	1.29	1.33
54	BA	1090	A	C5-C4	-5.15	1.35	1.38
54	BA	1319	C	C4-N4	-5.15	1.29	1.33
55	BB	79	G	C2-N2	-5.15	1.29	1.34
55	BB	86	G	C6-N1	-5.15	1.35	1.39
21	AA	730	G	C6-N1	-5.15	1.35	1.39
21	AA	770	C	C4'-C3'	-5.15	1.47	1.52
21	AA	1129	C	C4-N4	-5.15	1.29	1.33
54	BA	733	G	C2-N2	-5.15	1.29	1.34
55	BB	85	G	C2-N2	-5.15	1.29	1.34
54	BA	2446	G	C6-N1	-5.15	1.35	1.39
54	BA	42	A	C5-C4	-5.14	1.35	1.38
54	BA	597	G	C2-N2	-5.14	1.29	1.34
54	BA	1371	G	C2-N2	-5.14	1.29	1.34
21	AA	156	C	N3-C4	-5.14	1.30	1.33
21	AA	840	C	C4-N4	-5.14	1.29	1.33
21	AA	1141	C	C4-N4	-5.14	1.29	1.33
22	A1	15	G	C2-N2	-5.14	1.29	1.34
22	A1	53	G	C2-N2	-5.14	1.29	1.34
54	BA	411	G	C6-N1	-5.14	1.35	1.39
21	AA	604	G	C6-N1	-5.14	1.35	1.39
54	BA	2885	G	C2-N2	-5.14	1.29	1.34
21	AA	395	C	N3-C4	-5.14	1.30	1.33
21	AA	1071	C	N3-C4	-5.14	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	731	C	C4-N4	-5.14	1.29	1.33
54	BA	1530	G	C2-N2	-5.14	1.29	1.34
54	BA	2306	C	C4-N4	-5.14	1.29	1.33
21	AA	113	G	C2-N2	-5.14	1.29	1.34
54	BA	1536	C	C4-N4	-5.14	1.29	1.33
54	BA	1929	G	C2-N2	-5.14	1.29	1.34
54	BA	2362	C	C4-N4	-5.14	1.29	1.33
21	AA	1415	G	C2-N2	-5.14	1.29	1.34
54	BA	484	C	C4-N4	-5.14	1.29	1.33
54	BA	1821	A	C5-C4	-5.14	1.35	1.38
54	BA	1874	C	C4-N4	-5.14	1.29	1.33
54	BA	142	A	C6-N1	-5.13	1.31	1.35
54	BA	718	A	C5-C4	-5.13	1.35	1.38
54	BA	1451	C	N3-C4	-5.13	1.30	1.33
54	BA	1461	C	C4-N4	-5.13	1.29	1.33
54	BA	2545	G	C2-N2	-5.13	1.29	1.34
54	BA	2761	A	C6-N1	-5.13	1.31	1.35
54	BA	2062	A	C6-N1	-5.13	1.31	1.35
21	AA	386	C	C4-N4	-5.13	1.29	1.33
21	AA	1519	A	C5-C4	-5.13	1.35	1.38
54	BA	424	G	C2-N2	-5.13	1.29	1.34
21	AA	272	C	C4-N4	-5.13	1.29	1.33
21	AA	988	G	C2-N2	-5.13	1.29	1.34
54	BA	675	A	C6-N1	-5.13	1.31	1.35
54	BA	1746	A	C6-N1	-5.13	1.31	1.35
21	AA	292	G	C2-N2	-5.12	1.29	1.34
54	BA	2625	G	N1-C2	-5.12	1.33	1.37
21	AA	105	G	C2-N2	-5.12	1.29	1.34
22	A1	9	A	C6-N1	-5.12	1.31	1.35
54	BA	1434	A	C6-N6	-5.12	1.29	1.33
21	AA	370	C	N3-C4	-5.12	1.30	1.33
21	AA	228	A	C6-N6	-5.12	1.29	1.33
21	AA	853	C	C4-N4	-5.12	1.29	1.33
21	AA	1320	C	C4-N4	-5.12	1.29	1.33
54	BA	1	G	C2-N2	-5.12	1.29	1.34
54	BA	1112	G	C6-N1	-5.12	1.35	1.39
54	BA	2379	G	C2-N2	-5.12	1.29	1.34
21	AA	348	G	C6-N1	-5.12	1.35	1.39
21	AA	655	A	C6-N1	-5.12	1.31	1.35
21	AA	823	C	C4-N4	-5.12	1.29	1.33
21	AA	1178	G	N1-C2	-5.12	1.33	1.37
24	A3	58	A	C6-N6	-5.12	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	275	C	C4-N4	-5.12	1.29	1.33
21	AA	424	G	C2-N2	-5.11	1.29	1.34
54	BA	1973	G	C6-N1	-5.11	1.35	1.39
21	AA	312	C	C4-N4	-5.11	1.29	1.33
54	BA	39	G	C2-N2	-5.11	1.29	1.34
54	BA	1975	G	N1-C2	-5.11	1.33	1.37
54	BA	23	G	C2-N2	-5.11	1.29	1.34
54	BA	1514	G	C6-N1	-5.11	1.35	1.39
54	BA	2308	G	N1-C2	-5.11	1.33	1.37
21	AA	440	C	C4-N4	-5.11	1.29	1.33
21	AA	1187	G	C2-N2	-5.11	1.29	1.34
21	AA	1336	C	N3-C4	-5.11	1.30	1.33
21	AA	1396	A	C6-N1	-5.11	1.31	1.35
54	BA	797	G	N1-C2	-5.11	1.33	1.37
55	BB	97	C	C4-N4	-5.11	1.29	1.33
21	AA	570	G	N1-C2	-5.11	1.33	1.37
21	AA	575	G	C2-N2	-5.11	1.29	1.34
21	AA	1432	G	C2-N2	-5.11	1.29	1.34
54	BA	381	G	C6-N1	-5.11	1.35	1.39
54	BA	2767	C	C4-N4	-5.11	1.29	1.33
21	AA	611	C	C4-N4	-5.10	1.29	1.33
54	BA	1957	C	C4-N4	-5.10	1.29	1.33
21	AA	334	C	N3-C4	-5.10	1.30	1.33
54	BA	679	C	N3-C4	-5.10	1.30	1.33
21	AA	145	G	C6-N1	-5.10	1.35	1.39
21	AA	803	G	C6-N1	-5.10	1.35	1.39
54	BA	1743	G	C2-N2	-5.10	1.29	1.34
21	AA	443	C	N3-C4	-5.10	1.30	1.33
54	BA	1377	G	C2-N2	-5.10	1.29	1.34
54	BA	2015	A	C6-N1	-5.10	1.31	1.35
54	BA	2142	A	C6-N1	-5.10	1.31	1.35
21	AA	1107	C	C4-N4	-5.10	1.29	1.33
54	BA	1430	G	C6-N1	-5.10	1.35	1.39
55	BB	39	A	C6-N1	-5.10	1.31	1.35
21	AA	1484	C	C4-N4	-5.10	1.29	1.33
55	BB	69	G	C2-N2	-5.10	1.29	1.34
21	AA	494	G	C6-N1	-5.09	1.35	1.39
54	BA	1711	A	C6-N6	-5.09	1.29	1.33
54	BA	2174	C	C4-N4	-5.09	1.29	1.33
21	AA	1269	A	C6-N1	-5.09	1.31	1.35
21	AA	1346	A	C6-N6	-5.09	1.29	1.33
54	BA	2890	G	C2-N2	-5.09	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1084	G	C6-N1	-5.09	1.35	1.39
54	BA	563	A	C6-N1	-5.09	1.31	1.35
54	BA	2293	G	C2-N2	-5.09	1.29	1.34
21	AA	255	G	C2-N2	-5.09	1.29	1.34
21	AA	869	G	C2-N2	-5.09	1.29	1.34
22	A1	28	C	C4-N4	-5.09	1.29	1.33
54	BA	1084	A	C5-C4	-5.09	1.35	1.38
54	BA	1987	A	C6-N6	-5.09	1.29	1.33
21	AA	506	G	C2-N2	-5.08	1.29	1.34
54	BA	394	C	C4-N4	-5.08	1.29	1.33
54	BA	595	C	C4-N4	-5.08	1.29	1.33
54	BA	808	G	C2-N2	-5.08	1.29	1.34
54	BA	2606	C	N3-C4	-5.08	1.30	1.33
54	BA	972	A	O3'-P	-5.08	1.55	1.61
54	BA	1588	G	C2-N2	-5.08	1.29	1.34
54	BA	2791	G	C2-N2	-5.08	1.29	1.34
54	BA	795	C	N3-C4	-5.08	1.30	1.33
54	BA	1645	G	C2-N2	-5.08	1.29	1.34
55	BB	12	C	C4-N4	-5.08	1.29	1.33
21	AA	381	C	N3-C4	-5.08	1.30	1.33
21	AA	1267	C	C4-N4	-5.08	1.29	1.33
24	A3	69	C	C4'-C3'	-5.08	1.47	1.52
21	AA	179	A	C6-N1	-5.08	1.31	1.35
54	BA	1920	C	C4-N4	-5.08	1.29	1.33
54	BA	2237	G	C2-N2	-5.08	1.29	1.34
54	BA	1407	G	C6-N1	-5.08	1.35	1.39
21	AA	681	A	C6-N6	-5.08	1.29	1.33
21	AA	794	A	C6-N1	-5.08	1.31	1.35
21	AA	1385	G	C2-N2	-5.08	1.29	1.34
54	BA	74	A	C5-C4	-5.08	1.35	1.38
54	BA	74	A	C6-N6	-5.08	1.29	1.33
54	BA	423	A	C6-N1	-5.08	1.31	1.35
54	BA	1767	G	N1-C2	-5.08	1.33	1.37
54	BA	1813	G	C2-N2	-5.08	1.29	1.34
54	BA	1291	C	C4-N4	-5.07	1.29	1.33
54	BA	2215	C	N3-C4	-5.07	1.30	1.33
55	BB	30	C	N3-C4	-5.07	1.30	1.33
21	AA	16	A	C6-N6	-5.07	1.29	1.33
21	AA	1133	G	C2-N2	-5.07	1.29	1.34
54	BA	1374	G	N1-C2	-5.07	1.33	1.37
54	BA	89	A	C6-N1	-5.07	1.32	1.35
54	BA	876	C	C4-N4	-5.07	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1359	A	C5-C4	-5.07	1.35	1.38
54	BA	2736	A	C6-N1	-5.07	1.32	1.35
54	BA	2759	G	C2-N2	-5.07	1.29	1.34
55	BB	53	A	C6-N1	-5.07	1.32	1.35
21	AA	748	G	C2-N2	-5.07	1.29	1.34
54	BA	45	G	C6-N1	-5.07	1.36	1.39
54	BA	1809	A	C6-N1	-5.07	1.32	1.35
54	BA	2090	A	C5-C4	-5.07	1.35	1.38
54	BA	2169	A	C6-N1	-5.07	1.32	1.35
54	BA	2644	G	C6-N1	-5.07	1.36	1.39
22	A1	5	G	C2-N2	-5.06	1.29	1.34
54	BA	2280	G	C2-N2	-5.06	1.29	1.34
54	BA	2505	G	C6-N1	-5.06	1.36	1.39
54	BA	2549	G	C2-N2	-5.06	1.29	1.34
54	BA	2830	C	C4-N4	-5.06	1.29	1.33
54	BA	1361	G	C6-N1	-5.06	1.36	1.39
54	BA	1895	C	C4-N4	-5.06	1.29	1.33
54	BA	2354	C	N3-C4	-5.06	1.30	1.33
55	BB	37	C	C4-N4	-5.06	1.29	1.33
54	BA	2803	G	N1-C2	-5.06	1.33	1.37
54	BA	353	C	N3-C4	-5.06	1.30	1.33
54	BA	354	A	C5-C4	-5.06	1.35	1.38
54	BA	475	C	C4-N4	-5.06	1.29	1.33
54	BA	1803	A	C6-N1	-5.06	1.32	1.35
54	BA	2191	A	C5-C4	-5.06	1.35	1.38
54	BA	2729	G	C2-N2	-5.06	1.29	1.34
55	BB	2	G	C6-N1	-5.06	1.36	1.39
54	BA	1437	C	N3-C4	-5.06	1.30	1.33
54	BA	1970	A	C6-N1	-5.06	1.32	1.35
54	BA	1431	A	C5-C4	-5.06	1.35	1.38
54	BA	2060	A	C5-C4	-5.06	1.35	1.38
54	BA	977	G	C2-N2	-5.05	1.29	1.34
54	BA	1867	G	C2-N2	-5.05	1.29	1.34
54	BA	2544	G	C2-N2	-5.05	1.29	1.34
54	BA	2735	G	C2-N2	-5.05	1.29	1.34
54	BA	2757	A	C6-N6	-5.05	1.29	1.33
21	AA	738	C	C4-N4	-5.05	1.29	1.33
21	AA	846	G	C6-N1	-5.05	1.36	1.39
21	AA	440	C	N3-C4	-5.05	1.30	1.33
21	AA	1108	G	C6-N1	-5.05	1.36	1.39
54	BA	1351	C	N3-C4	-5.05	1.30	1.33
54	BA	1831	G	C6-N1	-5.05	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	139	A	C6-N1	-5.05	1.32	1.35
21	AA	339	C	N3-C4	-5.05	1.30	1.33
21	AA	457	G	C6-N1	-5.05	1.36	1.39
21	AA	650	G	C2-N2	-5.05	1.29	1.34
21	AA	784	A	C5-C4	-5.05	1.35	1.38
21	AA	1099	G	C2-N2	-5.05	1.29	1.34
21	AA	1111	A	C6-N1	-5.05	1.32	1.35
21	AA	1177	G	C2-N2	-5.05	1.29	1.34
54	BA	47	C	C4-N4	-5.05	1.29	1.33
54	BA	2590	A	C6-N1	-5.05	1.32	1.35
21	AA	211	G	N1-C2	-5.05	1.33	1.37
21	AA	729	A	C6-N6	-5.05	1.29	1.33
21	AA	1331	G	C2-N2	-5.05	1.29	1.34
21	AA	1411	C	C4-N4	-5.05	1.29	1.33
54	BA	1463	C	N3-C4	-5.05	1.30	1.33
21	AA	954	G	C2-N2	-5.04	1.29	1.34
54	BA	2315	G	C2-N2	-5.04	1.29	1.34
54	BA	351	C	C4-N4	-5.04	1.29	1.33
21	AA	578	C	N3-C4	-5.04	1.30	1.33
21	AA	1200	C	N3-C4	-5.04	1.30	1.33
54	BA	1441	G	C6-N1	-5.04	1.36	1.39
54	BA	2141	G	C2-N2	-5.04	1.29	1.34
54	BA	2153	C	N3-C4	-5.04	1.30	1.33
54	BA	2209	G	N1-C2	-5.04	1.33	1.37
54	BA	2367	G	C2-N2	-5.04	1.29	1.34
54	BA	2856	A	C6-N6	-5.04	1.29	1.33
55	BB	21	G	C2-N2	-5.04	1.29	1.34
21	AA	462	G	C6-N1	-5.04	1.36	1.39
21	AA	545	C	C4-N4	-5.04	1.29	1.33
21	AA	681	A	C5-C4	-5.04	1.35	1.38
21	AA	940	C	N3-C4	-5.04	1.30	1.33
21	AA	1150	A	C6-N1	-5.04	1.32	1.35
54	BA	2097	A	C6-N1	-5.04	1.32	1.35
54	BA	2633	G	C2-N2	-5.04	1.29	1.34
21	AA	882	C	C4-N4	-5.03	1.29	1.33
21	AA	1218	C	C4-N4	-5.03	1.29	1.33
54	BA	159	G	C2-N2	-5.03	1.29	1.34
54	BA	804	A	C6-N1	-5.03	1.32	1.35
54	BA	1587	G	C2-N2	-5.03	1.29	1.34
21	AA	376	G	C6-N1	-5.03	1.36	1.39
21	AA	39	G	C6-N1	-5.03	1.36	1.39
21	AA	177	G	N1-C2	-5.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	762	U	C4'-O4'	-5.03	1.39	1.45
21	AA	1207	G	C6-N1	-5.03	1.36	1.39
22	A1	52	G	C2-N2	-5.03	1.29	1.34
54	BA	432	A	C5-C4	-5.03	1.35	1.38
54	BA	2124	G	N1-C2	-5.03	1.33	1.37
54	BA	2890	G	C6-N1	-5.03	1.36	1.39
21	AA	237	G	C2-N2	-5.03	1.29	1.34
54	BA	447	A	C6-N6	-5.03	1.29	1.33
54	BA	510	C	C4-N4	-5.03	1.29	1.33
54	BA	2069	G	N1-C2	-5.03	1.33	1.37
54	BA	704	G	C2-N2	-5.02	1.29	1.34
54	BA	172	A	C5-C4	-5.02	1.35	1.38
54	BA	988	A	C6-N1	-5.02	1.32	1.35
54	BA	1582	C	C4-N4	-5.02	1.29	1.33
54	BA	2501	C	C4-N4	-5.02	1.29	1.33
54	BA	2587	A	C6-N1	-5.02	1.32	1.35
54	BA	1762	A	C6-N1	-5.02	1.32	1.35
21	AA	450	G	C2-N2	-5.02	1.29	1.34
21	AA	703	G	C2-N2	-5.02	1.29	1.34
21	AA	1521	C	N3-C4	-5.02	1.30	1.33
54	BA	210	C	C4-N4	-5.02	1.29	1.33
54	BA	1902	C	C4-N4	-5.02	1.29	1.33
54	BA	2792	A	C6-N1	-5.02	1.32	1.35
21	AA	553	A	C6-N6	-5.02	1.29	1.33
21	AA	647	C	C4-N4	-5.02	1.29	1.33
54	BA	201	C	C4-N4	-5.02	1.29	1.33
21	AA	1456	A	C6-N1	-5.01	1.32	1.35
54	BA	1936	A	C5-C4	-5.01	1.35	1.38
21	AA	1096	C	C4-N4	-5.01	1.29	1.33
54	BA	1869	G	C2-N2	-5.01	1.29	1.34
21	AA	993	G	C2-N2	-5.01	1.29	1.34
54	BA	2241	A	C5-C4	-5.01	1.35	1.38
21	AA	503	C	C4-N4	-5.00	1.29	1.33
54	BA	1925	C	C4-N4	-5.00	1.29	1.33
21	AA	428	G	C2-N2	-5.00	1.29	1.34
21	AA	560	A	C5-C4	-5.00	1.35	1.38
21	AA	1452	C	C4-N4	-5.00	1.29	1.33
54	BA	2760	C	N3-C4	-5.00	1.30	1.33
21	AA	1281	C	C4-N4	-5.00	1.29	1.33
54	BA	1900	A	C5-C4	-5.00	1.35	1.38
54	BA	1967	C	C4-N4	-5.00	1.29	1.33
54	BA	2255	G	N1-C2	-5.00	1.33	1.37

All (8067) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	34	A	N1-C6-N6	-13.76	110.34	118.60
54	BA	323	C	O4'-C1'-N1	13.51	119.01	108.20
54	BA	547	A	O4'-C1'-N9	12.98	118.58	108.20
54	BA	1943	U	O4'-C1'-N1	12.88	118.50	108.20
54	BA	1340	U	O4'-C1'-N1	12.80	118.44	108.20
54	BA	2284	A	N1-C6-N6	-12.62	111.03	118.60
54	BA	2176	A	N1-C6-N6	-12.59	111.05	118.60
21	AA	1188	A	N1-C6-N6	-12.29	111.23	118.60
54	BA	1566	A	N1-C6-N6	-12.28	111.23	118.60
21	AA	78	A	N1-C6-N6	-12.21	111.27	118.60
21	AA	914	A	N1-C6-N6	-12.18	111.29	118.60
54	BA	2439	A	N1-C6-N6	-12.10	111.34	118.60
54	BA	943	A	N1-C6-N6	-12.09	111.34	118.60
21	AA	397	A	N1-C6-N6	-12.07	111.36	118.60
54	BA	1815	A	N1-C6-N6	-12.07	111.36	118.60
54	BA	1427	A	N1-C6-N6	-12.06	111.36	118.60
54	BA	348	A	N1-C6-N6	-11.99	111.41	118.60
54	BA	280	U	O4'-C1'-N1	11.89	117.71	108.20
21	AA	749	A	N1-C6-N6	-11.87	111.48	118.60
54	BA	1021	A	N1-C6-N6	-11.86	111.48	118.60
21	AA	1398	A	N1-C6-N6	-11.84	111.50	118.60
24	A3	77	A	N1-C6-N6	-11.84	111.50	118.60
54	BA	346	A	N1-C6-N6	-11.82	111.50	118.60
54	BA	716	A	N1-C6-N6	-11.79	111.52	118.60
54	BA	2666	C	O4'-C1'-N1	11.78	117.62	108.20
54	BA	1088	A	N1-C6-N6	-11.73	111.56	118.60
54	BA	910	A	N1-C6-N6	-11.70	111.58	118.60
21	AA	408	A	N1-C6-N6	-11.69	111.58	118.60
21	AA	1005	A	N1-C6-N6	-11.67	111.60	118.60
54	BA	2297	A	N1-C6-N6	-11.65	111.61	118.60
54	BA	1783	A	N1-C6-N6	-11.63	111.62	118.60
54	BA	382	A	N1-C6-N6	-11.63	111.62	118.60
54	BA	1871	A	N1-C6-N6	-11.58	111.65	118.60
21	AA	129	A	N1-C6-N6	-11.54	111.67	118.60
54	BA	1505	A	N1-C6-N6	-11.48	111.71	118.60
54	BA	1285	A	N1-C6-N6	-11.47	111.72	118.60
21	AA	1502	A	N1-C6-N6	-11.47	111.72	118.60
54	BA	1272	A	N1-C6-N6	-11.46	111.73	118.60
54	BA	2513	A	N1-C6-N6	-11.44	111.74	118.60
54	BA	2241	A	N1-C6-N6	-11.43	111.74	118.60
55	BB	15	A	O4'-C1'-N9	11.42	117.33	108.20
21	AA	1246	A	N1-C6-N6	-11.41	111.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1257	A	N1-C6-N6	-11.41	111.75	118.60
54	BA	1679	A	N1-C6-N6	-11.40	111.76	118.60
21	AA	344	A	N1-C6-N6	-11.34	111.79	118.60
54	BA	925	A	N1-C6-N6	-11.32	111.81	118.60
54	BA	2733	A	N1-C6-N6	-11.32	111.81	118.60
54	BA	1960	A	N1-C6-N6	-11.31	111.82	118.60
21	AA	373	A	N1-C6-N6	-11.24	111.86	118.60
54	BA	945	A	N1-C6-N6	-11.23	111.86	118.60
54	BA	104	A	N1-C6-N6	-11.22	111.87	118.60
54	BA	2191	A	N1-C6-N6	-11.22	111.87	118.60
21	AA	546	A	N1-C6-N6	-11.19	111.89	118.60
21	AA	364	A	N1-C6-N6	-11.18	111.89	118.60
21	AA	728	A	N1-C6-N6	-11.17	111.90	118.60
39	BQ	12	ARG	NE-CZ-NH2	11.16	125.88	120.30
46	BX	71	ARG	NE-CZ-NH1	11.15	125.87	120.30
54	BA	1821	A	N1-C6-N6	-11.14	111.92	118.60
21	AA	1171	A	N1-C6-N6	-11.13	111.92	118.60
54	BA	2381	A	N1-C6-N6	-11.12	111.93	118.60
21	AA	1441	A	N1-C6-N6	-11.09	111.94	118.60
21	AA	1081	A	N1-C6-N6	-11.06	111.96	118.60
21	AA	363	A	N1-C6-N6	-11.03	111.98	118.60
54	BA	2109	U	O4'-C1'-N1	11.01	117.01	108.20
21	AA	452	A	N1-C6-N6	-11.00	112.00	118.60
54	BA	1204	A	N1-C6-N6	-10.99	112.00	118.60
54	BA	2590	A	N1-C6-N6	-10.97	112.02	118.60
21	AA	873	A	N1-C6-N6	-10.96	112.03	118.60
21	AA	1467	C	N3-C2-O2	-10.94	114.25	121.90
21	AA	807	A	N1-C6-N6	-10.91	112.06	118.60
54	BA	213	A	N1-C6-N6	-10.89	112.07	118.60
54	BA	1762	A	N1-C6-N6	-10.88	112.07	118.60
21	AA	466	A	N1-C6-N6	-10.88	112.07	118.60
46	BX	73	ARG	NE-CZ-NH1	10.87	125.74	120.30
21	AA	1346	A	N1-C6-N6	-10.87	112.08	118.60
54	BA	2311	A	N1-C6-N6	-10.86	112.08	118.60
54	BA	2031	A	N1-C6-N6	-10.86	112.09	118.60
54	BA	1509	A	N1-C6-N6	-10.84	112.09	118.60
54	BA	219	A	N1-C6-N6	-10.84	112.10	118.60
54	BA	83	A	N1-C6-N6	-10.83	112.10	118.60
21	AA	918	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	270	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	222	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	2358	A	N1-C6-N6	-10.79	112.13	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	481	G	O4'-C1'-N9	10.77	116.82	108.20
54	BA	1803	A	N1-C6-N6	-10.76	112.14	118.60
54	BA	1490	A	N1-C6-N6	-10.76	112.14	118.60
54	BA	1545	A	N1-C6-N6	-10.76	112.14	118.60
54	BA	233	A	N1-C6-N6	-10.75	112.15	118.60
2	AC	171	ARG	NE-CZ-NH1	10.74	125.67	120.30
54	BA	569	U	O4'-C1'-N1	10.73	116.78	108.20
54	BA	514	A	N1-C6-N6	-10.73	112.16	118.60
54	BA	1773	A	N1-C6-N6	-10.72	112.17	118.60
21	AA	130	A	N1-C6-N6	-10.69	112.19	118.60
11	AL	53	ARG	NE-CZ-NH1	10.68	125.64	120.30
25	BC	235	GLU	OE1-CD-OE2	-10.68	110.48	123.30
54	BA	847	U	O4'-C1'-N1	10.68	116.75	108.20
22	A1	41	A	N1-C6-N6	-10.67	112.20	118.60
54	BA	423	A	N1-C6-N6	-10.67	112.20	118.60
21	AA	499	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1496	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1635	A	N1-C6-N6	-10.65	112.21	118.60
21	AA	969	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1701	A	N1-C6-N6	-10.64	112.22	118.60
54	BA	2835	A	N1-C6-N6	-10.64	112.22	118.60
54	BA	1353	A	N1-C6-N6	-10.63	112.22	118.60
21	AA	1152	A	N1-C6-N6	-10.63	112.22	118.60
54	BA	1810	A	N1-C6-N6	-10.62	112.23	118.60
54	BA	980	A	N1-C6-N6	-10.61	112.23	118.60
21	AA	768	A	N1-C6-N6	-10.60	112.24	118.60
54	BA	1616	A	N1-C6-N6	-10.59	112.24	118.60
54	BA	1569	A	N1-C6-N6	-10.59	112.25	118.60
21	AA	26	A	N1-C6-N6	-10.58	112.25	118.60
54	BA	10	A	N1-C6-N6	-10.58	112.25	118.60
54	BA	2899	A	N1-C6-N6	-10.57	112.26	118.60
54	BA	2646	C	O4'-C1'-N1	10.57	116.65	108.20
21	AA	675	A	N1-C6-N6	-10.56	112.27	118.60
10	AK	92	ARG	NE-CZ-NH1	10.54	125.57	120.30
21	AA	236	A	N1-C6-N6	-10.54	112.28	118.60
54	BA	1352	U	O4'-C1'-N1	10.53	116.63	108.20
54	BA	2158	A	N1-C6-N6	-10.53	112.28	118.60
2	AC	10	ARG	NE-CZ-NH1	10.52	125.56	120.30
35	BM	40	ARG	NE-CZ-NH1	10.51	125.56	120.30
21	AA	509	A	N1-C6-N6	-10.51	112.29	118.60
21	AA	547	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	1784	A	N1-C6-N6	-10.49	112.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1396	A	N1-C6-N6	-10.49	112.31	118.60
54	BA	172	A	N1-C6-N6	-10.48	112.31	118.60
21	AA	288	A	N1-C6-N6	-10.45	112.33	118.60
54	BA	1713	A	N1-C6-N6	-10.45	112.33	118.60
21	AA	1467	C	N1-C2-O2	10.44	125.17	118.90
21	AA	1117	A	N1-C6-N6	-10.44	112.33	118.60
54	BA	602	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	2776	A	N1-C6-N6	-10.44	112.34	118.60
37	BO	9	ARG	NE-CZ-NH1	10.44	125.52	120.30
21	AA	205	A	N1-C6-N6	-10.44	112.34	118.60
54	BA	1969	A	N1-C6-N6	-10.43	112.34	118.60
37	BO	16	ARG	NE-CZ-NH1	10.42	125.51	120.30
21	AA	872	A	C1'-O4'-C4'	-10.40	101.58	109.90
21	AA	539	A	N1-C6-N6	-10.38	112.37	118.60
21	AA	968	A	N1-C6-N6	-10.38	112.37	118.60
2	AC	130	ARG	NE-CZ-NH1	10.37	125.48	120.30
21	AA	1519	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	821	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	1084	A	N1-C6-N6	-10.34	112.39	118.60
21	AA	1150	A	N1-C6-N6	-10.32	112.41	118.60
32	BJ	37	ARG	NE-CZ-NH1	10.32	125.46	120.30
54	BA	1901	A	N1-C6-N6	-10.32	112.41	118.60
21	AA	468	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	161	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	1690	A	N1-C6-N6	-10.30	112.42	118.60
54	BA	2270	A	N1-C6-N6	-10.29	112.43	118.60
7	AH	83	ARG	NE-CZ-NH1	10.29	125.44	120.30
54	BA	372	G	O4'-C1'-N9	10.28	116.43	108.20
38	BP	61	ARG	NE-CZ-NH1	10.26	125.43	120.30
54	BA	1226	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	1932	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	1434	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	1819	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	1789	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	2665	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	715	A	N1-C6-N6	-10.24	112.45	118.60
21	AA	845	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	673	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1021	A	N1-C6-N6	-10.23	112.46	118.60
14	AO	53	ARG	NE-CZ-NH1	10.23	125.41	120.30
54	BA	513	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1533	C	N3-C2-O2	-10.22	114.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2425	A	N1-C6-N6	-10.21	112.47	118.60
21	AA	1269	A	N1-C6-N6	-10.21	112.48	118.60
54	BA	920	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	13	A	N1-C6-N6	-10.20	112.48	118.60
21	AA	704	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	1847	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	2598	A	N1-C6-N6	-10.18	112.49	118.60
21	AA	33	A	N1-C6-N6	-10.16	112.50	118.60
39	BQ	91	ARG	NE-CZ-NH1	10.15	125.37	120.30
21	AA	715	A	N1-C6-N6	-10.14	112.51	118.60
54	BA	1532	A	N1-C6-N6	-10.14	112.52	118.60
54	BA	2900	A	N1-C6-N6	-10.14	112.52	118.60
12	AM	97	ARG	NE-CZ-NH2	10.12	125.36	120.30
21	AA	1105	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	1801	A	O4'-C1'-N9	10.11	116.29	108.20
54	BA	1626	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	676	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	609	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	1036	A	N1-C6-N6	-10.09	112.55	118.60
21	AA	356	A	N1-C6-N6	-10.09	112.55	118.60
21	AA	872	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	2163	A	N1-C6-N6	-10.09	112.55	118.60
21	AA	687	A	N1-C6-N6	-10.08	112.55	118.60
21	AA	1349	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	627	A	N1-C6-N6	-10.08	112.55	118.60
21	AA	1146	A	N1-C6-N6	-10.07	112.56	118.60
21	AA	161	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	825	A	N1-C6-N6	-10.07	112.56	118.60
21	AA	120	A	N1-C6-N6	-10.06	112.56	118.60
21	AA	915	A	C5-C6-N1	10.05	122.73	117.70
21	AA	1299	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	761	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	1084	A	C5-C6-N1	10.05	122.73	117.70
21	AA	414	A	N1-C6-N6	-10.05	112.57	118.60
21	AA	183	C	N3-C2-O2	-10.05	114.86	121.90
21	AA	344	A	C5-C6-N1	10.04	122.72	117.70
54	BA	2766	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	443	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	2813	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	197	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	1431	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	80	A	N1-C6-N6	-10.01	112.59	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	22	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	1637	A	N1-C6-N6	-10.00	112.60	118.60
55	BB	52	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	155	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	152	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	2635	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	681	A	N1-C6-N6	-9.99	112.60	118.60
54	BA	1746	A	N1-C6-N6	-9.99	112.61	118.60
54	BA	2721	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	412	A	N1-C6-N6	-9.97	112.61	118.60
54	BA	2080	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	2761	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	959	A	N1-C6-N6	-9.96	112.62	118.60
54	BA	1610	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	1216	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	1213	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	721	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	1528	A	N1-C6-N6	-9.93	112.64	118.60
27	BE	114	ARG	NE-CZ-NH1	9.93	125.26	120.30
54	BA	346	A	C5-C6-N1	9.92	122.66	117.70
54	BA	972	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	675	A	N1-C6-N6	-9.91	112.65	118.60
22	A1	38	A	N1-C6-N6	-9.91	112.66	118.60
54	BA	1089	A	N1-C6-N6	-9.91	112.65	118.60
21	AA	553	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	815	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	1785	A	N1-C6-N6	-9.89	112.66	118.60
54	BA	2126	A	N1-C6-N6	-9.89	112.66	118.60
54	BA	272	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	1889	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	1614	A	N1-C6-N6	-9.87	112.68	118.60
21	AA	1468	A	N1-C6-N6	-9.87	112.68	118.60
9	AJ	9	ARG	NE-CZ-NH1	9.86	125.23	120.30
55	BB	109	A	O4'-C1'-N9	9.85	116.08	108.20
10	AK	97	ARG	NE-CZ-NH1	9.85	125.22	120.30
21	AA	919	A	N1-C6-N6	-9.85	112.69	118.60
21	AA	1082	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	95	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	1205	A	N1-C6-N6	-9.85	112.69	118.60
21	AA	975	A	N1-C6-N6	-9.84	112.70	118.60
21	AA	1169	A	N1-C6-N6	-9.82	112.70	118.60
54	BA	1665	A	N1-C6-N6	-9.82	112.70	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1403	A	N1-C6-N6	-9.82	112.71	118.60
21	AA	1533	C	O4'-C1'-N1	9.82	116.05	108.20
56	B5	74	ARG	NE-CZ-NH1	9.81	125.21	120.30
9	AJ	68	ARG	NE-CZ-NH1	9.81	125.20	120.30
37	BO	10	ARG	NE-CZ-NH1	9.81	125.20	120.30
54	BA	429	A	N1-C6-N6	-9.81	112.72	118.60
24	A3	58	A	N1-C6-N6	-9.80	112.72	118.60
21	AA	19	A	N1-C6-N6	-9.79	112.72	118.60
54	BA	2750	A	N1-C6-N6	-9.79	112.72	118.60
55	BB	94	A	N1-C6-N6	-9.79	112.72	118.60
54	BA	482	A	N1-C6-N6	-9.79	112.73	118.60
54	BA	1928	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	1548	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	1456	A	N1-C6-N6	-9.76	112.74	118.60
54	BA	1630	A	N1-C6-N6	-9.76	112.75	118.60
15	AP	35	ARG	NE-CZ-NH1	9.75	125.18	120.30
21	AA	665	A	N1-C6-N6	-9.75	112.75	118.60
9	AJ	48	ARG	NE-CZ-NH1	9.74	125.17	120.30
34	BL	2	ARG	NE-CZ-NH1	9.74	125.17	120.30
21	AA	60	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	2450	A	N1-C6-N6	-9.74	112.76	118.60
21	AA	192	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2602	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1077	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	979	A	C5-C6-N1	9.72	122.56	117.70
54	BA	149	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	579	A	N1-C6-N6	-9.71	112.78	118.60
54	BA	730	A	N1-C6-N6	-9.71	112.78	118.60
54	BA	354	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	877	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	1196	A	N1-C6-N6	-9.70	112.78	118.60
21	AA	1428	A	N1-C6-N6	-9.69	112.79	118.60
18	AS	36	ARG	NE-CZ-NH1	9.69	125.14	120.30
54	BA	2833	U	O4'-C1'-N1	9.69	115.95	108.20
55	BB	29	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	592	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	2058	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	204	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	223	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	2287	A	N1-C6-N6	-9.67	112.80	118.60
10	AK	121	ARG	NE-CZ-NH2	9.66	125.13	120.30
21	AA	10	A	N1-C6-N6	-9.66	112.80	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1938	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	2170	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	1772	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	520	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	131	A	N1-C6-N6	-9.65	112.81	118.60
41	BS	84	ARG	NE-CZ-NH1	9.64	125.12	120.30
21	AA	116	A	N1-C6-N6	-9.64	112.82	118.60
21	AA	320	A	N1-C6-N6	-9.64	112.82	118.60
54	BA	91	A	O4'-C1'-N9	9.63	115.91	108.20
54	BA	1900	A	N1-C6-N6	-9.64	112.82	118.60
55	BB	59	A	N1-C6-N6	-9.63	112.82	118.60
8	AI	17	ARG	NE-CZ-NH1	9.62	125.11	120.30
54	BA	1359	A	N1-C6-N6	-9.62	112.83	118.60
55	BB	101	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	479	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2307	G	O4'-C1'-N9	9.62	115.90	108.20
54	BA	2851	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	909	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	2169	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	356	A	C5-C6-N1	9.61	122.50	117.70
54	BA	1204	A	C5-C6-N1	9.60	122.50	117.70
54	BA	1970	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	2317	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	2411	A	C5-C6-N1	9.59	122.50	117.70
54	BA	699	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	1088	A	C5-C6-N1	9.59	122.50	117.70
21	AA	746	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	125	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	900	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	372	C	N3-C2-O2	-9.58	115.19	121.90
15	AP	51	ARG	NE-CZ-NH1	9.58	125.09	120.30
54	BA	866	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	1046	A	O4'-C1'-N9	9.58	115.86	108.20
54	BA	670	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1365	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	2385	C	O4'-C1'-N1	9.55	115.84	108.20
13	AN	63	ARG	NE-CZ-NH1	9.55	125.07	120.30
54	BA	2015	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	2176	A	C5-C6-N1	9.55	122.47	117.70
21	AA	559	A	N1-C6-N6	-9.54	112.87	118.60
21	AA	336	A	N1-C6-N6	-9.54	112.88	118.60
22	A1	69	A	N1-C6-N6	-9.54	112.88	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	608	A	N1-C6-N6	-9.54	112.88	118.60
21	AA	243	A	N1-C6-N6	-9.54	112.88	118.60
21	AA	451	A	N1-C6-N6	-9.54	112.88	118.60
21	AA	949	A	N1-C6-N6	-9.53	112.88	118.60
55	BB	78	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	637	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2736	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	71	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	1549	A	C5-C6-N1	9.51	122.46	117.70
21	AA	366	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	983	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	2873	A	N1-C6-N6	-9.51	112.89	118.60
54	BA	1129	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	1251	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	1069	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	1780	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	973	A	N1-C6-N6	-9.49	112.90	118.60
54	BA	2814	A	N1-C6-N6	-9.49	112.90	118.60
21	AA	382	A	C5-C6-N1	9.49	122.44	117.70
21	AA	622	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	1503	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	42	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	629	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	1057	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	1654	A	N1-C6-N6	-9.47	112.92	118.60
55	BB	109	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1147	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1953	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	466	A	C5-C6-N1	9.46	122.43	117.70
21	AA	415	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1169	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	101	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	504	A	O4'-C1'-N9	9.45	115.76	108.20
54	BA	1010	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1783	A	C5-C6-N1	9.44	122.42	117.70
24	A3	60	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	1494	A	N1-C6-N6	-9.44	112.93	118.60
21	AA	728	A	C5-C6-N1	9.44	122.42	117.70
4	AE	67	ARG	NE-CZ-NH1	9.44	125.02	120.30
54	BA	2458	G	O4'-C1'-N9	9.44	115.75	108.20
54	BA	1535	A	O4'-C1'-N9	9.43	115.74	108.20
54	BA	1936	A	N1-C6-N6	-9.43	112.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	228	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	270	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	825	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	1111	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	2542	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	508	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1156	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	1327	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	527	C	N1-C2-O2	9.41	124.54	118.90
54	BA	141	G	O4'-C1'-N9	9.40	115.72	108.20
54	BA	735	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	845	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	977	A	N1-C6-N6	-9.39	112.96	118.60
21	AA	50	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	990	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	1493	A	C5-C6-N1	9.37	122.39	117.70
54	BA	2333	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	156	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	2765	A	N1-C6-N6	-9.36	112.99	118.60
54	BA	2566	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	2726	A	N1-C6-N6	-9.35	112.99	118.60
21	AA	1318	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	127	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1544	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	2497	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	2097	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	2212	A	O4'-C1'-N9	9.34	115.67	108.20
54	BA	368	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	608	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	1346	A	C5-C6-N1	9.33	122.36	117.70
54	BA	1246	A	N1-C6-N6	-9.33	113.00	118.60
54	BA	466	A	N1-C6-N6	-9.32	113.00	118.60
54	BA	1858	A	N1-C6-N6	-9.32	113.00	118.60
54	BA	756	A	N1-C6-N6	-9.32	113.01	118.60
55	BB	15	A	C5-C6-N1	9.32	122.36	117.70
21	AA	1046	A	C5-C6-N1	9.32	122.36	117.70
54	BA	1805	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	1418	A	C5-C6-N1	9.31	122.36	117.70
54	BA	541	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	759	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	1239	A	N1-C6-N6	-9.31	113.01	118.60
40	BR	90	ARG	NE-CZ-NH1	9.31	124.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	782	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	527	C	N3-C2-O2	-9.31	115.39	121.90
21	AA	143	A	N1-C6-N6	-9.30	113.02	118.60
21	AA	264	C	N3-C2-O2	-9.29	115.40	121.90
21	AA	300	A	N1-C6-N6	-9.29	113.03	118.60
42	BT	69	ARG	NE-CZ-NH1	9.28	124.94	120.30
21	AA	595	A	N1-C6-N6	-9.28	113.03	118.60
25	BC	211	ARG	NE-CZ-NH1	9.28	124.94	120.30
54	BA	988	A	N1-C6-N6	-9.27	113.04	118.60
26	BD	83	ARG	NE-CZ-NH1	9.27	124.94	120.30
54	BA	1872	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1098	A	N1-C6-N6	-9.26	113.04	118.60
21	AA	665	A	C5-C6-N1	9.26	122.33	117.70
54	BA	21	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	155	A	N1-C6-N6	-9.25	113.05	118.60
22	A1	66	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	144	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	947	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	896	A	N1-C6-N6	-9.25	113.05	118.60
55	BB	26	C	N3-C2-O2	-9.25	115.42	121.90
54	BA	2606	C	N3-C2-O2	-9.24	115.43	121.90
25	BC	181	ARG	NE-CZ-NH1	9.24	124.92	120.30
54	BA	2287	A	C5-C6-N1	9.24	122.32	117.70
54	BA	2589	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	574	A	N1-C6-N6	-9.23	113.06	118.60
22	A1	38	A	C5-C6-N1	9.22	122.31	117.70
54	BA	1284	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	2468	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	384	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	1322	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	1144	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	221	A	N1-C6-N6	-9.21	113.08	118.60
54	BA	241	A	N1-C6-N6	-9.21	113.08	118.60
56	B5	9	ARG	NE-CZ-NH1	9.21	124.90	120.30
54	BA	2451	A	N1-C6-N6	-9.20	113.08	118.60
21	AA	313	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	1009	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	2274	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	2577	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	911	A	N1-C6-N6	-9.19	113.08	118.60
21	AA	251	G	O4'-C1'-N9	9.19	115.55	108.20
54	BA	207	A	N1-C6-N6	-9.18	113.09	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2346	A	N1-C6-N6	-9.18	113.09	118.60
21	AA	784	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	101	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1451	C	N3-C2-O2	-9.17	115.48	121.90
54	BA	1853	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1591	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	228	A	C5-C6-N1	9.16	122.28	117.70
21	AA	129	A	C5-C6-N1	9.16	122.28	117.70
55	BB	50	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	2090	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	2872	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	2614	A	C5-C6-N1	9.16	122.28	117.70
54	BA	1320	C	N3-C2-O2	-9.16	115.49	121.90
54	BA	2748	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	441	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1420	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	1937	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	71	A	C5-C6-N1	9.13	122.27	117.70
55	BB	73	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	1393	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	938	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	160	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	1252	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	1885	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	1434	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	2154	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	364	A	C5-C6-N1	9.10	122.25	117.70
21	AA	1311	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	718	A	C5-C6-N1	9.09	122.24	117.70
21	AA	246	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	668	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	349	A	C5-C6-N1	9.08	122.24	117.70
54	BA	2872	A	C5-C6-N1	9.08	122.24	117.70
21	AA	978	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	2850	A	N1-C6-N6	-9.08	113.16	118.60
54	BA	599	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	412	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1374	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1016	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	322	A	C5-C6-N1	9.07	122.23	117.70
54	BA	1791	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	781	A	N1-C6-N6	-9.06	113.16	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	6	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	1302	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	1434	A	C5-C6-N1	9.06	122.23	117.70
21	AA	270	A	C5-C6-N1	9.05	122.23	117.70
54	BA	1711	A	C5-C6-N1	9.06	122.23	117.70
39	BQ	50	ARG	NE-CZ-NH2	9.05	124.83	120.30
54	BA	975	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	563	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	983	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1384	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	72	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	1287	A	N1-C6-N6	-9.04	113.17	118.60
21	AA	383	A	N1-C6-N6	-9.04	113.18	118.60
21	AA	1428	A	C5-C6-N1	9.04	122.22	117.70
54	BA	1403	A	C5-C6-N1	9.04	122.22	117.70
54	BA	2170	A	C5-C6-N1	9.04	122.22	117.70
22	A1	76	A	C4-C5-C6	-9.04	112.48	117.00
54	BA	1755	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2448	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2531	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2108	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	1368	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	183	C	N1-C2-O2	9.02	124.31	118.90
21	AA	873	A	C5-C6-N1	9.02	122.21	117.70
22	A1	23	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	614	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	1549	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	1392	A	N1-C6-N6	-9.01	113.19	118.60
1	AB	212	TYR	CB-CG-CD2	-9.01	115.59	121.00
54	BA	980	A	C5-C6-N1	9.01	122.20	117.70
54	BA	2171	A	C5-C6-N1	9.01	122.20	117.70
21	AA	430	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	518	C	N3-C2-O2	-9.00	115.60	121.90
21	AA	1398	A	C4-C5-C6	-9.00	112.50	117.00
23	A2	79	A	C5-C6-N1	9.00	122.20	117.70
21	AA	1534	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	2453	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	263	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	2450	A	C5-C6-N1	9.00	122.20	117.70
54	BA	751	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	250	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	1262	A	N1-C6-N6	-8.98	113.21	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1854	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2499	C	N3-C2-O2	-8.98	115.61	121.90
21	AA	1513	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	706	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2054	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	515	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	1459	G	O4'-C1'-N9	8.97	115.37	108.20
54	BA	294	A	C5-C6-N1	8.96	122.18	117.70
54	BA	1286	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1610	A	O4'-C1'-N9	8.96	115.37	108.20
54	BA	1089	A	C5-C6-N1	8.96	122.18	117.70
54	BA	74	A	C5-C6-N1	8.96	122.18	117.70
21	AA	1019	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	1260	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	432	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	1027	A	N1-C6-N6	-8.95	113.23	118.60
32	BJ	34	ARG	NE-CZ-NH1	8.95	124.77	120.30
54	BA	1668	A	N1-C6-N6	-8.94	113.23	118.60
21	AA	695	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1570	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	2062	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1802	A	N1-C6-N6	-8.94	113.24	118.60
10	AK	127	ARG	NE-CZ-NH1	8.93	124.77	120.30
21	AA	1082	A	C4-C5-C6	-8.93	112.53	117.00
54	BA	1711	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	468	A	C5-C6-N1	8.93	122.16	117.70
54	BA	203	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	1495	A	N1-C6-N6	-8.93	113.24	118.60
20	AU	32	ARG	NE-CZ-NH1	8.93	124.76	120.30
54	BA	531	C	O4'-C1'-N1	8.93	115.34	108.20
21	AA	1429	A	N1-C6-N6	-8.93	113.25	118.60
54	BA	547	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	2882	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	933	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1046	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1301	A	N1-C6-N6	-8.91	113.25	118.60
3	AD	110	ARG	NE-CZ-NH1	8.91	124.75	120.30
21	AA	502	A	C4-C5-C6	-8.91	112.55	117.00
21	AA	913	A	N1-C6-N6	-8.91	113.26	118.60
54	BA	2818	U	O4'-C1'-N1	8.91	115.33	108.20
21	AA	329	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2628	C	O4'-C1'-N1	8.90	115.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	26	A	C5-C6-N1	8.89	122.15	117.70
21	AA	498	A	C5-C6-N1	8.89	122.15	117.70
21	AA	546	A	C4-C5-C6	-8.89	112.55	117.00
54	BA	1772	A	C5-C6-N1	8.89	122.15	117.70
21	AA	1287	A	N1-C6-N6	-8.89	113.27	118.60
54	BA	1998	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	687	A	C5-C6-N1	8.89	122.14	117.70
54	BA	1420	A	C5-C6-N1	8.89	122.14	117.70
17	AR	72	ARG	NE-CZ-NH1	8.88	124.74	120.30
21	AA	1468	A	C5-C6-N1	8.88	122.14	117.70
54	BA	2003	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	1809	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	2734	A	N1-C6-N6	-8.88	113.27	118.60
21	AA	1329	A	N1-C6-N6	-8.88	113.27	118.60
24	A3	73	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	2675	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	1142	A	C5-C6-N1	8.87	122.14	117.70
54	BA	2733	A	C5-C6-N1	8.87	122.14	117.70
54	BA	1641	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1086	A	C5-C6-N1	8.87	122.14	117.70
21	AA	288	A	C5-C6-N1	8.87	122.13	117.70
54	BA	176	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	861	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	764	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	2391	G	O4'-C1'-N9	8.86	115.29	108.20
24	A3	74	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	63	A	C5-C6-N1	8.85	122.13	117.70
54	BA	2824	C	N3-C2-O2	-8.85	115.70	121.90
21	AA	1163	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	793	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	172	A	N1-C6-N6	-8.84	113.29	118.60
29	BG	68	ARG	NE-CZ-NH1	8.84	124.72	120.30
21	AA	1441	A	C5-C6-N1	8.83	122.12	117.70
54	BA	282	A	C5-C6-N1	8.83	122.12	117.70
54	BA	750	A	N1-C6-N6	-8.83	113.30	118.60
21	AA	371	A	C5-C6-N1	8.83	122.11	117.70
24	A3	1	C	N3-C2-O2	-8.83	115.72	121.90
54	BA	362	A	N1-C6-N6	-8.83	113.30	118.60
35	BM	6	ARG	NE-CZ-NH1	8.83	124.71	120.30
54	BA	1194	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	167	A	N1-C6-N6	-8.82	113.31	118.60
22	A1	21	A	N1-C6-N6	-8.82	113.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1785	A	C5-C6-N1	8.82	122.11	117.70
21	AA	44	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1556	C	N3-C2-O2	-8.81	115.73	121.90
21	AA	1151	A	N1-C6-N6	-8.81	113.31	118.60
18	AS	31	ARG	NE-CZ-NH1	8.81	124.71	120.30
21	AA	969	A	C5-C6-N1	8.81	122.11	117.70
54	BA	1758	U	O4'-C1'-N1	8.81	115.25	108.20
54	BA	2386	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1276	A	N1-C6-N6	-8.81	113.32	118.60
54	BA	2060	A	N1-C6-N6	-8.81	113.32	118.60
21	AA	262	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	313	A	C4-C5-C6	-8.80	112.60	117.00
21	AA	336	A	C4-C5-C6	-8.80	112.60	117.00
54	BA	1385	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	560	A	C5-C6-N1	8.80	122.10	117.70
21	AA	1519	A	C5-C6-N1	8.80	122.10	117.70
21	AA	553	A	C5-C6-N1	8.80	122.10	117.70
54	BA	2241	A	C5-C6-N1	8.80	122.10	117.70
21	AA	1350	A	C5-C6-N1	8.80	122.10	117.70
54	BA	2059	A	C5-C6-N1	8.80	122.10	117.70
54	BA	2080	A	C5-C6-N1	8.80	122.10	117.70
54	BA	693	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	1101	A	N1-C6-N6	-8.79	113.32	118.60
12	AM	89	ARG	NE-CZ-NH1	8.79	124.70	120.30
21	AA	1109	C	N3-C2-O2	-8.79	115.75	121.90
11	AL	49	ARG	NE-CZ-NH1	8.79	124.69	120.30
21	AA	996	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	573	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	909	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	2435	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	2820	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1515	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	792	A	C5-C6-N1	8.78	122.09	117.70
21	AA	1214	C	N3-C2-O2	-8.78	115.76	121.90
54	BA	472	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	1350	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2376	A	C5-C6-N1	8.78	122.09	117.70
54	BA	2711	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2657	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	1248	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	1271	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	546	A	C5-C6-N1	8.77	122.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	373	A	C5-C6-N1	8.77	122.08	117.70
54	BA	1593	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2154	A	C5-C6-N1	8.77	122.08	117.70
54	BA	19	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	1320	C	N3-C2-O2	-8.76	115.77	121.90
54	BA	1404	C	N3-C2-O2	-8.76	115.77	121.90
54	BA	2033	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	1067	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	1905	C	O4'-C1'-N1	8.76	115.20	108.20
54	BA	76	C	O4'-C1'-N1	8.76	115.20	108.20
54	BA	2266	A	N1-C6-N6	-8.76	113.35	118.60
26	BD	141	ARG	NE-CZ-NH1	8.75	124.68	120.30
54	BA	2823	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	958	A	C5-C6-N1	8.75	122.08	117.70
54	BA	1029	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	1987	A	C4-C5-C6	-8.75	112.62	117.00
54	BA	249	C	O4'-C1'-N1	8.75	115.20	108.20
54	BA	1936	A	C5-C6-N1	8.75	122.07	117.70
21	AA	937	A	C5-C6-N1	8.74	122.07	117.70
54	BA	2090	A	C5-C6-N1	8.74	122.07	117.70
21	AA	441	A	C5-C6-N1	8.74	122.07	117.70
54	BA	1665	A	C4-C5-C6	-8.74	112.63	117.00
21	AA	1431	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	344	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1829	A	C5-C6-N1	8.74	122.07	117.70
54	BA	199	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	1339	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1698	A	C5-C6-N1	8.73	122.06	117.70
21	AA	792	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1308	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	975	A	C5-C6-N1	8.72	122.06	117.70
21	AA	1533	C	N1-C2-O2	8.72	124.14	118.90
54	BA	347	A	N1-C6-N6	-8.72	113.36	118.60
54	BA	2469	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	1280	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	1654	A	C5-C6-N1	8.72	122.06	117.70
21	AA	1014	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	1336	C	N3-C2-O2	-8.72	115.80	121.90
24	A3	45	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	789	A	C5-C6-N1	8.72	122.06	117.70
54	BA	982	C	N3-C2-O2	-8.72	115.80	121.90
54	BA	1111	A	C5-C6-N1	8.72	122.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	729	A	C5-C6-N1	8.71	122.06	117.70
54	BA	510	C	N3-C2-O2	-8.71	115.80	121.90
21	AA	1518	A	N1-C6-N6	-8.71	113.37	118.60
54	BA	892	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	575	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	1899	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	2025	C	N3-C2-O2	-8.70	115.81	121.90
21	AA	328	C	N3-C2-O2	-8.70	115.81	121.90
54	BA	152	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	503	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	1759	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	10	A	C4-C5-C6	-8.68	112.66	117.00
54	BA	2284	A	C5-C6-N1	8.68	122.04	117.70
54	BA	1735	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1509	A	C5-C6-N1	8.67	122.03	117.70
26	BD	33	ARG	NE-CZ-NH1	8.66	124.63	120.30
21	AA	522	C	N3-C2-O2	-8.66	115.84	121.90
21	AA	802	A	N1-C6-N6	-8.66	113.41	118.60
54	BA	204	A	C4-C5-C6	-8.65	112.67	117.00
21	AA	143	A	C5-C6-N1	8.65	122.03	117.70
21	AA	238	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	2003	A	C5-C6-N1	8.65	122.03	117.70
54	BA	2814	A	C5-C6-N1	8.64	122.02	117.70
56	B5	134	ARG	NE-CZ-NH1	8.64	124.62	120.30
54	BA	789	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	51	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	354	A	C5-C6-N1	8.64	122.02	117.70
54	BA	1504	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	354	G	O4'-C1'-N9	8.63	115.11	108.20
21	AA	1169	A	C5-C6-N1	8.63	122.02	117.70
21	AA	1360	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1632	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1871	A	C5-C6-N1	8.63	122.02	117.70
8	AI	105	ARG	NE-CZ-NH1	8.63	124.62	120.30
54	BA	1073	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	510	A	C5-C6-N1	8.63	122.02	117.70
54	BA	2868	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	915	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	238	A	C5-C6-N1	8.62	122.01	117.70
54	BA	1899	A	C5-C6-N1	8.62	122.01	117.70
54	BA	1700	A	C5-C6-N1	8.62	122.01	117.70
54	BA	1354	A	N1-C6-N6	-8.62	113.43	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	15	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	2448	A	C5-C6-N1	8.61	122.01	117.70
54	BA	2781	A	C5-C6-N1	8.61	122.01	117.70
21	AA	1167	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	2856	A	C5-C6-N1	8.61	122.00	117.70
21	AA	414	A	C5-C6-N1	8.60	122.00	117.70
54	BA	626	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1383	A	N1-C6-N6	-8.60	113.44	118.60
15	AP	5	ARG	NE-CZ-NH1	8.60	124.60	120.30
19	AT	59	ARG	NE-CZ-NH1	8.60	124.60	120.30
54	BA	1080	A	N1-C6-N6	-8.60	113.44	118.60
6	AG	118	ARG	NE-CZ-NH1	8.59	124.60	120.30
54	BA	1189	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	1285	A	C5-C6-N1	8.59	122.00	117.70
54	BA	196	A	N1-C6-N6	-8.59	113.44	118.60
34	BL	41	ARG	NE-CZ-NH1	8.59	124.59	120.30
54	BA	719	C	N3-C2-O2	-8.59	115.89	121.90
54	BA	2009	A	N1-C6-N6	-8.59	113.45	118.60
25	BC	213	ARG	NE-CZ-NH1	8.59	124.59	120.30
54	BA	160	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	48	C	N3-C2-O2	-8.58	115.89	121.90
21	AA	781	A	C5-C6-N1	8.58	121.99	117.70
54	BA	750	A	C4-C5-C6	-8.58	112.71	117.00
9	AJ	37	ARG	NE-CZ-NH1	8.58	124.59	120.30
21	AA	1493	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	99	U	O4'-C1'-N1	8.58	115.06	108.20
54	BA	2451	A	C5-C6-N1	8.58	121.99	117.70
47	BY	29	ARG	NE-CZ-NH1	8.58	124.59	120.30
54	BA	204	A	C5-C6-N1	8.58	121.99	117.70
54	BA	1095	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	274	A	N1-C6-N6	-8.57	113.45	118.60
21	AA	1362	A	C5-C6-N1	8.57	121.99	117.70
54	BA	1525	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	192	C	N3-C2-O2	-8.57	115.90	121.90
54	BA	1142	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	483	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	582	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	831	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	371	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	766	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	1398	A	C5-C6-N1	8.55	121.98	117.70
54	BA	1757	A	C5-C6-N1	8.56	121.98	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1227	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	1698	A	C4-C5-C6	-8.55	112.72	117.00
55	BB	45	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2060	A	C5-C6-N1	8.55	121.98	117.70
21	AA	640	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2320	U	O4'-C1'-N1	8.55	115.04	108.20
21	AA	655	A	N1-C6-N6	-8.55	113.47	118.60
30	BH	50	ARG	NE-CZ-NH1	8.55	124.57	120.30
54	BA	371	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	1404	C	N1-C2-O2	8.55	124.03	118.90
54	BA	2851	A	C5-C6-N1	8.55	121.97	117.70
54	BA	739	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	1328	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	959	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	2886	A	C5-C6-N1	8.54	121.97	117.70
15	AP	28	ARG	NE-CZ-NH1	8.54	124.57	120.30
21	AA	983	A	C5-C6-N1	8.54	121.97	117.70
54	BA	64	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	104	A	C5-C6-N1	8.54	121.97	117.70
54	BA	1477	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	616	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	8	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	1324	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	980	A	O4'-C1'-N9	8.53	115.02	108.20
54	BA	1321	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	497	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	1789	A	C4-C5-C6	-8.53	112.74	117.00
21	AA	994	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	643	A	C5-C6-N1	8.52	121.96	117.70
21	AA	1155	A	N1-C6-N6	-8.52	113.49	118.60
52	B3	29	ARG	NE-CZ-NH1	8.52	124.56	120.30
54	BA	1981	A	C5-C6-N1	8.52	121.96	117.70
54	BA	2211	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	14	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	181	A	N1-C6-N6	-8.52	113.49	118.60
48	BZ	30	ARG	NE-CZ-NH1	8.51	124.56	120.30
54	BA	56	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	730	A	O4'-C1'-N9	8.51	115.01	108.20
54	BA	804	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1912	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	2459	A	C5-C6-N1	8.51	121.96	117.70
54	BA	1608	A	N1-C6-N6	-8.51	113.49	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	794	A	N1-C6-N6	-8.51	113.50	118.60
21	AA	80	A	C4-C5-C6	-8.51	112.75	117.00
24	A3	58	A	C5-C6-N1	8.50	121.95	117.70
54	BA	1451	C	O4'-C1'-N1	8.50	115.00	108.20
9	AJ	9	ARG	NE-CZ-NH2	-8.49	116.05	120.30
21	AA	1053	G	N3-C2-N2	-8.49	113.95	119.90
54	BA	492	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	996	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	172	A	C5-C6-N1	8.49	121.94	117.70
54	BA	1966	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	2407	A	N1-C6-N6	-8.49	113.51	118.60
12	AM	91	ARG	NE-CZ-NH1	8.48	124.54	120.30
21	AA	1346	A	C4-C5-C6	-8.48	112.76	117.00
7	AH	14	ARG	NE-CZ-NH1	8.48	124.54	120.30
21	AA	197	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1803	A	C5-C6-N1	8.48	121.94	117.70
31	BI	64	ARG	NE-CZ-NH1	8.47	124.54	120.30
54	BA	320	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	374	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	716	A	C5-C6-N1	8.47	121.94	117.70
13	AN	53	ARG	NE-CZ-NH1	8.47	124.53	120.30
35	BM	66	ARG	NE-CZ-NH1	8.47	124.53	120.30
21	AA	143	A	C4-C5-C6	-8.47	112.77	117.00
54	BA	73	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1722	A	C5-C6-N1	8.46	121.93	117.70
54	BA	2247	A	C4-C5-C6	-8.47	112.77	117.00
21	AA	298	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1597	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	342	A	N1-C6-N6	-8.46	113.52	118.60
24	A3	74	A	C5-C6-N1	8.46	121.93	117.70
54	BA	1155	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	2411	A	C4-C5-C6	-8.46	112.77	117.00
54	BA	2600	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	51	A	C5-C6-N1	8.46	121.93	117.70
54	BA	1665	A	C5-C6-N1	8.45	121.93	117.70
54	BA	2513	A	C5-C6-N1	8.45	121.93	117.70
21	AA	790	A	C5-C6-N1	8.45	121.92	117.70
54	BA	368	A	C5-C6-N1	8.45	121.92	117.70
27	BE	21	ARG	NE-CZ-NH1	8.44	124.52	120.30
54	BA	1134	A	N1-C6-N6	-8.44	113.53	118.60
27	BE	61	ARG	NE-CZ-NH1	8.44	124.52	120.30
54	BA	1008	A	N1-C6-N6	-8.44	113.53	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	432	A	C5-C6-N1	8.44	121.92	117.70
54	BA	1241	A	C5-C6-N1	8.44	121.92	117.70
21	AA	171	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	196	A	N1-C6-N6	-8.44	113.54	118.60
21	AA	1204	A	N1-C6-N6	-8.44	113.54	118.60
54	BA	2439	A	O4'-C1'-N9	8.44	114.95	108.20
21	AA	1100	C	N3-C2-O2	-8.44	115.99	121.90
54	BA	582	A	C5-C6-N1	8.44	121.92	117.70
21	AA	790	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	28	A	N1-C6-N6	-8.43	113.54	118.60
23	A2	79	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	177	G	O4'-C1'-N9	8.43	114.94	108.20
2	AC	87	ARG	NE-CZ-NH1	8.43	124.51	120.30
52	B3	7	ARG	NE-CZ-NH1	8.43	124.52	120.30
54	BA	482	A	C4-C5-C6	-8.43	112.79	117.00
54	BA	2700	A	C4-C5-C6	-8.43	112.79	117.00
21	AA	1105	A	C4-C5-C6	-8.43	112.79	117.00
54	BA	2169	A	O4'-C1'-N9	8.43	114.94	108.20
54	BA	1580	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	621	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	83	A	C5-C6-N1	8.42	121.91	117.70
54	BA	833	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2734	A	C5-C6-N1	8.42	121.91	117.70
54	BA	1111	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	1829	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	1552	A	C5-C6-N1	8.41	121.90	117.70
21	AA	74	A	C5-C6-N1	8.40	121.90	117.70
21	AA	131	A	C4-C5-C6	-8.40	112.80	117.00
21	AA	16	A	C5-C6-N1	8.40	121.90	117.70
21	AA	1333	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	1913	A	O4'-C1'-N9	8.40	114.92	108.20
54	BA	244	A	N1-C6-N6	-8.40	113.56	118.60
16	AQ	61	ARG	NE-CZ-NH1	8.40	124.50	120.30
21	AA	694	A	N1-C6-N6	-8.39	113.56	118.60
21	AA	728	A	C4-C5-C6	-8.39	112.80	117.00
43	BU	21	ARG	NE-CZ-NH1	8.39	124.50	120.30
54	BA	1427	A	C5-C6-N1	8.39	121.90	117.70
54	BA	1794	A	C4-C5-C6	-8.39	112.80	117.00
54	BA	2412	A	C5-C6-N1	8.39	121.90	117.70
54	BA	2887	A	N1-C6-N6	-8.39	113.57	118.60
21	AA	1102	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	1965	C	N3-C2-O2	-8.39	116.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2451	A	C4-C5-C6	-8.39	112.81	117.00
29	BG	162	ARG	NE-CZ-NH1	8.38	124.49	120.30
54	BA	2137	U	N3-C2-O2	-8.38	116.33	122.20
54	BA	1900	A	C5-C6-N1	8.38	121.89	117.70
54	BA	792	A	C5-C6-N1	8.38	121.89	117.70
55	BB	87	U	O4'-C1'-N1	8.38	114.91	108.20
54	BA	2226	C	N3-C2-O2	-8.38	116.04	121.90
54	BA	2346	A	C5-C6-N1	8.38	121.89	117.70
54	BA	2129	C	N3-C2-O2	-8.37	116.04	121.90
21	AA	181	A	C5-C6-N1	8.37	121.88	117.70
54	BA	1419	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1000	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1717	A	N1-C6-N6	-8.37	113.58	118.60
49	B0	9	ARG	NE-CZ-NH1	8.37	124.48	120.30
54	BA	2755	C	N3-C2-O2	-8.36	116.05	121.90
21	AA	681	A	C5-C6-N1	8.35	121.88	117.70
24	A3	45	A	C4-C5-C6	-8.35	112.82	117.00
21	AA	1375	A	C5-C6-N1	8.35	121.88	117.70
54	BA	2430	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	535	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1004	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	532	A	C5-C6-N1	8.34	121.87	117.70
54	BA	1689	A	C5-C6-N1	8.34	121.87	117.70
54	BA	2126	A	O4'-C1'-N9	8.34	114.88	108.20
21	AA	1267	C	N3-C2-O2	-8.34	116.06	121.90
19	AT	28	ARG	NE-CZ-NH1	8.34	124.47	120.30
21	AA	937	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	1848	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	2530	A	N1-C6-N6	-8.34	113.60	118.60
10	AK	52	ARG	NE-CZ-NH1	8.33	124.47	120.30
21	AA	1130	A	C4-C5-C6	-8.33	112.83	117.00
54	BA	5	A	C5-C6-N1	8.33	121.86	117.70
54	BA	223	A	C5-C6-N1	8.33	121.86	117.70
21	AA	33	A	C5-C6-N1	8.33	121.86	117.70
21	AA	77	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	253	A	N1-C6-N6	-8.33	113.60	118.60
21	AA	640	A	C5-C6-N1	8.33	121.86	117.70
21	AA	780	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	2091	C	N3-C2-O2	-8.33	116.07	121.90
21	AA	1513	A	C5-C6-N1	8.32	121.86	117.70
21	AA	1428	A	C4-C5-C6	-8.32	112.84	117.00
21	AA	510	A	N1-C6-N6	-8.32	113.61	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1188	A	C5-C6-N1	8.32	121.86	117.70
21	AA	422	C	N3-C2-O2	-8.32	116.08	121.90
54	BA	2030	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	342	A	C5-C6-N1	8.31	121.86	117.70
54	BA	219	A	C4-C5-C6	-8.31	112.84	117.00
54	BA	2058	A	C4-C5-C6	-8.31	112.84	117.00
21	AA	188	C	N3-C2-O2	-8.31	116.08	121.90
54	BA	126	A	N1-C6-N6	-8.31	113.62	118.60
54	BA	453	A	N1-C6-N6	-8.31	113.62	118.60
54	BA	1969	A	C4-C5-C6	-8.31	112.85	117.00
54	BA	2126	A	C5-C6-N1	8.31	121.85	117.70
54	BA	233	A	C5-C6-N1	8.30	121.85	117.70
54	BA	1134	A	C5-C6-N1	8.31	121.85	117.70
21	AA	498	A	N1-C6-N6	-8.30	113.62	118.60
21	AA	1238	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	2771	C	N3-C2-O2	-8.30	116.09	121.90
54	BA	2411	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	1640	A	C5-C6-N1	8.29	121.85	117.70
54	BA	2758	A	C5-C6-N1	8.29	121.85	117.70
21	AA	7	A	N1-C6-N6	-8.29	113.62	118.60
21	AA	73	C	N3-C2-O2	-8.29	116.10	121.90
54	BA	849	A	N1-C6-N6	-8.29	113.62	118.60
56	B5	122	ARG	NE-CZ-NH1	8.29	124.45	120.30
21	AA	161	A	C5-C6-N1	8.29	121.84	117.70
21	AA	1363	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	613	A	O4'-C1'-N9	8.29	114.83	108.20
54	BA	2170	A	C4-C5-C6	-8.29	112.85	117.00
54	BA	2628	C	N3-C2-O2	-8.29	116.10	121.90
21	AA	264	C	O4'-C1'-N1	8.29	114.83	108.20
13	AN	75	ARG	NE-CZ-NH1	8.29	124.44	120.30
21	AA	958	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1347	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1603	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1606	C	O4'-C1'-N1	8.29	114.83	108.20
54	BA	503	A	C5-C6-N1	8.29	121.84	117.70
21	AA	448	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	532	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	792	A	N1-C6-N6	-8.28	113.63	118.60
21	AA	16	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1981	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1522	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1789	A	C5-C6-N1	8.28	121.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	73	A	C5-C6-N1	8.28	121.84	117.70
54	BA	2062	A	O4'-C1'-N9	8.27	114.82	108.20
54	BA	222	A	C5-C6-N1	8.27	121.83	117.70
21	AA	768	A	C5-C6-N1	8.27	121.83	117.70
54	BA	1614	A	C5-C6-N1	8.27	121.83	117.70
7	AH	12	ARG	NE-CZ-NH1	8.27	124.43	120.30
36	BN	8	ARG	NE-CZ-NH1	8.27	124.43	120.30
54	BA	64	A	C5-C6-N1	8.27	121.83	117.70
54	BA	1672	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	2900	A	C5-C6-N1	8.27	121.83	117.70
56	B5	12	ARG	NE-CZ-NH1	8.27	124.43	120.30
54	BA	1819	A	C5-C6-N1	8.26	121.83	117.70
8	AI	98	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	1918	A	N1-C6-N6	-8.26	113.64	118.60
55	BB	109	A	C4-C5-C6	-8.26	112.87	117.00
54	BA	2369	A	C5-C6-N1	8.26	121.83	117.70
21	AA	325	A	N1-C6-N6	-8.26	113.65	118.60
21	AA	1507	A	C5-C6-N1	8.26	121.83	117.70
54	BA	447	A	C5-C6-N1	8.26	121.83	117.70
21	AA	787	A	N1-C6-N6	-8.26	113.65	118.60
21	AA	935	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2757	A	C5-C6-N1	8.25	121.83	117.70
26	BD	77	ARG	NE-CZ-NH1	8.25	124.42	120.30
54	BA	156	A	C4-C5-C6	-8.25	112.88	117.00
54	BA	218	A	C5-C6-N1	8.25	121.82	117.70
21	AA	1042	A	N1-C6-N6	-8.25	113.65	118.60
21	AA	1145	A	C5-C6-N1	8.25	121.82	117.70
54	BA	42	A	C5-C6-N1	8.25	121.82	117.70
54	BA	1439	A	O4'-C1'-N9	8.25	114.80	108.20
51	B2	14	ARG	NE-CZ-NH1	8.24	124.42	120.30
54	BA	49	A	C5-C6-N1	8.24	121.82	117.70
54	BA	1609	A	N1-C6-N6	-8.24	113.65	118.60
54	BA	2005	A	N1-C6-N6	-8.24	113.65	118.60
54	BA	441	U	O4'-C1'-N1	8.24	114.79	108.20
21	AA	702	A	C5-C6-N1	8.24	121.82	117.70
39	BQ	27	ARG	NE-CZ-NH1	8.24	124.42	120.30
54	BA	497	A	C5-C6-N1	8.24	121.82	117.70
54	BA	1354	A	C5-C6-N1	8.24	121.82	117.70
54	BA	2725	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	432	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	223	A	C4-C5-C6	-8.23	112.88	117.00
55	BB	70	C	N3-C2-O2	-8.23	116.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	335	C	N3-C2-O2	-8.23	116.14	121.90
54	BA	1969	A	C5-C6-N1	8.23	121.82	117.70
54	BA	21	A	C4-C5-C6	-8.23	112.89	117.00
54	BA	505	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	1392	A	C4-C5-C6	-8.23	112.89	117.00
54	BA	161	A	C5-C6-N1	8.23	121.81	117.70
54	BA	103	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2333	A	C4-C5-C6	-8.23	112.89	117.00
21	AA	1299	A	C5-C6-N1	8.22	121.81	117.70
54	BA	322	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1552	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1304	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	71	A	N1-C6-N6	-8.22	113.67	118.60
31	BI	102	ARG	NE-CZ-NH1	8.22	124.41	120.30
54	BA	142	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	526	A	C5-C6-N1	8.22	121.81	117.70
54	BA	661	A	N1-C6-N6	-8.22	113.67	118.60
22	A1	60	C	N3-C2-O2	-8.22	116.15	121.90
54	BA	1470	A	N1-C6-N6	-8.22	113.67	118.60
6	AG	137	ARG	NE-CZ-NH1	8.22	124.41	120.30
55	BB	108	A	N1-C6-N6	-8.21	113.67	118.60
54	BA	1616	A	C5-C6-N1	8.21	121.81	117.70
54	BA	2386	A	C5-C6-N1	8.21	121.81	117.70
21	AA	1110	A	N1-C6-N6	-8.21	113.68	118.60
54	BA	241	A	C5-C6-N1	8.21	121.80	117.70
54	BA	529	A	N1-C6-N6	-8.21	113.68	118.60
54	BA	1072	C	N3-C2-O2	-8.21	116.16	121.90
4	AE	19	ARG	NE-CZ-NH1	8.20	124.40	120.30
54	BA	1317	G	O4'-C1'-N9	8.21	114.76	108.20
21	AA	781	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	454	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	2418	A	N1-C6-N6	-8.20	113.68	118.60
46	BX	27	ARG	NE-CZ-NH1	8.19	124.40	120.30
19	AT	9	ARG	NE-CZ-NH1	8.19	124.40	120.30
21	AA	1256	A	N1-C6-N6	-8.19	113.69	118.60
3	AD	50	TYR	CB-CG-CD1	-8.19	116.09	121.00
21	AA	977	A	C5-C6-N1	8.19	121.79	117.70
21	AA	777	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	889	A	C5-C6-N1	8.19	121.79	117.70
21	AA	1375	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	655	A	C5-C6-N1	8.19	121.79	117.70
41	BS	18	ARG	NE-CZ-NH1	8.18	124.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	828	U	O4'-C1'-N1	8.18	114.75	108.20
54	BA	2700	A	N1-C6-N6	-8.18	113.69	118.60
55	BB	115	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	136	C	N3-C2-O2	-8.18	116.17	121.90
54	BA	889	C	N3-C2-O2	-8.18	116.17	121.90
54	BA	1275	A	C5-C6-N1	8.18	121.79	117.70
54	BA	2164	C	N3-C2-O2	-8.18	116.18	121.90
21	AA	715	A	C5-C6-N1	8.18	121.79	117.70
21	AA	795	C	N3-C2-O2	-8.18	116.18	121.90
22	A1	35	A	N1-C6-N6	-8.18	113.69	118.60
22	A1	38	A	C4-C5-C6	-8.18	112.91	117.00
54	BA	1690	A	C4-C5-C6	-8.18	112.91	117.00
5	AF	91	ARG	NE-CZ-NH1	8.17	124.39	120.30
6	AG	108	ARG	NE-CZ-NH1	8.17	124.39	120.30
21	AA	889	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2281	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2288	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2887	A	C5-C6-N1	8.17	121.78	117.70
21	AA	784	A	C5-C6-N1	8.17	121.78	117.70
54	BA	249	C	C1'-O4'-C4'	-8.17	103.37	109.90
54	BA	928	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	430	A	C5-C6-N1	8.17	121.78	117.70
54	BA	787	C	N3-C2-O2	-8.17	116.18	121.90
21	AA	139	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	764	A	C5-C6-N1	8.16	121.78	117.70
54	BA	715	A	C5-C6-N1	8.16	121.78	117.70
54	BA	1987	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	1410	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	2176	A	O4'-C1'-N9	8.16	114.73	108.20
21	AA	1213	A	C5-C6-N1	8.16	121.78	117.70
54	BA	119	A	C4-C5-C6	-8.15	112.92	117.00
54	BA	911	A	C5-C6-N1	8.15	121.78	117.70
54	BA	1090	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	374	A	C4-C5-C6	-8.15	112.92	117.00
21	AA	459	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	759	A	C5-C6-N1	8.15	121.78	117.70
54	BA	2142	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	356	A	C4-C5-C6	-8.14	112.93	117.00
21	AA	1197	A	C5-C6-N1	8.14	121.77	117.70
54	BA	1096	A	N1-C6-N6	-8.14	113.71	118.60
54	BA	1288	G	O4'-C1'-N9	8.14	114.71	108.20
54	BA	1571	A	N1-C6-N6	-8.14	113.72	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	529	A	C5-C6-N1	8.14	121.77	117.70
21	AA	421	U	N3-C2-O2	-8.14	116.50	122.20
54	BA	1427	A	C4-C5-C6	-8.14	112.93	117.00
21	AA	1054	C	N3-C2-O2	-8.13	116.21	121.90
39	BQ	49	ARG	NE-CZ-NH1	8.13	124.37	120.30
54	BA	749	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	721	A	C4-C5-C6	-8.13	112.93	117.00
54	BA	1021	A	C5-C6-N1	8.13	121.77	117.70
54	BA	1566	A	C5-C6-N1	8.13	121.77	117.70
54	BA	2564	A	C5-C6-N1	8.13	121.77	117.70
54	BA	2147	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	371	A	C4-C5-C6	-8.13	112.94	117.00
21	AA	1341	U	O4'-C1'-N1	8.13	114.70	108.20
54	BA	1336	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1433	A	C4-C5-C6	-8.13	112.94	117.00
54	BA	2070	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1741	C	N3-C2-O2	-8.12	116.21	121.90
54	BA	2158	A	C5-C6-N1	8.12	121.76	117.70
21	AA	1360	A	C4-C5-C6	-8.12	112.94	117.00
54	BA	460	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1403	A	C4-C5-C6	-8.12	112.94	117.00
21	AA	80	A	C5-C6-N1	8.12	121.76	117.70
21	AA	279	A	C5-C6-N1	8.12	121.76	117.70
21	AA	629	A	C4-C5-C6	-8.11	112.94	117.00
21	AA	1322	C	N3-C2-O2	-8.12	116.22	121.90
21	AA	1508	A	C5-C6-N1	8.11	121.76	117.70
54	BA	1135	C	N3-C2-O2	-8.11	116.22	121.90
54	BA	1009	A	C5-C6-N1	8.11	121.76	117.70
54	BA	2268	A	C5-C6-N1	8.11	121.75	117.70
21	AA	609	A	C5-C6-N1	8.11	121.75	117.70
54	BA	1054	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	1175	A	O4'-C1'-N9	8.11	114.69	108.20
54	BA	2058	A	C5-C6-N1	8.11	121.75	117.70
54	BA	2212	A	C5-C6-N1	8.11	121.75	117.70
21	AA	441	A	C4-C5-C6	-8.11	112.95	117.00
21	AA	313	A	C5-C6-N1	8.11	121.75	117.70
54	BA	2740	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	2860	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	2426	A	N1-C6-N6	-8.10	113.74	118.60
9	AJ	72	ARG	NE-CZ-NH1	8.10	124.35	120.30
7	AH	113	ARG	NE-CZ-NH1	8.10	124.35	120.30
54	BA	227	A	N1-C6-N6	-8.10	113.74	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	620	G	C8-N9-C4	-8.10	103.16	106.40
54	BA	1508	A	N1-C6-N6	-8.09	113.74	118.60
2	AC	53	ARG	NE-CZ-NH1	8.09	124.35	120.30
54	BA	480	A	N1-C6-N6	-8.09	113.75	118.60
21	AA	397	A	C5-C6-N1	8.09	121.75	117.70
26	BD	33	ARG	NE-CZ-NH2	-8.09	116.25	120.30
21	AA	366	A	C5-C6-N1	8.09	121.74	117.70
21	AA	814	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	1808	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	144	A	C5-C6-N1	8.08	121.74	117.70
54	BA	941	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	1938	A	C5-C6-N1	8.08	121.74	117.70
36	BN	64	ARG	NE-CZ-NH1	8.08	124.34	120.30
54	BA	2407	A	C5-C6-N1	8.08	121.74	117.70
21	AA	167	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	783	A	C5-C6-N1	8.08	121.74	117.70
21	AA	743	A	N1-C6-N6	-8.08	113.75	118.60
36	BN	63	ARG	NE-CZ-NH1	8.08	124.34	120.30
54	BA	456	C	N3-C2-O2	-8.08	116.25	121.90
54	BA	2598	A	C5-C6-N1	8.08	121.74	117.70
21	AA	493	A	N1-C6-N6	-8.07	113.75	118.60
54	BA	2171	A	N1-C6-N6	-8.07	113.75	118.60
40	BR	68	ARG	NE-CZ-NH1	8.07	124.34	120.30
21	AA	750	C	N3-C2-O2	-8.07	116.25	121.90
54	BA	119	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	197	A	C5-C6-N1	8.07	121.74	117.70
54	BA	613	A	C5-C6-N1	8.07	121.73	117.70
54	BA	1503	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	1012	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	460	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	783	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	918	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	642	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	981	A	C4-C5-C6	-8.06	112.97	117.00
54	BA	322	A	C4-C5-C6	-8.06	112.97	117.00
54	BA	2267	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	2886	A	N1-C6-N6	-8.06	113.76	118.60
21	AA	1105	A	C5-C6-N1	8.06	121.73	117.70
54	BA	428	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	2476	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	984	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	2322	A	N1-C6-N6	-8.06	113.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	BF	149	ARG	NE-CZ-NH1	8.06	124.33	120.30
54	BA	2377	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	730	A	C5-C6-N1	8.06	121.73	117.70
54	BA	119	A	C5-C6-N1	8.05	121.73	117.70
21	AA	374	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	1180	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	918	A	C5-C6-N1	8.05	121.73	117.70
55	BB	57	A	C5-C6-N1	8.05	121.73	117.70
21	AA	1130	A	C5-C6-N1	8.05	121.72	117.70
21	AA	329	A	C5-C6-N1	8.05	121.72	117.70
21	AA	469	C	N3-C2-O2	-8.05	116.27	121.90
54	BA	118	A	C5-C6-N1	8.05	121.72	117.70
54	BA	1264	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	146	A	C5-C6-N1	8.05	121.72	117.70
54	BA	2687	U	O4'-C1'-N1	8.05	114.64	108.20
21	AA	860	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1143	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	2727	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	779	C	N3-C2-O2	-8.04	116.28	121.90
54	BA	131	A	C5-C6-N1	8.04	121.72	117.70
54	BA	515	A	C5-C6-N1	8.04	121.72	117.70
54	BA	2326	C	N3-C2-O2	-8.04	116.28	121.90
54	BA	2726	A	C5-C6-N1	8.04	121.72	117.70
43	BU	93	ARG	NE-CZ-NH1	8.03	124.32	120.30
54	BA	1952	A	C5-C6-N1	8.03	121.72	117.70
21	AA	190	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	1067	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2322	A	C4-C5-C6	-8.03	112.98	117.00
54	BA	2887	A	C4-C5-C6	-8.03	112.98	117.00
27	BE	67	ARG	NE-CZ-NH1	8.03	124.31	120.30
54	BA	1916	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2278	A	C4-C5-C6	-8.03	112.99	117.00
21	AA	1274	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2335	A	C5-C6-N1	8.03	121.71	117.70
54	BA	2497	A	C5-C6-N1	8.03	121.71	117.70
1	AB	34	ARG	NE-CZ-NH1	8.02	124.31	120.30
21	AA	192	A	C5-C6-N1	8.02	121.71	117.70
54	BA	905	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	947	A	C5-C6-N1	8.02	121.71	117.70
45	BW	24	ARG	NE-CZ-NH1	8.02	124.31	120.30
54	BA	2448	A	C4-C5-C6	-8.02	112.99	117.00
21	AA	1204	A	C5-C6-N1	8.02	121.71	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	311	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	1057	A	C5-C6-N1	8.02	121.71	117.70
21	AA	600	A	C5-C6-N1	8.02	121.71	117.70
54	BA	1705	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	1035	A	C5-C6-N1	8.02	121.71	117.70
54	BA	990	A	C5-C6-N1	8.02	121.71	117.70
54	BA	2376	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	864	A	C5-C6-N1	8.01	121.71	117.70
54	BA	111	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	528	A	C5-C6-N1	8.01	121.71	117.70
21	AA	1248	A	C5-C6-N1	8.01	121.71	117.70
21	AA	1374	A	C5-C6-N1	8.01	121.71	117.70
21	AA	1437	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	447	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	2396	G	O4'-C1'-N9	8.01	114.61	108.20
44	BV	9	ARG	NE-CZ-NH1	8.01	124.31	120.30
21	AA	151	A	N1-C6-N6	-8.01	113.80	118.60
21	AA	560	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	2587	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	1535	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	2482	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	423	A	C5-C6-N1	8.00	121.70	117.70
54	BA	504	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1508	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2284	A	C4-C5-C6	-8.00	113.00	117.00
54	BA	528	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1086	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2753	A	C4-C5-C6	-8.00	113.00	117.00
54	BA	2810	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	1572	A	C5-C6-N1	8.00	121.70	117.70
54	BA	1732	C	N3-C2-O2	-8.00	116.30	121.90
54	BA	1359	A	C5-C6-N1	8.00	121.70	117.70
54	BA	2758	A	N1-C6-N6	-7.99	113.80	118.60
54	BA	199	A	C4-C5-C6	-7.99	113.00	117.00
54	BA	415	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	1050	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	1847	A	C5-C6-N1	7.99	121.69	117.70
54	BA	2705	A	C4-C5-C6	-7.99	113.01	117.00
14	AO	57	ARG	NE-CZ-NH1	7.99	124.29	120.30
54	BA	2014	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	1429	A	C4-C5-C6	-7.98	113.01	117.00
54	BA	1392	A	C5-C6-N1	7.98	121.69	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	872	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1987	A	C5-C6-N1	7.98	121.69	117.70
21	AA	702	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	696	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	348	A	C5-C6-N1	7.98	121.69	117.70
54	BA	2327	A	C4-C5-C6	-7.97	113.01	117.00
21	AA	303	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	600	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	938	A	C5-C6-N1	7.97	121.69	117.70
54	BA	2278	A	C5-C6-N1	7.97	121.69	117.70
21	AA	1531	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	2565	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	353	A	C5-C6-N1	7.96	121.68	117.70
21	AA	1179	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	633	A	N1-C6-N6	-7.96	113.82	118.60
21	AA	1250	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	2660	A	O4'-C1'-N9	7.96	114.57	108.20
54	BA	1744	A	C5-C6-N1	7.96	121.68	117.70
21	AA	355	C	N3-C2-O2	-7.96	116.33	121.90
54	BA	470	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1607	C	N3-C2-O2	-7.95	116.33	121.90
21	AA	101	A	C5-C6-N1	7.95	121.68	117.70
21	AA	864	A	C4-C5-C6	-7.95	113.02	117.00
21	AA	186	C	N3-C2-O2	-7.95	116.33	121.90
21	AA	282	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1127	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1794	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1008	A	C5-C6-N1	7.95	121.67	117.70
21	AA	1476	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	590	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1054	A	C5-C6-N1	7.95	121.67	117.70
54	BA	2792	A	N1-C6-N6	-7.95	113.83	118.60
46	BX	26	ARG	NE-CZ-NH1	7.94	124.27	120.30
21	AA	681	A	C4-C5-C6	-7.94	113.03	117.00
29	BG	169	ARG	NE-CZ-NH1	7.94	124.27	120.30
54	BA	740	C	N3-C2-O2	-7.94	116.34	121.90
54	BA	2752	C	N3-C2-O2	-7.94	116.34	121.90
21	AA	1219	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	2666	C	N3-C2-O2	-7.93	116.35	121.90
21	AA	583	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	1239	A	C5-C6-N1	7.93	121.66	117.70
54	BA	2856	A	N1-C6-N6	-7.93	113.84	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AD	12	ARG	NE-CZ-NH1	7.93	124.26	120.30
21	AA	32	A	N1-C6-N6	-7.93	113.84	118.60
21	AA	949	A	C5-C6-N1	7.93	121.66	117.70
54	BA	742	A	C5-C6-N1	7.93	121.66	117.70
54	BA	890	C	N3-C2-O2	-7.92	116.35	121.90
54	BA	2191	A	C5-C6-N1	7.92	121.66	117.70
54	BA	2358	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1916	A	C5-C6-N1	7.92	121.66	117.70
54	BA	330	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1302	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1151	A	C5-C6-N1	7.92	121.66	117.70
21	AA	1479	C	N3-C2-O2	-7.91	116.36	121.90
37	BO	81	ARG	NE-CZ-NH1	7.91	124.25	120.30
54	BA	2755	C	O4'-C1'-N1	7.91	114.53	108.20
21	AA	246	A	C5-C6-N1	7.91	121.65	117.70
21	AA	451	A	C5-C6-N1	7.91	121.65	117.70
54	BA	28	A	C5-C6-N1	7.91	121.66	117.70
54	BA	2003	A	C4-C5-C6	-7.91	113.05	117.00
54	BA	644	A	C5-C6-N1	7.91	121.65	117.70
54	BA	2882	A	C4-C5-C6	-7.91	113.05	117.00
21	AA	1357	A	C4-C5-C6	-7.90	113.05	117.00
54	BA	1821	A	C5-C6-N1	7.90	121.65	117.70
30	BH	68	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	689	A	C5-C6-N1	7.90	121.65	117.70
54	BA	752	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	753	A	C5-C6-N1	7.90	121.65	117.70
54	BA	1528	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2346	A	C4-C5-C6	-7.90	113.05	117.00
54	BA	301	G	O4'-C1'-N9	7.90	114.52	108.20
54	BA	401	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	227	A	C5-C6-N1	7.90	121.65	117.70
54	BA	341	C	N3-C2-O2	-7.90	116.37	121.90
54	BA	1585	C	N3-C2-O2	-7.90	116.37	121.90
55	BB	53	A	C5-C6-N1	7.89	121.65	117.70
21	AA	1239	A	C4-C5-C6	-7.89	113.05	117.00
24	A3	44	A	N1-C6-N6	-7.89	113.87	118.60
54	BA	2432	A	C5-C6-N1	7.89	121.64	117.70
24	A3	39	A	C5-C6-N1	7.88	121.64	117.70
54	BA	478	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	1365	A	C5-C6-N1	7.88	121.64	117.70
22	A1	66	A	C5-C6-N1	7.88	121.64	117.70
54	BA	482	A	C5-C6-N1	7.88	121.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	927	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	1247	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	1265	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	2095	A	C4-C5-C6	-7.88	113.06	117.00
44	BV	19	ARG	NE-CZ-NH1	7.88	124.24	120.30
54	BA	1301	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1387	A	C5-C6-N1	7.88	121.64	117.70
55	BB	118	C	N3-C2-O2	-7.88	116.39	121.90
54	BA	1320	C	N1-C2-O2	7.87	123.62	118.90
54	BA	2311	A	C5-C6-N1	7.87	121.64	117.70
21	AA	487	A	N1-C6-N6	-7.87	113.88	118.60
53	B4	12	ARG	NE-CZ-NH1	7.87	124.24	120.30
54	BA	2220	U	O4'-C1'-N1	7.87	114.50	108.20
21	AA	901	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	460	A	C5-C6-N1	7.87	121.64	117.70
54	BA	2776	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1321	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1784	A	C4-C5-C6	-7.87	113.07	117.00
54	BA	1870	C	N3-C2-O2	-7.87	116.39	121.90
21	AA	152	A	C5-C6-N1	7.87	121.63	117.70
21	AA	502	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	665	A	C4-C5-C6	-7.87	113.07	117.00
54	BA	1598	A	C5-C6-N1	7.87	121.63	117.70
54	BA	2900	A	C4-C5-C6	-7.87	113.07	117.00
21	AA	621	A	C5-C6-N1	7.86	121.63	117.70
54	BA	31	C	N3-C2-O2	-7.86	116.39	121.90
54	BA	1919	A	N1-C6-N6	-7.86	113.88	118.60
21	AA	383	A	C5-C6-N1	7.86	121.63	117.70
54	BA	430	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	487	C	N3-C2-O2	-7.86	116.40	121.90
21	AA	164	G	O4'-C1'-N9	7.86	114.49	108.20
21	AA	532	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	1630	A	C5-C6-N1	7.86	121.63	117.70
21	AA	726	C	N3-C2-O2	-7.85	116.41	121.90
21	AA	1500	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	173	A	C5-C6-N1	7.85	121.62	117.70
54	BA	1579	A	N1-C6-N6	-7.85	113.89	118.60
2	AC	126	ARG	NE-CZ-NH1	7.85	124.22	120.30
21	AA	1204	A	C4-C5-C6	-7.85	113.08	117.00
54	BA	2381	A	C4-C5-C6	-7.85	113.08	117.00
54	BA	609	A	N1-C6-N6	-7.84	113.89	118.60
27	BE	69	ARG	NE-CZ-NH1	7.84	124.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	386	C	N3-C2-O2	-7.84	116.41	121.90
21	AA	706	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	2090	A	C4-C5-C6	-7.84	113.08	117.00
21	AA	1216	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2825	G	O4'-C1'-N9	7.84	114.47	108.20
22	A1	35	A	C5-C6-N1	7.84	121.62	117.70
54	BA	756	A	C5-C6-N1	7.83	121.62	117.70
54	BA	2564	A	N1-C6-N6	-7.83	113.90	118.60
24	A3	39	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1717	A	C4-C5-C6	-7.83	113.08	117.00
54	BA	422	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	547	A	C5-C6-N1	7.83	121.61	117.70
54	BA	173	A	C4-C5-C6	-7.83	113.08	117.00
54	BA	1816	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	2171	A	C4-C5-C6	-7.83	113.09	117.00
54	BA	2406	A	C5-C6-N1	7.83	121.61	117.70
21	AA	50	A	C5-C6-N1	7.83	121.61	117.70
21	AA	448	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1126	A	N1-C6-N6	-7.83	113.91	118.60
54	BA	1213	A	N1-C6-N6	-7.83	113.91	118.60
21	AA	655	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1226	A	C5-C6-N1	7.82	121.61	117.70
54	BA	2654	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	155	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1313	U	O4'-C1'-N1	7.82	114.45	108.20
54	BA	655	A	C4-C5-C6	-7.82	113.09	117.00
54	BA	734	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	1439	A	C5-C6-N1	7.82	121.61	117.70
21	AA	892	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	2705	A	C5-C6-N1	7.81	121.61	117.70
21	AA	1342	C	N3-C2-O2	-7.81	116.43	121.90
21	AA	716	A	C4-C5-C6	-7.81	113.09	117.00
21	AA	1269	A	C5-C6-N1	7.81	121.61	117.70
54	BA	2134	A	N1-C6-N6	-7.81	113.92	118.60
21	AA	511	C	N3-C2-O2	-7.81	116.43	121.90
54	BA	603	A	C5-C6-N1	7.81	121.60	117.70
54	BA	2314	A	N1-C6-N6	-7.81	113.92	118.60
54	BA	2774	C	N3-C2-O2	-7.81	116.44	121.90
54	BA	502	A	N1-C6-N6	-7.81	113.92	118.60
54	BA	1353	A	C5-C6-N1	7.81	121.60	117.70
21	AA	345	C	N3-C2-O2	-7.80	116.44	121.90
21	AA	110	C	N3-C2-O2	-7.80	116.44	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	431	A	C5-C6-N1	7.80	121.60	117.70
22	A1	58	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	780	A	C4-C5-C6	-7.80	113.10	117.00
54	BA	1676	A	C4-C5-C6	-7.80	113.10	117.00
54	BA	896	A	C5-C6-N1	7.79	121.60	117.70
54	BA	900	A	C5-C6-N1	7.79	121.60	117.70
54	BA	941	A	C5-C6-N1	7.79	121.60	117.70
54	BA	972	A	C5-C6-N1	7.79	121.60	117.70
55	BB	36	C	N3-C2-O2	-7.79	116.44	121.90
54	BA	1678	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	1167	A	C5-C6-N1	7.79	121.59	117.70
12	AM	56	ARG	NE-CZ-NH1	7.79	124.19	120.30
21	AA	649	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	1152	A	C5-C6-N1	7.79	121.59	117.70
54	BA	599	A	C5-C6-N1	7.79	121.59	117.70
21	AA	74	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	1289	C	N3-C2-O2	-7.79	116.45	121.90
54	BA	2388	A	C4-C5-C6	-7.79	113.11	117.00
54	BA	2548	U	O4'-C1'-N1	7.79	114.43	108.20
54	BA	507	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	563	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	219	A	C5-C6-N1	7.78	121.59	117.70
54	BA	960	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	1073	A	C5-C6-N1	7.78	121.59	117.70
21	AA	53	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	415	A	C5-C6-N1	7.78	121.59	117.70
44	BV	93	ARG	NE-CZ-NH1	7.78	124.19	120.30
54	BA	1359	A	O4'-C1'-N9	7.78	114.42	108.20
54	BA	1932	A	C4-C5-C6	-7.78	113.11	117.00
21	AA	1191	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	1067	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1302	C	N3-C2-O2	-7.77	116.46	121.90
21	AA	1377	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	2051	A	C5-C6-N1	7.77	121.59	117.70
21	AA	349	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	1832	C	N3-C2-O2	-7.77	116.46	121.90
54	BA	975	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2498	C	N3-C2-O2	-7.77	116.46	121.90
6	AG	95	ARG	NE-CZ-NH1	7.77	124.18	120.30
21	AA	53	A	C4-C5-C6	-7.77	113.12	117.00
21	AA	554	A	C5-C6-N1	7.77	121.58	117.70
21	AA	1259	C	N3-C2-O2	-7.77	116.46	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	38	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	982	C	N1-C2-O2	7.77	123.56	118.90
54	BA	1336	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1773	A	C5-C6-N1	7.77	121.58	117.70
54	BA	91	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	2019	A	C4-C5-C6	-7.77	113.12	117.00
54	BA	2071	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	195	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	2639	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	162	A	C5-C6-N1	7.76	121.58	117.70
21	AA	1103	C	N3-C2-O2	-7.76	116.47	121.90
54	BA	1912	A	C5-C6-N1	7.76	121.58	117.70
54	BA	526	A	N1-C6-N6	-7.76	113.95	118.60
54	BA	1537	G	O4'-C1'-N9	7.76	114.41	108.20
21	AA	482	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	938	A	C4-C5-C6	-7.75	113.12	117.00
21	AA	270	A	C4-C5-C6	-7.75	113.12	117.00
54	BA	404	A	N1-C6-N6	-7.75	113.95	118.60
8	AI	48	ARG	NE-CZ-NH1	7.75	124.17	120.30
54	BA	793	A	C5-C6-N1	7.75	121.57	117.70
54	BA	1287	A	C5-C6-N1	7.75	121.57	117.70
54	BA	2740	A	C5-C6-N1	7.75	121.58	117.70
21	AA	819	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1238	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1285	A	N1-C6-N6	-7.75	113.95	118.60
40	BR	13	ARG	NE-CZ-NH1	7.75	124.17	120.30
54	BA	1495	A	C5-C6-N1	7.75	121.57	117.70
54	BA	1916	A	C4-C5-C6	-7.75	113.13	117.00
21	AA	1201	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	1227	A	C5-C6-N1	7.75	121.57	117.70
54	BA	1439	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	564	C	N3-C2-O2	-7.74	116.48	121.90
21	AA	1191	A	C5-C6-N1	7.74	121.57	117.70
9	AJ	89	ARG	NE-CZ-NH1	7.74	124.17	120.30
54	BA	1960	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1169	A	C4-C5-C6	-7.74	113.13	117.00
21	AA	1466	C	N3-C2-O2	-7.74	116.48	121.90
54	BA	477	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	1217	C	N3-C2-O2	-7.74	116.48	121.90
54	BA	1784	A	C5-C6-N1	7.74	121.57	117.70
21	AA	430	A	C5-C6-N1	7.74	121.57	117.70
22	A1	9	A	N1-C6-N6	-7.73	113.96	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	74	A	C4-C5-C6	-7.73	113.13	117.00
54	BA	5	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	586	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	2758	A	C4-C5-C6	-7.73	113.13	117.00
28	BF	79	ARG	NE-CZ-NH1	7.73	124.17	120.30
43	BU	5	ARG	NE-CZ-NH1	7.73	124.17	120.30
54	BA	1286	A	C5-C6-N1	7.73	121.56	117.70
54	BA	2826	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	223	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	2434	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	382	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	1211	C	N3-C2-O2	-7.73	116.49	121.90
24	A3	44	A	C5-C6-N1	7.72	121.56	117.70
54	BA	443	A	C5-C6-N1	7.72	121.56	117.70
48	BZ	37	ARG	NE-CZ-NH1	7.72	124.16	120.30
21	AA	238	A	P-O3'-C3'	7.72	128.97	119.70
21	AA	321	A	C5-C6-N1	7.72	121.56	117.70
21	AA	1031	C	N3-C2-O2	-7.72	116.50	121.90
26	BD	13	ARG	NE-CZ-NH1	7.72	124.16	120.30
54	BA	1069	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1085	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1363	C	N3-C2-O2	-7.72	116.50	121.90
54	BA	2063	C	N3-C2-O2	-7.72	116.50	121.90
21	AA	845	A	C5-C6-N1	7.71	121.56	117.70
24	A3	59	A	C5-C6-N1	7.71	121.56	117.70
54	BA	226	A	C5-C6-N1	7.71	121.56	117.70
54	BA	863	A	C5-C6-N1	7.71	121.56	117.70
54	BA	1700	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	338	A	N1-C6-N6	-7.71	113.97	118.60
22	A1	9	A	C5-C6-N1	7.71	121.56	117.70
54	BA	2749	A	N1-C6-N6	-7.71	113.97	118.60
14	AO	83	ARG	NE-CZ-NH1	7.71	124.16	120.30
54	BA	2021	C	N3-C2-O2	-7.71	116.50	121.90
54	BA	2031	A	C5-C6-N1	7.71	121.56	117.70
54	BA	2278	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	60	A	C5-C6-N1	7.71	121.56	117.70
21	AA	595	A	C5-C6-N1	7.71	121.55	117.70
54	BA	1978	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	2013	A	N1-C6-N6	-7.71	113.97	118.60
21	AA	1429	A	C5-C6-N1	7.71	121.55	117.70
24	A3	67	C	N3-C2-O2	-7.71	116.51	121.90
54	BA	1986	C	N3-C2-O2	-7.71	116.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1214	A	N1-C6-N6	-7.71	113.98	118.60
15	AP	28	ARG	NE-CZ-NH2	7.70	124.15	120.30
21	AA	1357	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	382	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1552	A	O4'-C1'-N9	7.70	114.36	108.20
54	BA	608	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1241	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1938	A	C4-C5-C6	-7.70	113.15	117.00
9	AJ	5	ARG	NE-CZ-NH1	7.70	124.15	120.30
21	AA	149	A	C5-C6-N1	7.70	121.55	117.70
54	BA	84	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1264	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	482	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1098	A	C5-C6-N1	7.70	121.55	117.70
55	BB	53	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	288	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	1170	A	C4-C5-C6	-7.70	113.15	117.00
54	BA	265	A	O4'-C1'-N9	7.70	114.36	108.20
54	BA	2055	C	O4'-C1'-N1	7.70	114.36	108.20
21	AA	737	C	N3-C2-O2	-7.69	116.51	121.90
54	BA	1650	A	N1-C6-N6	-7.69	113.98	118.60
5	AF	2	ARG	NE-CZ-NH1	7.69	124.15	120.30
21	AA	1137	C	N3-C2-O2	-7.69	116.52	121.90
54	BA	2541	A	C5-C6-N1	7.69	121.55	117.70
54	BA	2080	A	C4-C5-C6	-7.69	113.16	117.00
54	BA	479	A	C4-C5-C6	-7.69	113.16	117.00
54	BA	2015	A	C5-C6-N1	7.69	121.54	117.70
54	BA	2288	A	C5-C6-N1	7.69	121.54	117.70
11	AL	30	ARG	NE-CZ-NH1	7.69	124.14	120.30
21	AA	539	A	C5-C6-N1	7.69	121.54	117.70
21	AA	1044	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	1672	A	C5-C6-N1	7.68	121.54	117.70
54	BA	2866	U	O4'-C1'-N1	7.68	114.35	108.20
8	AI	44	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	345	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	808	C	N3-C2-O2	-7.68	116.52	121.90
54	BA	1808	A	C5-C6-N1	7.68	121.54	117.70
6	AG	110	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	2560	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2700	A	C5-C6-N1	7.68	121.54	117.70
21	AA	1130	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	614	A	C5-C6-N1	7.68	121.54	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	969	A	C4-C5-C6	-7.67	113.16	117.00
21	AA	1101	A	C4-C5-C6	-7.67	113.16	117.00
54	BA	739	A	C5-C6-N1	7.67	121.54	117.70
54	BA	2184	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2646	C	N3-C2-O2	-7.67	116.53	121.90
21	AA	370	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	324	A	C5-C6-N1	7.67	121.54	117.70
54	BA	2019	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	320	A	C5-C6-N1	7.67	121.54	117.70
21	AA	1197	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	240	C	N3-C2-O2	-7.67	116.53	121.90
34	BL	78	ARG	NE-CZ-NH1	7.67	124.14	120.30
54	BA	2327	A	N1-C6-N6	-7.67	114.00	118.60
3	AD	187	ARG	NE-CZ-NH1	7.67	124.13	120.30
21	AA	596	A	C5-C6-N1	7.67	121.53	117.70
22	A1	14	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	2480	C	O4'-C1'-N1	7.67	114.33	108.20
54	BA	2665	A	C5-C6-N1	7.67	121.53	117.70
21	AA	81	A	C5-C6-N1	7.67	121.53	117.70
54	BA	457	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	640	A	C4-C5-C6	-7.66	113.17	117.00
54	BA	655	A	N1-C6-N6	-7.66	114.00	118.60
54	BA	195	A	C5-C6-N1	7.66	121.53	117.70
12	AM	70	ARG	NE-CZ-NH1	7.66	124.13	120.30
55	BB	66	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2317	A	C5-C6-N1	7.66	121.53	117.70
26	BD	169	ARG	NE-CZ-NH1	7.66	124.13	120.30
21	AA	630	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	613	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	2021	C	O4'-C1'-N1	7.66	114.32	108.20
54	BA	863	A	N1-C6-N6	-7.65	114.01	118.60
1	AB	62	ARG	NE-CZ-NH1	7.65	124.12	120.30
24	A3	57	C	N3-C2-O2	-7.65	116.55	121.90
21	AA	1101	A	P-O3'-C3'	7.65	128.88	119.70
21	AA	510	A	C4-C5-C6	-7.65	113.18	117.00
54	BA	2050	C	N3-C2-O2	-7.65	116.55	121.90
21	AA	189	A	C4-C5-C6	-7.64	113.18	117.00
54	BA	2051	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	1092	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	743	A	C5-C6-N1	7.64	121.52	117.70
54	BA	750	A	C5-C6-N1	7.63	121.52	117.70
54	BA	2030	A	C4-C5-C6	-7.63	113.18	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1157	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	1213	A	C4-C5-C6	-7.63	113.18	117.00
54	BA	2222	C	N3-C2-O2	-7.63	116.56	121.90
55	BB	39	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	479	A	C5-C6-N1	7.63	121.52	117.70
5	AF	79	ARG	NE-CZ-NH1	7.63	124.11	120.30
8	AI	112	ARG	NE-CZ-NH1	7.63	124.11	120.30
21	AA	28	A	C5-C6-N1	7.63	121.51	117.70
21	AA	676	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	995	C	N3-C2-O2	-7.63	116.56	121.90
54	BA	2547	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	497	A	C4-C5-C6	-7.63	113.19	117.00
54	BA	1698	A	N1-C6-N6	-7.63	114.02	118.60
24	A3	77	A	C5-C6-N1	7.62	121.51	117.70
54	BA	819	A	C5-C6-N1	7.62	121.51	117.70
54	BA	947	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	2738	A	C5-C6-N1	7.62	121.51	117.70
54	BA	866	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2435	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1021	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	1640	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2534	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2666	C	N1-C2-O2	7.62	123.47	118.90
54	BA	2682	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	905	A	C5-C6-N1	7.62	121.51	117.70
54	BA	56	A	C4-C5-C6	-7.62	113.19	117.00
21	AA	528	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	1927	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	1264	A	C5-C6-N1	7.61	121.51	117.70
54	BA	270	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1090	A	C5-C6-N1	7.61	121.51	117.70
21	AA	1397	C	O4'-C1'-N1	7.61	114.29	108.20
54	BA	1686	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	2764	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1551	A	C4-C5-C6	-7.61	113.20	117.00
11	AL	55	ARG	NE-CZ-NH1	7.61	124.10	120.30
17	AR	42	ARG	NE-CZ-NH1	7.61	124.10	120.30
21	AA	984	C	N3-C2-O2	-7.61	116.58	121.90
21	AA	1434	A	C5-C6-N1	7.61	121.50	117.70
21	AA	1507	A	N1-C6-N6	-7.61	114.04	118.60
54	BA	1308	A	C5-C6-N1	7.61	121.50	117.70
54	BA	1610	A	C5-C6-N1	7.61	121.50	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2241	A	C4-C5-C6	-7.61	113.20	117.00
16	AQ	63	CYS	C-N-CA	7.60	140.71	121.70
21	AA	435	A	C4-C5-C6	-7.60	113.20	117.00
21	AA	819	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	1508	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	173	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	603	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	116	A	C5-C6-N1	7.60	121.50	117.70
21	AA	906	A	C5-C6-N1	7.60	121.50	117.70
54	BA	255	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	776	G	N3-C2-N2	-7.60	114.58	119.90
54	BA	784	G	O4'-C1'-N9	7.60	114.28	108.20
54	BA	1785	A	C4-C5-C6	-7.60	113.20	117.00
54	BA	2198	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	131	A	C5-C6-N1	7.60	121.50	117.70
54	BA	980	A	C4-C5-C6	-7.60	113.20	117.00
21	AA	162	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	2381	A	C5-C6-N1	7.59	121.50	117.70
21	AA	321	A	C4-C5-C6	-7.59	113.20	117.00
21	AA	865	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	1254	A	C4-C5-C6	-7.59	113.21	117.00
21	AA	414	A	C4-C5-C6	-7.59	113.21	117.00
21	AA	996	A	C5-C6-N1	7.59	121.49	117.70
55	BB	37	C	N3-C2-O2	-7.59	116.59	121.90
14	AO	88	ARG	NE-CZ-NH1	7.58	124.09	120.30
21	AA	199	A	N1-C6-N6	-7.58	114.05	118.60
21	AA	780	A	C5-C6-N1	7.58	121.49	117.70
41	BS	25	ARG	NE-CZ-NH1	7.58	124.09	120.30
21	AA	1328	C	N3-C2-O2	-7.58	116.59	121.90
54	BA	1531	C	O4'-C1'-N1	7.58	114.27	108.20
54	BA	1247	A	C5-C6-N1	7.58	121.49	117.70
54	BA	937	C	O4'-C1'-N1	7.58	114.26	108.20
54	BA	941	A	C4-C5-C6	-7.58	113.21	117.00
54	BA	1793	C	N3-C2-O2	-7.58	116.59	121.90
21	AA	393	A	C4-C5-C6	-7.58	113.21	117.00
54	BA	1953	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2434	A	C5-C6-N1	7.58	121.49	117.70
47	BY	47	ARG	NE-CZ-NH1	7.57	124.09	120.30
54	BA	149	A	C5-C6-N1	7.57	121.49	117.70
54	BA	265	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	2116	G	N3-C2-N2	-7.57	114.60	119.90
15	AP	28	ARG	NH1-CZ-NH2	-7.57	111.07	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	706	A	C4-C5-C6	-7.57	113.21	117.00
21	AA	59	A	C5-C6-N1	7.57	121.48	117.70
21	AA	74	A	C4-C5-C6	-7.57	113.21	117.00
24	A3	73	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1385	A	C5-C6-N1	7.57	121.48	117.70
21	AA	1317	C	N3-C2-O2	-7.57	116.60	121.90
54	BA	1668	A	C4-C5-C6	-7.57	113.22	117.00
21	AA	523	A	C4-C5-C6	-7.56	113.22	117.00
54	BA	2030	A	C5-C6-N1	7.56	121.48	117.70
54	BA	429	A	C5-C6-N1	7.56	121.48	117.70
20	AU	17	ARG	NE-CZ-NH1	7.56	124.08	120.30
21	AA	1287	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2392	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	892	A	C5-C6-N1	7.56	121.48	117.70
21	AA	1005	A	C4-C5-C6	-7.56	113.22	117.00
24	A3	69	C	P-O3'-C3'	7.56	128.77	119.70
54	BA	1128	G	O4'-C1'-N9	7.56	114.25	108.20
54	BA	2264	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	2433	A	C5-C6-N1	7.56	121.48	117.70
21	AA	246	A	C4-C5-C6	-7.55	113.22	117.00
54	BA	368	A	C4-C5-C6	-7.55	113.22	117.00
54	BA	1299	G	O4'-C1'-N9	7.55	114.24	108.20
21	AA	466	A	C4-C5-C6	-7.55	113.22	117.00
54	BA	973	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2114	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	645	C	N3-C2-O2	-7.55	116.61	121.90
54	BA	920	A	C5-C6-N1	7.55	121.48	117.70
21	AA	706	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1082	A	C5-C6-N1	7.55	121.47	117.70
54	BA	457	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2328	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	2368	C	N3-C2-O2	-7.55	116.61	121.90
21	AA	600	A	C4-C5-C6	-7.55	113.23	117.00
21	AA	718	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1350	A	C4-C5-C6	-7.55	113.23	117.00
54	BA	1114	C	N3-C2-O2	-7.55	116.62	121.90
55	BB	52	A	C5-C6-N1	7.55	121.47	117.70
21	AA	1446	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	961	C	N3-C2-O2	-7.54	116.62	121.90
45	BW	54	ARG	NE-CZ-NH1	7.54	124.07	120.30
54	BA	199	A	C5-C6-N1	7.54	121.47	117.70
21	AA	167	A	C4-C5-C6	-7.54	113.23	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	532	A	C5-C6-N1	7.54	121.47	117.70
21	AA	1462	C	N3-C2-O2	-7.54	116.62	121.90
54	BA	1067	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	2037	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	2247	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	1197	A	C4-C5-C6	-7.53	113.23	117.00
54	BA	900	A	C4-C5-C6	-7.53	113.23	117.00
54	BA	1912	A	C4-C5-C6	-7.53	113.23	117.00
54	BA	2675	A	C5-C6-N1	7.53	121.47	117.70
21	AA	574	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	1810	A	C5-C6-N1	7.53	121.47	117.70
21	AA	465	A	C5-C6-N1	7.53	121.46	117.70
21	AA	1132	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	1362	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	2610	C	N3-C2-O2	-7.53	116.63	121.90
21	AA	408	A	C5-C6-N1	7.53	121.46	117.70
54	BA	1676	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	2327	A	C5-C6-N1	7.53	121.46	117.70
54	BA	1941	C	N3-C2-O2	-7.52	116.63	121.90
21	AA	16	A	C4-C5-C6	-7.52	113.24	117.00
54	BA	742	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2052	A	C5-C6-N1	7.52	121.46	117.70
21	AA	716	A	C5-C6-N1	7.52	121.46	117.70
23	A2	82	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1254	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	1676	A	C5-C6-N1	7.52	121.46	117.70
21	AA	320	A	C4-C5-C6	-7.51	113.24	117.00
21	AA	1256	A	C5-C6-N1	7.51	121.46	117.70
21	AA	1362	A	N1-C6-N6	-7.51	114.09	118.60
33	BK	105	ARG	NE-CZ-NH1	7.51	124.06	120.30
54	BA	1084	A	C4-C5-C6	-7.51	113.24	117.00
21	AA	248	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	1634	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2095	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	1500	A	C4-C5-C6	-7.51	113.25	117.00
54	BA	2468	A	C5-C6-N1	7.51	121.45	117.70
21	AA	374	A	C5-C6-N1	7.51	121.45	117.70
21	AA	1431	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2092	U	N3-C2-O2	-7.51	116.94	122.20
54	BA	1936	A	C4-C5-C6	-7.50	113.25	117.00
42	BT	6	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	749	A	C5-C6-N1	7.50	121.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2478	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	839	U	O4'-C1'-N1	7.50	114.20	108.20
54	BA	1876	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	1360	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1000	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1156	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1854	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2572	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2835	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2765	A	C5-C6-N1	7.50	121.45	117.70
54	BA	190	A	N1-C6-N6	-7.49	114.10	118.60
21	AA	300	A	C5-C6-N1	7.49	121.45	117.70
54	BA	959	A	C5-C6-N1	7.49	121.44	117.70
54	BA	981	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	1393	A	C4-C5-C6	-7.49	113.25	117.00
4	AE	149	PRO	CA-N-CD	-7.49	101.02	111.50
21	AA	1496	C	N3-C2-O2	-7.49	116.66	121.90
21	AA	327	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	1382	G	O4'-C1'-N9	7.49	114.19	108.20
54	BA	63	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	1489	C	N3-C2-O2	-7.48	116.66	121.90
54	BA	1801	A	C5-C6-N1	7.48	121.44	117.70
54	BA	5	A	C4-C5-C6	-7.48	113.26	117.00
54	BA	1243	C	N3-C2-O2	-7.48	116.67	121.90
54	BA	1603	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2051	A	C4-C5-C6	-7.47	113.26	117.00
21	AA	1180	A	C4-C5-C6	-7.47	113.26	117.00
54	BA	49	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	895	U	O4'-C1'-N1	7.47	114.18	108.20
54	BA	981	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1433	A	C5-C6-N1	7.47	121.44	117.70
54	BA	2886	A	C4-C5-C6	-7.47	113.27	117.00
3	AD	55	ARG	NE-CZ-NH1	7.47	124.03	120.30
21	AA	743	A	C4-C5-C6	-7.47	113.27	117.00
54	BA	1236	G	O4'-C1'-N9	7.47	114.17	108.20
54	BA	1669	A	N1-C6-N6	-7.47	114.12	118.60
21	AA	573	A	C4-C5-C6	-7.47	113.27	117.00
54	BA	1812	U	O4'-C1'-N1	7.47	114.17	108.20
8	AI	121	ARG	NE-CZ-NH1	7.47	124.03	120.30
21	AA	502	A	C5-C6-N1	7.47	121.43	117.70
21	AA	815	A	C5-C6-N1	7.47	121.43	117.70
54	BA	796	C	N3-C2-O2	-7.47	116.67	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2070	A	C4-C5-C6	-7.47	113.27	117.00
54	BA	2235	G	N1-C6-O6	-7.47	115.42	119.90
16	AQ	5	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	1354	A	C4-C5-C6	-7.46	113.27	117.00
54	BA	1050	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2229	U	O4'-C1'-N1	7.46	114.17	108.20
54	BA	2749	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1493	A	C4-C5-C6	-7.46	113.27	117.00
55	BB	101	A	C5-C6-N1	7.46	121.43	117.70
54	BA	53	A	N1-C6-N6	-7.46	114.13	118.60
54	BA	1490	A	C5-C6-N1	7.46	121.43	117.70
54	BA	687	C	O4'-C1'-N1	7.45	114.16	108.20
54	BA	931	U	O4'-C1'-N1	7.45	114.16	108.20
55	BB	78	A	C4-C5-C6	-7.45	113.27	117.00
21	AA	609	A	C4-C5-C6	-7.45	113.27	117.00
21	AA	900	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	689	A	C4-C5-C6	-7.45	113.28	117.00
54	BA	1032	A	C5-C6-N1	7.45	121.42	117.70
54	BA	945	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2317	A	C4-C5-C6	-7.45	113.28	117.00
24	A3	45	A	C5-C6-N1	7.45	121.42	117.70
54	BA	38	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	217	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	343	C	N3-C2-O2	-7.45	116.69	121.90
54	BA	2750	A	C5-C6-N1	7.44	121.42	117.70
3	AD	2	ARG	NE-CZ-NH1	7.44	124.02	120.30
19	AT	24	ARG	NE-CZ-NH1	7.44	124.02	120.30
21	AA	554	A	N1-C6-N6	-7.44	114.13	118.60
32	BJ	120	ARG	NE-CZ-NH1	7.44	124.02	120.30
54	BA	627	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2385	C	N3-C2-O2	-7.44	116.69	121.90
21	AA	900	A	C5-C6-N1	7.44	121.42	117.70
54	BA	2044	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	2614	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	1146	C	N3-C2-O2	-7.44	116.69	121.90
21	AA	172	A	C5-C6-N1	7.44	121.42	117.70
54	BA	505	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	229	C	N3-C2-O2	-7.43	116.69	121.90
21	AA	223	A	C5-C6-N1	7.43	121.42	117.70
54	BA	9	G	O4'-C1'-N9	7.43	114.15	108.20
54	BA	1551	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	10	A	C5-C6-N1	7.43	121.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1229	A	C4-C5-C6	-7.43	113.28	117.00
54	BA	172	A	C4-C5-C6	-7.43	113.29	117.00
54	BA	631	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	2342	C	N3-C2-O2	-7.43	116.70	121.90
21	AA	968	A	C5-C6-N1	7.43	121.41	117.70
30	BH	27	ARG	NE-CZ-NH1	7.43	124.01	120.30
54	BA	1792	G	O4'-C1'-N9	7.43	114.14	108.20
21	AA	1000	A	N1-C6-N6	-7.42	114.14	118.60
54	BA	1967	C	N3-C2-O2	-7.42	116.70	121.90
21	AA	1005	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1363	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1783	A	C4-C5-C6	-7.42	113.29	117.00
21	AA	1145	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	563	A	C5-C6-N1	7.42	121.41	117.70
54	BA	2757	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	226	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	2564	A	C4-C5-C6	-7.42	113.29	117.00
54	BA	2781	A	C4-C5-C6	-7.42	113.29	117.00
54	BA	1788	C	N3-C2-O2	-7.41	116.71	121.90
21	AA	495	A	N1-C6-N6	-7.41	114.15	118.60
15	AP	70	ARG	NE-CZ-NH1	7.41	124.00	120.30
21	AA	1368	A	C5-C6-N1	7.41	121.40	117.70
21	AA	1055	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	689	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	1717	A	C5-C6-N1	7.41	121.40	117.70
22	A1	32	C	N3-C2-O2	-7.41	116.72	121.90
54	BA	522	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	1598	A	N1-C6-N6	-7.41	114.16	118.60
54	BA	2335	A	N1-C6-N6	-7.41	114.16	118.60
21	AA	631	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	1499	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2443	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	499	A	C5-C6-N1	7.40	121.40	117.70
21	AA	576	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	1418	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	1690	A	C5-C6-N1	7.40	121.40	117.70
54	BA	742	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	2516	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1254	A	C5-C6-N1	7.40	121.40	117.70
21	AA	182	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1045	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	89	A	N1-C6-N6	-7.40	114.16	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1111	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	309	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1230	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	1791	A	C5-C6-N1	7.39	121.40	117.70
54	BA	2377	A	C5-C6-N1	7.39	121.40	117.70
54	BA	2591	C	N3-C2-O2	-7.39	116.72	121.90
54	BA	2611	C	N3-C2-O2	-7.39	116.72	121.90
21	AA	20	U	O4'-C1'-N1	7.39	114.11	108.20
54	BA	143	C	N3-C2-O2	-7.39	116.73	121.90
54	BA	56	A	C5-C6-N1	7.39	121.39	117.70
21	AA	228	A	C4-C5-C6	-7.39	113.31	117.00
54	BA	718	A	N1-C6-N6	-7.39	114.17	118.60
54	BA	1532	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1821	A	C4-C5-C6	-7.39	113.31	117.00
54	BA	1477	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1754	A	C4-C5-C6	-7.38	113.31	117.00
21	AA	263	A	C5-C6-N1	7.38	121.39	117.70
30	BH	116	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	754	C	N3-C2-O2	-7.38	116.73	121.90
24	A3	62	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	2205	A	N1-C6-N6	-7.38	114.17	118.60
6	AG	77	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	879	C	N3-C2-O2	-7.38	116.74	121.90
54	BA	1736	U	O4'-C1'-N1	7.38	114.10	108.20
4	AE	156	ARG	NE-CZ-NH1	7.37	123.99	120.30
21	AA	475	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	663	A	C5-C6-N1	7.37	121.39	117.70
21	AA	1158	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	765	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	1990	C	O4'-C1'-N1	7.37	114.10	108.20
54	BA	2810	A	C5-C6-N1	7.37	121.39	117.70
21	AA	264	C	N1-C2-O2	7.37	123.32	118.90
54	BA	794	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	920	A	C4-C5-C6	-7.37	113.31	117.00
21	AA	55	A	N1-C6-N6	-7.37	114.18	118.60
35	BM	51	ARG	NE-CZ-NH1	7.37	123.98	120.30
54	BA	2654	A	C5-C6-N1	7.37	121.38	117.70
21	AA	1170	A	N1-C6-N6	-7.37	114.18	118.60
21	AA	393	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1004	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1378	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	128	C	N3-C2-O2	-7.36	116.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	478	A	C5-C6-N1	7.36	121.38	117.70
54	BA	556	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	610	C	O4'-C1'-N1	7.36	114.09	108.20
54	BA	632	A	C4-C5-C6	-7.36	113.32	117.00
54	BA	917	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2287	A	O4'-C1'-N9	7.36	114.09	108.20
21	AA	718	A	N1-C6-N6	-7.36	114.18	118.60
46	BX	2	ARG	NE-CZ-NH2	-7.36	116.62	120.30
54	BA	190	A	C5-C6-N1	7.36	121.38	117.70
54	BA	644	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	1276	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1829	A	C4-C5-C6	-7.36	113.32	117.00
21	AA	694	A	C5-C6-N1	7.36	121.38	117.70
54	BA	611	C	O4'-C1'-N1	7.36	114.08	108.20
54	BA	1453	A	O4'-C1'-N9	7.36	114.09	108.20
54	BA	1996	C	N3-C2-O2	-7.36	116.75	121.90
3	AD	62	ARG	NE-CZ-NH1	7.36	123.98	120.30
54	BA	1596	A	C4-C5-C6	-7.35	113.32	117.00
54	BA	2374	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	749	A	C5-C6-N1	7.35	121.38	117.70
54	BA	181	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2829	A	C4-C5-C6	-7.35	113.32	117.00
40	BR	79	ARG	NE-CZ-NH1	7.35	123.98	120.30
46	BX	49	ARG	NE-CZ-NH1	7.35	123.98	120.30
54	BA	94	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1641	A	C5-C6-N1	7.35	121.37	117.70
54	BA	2565	A	C5-C6-N1	7.35	121.38	117.70
54	BA	38	A	C4-C5-C6	-7.35	113.33	117.00
54	BA	2434	A	C4-C5-C6	-7.35	113.33	117.00
54	BA	2727	A	C5-C6-N1	7.35	121.37	117.70
25	BC	101	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	1102	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2084	C	N3-C2-O2	-7.34	116.76	121.90
21	AA	1319	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	531	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2104	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2799	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	2809	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	1275	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	1606	C	N3-C2-O2	-7.34	116.77	121.90
54	BA	2587	A	C5-C6-N1	7.33	121.37	117.70
8	AI	32	ARG	NE-CZ-NH1	7.33	123.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	7	A	C5-C6-N1	7.33	121.37	117.70
54	BA	675	A	C5-C6-N1	7.33	121.37	117.70
54	BA	676	A	C5-C6-N1	7.33	121.37	117.70
54	BA	2388	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	294	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	1035	U	O4'-C1'-N1	7.33	114.06	108.20
54	BA	1585	C	O4'-C1'-N1	7.33	114.06	108.20
54	BA	2499	C	O4'-C1'-N1	7.33	114.06	108.20
21	AA	190	A	C4-C5-C6	-7.33	113.34	117.00
21	AA	513	C	N3-C2-O2	-7.33	116.77	121.90
21	AA	1413	A	C5-C6-N1	7.33	121.36	117.70
54	BA	1679	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2762	C	N3-C2-O2	-7.33	116.77	121.90
21	AA	1252	A	C5-C6-N1	7.32	121.36	117.70
54	BA	761	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2135	A	O4'-C1'-N9	7.32	114.06	108.20
54	BA	1419	A	C5-C6-N1	7.32	121.36	117.70
54	BA	315	G	O4'-C1'-N9	7.32	114.06	108.20
54	BA	391	A	C5-C6-N1	7.32	121.36	117.70
54	BA	471	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	2208	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	2212	A	N1-C6-N6	-7.32	114.21	118.60
12	AM	108	ARG	NE-CZ-NH1	7.32	123.96	120.30
21	AA	393	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	182	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	1096	A	C5-C6-N1	7.32	121.36	117.70
21	AA	695	A	C5-C6-N1	7.31	121.36	117.70
21	AA	501	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	2175	C	N3-C2-O2	-7.31	116.78	121.90
3	AD	127	ARG	NE-CZ-NH1	7.31	123.96	120.30
8	AI	84	ARG	NE-CZ-NH1	7.31	123.95	120.30
54	BA	984	A	C5-C6-N1	7.31	121.36	117.70
54	BA	1827	U	O4'-C1'-N1	7.31	114.05	108.20
21	AA	421	U	O4'-C1'-N1	7.31	114.05	108.20
54	BA	1613	G	N1-C6-O6	-7.31	115.52	119.90
54	BA	2829	A	N1-C6-N6	-7.31	114.22	118.60
21	AA	156	C	N3-C2-O2	-7.31	116.79	121.90
21	AA	1081	A	C5-C6-N1	7.31	121.35	117.70
54	BA	620	G	N3-C2-N2	-7.31	114.79	119.90
21	AA	189	A	C5-C6-N1	7.30	121.35	117.70
54	BA	471	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1533	C	N3-C2-O2	-7.30	116.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2062	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2740	A	C4-C5-C6	-7.30	113.35	117.00
21	AA	389	A	N1-C6-N6	-7.30	114.22	118.60
21	AA	1382	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	751	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1954	G	N1-C6-O6	-7.30	115.52	119.90
54	BA	2899	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2114	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2861	U	O4'-C1'-N1	7.30	114.04	108.20
21	AA	1413	A	C4-C5-C6	-7.29	113.35	117.00
54	BA	910	A	C5-C6-N1	7.29	121.35	117.70
54	BA	2137	U	O4'-C1'-N1	7.29	114.04	108.20
54	BA	2428	G	C8-N9-C4	-7.29	103.48	106.40
12	AM	69	ARG	NE-CZ-NH1	7.29	123.95	120.30
21	AA	440	C	N3-C2-O2	-7.29	116.80	121.90
21	AA	878	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	880	C	N3-C2-O2	-7.29	116.80	121.90
21	AA	1319	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1040	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	1045	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	505	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1618	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	2766	A	C5-C6-N1	7.29	121.34	117.70
54	BA	1787	A	N1-C6-N6	-7.29	114.23	118.60
21	AA	1411	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	776	G	O4'-C1'-N9	7.29	114.03	108.20
54	BA	1677	A	N1-C6-N6	-7.29	114.23	118.60
21	AA	382	A	C4-C5-C6	-7.29	113.36	117.00
21	AA	782	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	145	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	2386	A	C4-C5-C6	-7.29	113.36	117.00
22	A1	76	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	129	C	N3-C2-O2	-7.28	116.80	121.90
54	BA	2542	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2340	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	130	A	C5-C6-N1	7.27	121.34	117.70
3	AD	50	TYR	CB-CG-CD2	7.27	125.36	121.00
21	AA	28	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	59	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	363	A	C5-C6-N1	7.27	121.34	117.70
54	BA	1165	A	N1-C6-N6	-7.27	114.24	118.60
54	BA	1966	A	C5-C6-N1	7.27	121.34	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2054	A	C5-C6-N1	7.27	121.34	117.70
54	BA	1431	A	O4'-C1'-N9	7.27	114.02	108.20
54	BA	2322	A	C5-C6-N1	7.27	121.34	117.70
56	B5	162	ARG	NE-CZ-NH1	7.27	123.94	120.30
54	BA	11	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	69	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	1285	A	C4-C5-C6	-7.27	113.37	117.00
54	BA	2022	U	O4'-C1'-N1	7.27	114.01	108.20
54	BA	2726	A	C4-C5-C6	-7.27	113.37	117.00
21	AA	182	A	N1-C6-N6	-7.27	114.24	118.60
21	AA	389	A	C5-C6-N1	7.26	121.33	117.70
21	AA	716	A	N1-C6-N6	-7.26	114.24	118.60
54	BA	1244	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1414	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	2453	A	C4-C5-C6	-7.26	113.37	117.00
21	AA	1022	A	N1-C6-N6	-7.26	114.24	118.60
11	AL	13	ARG	NE-CZ-NH1	7.26	123.93	120.30
19	AT	73	ARG	NE-CZ-NH1	7.26	123.93	120.30
21	AA	238	A	C3'-C2'-C1'	-7.26	95.69	101.50
40	BR	84	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	1794	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2091	C	N1-C2-O2	7.26	123.25	118.90
54	BA	143	C	O4'-C1'-N1	7.26	114.01	108.20
54	BA	352	A	N1-C6-N6	-7.26	114.25	118.60
54	BA	988	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1085	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	1550	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	32	A	C5-C6-N1	7.25	121.33	117.70
37	BO	25	ARG	NE-CZ-NH1	7.25	123.93	120.30
54	BA	2362	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	1404	C	N3-C2-O2	-7.25	116.82	121.90
54	BA	547	A	C5-C6-N1	7.25	121.33	117.70
54	BA	2298	A	C5-C6-N1	7.25	121.33	117.70
21	AA	768	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	1260	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	2665	A	O4'-C1'-N9	7.25	114.00	108.20
21	AA	1054	C	N1-C2-O2	7.25	123.25	118.90
21	AA	1480	A	C4-C5-C6	-7.25	113.38	117.00
39	BQ	57	ARG	NE-CZ-NH1	7.25	123.92	120.30
54	BA	1866	A	C5-C6-N1	7.25	121.32	117.70
54	BA	2104	C	O4'-C1'-N1	7.25	114.00	108.20
54	BA	2602	A	O4'-C1'-N9	7.25	114.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2676	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	1357	A	C5-C6-N1	7.25	121.32	117.70
54	BA	391	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	1979	U	O4'-C1'-N1	7.25	114.00	108.20
54	BA	111	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1545	A	C5-C6-N1	7.24	121.32	117.70
21	AA	179	A	N1-C6-N6	-7.24	114.25	118.60
21	AA	1322	C	N1-C2-O2	7.24	123.24	118.90
54	BA	602	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1253	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	1808	A	O4'-C1'-N9	7.24	113.99	108.20
55	BB	60	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	10	A	C5-C6-N1	7.24	121.32	117.70
54	BA	225	C	O4'-C1'-N1	7.24	113.99	108.20
54	BA	2126	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	2512	C	O4'-C1'-N1	7.24	113.99	108.20
21	AA	602	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	933	A	C5-C6-N1	7.24	121.32	117.70
21	AA	336	A	C5-C6-N1	7.23	121.32	117.70
54	BA	936	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	2738	A	N1-C6-N6	-7.23	114.26	118.60
21	AA	1274	A	C5-C6-N1	7.23	121.32	117.70
21	AA	1412	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	886	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	1757	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	2060	A	C4-C5-C6	-7.23	113.38	117.00
54	BA	1431	A	C5-C6-N1	7.23	121.31	117.70
5	AF	2	ARG	NE-CZ-NH2	-7.23	116.69	120.30
21	AA	52	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	1504	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2052	A	C4-C5-C6	-7.23	113.39	117.00
21	AA	58	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	1503	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2541	A	N1-C6-N6	-7.22	114.27	118.60
21	AA	811	C	N3-C2-O2	-7.22	116.84	121.90
21	AA	85	U	O4'-C1'-N1	7.22	113.98	108.20
21	AA	262	A	C5-C6-N1	7.22	121.31	117.70
21	AA	535	A	C5-C6-N1	7.22	121.31	117.70
21	AA	622	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	669	G	O4'-C1'-N9	7.22	113.98	108.20
54	BA	1357	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	978	A	C5-C6-N1	7.22	121.31	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1553	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	347	A	C5-C6-N1	7.21	121.31	117.70
54	BA	470	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1205	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1735	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1913	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	2288	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	2821	A	N1-C6-N6	-7.21	114.27	118.60
21	AA	162	A	C4-C5-C6	-7.21	113.39	117.00
21	AA	1163	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1151	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	2378	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	2403	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	281	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	849	A	C5-C6-N1	7.21	121.30	117.70
54	BA	146	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	1251	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	1454	C	N3-C2-O2	-7.20	116.86	121.90
21	AA	554	A	C4-C5-C6	-7.20	113.40	117.00
21	AA	924	C	N3-C2-O2	-7.20	116.86	121.90
21	AA	736	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	299	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	2546	U	O4'-C1'-N1	7.20	113.96	108.20
21	AA	1209	C	N3-C2-O2	-7.19	116.86	121.90
54	BA	167	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1952	A	N1-C6-N6	-7.19	114.28	118.60
54	BA	909	A	C5-C6-N1	7.19	121.29	117.70
54	BA	2761	A	C5-C6-N1	7.19	121.29	117.70
54	BA	453	A	C5-C6-N1	7.19	121.29	117.70
54	BA	445	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	1632	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2380	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	2778	A	N1-C6-N6	-7.18	114.29	118.60
18	AS	2	ARG	NE-CZ-NH1	7.18	123.89	120.30
21	AA	169	C	C1'-O4'-C4'	-7.18	104.16	109.90
21	AA	312	C	N3-C2-O2	-7.18	116.87	121.90
21	AA	1016	A	C5-C6-N1	7.18	121.29	117.70
52	B3	12	ARG	NE-CZ-NH1	7.18	123.89	120.30
54	BA	2108	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2175	C	O4'-C1'-N1	7.18	113.95	108.20
21	AA	465	A	O4'-C1'-N9	7.18	113.94	108.20
21	AA	1275	A	N1-C6-N6	-7.18	114.29	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1098	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1126	A	C5-C6-N1	7.18	121.29	117.70
21	AA	509	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	1250	A	C5-C6-N1	7.18	121.29	117.70
54	BA	572	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	792	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1502	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	2450	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	2634	A	C5-C6-N1	7.18	121.29	117.70
21	AA	411	A	N1-C6-N6	-7.17	114.30	118.60
21	AA	1236	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1248	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	833	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	1010	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1088	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	1928	A	C5-C6-N1	7.17	121.29	117.70
54	BA	2412	A	N1-C6-N6	-7.17	114.30	118.60
21	AA	78	A	C5-C6-N1	7.17	121.29	117.70
21	AA	215	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	767	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	1496	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	1981	A	C4-C5-C6	-7.17	113.42	117.00
21	AA	913	A	P-O3'-C3'	7.17	128.30	119.70
21	AA	1339	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	323	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	422	C	N1-C2-O2	7.17	123.20	118.90
54	BA	985	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	1990	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	1110	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	911	A	C4-C5-C6	-7.17	113.42	117.00
23	A2	91	A	N1-C6-N6	-7.16	114.30	118.60
54	BA	587	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	2781	A	N1-C6-N6	-7.16	114.30	118.60
54	BA	2045	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	1159	U	C1'-O4'-C4'	-7.16	104.17	109.90
46	BX	44	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	2868	A	C5-C6-N1	7.16	121.28	117.70
6	AG	118	ARG	NE-CZ-NH2	-7.16	116.72	120.30
21	AA	860	A	C4-C5-C6	-7.16	113.42	117.00
25	BC	47	ARG	NE-CZ-NH1	7.16	123.88	120.30
21	AA	217	C	N3-C2-O2	-7.16	116.89	121.90
21	AA	853	C	N3-C2-O2	-7.16	116.89	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	BP	61	ARG	NE-CZ-NH2	-7.16	116.72	120.30
54	BA	2734	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	1011	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	504	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2755	C	C3'-C2'-C1'	7.15	107.22	101.50
8	AI	17	ARG	NE-CZ-NH2	-7.15	116.72	120.30
21	AA	729	A	C4-C5-C6	-7.15	113.42	117.00
21	AA	765	G	O4'-C1'-N9	7.15	113.92	108.20
54	BA	603	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	960	A	C5-C6-N1	7.15	121.28	117.70
54	BA	2761	A	O4'-C1'-N9	7.15	113.92	108.20
22	A1	26	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	1447	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	671	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	1367	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	2439	A	C5-C6-N1	7.15	121.27	117.70
21	AA	1377	A	C5-C6-N1	7.14	121.27	117.70
26	BD	46	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	1953	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	2764	A	C4-C5-C6	-7.14	113.43	117.00
22	A1	28	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	131	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1070	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	1472	C	N3-C2-O2	-7.14	116.90	121.90
55	BB	3	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	826	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1383	A	C5-C6-N1	7.14	121.27	117.70
54	BA	735	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1549	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1652	A	N1-C6-N6	-7.14	114.32	118.60
54	BA	1947	C	N3-C2-O2	-7.14	116.90	121.90
21	AA	308	C	N3-C2-O2	-7.14	116.90	121.90
46	BX	17	ARG	NE-CZ-NH1	7.14	123.87	120.30
21	AA	109	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1183	U	O4'-C1'-N1	7.14	113.91	108.20
41	BS	110	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	2267	A	C5-C6-N1	7.14	121.27	117.70
21	AA	40	C	N3-C2-O2	-7.13	116.91	121.90
21	AA	995	C	N3-C2-O2	-7.13	116.91	121.90
22	A1	23	A	C5-C6-N1	7.13	121.27	117.70
54	BA	979	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	2263	C	N3-C2-O2	-7.13	116.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1172	C	N3-C2-O2	-7.13	116.91	121.90
46	BX	56	ARG	NE-CZ-NH1	7.13	123.87	120.30
21	AA	783	C	N3-C2-O2	-7.13	116.91	121.90
21	AA	1226	C	N3-C2-O2	-7.13	116.91	121.90
55	BB	109	A	C5-C6-N1	7.13	121.27	117.70
21	AA	523	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	1877	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	98	A	C4-C5-C6	-7.13	113.44	117.00
21	AA	321	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	1499	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	439	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	1020	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1352	U	N3-C2-O2	-7.13	117.21	122.20
54	BA	1580	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1885	A	C5-C6-N1	7.13	121.26	117.70
21	AA	1203	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	83	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	104	A	C4-C5-C6	-7.13	113.44	117.00
54	BA	1496	A	C5-C6-N1	7.13	121.26	117.70
54	BA	115	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	590	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	820	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2471	A	N1-C6-N6	-7.12	114.33	118.60
51	B2	34	ARG	NE-CZ-NH1	7.12	123.86	120.30
54	BA	528	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	734	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2352	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	76	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	332	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	609	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1304	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1637	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1925	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	996	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1654	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	155	A	C5-C6-N1	7.11	121.26	117.70
21	AA	478	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	792	A	C4-C5-C6	-7.11	113.44	117.00
54	BA	2477	U	O4'-C1'-N1	7.11	113.89	108.20
54	BA	2879	A	N1-C6-N6	-7.11	114.33	118.60
54	BA	456	C	N1-C2-O2	7.11	123.17	118.90
54	BA	2377	A	C4-C5-C6	-7.11	113.44	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1237	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	213	A	C5-C6-N1	7.11	121.25	117.70
54	BA	279	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	1140	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	2309	A	N1-C6-N6	-7.11	114.34	118.60
21	AA	1394	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	118	A	C4-C5-C6	-7.11	113.45	117.00
24	A3	59	A	C4-C5-C6	-7.10	113.45	117.00
21	AA	651	C	N3-C2-O2	-7.10	116.93	121.90
25	BC	237	ARG	NE-CZ-NH1	7.10	123.85	120.30
33	BK	78	ARG	NE-CZ-NH1	7.10	123.85	120.30
21	AA	411	A	C4-C5-C6	-7.10	113.45	117.00
21	AA	1066	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	1554	U	O4'-C1'-N1	7.10	113.88	108.20
24	A3	68	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	632	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	2073	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	699	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	2820	A	C5-C6-N1	7.10	121.25	117.70
21	AA	431	A	N1-C6-N6	-7.09	114.34	118.60
21	AA	1261	A	C5-C6-N1	7.09	121.25	117.70
25	BC	12	ARG	NE-CZ-NH1	7.09	123.85	120.30
54	BA	1801	A	N1-C6-N6	-7.09	114.34	118.60
9	AJ	68	ARG	NE-CZ-NH2	-7.09	116.75	120.30
21	AA	5	U	O4'-C1'-N1	7.09	113.87	108.20
54	BA	1591	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2336	A	N1-C6-N6	-7.09	114.35	118.60
55	BB	104	A	N1-C6-N6	-7.09	114.35	118.60
1	AB	221	ARG	NE-CZ-NH1	7.09	123.84	120.30
21	AA	994	A	C5-C6-N1	7.09	121.24	117.70
56	B5	164	ARG	NE-CZ-NH1	7.09	123.84	120.30
34	BL	21	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	1469	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	2634	A	N1-C6-N6	-7.08	114.35	118.60
55	BB	66	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	1833	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	2552	U	O4'-C1'-N1	7.08	113.86	108.20
21	AA	1146	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1579	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2705	A	N1-C6-N6	-7.08	114.35	118.60
21	AA	277	C	N3-C2-O2	-7.08	116.94	121.90
51	B2	21	ARG	NE-CZ-NH1	7.08	123.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	9	G	N1-C6-O6	-7.08	115.65	119.90
54	BA	1787	A	C5-C6-N1	7.08	121.24	117.70
21	AA	120	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	233	C	N3-C2-O2	-7.08	116.95	121.90
21	AA	279	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	583	A	C4-C5-C6	-7.08	113.46	117.00
21	AA	1042	A	C5-C6-N1	7.08	121.24	117.70
24	A3	22	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1879	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	2527	C	N3-C2-O2	-7.08	116.95	121.90
54	BA	2679	A	N1-C6-N6	-7.08	114.35	118.60
21	AA	98	A	C5-C6-N1	7.07	121.24	117.70
54	BA	439	A	C5-C6-N1	7.07	121.24	117.70
54	BA	1181	U	O4'-C1'-N1	7.07	113.86	108.20
55	BB	73	A	C4-C5-C6	-7.07	113.46	117.00
21	AA	119	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	174	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	435	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	660	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	2794	C	N3-C2-O2	-7.07	116.95	121.90
24	A3	36	A	N1-C6-N6	-7.07	114.36	118.60
25	BC	68	ARG	NE-CZ-NH1	7.07	123.83	120.30
54	BA	299	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	502	A	C5-C6-N1	7.07	121.23	117.70
21	AA	816	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	1575	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	2715	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	815	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	1318	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2710	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	456	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	140	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	1452	C	P-O3'-C3'	7.06	128.17	119.70
54	BA	861	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1142	A	C4-C5-C6	-7.06	113.47	117.00
55	BB	47	C	O4'-C1'-N1	7.06	113.85	108.20
54	BA	1815	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2716	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	344	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1553	A	C4-C5-C6	-7.05	113.47	117.00
54	BA	165	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	1244	A	N1-C6-N6	-7.05	114.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1655	A	C5-C6-N1	7.05	121.23	117.70
21	AA	559	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1822	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	731	C	N3-C2-O2	-7.05	116.97	121.90
55	BB	45	A	C5-C6-N1	7.05	121.22	117.70
21	AA	919	A	C5-C6-N1	7.05	121.22	117.70
54	BA	244	A	C5-C6-N1	7.05	121.22	117.70
54	BA	461	C	O4'-C1'-N1	7.05	113.84	108.20
54	BA	2518	A	N1-C6-N6	-7.05	114.37	118.60
9	AJ	31	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	1095	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2297	A	C5-C6-N1	7.04	121.22	117.70
54	BA	2338	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	106	C	N3-C2-O2	-7.04	116.97	121.90
33	BK	31	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	272	A	C5-C6-N1	7.04	121.22	117.70
21	AA	509	A	C5-C6-N1	7.03	121.22	117.70
21	AA	907	A	C5-C6-N1	7.03	121.22	117.70
21	AA	1035	A	N1-C6-N6	-7.03	114.38	118.60
24	A3	14	A	N1-C6-N6	-7.03	114.38	118.60
35	BM	18	ARG	NE-CZ-NH1	7.03	123.82	120.30
54	BA	1434	A	O4'-C1'-N9	7.03	113.83	108.20
54	BA	1606	C	N1-C2-O2	7.03	123.12	118.90
28	BF	109	ARG	NE-CZ-NH1	7.03	123.82	120.30
54	BA	2173	A	C4-C5-C6	-7.03	113.48	117.00
21	AA	1191	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	1749	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	2654	A	C4-C5-C6	-7.03	113.49	117.00
54	BA	840	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1383	A	C4-C5-C6	-7.03	113.49	117.00
21	AA	175	C	N3-C2-O2	-7.02	116.98	121.90
54	BA	838	C	N3-C2-O2	-7.02	116.98	121.90
21	AA	915	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	218	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	699	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	1866	A	N1-C6-N6	-7.02	114.39	118.60
21	AA	149	A	C4-C5-C6	-7.02	113.49	117.00
21	AA	109	A	N1-C6-N6	-7.02	114.39	118.60
21	AA	937	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	928	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1085	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	2006	C	N3-C2-O2	-7.02	116.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	886	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1977	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	2406	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	523	C	N3-C2-O2	-7.02	116.99	121.90
30	BH	123	ARG	NE-CZ-NH1	7.01	123.81	120.30
54	BA	1522	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1805	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2094	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1274	A	C5-C6-N1	7.01	121.21	117.70
54	BA	2433	A	C4-C5-C6	-7.01	113.49	117.00
21	AA	1195	C	N3-C2-O2	-7.01	116.99	121.90
24	A3	11	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1008	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2352	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	1289	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	228	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	661	A	C5-C6-N1	7.01	121.20	117.70
54	BA	802	A	C4-C5-C6	-7.01	113.50	117.00
54	BA	2099	U	N3-C2-O2	-7.01	117.29	122.20
54	BA	2635	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2860	A	C4-C5-C6	-7.01	113.50	117.00
54	BA	1140	C	O4'-C1'-N1	7.01	113.81	108.20
21	AA	696	A	C5-C6-N1	7.01	121.20	117.70
21	AA	756	C	N3-C2-O2	-7.01	117.00	121.90
34	BL	60	ARG	NE-CZ-NH1	7.01	123.80	120.30
54	BA	541	A	C4-C5-C6	-7.01	113.50	117.00
54	BA	942	G	N3-C2-N2	-7.01	115.00	119.90
54	BA	1571	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2247	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2275	C	N3-C2-O2	-7.01	117.00	121.90
21	AA	932	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2162	G	C8-N9-C4	-7.00	103.60	106.40
54	BA	1257	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2558	C	N3-C2-O2	-7.00	117.00	121.90
18	AS	77	ARG	NE-CZ-NH1	7.00	123.80	120.30
21	AA	1196	A	C5-C6-N1	7.00	121.20	117.70
54	BA	693	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1562	U	O4'-C1'-N1	7.00	113.80	108.20
3	AD	153	ARG	NE-CZ-NH1	7.00	123.80	120.30
54	BA	1804	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2183	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	2507	C	N3-C2-O2	-7.00	117.00	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	431	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	192	C	N1-C2-O2	7.00	123.10	118.90
55	BB	58	A	C5-C6-N1	7.00	121.20	117.70
21	AA	931	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	996	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	1046	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1937	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2295	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2531	A	C5-C6-N1	7.00	121.20	117.70
55	BB	80	U	O4'-C1'-N1	7.00	113.80	108.20
21	AA	715	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1655	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	2482	A	C5-C6-N1	7.00	121.20	117.70
8	AI	123	ARG	NE-CZ-NH1	6.99	123.80	120.30
21	AA	1271	A	C5-C6-N1	6.99	121.20	117.70
54	BA	433	C	N3-C2-O2	-6.99	117.00	121.90
54	BA	1700	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	2117	A	C5-C6-N1	6.99	121.20	117.70
54	BA	2520	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	1596	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1985	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	2094	A	N1-C6-N6	-6.99	114.41	118.60
21	AA	1219	A	C5-C6-N1	6.99	121.19	117.70
54	BA	602	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	1039	A	C5-C6-N1	6.99	121.19	117.70
54	BA	1322	A	C5-C6-N1	6.99	121.19	117.70
54	BA	302	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	155	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	1393	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2019	A	C5-C6-N1	6.99	121.19	117.70
54	BA	126	A	C5-C6-N1	6.98	121.19	117.70
54	BA	844	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	800	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1266	G	O4'-C1'-N9	6.98	113.78	108.20
54	BA	1268	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	2670	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2727	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1714	U	O4'-C1'-N1	6.98	113.78	108.20
54	BA	41	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	1711	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	2025	C	N1-C2-O2	6.98	123.09	118.90
54	BA	2503	A	N1-C6-N6	-6.98	114.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	699	A	C5-C6-N1	6.98	121.19	117.70
21	AA	65	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	207	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	629	A	C5-C6-N1	6.97	121.19	117.70
54	BA	131	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	262	A	C5-C6-N1	6.97	121.19	117.70
54	BA	721	A	C5-C6-N1	6.97	121.19	117.70
54	BA	743	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	1701	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2788	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	1179	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1439	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	2020	A	C5-C6-N1	6.97	121.19	117.70
54	BA	821	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1472	C	N1-C2-O2	6.97	123.08	118.90
54	BA	1780	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	990	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	156	A	C5-C6-N1	6.97	121.19	117.70
54	BA	698	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2350	C	N3-C2-O2	-6.97	117.02	121.90
55	BB	110	C	N3-C2-O2	-6.97	117.02	121.90
5	AF	44	ARG	NE-CZ-NH1	6.97	123.78	120.30
12	AM	112	ARG	NE-CZ-NH1	6.97	123.78	120.30
21	AA	607	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	622	A	C5-C6-N1	6.97	121.18	117.70
54	BA	251	A	C5-C6-N1	6.97	121.18	117.70
54	BA	1304	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	192	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1054	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	2225	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	766	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1246	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	53	A	C5-C6-N1	6.96	121.18	117.70
54	BA	197	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	1251	A	C5-C6-N1	6.96	121.18	117.70
24	A3	72	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	299	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1269	A	N1-C6-N6	-6.96	114.43	118.60
3	AD	43	ARG	NE-CZ-NH1	6.96	123.78	120.30
21	AA	298	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	374	A	C5-C6-N1	6.96	121.18	117.70
54	BA	444	C	O4'-C1'-N1	6.96	113.76	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	474	G	O4'-C1'-N9	6.96	113.76	108.20
54	BA	1213	A	C5-C6-N1	6.96	121.18	117.70
21	AA	564	C	N3-C2-O2	-6.95	117.03	121.90
22	A1	71	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	63	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	323	C	C3'-C2'-C1'	6.95	107.06	101.50
54	BA	2198	A	C5-C6-N1	6.95	121.18	117.70
20	AU	20	ARG	NE-CZ-NH1	6.95	123.78	120.30
21	AA	738	C	N3-C2-O2	-6.95	117.03	121.90
22	A1	72	C	N3-C2-O2	-6.95	117.03	121.90
50	B1	5	ARG	NE-CZ-NH1	6.95	123.78	120.30
54	BA	1020	A	N1-C6-N6	-6.95	114.43	118.60
54	BA	1974	C	N3-C2-O2	-6.95	117.03	121.90
21	AA	325	A	C5-C6-N1	6.95	121.17	117.70
54	BA	791	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	1760	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	1927	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2698	U	O4'-C1'-N1	6.95	113.76	108.20
54	BA	886	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	381	C	N3-C2-O2	-6.95	117.04	121.90
21	AA	959	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2427	C	N3-C2-O2	-6.95	117.04	121.90
21	AA	1375	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	1327	A	C5-C6-N1	6.94	121.17	117.70
54	BA	587	C	N1-C2-O2	6.94	123.06	118.90
54	BA	1722	A	N1-C6-N6	-6.94	114.44	118.60
54	BA	2793	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	345	C	N1-C2-O2	6.94	123.06	118.90
48	BZ	44	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	71	A	C4-C5-C6	-6.94	113.53	117.00
1	AB	20	ARG	NE-CZ-NH1	6.94	123.77	120.30
21	AA	643	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	1037	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	472	A	C5-C6-N1	6.94	121.17	117.70
54	BA	591	U	O4'-C1'-N1	6.94	113.75	108.20
54	BA	983	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1675	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	1332	A	N1-C6-N6	-6.94	114.44	118.60
22	A1	14	A	C5-C6-N1	6.94	121.17	117.70
54	BA	2008	C	N3-C2-O2	-6.94	117.05	121.90
54	BA	2153	C	N3-C2-O2	-6.94	117.05	121.90
21	AA	353	A	O4'-C1'-N9	6.93	113.75	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	26	A	C5-C6-N1	6.93	121.17	117.70
21	AA	889	A	C4-C5-C6	-6.93	113.53	117.00
24	A3	14	A	C5-C6-N1	6.93	121.17	117.70
54	BA	806	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	1548	A	C5-C6-N1	6.93	121.17	117.70
54	BA	2629	U	O4'-C1'-N1	6.93	113.75	108.20
25	BC	155	ARG	NE-CZ-NH1	6.93	123.76	120.30
54	BA	1890	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	2767	C	N3-C2-O2	-6.93	117.05	121.90
38	BP	102	ARG	NE-CZ-NH1	6.93	123.76	120.30
54	BA	2883	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	1000	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2009	A	C5-C6-N1	6.92	121.16	117.70
21	AA	1012	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	819	A	N1-C6-N6	-6.92	114.45	118.60
21	AA	790	A	C4-C5-C6	-6.92	113.54	117.00
11	AL	98	ARG	NE-CZ-NH1	6.92	123.76	120.30
21	AA	901	A	C5-C6-N1	6.92	121.16	117.70
21	AA	1427	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	878	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	1832	C	N1-C2-O2	6.92	123.05	118.90
21	AA	746	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	908	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	1155	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1307	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2225	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2418	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2420	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	599	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1689	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	1805	A	C5-C6-N1	6.92	121.16	117.70
54	BA	294	A	C4-C5-C6	-6.91	113.54	117.00
54	BA	1373	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1626	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1956	U	C5-C6-N1	-6.91	119.24	122.70
55	BB	59	A	C5-C6-N1	6.91	121.16	117.70
54	BA	685	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1586	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1944	U	O4'-C1'-N1	6.91	113.73	108.20
54	BA	1998	A	C5-C6-N1	6.91	121.16	117.70
54	BA	2499	C	N1-C2-O2	6.91	123.05	118.90
13	AN	13	ARG	NE-CZ-NH1	6.91	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2471	A	C5-C6-N1	6.91	121.15	117.70
21	AA	936	C	N3-C2-O2	-6.91	117.07	121.90
54	BA	2227	A	C4-C5-C6	-6.91	113.55	117.00
21	AA	767	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1092	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	1140	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2117	A	O4'-C1'-N9	6.90	113.72	108.20
54	BA	1997	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2635	A	C4-C5-C6	-6.90	113.55	117.00
55	BB	113	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	404	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1143	A	C5-C6-N1	6.90	121.15	117.70
21	AA	315	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	1169	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2855	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	2799	A	O4'-C1'-N9	6.90	113.72	108.20
54	BA	2813	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1078	U	C1'-O4'-C4'	-6.89	104.39	109.90
55	BB	45	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	925	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1331	G	N1-C6-O6	-6.89	115.77	119.90
21	AA	306	A	C5-C6-N1	6.89	121.15	117.70
21	AA	977	A	C4-C5-C6	-6.89	113.55	117.00
21	AA	1141	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	33	A	C4-C5-C6	-6.89	113.56	117.00
40	BR	80	ARG	NE-CZ-NH1	6.89	123.75	120.30
54	BA	1266	G	N3-C4-C5	-6.89	125.16	128.60
55	BB	19	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	2326	C	N1-C2-O2	6.89	123.03	118.90
54	BA	315	G	N1-C6-O6	-6.89	115.77	119.90
54	BA	1336	A	C4-C5-C6	-6.89	113.56	117.00
21	AA	1168	U	N3-C2-O2	-6.88	117.38	122.20
22	A1	11	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	1043	C	N1-C2-O2	6.88	123.03	118.90
54	BA	1605	C	N3-C2-O2	-6.88	117.08	121.90
12	AM	92	ARG	NE-CZ-NH1	6.88	123.74	120.30
21	AA	949	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	742	G	N1-C6-O6	-6.88	115.77	119.90
54	BA	1009	A	O4'-C1'-N9	6.88	113.70	108.20
54	BA	643	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2342	C	O4'-C1'-N1	6.88	113.70	108.20
54	BA	2432	A	O4'-C1'-N9	6.88	113.70	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2602	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2723	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	222	C	N3-C2-O2	-6.88	117.09	121.90
21	AA	448	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	337	C	N3-C2-O2	-6.88	117.09	121.90
21	AA	1126	U	N3-C2-O2	-6.88	117.39	122.20
54	BA	2335	A	C4-C5-C6	-6.88	113.56	117.00
4	AE	137	ARG	NE-CZ-NH1	6.87	123.74	120.30
21	AA	1524	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	11	C	N1-C2-O2	6.87	123.02	118.90
54	BA	378	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1189	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1357	C	O4'-C1'-N1	6.87	113.70	108.20
54	BA	1977	A	C5-C6-N1	6.87	121.14	117.70
54	BA	2255	G	N1-C6-O6	-6.87	115.78	119.90
54	BA	2300	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	1433	A	N1-C6-N6	-6.87	114.48	118.60
21	AA	1469	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1398	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	1344	C	N1-C2-O2	6.87	123.02	118.90
24	A3	11	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	764	A	O4'-C1'-N9	6.87	113.69	108.20
21	AA	175	C	O4'-C1'-N1	6.87	113.69	108.20
54	BA	623	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1328	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1889	A	C5-C6-N1	6.87	121.13	117.70
21	AA	563	A	C5-C6-N1	6.87	121.13	117.70
54	BA	2711	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	2733	A	C4-C5-C6	-6.87	113.57	117.00
21	AA	1208	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	1320	C	N1-C2-O2	6.86	123.02	118.90
28	BF	147	ARG	NE-CZ-NH1	6.86	123.73	120.30
36	BN	96	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	164	C	N3-C2-O2	-6.86	117.10	121.90
25	BC	100	ARG	NE-CZ-NH1	6.86	123.73	120.30
55	BB	78	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1345	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2146	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	866	C	O4'-C1'-N1	6.86	113.68	108.20
54	BA	84	A	C5-C6-N1	6.86	121.13	117.70
54	BA	216	A	N1-C6-N6	-6.86	114.49	118.60
54	BA	1134	A	C4-C5-C6	-6.86	113.57	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2147	A	C5-C6-N1	6.86	121.13	117.70
21	AA	946	A	N1-C6-N6	-6.85	114.49	118.60
54	BA	2227	A	N1-C6-N6	-6.85	114.49	118.60
16	AQ	10	ARG	NE-CZ-NH1	6.85	123.73	120.30
21	AA	596	A	N1-C6-N6	-6.85	114.49	118.60
28	BF	177	ARG	NE-CZ-NH2	6.85	123.73	120.30
51	B2	33	ARG	NE-CZ-NH1	6.85	123.73	120.30
54	BA	644	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	2174	C	N3-C2-O2	-6.85	117.10	121.90
2	AC	163	ARG	NE-CZ-NH1	6.85	123.72	120.30
21	AA	81	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	840	C	N3-C2-O2	-6.85	117.10	121.90
22	A1	73	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	899	A	C5-C6-N1	6.85	121.12	117.70
54	BA	345	A	C5-C6-N1	6.85	121.12	117.70
54	BA	412	A	C5-C6-N1	6.85	121.12	117.70
54	BA	2542	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	2572	A	C4-C5-C6	-6.85	113.58	117.00
10	AK	12	ARG	NE-CZ-NH1	6.85	123.72	120.30
21	AA	962	C	N3-C2-O2	-6.85	117.11	121.90
21	AA	1441	A	C4-C5-C6	-6.85	113.58	117.00
24	A3	36	A	C4-C5-C6	-6.85	113.58	117.00
24	A3	59	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	67	C	N3-C2-O2	-6.85	117.11	121.90
54	BA	710	U	O4'-C1'-N1	6.85	113.68	108.20
54	BA	1630	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	267	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1147	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1689	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1890	A	C5-C6-N1	6.84	121.12	117.70
37	BO	33	ARG	NE-CZ-NH2	6.84	123.72	120.30
54	BA	449	A	N1-C6-N6	-6.84	114.49	118.60
21	AA	676	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1281	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	1289	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1332	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2498	C	N1-C2-O2	6.84	123.00	118.90
54	BA	2875	C	N3-C2-O2	-6.84	117.11	121.90
20	AU	30	GLU	C-N-CA	6.84	138.80	121.70
21	AA	539	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	641	U	O4'-C1'-N1	6.84	113.67	108.20
54	BA	2094	A	C4-C5-C6	-6.84	113.58	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	519	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	800	A	C5-C6-N1	6.84	121.12	117.70
54	BA	580	U	O4'-C1'-N1	6.83	113.67	108.20
54	BA	2469	A	C5-C6-N1	6.83	121.12	117.70
21	AA	523	A	C5-C6-N1	6.83	121.12	117.70
21	AA	753	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1036	A	C4-C5-C6	-6.83	113.58	117.00
24	A3	29	C	N3-C2-O2	-6.83	117.12	121.90
32	BJ	116	ARG	NE-CZ-NH1	6.83	123.72	120.30
54	BA	1762	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2738	A	C4-C5-C6	-6.83	113.58	117.00
21	AA	908	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1186	G	N3-C2-N2	-6.83	115.12	119.90
54	BA	2581	G	O4'-C1'-N9	6.83	113.66	108.20
54	BA	2809	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1278	G	N3-C2-N2	-6.83	115.12	119.90
54	BA	146	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	514	A	C5-C6-N1	6.83	121.11	117.70
54	BA	861	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	1226	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	2038	G	O4'-C1'-N9	6.83	113.66	108.20
54	BA	2576	G	N3-C2-N2	-6.83	115.12	119.90
21	AA	764	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	428	A	C5-C6-N1	6.82	121.11	117.70
54	BA	817	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	1044	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	1335	C	N3-C2-O2	-6.82	117.12	121.90
54	BA	2176	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	2873	A	C5-C6-N1	6.82	121.11	117.70
4	AE	111	ARG	NE-CZ-NH1	6.82	123.71	120.30
21	AA	383	A	C4-C5-C6	-6.82	113.59	117.00
41	BS	8	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	16	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	582	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	917	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	2741	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	2282	G	N9-C4-C5	6.82	108.13	105.40
54	BA	2893	A	N1-C6-N6	-6.82	114.51	118.60
21	AA	280	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	992	U	O4'-C1'-N1	6.82	113.65	108.20
54	BA	2079	U	O4'-C1'-N1	6.82	113.65	108.20
21	AA	566	G	C5-C6-N1	6.82	114.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1071	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	1214	C	N1-C2-O2	6.82	122.99	118.90
21	AA	1344	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	2530	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1014	A	C5-C6-N1	6.81	121.11	117.70
6	AG	142	ARG	NE-CZ-NH1	6.81	123.71	120.30
21	AA	214	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	675	A	C5-C6-N1	6.81	121.11	117.70
21	AA	807	A	C5-C6-N1	6.81	121.11	117.70
21	AA	1229	A	N1-C6-N6	-6.81	114.51	118.60
22	A1	76	A	C5-C6-N1	6.81	121.11	117.70
54	BA	982	C	C6-N1-C2	-6.81	117.58	120.30
54	BA	2829	A	C5-C6-N1	6.81	121.10	117.70
8	AI	108	ARG	NE-CZ-NH1	6.81	123.70	120.30
23	A2	80	C	N3-C4-C5	6.81	124.62	121.90
54	BA	782	A	C5-C6-N1	6.81	121.10	117.70
54	BA	1323	C	N3-C2-O2	-6.81	117.14	121.90
54	BA	1453	A	N1-C6-N6	-6.81	114.52	118.60
54	BA	1556	C	N1-C2-O2	6.81	122.98	118.90
54	BA	2169	A	C5-C6-N1	6.81	121.10	117.70
54	BA	1558	C	N1-C2-O2	6.80	122.98	118.90
54	BA	1664	A	N1-C6-N6	-6.80	114.52	118.60
24	A3	17	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	160	A	C5-C6-N1	6.80	121.10	117.70
54	BA	217	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2059	A	C4-C5-C6	-6.80	113.60	117.00
55	BB	108	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	85	U	N3-C2-O2	-6.80	117.44	122.20
54	BA	116	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	182	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2324	U	O4'-C1'-N1	6.80	113.64	108.20
1	AB	73	ARG	NE-CZ-NH1	6.80	123.70	120.30
54	BA	1706	C	O4'-C1'-N1	6.80	113.64	108.20
21	AA	1394	A	C5-C6-N1	6.80	121.10	117.70
51	B2	19	ARG	NE-CZ-NH1	6.80	123.70	120.30
54	BA	330	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1725	U	O4'-C1'-N1	6.80	113.64	108.20
54	BA	866	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	1558	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	1237	A	C5-C6-N1	6.79	121.10	117.70
54	BA	2009	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	2416	C	N3-C2-O2	-6.79	117.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	964	A	C5-C6-N1	6.79	121.10	117.70
18	AS	80	ARG	NE-CZ-NH1	6.79	123.69	120.30
54	BA	1583	A	N1-C6-N6	-6.79	114.53	118.60
54	BA	1578	U	O4'-C1'-N1	6.79	113.63	108.20
21	AA	396	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	533	A	C5-C6-N1	6.79	121.09	117.70
54	BA	398	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	1039	A	N1-C6-N6	-6.79	114.53	118.60
54	BA	1932	A	C5-C6-N1	6.79	121.09	117.70
21	AA	1377	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	52	A	C5-C6-N1	6.78	121.09	117.70
54	BA	634	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	1685	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	1340	A	N1-C6-N6	-6.78	114.53	118.60
52	B3	44	ARG	NE-CZ-NH1	6.78	123.69	120.30
54	BA	218	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2082	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	1397	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	213	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	343	C	N1-C2-O2	6.78	122.97	118.90
54	BA	1086	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2266	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2789	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	1329	A	C5-C6-N1	6.78	121.09	117.70
54	BA	554	U	O4'-C1'-N1	6.78	113.62	108.20
54	BA	556	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1183	U	O4'-C1'-N1	6.78	113.62	108.20
54	BA	1672	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2856	A	C4-C5-C6	-6.78	113.61	117.00
55	BB	99	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1014	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	2070	A	C5-C6-N1	6.78	121.09	117.70
21	AA	250	A	C5-C6-N1	6.77	121.09	117.70
54	BA	67	U	O4'-C1'-N1	6.77	113.62	108.20
54	BA	2814	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	120	A	C5-C6-N1	6.77	121.08	117.70
21	AA	592	G	O4'-C1'-N9	6.77	113.62	108.20
21	AA	1036	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2433	A	N1-C6-N6	-6.77	114.54	118.60
54	BA	626	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	2660	A	N1-C6-N6	-6.77	114.54	118.60
21	AA	1363	A	C4-C5-C6	-6.77	113.62	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	334	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	421	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	892	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	1285	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1485	U	O4'-C1'-N1	6.77	113.61	108.20
54	BA	2566	A	C5-C6-N1	6.77	121.08	117.70
3	AD	103	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	147	G	C5-C6-N1	6.76	114.88	111.50
21	AA	451	A	P-O3'-C3'	6.76	127.82	119.70
54	BA	1532	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1595	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2547	A	C5-C6-N1	6.76	121.08	117.70
21	AA	392	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2632	A	N1-C6-N6	-6.76	114.54	118.60
40	BR	21	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	1043	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	28	A	N1-C6-N6	-6.76	114.55	118.60
34	BL	59	ARG	NE-CZ-NH1	6.76	123.68	120.30
56	B5	7	ARG	NE-CZ-NH1	6.76	123.68	120.30
6	AG	78	ARG	NE-CZ-NH1	6.76	123.68	120.30
21	AA	435	A	C5-C6-N1	6.76	121.08	117.70
54	BA	575	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1027	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1367	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1210	C	N3-C2-O2	-6.75	117.17	121.90
21	AA	1363	A	O4'-C1'-N9	6.75	113.60	108.20
54	BA	95	A	C5-C6-N1	6.75	121.08	117.70
54	BA	130	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	2827	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	1586	A	N1-C6-N6	-6.75	114.55	118.60
54	BA	221	A	C5-C6-N1	6.75	121.07	117.70
54	BA	581	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	1480	C	O4'-C1'-N1	6.75	113.60	108.20
54	BA	300	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	595	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	899	A	N1-C6-N6	-6.75	114.55	118.60
9	AJ	16	ARG	NE-CZ-NH1	6.75	123.67	120.30
24	A3	60	A	C5-C6-N1	6.75	121.07	117.70
54	BA	885	C	N3-C2-O2	-6.75	117.18	121.90
17	AR	52	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	1870	C	N1-C2-O2	6.74	122.94	118.90
21	AA	489	C	N3-C2-O2	-6.74	117.18	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2331	G	C5-C6-N1	6.74	114.87	111.50
55	BB	113	C	N1-C2-O2	6.74	122.94	118.90
20	AU	16	ARG	NE-CZ-NH1	6.74	123.67	120.30
21	AA	8	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1180	A	C5-C6-N1	6.74	121.07	117.70
54	BA	492	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1551	A	C5-C6-N1	6.74	121.07	117.70
54	BA	208	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	2014	A	C5-C6-N1	6.73	121.07	117.70
54	BA	2353	G	N3-C2-N2	-6.73	115.19	119.90
54	BA	2422	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1070	A	C5-C6-N1	6.73	121.07	117.70
55	BB	71	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2396	G	C8-N9-C4	-6.73	103.71	106.40
54	BA	2649	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	670	A	P-O3'-C3'	6.73	127.77	119.70
54	BA	1635	A	C5-C6-N1	6.73	121.06	117.70
54	BA	2268	A	N1-C6-N6	-6.73	114.56	118.60
55	BB	8	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	1179	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	680	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1118	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1638	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2298	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	2478	A	C5-C6-N1	6.73	121.06	117.70
54	BA	2883	A	C4-C5-C6	-6.73	113.64	117.00
30	BH	97	ARG	NE-CZ-NH1	6.73	123.66	120.30
21	AA	784	A	C4-C5-C6	-6.72	113.64	117.00
40	BR	78	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	1525	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2173	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2712	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	545	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	1520	U	O4'-C1'-N1	6.72	113.58	108.20
21	AA	401	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	201	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	1362	C	O4'-C1'-N1	6.72	113.58	108.20
21	AA	635	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	574	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2165	C	N3-C2-O2	-6.72	117.20	121.90
38	BP	100	ARG	NE-CZ-NH1	6.71	123.66	120.30
54	BA	919	U	O4'-C1'-N1	6.71	113.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1194	A	C5-C6-N1	6.71	121.06	117.70
54	BA	2339	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	621	A	N1-C6-N6	-6.71	114.57	118.60
54	BA	793	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1330	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1793	C	N1-C2-O2	6.71	122.93	118.90
54	BA	2776	A	C4-C5-C6	-6.71	113.64	117.00
56	B5	53	ARG	NE-CZ-NH1	6.71	123.66	120.30
54	BA	896	A	O4'-C1'-N9	6.71	113.57	108.20
54	BA	2430	A	C5-C6-N1	6.71	121.06	117.70
21	AA	129	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	1201	A	C5-C6-N1	6.71	121.06	117.70
21	AA	1483	A	N1-C6-N6	-6.71	114.58	118.60
54	BA	6	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1370	C	N3-C4-C5	6.71	124.58	121.90
54	BA	1387	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1962	C	N3-C2-O2	-6.71	117.20	121.90
34	BL	48	ARG	NE-CZ-NH2	-6.71	116.95	120.30
54	BA	1366	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1808	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	205	G	O4'-C1'-N9	6.70	113.56	108.20
54	BA	1189	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2388	A	C5-C6-N1	6.70	121.05	117.70
21	AA	923	A	C5-C6-N1	6.70	121.05	117.70
21	AA	325	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1113	U	O4'-C1'-N1	6.70	113.56	108.20
21	AA	533	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	670	A	C5-C6-N1	6.70	121.05	117.70
21	AA	1254	A	C5-C6-N1	6.70	121.05	117.70
54	BA	323	C	N1-C2-O2	6.70	122.92	118.90
13	AN	9	ARG	NE-CZ-NH1	6.70	123.65	120.30
21	AA	985	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	118	A	N1-C6-N6	-6.70	114.58	118.60
54	BA	125	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1772	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2281	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2632	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2134	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	2204	G	C5-C6-N1	6.69	114.85	111.50
54	BA	2518	A	C5-C6-N1	6.69	121.05	117.70
21	AA	342	C	N1-C2-O2	6.69	122.92	118.90
21	AA	732	C	N3-C2-O2	-6.69	117.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	135	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	348	G	O4'-C1'-N9	6.69	113.55	108.20
21	AA	1479	C	N1-C2-O2	6.69	122.91	118.90
54	BA	125	A	P-O3'-C3'	6.69	127.73	119.70
54	BA	196	A	O4'-C1'-N9	6.69	113.55	108.20
54	BA	503	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	506	G	O4'-C1'-N9	6.69	113.55	108.20
54	BA	1893	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2352	A	C5-C6-N1	6.69	121.05	117.70
54	BA	2799	A	C5-C6-N1	6.69	121.05	117.70
54	BA	96	C	O4'-C1'-N1	6.69	113.55	108.20
21	AA	1277	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	1413	A	N1-C6-N6	-6.69	114.59	118.60
54	BA	2421	G	N3-C2-N2	-6.69	115.22	119.90
21	AA	1019	A	C5-C6-N1	6.69	121.04	117.70
54	BA	461	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	1652	A	C5-C6-N1	6.69	121.04	117.70
21	AA	1368	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	654	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	1115	G	C5-C6-N1	6.68	114.84	111.50
54	BA	2753	A	C5-C6-N1	6.68	121.04	117.70
21	AA	913	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1093	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	2619	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	694	U	N3-C2-O2	-6.68	117.52	122.20
54	BA	1664	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1306	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	2088	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	2332	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	2506	U	O4'-C1'-N1	6.68	113.54	108.20
55	BB	66	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1029	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1359	C	N3-C2-O2	-6.68	117.23	121.90
39	BQ	91	ARG	NE-CZ-NH2	-6.68	116.96	120.30
54	BA	611	C	N3-C2-O2	-6.68	117.23	121.90
54	BA	909	A	C4-C5-C6	-6.68	113.66	117.00
19	AT	23	ARG	NE-CZ-NH1	6.67	123.64	120.30
21	AA	1251	A	C4-C5-C6	-6.67	113.66	117.00
22	A1	73	A	C5-C6-N1	6.67	121.04	117.70
24	A3	24	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	399	U	O4'-C1'-N1	6.67	113.54	108.20
54	BA	668	A	C5-C6-N1	6.67	121.04	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2215	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2266	A	C5-C6-N1	6.67	121.04	117.70
54	BA	2660	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1989	G	C8-N9-C4	-6.67	103.73	106.40
54	BA	72	U	O4'-C1'-N1	6.67	113.54	108.20
54	BA	421	C	P-O3'-C3'	6.67	127.70	119.70
54	BA	821	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	1194	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	1335	C	O4'-C1'-N1	6.67	113.54	108.20
54	BA	1493	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	190	A	C5-C6-N1	6.67	121.03	117.70
21	AA	409	U	C5-C6-N1	-6.67	119.36	122.70
21	AA	1447	A	N1-C6-N6	-6.67	114.60	118.60
37	BO	13	ARG	NE-CZ-NH1	6.67	123.64	120.30
54	BA	1268	A	C5-C6-N1	6.67	121.03	117.70
21	AA	1234	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1268	A	N1-C6-N6	-6.67	114.60	118.60
54	BA	1413	A	C5-C6-N1	6.67	121.03	117.70
54	BA	1748	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1615	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1847	A	O4'-C1'-N9	6.66	113.53	108.20
21	AA	1117	A	C5-C6-N1	6.66	121.03	117.70
54	BA	635	C	N3-C2-O2	-6.66	117.24	121.90
10	AK	126	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	400	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1340	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1408	G	N1-C6-O6	-6.66	115.90	119.90
54	BA	2199	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	583	A	C5-C6-N1	6.66	121.03	117.70
54	BA	899	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2803	G	N1-C6-O6	-6.66	115.91	119.90
21	AA	1070	U	O4'-C1'-N1	6.66	113.53	108.20
54	BA	781	A	C5-C6-N1	6.66	121.03	117.70
54	BA	898	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	498	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	447	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	480	A	C5-C6-N1	6.65	121.03	117.70
21	AA	298	A	C5-C6-N1	6.65	121.03	117.70
54	BA	330	A	O4'-C1'-N9	6.65	113.52	108.20
54	BA	572	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	852	G	N1-C6-O6	-6.65	115.91	119.90
54	BA	802	A	C5-C6-N1	6.65	121.03	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1320	C	O4'-C1'-N1	6.65	113.52	108.20
54	BA	1246	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	2369	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	2778	A	C5-C6-N1	6.65	121.02	117.70
16	AQ	64	ARG	NE-CZ-NH1	6.65	123.62	120.30
21	AA	389	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	477	A	C5-C6-N1	6.65	121.02	117.70
32	BJ	69	ARG	NE-CZ-NH1	6.65	123.62	120.30
21	AA	345	C	O4'-C1'-N1	6.64	113.52	108.20
21	AA	553	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2560	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2577	A	C5-C6-N1	6.64	121.02	117.70
21	AA	395	C	N3-C2-O2	-6.64	117.25	121.90
39	BQ	47	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	127	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2007	U	O4'-C1'-N1	6.64	113.51	108.20
54	BA	2882	A	C5-C6-N1	6.64	121.02	117.70
54	BA	484	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1070	A	C4-C5-C6	-6.64	113.68	117.00
55	BB	24	G	N9-C4-C5	6.64	108.06	105.40
55	BB	99	A	N1-C6-N6	-6.64	114.62	118.60
20	AU	20	ARG	NE-CZ-NH2	-6.63	116.98	120.30
54	BA	1366	A	C4-C5-C6	-6.63	113.68	117.00
21	AA	1022	A	C5-C6-N1	6.63	121.02	117.70
43	BU	81	ARG	NE-CZ-NH1	6.63	123.61	120.30
54	BA	888	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1524	G	C5-C6-N1	6.63	114.82	111.50
55	BB	26	C	N1-C2-O2	6.63	122.88	118.90
54	BA	2827	C	O4'-C1'-N1	6.63	113.50	108.20
21	AA	747	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	1792	G	N1-C6-O6	-6.63	115.92	119.90
54	BA	2191	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	1366	A	N1-C6-N6	-6.62	114.62	118.60
21	AA	766	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	980	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	982	C	C2-N1-C1'	6.62	126.08	118.80
55	BB	94	A	C5-C6-N1	6.62	121.01	117.70
21	AA	196	A	C5-C6-N1	6.62	121.01	117.70
21	AA	754	C	N1-C2-O2	6.62	122.87	118.90
43	BU	6	ARG	NE-CZ-NH1	6.62	123.61	120.30
54	BA	1454	C	N1-C2-O2	6.62	122.87	118.90
5	AF	24	ARG	NE-CZ-NH1	6.62	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	946	A	C5-C6-N1	6.62	121.01	117.70
21	AA	1288	A	C5-C6-N1	6.62	121.01	117.70
21	AA	1518	A	C5-C6-N1	6.62	121.01	117.70
22	A1	41	A	C5-C6-N1	6.62	121.01	117.70
54	BA	538	A	N1-C6-N6	-6.62	114.63	118.60
54	BA	1967	C	N1-C2-O2	6.62	122.87	118.90
54	BA	2393	U	O4'-C1'-N1	6.62	113.49	108.20
54	BA	2828	G	C5-C6-N1	6.62	114.81	111.50
21	AA	1281	C	N1-C2-O2	6.61	122.87	118.90
54	BA	849	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	2879	A	C5-C6-N1	6.61	121.01	117.70
21	AA	680	C	N3-C2-O2	-6.61	117.27	121.90
22	A1	61	C	N3-C2-O2	-6.61	117.27	121.90
29	BG	152	ARG	NE-CZ-NH1	6.61	123.61	120.30
54	BA	2258	C	N3-C2-O2	-6.61	117.27	121.90
11	AL	11	ARG	NE-CZ-NH1	6.61	123.61	120.30
21	AA	758	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	1014	A	C5-C6-N1	6.61	121.00	117.70
21	AA	1170	A	C5-C6-N1	6.61	121.01	117.70
33	BK	18	ARG	NE-CZ-NH1	6.61	123.61	120.30
54	BA	6	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	255	A	C5-C6-N1	6.61	121.00	117.70
54	BA	620	G	N9-C4-C5	6.61	108.04	105.40
22	A1	56	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	241	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	990	A	C4-C5-C6	-6.61	113.69	117.00
25	BC	62	ARG	NE-CZ-NH1	6.61	123.60	120.30
48	BZ	29	ARG	NE-CZ-NH1	6.61	123.60	120.30
54	BA	1980	G	N1-C6-O6	-6.61	115.94	119.90
54	BA	2183	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	1408	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	902	C	O4'-C1'-N1	6.60	113.48	108.20
54	BA	994	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	1054	C	N3-C4-C5	6.60	124.54	121.90
54	BA	444	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	632	A	C5-C6-N1	6.60	121.00	117.70
21	AA	279	A	N1-C6-N6	-6.60	114.64	118.60
54	BA	1013	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	364	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	96	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	101	A	C5-C6-N1	6.60	121.00	117.70
21	AA	266	G	C1'-O4'-C4'	-6.60	104.62	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	493	A	C5-C6-N1	6.59	121.00	117.70
21	AA	841	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	1484	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1848	A	C5-C6-N1	6.59	121.00	117.70
54	BA	1991	U	O4'-C1'-N1	6.59	113.47	108.20
21	AA	1533	C	P-O3'-C3'	6.59	127.61	119.70
36	BN	46	ARG	NE-CZ-NH1	6.59	123.59	120.30
54	BA	2703	C	N3-C2-O2	-6.59	117.29	121.90
24	A3	76	C	C6-N1-C2	-6.59	117.67	120.30
54	BA	2668	G	P-O3'-C3'	6.59	127.60	119.70
21	AA	536	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	689	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	531	C	C1'-O4'-C4'	-6.58	104.63	109.90
54	BA	2114	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2822	G	O4'-C1'-N9	6.58	113.47	108.20
54	BA	1538	G	N1-C6-O6	-6.58	115.95	119.90
54	BA	2059	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	2612	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	1885	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1158	C	N1-C2-O2	6.58	122.85	118.90
21	AA	1336	C	C1'-O4'-C4'	-6.58	104.64	109.90
24	A3	75	C	N3-C4-N4	-6.58	113.39	118.00
54	BA	784	G	N3-C4-C5	-6.58	125.31	128.60
54	BA	1616	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2321	U	O4'-C1'-N1	6.58	113.46	108.20
21	AA	373	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1040	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1920	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1970	A	C5-C6-N1	6.58	120.99	117.70
21	AA	303	A	C5-C6-N1	6.57	120.99	117.70
22	A1	58	A	C5-C6-N1	6.57	120.99	117.70
21	AA	432	A	C5-C6-N1	6.57	120.99	117.70
54	BA	282	A	N1-C6-N6	-6.57	114.66	118.60
54	BA	964	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1147	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2618	G	N3-C4-C5	-6.57	125.31	128.60
11	AL	8	ARG	NE-CZ-NH1	6.57	123.58	120.30
21	AA	1051	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	1446	A	C5-C6-N1	6.57	120.98	117.70
54	BA	282	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	2741	A	C5-C6-N1	6.57	120.98	117.70
54	BA	292	U	C5-C6-N1	-6.57	119.42	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1005	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2704	C	N3-C2-O2	-6.57	117.30	121.90
24	A3	42	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1060	U	O4'-C1'-N1	6.57	113.45	108.20
54	BA	1924	C	N3-C2-O2	-6.57	117.31	121.90
54	BA	2117	A	N1-C6-N6	-6.57	114.66	118.60
54	BA	371	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2359	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2717	C	N3-C2-O2	-6.56	117.31	121.90
36	BN	71	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	2632	A	C5-C6-N1	6.56	120.98	117.70
21	AA	250	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	466	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	1104	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1175	A	N1-C6-N6	-6.56	114.66	118.60
54	BA	2082	A	C5-C6-N1	6.56	120.98	117.70
54	BA	372	G	C1'-O4'-C4'	-6.56	104.66	109.90
54	BA	549	G	N3-C4-C5	-6.56	125.32	128.60
54	BA	1274	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	1259	C	N1-C2-O2	6.55	122.83	118.90
54	BA	2874	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1404	C	O4'-C1'-N1	6.55	113.44	108.20
54	BA	2880	C	N3-C2-O2	-6.55	117.31	121.90
25	BC	86	ARG	NE-CZ-NH1	6.55	123.57	120.30
54	BA	1221	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1451	C	P-O3'-C3'	6.55	127.56	119.70
54	BA	1655	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	2207	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	2800	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	804	A	C5-C6-N1	6.55	120.97	117.70
54	BA	815	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	893	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2212	A	C4-C5-C6	-6.55	113.73	117.00
31	BI	126	ARG	NE-CZ-NH1	6.55	123.57	120.30
54	BA	1577	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2013	A	C5-C6-N1	6.55	120.97	117.70
54	BA	2835	A	C4-C5-C6	-6.54	113.73	117.00
24	A3	58	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	430	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	669	G	C5-C6-N1	6.54	114.77	111.50
54	BA	2287	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2362	C	O4'-C1'-N1	6.54	113.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	71	C	O4'-C1'-N1	6.54	113.44	108.20
21	AA	496	A	N1-C6-N6	-6.54	114.67	118.60
21	AA	530	G	N3-C4-C5	-6.54	125.33	128.60
54	BA	103	A	C5-C6-N1	6.54	120.97	117.70
54	BA	2731	G	N1-C6-O6	-6.54	115.98	119.90
21	AA	26	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1475	G	N1-C6-O6	-6.54	115.98	119.90
54	BA	2576	G	N3-C4-C5	-6.54	125.33	128.60
21	AA	607	A	C5-C6-N1	6.54	120.97	117.70
21	AA	864	A	N1-C6-N6	-6.54	114.68	118.60
54	BA	1744	A	N1-C6-N6	-6.54	114.68	118.60
21	AA	171	A	C5-C6-N1	6.53	120.97	117.70
21	AA	1492	A	C5-C6-N1	6.53	120.97	117.70
54	BA	1420	A	C4-C5-C6	-6.53	113.73	117.00
21	AA	1367	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1678	A	C5-C6-N1	6.53	120.97	117.70
1	AB	212	TYR	CB-CG-CD1	6.53	124.92	121.00
21	AA	642	A	C5-C6-N1	6.53	120.97	117.70
21	AA	1288	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	2183	A	C5-C6-N1	6.53	120.97	117.70
21	AA	490	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1566	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	2469	A	C4-C5-C6	-6.53	113.73	117.00
24	A3	38	A	C5-C6-N1	6.53	120.96	117.70
54	BA	972	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1347	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1609	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1864	U	O4'-C1'-N1	6.53	113.42	108.20
54	BA	677	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	814	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	965	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	948	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	1598	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	507	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1726	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	2333	A	C5-C6-N1	6.52	120.96	117.70
21	AA	65	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	1044	A	C5-C6-N1	6.52	120.96	117.70
21	AA	814	A	C5-C6-N1	6.52	120.96	117.70
21	AA	895	G	N1-C6-O6	-6.52	115.99	119.90
34	BL	18	ARG	NE-CZ-NH1	6.52	123.56	120.30
54	BA	348	A	C4-C5-C6	-6.52	113.74	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	353	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	1270	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	1692	U	N3-C2-O2	-6.52	117.64	122.20
54	BA	1978	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2790	U	N3-C2-O2	-6.52	117.64	122.20
55	BB	34	A	C5-C6-N6	6.52	128.91	123.70
54	BA	1722	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	694	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1755	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1272	A	C5-C6-N1	6.51	120.96	117.70
55	BB	23	G	N1-C6-O6	-6.51	115.99	119.90
21	AA	993	G	N3-C4-C5	-6.51	125.34	128.60
54	BA	743	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1153	C	O4'-C1'-N1	6.51	113.41	108.20
54	BA	1505	A	C5-C6-N1	6.51	120.96	117.70
54	BA	2042	A	N1-C6-N6	-6.51	114.69	118.60
21	AA	797	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	300	A	C5-C6-N1	6.51	120.95	117.70
54	BA	706	A	O4'-C1'-N9	6.51	113.41	108.20
54	BA	1637	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1866	A	C4-C5-C6	-6.51	113.75	117.00
21	AA	108	G	O4'-C1'-N9	6.51	113.41	108.20
54	BA	433	C	N1-C2-O2	6.51	122.81	118.90
21	AA	66	A	N1-C6-N6	-6.51	114.70	118.60
54	BA	1499	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	25	C	N3-C2-O2	-6.50	117.35	121.90
46	BX	2	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	191	A	C5-C6-N1	6.50	120.95	117.70
21	AA	320	A	C3'-C2'-C1'	6.50	106.70	101.50
54	BA	2282	G	O4'-C1'-N9	6.50	113.40	108.20
54	BA	2541	A	C4-C5-C6	-6.50	113.75	117.00
55	BB	15	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	55	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	353	A	N1-C6-N6	-6.50	114.70	118.60
37	BO	111	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	1555	G	C5-C6-N1	6.50	114.75	111.50
21	AA	195	A	C1'-O4'-C4'	-6.50	104.70	109.90
26	BD	59	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	251	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	905	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1451	C	C6-N1-C2	-6.50	117.70	120.30
54	BA	2539	C	N3-C2-O2	-6.50	117.35	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	223	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	550	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1446	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2179	C	N3-C2-O2	-6.49	117.35	121.90
21	AA	65	A	C5-C6-N1	6.49	120.94	117.70
21	AA	195	A	N1-C6-N6	-6.49	114.71	118.60
21	AA	1410	A	C5-C6-N1	6.49	120.95	117.70
54	BA	678	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1853	A	C5-C6-N1	6.49	120.94	117.70
54	BA	2420	C	N1-C2-O2	6.49	122.79	118.90
21	AA	599	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	1531	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	207	A	C5-C6-N1	6.49	120.94	117.70
54	BA	366	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	436	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	722	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	2196	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1342	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	2748	A	C5-C6-N1	6.49	120.94	117.70
21	AA	908	A	N1-C6-N6	-6.48	114.71	118.60
54	BA	402	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1030	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1553	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2142	A	C5-C6-N1	6.48	120.94	117.70
54	BA	590	A	C5-C6-N1	6.48	120.94	117.70
54	BA	927	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2461	A	N1-C6-N6	-6.48	114.71	118.60
21	AA	563	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1609	A	C1'-O4'-C4'	-6.48	104.72	109.90
21	AA	412	A	C5-C6-N1	6.48	120.94	117.70
21	AA	779	C	N1-C2-O2	6.48	122.79	118.90
23	A2	79	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2374	C	N1-C2-O2	6.48	122.79	118.90
54	BA	2547	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	565	U	O4'-C1'-N1	6.48	113.38	108.20
54	BA	1247	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	948	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1157	A	C5-C6-N1	6.47	120.94	117.70
54	BA	829	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	1321	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1999	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	415	A	O4'-C1'-N9	6.47	113.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	621	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1705	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	1071	C	O4'-C1'-N1	6.47	113.38	108.20
54	BA	2103	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	630	G	N1-C6-O6	-6.47	116.02	119.90
54	BA	825	A	C5-C6-N1	6.47	120.94	117.70
54	BA	1367	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	2000	C	N3-C2-O2	-6.47	117.37	121.90
22	A1	6	A	C5-C6-N1	6.47	120.93	117.70
54	BA	2373	G	O4'-C1'-N9	6.47	113.37	108.20
21	AA	1257	A	C5-C6-N1	6.47	120.93	117.70
22	A1	60	C	N1-C2-O2	6.47	122.78	118.90
41	BS	92	ARG	NE-CZ-NH1	6.47	123.53	120.30
54	BA	412	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1502	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	2462	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2872	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	1080	A	N1-C6-N6	-6.46	114.72	118.60
28	BF	70	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	1230	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1950	G	N9-C4-C5	6.46	107.99	105.40
15	AP	25	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	231	A	C5-C6-N1	6.46	120.93	117.70
54	BA	592	A	C5-C6-N1	6.46	120.93	117.70
54	BA	621	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1894	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	656	G	N1-C6-O6	-6.46	116.02	119.90
21	AA	1480	A	C5-C6-N1	6.46	120.93	117.70
54	BA	753	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1800	C	N3-C2-O2	-6.46	117.38	121.90
15	AP	56	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	251	G	P-O3'-C3'	6.46	127.45	119.70
21	AA	253	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	906	A	C4-C5-C6	-6.46	113.77	117.00
22	A1	21	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1597	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1779	U	C5-C6-N1	-6.46	119.47	122.70
54	BA	1895	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2006	C	N1-C2-O2	6.46	122.78	118.90
21	AA	1246	A	C5-C6-N1	6.46	120.93	117.70
24	A3	7	G	O4'-C1'-N9	6.46	113.36	108.20
54	BA	2287	A	C2-N3-C4	6.46	113.83	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2601	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	716	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	176	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	825	A	C5-C6-N1	6.45	120.93	117.70
54	BA	2652	C	N3-C2-O2	-6.45	117.38	121.90
6	AG	101	ARG	NE-CZ-NH1	6.45	123.53	120.30
54	BA	184	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	684	G	N3-C2-N2	-6.45	115.38	119.90
54	BA	915	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1150	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1322	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	2295	C	O4'-C1'-N1	6.45	113.36	108.20
54	BA	2412	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	979	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1218	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	1480	A	N1-C6-N6	-6.45	114.73	118.60
24	A3	35	C	N3-C2-O2	-6.45	117.39	121.90
29	BG	2	ARG	NE-CZ-NH1	6.45	123.52	120.30
54	BA	671	C	N3-C4-C5	6.45	124.48	121.90
54	BA	829	A	C5-C6-N1	6.45	120.92	117.70
54	BA	945	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1156	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1544	A	C5-C6-N1	6.44	120.92	117.70
21	AA	461	A	N1-C6-N6	-6.44	114.73	118.60
21	AA	705	G	N1-C6-O6	-6.44	116.03	119.90
54	BA	2191	A	O4'-C1'-N9	6.44	113.35	108.20
12	AM	86	ARG	NE-CZ-NH1	6.44	123.52	120.30
3	AD	80	ARG	NE-CZ-NH1	6.44	123.52	120.30
21	AA	1287	A	C4-C5-C6	-6.44	113.78	117.00
24	A3	16	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	342	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	1461	G	N1-C6-O6	-6.44	116.04	119.90
54	BA	233	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1340	U	P-O3'-C3'	6.44	127.42	119.70
54	BA	2274	A	C5-C6-N1	6.44	120.92	117.70
21	AA	635	A	C5-C6-N1	6.44	120.92	117.70
54	BA	996	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2517	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	391	G	O4'-C1'-N9	6.43	113.35	108.20
54	BA	401	A	C5-C6-N1	6.43	120.92	117.70
54	BA	631	A	C5-C6-N1	6.43	120.92	117.70
21	AA	90	C	N3-C2-O2	-6.43	117.40	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	724	U	O4'-C1'-N1	6.43	113.35	108.20
54	BA	1428	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2534	A	C5-C6-N1	6.43	120.92	117.70
54	BA	558	U	O4'-C1'-N1	6.43	113.34	108.20
54	BA	1311	G	O4'-C1'-N9	6.43	113.34	108.20
21	AA	1219	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	661	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	81	A	N1-C6-N6	-6.43	114.74	118.60
22	A1	57	G	C1'-O4'-C4'	-6.43	104.76	109.90
54	BA	574	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	271	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	1446	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	2442	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2497	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	2860	A	C5-C6-N1	6.43	120.91	117.70
21	AA	403	C	N3-C2-O2	-6.42	117.40	121.90
54	BA	943	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1020	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2468	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2614	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	1151	A	C4-C5-C6	-6.42	113.79	117.00
22	A1	36	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	457	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2013	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	264	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1590	A	C5-C6-N1	6.42	120.91	117.70
21	AA	1028	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1151	A	P-O3'-C3'	6.42	127.40	119.70
21	AA	1465	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1384	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2636	C	N3-C2-O2	-6.42	117.41	121.90
55	BB	19	C	N1-C2-O2	6.42	122.75	118.90
21	AA	78	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	193	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1430	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	845	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2200	C	O4'-C1'-N1	6.42	113.33	108.20
46	BX	36	ARG	NE-CZ-NH1	6.42	123.51	120.30
54	BA	384	A	C5-C6-N1	6.42	120.91	117.70
21	AA	183	C	N3-C4-N4	-6.41	113.51	118.00
21	AA	1298	U	N3-C2-O2	-6.41	117.71	122.20
24	A3	66	C	N3-C2-O2	-6.41	117.41	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	195	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	1639	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	2270	A	C5-C6-N1	6.41	120.91	117.70
21	AA	194	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	374	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2606	C	N1-C2-O2	6.41	122.75	118.90
54	BA	557	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	220	G	N3-C2-N2	-6.41	115.42	119.90
21	AA	1314	C	N3-C2-O2	-6.41	117.42	121.90
23	A2	82	A	N1-C6-N6	-6.41	114.76	118.60
54	BA	1349	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	998	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2512	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	94	A	C5-C6-N1	6.40	120.90	117.70
54	BA	95	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	355	U	O4'-C1'-N1	6.40	113.32	108.20
21	AA	1147	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2145	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2205	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	696	A	C4-C5-C6	-6.40	113.80	117.00
25	BC	176	ARG	NE-CZ-NH1	6.40	123.50	120.30
54	BA	6	A	N1-C6-N6	-6.40	114.76	118.60
54	BA	510	C	N1-C2-O2	6.40	122.74	118.90
54	BA	637	A	C5-C6-N1	6.40	120.90	117.70
54	BA	1494	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2646	C	N1-C2-O2	6.40	122.74	118.90
54	BA	238	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	788	A	N1-C6-N6	-6.40	114.76	118.60
21	AA	618	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	198	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	20	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	252	G	N1-C6-O6	-6.39	116.06	119.90
54	BA	1317	G	N1-C6-O6	-6.39	116.06	119.90
54	BA	1536	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1646	C	N1-C2-O2	6.39	122.73	118.90
21	AA	807	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	1735	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	1767	G	O4'-C1'-N9	6.39	113.31	108.20
21	AA	44	A	C5-C6-N1	6.39	120.89	117.70
54	BA	513	A	C5-C6-N1	6.39	120.89	117.70
54	BA	1204	A	C2-N3-C4	6.39	113.80	110.60
54	BA	2173	A	N1-C6-N6	-6.39	114.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2498	C	O4'-C1'-N1	6.39	113.31	108.20
54	BA	275	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	727	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2061	G	N3-C2-N2	-6.39	115.43	119.90
21	AA	34	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	124	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	1453	G	O4'-C1'-N9	6.38	113.31	108.20
54	BA	2037	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2590	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2793	C	O4'-C1'-N1	6.38	113.31	108.20
54	BA	1503	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2824	C	N3-C4-N4	-6.38	113.53	118.00
21	AA	413	G	O4'-C1'-N9	6.38	113.30	108.20
21	AA	669	G	N1-C6-O6	-6.38	116.07	119.90
21	AA	974	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2321	U	N3-C2-O2	-6.38	117.74	122.20
54	BA	2771	C	N1-C2-O2	6.38	122.73	118.90
21	AA	912	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	616	A	C5-C6-N1	6.38	120.89	117.70
54	BA	835	C	O4'-C1'-N1	6.38	113.30	108.20
54	BA	946	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	1475	G	C5-C6-N1	6.38	114.69	111.50
54	BA	1900	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2392	A	C5-C6-N1	6.38	120.89	117.70
9	AJ	16	ARG	NE-CZ-NH2	-6.38	117.11	120.30
54	BA	1697	G	C8-N9-C4	-6.38	103.85	106.40
54	BA	2273	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	490	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1048	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	1749	A	N1-C6-N6	-6.37	114.78	118.60
54	BA	2747	G	N3-C4-C5	-6.37	125.41	128.60
53	B4	24	ARG	NE-CZ-NH2	-6.37	117.11	120.30
54	BA	610	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1253	A	C5-C6-N1	6.37	120.89	117.70
54	BA	1668	A	C5-C6-N1	6.37	120.89	117.70
4	AE	53	ARG	NE-CZ-NH1	6.37	123.48	120.30
22	A1	27	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1385	G	N1-C6-O6	-6.37	116.08	119.90
54	BA	14	A	C5-C6-N1	6.37	120.88	117.70
54	BA	643	A	N1-C6-N6	-6.37	114.78	118.60
54	BA	1644	C	O4'-C1'-N1	6.37	113.30	108.20
54	BA	1786	A	C5-C6-N1	6.37	120.88	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2846	G	N3-C2-N2	-6.37	115.44	119.90
21	AA	1080	A	C5-C6-N1	6.37	120.88	117.70
21	AA	1397	C	N1-C2-O2	6.37	122.72	118.90
21	AA	1513	A	C4-C5-C6	-6.36	113.82	117.00
22	A1	72	C	N1-C2-O2	6.36	122.72	118.90
54	BA	185	G	N7-C8-N9	6.36	116.28	113.10
54	BA	2226	C	O4'-C1'-N1	6.36	113.29	108.20
54	BA	2683	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	44	A	N1-C6-N6	-6.36	114.78	118.60
54	BA	346	A	C2-N3-C4	6.36	113.78	110.60
54	BA	670	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1876	A	C5-C6-N1	6.36	120.88	117.70
54	BA	109	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2283	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	13	U	C5'-C4'-C3'	-6.36	105.83	116.00
21	AA	1456	A	C5-C6-N1	6.36	120.88	117.70
54	BA	640	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	630	A	C5-C6-N1	6.36	120.88	117.70
21	AA	1263	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1745	A	N1-C6-N6	-6.36	114.79	118.60
54	BA	2752	C	N1-C2-O2	6.36	122.71	118.90
54	BA	2753	A	N1-C6-N6	-6.36	114.79	118.60
54	BA	2805	C	O4'-C1'-N1	6.36	113.28	108.20
54	BA	1165	A	C5-C6-N1	6.35	120.88	117.70
21	AA	269	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	1284	A	C5-C6-N1	6.35	120.88	117.70
21	AA	1496	C	N1-C2-O2	6.35	122.71	118.90
54	BA	462	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2199	A	C5-C6-N1	6.35	120.88	117.70
55	BB	65	U	C5-C6-N1	-6.35	119.53	122.70
21	AA	339	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	420	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	432	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	1241	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	1768	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2454	G	O4'-C1'-N9	6.35	113.28	108.20
54	BA	2822	G	C1'-O4'-C4'	-6.35	104.82	109.90
21	AA	348	G	C1'-O4'-C4'	-6.35	104.82	109.90
21	AA	1365	G	N3-C2-N2	-6.35	115.46	119.90
54	BA	181	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	515	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	532	A	C4-C5-C6	-6.35	113.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1593	A	C5-C6-N1	6.35	120.87	117.70
54	BA	2486	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	315	A	C5-C6-N1	6.34	120.87	117.70
21	AA	608	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1858	A	C5-C6-N1	6.34	120.87	117.70
54	BA	2284	A	C6-C5-N7	6.34	136.74	132.30
21	AA	161	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	964	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	788	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1610	A	C1'-O4'-C4'	-6.34	104.83	109.90
54	BA	338	G	N3-C4-C5	-6.34	125.43	128.60
54	BA	633	A	C5-C6-N1	6.34	120.87	117.70
54	BA	903	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1515	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1871	A	O4'-C1'-N9	6.34	113.27	108.20
54	BA	2143	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2425	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	355	C	N1-C2-O2	6.34	122.70	118.90
21	AA	602	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	574	A	C5-C6-N1	6.34	120.87	117.70
21	AA	963	G	N1-C6-O6	-6.34	116.10	119.90
54	BA	705	A	N1-C6-N6	-6.33	114.80	118.60
54	BA	1099	G	C8-N9-C4	-6.33	103.87	106.40
21	AA	77	A	C5-C6-N1	6.33	120.87	117.70
21	AA	1104	G	N1-C6-O6	-6.33	116.10	119.90
54	BA	147	C	O4'-C1'-N1	6.33	113.27	108.20
54	BA	705	A	C5-C6-N1	6.33	120.87	117.70
21	AA	6	G	N3-C4-C5	-6.33	125.44	128.60
21	AA	624	C	N3-C2-O2	-6.33	117.47	121.90
39	BQ	69	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	717	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	2163	A	C5-C6-N1	6.33	120.86	117.70
21	AA	60	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	181	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	1324	A	C5-C6-N1	6.33	120.86	117.70
54	BA	542	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	814	C	O4'-C1'-N1	6.33	113.26	108.20
54	BA	1328	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	1889	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	2273	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	130	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	478	A	C5-C6-N1	6.33	120.86	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	612	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	686	U	N1-C2-N3	6.33	118.70	114.90
54	BA	97	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	389	G	N9-C4-C5	6.32	107.93	105.40
54	BA	415	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1625	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	2516	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2001	C	N3-C2-O2	-6.32	117.47	121.90
22	A1	35	A	C4-C5-C6	-6.32	113.84	117.00
27	BE	88	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	AA	610	U	N3-C2-O2	-6.32	117.78	122.20
21	AA	1112	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	413	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	414	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2862	G	O4'-C1'-N9	6.32	113.25	108.20
21	AA	117	G	N1-C6-O6	-6.32	116.11	119.90
21	AA	578	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	719	C	N1-C2-O2	6.32	122.69	118.90
54	BA	1032	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	2078	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2756	U	C5-C6-N1	-6.32	119.54	122.70
21	AA	1256	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1579	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	572	A	C5-C6-N1	6.31	120.86	117.70
54	BA	647	G	C5-C6-N1	6.31	114.66	111.50
54	BA	2483	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	1395	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	316	C	O4'-C1'-N1	6.31	113.25	108.20
54	BA	711	G	C8-N9-C4	-6.31	103.88	106.40
54	BA	749	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	866	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	1342	C	N1-C2-O2	6.31	122.68	118.90
54	BA	1123	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1650	A	C5-C6-N1	6.31	120.85	117.70
22	A1	74	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	31	C	N1-C2-O2	6.31	122.68	118.90
21	AA	181	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1249	U	O4'-C1'-N1	6.30	113.24	108.20
54	BA	1671	U	C5-C6-N1	-6.30	119.55	122.70
54	BA	2471	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2657	A	C5-C6-N1	6.30	120.85	117.70
21	AA	961	U	O4'-C1'-N1	6.30	113.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1319	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	191	A	N1-C6-N6	-6.30	114.82	118.60
54	BA	402	A	N1-C6-N6	-6.30	114.82	118.60
21	AA	1000	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1836	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2461	A	C5-C6-N1	6.30	120.85	117.70
21	AA	149	A	N1-C6-N6	-6.30	114.82	118.60
54	BA	1403	A	C6-C5-N7	6.29	136.71	132.30
39	BQ	54	ARG	NE-CZ-NH1	6.29	123.45	120.30
54	BA	2236	U	O4'-C1'-N1	6.29	113.23	108.20
21	AA	101	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	1112	C	O4'-C1'-N1	6.29	113.23	108.20
54	BA	758	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1640	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1745	A	C5-C6-N1	6.29	120.84	117.70
54	BA	1754	A	C5-C6-N1	6.29	120.84	117.70
54	BA	1991	U	C5-C6-N1	-6.29	119.56	122.70
21	AA	327	A	C5-C6-N1	6.29	120.84	117.70
21	AA	349	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	803	G	N1-C6-O6	-6.29	116.13	119.90
21	AA	1311	A	C5-C6-N1	6.29	120.84	117.70
21	AA	1366	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	316	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2254	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2600	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1300	G	P-O3'-C3'	6.29	127.25	119.70
55	BB	110	C	O4'-C1'-N1	6.29	113.23	108.20
21	AA	67	C	O4'-C1'-N1	6.29	113.23	108.20
21	AA	73	C	N1-C2-O2	6.29	122.67	118.90
21	AA	712	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1293	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1960	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	910	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1303	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	460	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1670	C	O4'-C1'-N1	6.28	113.23	108.20
54	BA	2235	G	O4'-C1'-N9	6.28	113.23	108.20
54	BA	2355	G	N1-C6-O6	-6.28	116.13	119.90
21	AA	1369	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2899	A	C4-C5-C6	-6.28	113.86	117.00
13	AN	90	ARG	NE-CZ-NH1	6.28	123.44	120.30
46	BX	10	ARG	NE-CZ-NH1	6.28	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	573	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1681	G	O4'-C1'-N9	6.28	113.22	108.20
54	BA	1771	C	N3-C2-O2	-6.28	117.50	121.90
55	BB	2	G	N3-C4-C5	-6.28	125.46	128.60
21	AA	907	A	N1-C6-N6	-6.28	114.83	118.60
54	BA	163	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	203	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1158	C	N3-C2-O2	-6.28	117.51	121.90
2	AC	155	ARG	NE-CZ-NH1	6.27	123.44	120.30
54	BA	38	A	C5-C6-N1	6.27	120.84	117.70
21	AA	234	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	634	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	301	G	N3-C4-C5	-6.27	125.46	128.60
54	BA	937	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	862	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1151	A	C5-C6-N1	6.27	120.83	117.70
54	BA	435	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1057	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	311	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	461	A	C5-C6-N1	6.27	120.83	117.70
39	BQ	52	ARG	NE-CZ-NH1	6.27	123.44	120.30
54	BA	191	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	944	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2095	A	C5-C6-N1	6.27	120.83	117.70
54	BA	538	A	C5-C6-N1	6.27	120.83	117.70
54	BA	1233	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1334	G	N1-C6-O6	-6.27	116.14	119.90
54	BA	1368	G	O4'-C1'-N9	6.27	113.21	108.20
8	AI	10	ARG	NE-CZ-NH1	6.27	123.43	120.30
54	BA	1749	A	C5-C6-N1	6.27	120.83	117.70
21	AA	487	A	C5-C6-N1	6.26	120.83	117.70
54	BA	13	A	C5-C6-N1	6.26	120.83	117.70
54	BA	483	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2052	A	N1-C6-N6	-6.26	114.84	118.60
54	BA	2358	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	1333	A	C5-C6-N1	6.26	120.83	117.70
21	AA	1473	G	N1-C6-O6	-6.26	116.14	119.90
54	BA	1901	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2035	G	O4'-C1'-N9	6.26	113.21	108.20
54	BA	2589	A	C5-C6-N1	6.26	120.83	117.70
54	BA	479	A	C6-C5-N7	6.26	136.68	132.30
54	BA	1169	A	C4-C5-C6	-6.26	113.87	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1936	A	P-O3'-C3'	6.26	127.21	119.70
54	BA	2446	G	O4'-C4'-C3'	6.26	111.11	106.10
24	A3	1	C	N1-C2-O2	6.26	122.66	118.90
54	BA	718	A	O4'-C1'-N9	6.26	113.21	108.20
54	BA	1504	A	C4-C5-C6	-6.26	113.87	117.00
8	AI	11	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	1046	A	C5-C6-N1	6.26	120.83	117.70
54	BA	1998	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	125	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	221	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	1113	U	C5-C6-N1	-6.25	119.57	122.70
54	BA	1505	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	2515	C	N3-C2-O2	-6.25	117.52	121.90
24	A3	76	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	314	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	331	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	328	C	N1-C2-O2	6.25	122.65	118.90
54	BA	251	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2773	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	814	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	522	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	666	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	943	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	1319	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1658	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	900	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	327	G	N3-C2-N2	-6.25	115.53	119.90
54	BA	753	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	788	A	C5-C6-N1	6.25	120.82	117.70
54	BA	1033	U	O4'-C1'-N1	6.25	113.20	108.20
54	BA	2736	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	28	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	237	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1614	A	C4-C5-C6	-6.25	113.88	117.00
6	AG	2	ARG	NE-CZ-NH1	6.24	123.42	120.30
21	AA	1497	G	N1-C6-O6	-6.24	116.15	119.90
22	A1	69	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	820	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1507	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2459	A	N1-C6-N6	-6.24	114.85	118.60
54	BA	2815	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1144	A	C5-C6-N1	6.24	120.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1343	G	C8-N9-C4	-6.24	103.90	106.40
21	AA	1176	A	N1-C6-N6	-6.24	114.86	118.60
54	BA	957	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	736	C	N3-C4-N4	-6.24	113.63	118.00
31	BI	133	ARG	NE-CZ-NH1	6.24	123.42	120.30
55	BB	30	C	N3-C2-O2	-6.24	117.53	121.90
55	BB	35	C	N3-C2-O2	-6.24	117.53	121.90
55	BB	41	G	O4'-C1'-N9	6.24	113.19	108.20
2	AC	39	ARG	NE-CZ-NH1	6.24	123.42	120.30
21	AA	791	G	N3-C2-N2	-6.24	115.53	119.90
21	AA	990	C	N1-C2-O2	6.24	122.64	118.90
21	AA	1533	C	C2-N1-C1'	6.24	125.66	118.80
54	BA	8	C	O4'-C1'-N1	6.24	113.19	108.20
54	BA	364	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	415	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1441	G	N1-C6-O6	-6.24	116.16	119.90
54	BA	2158	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	1001	A	N1-C6-N6	-6.23	114.86	118.60
54	BA	2016	U	C5-C6-N1	-6.23	119.58	122.70
21	AA	501	C	N1-C2-O2	6.23	122.64	118.90
21	AA	549	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	580	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1029	U	O4'-C1'-N1	6.23	113.19	108.20
54	BA	1001	A	C5-C6-N1	6.23	120.82	117.70
54	BA	2286	G	C1'-O4'-C4'	-6.23	104.91	109.90
21	AA	935	A	C5-C6-N1	6.23	120.81	117.70
21	AA	1157	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	1438	U	O4'-C1'-N1	6.23	113.19	108.20
54	BA	2276	G	C5'-C4'-C3'	-6.23	106.03	116.00
22	A1	14	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	243	A	C5-C6-N1	6.23	120.81	117.70
21	AA	1012	A	C5-C6-N1	6.23	120.81	117.70
54	BA	19	A	C5-C6-N1	6.23	120.81	117.70
54	BA	178	G	N7-C8-N9	6.23	116.21	113.10
54	BA	1286	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	2736	A	C5-C6-N1	6.23	120.81	117.70
21	AA	379	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	658	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	834	G	N7-C8-N9	6.23	116.21	113.10
54	BA	9	G	N3-C2-N2	-6.22	115.54	119.90
54	BA	68	G	N1-C6-O6	-6.22	116.17	119.90
21	AA	221	C	N3-C2-O2	-6.22	117.54	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	341	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1419	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1973	G	N1-C6-O6	-6.22	116.17	119.90
21	AA	186	C	N1-C2-O2	6.22	122.63	118.90
21	AA	1331	G	N3-C2-N2	-6.22	115.55	119.90
54	BA	183	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	253	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	324	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	565	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1746	A	C5-C6-N1	6.22	120.81	117.70
54	BA	2675	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	605	U	C5-C6-N1	-6.22	119.59	122.70
21	AA	1384	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	1418	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	262	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	787	C	N1-C2-O2	6.22	122.63	118.90
21	AA	459	A	C5-C6-N1	6.21	120.81	117.70
21	AA	1133	G	N1-C6-O6	-6.21	116.17	119.90
54	BA	1211	C	N1-C2-O2	6.21	122.63	118.90
54	BA	1617	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2417	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1307	A	N1-C6-N6	-6.21	114.87	118.60
54	BA	2783	U	C5-C6-N1	-6.21	119.59	122.70
21	AA	1509	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1246	A	C5-C6-N1	6.21	120.81	117.70
54	BA	2176	A	C6-C5-N7	6.21	136.65	132.30
55	BB	91	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	306	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1588	G	N1-C6-O6	-6.21	116.17	119.90
54	BA	2238	G	N3-C4-C5	-6.21	125.50	128.60
21	AA	1229	A	C5-C6-N1	6.21	120.80	117.70
54	BA	51	G	N1-C6-O6	-6.21	116.18	119.90
54	BA	1434	A	C2-N3-C4	6.21	113.70	110.60
54	BA	1434	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1498	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	1603	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	893	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	1022	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	870	U	O4'-C1'-N1	6.21	113.16	108.20
54	BA	1597	A	C4-C5-C6	-6.21	113.90	117.00
1	AB	19	THR	C-N-CA	6.20	137.21	121.70
21	AA	1223	C	N3-C4-C5	6.20	124.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1263	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1480	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	923	A	N1-C6-N6	-6.20	114.88	118.60
54	BA	247	G	C5'-C4'-O4'	6.20	116.54	109.10
54	BA	1175	A	C5-C6-N1	6.20	120.80	117.70
54	BA	1290	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1934	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1492	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	466	A	C5-C6-N1	6.20	120.80	117.70
54	BA	502	A	O4'-C1'-N9	6.20	113.16	108.20
21	AA	873	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1111	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	145	C	N1-C2-O2	6.20	122.62	118.90
54	BA	2503	A	C5-C6-N1	6.19	120.80	117.70
36	BN	30	ARG	NE-CZ-NH1	6.19	123.40	120.30
54	BA	1313	U	N3-C2-O2	-6.19	117.86	122.20
54	BA	2103	C	O4'-C1'-N1	6.19	113.15	108.20
21	AA	1066	C	N3-C4-C5	6.19	124.38	121.90
54	BA	574	A	C5-C6-N1	6.19	120.80	117.70
54	BA	626	A	C5-C6-N1	6.19	120.80	117.70
21	AA	532	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	1302	C	N1-C2-O2	6.19	122.61	118.90
4	AE	92	ARG	NE-CZ-NH2	-6.19	117.21	120.30
21	AA	647	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	708	C	N3-C2-O2	-6.19	117.57	121.90
22	A1	38	A	C6-C5-N7	6.19	136.63	132.30
55	BB	81	G	N1-C6-O6	-6.19	116.19	119.90
21	AA	817	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	983	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	1236	A	N1-C6-N6	-6.18	114.89	118.60
54	BA	877	A	C5-C6-N1	6.18	120.79	117.70
54	BA	959	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2048	G	N9-C4-C5	6.18	107.87	105.40
24	A3	11	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	276	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	1237	A	N1-C6-N6	-6.18	114.89	118.60
54	BA	2088	A	C5-C6-N1	6.18	120.79	117.70
54	BA	2760	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	560	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1641	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1715	G	C5-C6-N1	6.18	114.59	111.50
54	BA	2518	A	C4-C5-C6	-6.18	113.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	113	C	N3-C4-C5	6.18	124.37	121.90
54	BA	362	A	C5-C6-N1	6.18	120.79	117.70
54	BA	1344	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2851	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2227	A	C5-C6-N1	6.18	120.79	117.70
54	BA	2427	C	O4'-C1'-N1	6.18	113.14	108.20
21	AA	169	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	182	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	1295	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1435	G	N3-C2-N2	-6.17	115.58	119.90
54	BA	2476	A	C5-C6-N1	6.17	120.79	117.70
21	AA	586	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1837	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1196	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1451	C	N1-C2-O2	6.17	122.60	118.90
54	BA	2436	G	N1-C6-O6	-6.17	116.20	119.90
54	BA	2513	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	712	A	C5-C6-N1	6.17	120.78	117.70
54	BA	349	U	C5-C6-N1	-6.17	119.62	122.70
54	BA	540	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	823	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2560	A	C5-C6-N1	6.17	120.78	117.70
21	AA	846	G	N3-C4-C5	-6.17	125.52	128.60
21	AA	1101	A	C5-C6-N1	6.17	120.78	117.70
21	AA	1225	A	C5-C6-N1	6.17	120.78	117.70
54	BA	718	A	C2-N3-C4	6.17	113.68	110.60
54	BA	1082	U	C5-C6-N1	-6.17	119.62	122.70
54	BA	1744	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	1886	U	O4'-C1'-N1	6.17	113.13	108.20
54	BA	1909	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2309	A	C5-C6-N1	6.17	120.78	117.70
21	AA	648	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	272	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	1061	G	N1-C6-O6	-6.16	116.20	119.90
21	AA	1465	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	177	G	N3-C2-N2	-6.16	115.59	119.90
54	BA	1217	U	O4'-C1'-N1	6.16	113.13	108.20
54	BA	1759	A	C5-C6-N1	6.16	120.78	117.70
54	BA	2603	G	C5-C6-N1	6.16	114.58	111.50
54	BA	1306	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1431	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	795	C	N1-C2-O2	6.16	122.60	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	847	U	C3'-C2'-C1'	6.16	106.43	101.50
54	BA	2525	G	N1-C6-O6	-6.16	116.20	119.90
21	AA	967	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	61	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1495	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1849	G	N1-C6-O6	-6.16	116.20	119.90
54	BA	1583	A	C5-C6-N1	6.16	120.78	117.70
38	BP	50	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	311	A	C5-C6-N1	6.16	120.78	117.70
54	BA	354	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1438	U	C5-C6-N1	-6.16	119.62	122.70
54	BA	1699	G	N3-C2-N2	-6.16	115.59	119.90
54	BA	1798	U	C5-C6-N1	-6.16	119.62	122.70
1	AB	112	ARG	NE-CZ-NH1	6.15	123.38	120.30
21	AA	1399	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2067	G	N1-C6-O6	-6.15	116.21	119.90
54	BA	397	U	N3-C2-O2	-6.15	117.89	122.20
54	BA	620	G	N7-C8-N9	6.15	116.18	113.10
54	BA	1001	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1918	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	1918	A	C5-C6-N1	6.15	120.78	117.70
54	BA	1417	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1860	G	N1-C6-O6	-6.15	116.21	119.90
54	BA	2268	A	C5'-C4'-O4'	6.15	116.48	109.10
54	BA	2350	C	O4'-C1'-N1	6.15	113.12	108.20
21	AA	1413	A	N1-C6-N6	-6.15	114.91	118.60
54	BA	1862	G	N3-C2-N2	-6.15	115.59	119.90
54	BA	2289	G	N3-C4-C5	-6.15	125.53	128.60
21	AA	1289	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	192	C	O4'-C1'-N1	6.15	113.12	108.20
54	BA	1305	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	1834	U	O4'-C4'-C3'	6.15	111.02	106.10
54	BA	64	A	C4-C5-C6	-6.15	113.93	117.00
45	BW	38	ARG	NE-CZ-NH1	6.14	123.37	120.30
55	BB	27	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	497	G	C5-C6-N1	6.14	114.57	111.50
54	BA	320	A	C5-C6-N1	6.14	120.77	117.70
54	BA	541	A	O4'-C1'-N9	6.14	113.11	108.20
54	BA	1385	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2356	U	C5-C6-N1	-6.14	119.63	122.70
54	BA	1929	G	N1-C6-O6	-6.14	116.22	119.90
21	AA	286	C	N3-C2-O2	-6.14	117.60	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	457	G	N1-C6-O6	-6.14	116.22	119.90
21	AA	1396	A	C5-C6-N1	6.14	120.77	117.70
54	BA	609	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1669	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1098	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	865	C	N3-C2-O2	-6.14	117.60	121.90
42	BT	3	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	229	C	N1-C2-O2	6.14	122.58	118.90
54	BA	812	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1036	G	N3-C4-C5	-6.14	125.53	128.60
54	BA	2717	C	N1-C2-O2	6.14	122.58	118.90
55	BB	106	G	C5-C6-N1	6.14	114.57	111.50
7	AH	76	ARG	NE-CZ-NH1	6.13	123.37	120.30
21	AA	795	C	O4'-C1'-N1	6.13	113.11	108.20
21	AA	892	A	C5-C6-N1	6.13	120.77	117.70
24	A3	73	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	278	A	N1-C6-N6	-6.13	114.92	118.60
21	AA	859	G	N1-C6-O6	-6.13	116.22	119.90
54	BA	581	C	O4'-C1'-N1	6.13	113.11	108.20
54	BA	1768	C	N3-C4-C5	6.13	124.35	121.90
54	BA	1265	A	C5-C6-N1	6.13	120.77	117.70
54	BA	1768	C	N1-C2-O2	6.13	122.58	118.90
54	BA	2184	A	C5-C6-N1	6.13	120.77	117.70
21	AA	1113	C	N1-C2-O2	6.13	122.58	118.90
27	BE	40	ARG	NE-CZ-NH1	6.13	123.36	120.30
29	BG	148	ARG	NE-CZ-NH1	6.13	123.36	120.30
21	AA	909	A	C5-C6-N1	6.13	120.77	117.70
21	AA	1403	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	925	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	1706	C	N3-C2-O2	-6.13	117.61	121.90
56	B5	71	ARG	NE-CZ-NH1	6.13	123.36	120.30
24	A3	66	C	O4'-C1'-N1	6.13	113.10	108.20
28	BF	111	ARG	NE-CZ-NH1	6.13	123.36	120.30
54	BA	1661	G	C5'-C4'-O4'	6.13	116.45	109.10
21	AA	15	G	C5-C6-N1	6.12	114.56	111.50
21	AA	1030	U	N3-C2-O2	-6.12	117.91	122.20
54	BA	801	G	N3-C2-N2	-6.12	115.61	119.90
54	BA	2602	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2863	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	669	G	N1-C6-O6	-6.12	116.23	119.90
54	BA	2576	G	N1-C6-O6	-6.12	116.23	119.90
54	BA	153	U	O4'-C1'-N1	6.12	113.10	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	951	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	1021	A	C4-C5-C6	-6.12	113.94	117.00
34	BL	33	ARG	NE-CZ-NH1	6.12	123.36	120.30
54	BA	227	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	284	U	O4'-C1'-N1	6.12	113.10	108.20
54	BA	2837	A	C5-C6-N1	6.12	120.76	117.70
55	BB	91	C	N1-C2-O2	6.12	122.57	118.90
21	AA	874	G	C5-C6-N1	6.12	114.56	111.50
54	BA	2627	G	N3-C2-N2	-6.12	115.62	119.90
54	BA	305	C	O4'-C1'-N1	6.12	113.09	108.20
54	BA	488	G	C5-C6-N1	6.12	114.56	111.50
54	BA	501	A	C5-C6-N1	6.12	120.76	117.70
21	AA	304	U	O4'-C1'-N1	6.12	113.09	108.20
21	AA	306	A	N1-C6-N6	-6.12	114.93	118.60
21	AA	663	A	N1-C6-N6	-6.12	114.93	118.60
21	AA	958	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	1306	A	C5-C6-N1	6.12	120.76	117.70
54	BA	1307	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2082	A	N1-C6-N6	-6.12	114.93	118.60
21	AA	1306	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	256	A	C5-C6-N1	6.11	120.76	117.70
54	BA	2055	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	692	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2071	A	C4-C5-C6	-6.11	113.94	117.00
55	BB	63	C	O4'-C1'-N1	6.11	113.09	108.20
21	AA	670	G	O4'-C1'-N9	6.11	113.09	108.20
54	BA	1064	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1135	C	N1-C2-O2	6.11	122.57	118.90
54	BA	1167	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2045	C	N1-C2-O2	6.11	122.57	118.90
18	AS	40	PHE	CB-CG-CD2	-6.11	116.52	120.80
54	BA	1294	U	O4'-C1'-N1	6.11	113.09	108.20
54	BA	1516	G	N1-C6-O6	-6.11	116.23	119.90
21	AA	372	C	N1-C2-O2	6.11	122.56	118.90
54	BA	442	G	N9-C4-C5	6.11	107.84	105.40
54	BA	2551	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2597	G	N1-C6-O6	-6.11	116.24	119.90
54	BA	2893	A	C5-C6-N1	6.11	120.75	117.70
55	BB	50	A	C4-C5-C6	-6.11	113.95	117.00
21	AA	334	C	O4'-C1'-N1	6.11	113.08	108.20
21	AA	1234	C	N1-C2-O2	6.11	122.56	118.90
25	BC	181	ARG	NE-CZ-NH2	-6.11	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	32	C	N3-C4-C5	6.11	124.34	121.90
54	BA	257	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	1928	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	2339	C	N1-C2-O2	6.11	122.56	118.90
21	AA	777	A	C5-C6-N1	6.10	120.75	117.70
54	BA	809	G	C8-N9-C4	-6.10	103.96	106.40
21	AA	964	A	N1-C6-N6	-6.10	114.94	118.60
21	AA	1390	U	N1-C2-N3	6.10	118.56	114.90
54	BA	97	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	2901	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	974	A	N1-C6-N6	-6.10	114.94	118.60
54	BA	1015	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	1340	U	N3-C2-O2	-6.10	117.93	122.20
54	BA	2226	C	N3-C4-N4	-6.10	113.73	118.00
54	BA	2669	G	O4'-C1'-N9	6.10	113.08	108.20
55	BB	97	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1150	A	C4-C5-C6	-6.10	113.95	117.00
44	BV	18	ARG	NE-CZ-NH1	6.10	123.35	120.30
54	BA	222	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	442	G	O4'-C1'-N9	6.10	113.08	108.20
54	BA	594	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	1010	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	2424	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	946	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	1279	G	O4'-C1'-N9	6.09	113.08	108.20
54	BA	2432	A	N1-C6-N6	-6.09	114.94	118.60
54	BA	290	U	O4'-C1'-N1	6.09	113.08	108.20
54	BA	2805	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	560	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	1275	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	2330	G	O4'-C1'-N9	6.09	113.07	108.20
54	BA	2473	U	O4'-C1'-N1	6.09	113.07	108.20
54	BA	2645	G	C5-C6-N1	6.09	114.55	111.50
21	AA	117	G	C5-C6-N1	6.09	114.54	111.50
21	AA	408	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	702	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	1274	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	921	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	1526	C	N3-C2-O2	-6.09	117.64	121.90
6	AG	94	ARG	NE-CZ-NH1	6.09	123.34	120.30
54	BA	794	A	C5-C6-N1	6.09	120.74	117.70
54	BA	2505	G	N1-C6-O6	-6.09	116.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	432	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	1325	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	74	A	N1-C6-N6	-6.09	114.95	118.60
54	BA	203	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	69	C	N1-C2-O2	6.08	122.55	118.90
54	BA	1100	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	78	A	C6-C5-N7	6.08	136.56	132.30
21	AA	648	A	N1-C6-N6	-6.08	114.95	118.60
22	A1	26	A	C4-C5-C6	-6.08	113.96	117.00
24	A3	69	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	752	A	C5-C6-N1	6.08	120.74	117.70
55	BB	58	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	71	A	C5-C6-N1	6.08	120.74	117.70
21	AA	726	C	N1-C2-O2	6.08	122.55	118.90
21	AA	896	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	1502	A	C5-C6-N1	6.08	120.74	117.70
54	BA	592	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2020	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2238	G	N1-C6-O6	-6.08	116.25	119.90
54	BA	1127	A	C5-C6-N1	6.08	120.74	117.70
21	AA	872	A	O4'-C1'-N9	6.08	113.06	108.20
54	BA	1130	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	1557	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	782	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1345	C	N1-C2-O2	6.08	122.55	118.90
21	AA	274	A	C5-C6-N1	6.08	120.74	117.70
21	AA	1341	U	N3-C2-O2	-6.08	117.95	122.20
54	BA	1382	G	C8-N9-C4	-6.08	103.97	106.40
54	BA	1569	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2778	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	9	G	N9-C4-C5	6.07	107.83	105.40
54	BA	37	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2129	C	O4'-C1'-N1	6.07	113.06	108.20
36	BN	17	ARG	NE-CZ-NH1	6.07	123.34	120.30
54	BA	267	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1942	C	O4'-C1'-N1	6.07	113.06	108.20
54	BA	2699	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2885	G	N1-C6-O6	-6.07	116.26	119.90
54	BA	246	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	426	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1028	A	C5-C6-N1	6.07	120.73	117.70
22	A1	25	C	N3-C2-O2	-6.07	117.65	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	109	C	O4'-C1'-N1	6.07	113.06	108.20
21	AA	206	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	596	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	897	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	1531	A	C5-C6-N1	6.07	120.73	117.70
33	BK	98	ARG	NE-CZ-NH1	6.07	123.33	120.30
54	BA	890	C	N1-C2-O2	6.07	122.54	118.90
24	A3	22	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	358	U	C3'-C2'-C1'	6.06	106.35	101.50
54	BA	787	C	C5'-C4'-O4'	6.06	116.37	109.10
54	BA	1287	A	C4-C5-C6	-6.06	113.97	117.00
55	BB	34	A	C5-C6-N1	6.06	120.73	117.70
21	AA	1084	G	N9-C4-C5	6.06	107.83	105.40
21	AA	68	G	C5-C6-N1	6.06	114.53	111.50
54	BA	119	A	O4'-C1'-N9	6.06	113.05	108.20
54	BA	1542	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	1857	G	O4'-C1'-N9	6.06	113.05	108.20
54	BA	2201	G	O4'-C1'-N9	6.06	113.05	108.20
54	BA	2222	C	N1-C2-O2	6.06	122.54	118.90
54	BA	2473	U	N3-C2-O2	-6.06	117.96	122.20
54	BA	2565	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	136	C	N1-C2-O2	6.06	122.53	118.90
21	AA	806	C	N3-C2-O2	-6.06	117.66	121.90
33	BK	70	ARG	NE-CZ-NH1	6.06	123.33	120.30
54	BA	1155	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1612	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1892	C	N3-C2-O2	-6.06	117.66	121.90
1	AB	138	ARG	NE-CZ-NH1	6.06	123.33	120.30
54	BA	1126	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2466	C	N3-C2-O2	-6.06	117.66	121.90
55	BB	47	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	1280	A	C1'-O4'-C4'	-6.05	105.06	109.90
54	BA	344	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1902	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	2559	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	23	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	701	U	C5-C6-N1	-6.05	119.67	122.70
21	AA	1250	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2313	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	2535	G	N3-C2-N2	-6.05	115.66	119.90
23	A2	82	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	979	A	C4-C5-C6	-6.05	113.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1531	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	810	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	74	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1241	A	C2-N3-C4	6.05	113.62	110.60
54	BA	1626	A	C4-C5-C6	-6.05	113.98	117.00
55	BB	51	G	N1-C6-O6	-6.05	116.27	119.90
54	BA	1275	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1386	C	N3-C2-O2	-6.04	117.67	121.90
55	BB	87	U	N3-C2-O2	-6.04	117.97	122.20
21	AA	1520	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	93	G	O4'-C1'-N9	6.04	113.04	108.20
54	BA	2508	G	C5-C6-N1	6.04	114.52	111.50
21	AA	452	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	572	A	N1-C6-N6	-6.04	114.97	118.60
27	BE	49	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	165	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2505	G	C8-N9-C4	-6.04	103.98	106.40
21	AA	750	C	N1-C2-O2	6.04	122.52	118.90
54	BA	1914	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2309	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	412	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	595	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	608	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1462	C	O4'-C1'-N1	6.04	113.03	108.20
54	BA	727	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	360	G	C5-C6-N1	6.04	114.52	111.50
54	BA	2430	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	52	C	N1-C2-O2	6.04	122.52	118.90
22	A1	65	C	N3-C2-O2	-6.04	117.68	121.90
54	BA	671	C	N1-C2-O2	6.04	122.52	118.90
54	BA	973	A	C4-C5-C6	-6.04	113.98	117.00
55	BB	27	C	N1-C2-O2	6.04	122.52	118.90
21	AA	487	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	746	A	C5-C6-N1	6.03	120.72	117.70
54	BA	546	U	O4'-C1'-N1	6.03	113.03	108.20
54	BA	791	C	O4'-C1'-N1	6.03	113.03	108.20
54	BA	1080	A	C5-C6-N1	6.03	120.72	117.70
54	BA	1800	C	C2-N3-C4	-6.03	116.88	119.90
54	BA	1871	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	307	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	584	G	N3-C4-C5	-6.03	125.58	128.60
21	AA	1021	A	C5-C6-N1	6.03	120.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1184	G	C5-C6-N1	6.03	114.52	111.50
21	AA	1500	A	C5-C6-N1	6.03	120.72	117.70
32	BJ	27	ARG	NE-CZ-NH1	6.03	123.32	120.30
54	BA	922	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1821	A	C6-C5-N7	6.03	136.52	132.30
55	BB	11	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	205	A	C5-C6-N1	6.03	120.72	117.70
21	AA	736	C	O4'-C1'-N1	6.03	113.02	108.20
54	BA	389	G	C8-N9-C4	-6.03	103.99	106.40
54	BA	1207	C	O4'-C1'-N1	6.03	113.02	108.20
21	AA	417	G	N1-C6-O6	-6.03	116.28	119.90
21	AA	635	A	N1-C6-N6	-6.03	114.98	118.60
21	AA	884	U	C3'-C2'-C1'	6.03	106.32	101.50
21	AA	1228	C	N3-C4-C5	6.03	124.31	121.90
47	BY	52	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	472	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	650	C	C6-N1-C2	-6.03	117.89	120.30
54	BA	1428	C	N1-C2-O2	6.03	122.52	118.90
21	AA	770	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	972	C	N3-C2-O2	-6.03	117.68	121.90
37	BO	10	ARG	NH1-CZ-NH2	-6.03	112.77	119.40
54	BA	832	U	O4'-C1'-N1	6.03	113.02	108.20
54	BA	1765	U	O4'-C1'-N1	6.03	113.02	108.20
54	BA	1929	G	N3-C4-C5	-6.03	125.59	128.60
54	BA	372	G	N3-C4-C5	-6.02	125.59	128.60
54	BA	402	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	355	U	C5-C6-N1	-6.02	119.69	122.70
54	BA	1674	G	O4'-C1'-N9	6.02	113.02	108.20
21	AA	1081	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	575	A	C5-C6-N1	6.02	120.71	117.70
54	BA	735	A	O4'-C1'-N9	6.02	113.02	108.20
54	BA	2520	C	N1-C2-O2	6.02	122.51	118.90
54	BA	2691	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	812	G	N3-C4-C5	-6.02	125.59	128.60
21	AA	1437	A	C5-C6-N1	6.02	120.71	117.70
54	BA	812	C	O4'-C1'-N1	6.02	113.01	108.20
54	BA	1395	A	N1-C6-N6	-6.02	114.99	118.60
54	BA	2069	G	C5-C6-N1	6.02	114.51	111.50
54	BA	2679	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2711	A	C5-C6-N1	6.02	120.71	117.70
21	AA	208	U	C5-C6-N1	-6.01	119.69	122.70
21	AA	1059	C	N3-C2-O2	-6.01	117.69	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1150	A	C5-C6-N1	6.01	120.71	117.70
21	AA	1254	A	N1-C6-N6	-6.01	114.99	118.60
21	AA	1378	C	O4'-C1'-N1	6.01	113.01	108.20
33	BK	64	ARG	NE-CZ-NH1	6.01	123.31	120.30
54	BA	355	U	N3-C2-O2	-6.01	117.99	122.20
54	BA	1420	A	O4'-C1'-N9	6.01	113.01	108.20
17	AR	52	ARG	NE-CZ-NH2	-6.01	117.29	120.30
54	BA	2282	G	N1-C6-O6	-6.01	116.29	119.90
21	AA	303	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	1339	A	C5-C6-N1	6.01	120.71	117.70
54	BA	210	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1514	G	N1-C6-O6	-6.01	116.29	119.90
54	BA	1604	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	1961	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1978	A	C5-C6-N1	6.01	120.71	117.70
21	AA	740	U	O4'-C1'-N1	6.01	113.01	108.20
21	AA	1383	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	160	A	C5-C6-N1	6.01	120.70	117.70
21	AA	857	C	N3-C2-O2	-6.01	117.70	121.90
21	AA	1262	C	N3-C2-O2	-6.01	117.70	121.90
21	AA	1293	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	1415	G	C5'-C4'-C3'	-6.01	106.39	116.00
21	AA	1529	G	N3-C2-N2	-6.01	115.70	119.90
54	BA	723	C	N3-C2-O2	-6.01	117.70	121.90
54	BA	2135	A	N1-C6-N6	-6.01	115.00	118.60
54	BA	2699	C	N3-C4-C5	6.01	124.30	121.90
54	BA	231	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	244	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	564	C	N1-C2-O2	6.00	122.50	118.90
55	BB	4	C	N3-C2-O2	-6.00	117.70	121.90
55	BB	57	A	N1-C6-N6	-6.00	115.00	118.60
21	AA	673	A	C5-C6-N1	6.00	120.70	117.70
21	AA	732	C	N3-C4-C5	6.00	124.30	121.90
21	AA	749	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	989	U	C5-C6-N1	-6.00	119.70	122.70
21	AA	1216	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1437	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2093	G	C5-C6-N1	6.00	114.50	111.50
54	BA	685	A	C5-C6-N1	6.00	120.70	117.70
54	BA	2134	A	C5-C6-N1	6.00	120.70	117.70
54	BA	2241	A	C6-C5-N7	6.00	136.50	132.30
54	BA	2202	U	N3-C2-O2	-6.00	118.00	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	615	G	C5-C6-N1	6.00	114.50	111.50
54	BA	652	U	C5'-C4'-O4'	6.00	116.30	109.10
54	BA	1799	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	2136	G	N3-C2-N2	-6.00	115.70	119.90
21	AA	637	C	N3-C2-O2	-6.00	117.70	121.90
38	BP	87	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	87	U	O4'-C1'-N1	6.00	113.00	108.20
54	BA	1752	C	N3-C2-O2	-6.00	117.70	121.90
24	A3	23	G	N3-C2-N2	-6.00	115.70	119.90
54	BA	1650	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1342	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1741	C	N1-C2-O2	5.99	122.50	118.90
55	BB	8	C	O4'-C1'-N1	5.99	113.00	108.20
54	BA	342	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1790	C	N1-C2-O2	5.99	122.50	118.90
54	BA	1930	G	O4'-C1'-N9	5.99	112.99	108.20
21	AA	626	G	N1-C6-O6	-5.99	116.31	119.90
21	AA	1078	U	C5-C6-N1	-5.99	119.70	122.70
21	AA	1155	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	1390	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	2097	A	C5-C6-N1	5.99	120.69	117.70
21	AA	347	G	O4'-C1'-N9	5.99	112.99	108.20
24	A3	13	C	N3-C2-O2	-5.99	117.71	121.90
34	BL	47	ARG	NE-CZ-NH1	5.99	123.29	120.30
54	BA	1006	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1178	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2198	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	1035	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	99	U	N3-C2-O2	-5.99	118.01	122.20
54	BA	2089	C	N3-C2-O2	-5.99	117.71	121.90
13	AN	41	ARG	NE-CZ-NH1	5.99	123.29	120.30
21	AA	385	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	465	A	C4-C5-C6	-5.99	114.01	117.00
29	BG	54	ARG	NE-CZ-NH1	5.99	123.29	120.30
54	BA	225	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	378	C	N1-C2-O2	5.99	122.49	118.90
54	BA	1095	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1937	A	O4'-C1'-N9	5.99	112.99	108.20
54	BA	2630	G	C5-C6-N1	5.99	114.49	111.50
54	BA	2766	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	1086	U	N3-C2-O2	-5.98	118.01	122.20
24	A3	57	C	N1-C2-O2	5.98	122.49	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	969	G	O4'-C1'-N9	5.98	112.99	108.20
54	BA	1230	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1632	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2119	A	N1-C6-N6	-5.98	115.01	118.60
54	BA	2211	A	C5-C6-N1	5.98	120.69	117.70
4	AE	92	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	615	G	N3-C2-N2	-5.98	115.71	119.90
54	BA	19	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	231	A	N1-C6-N6	-5.98	115.01	118.60
54	BA	2746	U	O4'-C1'-N1	5.98	112.98	108.20
54	BA	2810	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	58	G	C8-N9-C4	-5.98	104.01	106.40
54	BA	2420	C	N3-C4-C5	5.98	124.29	121.90
54	BA	1476	U	O4'-C1'-N1	5.98	112.98	108.20
54	BA	1802	A	C5-C6-N1	5.98	120.69	117.70
54	BA	2191	A	C6-C5-N7	5.98	136.49	132.30
54	BA	2661	G	N1-C6-O6	-5.98	116.31	119.90
21	AA	169	C	O4'-C1'-N1	5.97	112.98	108.20
54	BA	449	A	C5-C6-N1	5.97	120.69	117.70
54	BA	1773	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	2407	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	36	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	533	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	1048	A	N1-C6-N6	-5.97	115.02	118.60
54	BA	1278	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	290	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1782	U	N1-C2-N3	5.97	118.48	114.90
21	AA	98	A	N1-C6-N6	-5.97	115.02	118.60
21	AA	499	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	1317	C	N1-C2-O2	5.97	122.48	118.90
54	BA	565	C	N3-C4-C5	5.97	124.29	121.90
54	BA	633	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2154	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	1077	G	C5-C6-N1	5.97	114.48	111.50
21	AA	1239	A	O4'-C1'-N9	5.97	112.97	108.20
54	BA	256	A	N1-C6-N6	-5.97	115.02	118.60
54	BA	717	C	N1-C2-O2	5.97	122.48	118.90
54	BA	1102	C	N1-C2-O2	5.97	122.48	118.90
54	BA	1433	A	N1-C6-N6	-5.97	115.02	118.60
21	AA	314	C	N3-C4-C5	5.97	124.29	121.90
21	AA	1328	C	N1-C2-O2	5.97	122.48	118.90
54	BA	60	G	N3-C4-C5	-5.97	125.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1946	U	O4'-C1'-N1	5.97	112.97	108.20
8	AI	94	ARG	NE-CZ-NH2	-5.96	117.32	120.30
21	AA	211	G	N1-C6-O6	-5.96	116.32	119.90
54	BA	22	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	51	G	N9-C4-C5	5.96	107.79	105.40
54	BA	485	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	2394	C	N3-C2-O2	-5.96	117.72	121.90
21	AA	490	C	N1-C2-O2	5.96	122.48	118.90
54	BA	1258	U	O4'-C1'-N1	5.96	112.97	108.20
54	BA	1427	A	C6-C5-N7	5.96	136.47	132.30
54	BA	1586	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1609	A	C5-C6-N1	5.96	120.68	117.70
54	BA	2800	A	C5-C6-N1	5.96	120.68	117.70
21	AA	930	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	994	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1164	C	O4'-C1'-N1	5.96	112.97	108.20
21	AA	236	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	653	U	O4'-C1'-N1	5.96	112.97	108.20
21	AA	1136	C	N3-C2-O2	-5.96	117.73	121.90
24	A3	63	C	N1-C2-O2	5.96	122.47	118.90
28	BF	166	ARG	NE-CZ-NH1	5.96	123.28	120.30
54	BA	1045	C	N1-C2-O2	5.96	122.47	118.90
54	BA	8	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	53	A	C5-C6-N1	5.96	120.68	117.70
54	BA	487	C	N1-C2-O2	5.96	122.47	118.90
54	BA	2499	C	N3-C4-C5	5.96	124.28	121.90
54	BA	2722	G	N1-C6-O6	-5.96	116.33	119.90
21	AA	114	U	O4'-C1'-N1	5.95	112.96	108.20
21	AA	418	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	848	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	1224	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	1857	G	C8-N9-C4	-5.95	104.02	106.40
54	BA	2533	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	2682	A	C5-C6-N1	5.95	120.68	117.70
54	BA	2741	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	547	A	C1'-O4'-C4'	-5.95	105.14	109.90
21	AA	51	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	132	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	1327	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	1508	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	666	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1285	A	C6-C5-N7	5.95	136.47	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1298	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	1602	U	C5-C6-N1	-5.95	119.72	122.70
54	BA	1770	G	N3-C2-N2	-5.95	115.73	119.90
54	BA	2273	A	C5-C6-N1	5.95	120.67	117.70
54	BA	2540	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	2667	C	N3-C2-O2	-5.95	117.73	121.90
55	BB	108	A	C5-C6-N1	5.95	120.67	117.70
54	BA	340	A	N1-C6-N6	-5.95	115.03	118.60
54	BA	571	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	2538	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	2658	C	N3-C2-O2	-5.95	117.74	121.90
21	AA	493	A	O4'-C1'-N9	5.95	112.96	108.20
24	A3	63	C	N3-C4-C5	5.95	124.28	121.90
54	BA	2732	G	C1'-O4'-C4'	-5.95	105.14	109.90
55	BB	111	U	C5-C6-N1	-5.95	119.73	122.70
54	BA	968	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	2519	U	O4'-C1'-N1	5.95	112.96	108.20
55	BB	106	G	N1-C6-O6	-5.95	116.33	119.90
22	A1	72	C	N3-C4-C5	5.94	124.28	121.90
54	BA	182	A	N1-C6-N6	-5.94	115.03	118.60
54	BA	822	G	N1-C6-O6	-5.94	116.33	119.90
54	BA	1128	G	C1'-O4'-C4'	-5.94	105.14	109.90
21	AA	611	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	818	G	O4'-C1'-N9	5.94	112.95	108.20
21	AA	926	G	N1-C6-O6	-5.94	116.33	119.90
51	B2	41	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	209	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	305	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	650	C	C4'-C3'-C2'	-5.94	96.66	102.60
54	BA	873	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1550	C	N1-C2-O2	5.94	122.47	118.90
54	BA	1665	A	C6-C5-N7	5.94	136.46	132.30
54	BA	2200	C	N3-C2-O2	-5.94	117.74	121.90
22	A1	69	A	C5-C6-N1	5.94	120.67	117.70
54	BA	212	G	O4'-C1'-N9	5.94	112.95	108.20
54	BA	1092	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1165	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2757	A	C4-C5-C6	-5.94	114.03	117.00
55	BB	12	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	920	U	N3-C2-O2	-5.94	118.04	122.20
27	BE	170	ARG	NE-CZ-NH1	5.94	123.27	120.30
54	BA	719	C	N1-C2-O2	5.94	122.46	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1562	U	C5-C6-N1	-5.94	119.73	122.70
54	BA	1874	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2426	A	C5-C6-N1	5.94	120.67	117.70
21	AA	941	G	N1-C6-O6	-5.94	116.34	119.90
22	A1	70	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	613	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	2092	U	N1-C2-N3	5.94	118.46	114.90
54	BA	2190	G	C8-N9-C4	-5.94	104.03	106.40
21	AA	1005	A	C6-C5-N7	5.93	136.45	132.30
42	BT	77	ARG	NE-CZ-NH1	5.93	123.27	120.30
54	BA	43	G	C5-C6-N1	5.93	114.47	111.50
54	BA	246	C	O4'-C1'-N1	5.93	112.95	108.20
54	BA	1081	U	C5-C6-N1	-5.93	119.73	122.70
54	BA	1981	A	O4'-C1'-N9	5.93	112.95	108.20
54	BA	2299	U	O4'-C1'-N1	5.93	112.95	108.20
54	BA	2799	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	38	G	N9-C1'-C2'	-5.93	105.47	112.00
21	AA	57	G	N1-C6-O6	-5.93	116.34	119.90
21	AA	658	C	N3-C4-C5	5.93	124.27	121.90
21	AA	821	G	C5-C6-N1	5.93	114.47	111.50
21	AA	1228	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1271	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	541	A	C5-C6-N1	5.93	120.67	117.70
54	BA	1481	U	C5-C6-N1	-5.93	119.73	122.70
54	BA	2336	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	99	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	334	C	N3-C2-O2	-5.93	117.75	121.90
24	A3	3	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	727	G	C5-C6-N1	5.93	114.47	111.50
54	BA	967	U	O4'-C1'-N1	5.93	112.94	108.20
21	AA	680	C	O4'-C1'-N1	5.93	112.94	108.20
54	BA	1241	A	O4'-C1'-N9	5.93	112.94	108.20
54	BA	1705	A	C5-C6-N1	5.93	120.66	117.70
54	BA	2806	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	8	A	C4-C5-C6	-5.93	114.04	117.00
22	A1	28	C	O4'-C1'-N1	5.93	112.94	108.20
25	BC	174	ARG	NE-CZ-NH1	5.93	123.26	120.30
54	BA	677	A	C5-C6-N1	5.93	120.66	117.70
54	BA	817	C	O4'-C1'-N1	5.93	112.94	108.20
54	BA	1347	A	C5-C6-N1	5.93	120.66	117.70
21	AA	913	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	1509	C	N1-C2-O2	5.92	122.45	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	48	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1680	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2174	C	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2516	A	C4-C5-C6	-5.92	114.04	117.00
55	BB	37	C	O4'-C1'-N1	5.92	112.94	108.20
55	BB	102	G	C5-C6-N1	5.92	114.46	111.50
21	AA	197	A	C5-C6-N1	5.92	120.66	117.70
21	AA	210	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	619	U	N3-C2-O2	-5.92	118.05	122.20
54	BA	42	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1515	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1699	G	C5-C6-N1	5.92	114.46	111.50
54	BA	1804	C	N1-C2-O2	5.92	122.45	118.90
21	AA	344	A	C2-N3-C4	5.92	113.56	110.60
54	BA	732	C	O4'-C1'-N1	5.92	112.94	108.20
54	BA	1351	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1513	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	1980	G	C5-C6-N1	5.92	114.46	111.50
54	BA	2802	G	N1-C6-O6	-5.92	116.35	119.90
21	AA	702	A	C3'-C2'-C1'	5.92	106.24	101.50
21	AA	1408	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	1499	A	N1-C6-N6	-5.92	115.05	118.60
21	AA	642	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	79	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	526	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2762	C	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2764	A	N1-C6-N6	-5.92	115.05	118.60
54	BA	2862	G	C5-C6-N1	5.92	114.46	111.50
21	AA	1391	U	C5-C6-N1	-5.92	119.74	122.70
54	BA	577	G	N3-C4-C5	-5.92	125.64	128.60
21	AA	1284	C	O4'-C1'-N1	5.91	112.93	108.20
54	BA	1255	U	C1'-O4'-C4'	-5.91	105.17	109.90
54	BA	1442	U	N3-C2-O2	-5.91	118.06	122.20
54	BA	1646	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1735	A	O4'-C1'-N9	5.91	112.93	108.20
43	BU	85	ARG	NE-CZ-NH1	5.91	123.26	120.30
54	BA	578	G	C5-C6-N1	5.91	114.46	111.50
54	BA	1502	A	C5-C6-N1	5.91	120.66	117.70
21	AA	199	A	C5-C6-N1	5.91	120.66	117.70
21	AA	582	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	794	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1123	C	C6-N1-C2	-5.91	117.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2050	C	N1-C2-O2	5.91	122.45	118.90
55	BB	111	U	O4'-C1'-N1	5.91	112.93	108.20
21	AA	309	A	C5-C6-N1	5.91	120.66	117.70
54	BA	740	C	N1-C2-O2	5.91	122.44	118.90
54	BA	1435	G	C8-N9-C4	-5.91	104.04	106.40
54	BA	1512	C	O4'-C1'-N1	5.91	112.93	108.20
21	AA	518	C	N1-C2-O2	5.91	122.44	118.90
3	AD	72	ARG	NE-CZ-NH1	5.91	123.25	120.30
21	AA	315	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	796	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	2077	A	C5-C6-N1	5.91	120.65	117.70
54	BA	2575	C	N3-C4-C5	5.91	124.26	121.90
21	AA	353	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	1232	U	C5-C6-N1	-5.90	119.75	122.70
54	BA	2170	A	C6-C5-N7	5.90	136.43	132.30
54	BA	2475	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1067	A	C4-C5-C6	-5.90	114.05	117.00
34	BL	123	ARG	NE-CZ-NH1	5.90	123.25	120.30
54	BA	601	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	833	A	C5-C6-N1	5.90	120.65	117.70
54	BA	908	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	2267	A	O4'-C4'-C3'	5.90	110.82	106.10
21	AA	839	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1279	G	N1-C6-O6	-5.90	116.36	119.90
54	BA	897	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	2346	A	C6-C5-N7	5.90	136.43	132.30
54	BA	2505	G	N3-C4-C5	-5.90	125.65	128.60
54	BA	2858	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1432	G	N1-C6-O6	-5.90	116.36	119.90
35	BM	114	ARG	NE-CZ-NH1	5.90	123.25	120.30
54	BA	262	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	2692	G	N3-C4-C5	-5.90	125.65	128.60
21	AA	96	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	1019	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	1282	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	346	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1940	U	N3-C2-O2	-5.90	118.07	122.20
54	BA	2394	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	1535	A	C5-C6-N1	5.90	120.65	117.70
21	AA	1109	C	N1-C2-O2	5.89	122.44	118.90
24	A3	20	G	C5-C6-N1	5.89	114.45	111.50
55	BB	43	C	N3-C2-O2	-5.89	117.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	60	A	P-O3'-C3'	5.89	126.77	119.70
21	AA	1252	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	199	A	O4'-C1'-N9	5.89	112.91	108.20
54	BA	1113	U	N1-C2-N3	5.89	118.44	114.90
54	BA	1713	A	C5-C6-N1	5.89	120.65	117.70
54	BA	176	A	C5-C6-N1	5.89	120.65	117.70
54	BA	2199	A	N1-C6-N6	-5.89	115.07	118.60
21	AA	695	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	1045	C	N1-C2-O2	5.89	122.43	118.90
53	B4	24	ARG	NE-CZ-NH1	5.89	123.25	120.30
54	BA	481	G	C1'-O4'-C4'	-5.89	105.19	109.90
54	BA	1072	C	N1-C2-O2	5.89	122.43	118.90
21	AA	48	C	N1-C2-O2	5.89	122.43	118.90
21	AA	1412	C	N1-C2-O2	5.89	122.43	118.90
54	BA	552	U	C5'-C4'-O4'	5.89	116.17	109.10
54	BA	1584	U	C5-C6-N1	-5.89	119.76	122.70
54	BA	1919	A	C5-C6-N1	5.89	120.64	117.70
21	AA	575	G	P-O3'-C3'	5.89	126.76	119.70
21	AA	705	G	C5-C6-N1	5.89	114.44	111.50
54	BA	34	U	O4'-C1'-N1	5.89	112.91	108.20
54	BA	1039	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	1052	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	968	A	C4-C5-C6	-5.88	114.06	117.00
22	A1	49	G	C5-C6-N1	5.88	114.44	111.50
54	BA	1208	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1708	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	2459	A	C4-C5-C6	-5.88	114.06	117.00
24	A3	36	A	C5-C6-N1	5.88	120.64	117.70
33	BK	71	ARG	NE-CZ-NH1	5.88	123.24	120.30
21	AA	556	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1113	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1152	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	126	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	59	A	N1-C6-N6	-5.88	115.07	118.60
21	AA	163	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	209	U	N3-C2-O2	-5.88	118.08	122.20
21	AA	744	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	914	A	C5-C6-N1	5.88	120.64	117.70
21	AA	1049	U	P-O3'-C3'	5.88	126.75	119.70
21	AA	1096	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	1102	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	24	G	C8-N9-C4	-5.88	104.05	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	188	C	N1-C2-O2	5.88	122.43	118.90
21	AA	1523	G	C5-C6-N1	5.88	114.44	111.50
54	BA	508	A	C5-C6-N1	5.88	120.64	117.70
54	BA	1384	A	C5-C6-N1	5.88	120.64	117.70
55	BB	115	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	945	G	C5-C6-N1	5.87	114.44	111.50
21	AA	1046	A	N1-C6-N6	-5.87	115.08	118.60
21	AA	1082	A	C6-C5-N7	5.87	136.41	132.30
21	AA	1120	C	O4'-C1'-N1	5.87	112.90	108.20
54	BA	1826	G	C8-N9-C4	-5.87	104.05	106.40
21	AA	1061	G	N9-C4-C5	5.87	107.75	105.40
21	AA	1238	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	1522	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2074	U	C5-C6-N1	-5.87	119.77	122.70
54	BA	2123	G	N1-C6-O6	-5.87	116.38	119.90
54	BA	2340	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2511	U	O4'-C1'-N1	5.87	112.90	108.20
21	AA	1273	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2298	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2320	U	C1'-O4'-C4'	-5.87	105.20	109.90
21	AA	1495	U	O4'-C1'-N1	5.87	112.89	108.20
54	BA	240	C	N1-C2-O2	5.87	122.42	118.90
54	BA	1382	G	N3-C4-C5	-5.87	125.67	128.60
54	BA	1945	G	C3'-C2'-C1'	5.87	106.19	101.50
54	BA	2160	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1830	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2847	U	O4'-C1'-N1	5.87	112.89	108.20
55	BB	3	C	O4'-C1'-N1	5.87	112.89	108.20
54	BA	159	G	C5-C6-N1	5.87	114.43	111.50
54	BA	443	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	544	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1575	C	O4'-C1'-N1	5.87	112.89	108.20
54	BA	2662	A	C5-C6-N1	5.87	120.63	117.70
54	BA	2832	U	O4'-C1'-N1	5.87	112.89	108.20
54	BA	987	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1977	A	N1-C6-N6	-5.86	115.08	118.60
55	BB	34	A	C4-C5-C6	-5.86	114.07	117.00
12	AM	2	ARG	NE-CZ-NH1	5.86	123.23	120.30
21	AA	620	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	704	A	C5-C6-N1	5.86	120.63	117.70
21	AA	980	C	N3-C4-C5	5.86	124.25	121.90
54	BA	1780	A	C5-C6-N1	5.86	120.63	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2500	U	C1'-O4'-C4'	-5.86	105.21	109.90
54	BA	2824	C	N1-C2-O2	5.86	122.42	118.90
21	AA	831	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	786	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1145	C	O4'-C1'-N1	5.86	112.89	108.20
54	BA	1379	U	N3-C2-O2	-5.86	118.10	122.20
54	BA	1582	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2039	U	O4'-C1'-N1	5.86	112.89	108.20
54	BA	2900	A	C6-C5-N7	5.86	136.40	132.30
3	AD	153	ARG	NE-CZ-NH2	-5.86	117.37	120.30
21	AA	451	A	O4'-C1'-N9	5.86	112.89	108.20
21	AA	1430	A	C5-C6-N1	5.86	120.63	117.70
54	BA	4	U	C5-C6-N1	-5.86	119.77	122.70
54	BA	1893	C	O4'-C1'-N1	5.86	112.89	108.20
55	BB	95	U	N3-C2-O2	-5.86	118.10	122.20
23	A2	91	A	C5-C6-N1	5.86	120.63	117.70
24	A3	44	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	52	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	795	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	915	C	O4'-C1'-N1	5.86	112.88	108.20
54	BA	986	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1947	C	N1-C2-O2	5.86	122.41	118.90
54	BA	2391	G	N1-C6-O6	-5.86	116.39	119.90
21	AA	216	U	C5-C6-N1	-5.85	119.77	122.70
54	BA	130	C	N1-C2-O2	5.85	122.41	118.90
54	BA	1585	C	N1-C2-O2	5.85	122.41	118.90
55	BB	51	G	C8-N9-C4	-5.85	104.06	106.40
21	AA	465	A	N1-C6-N6	-5.85	115.09	118.60
21	AA	842	U	N3-C2-O2	-5.85	118.10	122.20
22	A1	75	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	806	C	N3-C4-C5	5.85	124.24	121.90
54	BA	1786	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	1879	C	N1-C2-O2	5.85	122.41	118.90
21	AA	1055	A	C5'-C4'-C3'	-5.85	106.64	116.00
31	BI	64	ARG	NE-CZ-NH2	-5.85	117.38	120.30
54	BA	1327	A	C4-C5-C6	-5.85	114.08	117.00
21	AA	34	C	C3'-C2'-C1'	-5.85	96.82	101.50
21	AA	164	G	C8-N9-C4	-5.85	104.06	106.40
21	AA	344	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	21	A	C5-C6-N1	5.85	120.62	117.70
54	BA	382	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	654	A	O4'-C1'-N9	5.85	112.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1455	G	N1-C6-O6	-5.85	116.39	119.90
54	BA	1607	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2091	C	N3-C4-C5	5.85	124.24	121.90
54	BA	2285	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	735	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	878	A	C4-C5-C6	-5.85	114.08	117.00
21	AA	1120	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	833	A	O4'-C1'-N9	5.84	112.88	108.20
54	BA	1248	G	C5-C6-N1	5.84	114.42	111.50
54	BA	1363	C	N1-C2-O2	5.84	122.41	118.90
21	AA	340	U	O4'-C1'-N1	5.84	112.88	108.20
21	AA	521	G	N1-C6-O6	-5.84	116.39	119.90
54	BA	2742	G	N1-C6-O6	-5.84	116.39	119.90
21	AA	802	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1791	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1810	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1942	C	N3-C2-O2	-5.84	117.81	121.90
55	BB	15	A	C1'-O4'-C4'	-5.84	105.23	109.90
21	AA	728	A	C2-N3-C4	5.84	113.52	110.60
21	AA	1024	G	N1-C6-O6	-5.84	116.40	119.90
28	BF	94	ARG	NE-CZ-NH1	5.84	123.22	120.30
54	BA	564	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	1974	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	2083	G	C8-N9-C4	-5.84	104.06	106.40
54	BA	2202	U	C5-C6-N1	-5.84	119.78	122.70
54	BA	2226	C	N1-C2-O2	5.84	122.40	118.90
22	A1	53	G	N1-C6-O6	-5.84	116.40	119.90
21	AA	658	C	N1-C2-O2	5.84	122.40	118.90
54	BA	55	G	N1-C6-O6	-5.84	116.40	119.90
54	BA	1692	U	N1-C2-N3	5.84	118.40	114.90
54	BA	1774	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2496	C	N3-C2-O2	-5.84	117.81	121.90
55	BB	49	C	O4'-C1'-N1	5.84	112.87	108.20
21	AA	653	U	N3-C2-O2	-5.83	118.12	122.20
54	BA	2067	G	O4'-C1'-N9	5.83	112.87	108.20
21	AA	1110	A	C5-C6-N1	5.83	120.62	117.70
54	BA	557	C	O4'-C1'-N1	5.83	112.87	108.20
54	BA	2330	G	N1-C6-O6	-5.83	116.40	119.90
21	AA	212	G	C5-C6-N1	5.83	114.42	111.50
21	AA	440	C	O4'-C1'-N1	5.83	112.86	108.20
21	AA	728	A	C6-C5-N7	5.83	136.38	132.30
54	BA	73	A	C5-C6-N1	5.83	120.62	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	732	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2815	C	O4'-C1'-N1	5.83	112.87	108.20
55	BB	116	G	C8-N9-C4	-5.83	104.07	106.40
21	AA	346	G	N3-C4-C5	-5.83	125.69	128.60
21	AA	687	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	868	C	N1-C2-O2	5.83	122.40	118.90
54	BA	397	U	C5-C6-N1	-5.83	119.79	122.70
21	AA	108	G	N3-C4-C5	-5.83	125.69	128.60
21	AA	531	U	N3-C2-O2	-5.83	118.12	122.20
21	AA	1404	C	C6-N1-C2	-5.83	117.97	120.30
54	BA	1453	A	C5-C6-N1	5.83	120.61	117.70
54	BA	2838	G	O4'-C1'-N9	5.83	112.86	108.20
21	AA	174	A	C5-C6-N1	5.83	120.61	117.70
21	AA	718	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	819	A	C4-C5-C6	-5.83	114.09	117.00
22	A1	30	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	340	A	C5-C6-N1	5.83	120.61	117.70
54	BA	353	C	O4'-C1'-N1	5.83	112.86	108.20
54	BA	2358	A	C6-C5-N7	5.83	136.38	132.30
12	AM	106	ARG	NE-CZ-NH1	5.82	123.21	120.30
24	A3	17	C	N1-C2-O2	5.82	122.39	118.90
54	BA	1076	C	N3-C2-O2	-5.82	117.82	121.90
54	BA	1213	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1679	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	1121	U	C5-C6-N1	-5.82	119.79	122.70
21	AA	368	U	C1'-O4'-C4'	-5.82	105.24	109.90
21	AA	685	G	N3-C4-C5	-5.82	125.69	128.60
54	BA	624	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1594	U	C5-C6-N1	-5.82	119.79	122.70
54	BA	2611	C	C6-N1-C2	-5.82	117.97	120.30
16	AQ	63	CYS	CA-C-N	5.82	130.00	117.20
21	AA	287	U	O4'-C1'-N1	5.82	112.86	108.20
21	AA	452	A	C5-C6-N1	5.82	120.61	117.70
54	BA	2038	G	N3-C4-C5	-5.82	125.69	128.60
54	BA	2687	U	N3-C2-O2	-5.82	118.13	122.20
22	A1	19	G	N1-C6-O6	-5.82	116.41	119.90
54	BA	55	G	C5-C6-N1	5.82	114.41	111.50
54	BA	847	U	N3-C2-O2	-5.82	118.13	122.20
54	BA	1133	A	C5-C6-N1	5.82	120.61	117.70
54	BA	1262	A	C5-C6-N1	5.82	120.61	117.70
54	BA	1293	C	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2285	C	N1-C2-O2	5.82	122.39	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2840	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	37	U	N3-C2-O2	-5.82	118.13	122.20
21	AA	405	U	O4'-C1'-N1	5.82	112.85	108.20
21	AA	1076	U	C5-C6-N1	-5.82	119.79	122.70
54	BA	144	A	O4'-C1'-N9	5.82	112.85	108.20
54	BA	486	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1786	A	N1-C6-N6	-5.82	115.11	118.60
54	BA	2084	C	O4'-C1'-N1	5.82	112.85	108.20
54	BA	2213	U	O4'-C1'-N1	5.82	112.85	108.20
21	AA	6	G	C1'-O4'-C4'	-5.81	105.25	109.90
21	AA	90	C	O4'-C1'-N1	5.81	112.85	108.20
54	BA	1408	G	N3-C4-C5	-5.81	125.69	128.60
54	BA	1726	C	N1-C2-O2	5.81	122.39	118.90
54	BA	1819	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2534	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	50	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	119	A	C5-C6-N1	5.81	120.61	117.70
54	BA	239	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	396	G	N9-C4-C5	5.81	107.72	105.40
54	BA	804	A	C3'-C2'-C1'	5.81	106.15	101.50
54	BA	1572	A	N1-C6-N6	-5.81	115.11	118.60
54	BA	2792	A	C5-C6-N1	5.81	120.61	117.70
54	BA	928	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1442	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	2427	C	N1-C2-O2	5.81	122.39	118.90
21	AA	13	U	O4'-C1'-N1	5.81	112.85	108.20
21	AA	978	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	998	C	N3-C2-O2	-5.81	117.83	121.90
31	BI	102	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
54	BA	357	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	508	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	680	C	O4'-C1'-N1	5.81	112.85	108.20
6	AG	3	ARG	NE-CZ-NH1	5.81	123.20	120.30
7	AH	79	ARG	NE-CZ-NH1	5.81	123.20	120.30
21	AA	460	A	C5-C6-N1	5.81	120.60	117.70
21	AA	918	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	2403	C	N1-C2-O2	5.81	122.39	118.90
54	BA	2670	A	N1-C6-N6	-5.81	115.11	118.60
55	BB	118	C	N3-C4-C5	5.81	124.22	121.90
54	BA	1783	A	C6-C5-N7	5.81	136.36	132.30
21	AA	512	U	C5-C6-N1	-5.80	119.80	122.70
21	AA	1521	C	N3-C2-O2	-5.80	117.84	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	493	G	C5-C6-N1	5.80	114.40	111.50
54	BA	681	G	C5-C6-N1	5.80	114.40	111.50
54	BA	1855	U	O4'-C1'-N1	5.80	112.84	108.20
55	BB	95	U	C5-C6-N1	-5.80	119.80	122.70
24	A3	68	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2079	U	C5-C6-N1	-5.80	119.80	122.70
55	BB	13	G	N3-C2-N2	-5.80	115.84	119.90
21	AA	437	U	O4'-C1'-N1	5.80	112.84	108.20
21	AA	557	G	N1-C6-O6	-5.80	116.42	119.90
21	AA	1239	A	C6-C5-N7	5.80	136.36	132.30
21	AA	1299	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1053	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1174	U	O4'-C1'-N1	5.80	112.84	108.20
54	BA	1214	A	C5-C6-N1	5.80	120.60	117.70
54	BA	2215	C	O4'-C1'-N1	5.80	112.84	108.20
54	BA	59	U	C5-C6-N1	-5.80	119.80	122.70
54	BA	105	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	2217	G	C5-C6-N1	5.80	114.40	111.50
54	BA	2826	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	758	C	N1-C2-O2	5.80	122.38	118.90
54	BA	1561	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	318	G	C5-C6-N1	5.80	114.40	111.50
21	AA	579	A	C5-C6-N1	5.80	120.60	117.70
54	BA	53	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	139	U	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2608	G	N3-C4-C5	-5.80	125.70	128.60
21	AA	454	G	N3-C4-C5	-5.79	125.70	128.60
21	AA	660	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	1888	G	O4'-C1'-N9	5.79	112.84	108.20
54	BA	1895	C	N1-C2-O2	5.79	122.38	118.90
54	BA	2723	C	N1-C2-O2	5.79	122.38	118.90
21	AA	83	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	183	C	N3-C4-C5	5.79	124.22	121.90
21	AA	1094	G	O4'-C1'-N9	5.79	112.83	108.20
21	AA	1100	C	C2-N3-C4	-5.79	117.00	119.90
21	AA	1523	G	N1-C6-O6	-5.79	116.42	119.90
54	BA	706	A	C5-C6-N1	5.79	120.60	117.70
54	BA	914	G	N1-C6-O6	-5.79	116.42	119.90
54	BA	1877	A	C5-C6-N1	5.79	120.60	117.70
54	BA	2043	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	2166	U	C5-C6-N1	-5.79	119.80	122.70
54	BA	2369	A	N1-C6-N6	-5.79	115.12	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2427	C	N3-C4-C5	5.79	124.22	121.90
21	AA	95	C	N3-C2-O2	-5.79	117.84	121.90
21	AA	330	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	171	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1103	A	C5-C6-N1	5.79	120.60	117.70
54	BA	1229	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	416	U	O4'-C1'-N1	5.79	112.83	108.20
21	AA	1352	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1264	A	O4'-C1'-N9	5.79	112.83	108.20
54	BA	1754	A	N1-C6-N6	-5.79	115.13	118.60
54	BA	2725	A	C5-C6-N1	5.79	120.59	117.70
54	BA	193	U	N1-C2-N3	5.79	118.37	114.90
54	BA	1929	G	O4'-C1'-N9	5.79	112.83	108.20
54	BA	2730	C	N3-C2-O2	-5.79	117.85	121.90
47	BY	7	ARG	NE-CZ-NH1	5.79	123.19	120.30
54	BA	394	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	885	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2725	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	906	A	N1-C6-N6	-5.78	115.13	118.60
21	AA	1509	C	N3-C4-C5	5.78	124.21	121.90
54	BA	78	U	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2210	U	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2480	C	N3-C2-O2	-5.78	117.85	121.90
10	AK	36	ARG	NE-CZ-NH1	5.78	123.19	120.30
21	AA	97	G	C5-C6-N1	5.78	114.39	111.50
54	BA	480	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	975	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	335	C	O4'-C1'-N1	5.78	112.82	108.20
21	AA	653	U	C3'-C2'-C1'	5.78	106.12	101.50
21	AA	1400	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	1412	C	N3-C4-C5	5.78	124.21	121.90
54	BA	1121	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	1402	U	C5-C6-N1	-5.78	119.81	122.70
54	BA	1952	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2018	G	N1-C6-O6	-5.78	116.43	119.90
2	AC	10	ARG	NE-CZ-NH2	-5.78	117.41	120.30
21	AA	1064	G	C8-N9-C4	-5.78	104.09	106.40
54	BA	1099	G	N7-C8-N9	5.78	115.99	113.10
54	BA	2128	G	C8-N9-C4	-5.78	104.09	106.40
21	AA	1161	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	811	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	1960	A	C6-C5-N7	5.78	136.34	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2651	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	2760	C	O4'-C1'-N1	5.78	112.82	108.20
15	AP	8	ARG	NE-CZ-NH1	5.78	123.19	120.30
21	AA	715	A	O4'-C1'-N9	5.78	112.82	108.20
21	AA	1063	C	N3-C4-C5	5.78	124.21	121.90
35	BM	114	ARG	NE-CZ-NH2	-5.78	117.41	120.30
51	B2	28	ARG	NE-CZ-NH1	5.78	123.19	120.30
54	BA	1149	G	C5'-C4'-O4'	5.78	116.03	109.10
54	BA	1589	U	C5-C6-N1	-5.78	119.81	122.70
54	BA	1797	G	O4'-C1'-N9	5.78	112.82	108.20
54	BA	2111	U	O4'-C1'-N1	5.78	112.82	108.20
55	BB	118	C	N1-C2-O2	5.78	122.36	118.90
21	AA	833	G	N1-C6-O6	-5.77	116.44	119.90
24	A3	63	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	485	C	N1-C2-O2	5.77	122.36	118.90
54	BA	2029	G	O4'-C1'-N9	5.77	112.82	108.20
2	AC	71	ARG	NE-CZ-NH1	5.77	123.19	120.30
21	AA	508	U	C5-C6-N1	-5.77	119.81	122.70
21	AA	917	G	N7-C8-N9	5.77	115.99	113.10
21	AA	1371	G	N3-C2-N2	-5.77	115.86	119.90
21	AA	1465	A	N1-C6-N6	-5.77	115.14	118.60
22	A1	73	A	N1-C6-N6	-5.77	115.14	118.60
54	BA	698	C	N1-C2-O2	5.77	122.36	118.90
54	BA	1697	G	N7-C8-N9	5.77	115.99	113.10
54	BA	2616	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	1477	U	C5-C6-N1	-5.77	119.81	122.70
54	BA	1772	A	O4'-C1'-N9	5.77	112.82	108.20
54	BA	2428	G	N9-C4-C5	5.77	107.71	105.40
4	AE	28	ARG	NE-CZ-NH1	5.77	123.19	120.30
23	A2	88	U	C5-C6-N1	-5.77	119.81	122.70
54	BA	587	C	N3-C4-C5	5.77	124.21	121.90
54	BA	1456	G	N1-C6-O6	-5.77	116.44	119.90
54	BA	2446	G	C8-N9-C4	-5.77	104.09	106.40
21	AA	926	G	N3-C4-C5	-5.77	125.72	128.60
54	BA	10	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	1767	G	C5-C6-N1	5.77	114.38	111.50
21	AA	19	A	C5-C6-N1	5.77	120.58	117.70
21	AA	1349	A	C5-C6-N1	5.77	120.58	117.70
54	BA	1029	A	O4'-C1'-N9	5.77	112.81	108.20
21	AA	86	G	N3-C2-N2	-5.76	115.86	119.90
21	AA	483	C	N3-C2-O2	-5.76	117.86	121.90
23	A2	87	U	N1-C2-N3	5.76	118.36	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	272	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	863	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	961	C	O4'-C1'-N1	5.76	112.81	108.20
54	BA	1324	G	N1-C6-O6	-5.76	116.44	119.90
21	AA	1308	U	N3-C2-O2	-5.76	118.17	122.20
21	AA	1519	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1153	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2197	U	C5-C6-N1	-5.76	119.82	122.70
54	BA	2376	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	997	U	O4'-C1'-N1	5.76	112.81	108.20
21	AA	1476	A	C4-C5-C6	-5.76	114.12	117.00
24	A3	2	G	C5-C6-N1	5.76	114.38	111.50
54	BA	360	U	C5-C6-N1	-5.76	119.82	122.70
54	BA	501	A	N1-C6-N6	-5.76	115.14	118.60
54	BA	385	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2250	G	O4'-C1'-C2'	-5.76	100.04	105.80
21	AA	1181	G	O4'-C1'-N9	5.76	112.81	108.20
54	BA	593	U	O4'-C1'-N1	5.76	112.81	108.20
54	BA	1204	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1332	G	C5-C6-N1	5.76	114.38	111.50
54	BA	2354	C	O4'-C1'-N1	5.76	112.81	108.20
21	AA	282	A	C5-C6-N1	5.76	120.58	117.70
21	AA	422	C	N3-C4-C5	5.76	124.20	121.90
54	BA	309	A	C5-C6-N1	5.76	120.58	117.70
54	BA	2356	U	O4'-C1'-N1	5.76	112.81	108.20
54	BA	2425	A	C5-C6-N1	5.76	120.58	117.70
55	BB	24	G	C3'-C2'-C1'	5.76	106.11	101.50
21	AA	20	U	C5-C6-N1	-5.75	119.82	122.70
21	AA	848	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	883	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	2378	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	164	G	C1'-O4'-C4'	-5.75	105.30	109.90
21	AA	1426	G	C8-N9-C4	-5.75	104.10	106.40
33	BK	17	ARG	NE-CZ-NH1	5.75	123.18	120.30
54	BA	439	A	N1-C6-N6	-5.75	115.15	118.60
54	BA	1314	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	1814	G	N1-C6-O6	-5.75	116.45	119.90
54	BA	2821	A	C5-C6-N1	5.75	120.58	117.70
1	AB	207	ARG	NE-CZ-NH1	5.75	123.18	120.30
54	BA	1089	A	C2-N3-C4	5.75	113.47	110.60
21	AA	1128	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	1261	C	O4'-C1'-N1	5.75	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1887	C	C6-N1-C2	-5.75	118.00	120.30
21	AA	421	U	C2-N1-C1'	5.75	124.60	117.70
54	BA	2234	G	C8-N9-C4	-5.75	104.10	106.40
25	BC	101	ARG	NE-CZ-NH2	-5.75	117.43	120.30
54	BA	1216	G	C5-C6-N1	5.75	114.37	111.50
54	BA	1260	A	C5-C6-N1	5.75	120.57	117.70
54	BA	1585	C	N3-C4-C5	5.75	124.20	121.90
21	AA	427	U	N3-C2-O2	-5.75	118.18	122.20
21	AA	1296	C	N3-C2-O2	-5.75	117.88	121.90
3	AD	72	ARG	NE-CZ-NH2	-5.74	117.43	120.30
10	AK	68	ARG	NE-CZ-NH1	5.74	123.17	120.30
21	AA	148	G	C5-C6-N1	5.74	114.37	111.50
21	AA	209	U	C1'-O4'-C4'	-5.74	105.31	109.90
21	AA	274	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2530	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	55	A	C5-C6-N1	5.74	120.57	117.70
54	BA	420	C	C6-N1-C2	-5.74	118.00	120.30
54	BA	1319	C	N1-C2-O2	5.74	122.34	118.90
54	BA	2496	C	O4'-C1'-N1	5.74	112.79	108.20
21	AA	1067	A	C5-C6-N1	5.74	120.57	117.70
54	BA	527	C	N1-C1'-C2'	5.74	121.46	114.00
54	BA	1334	G	O4'-C1'-N9	5.74	112.79	108.20
21	AA	122	G	N1-C6-O6	-5.74	116.46	119.90
21	AA	865	A	C5-C6-N1	5.74	120.57	117.70
21	AA	1320	C	N3-C4-N4	-5.74	113.98	118.00
54	BA	310	A	C5-C6-N1	5.74	120.57	117.70
54	BA	324	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2060	A	P-O3'-C3'	5.74	126.58	119.70
21	AA	1280	A	C5-C6-N1	5.74	120.57	117.70
21	AA	1288	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2051	A	C3'-C2'-C1'	5.74	106.09	101.50
21	AA	113	G	C8-N9-C4	-5.74	104.11	106.40
21	AA	199	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	775	G	N3-C2-N2	-5.74	115.89	119.90
54	BA	270	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	679	C	N3-C2-O2	-5.74	117.89	121.90
54	BA	1531	C	C3'-C2'-C1'	5.74	106.09	101.50
54	BA	1533	C	N3-C4-C5	5.74	124.19	121.90
54	BA	2301	C	N3-C2-O2	-5.74	117.89	121.90
21	AA	227	G	N3-C4-C5	-5.73	125.73	128.60
21	AA	336	A	C6-C5-N7	5.73	136.31	132.30
54	BA	1600	C	O4'-C1'-N1	5.73	112.79	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2837	A	N1-C6-N6	-5.73	115.16	118.60
21	AA	285	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	575	G	N1-C6-O6	-5.73	116.46	119.90
54	BA	201	C	N3-C4-C5	5.73	124.19	121.90
54	BA	2306	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2465	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2521	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2755	C	C6-N1-C2	-5.73	118.01	120.30
21	AA	138	G	C1'-O4'-C4'	-5.73	105.32	109.90
44	BV	21	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	1009	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1152	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1587	G	O4'-C1'-N9	5.73	112.78	108.20
54	BA	1801	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1477	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	1511	G	O4'-C1'-N9	5.73	112.78	108.20
55	BB	62	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1913	A	C5-C6-N1	5.73	120.56	117.70
54	BA	2101	A	N1-C6-N6	-5.73	115.16	118.60
22	A1	66	A	C4-C5-C6	-5.72	114.14	117.00
51	B2	35	ARG	NE-CZ-NH1	5.72	123.16	120.30
54	BA	650	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	274	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	902	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	960	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1881	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	2042	A	C5-C6-N1	5.72	120.56	117.70
21	AA	34	C	C5'-C4'-C3'	-5.72	106.85	116.00
21	AA	755	G	C3'-C2'-C1'	5.72	106.08	101.50
21	AA	977	A	C2-N3-C4	5.72	113.46	110.60
21	AA	1492	A	N1-C6-N6	-5.72	115.17	118.60
54	BA	2274	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	209	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	379	C	N1-C2-O2	5.72	122.33	118.90
21	AA	735	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	1437	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	782	A	O4'-C1'-N9	5.72	112.78	108.20
54	BA	1499	C	O4'-C1'-N1	5.72	112.78	108.20
54	BA	1556	C	N3-C4-C5	5.72	124.19	121.90
21	AA	1006	G	N3-C2-N2	-5.72	115.90	119.90
54	BA	748	G	N9-C4-C5	5.72	107.69	105.40
54	BA	1144	A	C4-C5-C6	-5.72	114.14	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	781	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	1501	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	32	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	2020	A	C5'-C4'-C3'	-5.72	106.86	116.00
54	BA	2639	A	C5-C6-N1	5.72	120.56	117.70
21	AA	233	C	N1-C2-O2	5.71	122.33	118.90
21	AA	666	G	N3-C2-N2	-5.71	115.90	119.90
21	AA	969	A	C6-C5-N7	5.71	136.30	132.30
54	BA	586	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1042	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1262	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1508	A	O4'-C1'-N9	5.71	112.77	108.20
55	BB	36	C	N1-C2-O2	5.71	122.33	118.90
55	BB	57	A	C4-C5-C6	-5.71	114.14	117.00
21	AA	732	C	N1-C2-O2	5.71	122.33	118.90
21	AA	859	G	C5-C6-N1	5.71	114.36	111.50
50	B1	27	ARG	NE-CZ-NH1	5.71	123.16	120.30
54	BA	309	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	748	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1271	G	C5-C6-N1	5.71	114.36	111.50
54	BA	1342	A	C5-C6-N1	5.71	120.56	117.70
54	BA	1343	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1541	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	2119	A	C5-C6-N1	5.71	120.56	117.70
54	BA	2425	A	O4'-C1'-N9	5.71	112.77	108.20
54	BA	2575	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	488	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	2055	C	C3'-C2'-C1'	-5.71	96.93	101.50
3	AD	114	ARG	NE-CZ-NH1	5.71	123.15	120.30
21	AA	179	A	C5-C6-N1	5.71	120.55	117.70
21	AA	1063	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1463	U	C5-C6-N1	-5.71	119.85	122.70
22	A1	58	A	C4-C5-C6	-5.71	114.14	117.00
39	BQ	2	ARG	NE-CZ-NH1	5.71	123.15	120.30
54	BA	623	C	N1-C2-O2	5.71	122.33	118.90
54	BA	810	U	C5-C6-N1	-5.71	119.85	122.70
14	AO	71	ARG	NE-CZ-NH1	5.71	123.15	120.30
21	AA	372	C	N3-C4-C5	5.71	124.18	121.90
23	A2	79	A	C2-N3-C4	5.71	113.45	110.60
21	AA	865	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	948	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1164	C	N3-C2-O2	-5.70	117.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2127	G	O4'-C1'-N9	5.70	112.76	108.20
6	AG	137	ARG	NE-CZ-NH2	-5.70	117.45	120.30
21	AA	528	C	N1-C2-O2	5.70	122.32	118.90
21	AA	1078	U	O4'-C1'-N1	5.70	112.76	108.20
21	AA	1528	U	C5-C6-N1	-5.70	119.85	122.70
7	AH	116	ARG	NE-CZ-NH1	5.70	123.15	120.30
21	AA	749	A	C6-C5-N7	5.70	136.29	132.30
21	AA	1285	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	331	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1378	A	N1-C6-N6	-5.70	115.18	118.60
54	BA	1979	U	C5-C6-N1	-5.70	119.85	122.70
54	BA	2427	C	C1'-O4'-C4'	-5.70	105.34	109.90
21	AA	1020	G	N1-C6-O6	-5.70	116.48	119.90
54	BA	168	G	C5-C6-N1	5.70	114.35	111.50
54	BA	437	U	N3-C2-O2	-5.70	118.21	122.20
54	BA	776	G	C8-N9-C4	-5.70	104.12	106.40
21	AA	466	A	C2-N3-C4	5.70	113.45	110.60
21	AA	1063	C	N1-C2-O2	5.70	122.32	118.90
54	BA	435	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1122	G	N3-C2-N2	-5.70	115.91	119.90
54	BA	1830	C	C6-N1-C2	-5.70	118.02	120.30
21	AA	189	A	N1-C6-N6	-5.70	115.18	118.60
54	BA	265	A	C5-C6-N1	5.70	120.55	117.70
54	BA	825	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1207	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	1454	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1761	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	124	C	N1-C2-O2	5.69	122.32	118.90
21	AA	167	A	C5-C6-N1	5.69	120.55	117.70
39	BQ	32	ARG	NE-CZ-NH2	5.69	123.15	120.30
54	BA	359	G	O4'-C1'-N9	5.69	112.75	108.20
54	BA	478	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2710	C	N1-C2-O2	5.69	122.32	118.90
21	AA	151	A	C5-C6-N1	5.69	120.55	117.70
21	AA	844	G	N7-C8-N9	5.69	115.95	113.10
21	AA	1428	A	C6-C5-N7	5.69	136.28	132.30
54	BA	148	U	C3'-C2'-C1'	5.69	106.06	101.50
54	BA	180	G	N1-C6-O6	-5.69	116.48	119.90
54	BA	1539	U	N3-C2-O2	-5.69	118.22	122.20
54	BA	2807	U	O4'-C1'-N1	5.69	112.75	108.20
21	AA	618	C	N1-C2-O2	5.69	122.31	118.90
24	A3	47	G	C3'-C2'-C1'	5.69	106.05	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	730	A	C5'-C4'-O4'	5.69	115.93	109.10
54	BA	859	G	C4'-C3'-C2'	-5.69	96.91	102.60
54	BA	2794	C	N1-C2-O2	5.69	122.31	118.90
21	AA	129	A	C6-C5-N7	5.69	136.28	132.30
21	AA	720	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1409	U	O4'-C1'-N1	5.69	112.75	108.20
54	BA	1727	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1963	U	N3-C2-O2	-5.69	118.22	122.20
54	BA	2277	G	N1-C6-O6	-5.69	116.49	119.90
54	BA	2442	C	N1-C2-O2	5.69	122.31	118.90
21	AA	892	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1833	C	N1-C2-O2	5.69	122.31	118.90
54	BA	1969	A	C6-C5-N7	5.69	136.28	132.30
13	AN	69	ARG	NE-CZ-NH1	5.68	123.14	120.30
21	AA	165	G	N1-C6-O6	-5.68	116.49	119.90
21	AA	309	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	558	G	C5-C6-N1	5.68	114.34	111.50
54	BA	431	U	N3-C2-O2	-5.68	118.22	122.20
54	BA	1359	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	246	A	C1'-O4'-C4'	-5.68	105.35	109.90
21	AA	985	C	N1-C2-O2	5.68	122.31	118.90
21	AA	1153	G	C5-C6-N1	5.68	114.34	111.50
54	BA	64	A	C2-N3-C4	5.68	113.44	110.60
54	BA	348	A	C6-C5-N7	5.68	136.28	132.30
54	BA	1775	U	O4'-C1'-N1	5.68	112.75	108.20
55	BB	2	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	1732	C	N1-C2-O2	5.68	122.31	118.90
54	BA	2290	G	C5-C6-N1	5.68	114.34	111.50
54	BA	2476	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	9	G	C5-C6-N1	5.68	114.34	111.50
21	AA	827	U	C5-C6-N1	-5.68	119.86	122.70
21	AA	844	G	C8-N9-C4	-5.68	104.13	106.40
54	BA	184	C	O4'-C1'-N1	5.68	112.74	108.20
54	BA	564	C	N3-C4-C5	5.68	124.17	121.90
54	BA	797	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	1209	U	C5-C6-N1	-5.68	119.86	122.70
54	BA	1597	A	O4'-C4'-C3'	5.68	110.64	106.10
21	AA	874	G	N3-C4-C5	-5.68	125.76	128.60
21	AA	1092	A	C5-C6-N1	5.68	120.54	117.70
24	A3	52	C	N3-C2-O2	-5.68	117.93	121.90
26	BD	179	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	851	C	N3-C2-O2	-5.68	117.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	90	C	N3-C2-O2	-5.68	117.92	121.90
21	AA	509	A	O4'-C1'-N9	5.68	112.74	108.20
21	AA	1225	A	N1-C6-N6	-5.68	115.19	118.60
21	AA	1297	G	O4'-C1'-N9	5.68	112.74	108.20
21	AA	1497	G	C5-C6-N1	5.68	114.34	111.50
54	BA	161	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	300	A	N1-C6-N6	-5.68	115.19	118.60
54	BA	359	G	N1-C6-O6	-5.68	116.49	119.90
54	BA	438	G	C5-C6-N1	5.68	114.34	111.50
21	AA	177	G	O4'-C1'-N9	5.67	112.74	108.20
21	AA	192	A	C6-C5-N7	5.67	136.27	132.30
21	AA	204	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	803	G	C5-C6-N1	5.67	114.34	111.50
21	AA	933	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	1217	C	N1-C2-O2	5.67	122.31	118.90
21	AA	1468	A	C4-C5-C6	-5.67	114.16	117.00
35	BM	10	ARG	NE-CZ-NH1	5.67	123.14	120.30
54	BA	1728	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1872	A	C5-C6-N1	5.67	120.54	117.70
54	BA	2636	C	N1-C2-O2	5.67	122.31	118.90
54	BA	2823	A	C5-C6-N1	5.67	120.54	117.70
55	BB	24	G	C4-C5-N7	-5.67	108.53	110.80
55	BB	99	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1472	C	N3-C4-C5	5.67	124.17	121.90
54	BA	1527	G	N3-C4-C5	-5.67	125.76	128.60
54	BA	2022	U	C5-C6-N1	-5.67	119.86	122.70
54	BA	2353	G	C4'-C3'-C2'	-5.67	96.93	102.60
21	AA	919	A	C4-C5-C6	-5.67	114.16	117.00
21	AA	1458	G	N3-C4-C5	-5.67	125.76	128.60
40	BR	21	ARG	NE-CZ-NH2	-5.67	117.47	120.30
54	BA	392	U	N3-C2-O2	-5.67	118.23	122.20
54	BA	1657	U	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2090	A	C6-C5-N7	5.67	136.27	132.30
54	BA	2625	G	C5-C6-N1	5.67	114.34	111.50
21	AA	1450	U	N3-C2-O2	-5.67	118.23	122.20
54	BA	41	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2378	A	C5-C6-N1	5.67	120.53	117.70
8	AI	79	ARG	NE-CZ-NH1	5.67	123.13	120.30
54	BA	396	G	N1-C6-O6	-5.67	116.50	119.90
54	BA	471	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	2844	G	C5-C6-N1	5.67	114.33	111.50
21	AA	398	U	C5-C6-N1	-5.67	119.87	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	525	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	776	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	1408	A	C5-C6-N1	5.67	120.53	117.70
54	BA	793	A	C6-C5-N7	5.67	136.27	132.30
54	BA	1162	G	N1-C6-O6	-5.67	116.50	119.90
54	BA	1790	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2246	G	C5-C6-N1	5.67	114.33	111.50
54	BA	2314	A	C5-C6-N1	5.67	120.53	117.70
54	BA	787	C	O4'-C1'-N1	5.67	112.73	108.20
54	BA	885	C	N1-C2-O2	5.67	122.30	118.90
54	BA	1121	C	N1-C2-O2	5.67	122.30	118.90
54	BA	1302	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	1798	U	O4'-C1'-N1	5.67	112.73	108.20
54	BA	2102	G	C8-N9-C4	-5.67	104.13	106.40
54	BA	1259	G	C5-C6-N1	5.66	114.33	111.50
54	BA	2336	A	C5-C6-N1	5.66	120.53	117.70
54	BA	2620	C	N3-C4-C5	5.66	124.17	121.90
54	BA	783	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	893	C	N1-C2-O2	5.66	122.30	118.90
21	AA	1430	A	N1-C6-N6	-5.66	115.20	118.60
54	BA	60	G	C5-C6-N1	5.66	114.33	111.50
54	BA	343	C	N3-C4-C5	5.66	124.16	121.90
54	BA	1211	C	N3-C4-C5	5.66	124.16	121.90
54	BA	1730	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	953	G	C8-N9-C4	-5.66	104.14	106.40
21	AA	1093	A	C1'-O4'-C4'	-5.66	105.37	109.90
54	BA	1369	G	N1-C6-O6	-5.66	116.51	119.90
54	BA	2267	A	C3'-C2'-C1'	5.66	106.03	101.50
8	AI	121	ARG	NE-CZ-NH2	-5.66	117.47	120.30
21	AA	646	G	N1-C6-O6	-5.66	116.51	119.90
54	BA	128	C	O4'-C1'-N1	5.66	112.72	108.20
54	BA	839	U	N1-C2-N3	5.66	118.29	114.90
54	BA	2209	G	C5-C6-N1	5.66	114.33	111.50
54	BA	2576	G	C2-N3-C4	5.66	114.73	111.90
54	BA	522	A	C5-C6-N1	5.65	120.53	117.70
21	AA	729	A	N1-C6-N6	-5.65	115.21	118.60
21	AA	863	U	N1-C2-N3	5.65	118.29	114.90
54	BA	49	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	101	A	O4'-C1'-N9	5.65	112.72	108.20
54	BA	542	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1180	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	2029	G	C5-C6-N1	5.65	114.33	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2230	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	2707	U	O4'-C1'-N1	5.65	112.72	108.20
21	AA	234	C	N1-C2-O2	5.65	122.29	118.90
21	AA	759	A	C4-C5-C6	-5.65	114.17	117.00
49	B0	39	ARG	NE-CZ-NH1	5.65	123.12	120.30
54	BA	274	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	401	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1436	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	2268	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	82	U	N1-C2-N3	5.65	118.29	114.90
21	AA	1201	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	1373	G	C5-C6-N1	5.65	114.32	111.50
31	BI	126	ARG	NE-CZ-NH2	-5.65	117.48	120.30
54	BA	340	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	2730	C	O4'-C1'-N1	5.65	112.72	108.20
55	BB	70	C	N1-C2-O2	5.65	122.29	118.90
54	BA	27	G	N3-C4-C5	-5.65	125.78	128.60
54	BA	152	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	393	C	N3-C2-O2	-5.65	117.95	121.90
54	BA	884	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1590	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	66	A	C5-C6-N1	5.64	120.52	117.70
21	AA	84	U	N3-C2-O2	-5.64	118.25	122.20
21	AA	204	G	N3-C4-C5	-5.64	125.78	128.60
21	AA	429	U	C5-C6-N1	-5.64	119.88	122.70
21	AA	522	C	N1-C2-O2	5.64	122.29	118.90
54	BA	738	G	N3-C4-C5	-5.64	125.78	128.60
54	BA	1199	U	O4'-C1'-N1	5.64	112.72	108.20
54	BA	1574	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1956	U	O4'-C1'-N1	5.64	112.72	108.20
54	BA	2540	C	N1-C2-O2	5.64	122.29	118.90
21	AA	734	G	C8-N9-C4	-5.64	104.14	106.40
54	BA	1994	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	2863	C	N3-C4-C5	5.64	124.16	121.90
21	AA	639	G	C5-C6-N1	5.64	114.32	111.50
21	AA	970	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	1341	U	N1-C2-N3	5.64	118.28	114.90
54	BA	207	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1210	G	N1-C6-O6	-5.64	116.52	119.90
54	BA	1314	C	N1-C2-O2	5.64	122.28	118.90
54	BA	1353	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1882	U	N1-C2-N3	5.64	118.28	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2054	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2083	G	N9-C4-C5	5.64	107.66	105.40
21	AA	1050	G	C5-C6-N1	5.64	114.32	111.50
52	B3	41	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	44	A	C5-C6-N1	5.64	120.52	117.70
54	BA	160	A	C5'-C4'-O4'	5.64	115.86	109.10
54	BA	816	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	1189	U	N3-C2-O2	-5.64	118.25	122.20
21	AA	1396	A	O4'-C1'-N9	5.64	112.71	108.20
54	BA	1869	G	N3-C4-C5	-5.64	125.78	128.60
54	BA	2250	G	N3-C2-N2	-5.64	115.95	119.90
21	AA	1184	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	1401	G	C5-C6-N1	5.63	114.32	111.50
25	BC	166	ARG	NE-CZ-NH1	5.63	123.12	120.30
54	BA	855	G	N3-C2-N2	-5.63	115.96	119.90
54	BA	1225	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	1594	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	2562	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	2661	G	C5-C6-N1	5.63	114.32	111.50
21	AA	20	U	N1-C2-N3	5.63	118.28	114.90
21	AA	1337	G	C5-C6-N1	5.63	114.32	111.50
54	BA	1964	G	C5-C6-N1	5.63	114.32	111.50
21	AA	794	A	C5-C6-N1	5.63	120.52	117.70
21	AA	1016	A	C4-C5-C6	-5.63	114.18	117.00
22	A1	75	C	N3-C4-C5	5.63	124.15	121.90
54	BA	100	U	O4'-C1'-N1	5.63	112.71	108.20
54	BA	620	G	O4'-C1'-N9	5.63	112.70	108.20
54	BA	1029	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	1253	A	O4'-C1'-N9	5.63	112.70	108.20
54	BA	2439	A	C4-C5-C6	-5.63	114.18	117.00
5	AF	38	ARG	NE-CZ-NH1	5.63	123.11	120.30
54	BA	806	C	N1-C2-O2	5.63	122.28	118.90
21	AA	342	C	N3-C4-C5	5.63	124.15	121.90
21	AA	1182	G	N9-C4-C5	5.63	107.65	105.40
54	BA	358	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	620	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	2417	C	O4'-C1'-N1	5.63	112.70	108.20
3	AD	12	ARG	NH1-CZ-NH2	-5.63	113.21	119.40
21	AA	767	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	847	G	N1-C6-O6	-5.63	116.52	119.90
24	A3	49	C	O4'-C1'-N1	5.63	112.70	108.20
54	BA	823	C	N1-C2-O2	5.63	122.28	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1457	U	O4'-C1'-N1	5.63	112.70	108.20
21	AA	272	C	N1-C2-O2	5.62	122.28	118.90
54	BA	1508	A	C4-C5-C6	-5.62	114.19	117.00
55	BB	68	C	N3-C2-O2	-5.62	117.96	121.90
3	AD	45	PRO	C-N-CA	5.62	135.76	121.70
21	AA	155	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	202	G	C5-C6-N1	5.62	114.31	111.50
21	AA	328	C	P-O3'-C3'	5.62	126.45	119.70
21	AA	1085	U	N3-C2-O2	-5.62	118.26	122.20
54	BA	743	A	C5-C6-N1	5.62	120.51	117.70
54	BA	992	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	1351	C	O4'-C1'-N1	5.62	112.70	108.20
54	BA	1381	G	N3-C2-N2	-5.62	115.96	119.90
21	AA	602	A	C5-C6-N1	5.62	120.51	117.70
22	A1	17	U	N1-C2-N3	5.62	118.27	114.90
54	BA	3	U	O4'-C1'-N1	5.62	112.70	108.20
54	BA	111	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	695	G	N3-C2-N2	-5.62	115.97	119.90
54	BA	1161	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1432	G	C5-C6-N1	5.62	114.31	111.50
54	BA	2028	U	C4-C5-C6	5.62	123.07	119.70
54	BA	2854	G	O4'-C1'-N9	5.62	112.70	108.20
21	AA	96	U	C5-C6-N1	-5.62	119.89	122.70
21	AA	1450	U	C5-C6-N1	-5.62	119.89	122.70
22	A1	40	G	N3-C2-N2	-5.62	115.97	119.90
54	BA	170	U	O4'-C1'-N1	5.62	112.69	108.20
54	BA	565	C	N1-C2-O2	5.62	122.27	118.90
54	BA	608	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2112	G	N3-C2-N2	-5.62	115.97	119.90
54	BA	2482	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	109	A	O4'-C1'-N9	5.62	112.69	108.20
21	AA	1036	A	O4'-C1'-N9	5.62	112.69	108.20
54	BA	2545	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	2772	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	2846	G	N9-C4-C5	5.62	107.65	105.40
21	AA	890	G	O4'-C1'-N9	5.62	112.69	108.20
21	AA	1089	G	N3-C2-N2	-5.62	115.97	119.90
21	AA	1472	U	O4'-C1'-N1	5.62	112.69	108.20
33	BK	108	ARG	NE-CZ-NH1	5.62	123.11	120.30
36	BN	22	ARG	NE-CZ-NH1	5.62	123.11	120.30
49	B0	51	ARG	NE-CZ-NH1	5.62	123.11	120.30
54	BA	1345	C	N3-C4-C5	5.62	124.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1796	U	O4'-C1'-N1	5.62	112.69	108.20
54	BA	2080	A	C6-C5-N7	5.62	136.23	132.30
21	AA	289	G	C5-C6-N1	5.61	114.31	111.50
21	AA	843	U	N3-C2-O2	-5.61	118.27	122.20
54	BA	33	C	N3-C4-C5	5.61	124.14	121.90
54	BA	211	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	475	C	N3-C4-C5	5.61	124.15	121.90
54	BA	1537	G	C5-C6-N1	5.61	114.31	111.50
54	BA	1873	G	O4'-C1'-N9	5.61	112.69	108.20
54	BA	2869	G	O4'-C1'-N9	5.61	112.69	108.20
21	AA	989	U	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1711	A	C6-C5-N7	5.61	136.23	132.30
54	BA	2208	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2531	A	C4-C5-C6	-5.61	114.19	117.00
8	AI	94	ARG	NE-CZ-NH1	5.61	123.11	120.30
21	AA	638	U	O4'-C1'-N1	5.61	112.69	108.20
21	AA	993	G	O4'-C1'-N9	5.61	112.69	108.20
34	BL	126	ARG	NE-CZ-NH1	5.61	123.11	120.30
54	BA	341	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1090	A	C4-C5-C6	-5.61	114.19	117.00
24	A3	50	G	N1-C6-O6	-5.61	116.53	119.90
54	BA	332	A	C5-C6-N1	5.61	120.50	117.70
54	BA	1200	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	2602	A	O4'-C1'-C2'	-5.61	100.19	105.80
21	AA	87	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	1004	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	1068	G	C5-C6-N1	5.61	114.30	111.50
21	AA	277	C	N1-C2-O2	5.61	122.26	118.90
21	AA	942	G	C5-C6-N1	5.61	114.30	111.50
21	AA	1105	A	C6-C5-N7	5.61	136.22	132.30
24	A3	45	A	C6-C5-N7	5.61	136.22	132.30
54	BA	1378	A	C5-C6-N1	5.61	120.50	117.70
54	BA	2201	G	N3-C4-C5	-5.61	125.80	128.60
54	BA	2225	A	N1-C6-N6	-5.61	115.24	118.60
55	BB	63	C	P-O3'-C3'	5.61	126.43	119.70
21	AA	1190	G	P-O3'-C3'	5.60	126.42	119.70
54	BA	2757	A	C5'-C4'-C3'	-5.60	107.03	116.00
21	AA	271	C	N1-C2-O2	5.60	122.26	118.90
21	AA	283	U	N3-C2-O2	-5.60	118.28	122.20
21	AA	647	C	N1-C2-O2	5.60	122.26	118.90
32	BJ	96	ARG	NE-CZ-NH1	5.60	123.10	120.30
54	BA	188	G	N1-C6-O6	-5.60	116.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	648	G	C5-C6-N1	5.60	114.30	111.50
54	BA	2205	A	C5-C6-N1	5.60	120.50	117.70
54	BA	679	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2336	A	O4'-C1'-N9	5.60	112.68	108.20
21	AA	1275	A	C5-C6-N1	5.60	120.50	117.70
54	BA	451	U	O4'-C1'-N1	5.60	112.68	108.20
54	BA	789	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	970	U	C5'-C4'-O4'	5.60	115.82	109.10
54	BA	1947	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2128	G	O4'-C1'-N9	5.60	112.68	108.20
21	AA	415	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	856	C	O4'-C1'-N1	5.60	112.68	108.20
21	AA	1447	A	C5-C6-N1	5.60	120.50	117.70
54	BA	601	C	N1-C2-O2	5.60	122.26	118.90
54	BA	1050	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1382	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	2628	C	N1-C2-O2	5.60	122.26	118.90
54	BA	450	G	N3-C4-C5	-5.60	125.80	128.60
54	BA	678	C	N1-C2-O2	5.60	122.26	118.90
54	BA	2332	C	N1-C2-O2	5.60	122.26	118.90
54	BA	2406	A	O4'-C1'-N9	5.60	112.68	108.20
36	BN	118	ARG	NE-CZ-NH1	5.59	123.10	120.30
54	BA	233	A	C6-C5-N7	5.59	136.22	132.30
54	BA	614	A	O4'-C1'-N9	5.59	112.67	108.20
54	BA	762	U	P-O3'-C3'	5.59	126.41	119.70
54	BA	1104	C	O4'-C1'-N1	5.59	112.68	108.20
54	BA	1815	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	2337	G	N1-C6-O6	-5.59	116.54	119.90
54	BA	2354	C	N3-C2-O2	-5.59	117.98	121.90
54	BA	2498	C	C3'-C2'-C1'	5.59	105.98	101.50
54	BA	2502	G	N7-C8-N9	5.59	115.90	113.10
54	BA	91	A	C5-C6-N1	5.59	120.50	117.70
54	BA	1591	A	C5-C6-N1	5.59	120.50	117.70
13	AN	24	ARG	NE-CZ-NH1	5.59	123.10	120.30
21	AA	305	G	N1-C6-O6	-5.59	116.55	119.90
21	AA	316	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1338	G	C5-C6-N1	5.59	114.30	111.50
54	BA	1864	U	C5-C6-N1	-5.59	119.90	122.70
54	BA	2071	A	C5-C6-N1	5.59	120.50	117.70
21	AA	546	A	C6-C5-N7	5.59	136.21	132.30
21	AA	1370	G	N3-C2-N2	-5.59	115.99	119.90
22	A1	8	U	N3-C2-O2	-5.59	118.29	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	41	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	382	A	C6-C5-N7	5.59	136.21	132.30
54	BA	410	G	C8-N9-C4	-5.59	104.16	106.40
54	BA	593	U	N1-C2-N3	5.59	118.25	114.90
54	BA	1274	A	N1-C6-N6	-5.59	115.25	118.60
54	BA	2085	U	O4'-C1'-N1	5.59	112.67	108.20
55	BB	34	A	C6-C5-N7	5.59	136.21	132.30
55	BB	58	A	N1-C6-N6	-5.59	115.25	118.60
21	AA	48	C	C2-N3-C4	-5.59	117.11	119.90
54	BA	2478	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	456	A	C5-C6-N1	5.59	120.49	117.70
21	AA	940	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1245	C	N3-C2-O2	-5.59	117.99	121.90
22	A1	52	G	N3-C4-C5	-5.59	125.81	128.60
54	BA	278	A	C5-C6-N1	5.59	120.49	117.70
54	BA	1667	G	C8-N9-C4	-5.59	104.17	106.40
54	BA	2721	A	C5-C6-N1	5.59	120.49	117.70
54	BA	2899	A	C6-C5-N7	5.59	136.21	132.30
54	BA	1289	C	O4'-C1'-N1	5.58	112.67	108.20
54	BA	1999	C	O4'-C1'-N1	5.58	112.67	108.20
54	BA	2623	G	N3-C4-C5	-5.58	125.81	128.60
21	AA	450	G	O4'-C1'-N9	5.58	112.67	108.20
21	AA	617	G	C1'-O4'-C4'	-5.58	105.43	109.90
54	BA	634	C	O4'-C1'-N1	5.58	112.67	108.20
21	AA	731	G	C5-C6-N1	5.58	114.29	111.50
21	AA	1103	C	O4'-C1'-N1	5.58	112.67	108.20
50	B1	43	ARG	NE-CZ-NH1	5.58	123.09	120.30
54	BA	279	A	C5-C6-N1	5.58	120.49	117.70
54	BA	585	G	C8-N9-C4	-5.58	104.17	106.40
54	BA	938	G	N1-C6-O6	-5.58	116.55	119.90
54	BA	1048	A	C5-C6-N1	5.58	120.49	117.70
54	BA	1101	U	O4'-C1'-N1	5.58	112.67	108.20
54	BA	2048	G	C8-N9-C4	-5.58	104.17	106.40
54	BA	2145	C	N1-C2-O2	5.58	122.25	118.90
54	BA	1248	G	N3-C4-C5	-5.58	125.81	128.60
54	BA	1386	C	N3-C4-C5	5.58	124.13	121.90
54	BA	1460	U	O4'-C1'-N1	5.58	112.66	108.20
54	BA	2250	G	N7-C8-N9	5.58	115.89	113.10
54	BA	2729	G	C8-N9-C4	-5.58	104.17	106.40
21	AA	493	A	C8-N9-C4	-5.58	103.57	105.80
21	AA	737	C	N1-C2-O2	5.58	122.25	118.90
54	BA	658	U	C5-C6-N1	-5.58	119.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1044	C	C4'-C3'-C2'	-5.58	97.02	102.60
54	BA	1055	G	C5-C6-N1	5.58	114.29	111.50
54	BA	2786	U	O4'-C1'-N1	5.58	112.66	108.20
55	BB	9	G	C5-C6-N1	5.58	114.29	111.50
9	AJ	7	ARG	NE-CZ-NH1	5.58	123.09	120.30
21	AA	682	G	C5-C6-N1	5.58	114.29	111.50
21	AA	1069	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	982	C	N1-C1'-C2'	5.58	121.25	114.00
54	BA	1793	C	N3-C4-C5	5.58	124.13	121.90
54	BA	2756	U	N3-C2-O2	-5.58	118.30	122.20
54	BA	2770	G	N1-C6-O6	-5.58	116.55	119.90
21	AA	238	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	838	C	N1-C2-O2	5.58	122.25	118.90
54	BA	1607	C	N1-C2-O2	5.58	122.25	118.90
21	AA	52	C	N3-C4-C5	5.57	124.13	121.90
21	AA	999	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1021	A	C6-C5-N7	5.57	136.20	132.30
54	BA	2515	C	C4'-C3'-C2'	-5.57	97.03	102.60
54	BA	2870	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	572	A	C5-C6-N1	5.57	120.49	117.70
54	BA	2284	A	O4'-C1'-N9	5.57	112.66	108.20
9	AJ	45	ARG	NE-CZ-NH1	5.57	123.08	120.30
21	AA	244	U	N3-C2-O2	-5.57	118.30	122.20
54	BA	826	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	1566	A	C6-C5-N7	5.57	136.20	132.30
54	BA	2353	G	N9-C4-C5	5.57	107.63	105.40
54	BA	2429	G	C5-C6-N1	5.57	114.28	111.50
54	BA	2023	C	O4'-C1'-N1	5.57	112.66	108.20
21	AA	874	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	419	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	549	G	C5-C6-N1	5.57	114.28	111.50
54	BA	1359	A	C6-C5-N7	5.57	136.20	132.30
54	BA	1446	C	O4'-C1'-N1	5.57	112.65	108.20
54	BA	1577	C	N1-C2-O2	5.57	122.24	118.90
54	BA	1757	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	1364	U	N3-C2-O2	-5.57	118.31	122.20
22	A1	62	C	C5-C4-N4	-5.57	116.30	120.20
54	BA	297	G	C5-C6-N1	5.57	114.28	111.50
54	BA	556	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	976	G	N9-C4-C5	5.56	107.63	105.40
54	BA	2883	A	C5-C6-N1	5.56	120.48	117.70
54	BA	285	G	N9-C4-C5	5.56	107.62	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1114	C	N1-C2-O2	5.56	122.24	118.90
54	BA	1118	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	1263	U	C3'-C2'-C1'	5.56	105.95	101.50
54	BA	2739	U	C5-C6-N1	-5.56	119.92	122.70
54	BA	914	G	N3-C4-C5	-5.56	125.82	128.60
54	BA	1519	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	1779	U	N3-C2-O2	-5.56	118.31	122.20
54	BA	2331	G	O4'-C1'-N9	5.56	112.65	108.20
55	BB	60	C	C2-N3-C4	-5.56	117.12	119.90
21	AA	500	G	N3-C4-C5	-5.56	125.82	128.60
21	AA	564	C	N1-C2-O2	5.56	122.24	118.90
21	AA	586	C	N1-C2-O2	5.56	122.23	118.90
21	AA	1091	U	N1-C2-N3	5.56	118.23	114.90
21	AA	1317	C	N3-C4-N4	-5.56	114.11	118.00
21	AA	1407	C	N3-C2-O2	-5.56	118.01	121.90
24	A3	68	C	N3-C4-C5	5.56	124.12	121.90
38	BP	20	ARG	NE-CZ-NH1	5.56	123.08	120.30
55	BB	40	U	O4'-C4'-C3'	5.56	110.55	106.10
21	AA	681	A	C6-C5-N7	5.56	136.19	132.30
54	BA	594	U	C5-C6-N1	-5.56	119.92	122.70
54	BA	1170	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1648	U	C5-C6-N1	-5.56	119.92	122.70
54	BA	1370	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	2474	U	C5-C6-N1	-5.56	119.92	122.70
35	BM	38	ARG	NE-CZ-NH2	-5.55	117.52	120.30
54	BA	54	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	1119	U	C5-C6-N1	-5.55	119.92	122.70
54	BA	1595	C	N1-C2-O2	5.55	122.23	118.90
54	BA	2787	C	C5'-C4'-O4'	5.55	115.77	109.10
10	AK	127	ARG	NE-CZ-NH2	-5.55	117.52	120.30
21	AA	1083	U	C1'-O4'-C4'	-5.55	105.46	109.90
24	A3	39	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	179	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	476	G	C5'-C4'-O4'	5.55	115.76	109.10
54	BA	1276	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1674	G	C5-C6-N1	5.55	114.28	111.50
21	AA	670	G	N1-C6-O6	-5.55	116.57	119.90
21	AA	860	A	N1-C6-N6	-5.55	115.27	118.60
21	AA	1448	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	163	C	O4'-C1'-N1	5.55	112.64	108.20
21	AA	585	G	C5-C6-N1	5.55	114.28	111.50
21	AA	747	A	C5-C6-N1	5.55	120.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	768	A	C6-C5-N7	5.55	136.19	132.30
54	BA	129	C	N1-C2-O2	5.55	122.23	118.90
54	BA	800	A	N1-C6-N6	-5.55	115.27	118.60
54	BA	1257	C	C6-N1-C2	-5.55	118.08	120.30
54	BA	1670	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	1851	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	2294	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	383	C	N3-C2-O2	-5.55	118.02	121.90
21	AA	453	G	N3-C4-C5	-5.55	125.83	128.60
21	AA	755	G	C8-N9-C4	-5.55	104.18	106.40
21	AA	1478	U	C5-C6-N1	-5.55	119.93	122.70
54	BA	123	G	O4'-C1'-N9	5.55	112.64	108.20
54	BA	147	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	824	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	854	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	1402	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1950	G	C8-N9-C4	-5.55	104.18	106.40
54	BA	2229	U	P-O3'-C3'	5.55	126.36	119.70
54	BA	518	G	N7-C8-N9	5.54	115.87	113.10
54	BA	2572	A	N1-C6-N6	-5.54	115.27	118.60
54	BA	2733	A	C6-C5-N7	5.54	136.18	132.30
9	AJ	62	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	191	G	N1-C6-O6	-5.54	116.57	119.90
21	AA	488	C	O4'-C1'-N1	5.54	112.64	108.20
24	A3	70	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	220	G	C8-N9-C4	-5.54	104.18	106.40
54	BA	1618	A	C5-C6-N1	5.54	120.47	117.70
54	BA	1751	U	O4'-C1'-N1	5.54	112.64	108.20
54	BA	1817	G	N3-C4-C5	-5.54	125.83	128.60
22	A1	61	C	N1-C2-O2	5.54	122.22	118.90
54	BA	1065	U	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1161	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1772	A	C6-C5-N7	5.54	136.18	132.30
54	BA	2790	U	C5-C6-N1	-5.54	119.93	122.70
21	AA	613	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	1109	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2384	U	O4'-C1'-N1	5.54	112.63	108.20
22	A1	44	G	C5-C6-N1	5.54	114.27	111.50
54	BA	2349	G	N1-C6-O6	-5.54	116.58	119.90
21	AA	43	C	N3-C2-O2	-5.54	118.03	121.90
21	AA	648	A	C5-C6-N1	5.54	120.47	117.70
21	AA	1037	C	N1-C2-O2	5.54	122.22	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1228	C	N1-C2-O2	5.54	122.22	118.90
54	BA	404	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	701	G	N1-C6-O6	-5.54	116.58	119.90
54	BA	1339	G	N3-C4-C5	-5.54	125.83	128.60
54	BA	2020	A	N1-C6-N6	-5.54	115.28	118.60
22	A1	47	U	C1'-O4'-C4'	-5.53	105.47	109.90
54	BA	123	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	727	A	N1-C6-N6	-5.53	115.28	118.60
54	BA	1552	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1781	U	N3-C2-O2	-5.53	118.33	122.20
54	BA	1921	G	C3'-C2'-C1'	5.53	105.93	101.50
54	BA	2285	C	N3-C4-C5	5.53	124.11	121.90
21	AA	313	A	C6-C5-N7	5.53	136.17	132.30
21	AA	816	A	C5-C6-N1	5.53	120.47	117.70
21	AA	1385	G	C5-C6-N1	5.53	114.27	111.50
36	BN	86	ARG	NE-CZ-NH1	5.53	123.07	120.30
54	BA	44	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1028	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1368	G	N1-C6-O6	-5.53	116.58	119.90
21	AA	308	C	N3-C4-C5	5.53	124.11	121.90
21	AA	941	G	C5'-C4'-C3'	-5.53	107.15	116.00
21	AA	1218	C	N1-C2-O2	5.53	122.22	118.90
54	BA	420	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	1814	G	C5-C6-N1	5.53	114.27	111.50
54	BA	2716	C	N1-C2-O2	5.53	122.22	118.90
54	BA	222	A	O4'-C1'-N9	5.53	112.62	108.20
21	AA	330	C	N3-C4-C5	5.53	124.11	121.90
21	AA	793	U	C3'-C2'-C1'	5.53	105.92	101.50
35	BM	38	ARG	NE-CZ-NH1	5.53	123.06	120.30
54	BA	365	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	586	A	C5-C6-N1	5.53	120.46	117.70
54	BA	672	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	1316	U	N3-C2-O2	-5.53	118.33	122.20
54	BA	1397	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	2395	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	2783	U	O4'-C1'-N1	5.53	112.62	108.20
54	BA	2361	G	N3-C2-N2	-5.53	116.03	119.90
21	AA	1164	G	C5-C6-N1	5.52	114.26	111.50
21	AA	1389	C	C6-N1-C2	-5.52	118.09	120.30
21	AA	978	A	C3'-C2'-C1'	5.52	105.92	101.50
21	AA	1371	G	C8-N9-C4	-5.52	104.19	106.40
54	BA	1035	U	N1-C2-N3	5.52	118.21	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1828	G	C3'-C2'-C1'	-5.52	97.08	101.50
54	BA	2301	C	O4'-C1'-N1	5.52	112.62	108.20
54	BA	2361	G	N9-C4-C5	5.52	107.61	105.40
54	BA	2391	G	N3-C4-C5	-5.52	125.84	128.60
21	AA	143	A	C6-C5-N7	5.52	136.16	132.30
21	AA	289	G	C1'-O4'-C4'	-5.52	105.48	109.90
54	BA	845	A	O4'-C1'-N9	5.52	112.62	108.20
54	BA	2250	G	C8-N9-C4	-5.52	104.19	106.40
55	BB	86	G	N9-C4-C5	5.52	107.61	105.40
11	AL	85	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	AA	125	U	O4'-C1'-N1	5.52	112.61	108.20
21	AA	217	C	N1-C2-O2	5.52	122.21	118.90
24	A3	19	G	C8-N9-C4	-5.52	104.19	106.40
54	BA	267	C	N1-C2-O2	5.52	122.21	118.90
54	BA	530	G	C5-C6-N1	5.52	114.26	111.50
54	BA	2450	A	C6-C5-N7	5.52	136.16	132.30
54	BA	2662	A	N1-C6-N6	-5.52	115.29	118.60
21	AA	211	G	N3-C4-C5	-5.52	125.84	128.60
21	AA	288	A	C6-C5-N7	5.52	136.16	132.30
21	AA	357	G	C3'-C2'-C1'	5.52	105.91	101.50
21	AA	1226	C	N1-C2-O2	5.52	122.21	118.90
54	BA	33	C	N1-C2-O2	5.52	122.21	118.90
54	BA	423	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1109	C	C3'-C2'-C1'	5.52	105.91	101.50
54	BA	1369	G	C5-C6-N1	5.52	114.26	111.50
54	BA	1806	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	2245	U	O4'-C1'-N1	5.52	112.61	108.20
54	BA	2573	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	2752	C	O4'-C1'-N1	5.52	112.61	108.20
55	BB	115	A	C5-C6-N1	5.52	120.46	117.70
54	BA	1677	A	C5-C6-N1	5.52	120.46	117.70
54	BA	2338	C	N1-C2-O2	5.52	122.21	118.90
14	AO	63	ARG	NE-CZ-NH1	5.51	123.06	120.30
21	AA	290	C	N1-C2-O2	5.51	122.21	118.90
21	AA	665	A	C6-C5-N7	5.51	136.16	132.30
21	AA	1398	A	N1-C2-N3	-5.51	126.54	129.30
54	BA	2601	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	237	G	C8-N9-C4	-5.51	104.19	106.40
54	BA	257	C	O4'-C1'-N1	5.51	112.61	108.20
54	BA	520	G	N1-C6-O6	-5.51	116.59	119.90
54	BA	1442	U	C5-C6-N1	-5.51	119.94	122.70
21	AA	714	G	O4'-C1'-N9	5.51	112.61	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	720	C	N1-C2-O2	5.51	122.21	118.90
21	AA	811	C	C3'-C2'-C1'	5.51	105.91	101.50
21	AA	1129	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	1140	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	1174	G	C5-C6-N1	5.51	114.26	111.50
21	AA	1227	A	O4'-C1'-N9	5.51	112.61	108.20
21	AA	1389	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	431	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	1550	C	N3-C4-C5	5.51	124.10	121.90
54	BA	2624	G	C5-C6-N1	5.51	114.26	111.50
21	AA	101	A	O4'-C1'-N9	5.51	112.61	108.20
21	AA	785	G	C5-C6-N1	5.51	114.25	111.50
54	BA	971	G	C3'-C2'-C1'	-5.51	97.09	101.50
54	BA	1464	G	N1-C6-O6	-5.51	116.59	119.90
54	BA	1582	C	N1-C2-O2	5.51	122.21	118.90
54	BA	2189	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	2211	A	O4'-C1'-N9	5.51	112.61	108.20
54	BA	2850	A	C5-C6-N1	5.51	120.45	117.70
54	BA	386	G	P-O3'-C3'	5.51	126.31	119.70
54	BA	1176	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	1538	G	N9-C4-C5	5.51	107.60	105.40
54	BA	2599	G	N7-C8-N9	5.51	115.85	113.10
55	BB	54	G	N1-C6-O6	-5.51	116.59	119.90
21	AA	877	G	N7-C8-N9	5.51	115.85	113.10
39	BQ	63	ARG	NE-CZ-NH1	5.51	123.05	120.30
54	BA	1441	G	N9-C4-C5	5.51	107.60	105.40
54	BA	1916	A	C6-C5-N7	5.51	136.16	132.30
54	BA	2486	C	N1-C2-O2	5.51	122.20	118.90
55	BB	67	G	C5-C6-N1	5.51	114.25	111.50
54	BA	183	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	377	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	1318	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	2039	U	N3-C2-O2	-5.50	118.35	122.20
21	AA	115	G	C5-C6-N1	5.50	114.25	111.50
21	AA	1490	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	79	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1033	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	1638	C	N1-C2-O2	5.50	122.20	118.90
21	AA	139	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	802	A	C5-C6-N1	5.50	120.45	117.70
21	AA	1443	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	1476	A	C5-C6-N1	5.50	120.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	60	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	797	G	C5-C6-N1	5.50	114.25	111.50
54	BA	1583	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1588	G	C5-C6-N1	5.50	114.25	111.50
54	BA	1844	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	2803	G	N3-C4-C5	-5.50	125.85	128.60
54	BA	1133	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1533	C	N1-C2-O2	5.50	122.20	118.90
54	BA	1645	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	2418	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	2443	C	N3-C4-C5	5.50	124.10	121.90
54	BA	2665	A	C4-C5-C6	-5.50	114.25	117.00
55	BB	109	A	C1'-O4'-C4'	-5.50	105.50	109.90
21	AA	69	G	C5-C6-N1	5.50	114.25	111.50
54	BA	481	G	N3-C4-C5	-5.50	125.85	128.60
54	BA	1563	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	2676	C	N1-C2-O2	5.50	122.20	118.90
54	BA	1202	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	1523	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1764	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1931	U	O4'-C1'-N1	5.50	112.60	108.20
21	AA	1398	A	C6-C5-N7	5.49	136.15	132.30
27	BE	102	ARG	NE-CZ-NH1	5.49	123.05	120.30
54	BA	606	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	830	G	N3-C2-N2	-5.49	116.06	119.90
54	BA	2150	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	2655	G	C8-N9-C4	-5.49	104.20	106.40
21	AA	369	G	N3-C4-C5	-5.49	125.85	128.60
21	AA	1469	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1041	G	C5'-C4'-O4'	5.49	115.69	109.10
54	BA	1077	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	1459	G	N3-C4-C5	-5.49	125.85	128.60
54	BA	730	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	958	U	C5-C6-N1	-5.49	119.95	122.70
54	BA	1079	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	2779	U	O4'-C1'-N1	5.49	112.59	108.20
21	AA	246	A	C6-C5-N7	5.49	136.14	132.30
21	AA	511	C	O4'-C1'-N1	5.49	112.59	108.20
54	BA	337	C	N1-C2-O2	5.49	122.19	118.90
54	BA	435	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1092	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1876	A	C4-C5-C6	-5.49	114.25	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2441	U	O4'-C1'-N1	5.49	112.59	108.20
21	AA	91	U	C5-C6-N1	-5.49	119.96	122.70
54	BA	393	C	N1-C2-O2	5.49	122.19	118.90
21	AA	197	A	C5'-C4'-C3'	-5.49	107.22	116.00
21	AA	1070	U	N1-C2-N3	5.49	118.19	114.90
54	BA	228	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1266	G	N3-C4-N9	5.49	129.29	126.00
54	BA	1288	G	N3-C4-C5	-5.49	125.86	128.60
54	BA	2712	C	N1-C2-O2	5.49	122.19	118.90
54	BA	2549	G	C8-N9-C4	-5.48	104.21	106.40
54	BA	2657	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2832	U	C3'-C2'-C1'	5.48	105.89	101.50
21	AA	634	C	N1-C2-O2	5.48	122.19	118.90
21	AA	901	A	C4-C5-C6	-5.48	114.26	117.00
22	A1	52	G	C8-N9-C4	-5.48	104.21	106.40
45	BW	10	ARG	NE-CZ-NH2	5.48	123.04	120.30
54	BA	595	C	N1-C2-O2	5.48	122.19	118.90
54	BA	774	G	C8-N9-C4	-5.48	104.21	106.40
54	BA	1494	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2556	C	C5'-C4'-O4'	5.48	115.68	109.10
21	AA	566	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	1919	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2443	C	N1-C2-O2	5.48	122.19	118.90
54	BA	2645	G	N3-C4-C5	-5.48	125.86	128.60
54	BA	2825	G	N3-C4-C5	-5.48	125.86	128.60
21	AA	559	A	O4'-C1'-N9	5.48	112.58	108.20
21	AA	634	C	N3-C4-C5	5.48	124.09	121.90
54	BA	2847	U	C5-C6-N1	-5.48	119.96	122.70
21	AA	212	G	N3-C4-C5	-5.48	125.86	128.60
22	A1	42	G	N3-C4-C5	-5.48	125.86	128.60
54	BA	293	U	C5-C6-N1	-5.48	119.96	122.70
54	BA	453	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	507	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1007	C	N3-C2-O2	-5.48	118.07	121.90
54	BA	1244	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2467	C	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2902	C	N3-C2-O2	-5.48	118.06	121.90
16	AQ	39	ARG	NE-CZ-NH1	5.48	123.04	120.30
21	AA	495	A	C5-C6-N1	5.48	120.44	117.70
21	AA	514	C	N3-C2-O2	-5.48	118.07	121.90
26	BD	33	ARG	CD-NE-CZ	5.48	131.27	123.60
54	BA	712	G	C5-C6-N1	5.48	114.24	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2456	C	N3-C2-O2	-5.48	118.07	121.90
54	BA	2863	C	N1-C2-O2	5.48	122.19	118.90
21	AA	146	G	N3-C4-C5	-5.47	125.86	128.60
21	AA	265	G	N1-C6-O6	-5.47	116.61	119.90
21	AA	920	U	C5-C6-N1	-5.47	119.96	122.70
21	AA	1031	C	C6-N1-C2	-5.47	118.11	120.30
21	AA	1268	G	N3-C4-C5	-5.47	125.86	128.60
54	BA	776	G	N9-C4-C5	5.47	107.59	105.40
54	BA	1961	C	N1-C2-O2	5.47	122.18	118.90
54	BA	2795	C	N3-C2-O2	-5.47	118.07	121.90
24	A3	19	G	N9-C4-C5	5.47	107.59	105.40
54	BA	1430	G	N9-C4-C5	5.47	107.59	105.40
54	BA	1710	G	C8-N9-C4	-5.47	104.21	106.40
54	BA	2031	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	2068	U	O4'-C1'-N1	5.47	112.58	108.20
55	BB	46	A	C5-C6-N1	5.47	120.44	117.70
21	AA	564	C	C3'-C2'-C1'	5.47	105.88	101.50
22	A1	20	G	O4'-C1'-N9	5.47	112.58	108.20
54	BA	1077	A	C5-C6-N1	5.47	120.44	117.70
54	BA	2571	U	C5-C6-N1	-5.47	119.96	122.70
15	AP	5	ARG	NE-CZ-NH2	-5.47	117.56	120.30
21	AA	22	G	C5-C6-N1	5.47	114.23	111.50
21	AA	1521	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	663	G	N3-C4-C5	-5.47	125.86	128.60
54	BA	741	U	N3-C2-O2	-5.47	118.37	122.20
54	BA	1095	A	C5-N7-C8	-5.47	101.17	103.90
54	BA	1120	G	C5-C6-N1	5.47	114.23	111.50
54	BA	1679	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	2028	U	O4'-C1'-N1	5.47	112.58	108.20
55	BB	82	U	C3'-C2'-C1'	5.47	105.88	101.50
19	AT	17	ARG	NE-CZ-NH1	5.47	123.03	120.30
21	AA	606	G	C5-C6-N1	5.47	114.23	111.50
21	AA	1076	U	O4'-C1'-N1	5.47	112.57	108.20
54	BA	1281	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	2235	G	C5-C6-N1	5.47	114.23	111.50
54	BA	2719	G	C8-N9-C4	-5.47	104.21	106.40
21	AA	177	G	N3-C4-C5	-5.47	125.87	128.60
21	AA	686	U	C4-C5-C6	5.47	122.98	119.70
21	AA	1458	G	C5-C6-N1	5.47	114.23	111.50
54	BA	1370	C	N1-C2-O2	5.47	122.18	118.90
54	BA	2708	G	N3-C4-C5	-5.47	125.87	128.60
21	AA	540	G	C5-C6-N1	5.46	114.23	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1221	G	N1-C6-O6	-5.46	116.62	119.90
21	AA	566	G	N3-C4-C5	-5.46	125.87	128.60
21	AA	593	U	N1-C2-N3	5.46	118.18	114.90
21	AA	1056	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1878	G	C5-C6-N1	5.46	114.23	111.50
3	AD	46	ARG	NE-CZ-NH1	5.46	123.03	120.30
21	AA	115	G	N3-C4-C5	-5.46	125.87	128.60
21	AA	914	A	C5-C6-N6	5.46	128.07	123.70
21	AA	1342	C	O4'-C1'-N1	5.46	112.57	108.20
36	BN	12	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	2702	G	N3-C2-N2	-5.46	116.08	119.90
21	AA	848	C	N1-C2-O2	5.46	122.18	118.90
21	AA	1386	G	C5-C6-N1	5.46	114.23	111.50
54	BA	421	C	C2'-C3'-O3'	5.46	122.44	113.70
21	AA	1379	G	N1-C6-O6	-5.46	116.62	119.90
21	AA	1510	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	437	U	C5-C6-N1	-5.46	119.97	122.70
54	BA	1339	G	C8-N9-C4	-5.46	104.22	106.40
54	BA	2706	A	N7-C8-N9	5.46	116.53	113.80
21	AA	848	C	N3-C4-C5	5.46	124.08	121.90
54	BA	576	U	O4'-C1'-N1	5.46	112.56	108.20
54	BA	796	C	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1965	C	N1-C2-O2	5.46	122.17	118.90
54	BA	2461	A	C4-C5-C6	-5.46	114.27	117.00
55	BB	76	G	N3-C4-C5	-5.46	125.87	128.60
21	AA	1072	G	C5-C6-N1	5.46	114.23	111.50
21	AA	784	A	C6-C5-N7	5.45	136.12	132.30
21	AA	1111	A	C5-C6-N1	5.45	120.43	117.70
54	BA	13	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	1707	G	C5-C6-N1	5.45	114.23	111.50
54	BA	1789	A	C6-C5-N7	5.45	136.12	132.30
54	BA	1908	C	N3-C2-O2	-5.45	118.08	121.90
55	BB	62	C	N1-C2-O2	5.45	122.17	118.90
21	AA	1113	C	N3-C4-C5	5.45	124.08	121.90
54	BA	287	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	1426	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	2640	G	N1-C6-O6	-5.45	116.63	119.90
55	BB	76	G	N1-C6-O6	-5.45	116.63	119.90
21	AA	226	G	C8-N9-C4	-5.45	104.22	106.40
21	AA	235	C	N3-C4-C5	5.45	124.08	121.90
21	AA	438	U	C4-C5-C6	5.45	122.97	119.70
21	AA	807	A	C6-C5-N7	5.45	136.12	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1394	A	N1-C6-N6	-5.45	115.33	118.60
22	A1	9	A	O4'-C1'-N9	5.45	112.56	108.20
24	A3	26	C	N3-C2-O2	-5.45	118.08	121.90
54	BA	102	U	O4'-C1'-N1	5.45	112.56	108.20
54	BA	1329	U	O4'-C4'-C3'	5.45	110.46	106.10
54	BA	1389	G	O4'-C1'-N9	5.45	112.56	108.20
54	BA	2073	C	O4'-C1'-N1	5.45	112.56	108.20
54	BA	2546	U	N3-C2-O2	-5.45	118.39	122.20
21	AA	71	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	1240	U	N3-C2-O2	-5.45	118.39	122.20
21	AA	1406	U	C5-C6-N1	-5.45	119.98	122.70
54	BA	1463	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	1512	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	2576	G	N9-C4-C5	5.45	107.58	105.40
11	AL	55	ARG	NE-CZ-NH2	-5.45	117.58	120.30
54	BA	770	G	C5-C6-N1	5.45	114.22	111.50
54	BA	1159	U	O4'-C1'-N1	5.45	112.56	108.20
21	AA	152	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	734	G	O4'-C4'-C3'	5.45	110.46	106.10
54	BA	114	U	N1-C2-N3	5.45	118.17	114.90
54	BA	1332	G	O4'-C1'-N9	5.45	112.56	108.20
54	BA	1826	G	N3-C4-C5	-5.45	125.88	128.60
54	BA	2339	C	N3-C4-C5	5.45	124.08	121.90
21	AA	234	C	N3-C4-C5	5.44	124.08	121.90
54	BA	109	C	N1-C2-O2	5.44	122.17	118.90
54	BA	650	C	O4'-C1'-N1	5.44	112.56	108.20
54	BA	1269	A	C5-C6-N1	5.44	120.42	117.70
54	BA	2313	C	C1'-O4'-C4'	-5.44	105.55	109.90
11	AL	13	ARG	NH1-CZ-NH2	-5.44	113.41	119.40
18	AS	54	ARG	NE-CZ-NH1	5.44	123.02	120.30
21	AA	142	G	N1-C6-O6	-5.44	116.64	119.90
21	AA	201	G	N1-C6-O6	-5.44	116.63	119.90
54	BA	102	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	116	C	O4'-C1'-N1	5.44	112.56	108.20
54	BA	368	A	C6-C5-N7	5.44	136.11	132.30
54	BA	1589	U	O4'-C1'-N1	5.44	112.56	108.20
54	BA	1674	G	C3'-C2'-C1'	5.44	105.85	101.50
54	BA	2527	C	N1-C2-O2	5.44	122.17	118.90
55	BB	30	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	172	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	308	C	C3'-C2'-C1'	5.44	105.85	101.50
21	AA	473	U	C3'-C2'-C1'	5.44	105.85	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	738	C	N1-C2-O2	5.44	122.17	118.90
23	A2	89	U	C5-C6-N1	-5.44	119.98	122.70
54	BA	947	A	C6-C5-N7	5.44	136.11	132.30
54	BA	1460	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	1546	G	C4'-C3'-C2'	-5.44	97.16	102.60
54	BA	1748	C	N1-C2-O2	5.44	122.16	118.90
54	BA	2069	G	C5'-C4'-O4'	5.44	115.63	109.10
54	BA	2689	U	O4'-C1'-N1	5.44	112.55	108.20
55	BB	60	C	O4'-C1'-N1	5.44	112.55	108.20
55	BB	4	C	N1-C2-O2	5.44	122.16	118.90
12	AM	78	ARG	NE-CZ-NH1	5.44	123.02	120.30
21	AA	931	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	932	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	1051	C	N1-C2-O2	5.44	122.16	118.90
21	AA	1457	G	N9-C4-C5	5.44	107.58	105.40
24	A3	17	C	N3-C4-C5	5.44	124.08	121.90
54	BA	125	A	C6-C5-N7	5.44	136.11	132.30
54	BA	193	U	C4-C5-C6	5.44	122.96	119.70
54	BA	1305	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	2165	C	N3-C4-C5	5.44	124.08	121.90
54	BA	2473	U	C5-C6-N1	-5.44	119.98	122.70
55	BB	41	G	C5-C6-N1	5.44	114.22	111.50
21	AA	938	A	O4'-C1'-N9	5.44	112.55	108.20
21	AA	1372	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	685	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1708	C	N1-C2-O2	5.44	122.16	118.90
54	BA	2054	A	O4'-C1'-N9	5.44	112.55	108.20
54	BA	83	A	C6-C5-N7	5.43	136.10	132.30
54	BA	306	U	O4'-C1'-N1	5.43	112.55	108.20
54	BA	2124	G	N1-C6-O6	-5.43	116.64	119.90
55	BB	90	C	N3-C4-C5	5.43	124.07	121.90
21	AA	340	U	C5-C6-N1	-5.43	119.98	122.70
21	AA	868	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	949	A	C6-C5-N7	5.43	136.10	132.30
21	AA	1396	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	142	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	1415	G	C8-N9-C4	-5.43	104.23	106.40
54	BA	1634	A	C5-C6-N1	5.43	120.42	117.70
21	AA	439	U	O4'-C1'-N1	5.43	112.54	108.20
21	AA	1194	U	C5-C6-N1	-5.43	119.98	122.70
54	BA	711	G	N7-C8-N9	5.43	115.81	113.10
54	BA	961	C	N1-C2-O2	5.43	122.16	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1318	U	N3-C2-O2	-5.43	118.40	122.20
54	BA	2661	G	O4'-C1'-N9	5.43	112.54	108.20
21	AA	664	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	685	G	C5-C6-N1	5.43	114.21	111.50
54	BA	461	C	N3-C4-N4	-5.43	114.20	118.00
54	BA	1558	C	N3-C4-C5	5.43	124.07	121.90
54	BA	2132	U	C5-C6-N1	-5.43	119.99	122.70
21	AA	115	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	220	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	703	G	N3-C4-C5	-5.43	125.89	128.60
21	AA	907	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	1139	G	N3-C2-N2	-5.43	116.10	119.90
21	AA	1231	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	1311	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	1379	G	C5-C6-N1	5.43	114.21	111.50
52	B3	44	ARG	NE-CZ-NH2	-5.43	117.59	120.30
54	BA	208	C	O4'-C1'-N1	5.43	112.54	108.20
54	BA	855	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1482	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1874	C	O4'-C1'-N1	5.43	112.54	108.20
54	BA	2520	C	N3-C4-C5	5.43	124.07	121.90
21	AA	585	G	N1-C6-O6	-5.42	116.65	119.90
21	AA	827	U	N3-C2-O2	-5.42	118.40	122.20
21	AA	1081	A	C6-C5-N7	5.42	136.10	132.30
21	AA	1471	U	O4'-C1'-N1	5.42	112.54	108.20
24	A3	3	C	N1-C2-O2	5.42	122.15	118.90
54	BA	1374	G	N1-C6-O6	-5.42	116.64	119.90
54	BA	1724	G	C8-N9-C4	-5.42	104.23	106.40
54	BA	2016	U	N3-C2-O2	-5.42	118.40	122.20
54	BA	2359	C	N3-C4-C5	5.42	124.07	121.90
54	BA	2440	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	2542	A	O4'-C1'-N9	5.42	112.54	108.20
21	AA	394	G	N3-C2-N2	-5.42	116.10	119.90
21	AA	934	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	977	G	C8-N9-C4	-5.42	104.23	106.40
54	BA	1563	U	C5-C6-N1	-5.42	119.99	122.70
54	BA	2116	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	2359	C	N1-C2-O2	5.42	122.15	118.90
21	AA	233	C	N3-C4-C5	5.42	124.07	121.90
21	AA	423	G	O4'-C1'-N9	5.42	112.54	108.20
21	AA	863	U	N3-C2-O2	-5.42	118.41	122.20
21	AA	1265	C	N3-C2-O2	-5.42	118.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1269	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1507	A	C4-C5-C6	-5.42	114.29	117.00
38	BP	108	ARG	NE-CZ-NH2	5.42	123.01	120.30
54	BA	1570	A	C5-C6-N1	5.42	120.41	117.70
54	BA	1681	G	C8-N9-C4	-5.42	104.23	106.40
21	AA	1062	U	C5-C6-N1	-5.42	119.99	122.70
54	BA	668	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2124	G	N3-C4-C5	-5.42	125.89	128.60
21	AA	649	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1441	A	C6-C5-N7	5.42	136.09	132.30
21	AA	1477	U	O4'-C1'-N1	5.42	112.53	108.20
54	BA	878	A	C5-C6-N1	5.42	120.41	117.70
54	BA	1117	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	1129	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1452	G	N3-C4-C5	-5.42	125.89	128.60
54	BA	1957	C	N3-C2-O2	-5.42	118.11	121.90
55	BB	81	G	C5-C6-N1	5.42	114.21	111.50
21	AA	490	C	N3-C4-C5	5.42	124.07	121.90
21	AA	831	A	C5-C6-N1	5.42	120.41	117.70
21	AA	1171	A	C5-C6-N1	5.42	120.41	117.70
21	AA	1189	U	C5-C6-N1	-5.42	119.99	122.70
54	BA	2774	C	N1-C2-O2	5.42	122.15	118.90
54	BA	455	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	1453	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2270	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	176	C	N1-C2-O2	5.41	122.15	118.90
54	BA	40	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	101	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	437	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1000	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	2556	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	2854	G	N9-C4-C5	5.41	107.57	105.40
21	AA	275	G	N3-C4-C5	-5.41	125.89	128.60
21	AA	1511	G	N9-C4-C5	5.41	107.56	105.40
54	BA	2323	G	N3-C2-N2	-5.41	116.11	119.90
21	AA	1167	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1114	C	N3-C4-C5	5.41	124.06	121.90
54	BA	1436	G	N3-C4-C5	-5.41	125.89	128.60
54	BA	1615	C	N1-C2-O2	5.41	122.15	118.90
54	BA	1776	G	N3-C4-C5	-5.41	125.89	128.60
54	BA	1924	C	O4'-C1'-N1	5.41	112.53	108.20
21	AA	879	C	N1-C2-O2	5.41	122.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	17	U	C5-C6-N1	-5.41	120.00	122.70
54	BA	1527	G	N1-C6-O6	-5.41	116.66	119.90
54	BA	1728	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2816	G	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	632	U	O4'-C1'-N1	5.41	112.53	108.20
21	AA	1273	C	N1-C2-O2	5.41	122.14	118.90
54	BA	677	A	N1-C6-N6	-5.41	115.36	118.60
55	BB	24	G	N1-C6-O6	-5.41	116.66	119.90
54	BA	151	C	N3-C2-O2	-5.41	118.12	121.90
54	BA	352	A	C5-C6-N1	5.41	120.40	117.70
54	BA	606	U	N3-C2-O2	-5.41	118.42	122.20
54	BA	646	U	N1-C2-N3	5.41	118.14	114.90
54	BA	715	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	791	C	N1-C2-O2	5.41	122.14	118.90
54	BA	912	C	N3-C2-O2	-5.41	118.12	121.90
54	BA	2367	G	N1-C6-O6	-5.41	116.66	119.90
8	AI	118	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	975	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	523	C	N1-C2-O2	5.40	122.14	118.90
54	BA	1237	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1994	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	1701	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2306	C	N1-C2-O2	5.40	122.14	118.90
21	AA	262	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	1224	U	N3-C2-O2	-5.40	118.42	122.20
21	AA	1466	C	N1-C2-O2	5.40	122.14	118.90
54	BA	758	C	O4'-C1'-N1	5.40	112.52	108.20
55	BB	39	A	C5-C6-N1	5.40	120.40	117.70
21	AA	1207	G	N9-C4-C5	5.40	107.56	105.40
54	BA	502	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	809	G	N3-C4-C5	-5.40	125.90	128.60
54	BA	2415	G	N1-C6-O6	-5.40	116.66	119.90
55	BB	110	C	N3-C4-N4	-5.40	114.22	118.00
21	AA	236	A	C5-C6-N1	5.40	120.40	117.70
21	AA	346	G	C5-C6-N1	5.40	114.20	111.50
21	AA	402	G	N3-C4-C5	-5.40	125.90	128.60
21	AA	925	G	C5-C6-N1	5.40	114.20	111.50
22	A1	6	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1150	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	1193	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	2381	A	C6-C5-N7	5.40	136.08	132.30
55	BB	64	G	C8-N9-C4	-5.40	104.24	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	29	A	C5-C6-N1	5.40	120.40	117.70
55	BB	79	G	C8-N9-C4	-5.40	104.24	106.40
21	AA	204	G	N9-C4-C5	5.39	107.56	105.40
21	AA	365	U	C1'-O4'-C4'	-5.39	105.58	109.90
21	AA	1062	U	N3-C2-O2	-5.39	118.42	122.20
54	BA	285	G	C8-N9-C4	-5.39	104.24	106.40
54	BA	1343	G	N3-C2-N2	-5.39	116.12	119.90
54	BA	1520	U	C5-C6-N1	-5.39	120.00	122.70
54	BA	2305	U	C5-C6-N1	-5.39	120.00	122.70
54	BA	2825	G	C2-N3-C4	5.39	114.60	111.90
21	AA	521	G	C5-C6-N1	5.39	114.20	111.50
21	AA	536	C	N1-C2-O2	5.39	122.14	118.90
21	AA	1223	C	N3-C2-O2	-5.39	118.12	121.90
54	BA	744	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1236	G	C3'-C2'-C1'	5.39	105.81	101.50
54	BA	1543	G	N3-C2-N2	-5.39	116.12	119.90
54	BA	2018	G	C5-C6-N1	5.39	114.20	111.50
55	BB	31	C	N3-C2-O2	-5.39	118.12	121.90
21	AA	1099	G	N1-C6-O6	-5.39	116.67	119.90
54	BA	2422	C	N1-C2-O2	5.39	122.13	118.90
54	BA	2866	U	C5-C6-N1	-5.39	120.00	122.70
3	AD	183	ARG	NE-CZ-NH1	5.39	123.00	120.30
21	AA	530	G	N1-C6-O6	-5.39	116.67	119.90
21	AA	1439	G	C5-C6-N1	5.39	114.19	111.50
54	BA	310	A	N1-C6-N6	-5.39	115.37	118.60
54	BA	464	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1665	A	O4'-C1'-N9	5.39	112.51	108.20
54	BA	2406	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	2558	C	N1-C2-O2	5.39	122.13	118.90
55	BB	92	C	O4'-C1'-N1	5.39	112.51	108.20
21	AA	1163	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	84	A	C4-C5-C6	-5.39	114.31	117.00
21	AA	124	C	N3-C4-C5	5.39	124.06	121.90
21	AA	734	G	N7-C8-N9	5.39	115.79	113.10
54	BA	429	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	2049	G	O4'-C1'-N9	5.39	112.51	108.20
54	BA	2155	U	O4'-C1'-N1	5.39	112.51	108.20
21	AA	34	C	N3-C4-C5	5.38	124.05	121.90
21	AA	215	C	O4'-C1'-N1	5.38	112.51	108.20
21	AA	1284	C	N3-C2-O2	-5.38	118.13	121.90
21	AA	1332	A	C4-C5-C6	-5.38	114.31	117.00
41	BS	11	ARG	NE-CZ-NH1	5.38	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	286	U	N1-C2-N3	5.38	118.13	114.90
54	BA	1785	A	C6-C5-N7	5.38	136.07	132.30
21	AA	356	A	C6-C5-N7	5.38	136.07	132.30
54	BA	1597	A	C3'-C2'-C1'	5.38	105.81	101.50
54	BA	1827	U	N3-C2-O2	-5.38	118.43	122.20
55	BB	46	A	N1-C6-N6	-5.38	115.37	118.60
21	AA	479	U	N3-C2-O2	-5.38	118.43	122.20
21	AA	1430	A	C3'-C2'-C1'	5.38	105.81	101.50
54	BA	1317	G	C1'-O4'-C4'	-5.38	105.59	109.90
54	BA	1559	U	O4'-C1'-N1	5.38	112.50	108.20
55	BB	105	G	N3-C4-C5	-5.38	125.91	128.60
54	BA	1205	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	2064	C	N3-C2-O2	-5.38	118.13	121.90
55	BB	104	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	1467	C	N3-C4-C5	5.38	124.05	121.90
54	BA	890	C	O4'-C1'-N1	5.38	112.50	108.20
54	BA	949	G	N7-C8-N9	5.38	115.79	113.10
54	BA	1567	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1692	U	C5-C6-N1	-5.38	120.01	122.70
54	BA	2344	U	N3-C2-O2	-5.38	118.44	122.20
54	BA	2628	C	C6-N1-C2	-5.38	118.15	120.30
39	BQ	5	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BA	317	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1766	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	2323	G	C8-N9-C4	-5.38	104.25	106.40
54	BA	2342	C	N1-C2-O2	5.38	122.13	118.90
54	BA	2620	C	N3-C2-O2	-5.38	118.14	121.90
21	AA	1053	G	C8-N9-C4	-5.38	104.25	106.40
54	BA	1576	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	2678	C	O4'-C1'-N1	5.38	112.50	108.20
21	AA	284	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	679	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	803	G	N3-C4-C5	-5.37	125.91	128.60
21	AA	1138	G	C5-C6-N1	5.37	114.19	111.50
21	AA	1417	G	C5-C6-N1	5.37	114.19	111.50
22	A1	23	A	C4-C5-C6	-5.37	114.31	117.00
24	A3	53	G	C8-N9-C4	-5.37	104.25	106.40
54	BA	1290	C	N1-C2-O2	5.37	122.12	118.90
54	BA	1604	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1962	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2057	G	C5-C6-N1	5.37	114.19	111.50
21	AA	370	C	N1-C2-O2	5.37	122.12	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	639	G	N3-C4-C5	-5.37	125.91	128.60
21	AA	806	C	O4'-C1'-N1	5.37	112.50	108.20
21	AA	1011	C	N1-C2-O2	5.37	122.12	118.90
54	BA	209	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	910	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	1414	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	1782	U	N3-C2-O2	-5.37	118.44	122.20
54	BA	2610	C	N1-C2-O2	5.37	122.12	118.90
21	AA	335	C	N1-C2-O2	5.37	122.12	118.90
54	BA	2068	U	C5-C6-N1	-5.37	120.02	122.70
54	BA	2498	C	N3-C4-C5	5.37	124.05	121.90
54	BA	2590	A	C4-C5-C6	-5.37	114.31	117.00
55	BB	65	U	N3-C2-O2	-5.37	118.44	122.20
21	AA	5	U	C1'-O4'-C4'	-5.37	105.61	109.90
21	AA	82	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	777	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	1452	C	N3-C2-O2	-5.37	118.14	121.90
24	A3	29	C	N1-C2-O2	5.37	122.12	118.90
54	BA	172	A	C6-C5-N7	5.37	136.06	132.30
54	BA	427	U	C4-C5-C6	5.37	122.92	119.70
54	BA	1066	U	C5-C6-N1	-5.37	120.02	122.70
54	BA	1899	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	469	C	O4'-C1'-N1	5.37	112.49	108.20
24	A3	6	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	549	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	1295	C	C5'-C4'-O4'	5.37	115.54	109.10
21	AA	481	G	N3-C4-C5	-5.37	125.92	128.60
54	BA	335	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	377	G	C5-C6-N1	5.37	114.18	111.50
54	BA	2521	C	N3-C4-C5	5.37	124.05	121.90
54	BA	2785	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	269	C	N3-C2-O2	-5.36	118.14	121.90
54	BA	1875	G	C8-N9-C4	-5.36	104.25	106.40
54	BA	1888	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	2124	G	C5-C6-N1	5.36	114.18	111.50
54	BA	2146	C	N1-C2-O2	5.36	122.12	118.90
54	BA	2717	C	N3-C4-C5	5.36	124.05	121.90
21	AA	311	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	196	A	C5-C6-N1	5.36	120.38	117.70
21	AA	917	G	C8-N9-C4	-5.36	104.26	106.40
32	BJ	95	ARG	NE-CZ-NH1	5.36	122.98	120.30
46	BX	17	ARG	NH1-CZ-NH2	-5.36	113.50	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	11	C	N3-C4-C5	5.36	124.04	121.90
54	BA	1509	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1810	A	C6-C5-N7	5.36	136.05	132.30
54	BA	2644	G	N1-C6-O6	-5.36	116.68	119.90
21	AA	605	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	831	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	1464	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	1729	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	2229	U	C5-C6-N1	-5.36	120.02	122.70
21	AA	15	G	N1-C6-O6	-5.36	116.69	119.90
21	AA	72	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	418	C	N1-C2-O2	5.36	122.11	118.90
21	AA	605	U	N1-C2-N3	5.36	118.11	114.90
21	AA	1433	A	C5-C6-N1	5.36	120.38	117.70
22	A1	21	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2116	G	N9-C4-C5	5.36	107.54	105.40
21	AA	1534	A	C4-C5-C6	-5.36	114.32	117.00
23	A2	90	U	C5-C6-N1	-5.36	120.02	122.70
54	BA	561	G	N1-C6-O6	-5.36	116.69	119.90
54	BA	1317	G	N3-C4-C5	-5.36	125.92	128.60
54	BA	1430	G	C8-N9-C4	-5.36	104.26	106.40
54	BA	1832	C	N3-C4-C5	5.36	124.04	121.90
21	AA	151	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	777	G	C5-C6-N1	5.35	114.18	111.50
54	BA	2353	G	C8-N9-C4	-5.35	104.26	106.40
21	AA	116	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	166	U	N3-C2-O2	-5.35	118.45	122.20
21	AA	308	C	O4'-C4'-C3'	5.35	110.38	106.10
21	AA	397	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	692	U	N3-C2-O2	-5.35	118.45	122.20
21	AA	1183	U	N3-C2-O2	-5.35	118.45	122.20
54	BA	552	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	846	U	N3-C2-O2	-5.35	118.45	122.20
54	BA	2086	U	C5'-C4'-O4'	5.35	115.52	109.10
54	BA	2092	U	C5-C6-N1	-5.35	120.02	122.70
21	AA	539	A	C6-C5-N7	5.35	136.05	132.30
54	BA	1967	C	O4'-C1'-N1	5.35	112.48	108.20
6	AG	4	ARG	NE-CZ-NH1	5.35	122.97	120.30
21	AA	496	A	O4'-C1'-N9	5.35	112.48	108.20
21	AA	571	U	O4'-C4'-C3'	5.35	110.38	106.10
21	AA	1141	C	N1-C2-O2	5.35	122.11	118.90
21	AA	1314	C	O4'-C1'-N1	5.35	112.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	54	G	N3-C4-C5	-5.35	125.93	128.60
54	BA	659	G	C5-C6-N1	5.35	114.17	111.50
54	BA	2138	G	O4'-C1'-N9	5.35	112.48	108.20
55	BB	54	G	C5-C6-N1	5.35	114.17	111.50
20	AU	44	ARG	NE-CZ-NH1	5.35	122.97	120.30
21	AA	308	C	N1-C2-O2	5.35	122.11	118.90
21	AA	396	C	N1-C2-O2	5.35	122.11	118.90
21	AA	568	G	N3-C2-N2	-5.35	116.16	119.90
21	AA	912	C	N1-C2-O2	5.35	122.11	118.90
21	AA	1200	C	N3-C2-O2	-5.35	118.16	121.90
21	AA	1524	C	N1-C2-O2	5.35	122.11	118.90
24	A3	50	G	C5-C6-N1	5.35	114.17	111.50
54	BA	321	U	C5-C6-N1	-5.35	120.03	122.70
54	BA	381	G	N9-C4-C5	5.35	107.54	105.40
54	BA	597	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	1438	U	N3-C2-O2	-5.35	118.46	122.20
54	BA	2110	G	C5-C6-N1	5.35	114.17	111.50
54	BA	2130	U	N1-C2-N3	5.35	118.11	114.90
54	BA	1318	U	C3'-C2'-C1'	5.35	105.78	101.50
54	BA	2101	A	C4-C5-C6	-5.35	114.33	117.00
1	AB	73	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	AB	224	ARG	NE-CZ-NH1	5.34	122.97	120.30
21	AA	771	G	N1-C6-O6	-5.34	116.69	119.90
22	A1	67	U	N3-C2-O2	-5.34	118.46	122.20
54	BA	605	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	664	G	C5-C6-N1	5.34	114.17	111.50
54	BA	867	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1209	U	N1-C2-N3	5.34	118.11	114.90
54	BA	2432	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2890	G	C5-C6-N1	5.34	114.17	111.50
55	BB	114	C	N3-C2-O2	-5.34	118.16	121.90
21	AA	851	G	C8-N9-C4	-5.34	104.26	106.40
21	AA	1028	C	N1-C2-O2	5.34	122.11	118.90
54	BA	142	A	C5-C6-N1	5.34	120.37	117.70
54	BA	1539	U	C5-C6-N1	-5.34	120.03	122.70
54	BA	2650	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2715	C	O4'-C1'-N1	5.34	112.47	108.20
21	AA	1044	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	1066	C	N1-C2-O2	5.34	122.11	118.90
54	BA	159	G	N3-C4-C5	-5.34	125.93	128.60
54	BA	247	G	O4'-C1'-N9	5.34	112.47	108.20
54	BA	765	C	N1-C2-O2	5.34	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1389	G	C8-N9-C4	-5.34	104.26	106.40
54	BA	1702	G	N1-C6-O6	-5.34	116.69	119.90
55	BB	116	G	O4'-C1'-N9	5.34	112.47	108.20
21	AA	995	C	O4'-C1'-N1	5.34	112.47	108.20
25	BC	155	ARG	NE-CZ-NH2	-5.34	117.63	120.30
54	BA	383	C	N3-C4-C5	5.34	124.04	121.90
54	BA	1488	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1941	C	N1-C2-O2	5.34	122.10	118.90
21	AA	1308	U	C5-C6-N1	-5.34	120.03	122.70
54	BA	517	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1167	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1951	U	C5-C6-N1	-5.34	120.03	122.70
54	BA	2129	C	N1-C2-O2	5.34	122.10	118.90
21	AA	245	U	C5-C6-N1	-5.34	120.03	122.70
21	AA	263	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	878	A	C5-C6-N1	5.34	120.37	117.70
21	AA	899	C	N3-C2-O2	-5.34	118.16	121.90
21	AA	1115	U	N1-C2-N3	5.34	118.10	114.90
54	BA	32	C	N1-C2-O2	5.34	122.10	118.90
54	BA	90	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	774	G	N9-C4-C5	5.34	107.53	105.40
21	AA	1400	C	O4'-C4'-C3'	5.33	110.37	106.10
54	BA	37	C	N3-C4-C5	5.33	124.03	121.90
54	BA	914	G	C5-C6-N1	5.33	114.17	111.50
54	BA	2819	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	145	G	C8-N9-C4	-5.33	104.27	106.40
21	AA	664	G	C5-C6-N1	5.33	114.17	111.50
21	AA	1080	A	C4-C5-C6	-5.33	114.33	117.00
22	A1	11	C	N1-C2-O2	5.33	122.10	118.90
54	BA	15	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	236	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	377	G	O4'-C1'-N9	5.33	112.47	108.20
54	BA	1027	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	1562	U	N3-C2-O2	-5.33	118.47	122.20
54	BA	2092	U	C4-C5-C6	5.33	122.90	119.70
54	BA	2761	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	1030	U	N1-C2-N3	5.33	118.10	114.90
54	BA	468	G	C5-C6-N1	5.33	114.17	111.50
54	BA	651	G	N9-C4-C5	5.33	107.53	105.40
54	BA	657	U	N1-C2-N3	5.33	118.10	114.90
54	BA	856	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	1431	A	C6-C5-N7	5.33	136.03	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1904	G	C8-N9-C4	-5.33	104.27	106.40
54	BA	2361	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	2841	C	N3-C2-O2	-5.33	118.17	121.90
55	BB	92	C	C4'-C3'-C2'	-5.33	97.27	102.60
21	AA	422	C	C5'-C4'-C3'	-5.33	107.47	116.00
54	BA	106	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	156	A	C6-C5-N7	5.33	136.03	132.30
54	BA	427	U	N1-C2-N3	5.33	118.10	114.90
4	AE	68	ARG	NE-CZ-NH1	5.33	122.97	120.30
21	AA	408	A	C6-C5-N7	5.33	136.03	132.30
21	AA	677	U	N1-C2-N3	5.33	118.10	114.90
23	A2	87	U	C4-C5-C6	5.33	122.90	119.70
28	BF	79	ARG	NE-CZ-NH2	-5.33	117.64	120.30
54	BA	698	C	C3'-C2'-C1'	5.33	105.76	101.50
54	BA	755	U	C4'-C3'-C2'	-5.33	97.27	102.60
54	BA	1804	C	N3-C4-C5	5.33	124.03	121.90
54	BA	2137	U	N1-C2-O2	5.33	126.53	122.80
54	BA	2178	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	373	A	C2-N3-C4	5.33	113.26	110.60
21	AA	1077	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	1301	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	1739	A	C5-C6-N1	5.33	120.36	117.70
54	BA	1799	G	C5-C6-N1	5.33	114.16	111.50
21	AA	44	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	51	G	C8-N9-C4	-5.33	104.27	106.40
54	BA	599	A	C6-C5-N7	5.33	136.03	132.30
54	BA	1481	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	1509	A	C2-N3-C4	5.33	113.26	110.60
54	BA	1541	C	N1-C2-O2	5.33	122.09	118.90
54	BA	2074	U	N3-C2-O2	-5.33	118.47	122.20
28	BF	101	ARG	NE-CZ-NH1	5.32	122.96	120.30
54	BA	98	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	945	A	C6-C5-N7	5.32	136.03	132.30
54	BA	1030	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1481	U	N1-C2-N3	5.32	118.09	114.90
54	BA	1833	C	N3-C4-C5	5.32	124.03	121.90
54	BA	2240	U	N1-C2-N3	5.32	118.09	114.90
54	BA	2824	C	O4'-C1'-N1	5.32	112.46	108.20
21	AA	995	C	N1-C2-O2	5.32	122.09	118.90
22	A1	68	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	1679	A	C6-C5-N7	5.32	136.03	132.30
54	BA	1817	G	N3-C2-N2	-5.32	116.17	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2428	G	N3-C4-C5	-5.32	125.94	128.60
10	AK	124	LYS	C-N-CA	5.32	135.00	121.70
21	AA	232	G	C5-C6-N1	5.32	114.16	111.50
21	AA	715	A	C6-C5-N7	5.32	136.02	132.30
21	AA	1094	G	N3-C2-N2	-5.32	116.18	119.90
21	AA	1178	G	C5-C6-N1	5.32	114.16	111.50
54	BA	1125	G	C5-C6-N1	5.32	114.16	111.50
54	BA	1306	C	N1-C2-O2	5.32	122.09	118.90
54	BA	1390	U	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1656	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1816	C	N1-C2-O2	5.32	122.09	118.90
54	BA	2260	C	N3-C2-O2	-5.32	118.17	121.90
21	AA	485	U	C5-C6-N1	-5.32	120.04	122.70
21	AA	630	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	1078	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	280	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	412	A	O4'-C1'-N9	5.32	112.45	108.20
54	BA	1089	A	O4'-C1'-C2'	-5.32	100.48	105.80
54	BA	1291	C	N3-C2-O2	-5.32	118.18	121.90
21	AA	131	A	C6-C5-N7	5.32	136.02	132.30
21	AA	170	U	C5-C6-N1	-5.32	120.04	122.70
21	AA	475	C	N1-C2-O2	5.32	122.09	118.90
21	AA	544	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	1298	U	O4'-C1'-N1	5.32	112.45	108.20
21	AA	1300	G	P-O3'-C3'	5.32	126.08	119.70
34	BL	48	ARG	NE-CZ-NH1	5.32	122.96	120.30
54	BA	835	C	N3-C2-O2	-5.32	118.18	121.90
54	BA	1584	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	1972	G	C8-N9-C4	-5.32	104.27	106.40
54	BA	2101	A	C5-C6-N1	5.32	120.36	117.70
21	AA	418	C	N3-C4-C5	5.32	124.03	121.90
21	AA	582	C	N3-C4-C5	5.32	124.03	121.90
21	AA	939	G	C8-N9-C4	-5.32	104.27	106.40
49	B0	51	ARG	NE-CZ-NH2	-5.32	117.64	120.30
54	BA	810	U	N3-C2-O2	-5.32	118.48	122.20
21	AA	1318	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	647	G	N3-C4-C5	-5.31	125.94	128.60
21	AA	793	U	N3-C2-O2	-5.31	118.48	122.20
24	A3	49	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	201	C	N1-C2-O2	5.31	122.09	118.90
54	BA	890	C	C3'-C2'-C1'	-5.31	97.25	101.50
54	BA	989	G	O4'-C1'-N9	5.31	112.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1089	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	2049	G	N9-C4-C5	5.31	107.53	105.40
54	BA	2255	G	C5-C6-N1	5.31	114.16	111.50
54	BA	2117	A	C4-C5-C6	-5.31	114.34	117.00
21	AA	787	A	C5-C6-N1	5.31	120.36	117.70
21	AA	1335	U	O4'-C4'-C3'	5.31	110.35	106.10
33	BK	49	ARG	NE-CZ-NH1	5.31	122.95	120.30
54	BA	86	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	123	G	C5-C6-N1	5.31	114.16	111.50
54	BA	876	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	888	C	N1-C2-O2	5.31	122.08	118.90
54	BA	1937	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	2169	A	C8-N9-C4	-5.31	103.68	105.80
54	BA	2428	G	O4'-C1'-N9	5.31	112.45	108.20
21	AA	1432	G	C5-C6-N1	5.31	114.15	111.50
54	BA	516	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	1964	G	N3-C4-C5	-5.31	125.95	128.60
54	BA	2385	C	N1-C2-O2	5.31	122.08	118.90
54	BA	2390	U	C5-C6-N1	-5.31	120.05	122.70
21	AA	1249	C	N3-C2-O2	-5.31	118.19	121.90
21	AA	1333	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	548	G	C8-N9-C4	-5.31	104.28	106.40
21	AA	305	G	O4'-C1'-N9	5.30	112.44	108.20
21	AA	433	G	N3-C4-C5	-5.30	125.95	128.60
21	AA	701	U	N3-C2-O2	-5.30	118.49	122.20
21	AA	842	U	C5-C6-N1	-5.30	120.05	122.70
21	AA	1173	U	C5-C6-N1	-5.30	120.05	122.70
21	AA	1155	A	C5-C6-N1	5.30	120.35	117.70
54	BA	1474	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2737	G	N3-C4-C5	-5.30	125.95	128.60
21	AA	756	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1221	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1548	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1703	G	C5-C6-N1	5.30	114.15	111.50
54	BA	1868	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2618	G	C5'-C4'-O4'	5.30	115.46	109.10
21	AA	507	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	529	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	1559	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	2428	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	429	U	N1-C2-N3	5.30	118.08	114.90
54	BA	901	C	N3-C2-O2	-5.30	118.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2063	C	C2-N3-C4	-5.30	117.25	119.90
54	BA	2281	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	2383	G	C8-N9-C4	-5.30	104.28	106.40
21	AA	257	G	C5-C6-N1	5.30	114.15	111.50
21	AA	322	C	N3-C2-O2	-5.30	118.19	121.90
21	AA	403	C	N3-C4-C5	5.30	124.02	121.90
21	AA	1369	C	N1-C2-O2	5.30	122.08	118.90
21	AA	1450	U	N1-C2-N3	5.30	118.08	114.90
54	BA	330	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	446	G	O4'-C4'-C3'	5.30	110.34	106.10
54	BA	808	G	C3'-C2'-C1'	5.30	105.74	101.50
54	BA	1536	C	C5'-C4'-C3'	-5.30	107.53	116.00
54	BA	1669	A	C5-C6-N1	5.30	120.35	117.70
54	BA	2175	C	N3-C4-C5	5.30	124.02	121.90
54	BA	2515	C	N1-C2-O2	5.30	122.08	118.90
21	AA	327	A	O4'-C1'-N9	5.29	112.44	108.20
54	BA	394	C	N1-C2-O2	5.29	122.08	118.90
54	BA	948	C	N1-C2-O2	5.29	122.08	118.90
54	BA	2693	G	C5-C6-N1	5.29	114.15	111.50
21	AA	1126	U	C5-C6-N1	-5.29	120.05	122.70
54	BA	57	C	N3-C2-O2	-5.29	118.19	121.90
54	BA	427	U	C5-C6-N1	-5.29	120.05	122.70
54	BA	1112	G	C8-N9-C4	-5.29	104.28	106.40
54	BA	2047	C	C4'-C3'-C2'	-5.29	97.31	102.60
54	BA	2235	G	C4'-C3'-C2'	-5.29	97.31	102.60
54	BA	2374	C	N3-C4-C5	5.29	124.02	121.90
54	BA	2803	G	C5-C6-N1	5.29	114.15	111.50
54	BA	2830	C	N3-C2-O2	-5.29	118.19	121.90
21	AA	97	G	N3-C4-C5	-5.29	125.95	128.60
21	AA	1036	A	C6-C5-N7	5.29	136.00	132.30
54	BA	175	G	N3-C2-N2	-5.29	116.20	119.90
54	BA	445	C	N1-C2-O2	5.29	122.08	118.90
54	BA	2513	A	C6-C5-N7	5.29	136.00	132.30
54	BA	2602	A	C1'-O4'-C4'	-5.29	105.67	109.90
54	BA	2867	G	O4'-C1'-N9	5.29	112.43	108.20
22	A1	67	U	C5-C6-N1	-5.29	120.06	122.70
54	BA	2890	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	921	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1518	C	N3-C2-O2	-5.29	118.20	121.90
55	BB	105	G	C8-N9-C4	-5.29	104.28	106.40
21	AA	1478	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	136	G	C5-C6-N1	5.29	114.14	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1580	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	2002	G	N1-C6-O6	-5.29	116.73	119.90
21	AA	166	U	C5-C6-N1	-5.29	120.06	122.70
21	AA	267	C	C3'-C2'-C1'	5.29	105.73	101.50
22	A1	71	C	O4'-C1'-N1	5.29	112.43	108.20
28	BF	109	ARG	NE-CZ-NH2	-5.29	117.66	120.30
54	BA	149	A	O4'-C1'-N9	5.29	112.43	108.20
54	BA	761	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	943	A	C4-C5-C6	-5.29	114.36	117.00
21	AA	248	C	O4'-C1'-N1	5.28	112.43	108.20
21	AA	379	C	N3-C4-C5	5.28	124.01	121.90
54	BA	345	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	513	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1818	U	C5-C6-N1	-5.28	120.06	122.70
54	BA	1984	G	C8-N9-C4	-5.28	104.29	106.40
54	BA	2347	C	N3-C2-O2	-5.28	118.20	121.90
54	BA	2571	U	N3-C2-O2	-5.28	118.50	122.20
21	AA	1117	A	C6-C5-N7	5.28	136.00	132.30
54	BA	446	G	C3'-C2'-C1'	5.28	105.73	101.50
54	BA	734	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	916	G	N3-C4-C5	-5.28	125.96	128.60
54	BA	1585	C	C2-N3-C4	-5.28	117.26	119.90
54	BA	2085	U	C5-C6-N1	-5.28	120.06	122.70
54	BA	2820	A	C4-C5-C6	-5.28	114.36	117.00
55	BB	117	G	N9-C4-C5	5.28	107.51	105.40
21	AA	94	G	N3-C2-N2	-5.28	116.20	119.90
21	AA	164	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	802	A	N1-C6-N6	-5.28	115.43	118.60
54	BA	1041	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	1071	G	C3'-C2'-C1'	5.28	105.72	101.50
54	BA	2305	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2679	A	O4'-C1'-N9	5.28	112.42	108.20
54	BA	2699	C	N1-C2-O2	5.28	122.07	118.90
21	AA	725	G	C5'-C4'-C3'	-5.28	107.55	116.00
54	BA	1545	A	C6-C5-N7	5.28	136.00	132.30
21	AA	80	A	C6-C5-N7	5.28	136.00	132.30
21	AA	113	G	N7-C8-N9	5.28	115.74	113.10
24	A3	16	C	N1-C2-O2	5.28	122.07	118.90
24	A3	58	A	C6-C5-N7	5.28	136.00	132.30
54	BA	348	A	O4'-C1'-N9	5.28	112.42	108.20
54	BA	1714	U	N3-C2-O2	-5.28	118.51	122.20
21	AA	220	G	N9-C4-C5	5.28	107.51	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1370	G	O4'-C1'-N9	5.28	112.42	108.20
54	BA	1887	C	N3-C2-O2	-5.28	118.21	121.90
55	BB	112	G	C5-C6-N1	5.28	114.14	111.50
54	BA	210	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	456	C	N3-C4-N4	-5.27	114.31	118.00
54	BA	846	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	1248	G	O4'-C1'-N9	5.27	112.42	108.20
55	BB	17	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	1097	C	C1'-O4'-C4'	-5.27	105.68	109.90
21	AA	1176	A	C5-C6-N1	5.27	120.34	117.70
38	BP	88	ARG	NE-CZ-NH1	5.27	122.94	120.30
54	BA	130	C	N3-C4-C5	5.27	124.01	121.90
54	BA	518	G	C8-N9-C4	-5.27	104.29	106.40
54	BA	541	A	C6-C5-N7	5.27	135.99	132.30
54	BA	1036	G	C5-C6-N1	5.27	114.14	111.50
54	BA	1169	A	C6-C5-N7	5.27	135.99	132.30
54	BA	1979	U	N3-C2-O2	-5.27	118.51	122.20
54	BA	2583	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	2847	U	N1-C2-N3	5.27	118.06	114.90
55	BB	5	U	C4'-C3'-C2'	-5.27	97.33	102.60
21	AA	1460	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	1172	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	34	C	N1-C2-O2	5.27	122.06	118.90
21	AA	622	A	C6-C5-N7	5.27	135.99	132.30
21	AA	979	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2240	U	O4'-C1'-N1	5.27	112.42	108.20
21	AA	139	A	C5-C6-N1	5.27	120.33	117.70
21	AA	364	A	C6-C5-N7	5.27	135.99	132.30
21	AA	503	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	521	G	O4'-C1'-N9	5.27	112.41	108.20
21	AA	1097	C	N3-C2-O2	-5.27	118.21	121.90
21	AA	1184	G	N3-C4-C5	-5.27	125.97	128.60
21	AA	1342	C	N3-C4-C5	5.27	124.01	121.90
54	BA	994	C	N1-C2-O2	5.27	122.06	118.90
54	BA	1613	G	O4'-C1'-N9	5.27	112.41	108.20
54	BA	2138	G	N1-C6-O6	-5.27	116.74	119.90
21	AA	116	A	C6-C5-N7	5.27	135.99	132.30
21	AA	443	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	726	G	O4'-C1'-N9	5.27	112.41	108.20
54	BA	935	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	1489	C	N1-C2-O2	5.27	122.06	118.90
54	BA	2341	G	C4'-C3'-C2'	-5.27	97.33	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	187	G	C5-C6-N1	5.26	114.13	111.50
21	AA	204	G	C8-N9-C4	-5.26	104.29	106.40
21	AA	426	U	N1-C2-N3	5.26	118.06	114.90
21	AA	809	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	343	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	1841	U	O4'-C1'-N1	5.26	112.41	108.20
55	BB	117	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	872	A	C2-N3-C4	5.26	113.23	110.60
21	AA	40	C	N1-C2-O2	5.26	122.06	118.90
21	AA	1215	G	N9-C4-C5	5.26	107.50	105.40
21	AA	1276	G	N7-C8-N9	5.26	115.73	113.10
21	AA	1482	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	666	A	C5-C6-N1	5.26	120.33	117.70
54	BA	775	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	1624	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	2745	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	504	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	547	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	861	G	N7-C8-N9	5.26	115.73	113.10
21	AA	897	C	O4'-C1'-N1	5.26	112.41	108.20
21	AA	923	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1233	G	C5-C6-N1	5.26	114.13	111.50
21	AA	1487	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	1082	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	1462	C	N3-C2-O2	-5.26	118.22	121.90
54	BA	1725	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	1831	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	2065	C	N3-C2-O2	-5.26	118.22	121.90
54	BA	2131	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	2317	A	C6-C5-N7	5.26	135.98	132.30
54	BA	2813	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	33	A	C6-C5-N7	5.26	135.98	132.30
54	BA	1422	G	N1-C6-O6	-5.26	116.75	119.90
54	BA	2624	G	N1-C6-O6	-5.26	116.75	119.90
17	AR	47	ARG	NE-CZ-NH2	-5.26	117.67	120.30
21	AA	631	C	N1-C2-O2	5.26	122.05	118.90
21	AA	1387	G	C5-C6-N1	5.26	114.13	111.50
21	AA	1519	A	C6-C5-N7	5.26	135.98	132.30
54	BA	514	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1618	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2243	U	O4'-C1'-N1	5.26	112.41	108.20
55	BB	24	G	C8-N9-C4	-5.26	104.30	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2222	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2638	G	C8-N9-C4	-5.25	104.30	106.40
55	BB	59	A	C4-C5-C6	-5.25	114.37	117.00
21	AA	1085	U	C5-C6-N1	-5.25	120.07	122.70
21	AA	1528	U	N3-C2-O2	-5.25	118.52	122.20
54	BA	532	A	O4'-C1'-N9	5.25	112.40	108.20
54	BA	920	A	C6-C5-N7	5.25	135.98	132.30
54	BA	1084	A	C6-C5-N7	5.25	135.98	132.30
54	BA	1795	C	N3-C2-O2	-5.25	118.22	121.90
54	BA	2537	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2546	U	C5-C6-N1	-5.25	120.07	122.70
21	AA	248	C	N1-C2-O2	5.25	122.05	118.90
21	AA	764	C	N1-C2-O2	5.25	122.05	118.90
54	BA	410	G	N9-C4-C5	5.25	107.50	105.40
54	BA	1257	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1911	U	C5'-C4'-O4'	5.25	115.40	109.10
54	BA	2424	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	21	G	C5-C6-N1	5.25	114.12	111.50
21	AA	359	G	N3-C4-C5	-5.25	125.97	128.60
21	AA	426	U	N3-C2-O2	-5.25	118.53	122.20
54	BA	869	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	2611	C	O4'-C1'-N1	5.25	112.40	108.20
21	AA	494	G	N3-C4-C5	-5.25	125.97	128.60
21	AA	610	U	O4'-C1'-N1	5.25	112.40	108.20
21	AA	1432	G	C3'-C2'-C1'	5.25	105.70	101.50
21	AA	1502	A	O4'-C1'-N9	5.25	112.40	108.20
54	BA	2757	A	C5'-C4'-O4'	5.25	115.40	109.10
55	BB	82	U	C5-C6-N1	-5.25	120.08	122.70
21	AA	1380	U	C5-C6-N1	-5.25	120.08	122.70
21	AA	1392	G	C5-C6-N1	5.25	114.12	111.50
54	BA	721	A	C6-C5-N7	5.25	135.97	132.30
54	BA	2805	C	N1-C2-O2	5.25	122.05	118.90
55	BB	42	C	N3-C2-O2	-5.25	118.23	121.90
21	AA	501	C	N3-C4-C5	5.25	124.00	121.90
54	BA	47	C	N3-C2-O2	-5.25	118.23	121.90
21	AA	75	G	C5-C6-N1	5.24	114.12	111.50
21	AA	811	C	O4'-C1'-N1	5.24	112.39	108.20
21	AA	1093	A	C5-C6-N1	5.24	120.32	117.70
54	BA	171	U	C5-C6-N1	-5.24	120.08	122.70
54	BA	1888	G	C8-N9-C4	-5.24	104.30	106.40
54	BA	2196	C	C1'-O4'-C4'	-5.24	105.71	109.90
54	BA	2636	C	O4'-C1'-N1	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	AP	14	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BA	578	G	N1-C6-O6	-5.24	116.75	119.90
54	BA	702	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1129	A	C5-C6-N1	5.24	120.32	117.70
21	AA	253	A	C5-C6-N1	5.24	120.32	117.70
21	AA	816	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	1472	U	N3-C2-O2	-5.24	118.53	122.20
54	BA	37	C	N1-C2-O2	5.24	122.04	118.90
54	BA	505	A	O4'-C1'-N9	5.24	112.39	108.20
54	BA	1041	G	C5-C6-N1	5.24	114.12	111.50
54	BA	1088	A	C6-C5-N7	5.24	135.97	132.30
54	BA	2831	G	N1-C6-O6	-5.24	116.76	119.90
21	AA	572	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	701	U	P-O3'-C3'	5.24	125.98	119.70
21	AA	744	C	N1-C2-O2	5.24	122.04	118.90
21	AA	1001	C	N3-C2-O2	-5.24	118.23	121.90
21	AA	1067	A	P-O3'-C3'	5.24	125.99	119.70
21	AA	1405	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	59	U	N1-C2-N3	5.24	118.04	114.90
54	BA	504	A	C1'-O4'-C4'	-5.24	105.71	109.90
54	BA	1214	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1222	U	C5-C6-N1	-5.24	120.08	122.70
54	BA	2030	A	C6-C5-N7	5.24	135.97	132.30
55	BB	76	G	O4'-C1'-N9	5.24	112.39	108.20
21	AA	1121	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	1330	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	774	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	1639	C	N3-C4-N4	-5.24	114.33	118.00
15	AP	51	ARG	NE-CZ-NH2	-5.24	117.68	120.30
21	AA	747	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	755	G	O4'-C1'-N9	5.24	112.39	108.20
21	AA	818	G	N3-C2-N2	-5.24	116.23	119.90
24	A3	3	C	N3-C4-C5	5.24	124.00	121.90
54	BA	570	G	N3-C2-N2	-5.24	116.23	119.90
54	BA	948	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1281	G	C5'-C4'-O4'	5.24	115.38	109.10
54	BA	1316	U	N1-C2-N3	5.24	118.04	114.90
54	BA	1350	C	C4'-C3'-C2'	-5.24	97.36	102.60
54	BA	1351	C	C6-N1-C2	-5.24	118.21	120.30
54	BA	2077	A	N1-C6-N6	-5.24	115.46	118.60
54	BA	2557	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	370	C	N3-C4-C5	5.23	123.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	773	G	C5-C6-N1	5.23	114.12	111.50
21	AA	1300	G	O4'-C1'-N9	5.23	112.39	108.20
21	AA	1514	G	C5-C6-N1	5.23	114.12	111.50
54	BA	1033	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	1834	U	C3'-C2'-C1'	5.23	105.69	101.50
54	BA	2066	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	2168	G	C4'-C3'-C2'	-5.23	97.37	102.60
54	BA	2463	C	N3-C2-O2	-5.23	118.24	121.90
21	AA	146	G	C5-C6-N1	5.23	114.12	111.50
21	AA	719	C	N3-C2-O2	-5.23	118.24	121.90
21	AA	1237	C	N1-C2-O2	5.23	122.04	118.90
54	BA	860	U	O4'-C1'-N1	5.23	112.38	108.20
54	BA	874	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	1088	A	C2-N3-C4	5.23	113.22	110.60
54	BA	2563	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2809	A	C4-C5-C6	-5.23	114.38	117.00
54	BA	2890	G	N3-C4-C5	-5.23	125.98	128.60
54	BA	838	C	C5'-C4'-O4'	5.23	115.38	109.10
54	BA	1505	A	C6-C5-N7	5.23	135.96	132.30
54	BA	2323	G	N7-C8-N9	5.23	115.72	113.10
54	BA	2626	C	N3-C2-O2	-5.23	118.24	121.90
55	BB	64	G	N3-C4-C5	-5.23	125.99	128.60
54	BA	1378	A	C3'-C2'-C1'	5.23	105.68	101.50
20	AU	46	ARG	NE-CZ-NH1	5.23	122.91	120.30
21	AA	799	G	C5-C6-N1	5.23	114.11	111.50
21	AA	813	U	O4'-C1'-N1	5.23	112.38	108.20
24	A3	43	G	N9-C4-C5	5.23	107.49	105.40
54	BA	108	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	651	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	47	C	N3-C2-O2	-5.22	118.24	121.90
21	AA	918	A	C5-C6-N6	5.22	127.88	123.70
21	AA	1340	A	O4'-C1'-N9	5.22	112.38	108.20
27	BE	44	ARG	NE-CZ-NH1	5.22	122.91	120.30
54	BA	249	C	P-O3'-C3'	5.22	125.97	119.70
54	BA	676	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	1714	U	C1'-O4'-C4'	-5.22	105.72	109.90
54	BA	2197	U	N3-C2-O2	-5.22	118.54	122.20
21	AA	212	G	O4'-C1'-N9	5.22	112.38	108.20
21	AA	444	G	N3-C4-C5	-5.22	125.99	128.60
21	AA	799	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	1504	G	O4'-C1'-N9	5.22	112.38	108.20
22	A1	33	U	N3-C2-O2	-5.22	118.54	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A2	86	U	C5'-C4'-C3'	-5.22	107.64	116.00
54	BA	204	A	C6-C5-N7	5.22	135.96	132.30
54	BA	1646	C	N3-C4-C5	5.22	123.99	121.90
54	BA	1767	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	1100	C	N1-C2-O2	5.22	122.03	118.90
21	AA	1119	C	O4'-C1'-N1	5.22	112.38	108.20
21	AA	1139	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	122	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	810	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	1158	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1635	A	C4-C5-C6	-5.22	114.39	117.00
54	BA	1644	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	2417	C	C4'-C3'-C2'	-5.22	97.38	102.60
21	AA	531	U	C5-C6-N1	-5.22	120.09	122.70
21	AA	843	U	O4'-C1'-N1	5.22	112.37	108.20
22	A1	43	G	N1-C6-O6	-5.22	116.77	119.90
55	BB	63	C	N3-C2-O2	-5.22	118.25	121.90
21	AA	1192	C	N1-C2-O2	5.22	122.03	118.90
21	AA	1434	A	C6-C5-N7	5.22	135.95	132.30
54	BA	1850	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	420	U	N1-C2-N3	5.21	118.03	114.90
21	AA	883	C	C1'-O4'-C4'	-5.21	105.73	109.90
21	AA	1126	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1764	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	2689	U	C1'-O4'-C4'	-5.21	105.73	109.90
54	BA	1397	U	N1-C2-N3	5.21	118.03	114.90
54	BA	2246	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	2337	G	N3-C4-C5	-5.21	125.99	128.60
54	BA	2343	U	C5-C6-N1	-5.21	120.09	122.70
21	AA	155	A	C6-C5-N7	5.21	135.95	132.30
21	AA	428	G	N1-C6-O6	-5.21	116.77	119.90
21	AA	679	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	220	G	N3-C4-C5	-5.21	125.99	128.60
54	BA	660	C	C3'-C2'-C1'	5.21	105.67	101.50
54	BA	1989	G	N7-C8-N9	5.21	115.71	113.10
21	AA	176	C	N3-C4-C5	5.21	123.98	121.90
22	A1	56	C	N1-C2-O2	5.21	122.03	118.90
54	BA	1594	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	1806	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2229	U	N1-C2-N3	5.21	118.03	114.90
54	BA	2755	C	N1-C2-O2	5.21	122.03	118.90
11	AL	120	ARG	NE-CZ-NH1	5.21	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1023	U	O4'-C1'-N1	5.21	112.37	108.20
21	AA	1204	A	C6-C5-N7	5.21	135.94	132.30
21	AA	1364	U	N1-C2-N3	5.21	118.03	114.90
21	AA	1482	G	C8-N9-C4	-5.21	104.32	106.40
54	BA	35	G	N3-C4-C5	-5.21	126.00	128.60
54	BA	116	C	N1-C2-O2	5.21	122.03	118.90
54	BA	154	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1776	G	N1-C6-O6	-5.21	116.78	119.90
54	BA	2145	C	N3-C4-C5	5.21	123.98	121.90
54	BA	2338	C	N3-C4-C5	5.21	123.98	121.90
54	BA	2679	A	C5-C6-N1	5.21	120.30	117.70
55	BB	9	G	N1-C6-O6	-5.21	116.77	119.90
21	AA	34	C	C5'-C4'-O4'	5.21	115.35	109.10
21	AA	513	C	N1-C2-O2	5.21	122.02	118.90
21	AA	517	G	C5-C6-N1	5.21	114.10	111.50
21	AA	524	G	C5-C6-N1	5.21	114.10	111.50
21	AA	1432	G	N3-C4-C5	-5.21	126.00	128.60
24	A3	64	G	N7-C8-N9	5.21	115.70	113.10
54	BA	458	G	O4'-C1'-N9	5.21	112.36	108.20
54	BA	571	U	O4'-C1'-C2'	-5.21	100.59	105.80
54	BA	884	U	C5-C6-N1	-5.21	120.10	122.70
54	BA	1576	U	C5-C6-N1	-5.21	120.10	122.70
54	BA	2391	G	C5-C6-N1	5.21	114.10	111.50
54	BA	2743	U	C5-C6-N1	-5.21	120.10	122.70
54	BA	2862	G	N1-C6-O6	-5.21	116.78	119.90
21	AA	536	C	N3-C4-C5	5.21	123.98	121.90
21	AA	872	A	C4-C5-C6	-5.21	114.40	117.00
21	AA	984	C	N1-C2-O2	5.21	122.02	118.90
54	BA	422	A	C5-C6-N1	5.21	120.30	117.70
54	BA	1569	A	C5-C6-N1	5.21	120.30	117.70
54	BA	2697	G	C4'-C3'-C2'	-5.21	97.39	102.60
9	AJ	89	ARG	NE-CZ-NH2	-5.20	117.70	120.30
21	AA	1167	A	C3'-C2'-C1'	5.20	105.66	101.50
21	AA	1324	A	C4-C5-C6	-5.20	114.40	117.00
34	BL	69	ARG	NE-CZ-NH1	5.20	122.90	120.30
54	BA	104	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1228	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	1711	A	C2-N3-C4	5.20	113.20	110.60
54	BA	646	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1572	A	C4-C5-C6	-5.20	114.40	117.00
21	AA	1104	G	C5-C6-N1	5.20	114.10	111.50
21	AA	1251	A	C6-C5-N7	5.20	135.94	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1105	U	N1-C2-N3	5.20	118.02	114.90
54	BA	2234	G	N3-C4-C5	-5.20	126.00	128.60
54	BA	2894	G	C5-C6-N1	5.20	114.10	111.50
21	AA	177	G	C5-C6-N1	5.20	114.10	111.50
21	AA	434	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	548	G	N7-C8-N9	5.20	115.70	113.10
54	BA	583	G	C5-C6-N1	5.20	114.10	111.50
54	BA	616	A	O4'-C1'-N9	5.20	112.36	108.20
54	BA	680	C	C2-N3-C4	-5.20	117.30	119.90
54	BA	1793	C	C5'-C4'-O4'	5.20	115.34	109.10
54	BA	2617	U	O4'-C1'-N1	5.20	112.36	108.20
21	AA	411	A	C5-C6-N1	5.20	120.30	117.70
21	AA	652	U	C5-C6-N1	-5.20	120.10	122.70
54	BA	123	G	C5'-C4'-O4'	5.20	115.34	109.10
54	BA	2160	C	N1-C2-O2	5.20	122.02	118.90
21	AA	1027	C	N3-C2-O2	-5.20	118.26	121.90
22	A1	57	G	C5-C6-N1	5.20	114.10	111.50
54	BA	296	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	716	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1392	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1713	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2005	A	C5-C6-N1	5.20	120.30	117.70
54	BA	2056	G	C5-C6-N1	5.20	114.10	111.50
54	BA	2311	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2804	U	C5-C6-N1	-5.20	120.10	122.70
54	BA	637	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	1579	A	O4'-C1'-N9	5.19	112.36	108.20
54	BA	2165	C	N1-C2-O2	5.19	122.02	118.90
21	AA	847	G	C5-C6-N1	5.19	114.10	111.50
24	A3	54	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	28	A	O4'-C1'-N9	5.19	112.35	108.20
54	BA	371	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	433	C	N3-C4-C5	5.19	123.98	121.90
54	BA	1545	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	1567	G	C5-C6-N1	5.19	114.10	111.50
54	BA	1823	G	C5-C6-N1	5.19	114.10	111.50
54	BA	1843	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	1859	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	2135	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	2328	A	C5-C6-N1	5.19	120.30	117.70
21	AA	392	C	N3-C4-C5	5.19	123.98	121.90
54	BA	82	U	O4'-C1'-N1	5.19	112.35	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	239	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	509	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	795	C	C6-N1-C2	-5.19	118.22	120.30
54	BA	1503	A	C5-C6-N1	5.19	120.30	117.70
54	BA	1792	G	N9-C4-C5	5.19	107.48	105.40
21	AA	494	G	C8-N9-C4	-5.19	104.32	106.40
21	AA	1483	A	C5-C6-N1	5.19	120.30	117.70
54	BA	281	C	N1-C2-O2	5.19	122.01	118.90
54	BA	646	U	C4-C5-C6	5.19	122.81	119.70
21	AA	136	C	O4'-C1'-N1	5.19	112.35	108.20
21	AA	186	C	N3-C4-C5	5.19	123.97	121.90
21	AA	1246	A	C6-C5-N7	5.19	135.93	132.30
21	AA	1382	C	N1-C2-O2	5.19	122.01	118.90
21	AA	1534	A	C5-C6-N1	5.19	120.29	117.70
23	A2	81	U	N3-C2-O2	-5.19	118.57	122.20
54	BA	398	C	N1-C2-O2	5.19	122.01	118.90
54	BA	544	C	N3-C4-C5	5.19	123.97	121.90
54	BA	873	C	C5'-C4'-O4'	5.19	115.33	109.10
54	BA	1634	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	1797	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	1910	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	2029	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	2496	C	C1'-O4'-C4'	-5.19	105.75	109.90
54	BA	2706	A	C5-C6-N1	5.19	120.29	117.70
21	AA	367	U	O4'-C1'-N1	5.19	112.35	108.20
21	AA	772	U	N3-C2-O2	-5.19	118.57	122.20
24	A3	62	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1678	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	2416	C	N1-C2-O2	5.19	122.01	118.90
21	AA	49	U	C5-C6-N1	-5.18	120.11	122.70
21	AA	366	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	1147	C	C2-N3-C4	-5.18	117.31	119.90
54	BA	219	A	C6-C5-N7	5.18	135.93	132.30
54	BA	598	U	O4'-C1'-N1	5.18	112.35	108.20
54	BA	803	U	O4'-C1'-N1	5.18	112.35	108.20
54	BA	1140	C	N1-C2-O2	5.18	122.01	118.90
54	BA	1229	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	2868	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	108	G	C2-N3-C4	5.18	114.49	111.90
21	AA	593	U	N3-C2-O2	-5.18	118.57	122.20
21	AA	1364	U	C5-C6-N1	-5.18	120.11	122.70
21	AA	1473	G	C5-C6-N1	5.18	114.09	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	724	U	N3-C2-O2	-5.18	118.57	122.20
54	BA	939	G	C5'-C4'-C3'	-5.18	107.71	116.00
54	BA	1376	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	1873	G	C5-C6-N1	5.18	114.09	111.50
54	BA	2031	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2130	U	C5-C6-N1	-5.18	120.11	122.70
54	BA	2326	C	N3-C4-C5	5.18	123.97	121.90
54	BA	2589	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	497	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	936	C	O4'-C1'-N1	5.18	112.34	108.20
21	AA	1188	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	381	G	C8-N9-C4	-5.18	104.33	106.40
54	BA	1332	G	N3-C4-C5	-5.18	126.01	128.60
54	BA	2664	G	C5-C6-N1	5.18	114.09	111.50
55	BB	12	C	C2-N3-C4	-5.18	117.31	119.90
21	AA	79	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	253	A	C1'-O4'-C4'	-5.18	105.76	109.90
21	AA	329	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	778	G	O4'-C1'-N9	5.18	112.34	108.20
23	A2	87	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	1145	C	N3-C2-O2	-5.18	118.28	121.90
54	BA	1267	U	C5-C6-N1	-5.18	120.11	122.70
54	BA	1387	A	N1-C6-N6	-5.18	115.49	118.60
54	BA	1565	C	N3-C2-O2	-5.18	118.28	121.90
54	BA	1871	A	C2-N3-C4	5.18	113.19	110.60
54	BA	2839	G	C5-C6-N1	5.18	114.09	111.50
21	AA	5	U	P-O3'-C3'	5.17	125.91	119.70
21	AA	452	A	O4'-C1'-N9	5.17	112.34	108.20
21	AA	782	A	C4-C5-C6	-5.17	114.41	117.00
21	AA	823	C	N3-C2-O2	-5.17	118.28	121.90
21	AA	1089	G	C8-N9-C4	-5.17	104.33	106.40
21	AA	1162	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	292	U	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1168	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1461	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	2097	A	C4-C5-C6	-5.17	114.41	117.00
21	AA	378	G	C5-C6-N1	5.17	114.09	111.50
21	AA	469	C	C2-N3-C4	-5.17	117.31	119.90
54	BA	145	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	584	C	N3-C4-C5	5.17	123.97	121.90
54	BA	711	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1325	U	C5-C6-N1	-5.17	120.11	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	158	G	C5-C6-N1	5.17	114.08	111.50
21	AA	271	C	N3-C4-C5	5.17	123.97	121.90
54	BA	985	C	N1-C2-O2	5.17	122.00	118.90
54	BA	998	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1667	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1719	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	2104	C	C2-N3-C4	-5.17	117.31	119.90
54	BA	2767	C	O4'-C1'-N1	5.17	112.34	108.20
21	AA	201	G	C5-C6-N1	5.17	114.08	111.50
21	AA	421	U	N1-C2-O2	5.17	126.42	122.80
21	AA	1128	C	N3-C4-C5	5.17	123.97	121.90
21	AA	1243	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	152	A	C5-C6-N1	5.17	120.28	117.70
54	BA	281	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1040	A	C4-C5-C6	-5.17	114.42	117.00
54	BA	1049	C	N3-C2-O2	-5.17	118.28	121.90
21	AA	677	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	801	G	C5-C6-N1	5.17	114.08	111.50
54	BA	826	U	C5-C4-O4	-5.17	122.80	125.90
54	BA	1210	G	O4'-C1'-N9	5.17	112.33	108.20
21	AA	880	C	O4'-C1'-N1	5.17	112.33	108.20
54	BA	712	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1379	U	C3'-C2'-C1'	5.17	105.63	101.50
54	BA	2162	G	N9-C4-C5	5.17	107.47	105.40
54	BA	2364	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	2583	G	C5-C6-N1	5.17	114.08	111.50
21	AA	61	G	C5-C6-N1	5.17	114.08	111.50
21	AA	969	A	C2-N3-C4	5.17	113.18	110.60
21	AA	1361	G	N3-C4-C5	-5.17	126.02	128.60
21	AA	1453	G	N7-C8-N9	5.17	115.68	113.10
54	BA	1819	A	C6-C5-N7	5.17	135.92	132.30
54	BA	2193	G	O4'-C1'-N9	5.17	112.33	108.20
54	BA	2278	A	C1'-O4'-C4'	-5.16	105.77	109.90
54	BA	2638	G	N7-C8-N9	5.16	115.68	113.10
54	BA	2887	A	C6-C5-N7	5.16	135.91	132.30
54	BA	844	A	C5-C6-N1	5.16	120.28	117.70
54	BA	1143	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1835	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	2113	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	2331	G	N1-C6-O6	-5.16	116.80	119.90
21	AA	111	G	C5-C6-N1	5.16	114.08	111.50
21	AA	344	A	C3'-C2'-C1'	5.16	105.63	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	531	U	N1-C2-N3	5.16	118.00	114.90
21	AA	840	C	N1-C2-O2	5.16	122.00	118.90
21	AA	1144	G	O4'-C1'-N9	5.16	112.33	108.20
22	A1	1	G	N3-C4-C5	-5.16	126.02	128.60
28	BF	91	ARG	NE-CZ-NH1	5.16	122.88	120.30
32	BJ	37	ARG	CD-NE-CZ	5.16	130.82	123.60
54	BA	417	C	N3-C2-O2	-5.16	118.29	121.90
54	BA	516	C	N3-C4-C5	5.16	123.96	121.90
54	BA	1248	G	N3-C2-N2	-5.16	116.29	119.90
21	AA	722	G	O4'-C1'-N9	5.16	112.33	108.20
21	AA	909	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	1134	G	C5-C6-N1	5.16	114.08	111.50
23	A2	88	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	722	A	C5-C6-N1	5.16	120.28	117.70
54	BA	950	G	N3-C2-N2	-5.16	116.29	119.90
54	BA	1045	C	N3-C4-C5	5.16	123.96	121.90
54	BA	1662	U	O4'-C1'-N1	5.16	112.33	108.20
54	BA	1953	A	C6-C5-N7	5.16	135.91	132.30
54	BA	2655	G	N3-C2-N2	-5.16	116.29	119.90
54	BA	2698	U	N1-C2-N3	5.16	118.00	114.90
21	AA	1230	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1320	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1439	G	N1-C6-O6	-5.16	116.81	119.90
21	AA	1520	C	N1-C2-O2	5.16	121.99	118.90
54	BA	1124	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	2130	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	2681	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	614	C	N3-C2-O2	-5.16	118.29	121.90
21	AA	1430	A	O4'-C4'-C3'	5.16	110.22	106.10
54	BA	738	G	C8-N9-C4	-5.16	104.34	106.40
54	BA	1079	C	C6-N1-C2	-5.16	118.24	120.30
54	BA	1258	U	C5-C6-N1	-5.16	120.12	122.70
54	BA	1639	C	O4'-C1'-N1	5.16	112.33	108.20
54	BA	2487	G	P-O3'-C3'	5.16	125.89	119.70
54	BA	2708	G	O4'-C1'-N9	5.16	112.33	108.20
21	AA	191	G	N3-C4-C5	-5.15	126.02	128.60
54	BA	660	C	N1-C2-O2	5.15	121.99	118.90
21	AA	91	U	O4'-C1'-N1	5.15	112.32	108.20
21	AA	1221	G	C5-C6-N1	5.15	114.08	111.50
21	AA	1223	C	N1-C2-O2	5.15	121.99	118.90
54	BA	214	G	C5-C6-N1	5.15	114.08	111.50
54	BA	1319	C	O4'-C1'-N1	5.15	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1329	U	N3-C2-O2	-5.15	118.59	122.20
54	BA	1966	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	2080	A	C2-N3-C4	5.15	113.18	110.60
54	BA	2238	G	C8-N9-C4	-5.15	104.34	106.40
21	AA	10	A	C6-C5-N7	5.15	135.91	132.30
21	AA	18	C	N3-C2-O2	-5.15	118.30	121.90
24	A3	2	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	55	G	N3-C4-C5	-5.15	126.03	128.60
54	BA	107	G	N7-C8-N9	5.15	115.67	113.10
54	BA	707	G	C5-C6-N1	5.15	114.08	111.50
54	BA	1267	U	N3-C2-O2	-5.15	118.59	122.20
54	BA	1284	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	1559	U	C5-C6-N1	-5.15	120.12	122.70
54	BA	1781	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2854	G	C8-N9-C4	-5.15	104.34	106.40
55	BB	91	C	N3-C4-C5	5.15	123.96	121.90
21	AA	755	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1595	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2206	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	2207	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2503	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	805	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	1084	G	C8-N9-C4	-5.15	104.34	106.40
21	AA	1477	U	N1-C2-N3	5.15	117.99	114.90
54	BA	354	A	C6-C5-N7	5.15	135.90	132.30
54	BA	436	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	1890	A	C4-C5-C6	-5.15	114.43	117.00
54	BA	1905	C	N3-C2-O2	-5.15	118.30	121.90
21	AA	35	G	N3-C2-N2	-5.15	116.30	119.90
54	BA	144	A	C4-C5-C6	-5.15	114.43	117.00
54	BA	736	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	2222	C	N3-C4-C5	5.15	123.96	121.90
55	BB	93	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	980	A	C6-C5-N7	5.14	135.90	132.30
54	BA	1378	A	O4'-C4'-C3'	5.14	110.22	106.10
54	BA	1447	C	N3-C4-C5	5.14	123.96	121.90
54	BA	1756	G	C5-C6-N1	5.14	114.07	111.50
54	BA	1869	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	2100	G	C5-C6-N1	5.14	114.07	111.50
54	BA	2175	C	N1-C2-O2	5.14	121.99	118.90
21	AA	297	G	N3-C4-C5	-5.14	126.03	128.60
21	AA	441	A	C6-C5-N7	5.14	135.90	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	526	C	N3-C2-O2	-5.14	118.30	121.90
21	AA	849	G	C5-C6-N1	5.14	114.07	111.50
21	AA	980	C	N1-C2-O2	5.14	121.99	118.90
54	BA	69	C	N3-C4-C5	5.14	123.96	121.90
54	BA	329	G	C3'-C2'-C1'	5.14	105.61	101.50
54	BA	1368	G	N3-C4-C5	-5.14	126.03	128.60
54	BA	1389	G	N9-C4-C5	5.14	107.46	105.40
54	BA	1532	A	C6-C5-N7	5.14	135.90	132.30
54	BA	2539	C	N1-C2-O2	5.14	121.99	118.90
21	AA	101	A	C6-C5-N7	5.14	135.90	132.30
21	AA	601	G	C5-C6-N1	5.14	114.07	111.50
8	AI	105	ARG	CD-NE-CZ	5.14	130.80	123.60
21	AA	971	G	C5-C6-N1	5.14	114.07	111.50
22	A1	57	G	O4'-C1'-N9	5.14	112.31	108.20
24	A3	19	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	21	A	C6-C5-N7	5.14	135.90	132.30
54	BA	830	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	958	U	N1-C2-N3	5.14	117.98	114.90
54	BA	1334	G	C5-C6-N1	5.14	114.07	111.50
54	BA	1651	G	C5-C6-N1	5.14	114.07	111.50
54	BA	2202	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2500	U	C5'-C4'-O4'	5.14	115.27	109.10
55	BB	50	A	C5-C6-N1	5.14	120.27	117.70
2	AC	131	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	178	G	C8-N9-C4	-5.14	104.34	106.40
54	BA	2324	U	N3-C2-O2	-5.14	118.60	122.20
54	BA	2776	A	C6-C5-N7	5.14	135.90	132.30
21	AA	180	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	446	G	C5-C6-N1	5.14	114.07	111.50
21	AA	782	A	C5-C6-N1	5.14	120.27	117.70
54	BA	826	U	N3-C4-O4	5.14	123.00	119.40
54	BA	986	C	N1-C2-O2	5.14	121.98	118.90
54	BA	2093	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	2098	U	C5-C6-N1	-5.14	120.13	122.70
54	BA	2232	C	C4'-C3'-C2'	-5.14	97.46	102.60
54	BA	2500	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2600	A	C5-C6-N1	5.14	120.27	117.70
55	BB	82	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	1121	U	O4'-C1'-N1	5.13	112.31	108.20
21	AA	1302	C	N3-C4-C5	5.13	123.95	121.90
21	AA	1423	G	C5-C6-N1	5.13	114.07	111.50
21	AA	1472	U	N1-C2-N3	5.13	117.98	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	BO	15	ARG	NE-CZ-NH1	5.13	122.87	120.30
47	BY	48	ARG	NE-CZ-NH1	5.13	122.87	120.30
54	BA	149	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	758	C	N3-C4-C5	5.13	123.95	121.90
54	BA	1506	U	N3-C2-O2	-5.13	118.61	122.20
21	AA	371	A	C6-C5-N7	5.13	135.89	132.30
21	AA	869	G	N3-C4-C5	-5.13	126.03	128.60
54	BA	2100	G	C5'-C4'-O4'	5.13	115.26	109.10
54	BA	492	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	588	U	C5-C6-N1	-5.13	120.13	122.70
54	BA	745	G	O4'-C1'-N9	5.13	112.31	108.20
54	BA	1128	G	C5'-C4'-O4'	5.13	115.26	109.10
54	BA	1467	U	O4'-C1'-N1	5.13	112.31	108.20
54	BA	2577	A	C4-C5-C6	-5.13	114.43	117.00
21	AA	41	G	C5-C6-N1	5.13	114.06	111.50
54	BA	691	C	O4'-C1'-N1	5.13	112.30	108.20
54	BA	1242	U	N1-C2-N3	5.13	117.98	114.90
54	BA	1429	G	C8-N9-C4	-5.13	104.35	106.40
54	BA	1986	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2157	G	O4'-C1'-N9	5.13	112.30	108.20
54	BA	2319	G	N3-C4-C5	-5.13	126.03	128.60
21	AA	798	U	O4'-C1'-N1	5.13	112.30	108.20
21	AA	1353	G	C8-N9-C4	-5.13	104.35	106.40
21	AA	1397	C	C6-N1-C2	-5.13	118.25	120.30
54	BA	359	G	C5-C6-N1	5.13	114.06	111.50
54	BA	918	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	1677	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	1963	U	O4'-C1'-N1	5.13	112.30	108.20
54	BA	2626	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2850	A	C8-N9-C4	-5.13	103.75	105.80
21	AA	1091	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	1448	G	C4'-C3'-C2'	-5.13	97.47	102.60
54	BA	1608	A	C5-C6-N1	5.13	120.26	117.70
54	BA	1724	G	N3-C4-C5	-5.13	126.04	128.60
54	BA	2240	U	C5-C6-N1	-5.13	120.14	122.70
54	BA	2283	C	C2-N3-C4	-5.13	117.34	119.90
54	BA	2735	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	1469	C	N3-C4-C5	5.12	123.95	121.90
54	BA	1888	G	N7-C8-N9	5.12	115.66	113.10
6	AG	52	ARG	NE-CZ-NH1	5.12	122.86	120.30
21	AA	463	U	C5-C6-N1	-5.12	120.14	122.70
21	AA	761	G	O4'-C1'-N9	5.12	112.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1207	G	C8-N9-C4	-5.12	104.35	106.40
21	AA	1213	A	C6-C5-N7	5.12	135.89	132.30
21	AA	1390	U	C4-C5-C6	5.12	122.77	119.70
54	BA	738	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1527	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1854	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2215	C	C6-N1-C2	-5.12	118.25	120.30
54	BA	2310	C	N3-C2-O2	-5.12	118.31	121.90
54	BA	2830	C	N1-C2-O2	5.12	121.97	118.90
55	BB	44	G	N7-C8-N9	5.12	115.66	113.10
21	AA	295	C	N3-C2-O2	-5.12	118.31	121.90
21	AA	558	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	1484	C	N3-C4-N4	-5.12	114.42	118.00
54	BA	620	G	N3-C4-C5	-5.12	126.04	128.60
54	BA	1071	G	C8-N9-C4	-5.12	104.35	106.40
54	BA	1373	A	C5-C6-N1	5.12	120.26	117.70
54	BA	1853	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	1988	G	C4'-C3'-C2'	-5.12	97.48	102.60
54	BA	2895	G	C5-C6-N1	5.12	114.06	111.50
55	BB	104	A	C5-C6-N1	5.12	120.26	117.70
21	AA	1211	U	C1'-O4'-C4'	-5.12	105.80	109.90
54	BA	249	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	757	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	357	G	N7-C8-N9	5.12	115.66	113.10
21	AA	468	A	C2-N3-C4	5.12	113.16	110.60
54	BA	1459	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1869	G	C8-N9-C4	-5.12	104.35	106.40
54	BA	2033	A	C5-C6-N1	5.12	120.26	117.70
54	BA	2435	A	C4-C5-C6	-5.12	114.44	117.00
55	BB	49	C	N3-C2-O2	-5.12	118.32	121.90
21	AA	26	A	C6-C5-N7	5.12	135.88	132.30
21	AA	23	C	N1-C2-O2	5.12	121.97	118.90
21	AA	903	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	1117	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	127	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2062	A	C8-N9-C4	-5.12	103.75	105.80
54	BA	2086	U	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2897	U	O4'-C1'-N1	5.12	112.29	108.20
55	BB	68	C	O4'-C1'-N1	5.12	112.29	108.20
10	AK	105	ARG	NE-CZ-NH1	5.11	122.86	120.30
21	AA	429	U	C4-C5-C6	5.11	122.77	119.70
21	AA	742	G	N3-C4-C5	-5.11	126.04	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	985	C	N3-C4-C5	5.11	123.94	121.90
21	AA	1261	A	C4-C5-C6	-5.11	114.44	117.00
21	AA	1434	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	624	C	N1-C2-O2	5.11	121.97	118.90
54	BA	977	G	N7-C8-N9	5.11	115.66	113.10
54	BA	1014	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	1220	G	C8-N9-C4	-5.11	104.36	106.40
54	BA	1882	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	2072	C	N3-C2-O2	-5.11	118.32	121.90
54	BA	2253	G	C8-N9-C4	-5.11	104.35	106.40
21	AA	72	A	C5-C6-N1	5.11	120.26	117.70
21	AA	674	G	N9-C4-C5	5.11	107.44	105.40
54	BA	213	A	C6-C5-N7	5.11	135.88	132.30
54	BA	705	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	1305	C	N3-C4-C5	5.11	123.94	121.90
54	BA	2381	A	C4'-C3'-C2'	-5.11	97.49	102.60
2	AC	106	ARG	NE-CZ-NH1	5.11	122.86	120.30
21	AA	68	G	N3-C4-C5	-5.11	126.05	128.60
21	AA	1209	C	N3-C4-N4	-5.11	114.42	118.00
22	A1	12	U	C5'-C4'-O4'	5.11	115.23	109.10
54	BA	985	C	N3-C4-C5	5.11	123.94	121.90
54	BA	1131	G	C5-C6-N1	5.11	114.06	111.50
54	BA	1528	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	1809	A	C5-C6-N1	5.11	120.25	117.70
54	BA	2063	C	N1-C2-O2	5.11	121.97	118.90
54	BA	2365	G	N7-C8-N9	5.11	115.66	113.10
55	BB	93	C	O4'-C1'-N1	5.11	112.29	108.20
21	AA	808	C	N1-C2-O2	5.11	121.97	118.90
21	AA	957	U	O4'-C1'-N1	5.11	112.28	108.20
54	BA	621	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	2020	A	C1'-O4'-C4'	-5.11	105.81	109.90
54	BA	2667	C	O4'-C1'-N1	5.11	112.28	108.20
21	AA	1093	A	C4-C5-C6	-5.11	114.45	117.00
24	A3	7	G	N1-C6-O6	-5.11	116.84	119.90
54	BA	418	C	N3-C2-O2	-5.11	118.33	121.90
54	BA	484	C	O4'-C1'-N1	5.11	112.28	108.20
54	BA	808	G	O4'-C1'-N9	5.11	112.28	108.20
54	BA	1288	G	N1-C6-O6	-5.11	116.84	119.90
54	BA	1306	C	N3-C4-C5	5.11	123.94	121.90
21	AA	1438	G	N3-C2-N2	-5.10	116.33	119.90
54	BA	308	G	C5-C6-N1	5.10	114.05	111.50
54	BA	1297	C	N3-C2-O2	-5.10	118.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2403	C	N3-C4-C5	5.10	123.94	121.90
21	AA	30	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	514	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1126	U	N1-C2-N3	5.10	117.96	114.90
21	AA	1350	A	C6-C5-N7	5.10	135.87	132.30
54	BA	48	G	C8-N9-C4	-5.10	104.36	106.40
54	BA	536	G	N9-C4-C5	5.10	107.44	105.40
54	BA	1019	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	1272	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	1356	G	N3-C4-C5	-5.10	126.05	128.60
54	BA	2252	G	C5-C6-N1	5.10	114.05	111.50
21	AA	1434	A	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1445	U	C5-C6-N1	-5.10	120.15	122.70
21	AA	1506	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	809	G	N7-C8-N9	5.10	115.65	113.10
54	BA	1682	G	C5-C6-N1	5.10	114.05	111.50
21	AA	102	G	C5-C6-N1	5.10	114.05	111.50
21	AA	153	C	N3-C2-O2	-5.10	118.33	121.90
21	AA	284	C	N1-C2-O2	5.10	121.96	118.90
21	AA	525	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1114	C	N3-C2-O2	-5.10	118.33	121.90
24	A3	71	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	2780	G	C1'-O4'-C4'	-5.10	105.82	109.90
55	BB	41	G	N3-C4-C5	-5.10	126.05	128.60
21	AA	640	A	C6-C5-N7	5.10	135.87	132.30
21	AA	1192	C	N3-C2-O2	-5.10	118.33	121.90
22	A1	61	C	N3-C4-C5	5.10	123.94	121.90
54	BA	135	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	784	G	C8-N9-C4	-5.10	104.36	106.40
54	BA	1525	A	C5-C6-N1	5.10	120.25	117.70
54	BA	1612	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	1800	C	N3-C4-C5	5.10	123.94	121.90
54	BA	1828	G	C5-C6-N1	5.10	114.05	111.50
54	BA	1847	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	1857	G	N3-C2-N2	-5.10	116.33	119.90
54	BA	1874	C	N1-C2-O2	5.10	121.96	118.90
54	BA	2047	C	N3-C2-O2	-5.10	118.33	121.90
54	BA	2598	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2737	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	1411	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	42	A	C6-C5-N7	5.10	135.87	132.30
54	BA	2497	A	O4'-C1'-N9	5.10	112.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	369	G	C8-N9-C4	-5.09	104.36	106.40
21	AA	535	A	C4-C5-C6	-5.09	114.45	117.00
21	AA	939	G	N7-C8-N9	5.09	115.65	113.10
21	AA	1134	G	N1-C6-O6	-5.09	116.84	119.90
21	AA	1336	C	N1-C2-O2	5.09	121.96	118.90
54	BA	557	C	N3-C4-C5	5.09	123.94	121.90
54	BA	1592	C	N3-C2-O2	-5.09	118.33	121.90
54	BA	1925	C	O4'-C1'-N1	5.09	112.28	108.20
54	BA	2135	A	C5-C6-N1	5.09	120.25	117.70
54	BA	2307	G	C5-C6-N1	5.09	114.05	111.50
54	BA	2510	C	N3-C2-O2	-5.09	118.33	121.90
54	BA	2719	G	N7-C8-N9	5.09	115.65	113.10
54	BA	427	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2029	G	C3'-C2'-C1'	5.09	105.57	101.50
21	AA	419	C	N3-C2-O2	-5.09	118.34	121.90
21	AA	741	G	C8-N9-C4	-5.09	104.36	106.40
21	AA	1127	G	C5-C6-N1	5.09	114.05	111.50
54	BA	122	G	C4'-C3'-C2'	-5.09	97.51	102.60
54	BA	481	G	C8-N9-C4	-5.09	104.36	106.40
54	BA	523	C	C5'-C4'-O4'	5.09	115.21	109.10
54	BA	1656	C	N3-C2-O2	-5.09	118.33	121.90
54	BA	1990	C	N3-C4-N4	-5.09	114.44	118.00
54	BA	2240	U	C4-C5-C6	5.09	122.75	119.70
54	BA	2521	C	N1-C2-O2	5.09	121.95	118.90
54	BA	2590	A	C6-C5-N7	5.09	135.86	132.30
54	BA	2633	G	N3-C2-N2	-5.09	116.33	119.90
21	AA	213	G	C5-C6-N1	5.09	114.05	111.50
54	BA	36	G	C5-C6-N1	5.09	114.05	111.50
54	BA	412	A	C6-C5-N7	5.09	135.86	132.30
54	BA	1868	C	N3-C2-O2	-5.09	118.34	121.90
54	BA	2519	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	434	U	C5-C6-N1	-5.09	120.16	122.70
54	BA	484	C	N1-C2-O2	5.09	121.95	118.90
54	BA	1950	G	N3-C2-N2	-5.09	116.34	119.90
54	BA	2555	U	O4'-C1'-N1	5.09	112.27	108.20
2	AC	131	ARG	NE-CZ-NH2	-5.09	117.76	120.30
21	AA	363	A	C6-C5-N7	5.09	135.86	132.30
21	AA	425	G	C8-N9-C4	-5.09	104.37	106.40
21	AA	723	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	1466	C	N3-C4-C5	5.09	123.94	121.90
54	BA	126	A	O4'-C1'-N9	5.09	112.27	108.20
54	BA	164	C	N3-C4-C5	5.09	123.94	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	346	A	C6-C5-N7	5.09	135.86	132.30
54	BA	730	A	C6-C5-N7	5.09	135.86	132.30
54	BA	772	C	N3-C2-O2	-5.09	118.34	121.90
54	BA	1436	G	C8-N9-C4	-5.09	104.36	106.40
54	BA	1508	A	C1'-O4'-C4'	-5.09	105.83	109.90
21	AA	953	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	1489	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	730	A	C1'-O4'-C4'	-5.08	105.83	109.90
54	BA	2825	G	C5-C6-N1	5.08	114.04	111.50
21	AA	318	G	N3-C4-C5	-5.08	126.06	128.60
21	AA	621	A	O4'-C1'-N9	5.08	112.27	108.20
21	AA	825	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	898	G	N1-C6-O6	-5.08	116.85	119.90
21	AA	1119	C	N3-C2-O2	-5.08	118.34	121.90
21	AA	1482	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	455	C	O4'-C4'-C3'	5.08	110.17	106.10
54	BA	607	U	C5-C6-N1	-5.08	120.16	122.70
54	BA	819	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1071	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	1435	G	N7-C8-N9	5.08	115.64	113.10
54	BA	1510	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1637	A	C6-C5-N7	5.08	135.86	132.30
54	BA	2424	C	C5'-C4'-C3'	-5.08	107.87	116.00
21	AA	79	G	C5-C6-N1	5.08	114.04	111.50
21	AA	591	U	C5'-C4'-C3'	-5.08	107.87	116.00
22	A1	63	G	N7-C8-N9	5.08	115.64	113.10
22	A1	70	C	C5'-C4'-O4'	5.08	115.20	109.10
39	BQ	29	ARG	NE-CZ-NH1	5.08	122.84	120.30
54	BA	432	A	C6-C5-N7	5.08	135.86	132.30
54	BA	547	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	711	G	N9-C4-C5	5.08	107.43	105.40
54	BA	777	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	1443	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	1549	A	C6-C5-N7	5.08	135.86	132.30
54	BA	2573	C	C6-N1-C2	-5.08	118.27	120.30
21	AA	280	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2190	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	2276	G	C5-C6-N1	5.08	114.04	111.50
21	AA	683	G	C5-C6-N1	5.08	114.04	111.50
42	BT	12	ARG	NE-CZ-NH1	5.08	122.84	120.30
54	BA	157	C	N3-C2-O2	-5.08	118.34	121.90
54	BA	350	G	C5-C6-N1	5.08	114.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	389	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	506	G	N7-C8-N9	5.08	115.64	113.10
54	BA	1298	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1308	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1418	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2852	G	C5-C6-N1	5.08	114.04	111.50
21	AA	943	U	C5-C6-N1	-5.08	120.16	122.70
21	AA	281	G	N3-C4-C5	-5.08	126.06	128.60
21	AA	384	G	N3-C2-N2	-5.08	116.35	119.90
21	AA	429	U	N3-C2-O2	-5.08	118.65	122.20
21	AA	805	C	O4'-C1'-N1	5.08	112.26	108.20
21	AA	1169	A	C6-C5-N7	5.08	135.85	132.30
21	AA	1490	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	52	A	N1-C6-N6	-5.08	115.56	118.60
54	BA	1541	C	N3-C4-C5	5.08	123.93	121.90
54	BA	1648	U	N3-C2-O2	-5.08	118.65	122.20
21	AA	775	G	C8-N9-C4	-5.07	104.37	106.40
21	AA	993	G	O4'-C4'-C3'	5.07	110.16	106.10
21	AA	1003	G	O4'-C1'-N9	5.07	112.26	108.20
54	BA	33	C	N3-C2-O2	-5.07	118.35	121.90
54	BA	161	A	C6-C5-N7	5.07	135.85	132.30
54	BA	844	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	957	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1465	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	2443	C	C2-N3-C4	-5.07	117.36	119.90
21	AA	467	U	N3-C2-O2	-5.07	118.65	122.20
21	AA	1257	A	C4-C5-C6	-5.07	114.46	117.00
21	AA	1421	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1142	A	C6-C5-N7	5.07	135.85	132.30
21	AA	16	A	C2-N3-C4	5.07	113.14	110.60
21	AA	172	A	C3'-C2'-C1'	5.07	105.56	101.50
21	AA	239	U	N3-C2-O2	-5.07	118.65	122.20
21	AA	673	A	C4-C5-C6	-5.07	114.46	117.00
21	AA	712	A	N1-C6-N6	-5.07	115.56	118.60
21	AA	812	G	C5-C6-N1	5.07	114.04	111.50
21	AA	1355	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	358	U	N1-C2-N3	5.07	117.94	114.90
54	BA	1237	A	C4'-C3'-C2'	-5.07	97.53	102.60
54	BA	1555	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1674	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	1958	C	N3-C2-O2	-5.07	118.35	121.90
54	BA	2300	C	N1-C2-O2	5.07	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2618	G	C5-C6-N1	5.07	114.03	111.50
21	AA	921	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	170	U	C4'-C3'-C2'	-5.07	97.53	102.60
54	BA	2271	G	C5-C6-N1	5.07	114.03	111.50
54	BA	2510	C	O4'-C1'-N1	5.07	112.25	108.20
21	AA	463	U	O4'-C1'-N1	5.07	112.25	108.20
21	AA	1049	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	567	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	764	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	876	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1093	G	N3-C2-N2	-5.07	116.35	119.90
54	BA	1356	G	C8-N9-C4	-5.07	104.37	106.40
21	AA	976	G	N1-C6-O6	-5.07	116.86	119.90
22	A1	61	C	C5'-C4'-O4'	5.07	115.18	109.10
54	BA	1226	A	C6-C5-N7	5.07	135.84	132.30
54	BA	1281	G	C5-C6-N1	5.07	114.03	111.50
54	BA	2291	U	O4'-C1'-N1	5.07	112.25	108.20
55	BB	9	G	N3-C4-C5	-5.07	126.07	128.60
55	BB	22	U	N1-C2-N3	5.07	117.94	114.90
55	BB	86	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1758	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	156	C	N1-C2-O2	5.06	121.94	118.90
21	AA	267	C	N1-C2-O2	5.06	121.94	118.90
21	AA	1380	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1289	C	N1-C2-O2	5.06	121.94	118.90
54	BA	1408	G	C5-C6-N1	5.06	114.03	111.50
54	BA	1649	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	2413	G	N3-C2-N2	-5.06	116.36	119.90
54	BA	2873	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	887	G	N3-C2-N2	-5.06	116.36	119.90
21	AA	1152	A	C6-C5-N7	5.06	135.84	132.30
54	BA	2039	U	C5-C6-N1	-5.06	120.17	122.70
54	BA	2488	G	N1-C6-O6	-5.06	116.86	119.90
21	AA	606	G	N1-C6-O6	-5.06	116.86	119.90
21	AA	1129	C	N1-C2-O2	5.06	121.94	118.90
54	BA	122	G	C5-C6-N1	5.06	114.03	111.50
54	BA	360	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	397	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1269	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	1710	G	N9-C4-C5	5.06	107.42	105.40
54	BA	2538	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2739	U	O4'-C1'-N1	5.06	112.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	355	C	C5'-C4'-O4'	5.06	115.17	109.10
21	AA	612	C	N1-C2-O2	5.06	121.94	118.90
54	BA	14	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	1114	C	C2-N3-C4	-5.06	117.37	119.90
54	BA	1447	C	N1-C2-O2	5.06	121.93	118.90
54	BA	1741	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2453	A	C5-C6-N1	5.06	120.23	117.70
54	BA	2477	U	N1-C2-N3	5.06	117.94	114.90
54	BA	2851	A	C6-C5-N7	5.06	135.84	132.30
21	AA	659	U	O4'-C4'-C3'	5.06	110.14	106.10
21	AA	674	G	O4'-C1'-N9	5.06	112.25	108.20
54	BA	653	U	C1'-O4'-C4'	-5.06	105.86	109.90
54	BA	2078	C	C4'-C3'-C2'	-5.06	97.54	102.60
54	BA	2099	U	C5-C6-N1	-5.06	120.17	122.70
54	BA	2603	G	N1-C6-O6	-5.06	116.87	119.90
55	BB	14	U	C5-C6-N1	-5.06	120.17	122.70
55	BB	25	U	O4'-C1'-N1	5.06	112.25	108.20
11	AL	82	ARG	NE-CZ-NH1	5.05	122.83	120.30
21	AA	402	G	C5-C6-N1	5.05	114.03	111.50
54	BA	584	C	N3-C2-O2	-5.05	118.36	121.90
54	BA	642	U	C5-C6-N1	-5.05	120.17	122.70
54	BA	2122	U	N1-C2-N3	5.05	117.93	114.90
54	BA	2180	U	N3-C2-O2	-5.05	118.66	122.20
21	AA	664	G	N3-C4-C5	-5.05	126.07	128.60
54	BA	573	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	1294	U	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	1807	G	O4'-C1'-N9	5.05	112.24	108.20
54	BA	2056	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	2582	G	N3-C4-C5	-5.05	126.07	128.60
16	AQ	63	CYS	O-C-N	-5.05	114.62	122.70
21	AA	6	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	270	A	C6-C5-N7	5.05	135.84	132.30
21	AA	293	G	N3-C2-N2	-5.05	116.36	119.90
21	AA	572	A	C3'-C2'-C1'	5.05	105.54	101.50
21	AA	671	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	699	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1532	U	C1'-O4'-C4'	-5.05	105.86	109.90
54	BA	185	G	C8-N9-C4	-5.05	104.38	106.40
54	BA	817	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1343	G	N9-C4-C5	5.05	107.42	105.40
54	BA	1398	C	O4'-C4'-C3'	5.05	110.14	106.10
54	BA	1704	C	N3-C2-O2	-5.05	118.36	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1986	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2423	U	O4'-C1'-N1	5.05	112.24	108.20
21	AA	1409	C	N3-C2-O2	-5.05	118.37	121.90
54	BA	445	C	N3-C4-C5	5.05	123.92	121.90
54	BA	489	G	C5-C6-N1	5.05	114.03	111.50
54	BA	877	A	C4-C5-C6	-5.05	114.47	117.00
54	BA	1154	G	N3-C4-C5	-5.05	126.08	128.60
54	BA	1374	G	C5-C6-N1	5.05	114.03	111.50
54	BA	2160	C	N3-C4-C5	5.05	123.92	121.90
21	AA	326	G	C8-N9-C4	-5.05	104.38	106.40
26	BD	124	ARG	NE-CZ-NH1	5.05	122.82	120.30
54	BA	826	U	C4-C5-C6	5.05	122.73	119.70
54	BA	1238	G	C5-C6-N1	5.05	114.02	111.50
54	BA	2380	C	N1-C2-O2	5.05	121.93	118.90
21	AA	147	G	N3-C4-C5	-5.05	126.08	128.60
21	AA	914	A	C4-C5-C6	-5.05	114.48	117.00
21	AA	1277	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1476	U	C5-C6-N1	-5.05	120.18	122.70
54	BA	1817	G	C5-C6-N1	5.05	114.02	111.50
54	BA	2006	C	O4'-C1'-N1	5.05	112.24	108.20
21	AA	296	U	N1-C2-N3	5.04	117.93	114.90
21	AA	1226	C	C5'-C4'-C3'	-5.04	107.93	116.00
22	A1	20	G	N3-C4-C5	-5.04	126.08	128.60
54	BA	1388	G	N3-C2-N2	-5.04	116.37	119.90
54	BA	2824	C	N3-C4-C5	5.04	123.92	121.90
15	AP	25	ARG	NE-CZ-NH2	-5.04	117.78	120.30
21	AA	166	U	C5'-C4'-O4'	5.04	115.15	109.10
21	AA	403	C	N1-C2-O2	5.04	121.93	118.90
21	AA	549	C	N1-C2-O2	5.04	121.93	118.90
21	AA	1502	A	C8-N9-C4	-5.04	103.78	105.80
54	BA	874	G	C5-C6-N1	5.04	114.02	111.50
54	BA	1857	G	N9-C4-C5	5.04	107.42	105.40
54	BA	2365	G	C8-N9-C4	-5.04	104.38	106.40
21	AA	178	C	N3-C2-O2	-5.04	118.37	121.90
21	AA	1367	C	O4'-C1'-N1	5.04	112.23	108.20
21	AA	1496	C	N3-C4-C5	5.04	123.92	121.90
22	A1	8	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	286	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	706	A	C8-N9-C4	-5.04	103.78	105.80
54	BA	879	G	N9-C4-C5	5.04	107.42	105.40
54	BA	2122	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	2511	U	N1-C2-N3	5.04	117.92	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2567	G	C5-C6-N1	5.04	114.02	111.50
54	BA	2678	C	N3-C2-O2	-5.04	118.37	121.90
54	BA	2885	G	N9-C4-C5	5.04	107.42	105.40
55	BB	12	C	C3'-C2'-C1'	-5.04	97.47	101.50
21	AA	610	U	C1'-O4'-C4'	-5.04	105.87	109.90
54	BA	423	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1096	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	2844	G	N1-C6-O6	-5.04	116.88	119.90
21	AA	914	A	C6-C5-N7	5.04	135.83	132.30
54	BA	568	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	1954	G	C3'-C2'-C1'	5.04	105.53	101.50
54	BA	2305	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	2861	U	C4-C5-C6	5.04	122.72	119.70
21	AA	876	C	C1'-O4'-C4'	-5.04	105.87	109.90
54	BA	114	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	118	A	C5'-C4'-O4'	5.04	115.14	109.10
54	BA	285	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	657	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	2006	C	N3-C4-C5	5.04	123.92	121.90
54	BA	2756	U	N1-C1'-C2'	5.04	120.55	114.00
21	AA	390	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	776	G	N9-C4-C5	5.04	107.41	105.40
21	AA	1090	U	C4-C5-C6	5.04	122.72	119.70
54	BA	821	A	C6-C5-N7	5.04	135.82	132.30
54	BA	2777	G	C8-N9-C4	-5.04	104.39	106.40
21	AA	603	U	O4'-C1'-N1	5.03	112.23	108.20
54	BA	4	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	1209	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	1721	G	N7-C8-N9	5.03	115.62	113.10
55	BB	3	C	N3-C4-C5	5.03	123.91	121.90
21	AA	569	C	N3-C2-O2	-5.03	118.38	121.90
21	AA	803	G	N9-C4-C5	5.03	107.41	105.40
22	A1	42	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	676	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1186	G	O4'-C1'-N9	5.03	112.22	108.20
54	BA	1471	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	2021	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2076	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	2283	C	O4'-C1'-N1	5.03	112.23	108.20
54	BA	2651	C	O4'-C1'-N1	5.03	112.23	108.20
54	BA	2794	C	N3-C4-C5	5.03	123.91	121.90
55	BB	51	G	N9-C4-C5	5.03	107.41	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	638	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	686	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	911	U	C5-C6-N1	-5.03	120.19	122.70
21	AA	1203	C	O4'-C1'-N1	5.03	112.22	108.20
35	BM	59	ARG	NE-CZ-NH1	5.03	122.81	120.30
54	BA	266	G	C5-C6-N1	5.03	114.02	111.50
54	BA	1288	G	C1'-O4'-C4'	-5.03	105.88	109.90
54	BA	1365	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	1763	G	C5-C6-N1	5.03	114.02	111.50
54	BA	2162	G	N3-C4-C5	-5.03	126.08	128.60
54	BA	2850	A	C4'-C3'-C2'	-5.03	97.57	102.60
55	BB	71	C	N1-C2-O2	5.03	121.92	118.90
21	AA	223	A	C6-C5-N7	5.03	135.82	132.30
21	AA	1355	G	O4'-C1'-N9	5.03	112.22	108.20
21	AA	1398	A	C2-N3-C4	5.03	113.11	110.60
54	BA	90	U	N1-C2-N3	5.03	117.92	114.90
54	BA	687	C	N3-C2-O2	-5.03	118.38	121.90
54	BA	2086	U	C4'-C3'-C2'	-5.03	97.57	102.60
54	BA	2768	U	O4'-C1'-N1	5.03	112.22	108.20
21	AA	211	G	O4'-C1'-N9	5.03	112.22	108.20
21	AA	415	A	C2-N3-C4	5.03	113.11	110.60
21	AA	1139	G	N9-C4-C5	5.03	107.41	105.40
21	AA	1231	G	C8-N9-C4	-5.03	104.39	106.40
54	BA	114	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	216	A	C5-C6-N1	5.03	120.21	117.70
54	BA	731	C	N1-C2-O2	5.03	121.92	118.90
54	BA	1363	C	N3-C4-C5	5.03	123.91	121.90
54	BA	1459	G	C5'-C4'-O4'	5.03	115.13	109.10
54	BA	1704	C	N1-C2-O2	5.03	121.92	118.90
54	BA	1746	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	2853	C	O4'-C1'-N1	5.03	112.22	108.20
21	AA	21	G	N1-C6-O6	-5.03	116.89	119.90
21	AA	359	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	1182	G	N3-C4-C5	-5.03	126.09	128.60
54	BA	152	A	C4'-C3'-C2'	-5.03	97.58	102.60
54	BA	292	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	519	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1237	A	O4'-C1'-N9	5.03	112.22	108.20
54	BA	2045	C	N3-C4-C5	5.03	123.91	121.90
54	BA	2362	C	C2-N3-C4	-5.03	117.39	119.90
54	BA	2812	G	C8-N9-C4	-5.03	104.39	106.40
55	BB	34	A	O4'-C1'-N9	5.03	112.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1391	U	N3-C2-O2	-5.02	118.68	122.20
54	BA	95	A	O4'-C1'-N9	5.02	112.22	108.20
54	BA	440	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1305	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1360	G	O4'-C1'-N9	5.02	112.22	108.20
54	BA	2352	A	C4'-C3'-C2'	-5.02	97.58	102.60
55	BB	67	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	381	C	C3'-C2'-C1'	5.02	105.52	101.50
21	AA	846	G	C5-C6-N1	5.02	114.01	111.50
21	AA	1140	C	N1-C2-O2	5.02	121.91	118.90
21	AA	1253	G	C5-C6-N1	5.02	114.01	111.50
54	BA	159	G	C5'-C4'-O4'	5.02	115.13	109.10
54	BA	547	A	C5'-C4'-O4'	5.02	115.13	109.10
54	BA	1299	G	C5-C6-N1	5.02	114.01	111.50
54	BA	1554	U	N1-C2-N3	5.02	117.91	114.90
54	BA	1690	A	C6-C5-N7	5.02	135.81	132.30
54	BA	1943	U	N3-C2-O2	-5.02	118.68	122.20
54	BA	2010	G	C5-C6-N1	5.02	114.01	111.50
54	BA	2108	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	2120	G	C5-C6-N1	5.02	114.01	111.50
21	AA	56	U	N3-C2-O2	-5.02	118.69	122.20
21	AA	1188	A	C6-C5-N7	5.02	135.81	132.30
21	AA	1371	G	N7-C8-N9	5.02	115.61	113.10
54	BA	456	C	N3-C4-C5	5.02	123.91	121.90
54	BA	1291	C	N3-C4-C5	5.02	123.91	121.90
54	BA	2368	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2815	C	N1-C2-O2	5.02	121.91	118.90
21	AA	287	U	C5-C6-N1	-5.02	120.19	122.70
21	AA	924	C	N1-C2-O2	5.02	121.91	118.90
21	AA	1042	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	1762	A	C4'-C3'-C2'	-5.02	97.58	102.60
21	AA	1160	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	1366	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	264	C	C1'-O4'-C4'	-5.02	105.89	109.90
54	BA	445	C	N3-C4-N4	-5.02	114.49	118.00
54	BA	544	C	N1-C2-O2	5.02	121.91	118.90
54	BA	681	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	1091	G	C5-C6-N1	5.02	114.01	111.50
54	BA	1616	A	C6-C5-N7	5.02	135.81	132.30
54	BA	1954	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	431	U	N1-C2-N3	5.02	117.91	114.90
54	BA	1369	G	C4'-C3'-C2'	-5.02	97.58	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2069	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	2379	G	O4'-C1'-N9	5.02	112.21	108.20
21	AA	312	C	N1-C2-O2	5.01	121.91	118.90
21	AA	530	G	C5-C6-N1	5.01	114.01	111.50
21	AA	599	C	N1-C2-O2	5.01	121.91	118.90
21	AA	812	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	1193	G	C8-N9-C4	-5.01	104.39	106.40
21	AA	1491	G	C5'-C4'-C3'	-5.01	107.97	116.00
54	BA	2608	G	N1-C6-O6	-5.01	116.89	119.90
55	BB	7	G	C8-N9-C4	-5.01	104.39	106.40
21	AA	20	U	C4-C5-C6	5.01	122.71	119.70
21	AA	96	U	N1-C2-N3	5.01	117.91	114.90
54	BA	578	G	N3-C4-C5	-5.01	126.09	128.60
21	AA	235	C	N3-C2-O2	-5.01	118.39	121.90
21	AA	457	G	C5-C6-N1	5.01	114.01	111.50
21	AA	570	G	C5-C6-N1	5.01	114.01	111.50
21	AA	755	G	N9-C4-C5	5.01	107.40	105.40
46	BX	71	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
54	BA	590	A	C1'-O4'-C4'	-5.01	105.89	109.90
54	BA	1066	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	1124	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	1385	A	O4'-C1'-N9	5.01	112.21	108.20
54	BA	2176	A	C2-N3-C4	5.01	113.11	110.60
54	BA	2867	G	N3-C2-N2	-5.01	116.39	119.90
21	AA	1074	G	C8-N9-C4	-5.01	104.40	106.40
21	AA	1136	C	N1-C2-O2	5.01	121.91	118.90
22	A1	42	G	C5-C6-N1	5.01	114.00	111.50
24	A3	23	G	N9-C4-C5	5.01	107.40	105.40
24	A3	67	C	C2-N3-C4	-5.01	117.39	119.90
39	BQ	10	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	638	G	C5'-C4'-C3'	-5.01	107.98	116.00
54	BA	663	G	C5-C6-N1	5.01	114.00	111.50
54	BA	1379	U	P-O3'-C3'	5.01	125.71	119.70
54	BA	1450	G	C3'-C2'-C1'	5.01	105.51	101.50
54	BA	2113	U	C5-C6-N1	-5.01	120.19	122.70
54	BA	2415	G	C5-C6-N1	5.01	114.00	111.50
54	BA	2544	G	C8-N9-C4	-5.01	104.40	106.40
54	BA	2812	G	N7-C8-N9	5.01	115.60	113.10
21	AA	599	C	O4'-C1'-N1	5.01	112.21	108.20
54	BA	296	U	N1-C2-N3	5.01	117.91	114.90
54	BA	1398	C	N3-C4-C5	5.01	123.90	121.90
54	BA	1907	G	C5-C6-N1	5.01	114.00	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2102	G	C4'-C3'-C2'	-5.01	97.59	102.60
55	BB	23	G	N3-C4-C5	-5.01	126.10	128.60
21	AA	37	U	O4'-C1'-N1	5.01	112.20	108.20
21	AA	992	U	C1'-O4'-C4'	-5.01	105.89	109.90
21	AA	1361	G	C8-N9-C4	-5.01	104.40	106.40
54	BA	631	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	943	A	C6-C5-N7	5.01	135.81	132.30
54	BA	1338	G	C8-N9-C4	-5.01	104.40	106.40
54	BA	1605	C	N1-C2-O2	5.01	121.90	118.90
54	BA	1872	A	C4'-C3'-C2'	-5.01	97.59	102.60
54	BA	2087	G	N7-C8-N9	5.01	115.60	113.10
54	BA	2645	G	O4'-C1'-N9	5.01	112.20	108.20
54	BA	2659	G	N1-C6-O6	-5.01	116.90	119.90
54	BA	2745	C	N1-C2-O2	5.01	121.90	118.90
21	AA	293	G	C5-C6-N1	5.00	114.00	111.50
21	AA	341	C	N1-C2-O2	5.00	121.90	118.90
21	AA	789	U	N3-C2-O2	-5.00	118.70	122.20
21	AA	846	G	N1-C6-O6	-5.00	116.90	119.90
24	A3	70	C	N1-C2-O2	5.00	121.90	118.90
54	BA	2133	G	C8-N9-C4	-5.00	104.40	106.40
54	BA	2592	G	C5-C6-N1	5.00	114.00	111.50
54	BA	2705	A	C6-C5-N7	5.00	135.80	132.30
21	AA	182	A	C2-N3-C4	5.00	113.10	110.60
21	AA	545	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	1056	U	N1-C2-N3	5.00	117.90	114.90
22	A1	18	G	N3-C2-N2	-5.00	116.40	119.90
54	BA	275	C	N1-C2-O2	5.00	121.90	118.90
54	BA	287	G	C5-C6-N1	5.00	114.00	111.50
54	BA	747	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	807	U	C3'-C2'-C1'	5.00	105.50	101.50
54	BA	903	C	O4'-C1'-N1	5.00	112.20	108.20
54	BA	1011	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	1436	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	1755	A	C5-C6-N1	5.00	120.20	117.70
54	BA	2104	C	N3-C4-C5	5.00	123.90	121.90
54	BA	2373	G	C5-C6-N1	5.00	114.00	111.50
54	BA	2442	C	N3-C4-C5	5.00	123.90	121.90
55	BB	80	U	N1-C2-N3	5.00	117.90	114.90
55	BB	109	A	C6-C5-N7	5.00	135.80	132.30
21	AA	417	G	C5-C6-N1	5.00	114.00	111.50
54	BA	724	U	N1-C2-N3	5.00	117.90	114.90
54	BA	1852	U	O4'-C1'-N1	5.00	112.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1940	U	C4-C5-C6	5.00	122.70	119.70
54	BA	2221	G	N3-C4-C5	-5.00	126.10	128.60
55	BB	18	G	C5-C6-N1	5.00	114.00	111.50

There are no chirality outliers.

All (1054) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	16	C	Sidechain
22	A1	25	C	Sidechain
22	A1	29	U	Sidechain
22	A1	32	C	Sidechain
22	A1	33	U	Sidechain
22	A1	39	G	Sidechain
22	A1	45	G	Sidechain
22	A1	6	A	Sidechain
22	A1	62	C	Sidechain
22	A1	65	C	Sidechain
22	A1	74	C	Sidechain
22	A1	75	C	Sidechain
22	A1	76	A	Sidechain
23	A2	80	C	Sidechain
23	A2	81	U	Sidechain
23	A2	82	A	Sidechain
23	A2	83	U	Sidechain
23	A2	86	U	Sidechain
24	A3	11	A	Sidechain
24	A3	2	G	Sidechain
24	A3	22	A	Sidechain
24	A3	25	U	Sidechain
24	A3	26	C	Sidechain
24	A3	31	G	Sidechain
24	A3	32	G	Sidechain
24	A3	46	G	Sidechain
24	A3	54	G	Sidechain
24	A3	57	C	Sidechain
24	A3	64	G	Sidechain
24	A3	69	C	Sidechain
24	A3	70	C	Sidechain
24	A3	71	G	Sidechain
24	A3	73	A	Sidechain
24	A3	74	A	Sidechain

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Mol	Chain	Res	Type	Group
24	A3	75	C	Sidechain
24	A3	76	C	Sidechain
24	A3	77	A	Sidechain
21	AA	1000	A	Sidechain
21	AA	1012	A	Sidechain
21	AA	1016	A	Sidechain
21	AA	1017	U	Sidechain
21	AA	1029	U	Sidechain
21	AA	1031	C	Sidechain
21	AA	1038	C	Sidechain
21	AA	1046	A	Sidechain
21	AA	1053	G	Sidechain
21	AA	1055	A	Sidechain
21	AA	1057	G	Sidechain
21	AA	1065	U	Sidechain
21	AA	1072	G	Sidechain
21	AA	1076	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	1079	G	Sidechain
21	AA	1088	G	Sidechain
21	AA	1092	A	Sidechain
21	AA	1093	A	Sidechain
21	AA	1094	G	Sidechain
21	AA	1101	A	Sidechain
21	AA	1102	A	Sidechain
21	AA	1105	A	Sidechain
21	AA	1108	G	Sidechain
21	AA	1119	C	Sidechain
21	AA	1123	U	Sidechain
21	AA	1130	A	Sidechain
21	AA	1131	G	Sidechain
21	AA	1132	C	Sidechain
21	AA	1150	A	Sidechain
21	AA	1153	G	Sidechain
21	AA	1155	A	Sidechain
21	AA	1159	U	Sidechain
21	AA	1162	C	Sidechain
21	AA	1163	A	Sidechain
21	AA	1164	G	Sidechain
21	AA	1176	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1184	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1198	G	Sidechain
21	AA	12	U	Sidechain
21	AA	120	A	Sidechain
21	AA	1206	G	Sidechain
21	AA	1212	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1215	G	Sidechain
21	AA	1219	A	Sidechain
21	AA	122	G	Sidechain
21	AA	123	U	Sidechain
21	AA	1245	C	Sidechain
21	AA	1249	C	Sidechain
21	AA	125	U	Sidechain
21	AA	1256	A	Sidechain
21	AA	1264	U	Sidechain
21	AA	1266	G	Sidechain
21	AA	1276	G	Sidechain
21	AA	1278	G	Sidechain
21	AA	1279	G	Sidechain
21	AA	1280	A	Sidechain
21	AA	1282	C	Sidechain
21	AA	1285	A	Sidechain
21	AA	1288	A	Sidechain
21	AA	129	A	Sidechain
21	AA	1291	U	Sidechain
21	AA	1296	C	Sidechain
21	AA	1297	G	Sidechain
21	AA	1299	A	Sidechain
21	AA	13	U	Sidechain
21	AA	1300	G	Sidechain
21	AA	1307	U	Sidechain
21	AA	1316	G	Sidechain
21	AA	1319	A	Sidechain
21	AA	1321	U	Sidechain
21	AA	1329	A	Sidechain
21	AA	1331	G	Sidechain
21	AA	1335	U	Sidechain
21	AA	1337	G	Sidechain
21	AA	1343	G	Sidechain
21	AA	1358	U	Sidechain
21	AA	1359	C	Sidechain
21	AA	1363	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1364	U	Sidechain
21	AA	1367	C	Sidechain
21	AA	1370	G	Sidechain
21	AA	1374	A	Sidechain
21	AA	1376	U	Sidechain
21	AA	1382	C	Sidechain
21	AA	1383	C	Sidechain
21	AA	1391	U	Sidechain
21	AA	1406	U	Sidechain
21	AA	1412	C	Sidechain
21	AA	1414	U	Sidechain
21	AA	1418	A	Sidechain
21	AA	1424	U	Sidechain
21	AA	1425	U	Sidechain
21	AA	1430	A	Sidechain
21	AA	1432	G	Sidechain
21	AA	1435	G	Sidechain
21	AA	1436	U	Sidechain
21	AA	1438	G	Sidechain
21	AA	1446	A	Sidechain
21	AA	1450	U	Sidechain
21	AA	1460	C	Sidechain
21	AA	1468	A	Sidechain
21	AA	1483	A	Sidechain
21	AA	1487	G	Sidechain
21	AA	1488	G	Sidechain
21	AA	149	A	Sidechain
21	AA	1491	G	Sidechain
21	AA	1498	U	Sidechain
21	AA	1501	C	Sidechain
21	AA	1505	G	Sidechain
21	AA	1514	G	Sidechain
21	AA	1516	G	Sidechain
21	AA	1518	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1525	G	Sidechain
21	AA	1527	U	Sidechain
21	AA	153	C	Sidechain
21	AA	1530	G	Sidechain
21	AA	1532	U	Sidechain
21	AA	1533	C	Sidechain
21	AA	1534	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	154	U	Sidechain
21	AA	155	A	Sidechain
21	AA	159	G	Sidechain
21	AA	161	A	Sidechain
21	AA	163	C	Sidechain
21	AA	164	G	Sidechain
21	AA	171	A	Sidechain
21	AA	174	A	Sidechain
21	AA	176	C	Sidechain
21	AA	181	A	Sidechain
21	AA	182	A	Sidechain
21	AA	187	G	Sidechain
21	AA	188	C	Sidechain
21	AA	194	C	Sidechain
21	AA	197	A	Sidechain
21	AA	198	G	Sidechain
21	AA	20	U	Sidechain
21	AA	202	G	Sidechain
21	AA	203	G	Sidechain
21	AA	211	G	Sidechain
21	AA	215	C	Sidechain
21	AA	229	U	Sidechain
21	AA	230	G	Sidechain
21	AA	236	A	Sidechain
21	AA	237	G	Sidechain
21	AA	238	A	Sidechain
21	AA	249	U	Sidechain
21	AA	252	U	Sidechain
21	AA	257	G	Sidechain
21	AA	260	G	Sidechain
21	AA	264	C	Sidechain
21	AA	268	U	Sidechain
21	AA	270	A	Sidechain
21	AA	272	C	Sidechain
21	AA	277	C	Sidechain
21	AA	278	G	Sidechain
21	AA	279	A	Sidechain
21	AA	291	U	Sidechain
21	AA	292	G	Sidechain
21	AA	297	G	Sidechain
21	AA	309	A	Sidechain
21	AA	324	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	326	G	Sidechain
21	AA	331	G	Sidechain
21	AA	336	A	Sidechain
21	AA	337	G	Sidechain
21	AA	340	U	Sidechain
21	AA	343	U	Sidechain
21	AA	344	A	Sidechain
21	AA	347	G	Sidechain
21	AA	348	G	Sidechain
21	AA	350	G	Sidechain
21	AA	353	A	Sidechain
21	AA	355	C	Sidechain
21	AA	357	G	Sidechain
21	AA	36	C	Sidechain
21	AA	362	G	Sidechain
21	AA	365	U	Sidechain
21	AA	368	U	Sidechain
21	AA	376	G	Sidechain
21	AA	377	G	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	382	A	Sidechain
21	AA	387	U	Sidechain
21	AA	39	G	Sidechain
21	AA	394	G	Sidechain
21	AA	399	G	Sidechain
21	AA	40	C	Sidechain
21	AA	403	C	Sidechain
21	AA	405	U	Sidechain
21	AA	406	G	Sidechain
21	AA	409	U	Sidechain
21	AA	413	G	Sidechain
21	AA	427	U	Sidechain
21	AA	429	U	Sidechain
21	AA	436	C	Sidechain
21	AA	442	G	Sidechain
21	AA	449	G	Sidechain
21	AA	452	A	Sidechain
21	AA	455	G	Sidechain
21	AA	462	G	Sidechain
21	AA	464	U	Sidechain
21	AA	468	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	476	U	Sidechain
21	AA	477	C	Sidechain
21	AA	479	U	Sidechain
21	AA	480	U	Sidechain
21	AA	485	U	Sidechain
21	AA	491	G	Sidechain
21	AA	492	C	Sidechain
21	AA	493	A	Sidechain
21	AA	5	U	Sidechain
21	AA	50	A	Sidechain
21	AA	51	A	Sidechain
21	AA	510	A	Sidechain
21	AA	514	C	Sidechain
21	AA	516	U	Sidechain
21	AA	521	G	Sidechain
21	AA	527	G	Sidechain
21	AA	529	G	Sidechain
21	AA	530	G	Sidechain
21	AA	535	A	Sidechain
21	AA	537	G	Sidechain
21	AA	547	A	Sidechain
21	AA	557	G	Sidechain
21	AA	558	G	Sidechain
21	AA	562	U	Sidechain
21	AA	564	C	Sidechain
21	AA	566	G	Sidechain
21	AA	571	U	Sidechain
21	AA	572	A	Sidechain
21	AA	586	C	Sidechain
21	AA	588	G	Sidechain
21	AA	590	U	Sidechain
21	AA	597	G	Sidechain
21	AA	598	U	Sidechain
21	AA	6	G	Sidechain
21	AA	60	A	Sidechain
21	AA	61	G	Sidechain
21	AA	611	C	Sidechain
21	AA	613	C	Sidechain
21	AA	617	G	Sidechain
21	AA	623	C	Sidechain
21	AA	626	G	Sidechain
21	AA	635	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	636	U	Sidechain
21	AA	641	U	Sidechain
21	AA	646	G	Sidechain
21	AA	65	A	Sidechain
21	AA	653	U	Sidechain
21	AA	657	U	Sidechain
21	AA	660	C	Sidechain
21	AA	663	A	Sidechain
21	AA	670	G	Sidechain
21	AA	671	G	Sidechain
21	AA	68	G	Sidechain
21	AA	682	G	Sidechain
21	AA	688	G	Sidechain
21	AA	690	G	Sidechain
21	AA	691	G	Sidechain
21	AA	692	U	Sidechain
21	AA	696	A	Sidechain
21	AA	698	G	Sidechain
21	AA	699	C	Sidechain
21	AA	704	A	Sidechain
21	AA	710	G	Sidechain
21	AA	712	A	Sidechain
21	AA	715	A	Sidechain
21	AA	716	A	Sidechain
21	AA	722	G	Sidechain
21	AA	727	G	Sidechain
21	AA	728	A	Sidechain
21	AA	735	C	Sidechain
21	AA	740	U	Sidechain
21	AA	741	G	Sidechain
21	AA	742	G	Sidechain
21	AA	747	A	Sidechain
21	AA	751	U	Sidechain
21	AA	752	G	Sidechain
21	AA	754	C	Sidechain
21	AA	755	G	Sidechain
21	AA	760	G	Sidechain
21	AA	763	G	Sidechain
21	AA	776	G	Sidechain
21	AA	787	A	Sidechain
21	AA	791	G	Sidechain
21	AA	795	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	802	A	Sidechain
21	AA	809	G	Sidechain
21	AA	811	C	Sidechain
21	AA	812	G	Sidechain
21	AA	813	U	Sidechain
21	AA	818	G	Sidechain
21	AA	820	U	Sidechain
21	AA	826	C	Sidechain
21	AA	827	U	Sidechain
21	AA	828	U	Sidechain
21	AA	83	C	Sidechain
21	AA	830	G	Sidechain
21	AA	833	G	Sidechain
21	AA	844	G	Sidechain
21	AA	864	A	Sidechain
21	AA	873	A	Sidechain
21	AA	874	G	Sidechain
21	AA	882	C	Sidechain
21	AA	883	C	Sidechain
21	AA	886	G	Sidechain
21	AA	887	G	Sidechain
21	AA	890	G	Sidechain
21	AA	892	A	Sidechain
21	AA	894	G	Sidechain
21	AA	898	G	Sidechain
21	AA	90	C	Sidechain
21	AA	900	A	Sidechain
21	AA	901	A	Sidechain
21	AA	904	U	Sidechain
21	AA	914	A	Sidechain
21	AA	922	G	Sidechain
21	AA	926	G	Sidechain
21	AA	927	G	Sidechain
21	AA	928	G	Sidechain
21	AA	933	G	Sidechain
21	AA	938	A	Sidechain
21	AA	94	G	Sidechain
21	AA	944	G	Sidechain
21	AA	95	C	Sidechain
21	AA	954	G	Sidechain
21	AA	968	A	Sidechain
21	AA	97	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	971	G	Sidechain
21	AA	973	G	Sidechain
21	AA	976	G	Sidechain
21	AA	978	A	Sidechain
21	AA	99	C	Sidechain
21	AA	994	A	Sidechain
21	AA	995	C	Sidechain
21	AA	997	U	Sidechain
21	AA	998	C	Sidechain
3	AD	44	LYS	Peptide
4	AE	148	SER	Peptide
13	AN	69	ARG	Sidechain
14	AO	68	TYR	Sidechain
56	B5	21	TYR	Sidechain
54	BA	1008	A	Sidechain
54	BA	1012	U	Sidechain
54	BA	1016	G	Sidechain
54	BA	1023	U	Sidechain
54	BA	1024	G	Sidechain
54	BA	1035	U	Sidechain
54	BA	1048	A	Sidechain
54	BA	1051	G	Sidechain
54	BA	1052	C	Sidechain
54	BA	1058	U	Sidechain
54	BA	1067	A	Sidechain
54	BA	1071	G	Sidechain
54	BA	1073	A	Sidechain
54	BA	108	G	Sidechain
54	BA	1083	U	Sidechain
54	BA	1087	G	Sidechain
54	BA	1088	A	Sidechain
54	BA	1093	G	Sidechain
54	BA	1100	C	Sidechain
54	BA	1108	U	Sidechain
54	BA	111	A	Sidechain
54	BA	1123	C	Sidechain
54	BA	1125	G	Sidechain
54	BA	1126	A	Sidechain
54	BA	1127	A	Sidechain
54	BA	1134	A	Sidechain
54	BA	1140	C	Sidechain
54	BA	1142	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1147	A	Sidechain
54	BA	1149	G	Sidechain
54	BA	1151	A	Sidechain
54	BA	1155	A	Sidechain
54	BA	1156	A	Sidechain
54	BA	116	C	Sidechain
54	BA	1160	G	Sidechain
54	BA	1162	G	Sidechain
54	BA	1166	G	Sidechain
54	BA	1167	C	Sidechain
54	BA	1175	A	Sidechain
54	BA	1181	U	Sidechain
54	BA	1182	G	Sidechain
54	BA	1187	G	Sidechain
54	BA	1188	U	Sidechain
54	BA	1191	G	Sidechain
54	BA	1195	G	Sidechain
54	BA	1197	G	Sidechain
54	BA	1205	A	Sidechain
54	BA	1206	G	Sidechain
54	BA	1208	C	Sidechain
54	BA	1210	G	Sidechain
54	BA	1215	G	Sidechain
54	BA	1218	G	Sidechain
54	BA	1221	C	Sidechain
54	BA	1223	G	Sidechain
54	BA	1224	U	Sidechain
54	BA	1230	A	Sidechain
54	BA	1236	G	Sidechain
54	BA	1237	A	Sidechain
54	BA	1242	U	Sidechain
54	BA	1251	C	Sidechain
54	BA	1252	G	Sidechain
54	BA	1258	U	Sidechain
54	BA	1263	U	Sidechain
54	BA	1267	U	Sidechain
54	BA	1273	U	Sidechain
54	BA	1279	G	Sidechain
54	BA	1281	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	1307	A	Sidechain
54	BA	1309	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1312	U	Sidechain
54	BA	1313	U	Sidechain
54	BA	1315	C	Sidechain
54	BA	1317	G	Sidechain
54	BA	1320	C	Sidechain
54	BA	1326	U	Sidechain
54	BA	1330	C	Sidechain
54	BA	1334	G	Sidechain
54	BA	1336	A	Sidechain
54	BA	1343	G	Sidechain
54	BA	1344	U	Sidechain
54	BA	1345	C	Sidechain
54	BA	1351	C	Sidechain
54	BA	1360	G	Sidechain
54	BA	1364	G	Sidechain
54	BA	1366	A	Sidechain
54	BA	1373	A	Sidechain
54	BA	1376	C	Sidechain
54	BA	1377	G	Sidechain
54	BA	1378	A	Sidechain
54	BA	1384	A	Sidechain
54	BA	1386	C	Sidechain
54	BA	1388	G	Sidechain
54	BA	1389	G	Sidechain
54	BA	139	U	Sidechain
54	BA	1392	A	Sidechain
54	BA	1399	C	Sidechain
54	BA	14	A	Sidechain
54	BA	140	C	Sidechain
54	BA	1405	U	Sidechain
54	BA	1407	G	Sidechain
54	BA	141	G	Sidechain
54	BA	1415	U	Sidechain
54	BA	1422	G	Sidechain
54	BA	1426	G	Sidechain
54	BA	1434	A	Sidechain
54	BA	1437	C	Sidechain
54	BA	144	A	Sidechain
54	BA	1442	U	Sidechain
54	BA	1444	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1447	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1448	G	Sidechain
54	BA	1454	C	Sidechain
54	BA	1455	G	Sidechain
54	BA	1456	G	Sidechain
54	BA	1461	C	Sidechain
54	BA	1469	A	Sidechain
54	BA	1473	G	Sidechain
54	BA	1492	G	Sidechain
54	BA	1499	C	Sidechain
54	BA	150	U	Sidechain
54	BA	1502	A	Sidechain
54	BA	1507	C	Sidechain
54	BA	1519	G	Sidechain
54	BA	1520	U	Sidechain
54	BA	1527	G	Sidechain
54	BA	1528	A	Sidechain
54	BA	1530	G	Sidechain
54	BA	1532	A	Sidechain
54	BA	1534	U	Sidechain
54	BA	1535	A	Sidechain
54	BA	1544	A	Sidechain
54	BA	1546	G	Sidechain
54	BA	155	A	Sidechain
54	BA	1553	A	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1563	U	Sidechain
54	BA	1573	G	Sidechain
54	BA	1576	U	Sidechain
54	BA	1577	C	Sidechain
54	BA	158	U	Sidechain
54	BA	1586	A	Sidechain
54	BA	159	G	Sidechain
54	BA	1593	A	Sidechain
54	BA	1596	A	Sidechain
54	BA	160	A	Sidechain
54	BA	1600	C	Sidechain
54	BA	1602	U	Sidechain
54	BA	161	A	Sidechain
54	BA	1610	A	Sidechain
54	BA	1611	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1616	A	Sidechain
54	BA	1618	A	Sidechain
54	BA	1620	G	Sidechain
54	BA	1628	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1638	C	Sidechain
54	BA	1642	G	Sidechain
54	BA	1652	A	Sidechain
54	BA	1661	G	Sidechain
54	BA	1662	U	Sidechain
54	BA	1664	A	Sidechain
54	BA	1665	A	Sidechain
54	BA	1667	G	Sidechain
54	BA	1671	U	Sidechain
54	BA	1681	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1683	U	Sidechain
54	BA	1697	G	Sidechain
54	BA	17	G	Sidechain
54	BA	1701	A	Sidechain
54	BA	1702	G	Sidechain
54	BA	1703	G	Sidechain
54	BA	1704	C	Sidechain
54	BA	1706	C	Sidechain
54	BA	1708	C	Sidechain
54	BA	1713	A	Sidechain
54	BA	1731	G	Sidechain
54	BA	1733	G	Sidechain
54	BA	1734	G	Sidechain
54	BA	1738	G	Sidechain
54	BA	1739	A	Sidechain
54	BA	1744	A	Sidechain
54	BA	1747	U	Sidechain
54	BA	1749	A	Sidechain
54	BA	1751	U	Sidechain
54	BA	1754	A	Sidechain
54	BA	1758	U	Sidechain
54	BA	1760	C	Sidechain
54	BA	1762	A	Sidechain
54	BA	1770	G	Sidechain
54	BA	1774	C	Sidechain
54	BA	1785	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1787	A	Sidechain
54	BA	1789	A	Sidechain
54	BA	1791	A	Sidechain
54	BA	1792	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1820	U	Sidechain
54	BA	1826	G	Sidechain
54	BA	1827	U	Sidechain
54	BA	1828	G	Sidechain
54	BA	1837	C	Sidechain
54	BA	1840	G	Sidechain
54	BA	1854	A	Sidechain
54	BA	1857	G	Sidechain
54	BA	1858	A	Sidechain
54	BA	1860	G	Sidechain
54	BA	1869	G	Sidechain
54	BA	1870	C	Sidechain
54	BA	1883	U	Sidechain
54	BA	1887	C	Sidechain
54	BA	1888	G	Sidechain
54	BA	1890	A	Sidechain
54	BA	1893	C	Sidechain
54	BA	1894	C	Sidechain
54	BA	1897	G	Sidechain
54	BA	1903	G	Sidechain
54	BA	1905	C	Sidechain
54	BA	1910	G	Sidechain
54	BA	1914	C	Sidechain
54	BA	1927	A	Sidechain
54	BA	1932	A	Sidechain
54	BA	1945	G	Sidechain
54	BA	1956	U	Sidechain
54	BA	196	A	Sidechain
54	BA	1960	A	Sidechain
54	BA	1961	C	Sidechain
54	BA	1962	C	Sidechain
54	BA	1971	U	Sidechain
54	BA	1976	U	Sidechain
54	BA	198	C	Sidechain
54	BA	1983	G	Sidechain
54	BA	1989	G	Sidechain
54	BA	1993	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1995	U	Sidechain
54	BA	1997	C	Sidechain
54	BA	20	C	Sidechain
54	BA	2002	G	Sidechain
54	BA	2004	G	Sidechain
54	BA	2007	U	Sidechain
54	BA	2012	G	Sidechain
54	BA	2013	A	Sidechain
54	BA	2018	G	Sidechain
54	BA	2019	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2029	G	Sidechain
54	BA	2055	C	Sidechain
54	BA	2056	G	Sidechain
54	BA	2058	A	Sidechain
54	BA	2059	A	Sidechain
54	BA	206	U	Sidechain
54	BA	2062	A	Sidechain
54	BA	2066	C	Sidechain
54	BA	2067	G	Sidechain
54	BA	207	A	Sidechain
54	BA	2072	C	Sidechain
54	BA	2078	C	Sidechain
54	BA	2079	U	Sidechain
54	BA	2082	A	Sidechain
54	BA	2088	A	Sidechain
54	BA	2091	C	Sidechain
54	BA	2104	C	Sidechain
54	BA	2107	G	Sidechain
54	BA	2109	U	Sidechain
54	BA	2111	U	Sidechain
54	BA	2113	U	Sidechain
54	BA	2114	A	Sidechain
54	BA	2115	G	Sidechain
54	BA	2121	G	Sidechain
54	BA	2125	G	Sidechain
54	BA	2128	G	Sidechain
54	BA	2132	U	Sidechain
54	BA	2140	G	Sidechain
54	BA	2153	C	Sidechain
54	BA	2157	G	Sidechain
54	BA	2160	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2167	U	Sidechain
54	BA	2168	G	Sidechain
54	BA	2172	U	Sidechain
54	BA	2175	C	Sidechain
54	BA	2176	A	Sidechain
54	BA	2181	U	Sidechain
54	BA	2189	U	Sidechain
54	BA	2196	C	Sidechain
54	BA	2197	U	Sidechain
54	BA	2198	A	Sidechain
54	BA	2202	U	Sidechain
54	BA	2207	C	Sidechain
54	BA	2211	A	Sidechain
54	BA	2212	A	Sidechain
54	BA	2217	G	Sidechain
54	BA	2219	U	Sidechain
54	BA	2224	G	Sidechain
54	BA	2225	A	Sidechain
54	BA	2230	G	Sidechain
54	BA	2236	U	Sidechain
54	BA	2242	G	Sidechain
54	BA	2244	U	Sidechain
54	BA	2245	U	Sidechain
54	BA	2248	C	Sidechain
54	BA	2249	U	Sidechain
54	BA	2250	G	Sidechain
54	BA	2251	G	Sidechain
54	BA	2256	G	Sidechain
54	BA	2257	U	Sidechain
54	BA	2266	A	Sidechain
54	BA	2271	G	Sidechain
54	BA	2274	A	Sidechain
54	BA	2278	A	Sidechain
54	BA	2283	C	Sidechain
54	BA	2284	A	Sidechain
54	BA	2290	G	Sidechain
54	BA	2298	A	Sidechain
54	BA	2300	C	Sidechain
54	BA	2301	C	Sidechain
54	BA	2302	U	Sidechain
54	BA	2304	G	Sidechain
54	BA	2308	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	231	A	Sidechain
54	BA	2323	G	Sidechain
54	BA	2327	A	Sidechain
54	BA	2328	A	Sidechain
54	BA	2330	G	Sidechain
54	BA	2331	G	Sidechain
54	BA	2336	A	Sidechain
54	BA	2337	G	Sidechain
54	BA	2338	C	Sidechain
54	BA	234	U	Sidechain
54	BA	2344	U	Sidechain
54	BA	235	U	Sidechain
54	BA	2352	A	Sidechain
54	BA	2357	G	Sidechain
54	BA	2363	G	Sidechain
54	BA	2375	G	Sidechain
54	BA	2376	A	Sidechain
54	BA	238	C	Sidechain
54	BA	2389	G	Sidechain
54	BA	2391	G	Sidechain
54	BA	2392	A	Sidechain
54	BA	2396	G	Sidechain
54	BA	2399	G	Sidechain
54	BA	240	C	Sidechain
54	BA	2411	A	Sidechain
54	BA	2416	C	Sidechain
54	BA	2418	A	Sidechain
54	BA	2428	G	Sidechain
54	BA	2432	A	Sidechain
54	BA	2433	A	Sidechain
54	BA	2439	A	Sidechain
54	BA	2442	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2447	G	Sidechain
54	BA	2455	G	Sidechain
54	BA	2466	C	Sidechain
54	BA	2468	A	Sidechain
54	BA	2469	A	Sidechain
54	BA	247	G	Sidechain
54	BA	2478	A	Sidechain
54	BA	248	G	Sidechain
54	BA	2481	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2495	G	Sidechain
54	BA	2499	C	Sidechain
54	BA	250	G	Sidechain
54	BA	2500	U	Sidechain
54	BA	2504	U	Sidechain
54	BA	2505	G	Sidechain
54	BA	2508	G	Sidechain
54	BA	2512	C	Sidechain
54	BA	2516	A	Sidechain
54	BA	2517	C	Sidechain
54	BA	2519	U	Sidechain
54	BA	2523	G	Sidechain
54	BA	2527	C	Sidechain
54	BA	2529	G	Sidechain
54	BA	2532	G	Sidechain
54	BA	2543	G	Sidechain
54	BA	2564	A	Sidechain
54	BA	2566	A	Sidechain
54	BA	2567	G	Sidechain
54	BA	2572	A	Sidechain
54	BA	2576	G	Sidechain
54	BA	2579	C	Sidechain
54	BA	2581	G	Sidechain
54	BA	2588	G	Sidechain
54	BA	2596	U	Sidechain
54	BA	2597	G	Sidechain
54	BA	2598	A	Sidechain
54	BA	2600	A	Sidechain
54	BA	2601	C	Sidechain
54	BA	2603	G	Sidechain
54	BA	2606	C	Sidechain
54	BA	2607	G	Sidechain
54	BA	2611	C	Sidechain
54	BA	2614	A	Sidechain
54	BA	262	A	Sidechain
54	BA	2621	G	Sidechain
54	BA	2622	U	Sidechain
54	BA	2626	C	Sidechain
54	BA	2631	G	Sidechain
54	BA	2637	U	Sidechain
54	BA	2639	A	Sidechain
54	BA	264	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2640	G	Sidechain
54	BA	2644	G	Sidechain
54	BA	265	A	Sidechain
54	BA	2652	C	Sidechain
54	BA	2659	G	Sidechain
54	BA	2662	A	Sidechain
54	BA	2668	G	Sidechain
54	BA	2669	G	Sidechain
54	BA	2673	G	Sidechain
54	BA	2679	A	Sidechain
54	BA	2680	U	Sidechain
54	BA	2682	A	Sidechain
54	BA	2687	U	Sidechain
54	BA	27	G	Sidechain
54	BA	2701	U	Sidechain
54	BA	2710	C	Sidechain
54	BA	2711	A	Sidechain
54	BA	2716	C	Sidechain
54	BA	2733	A	Sidechain
54	BA	2737	G	Sidechain
54	BA	2750	A	Sidechain
54	BA	2756	U	Sidechain
54	BA	276	U	Sidechain
54	BA	2765	A	Sidechain
54	BA	2774	C	Sidechain
54	BA	2780	G	Sidechain
54	BA	2781	A	Sidechain
54	BA	2784	U	Sidechain
54	BA	2785	C	Sidechain
54	BA	2787	C	Sidechain
54	BA	2790	U	Sidechain
54	BA	2802	G	Sidechain
54	BA	2805	C	Sidechain
54	BA	2806	C	Sidechain
54	BA	2807	U	Sidechain
54	BA	2811	G	Sidechain
54	BA	2817	U	Sidechain
54	BA	2819	G	Sidechain
54	BA	2822	G	Sidechain
54	BA	2823	A	Sidechain
54	BA	2829	A	Sidechain
54	BA	283	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2832	U	Sidechain
54	BA	2839	G	Sidechain
54	BA	2852	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2859	G	Sidechain
54	BA	2861	U	Sidechain
54	BA	2868	A	Sidechain
54	BA	2871	U	Sidechain
54	BA	2873	A	Sidechain
54	BA	2874	C	Sidechain
54	BA	2879	A	Sidechain
54	BA	2883	A	Sidechain
54	BA	2886	A	Sidechain
54	BA	2887	A	Sidechain
54	BA	2888	C	Sidechain
54	BA	2895	G	Sidechain
54	BA	2903	U	Sidechain
54	BA	295	G	Sidechain
54	BA	297	G	Sidechain
54	BA	304	U	Sidechain
54	BA	305	C	Sidechain
54	BA	307	G	Sidechain
54	BA	308	G	Sidechain
54	BA	309	A	Sidechain
54	BA	313	G	Sidechain
54	BA	317	G	Sidechain
54	BA	32	C	Sidechain
54	BA	323	C	Sidechain
54	BA	325	G	Sidechain
54	BA	326	G	Sidechain
54	BA	327	G	Sidechain
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	339	U	Sidechain
54	BA	340	A	Sidechain
54	BA	344	A	Sidechain
54	BA	355	U	Sidechain
54	BA	36	G	Sidechain
54	BA	364	C	Sidechain
54	BA	367	G	Sidechain
54	BA	385	C	Sidechain
54	BA	39	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	392	U	Sidechain
54	BA	393	C	Sidechain
54	BA	394	C	Sidechain
54	BA	4	U	Sidechain
54	BA	401	A	Sidechain
54	BA	402	A	Sidechain
54	BA	404	A	Sidechain
54	BA	416	U	Sidechain
54	BA	418	C	Sidechain
54	BA	420	C	Sidechain
54	BA	422	A	Sidechain
54	BA	434	U	Sidechain
54	BA	442	G	Sidechain
54	BA	446	G	Sidechain
54	BA	45	G	Sidechain
54	BA	450	G	Sidechain
54	BA	458	G	Sidechain
54	BA	463	G	Sidechain
54	BA	467	G	Sidechain
54	BA	471	A	Sidechain
54	BA	473	G	Sidechain
54	BA	476	G	Sidechain
54	BA	477	A	Sidechain
54	BA	478	A	Sidechain
54	BA	479	A	Sidechain
54	BA	481	G	Sidechain
54	BA	49	A	Sidechain
54	BA	493	G	Sidechain
54	BA	494	G	Sidechain
54	BA	495	G	Sidechain
54	BA	496	G	Sidechain
54	BA	499	U	Sidechain
54	BA	5	A	Sidechain
54	BA	500	G	Sidechain
54	BA	501	A	Sidechain
54	BA	505	A	Sidechain
54	BA	508	A	Sidechain
54	BA	510	C	Sidechain
54	BA	514	A	Sidechain
54	BA	518	G	Sidechain
54	BA	521	U	Sidechain
54	BA	522	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	523	C	Sidechain
54	BA	525	U	Sidechain
54	BA	527	C	Sidechain
54	BA	528	A	Sidechain
54	BA	53	A	Sidechain
54	BA	531	C	Sidechain
54	BA	538	A	Sidechain
54	BA	543	G	Sidechain
54	BA	547	A	Sidechain
54	BA	567	U	Sidechain
54	BA	573	U	Sidechain
54	BA	576	U	Sidechain
54	BA	579	G	Sidechain
54	BA	58	G	Sidechain
54	BA	587	C	Sidechain
54	BA	589	U	Sidechain
54	BA	59	U	Sidechain
54	BA	590	A	Sidechain
54	BA	595	C	Sidechain
54	BA	597	G	Sidechain
54	BA	600	G	Sidechain
54	BA	603	A	Sidechain
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	614	A	Sidechain
54	BA	615	U	Sidechain
54	BA	628	G	Sidechain
54	BA	630	G	Sidechain
54	BA	632	A	Sidechain
54	BA	636	G	Sidechain
54	BA	637	A	Sidechain
54	BA	64	A	Sidechain
54	BA	65	U	Sidechain
54	BA	655	A	Sidechain
54	BA	659	G	Sidechain
54	BA	670	A	Sidechain
54	BA	687	C	Sidechain
54	BA	69	C	Sidechain
54	BA	693	A	Sidechain
54	BA	695	G	Sidechain
54	BA	703	U	Sidechain
54	BA	71	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	715	A	Sidechain
54	BA	716	A	Sidechain
54	BA	718	A	Sidechain
54	BA	722	A	Sidechain
54	BA	724	U	Sidechain
54	BA	725	G	Sidechain
54	BA	727	A	Sidechain
54	BA	737	C	Sidechain
54	BA	738	G	Sidechain
54	BA	74	A	Sidechain
54	BA	750	A	Sidechain
54	BA	752	A	Sidechain
54	BA	76	C	Sidechain
54	BA	760	G	Sidechain
54	BA	764	A	Sidechain
54	BA	765	C	Sidechain
54	BA	770	G	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain
54	BA	777	G	Sidechain
54	BA	792	A	Sidechain
54	BA	793	A	Sidechain
54	BA	794	A	Sidechain
54	BA	795	C	Sidechain
54	BA	8	C	Sidechain
54	BA	800	A	Sidechain
54	BA	801	G	Sidechain
54	BA	802	A	Sidechain
54	BA	804	A	Sidechain
54	BA	805	G	Sidechain
54	BA	806	C	Sidechain
54	BA	810	U	Sidechain
54	BA	811	U	Sidechain
54	BA	813	U	Sidechain
54	BA	827	U	Sidechain
54	BA	828	U	Sidechain
54	BA	830	G	Sidechain
54	BA	834	G	Sidechain
54	BA	857	G	Sidechain
54	BA	858	G	Sidechain
54	BA	860	U	Sidechain
54	BA	862	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	880	G	Sidechain
54	BA	886	A	Sidechain
54	BA	888	C	Sidechain
54	BA	889	C	Sidechain
54	BA	895	U	Sidechain
54	BA	899	A	Sidechain
54	BA	90	U	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	920	A	Sidechain
54	BA	925	A	Sidechain
54	BA	926	G	Sidechain
54	BA	929	U	Sidechain
54	BA	930	G	Sidechain
54	BA	931	U	Sidechain
54	BA	941	A	Sidechain
54	BA	942	G	Sidechain
54	BA	952	G	Sidechain
54	BA	956	G	Sidechain
54	BA	959	A	Sidechain
54	BA	96	C	Sidechain
54	BA	966	G	Sidechain
54	BA	97	C	Sidechain
54	BA	974	G	Sidechain
54	BA	975	A	Sidechain
54	BA	983	A	Sidechain
54	BA	984	A	Sidechain
54	BA	988	A	Sidechain
54	BA	993	G	Sidechain
54	BA	998	C	Sidechain
55	BB	106	G	Sidechain
55	BB	109	A	Sidechain
55	BB	112	G	Sidechain
55	BB	12	C	Sidechain
55	BB	13	G	Sidechain
55	BB	14	U	Sidechain
55	BB	15	A	Sidechain
55	BB	19	C	Sidechain
55	BB	23	G	Sidechain
55	BB	31	C	Sidechain
55	BB	35	C	Sidechain
55	BB	38	C	Sidechain

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Mol	Chain	Res	Type	Group
55	BB	39	A	Sidechain
55	BB	49	C	Sidechain
55	BB	50	A	Sidechain
55	BB	57	A	Sidechain
55	BB	6	G	Sidechain
55	BB	64	G	Sidechain
55	BB	66	A	Sidechain
55	BB	69	G	Sidechain
55	BB	75	G	Sidechain
55	BB	87	U	Sidechain
55	BB	96	G	Sidechain
46	BX	36	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1708	0	1736	0	0
2	AC	1625	0	1699	0	0
3	AD	1643	0	1710	0	0
4	AE	1109	0	1152	1	0
5	AF	818	0	808	1	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	1	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	1	0
21	AA	32828	0	16011	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A1	1627	0	802	0	0
23	A2	309	0	156	0	0
24	A3	1642	0	811	2	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	1	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	1	0
33	BK	939	0	1012	1	0
34	BL	1045	0	1117	2	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	0
38	BP	917	0	965	1	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	1	0
52	B3	504	0	574	3	0
53	B4	302	0	343	0	0
54	BA	62317	0	30495	12	0
55	BB	2504	0	1187	0	0
56	B5	1658	0	1751	1	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	98156	28	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 (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BL:64:PHE:CE2	52:B3:24:LYS:HE2	2.40	0.56
20:AU:30:GLU:H	20:AU:31:VAL:HG22	1.72	0.54
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.30	0.49
56:B5:19:LYS:HE3	56:B5:21:TYR:CE2	2.46	0.49
52:B3:2:LYS:HE3	54:BA:242:G:C8	2.51	0.45
54:BA:780:G:C6	54:BA:782:A:C2	3.05	0.45
24:A3:75:C:H2'	24:A3:76:C:C5'	2.46	0.44
33:BK:106:GLU:H	33:BK:106:GLU:CD	2.20	0.44
45:BW:35:ILE:HD12	45:BW:35:ILE:N	2.33	0.44
21:AA:901:A:N7	21:AA:902:G:H1'	2.34	0.43
21:AA:539:A:H2'	21:AA:540:G:C8	2.54	0.42
54:BA:669:G:H2'	54:BA:670:A:C5	2.54	0.42
4:AE:155:LYS:HE2	7:AH:44:PHE:CE1	2.54	0.42
51:B2:8:SER:HB3	54:BA:686:U:H3	1.85	0.42
54:BA:639:U:H2'	54:BA:640:C:C6	2.55	0.42
21:AA:493:A:H2'	21:AA:494:G:C4	2.55	0.42
29:BG:93:TYR:CE2	29:BG:159:LYS:HE2	2.54	0.41
54:BA:2210:U:C2	54:BA:2212:A:H2'	2.55	0.41
34:BL:64:PHE:CZ	52:B3:24:LYS:HE2	2.56	0.41
54:BA:139:U:H3'	54:BA:140:C:C5'	2.51	0.41
54:BA:1050:A:C2	54:BA:2751:G:C4	3.08	0.41
37:BO:5:SER:HA	37:BO:8:ILE:HG22	2.03	0.41
54:BA:2291:U:H2'	54:BA:2292:U:C6	2.56	0.41
32:BJ:13:ARG:HB3	32:BJ:53:TYR:CD2	2.56	0.40
21:AA:713:G:H2'	21:AA:714:G:C8	2.57	0.40
24:A3:75:C:H1'	54:BA:2602:A:H2'	2.04	0.40
38:BP:93:LYS:HE3	54:BA:1754:A:C8	2.57	0.40
54:BA:449:A:C8	54:BA:449:A:O5'	2.75	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%)	199 (91%)	17 (8%)	2 (1%)	17 57
2	AC	205/208 (99%)	187 (91%)	15 (7%)	3 (2%)	10 46
3	AD	203/206 (98%)	184 (91%)	14 (7%)	5 (2%)	5 32
4	AE	150/152 (99%)	132 (88%)	14 (9%)	4 (3%)	5 31
5	AF	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	4 28
6	AG	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	7 38
7	AH	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	6 33
8	AI	126/128 (98%)	113 (90%)	7 (6%)	6 (5%)	2 21
9	AJ	98/100 (98%)	90 (92%)	4 (4%)	4 (4%)	3 23
10	AK	116/118 (98%)	107 (92%)	8 (7%)	1 (1%)	17 57
11	AL	121/124 (98%)	108 (89%)	7 (6%)	6 (5%)	2 20
12	AM	112/115 (97%)	100 (89%)	9 (8%)	3 (3%)	5 31
13	AN	98/101 (97%)	83 (85%)	12 (12%)	3 (3%)	4 27
14	AO	86/89 (97%)	76 (88%)	8 (9%)	2 (2%)	6 34
15	AP	79/81 (98%)	67 (85%)	8 (10%)	4 (5%)	2 19
16	AQ	80/82 (98%)	75 (94%)	3 (4%)	2 (2%)	5 32
17	AR	55/57 (96%)	51 (93%)	4 (7%)	0	100 100
18	AS	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	12 48
19	AT	84/86 (98%)	76 (90%)	7 (8%)	1 (1%)	13 50
20	AU	51/53 (96%)	32 (63%)	9 (18%)	10 (20%)	0 2
25	BC	270/273 (99%)	246 (91%)	18 (7%)	6 (2%)	6 35
26	BD	207/209 (99%)	177 (86%)	19 (9%)	11 (5%)	2 19
27	BE	199/201 (99%)	179 (90%)	11 (6%)	9 (4%)	2 22
28	BF	176/179 (98%)	150 (85%)	20 (11%)	6 (3%)	3 26
29	BG	174/177 (98%)	156 (90%)	15 (9%)	3 (2%)	9 42
30	BH	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	11 46
31	BI	139/142 (98%)	130 (94%)	7 (5%)	2 (1%)	11 46
32	BJ	140/142 (99%)	122 (87%)	15 (11%)	3 (2%)	7 36
33	BK	121/123 (98%)	112 (93%)	9 (7%)	0	100 100
34	BL	141/144 (98%)	127 (90%)	10 (7%)	4 (3%)	5 30
35	BM	134/136 (98%)	118 (88%)	11 (8%)	5 (4%)	3 24
36	BN	119/121 (98%)	107 (90%)	10 (8%)	2 (2%)	9 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
37	BO	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	17 57
38	BP	112/115 (97%)	94 (84%)	11 (10%)	7 (6%)	1 17
39	BQ	115/118 (98%)	109 (95%)	3 (3%)	3 (3%)	5 31
40	BR	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	7 38
41	BS	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	17 57
42	BT	92/94 (98%)	71 (77%)	17 (18%)	4 (4%)	2 22
43	BU	101/104 (97%)	88 (87%)	10 (10%)	3 (3%)	4 28
44	BV	92/94 (98%)	90 (98%)	2 (2%)	0	100 100
45	BW	78/80 (98%)	60 (77%)	15 (19%)	3 (4%)	3 24
46	BX	75/79 (95%)	64 (85%)	9 (12%)	2 (3%)	5 31
47	BY	61/63 (97%)	53 (87%)	7 (12%)	1 (2%)	9 44
48	BZ	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	8 40
49	B0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	2 19
50	B1	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	3 23
51	B2	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
52	B3	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	9 44
53	B4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	2 19
56	B5	221/234 (94%)	207 (94%)	12 (5%)	2 (1%)	17 57
All	All	5876/6008 (98%)	5263 (90%)	456 (8%)	157 (3%)	8 31

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	149	PRO
6	AG	11	ILE
6	AG	56	SER
8	AI	110	VAL
9	AJ	57	VAL
13	AN	56	SER
14	AO	18	ALA
18	AS	4	LEU
20	AU	9	GLU
20	AU	37	TYR
25	BC	136	VAL
26	BD	80	TRP
26	BD	170	VAL

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Mol	Chain	Res	Type
28	BF	103	ILE
34	BL	36	LYS
36	BN	47	VAL
39	BQ	87	VAL
42	BT	68	LYS
50	B1	50	GLU
2	AC	167	TYR
3	AD	24	VAL
4	AE	105	ILE
5	AF	6	ILE
6	AG	5	VAL
7	AH	77	VAL
8	AI	119	LYS
9	AJ	74	VAL
12	AM	42	VAL
15	AP	17	TYR
15	AP	79	ASN
19	AT	3	ILE
20	AU	15	LEU
20	AU	27	VAL
27	BE	49	ARG
30	BH	121	VAL
34	BL	25	SER
34	BL	101	ILE
35	BM	36	VAL
35	BM	58	LYS
35	BM	70	ASP
38	BP	31	VAL
39	BQ	86	SER
41	BS	29	VAL
42	BT	61	LEU
43	BU	43	LYS
45	BW	68	PHE
46	BX	17	ARG
46	BX	27	ARG
49	B0	52	LYS
50	B1	6	GLU
3	AD	28	ASP
3	AD	84	ASN
5	AF	63	ASN
11	AL	68	GLY
11	AL	78	VAL

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Mol	Chain	Res	Type
13	AN	55	SER
15	AP	50	THR
16	AQ	27	PHE
20	AU	13	VAL
20	AU	25	ALA
20	AU	31	VAL
25	BC	37	SER
25	BC	196	ASN
25	BC	260	LYS
26	BD	2	ILE
26	BD	22	ILE
26	BD	51	THR
26	BD	77	ARG
26	BD	131	ASP
26	BD	150	GLN
27	BE	43	THR
27	BE	96	VAL
27	BE	123	LYS
28	BF	87	LYS
28	BF	132	ARG
29	BG	22	VAL
32	BJ	15	TRP
34	BL	125	LEU
35	BM	117	PHE
38	BP	74	GLN
40	BR	53	PHE
43	BU	5	ARG
43	BU	45	GLN
47	BY	37	LEU
56	B5	91	GLY
1	AB	11	ALA
1	AB	18	GLN
4	AE	38	VAL
7	AH	65	PHE
8	AI	31	GLN
8	AI	57	VAL
9	AJ	75	ASP
12	AM	60	ALA
14	AO	43	ALA
16	AQ	64	ARG
26	BD	15	PHE
26	BD	75	ALA

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Mol	Chain	Res	Type
27	BE	71	GLY
32	BJ	53	TYR
35	BM	134	THR
38	BP	26	GLU
38	BP	112	ARG
42	BT	3	ARG
45	BW	74	LYS
49	B0	5	ASN
52	B3	35	LYS
53	B4	32	LYS
56	B5	220	ALA
8	AI	55	ASP
11	AL	116	TYR
20	AU	3	ILE
25	BC	191	LEU
26	BD	112	THR
27	BE	165	HIS
30	BH	94	ILE
31	BI	37	PHE
32	BJ	45	THR
38	BP	32	VAL
39	BQ	2	ARG
40	BR	51	VAL
42	BT	66	LYS
53	B4	2	LYS
2	AC	195	ILE
3	AD	138	PRO
4	AE	54	GLU
5	AF	98	GLU
7	AH	78	SER
9	AJ	92	LEU
11	AL	33	CYS
13	AN	100	SER
20	AU	12	ASP
25	BC	36	ASN
27	BE	94	GLN
29	BG	101	VAL
38	BP	109	ILE
45	BW	53	GLY
48	BZ	31	ILE
8	AI	25	GLY
15	AP	40	ASN

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Mol	Chain	Res	Type
27	BE	81	GLY
28	BF	12	VAL
28	BF	75	GLY
38	BP	69	VAL
49	B0	24	VAL
3	AD	199	ILE
12	AM	63	VAL
27	BE	148	ILE
2	AC	144	GLY
10	AK	77	GLY
11	AL	84	GLY
28	BF	140	ILE
29	BG	116	LEU
11	AL	43	LYS
20	AU	52	VAL
31	BI	97	VAL
36	BN	84	GLY
37	BO	27	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%)	170 (100%)	0	100 100
3	AD	172/173 (99%)	169 (98%)	3 (2%)	60 78
4	AE	113/113 (100%)	111 (98%)	2 (2%)	59 77
5	AF	87/87 (100%)	85 (98%)	2 (2%)	50 70
6	AG	123/123 (100%)	121 (98%)	2 (2%)	62 79
7	AH	104/105 (99%)	104 (100%)	0	100 100
8	AI	105/105 (100%)	102 (97%)	3 (3%)	42 64
9	AJ	86/86 (100%)	86 (100%)	0	100 100
10	AK	90/90 (100%)	89 (99%)	1 (1%)	73 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	AL	103/104 (99%)	102 (99%)	1 (1%)	76 86
12	AM	91/92 (99%)	91 (100%)	0	100 100
13	AN	83/84 (99%)	82 (99%)	1 (1%)	71 83
14	AO	76/77 (99%)	74 (97%)	2 (3%)	46 66
15	AP	65/65 (100%)	65 (100%)	0	100 100
16	AQ	74/74 (100%)	73 (99%)	1 (1%)	67 80
17	AR	48/48 (100%)	48 (100%)	0	100 100
18	AS	70/70 (100%)	69 (99%)	1 (1%)	67 80
19	AT	65/65 (100%)	64 (98%)	1 (2%)	65 80
20	AU	44/44 (100%)	41 (93%)	3 (7%)	16 41
25	BC	216/217 (100%)	213 (99%)	3 (1%)	67 80
26	BD	164/164 (100%)	160 (98%)	4 (2%)	49 69
27	BE	165/165 (100%)	162 (98%)	3 (2%)	59 77
28	BF	149/150 (99%)	147 (99%)	2 (1%)	69 81
29	BG	137/138 (99%)	134 (98%)	3 (2%)	52 71
30	BH	114/114 (100%)	112 (98%)	2 (2%)	59 77
31	BI	109/110 (99%)	108 (99%)	1 (1%)	78 87
32	BJ	116/116 (100%)	115 (99%)	1 (1%)	78 87
33	BK	103/103 (100%)	103 (100%)	0	100 100
34	BL	102/103 (99%)	100 (98%)	2 (2%)	55 74
35	BM	109/109 (100%)	107 (98%)	2 (2%)	59 77
36	BN	100/100 (100%)	99 (99%)	1 (1%)	76 86
37	BO	86/87 (99%)	86 (100%)	0	100 100
38	BP	99/100 (99%)	97 (98%)	2 (2%)	55 74
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	73 84
40	BR	84/84 (100%)	82 (98%)	2 (2%)	49 69
41	BS	93/93 (100%)	92 (99%)	1 (1%)	73 84
42	BT	80/80 (100%)	80 (100%)	0	100 100
43	BU	83/84 (99%)	82 (99%)	1 (1%)	71 83
44	BV	78/78 (100%)	78 (100%)	0	100 100
45	BW	59/59 (100%)	57 (97%)	2 (3%)	37 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	BX	67/68 (98%)	67 (100%)	0	100 100
47	BY	55/55 (100%)	55 (100%)	0	100 100
48	BZ	48/49 (98%)	47 (98%)	1 (2%)	53 72
49	B0	47/48 (98%)	47 (100%)	0	100 100
50	B1	45/45 (100%)	44 (98%)	1 (2%)	52 71
51	B2	38/38 (100%)	35 (92%)	3 (8%)	12 35
52	B3	51/52 (98%)	51 (100%)	0	100 100
53	B4	34/34 (100%)	33 (97%)	1 (3%)	42 64
56	B5	173/181 (96%)	170 (98%)	3 (2%)	60 78
All	All	4842/4870 (99%)	4774 (99%)	68 (1%)	68 80

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	17	HIS
1	AB	106	VAL
1	AB	189	ASN
3	AD	50	TYR
3	AD	56	GLU
3	AD	181	PHE
4	AE	70	MET
4	AE	89	THR
5	AF	72	ASP
5	AF	97	THR
6	AG	12	LEU
6	AG	27	ASN
8	AI	53	LEU
8	AI	56	MET
8	AI	105	ARG
10	AK	100	ASN
11	AL	28	GLN
13	AN	81	ARG
14	AO	24	THR
14	AO	45	HIS
16	AQ	69	THR
18	AS	14	LEU
19	AT	30	PHE
20	AU	18	PHE
20	AU	20	ARG

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Mol	Chain	Res	Type
20	AU	27	VAL
25	BC	24	HIS
25	BC	86	ARG
25	BC	200	MET
26	BD	90	PHE
26	BD	91	THR
26	BD	103	ASP
26	BD	172	VAL
27	BE	122	GLU
27	BE	152	GLU
27	BE	163	ASN
28	BF	35	LEU
28	BF	134	GLN
29	BG	34	ARG
29	BG	154	GLU
29	BG	162	ARG
30	BH	68	ARG
30	BH	104	THR
31	BI	16	MET
32	BJ	30	THR
34	BL	77	ILE
34	BL	81	ASP
35	BM	1	MET
35	BM	126	ILE
36	BN	1	MET
38	BP	19	PHE
38	BP	75	THR
39	BQ	5	ARG
40	BR	31	GLU
40	BR	80	ARG
41	BS	81	SER
43	BU	8	ASP
45	BW	23	LYS
45	BW	39	GLN
48	BZ	37	ARG
50	B1	22	THR
51	B2	1	MET
51	B2	25	LYS
51	B2	34	ARG
53	B4	24	ARG
56	B5	12	ARG
56	B5	129	GLN

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Mol	Chain	Res	Type
56	B5	148	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
4	AE	96	GLN
10	AK	100	ASN
29	BG	110	HIS
44	BV	88	HIS
45	BW	56	HIS
46	BX	31	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	264 (17%)	77 (5%)
22	A1	74/76 (97%)	14 (18%)	6 (8%)
23	A2	14/15 (93%)	5 (35%)	2 (14%)
24	A3	76/77 (98%)	14 (18%)	7 (9%)
54	BA	2902/2903 (99%)	451 (15%)	146 (5%)
55	BB	116/118 (98%)	12 (10%)	3 (2%)
All	All	4711/4722 (99%)	760 (16%)	241 (5%)

All (760) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	61	G
21	AA	65	A
21	AA	66	A

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Mol	Chain	Res	Type
21	AA	70	U
21	AA	71	A
21	AA	84	U
21	AA	85	U
21	AA	94	G
21	AA	95	C
21	AA	109	A
21	AA	110	C
21	AA	121	U
21	AA	122	G
21	AA	131	A
21	AA	144	G
21	AA	165	G
21	AA	173	U
21	AA	181	A
21	AA	182	A
21	AA	191	G
21	AA	197	A
21	AA	198	G
21	AA	204	G
21	AA	212	G
21	AA	214	C
21	AA	238	A
21	AA	239	U
21	AA	240	G
21	AA	245	U
21	AA	246	A
21	AA	247	G
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	267	C
21	AA	289	G
21	AA	308	C
21	AA	309	A
21	AA	321	A
21	AA	328	C
21	AA	329	A
21	AA	330	C
21	AA	335	C
21	AA	343	U
21	AA	344	A

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Mol	Chain	Res	Type
21	AA	346	G
21	AA	347	G
21	AA	348	G
21	AA	352	C
21	AA	354	G
21	AA	356	A
21	AA	358	U
21	AA	367	U
21	AA	372	C
21	AA	381	C
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	412	A
21	AA	413	G
21	AA	414	A
21	AA	415	A
21	AA	421	U
21	AA	422	C
21	AA	429	U
21	AA	437	U
21	AA	438	U
21	AA	448	A
21	AA	449	G
21	AA	452	A
21	AA	461	A
21	AA	467	U
21	AA	468	A
21	AA	474	G
21	AA	481	G
21	AA	484	G
21	AA	493	A
21	AA	494	G
21	AA	500	G
21	AA	501	C
21	AA	505	G
21	AA	506	G
21	AA	508	U
21	AA	509	A
21	AA	511	C
21	AA	527	G
21	AA	532	A

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Mol	Chain	Res	Type
21	AA	533	A
21	AA	534	U
21	AA	535	A
21	AA	547	A
21	AA	550	G
21	AA	553	A
21	AA	559	A
21	AA	564	C
21	AA	565	U
21	AA	566	G
21	AA	571	U
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	619	U
21	AA	620	C
21	AA	625	U
21	AA	633	G
21	AA	654	G
21	AA	659	U
21	AA	660	C
21	AA	665	A
21	AA	671	G
21	AA	687	A
21	AA	700	G
21	AA	702	A
21	AA	718	A
21	AA	719	C
21	AA	724	G
21	AA	725	G
21	AA	755	G
21	AA	756	C
21	AA	761	G
21	AA	762	U
21	AA	777	A
21	AA	787	A
21	AA	793	U
21	AA	794	A
21	AA	808	C
21	AA	812	G
21	AA	817	C

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Mol	Chain	Res	Type
21	AA	819	A
21	AA	827	U
21	AA	828	U
21	AA	841	C
21	AA	843	U
21	AA	844	G
21	AA	846	G
21	AA	849	G
21	AA	885	G
21	AA	887	G
21	AA	889	A
21	AA	890	G
21	AA	914	A
21	AA	926	G
21	AA	927	G
21	AA	934	C
21	AA	939	G
21	AA	942	G
21	AA	945	G
21	AA	960	U
21	AA	961	U
21	AA	962	C
21	AA	968	A
21	AA	969	A
21	AA	972	C
21	AA	974	A
21	AA	976	G
21	AA	978	A
21	AA	979	C
21	AA	980	C
21	AA	993	G
21	AA	1004	A
21	AA	1006	G
21	AA	1031	C
21	AA	1033	G
21	AA	1042	A
21	AA	1050	G
21	AA	1053	G
21	AA	1054	C
21	AA	1055	A
21	AA	1056	U
21	AA	1065	U

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Mol	Chain	Res	Type
21	AA	1068	G
21	AA	1078	U
21	AA	1079	G
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1125	U
21	AA	1129	C
21	AA	1130	A
21	AA	1136	C
21	AA	1139	G
21	AA	1151	A
21	AA	1152	A
21	AA	1159	U
21	AA	1161	C
21	AA	1167	A
21	AA	1168	U
21	AA	1169	A
21	AA	1183	U
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1196	A
21	AA	1200	C
21	AA	1201	A
21	AA	1202	U
21	AA	1212	U
21	AA	1217	C
21	AA	1223	C
21	AA	1224	U
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1228	C
21	AA	1239	A
21	AA	1240	U
21	AA	1241	G
21	AA	1257	A
21	AA	1267	C
21	AA	1279	G
21	AA	1280	A

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Mol	Chain	Res	Type
21	AA	1281	C
21	AA	1282	C
21	AA	1285	A
21	AA	1287	A
21	AA	1301	U
21	AA	1303	C
21	AA	1305	G
21	AA	1308	U
21	AA	1309	G
21	AA	1319	A
21	AA	1320	C
21	AA	1322	C
21	AA	1336	C
21	AA	1337	G
21	AA	1338	G
21	AA	1345	U
21	AA	1360	A
21	AA	1363	A
21	AA	1364	U
21	AA	1378	C
21	AA	1382	C
21	AA	1383	C
21	AA	1432	G
21	AA	1446	A
21	AA	1453	G
21	AA	1466	C
21	AA	1471	U
21	AA	1484	C
21	AA	1492	A
21	AA	1493	A
21	AA	1494	G
21	AA	1499	A
21	AA	1503	A
21	AA	1504	G
21	AA	1505	G
21	AA	1506	U
21	AA	1529	G
21	AA	1530	G
21	AA	1533	C
21	AA	1534	A
22	A1	10	G
22	A1	17	U

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Mol	Chain	Res	Type
22	A1	20	G
22	A1	47	U
22	A1	48	C
22	A1	49	G
22	A1	56	C
22	A1	57	G
22	A1	58	A
22	A1	60	C
22	A1	62	C
22	A1	70	C
22	A1	75	C
22	A1	76	A
23	A2	80	C
23	A2	82	A
23	A2	89	U
23	A2	91	A
23	A2	92	U
24	A3	2	G
24	A3	9	G
24	A3	10	G
24	A3	18	U
24	A3	20	G
24	A3	22	A
24	A3	32	G
24	A3	49	C
24	A3	57	C
24	A3	58	A
24	A3	70	C
24	A3	75	C
24	A3	76	C
24	A3	77	A
54	BA	9	G
54	BA	14	A
54	BA	15	G
54	BA	20	C
54	BA	33	C
54	BA	34	U
54	BA	63	A
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	88	G

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Mol	Chain	Res	Type
54	BA	91	A
54	BA	92	U
54	BA	98	G
54	BA	100	U
54	BA	102	U
54	BA	110	G
54	BA	111	A
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	125	A
54	BA	126	A
54	BA	139	U
54	BA	140	C
54	BA	141	G
54	BA	142	A
54	BA	143	C
54	BA	145	C
54	BA	146	A
54	BA	147	C
54	BA	181	A
54	BA	196	A
54	BA	197	A
54	BA	199	A
54	BA	216	A
54	BA	222	A
54	BA	230	G
54	BA	233	A
54	BA	248	G
54	BA	250	G
54	BA	266	G
54	BA	278	A
54	BA	279	A
54	BA	294	A
54	BA	297	G
54	BA	299	A
54	BA	316	C
54	BA	323	C
54	BA	324	A
54	BA	330	A
54	BA	331	C

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Mol	Chain	Res	Type
54	BA	346	A
54	BA	370	G
54	BA	373	U
54	BA	374	A
54	BA	386	G
54	BA	387	U
54	BA	406	G
54	BA	411	G
54	BA	422	A
54	BA	428	A
54	BA	429	A
54	BA	430	A
54	BA	450	G
54	BA	451	U
54	BA	457	A
54	BA	473	G
54	BA	481	G
54	BA	491	G
54	BA	493	G
54	BA	504	A
54	BA	505	A
54	BA	507	A
54	BA	527	C
54	BA	528	A
54	BA	530	G
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	546	U
54	BA	547	A
54	BA	548	G
54	BA	549	G
54	BA	550	C
54	BA	573	U
54	BA	574	A
54	BA	588	U
54	BA	590	A
54	BA	603	A
54	BA	614	A
54	BA	627	A
54	BA	631	A
54	BA	637	A

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Mol	Chain	Res	Type
54	BA	645	C
54	BA	653	U
54	BA	655	A
54	BA	671	C
54	BA	686	U
54	BA	719	C
54	BA	727	A
54	BA	740	C
54	BA	747	U
54	BA	748	G
54	BA	750	A
54	BA	751	A
54	BA	752	A
54	BA	753	A
54	BA	763	G
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	791	C
54	BA	792	A
54	BA	805	G
54	BA	809	G
54	BA	812	C
54	BA	827	U
54	BA	828	U
54	BA	829	A
54	BA	830	G
54	BA	846	U
54	BA	858	G
54	BA	859	G
54	BA	866	A
54	BA	867	C
54	BA	889	C
54	BA	890	C
54	BA	891	G
54	BA	897	C
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	933	A

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Mol	Chain	Res	Type
54	BA	934	U
54	BA	941	A
54	BA	946	C
54	BA	959	A
54	BA	961	C
54	BA	974	G
54	BA	981	A
54	BA	982	C
54	BA	984	A
54	BA	989	G
54	BA	996	A
54	BA	1012	U
54	BA	1013	C
54	BA	1022	G
54	BA	1024	G
54	BA	1025	G
54	BA	1026	G
54	BA	1033	U
54	BA	1044	C
54	BA	1046	A
54	BA	1047	G
54	BA	1058	U
54	BA	1069	A
54	BA	1070	A
54	BA	1073	A
54	BA	1077	A
54	BA	1086	A
54	BA	1087	G
54	BA	1088	A
54	BA	1089	A
54	BA	1090	A
54	BA	1100	C
54	BA	1112	G
54	BA	1126	A
54	BA	1128	G
54	BA	1129	A
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1143	A
54	BA	1144	A
54	BA	1176	U

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Mol	Chain	Res	Type
54	BA	1204	A
54	BA	1205	A
54	BA	1206	G
54	BA	1237	A
54	BA	1242	U
54	BA	1253	A
54	BA	1256	G
54	BA	1265	A
54	BA	1266	G
54	BA	1271	G
54	BA	1272	A
54	BA	1276	A
54	BA	1288	G
54	BA	1289	C
54	BA	1300	G
54	BA	1301	A
54	BA	1302	A
54	BA	1313	U
54	BA	1317	G
54	BA	1325	U
54	BA	1326	U
54	BA	1327	A
54	BA	1341	G
54	BA	1342	A
54	BA	1350	C
54	BA	1365	A
54	BA	1379	U
54	BA	1385	A
54	BA	1388	G
54	BA	1390	U
54	BA	1396	U
54	BA	1416	G
54	BA	1417	C
54	BA	1419	A
54	BA	1420	A
54	BA	1428	C
54	BA	1440	U
54	BA	1452	G
54	BA	1454	C
54	BA	1455	G
54	BA	1458	U
54	BA	1459	G

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Mol	Chain	Res	Type
54	BA	1461	C
54	BA	1468	U
54	BA	1482	G
54	BA	1487	U
54	BA	1490	A
54	BA	1493	C
54	BA	1523	U
54	BA	1528	A
54	BA	1535	A
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1540	G
54	BA	1549	A
54	BA	1552	A
54	BA	1553	A
54	BA	1566	A
54	BA	1569	A
54	BA	1584	U
54	BA	1607	C
54	BA	1608	A
54	BA	1609	A
54	BA	1610	A
54	BA	1611	C
54	BA	1616	A
54	BA	1618	A
54	BA	1639	C
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1651	G
54	BA	1652	A
54	BA	1654	A
54	BA	1663	G
54	BA	1670	C
54	BA	1674	G
54	BA	1675	C
54	BA	1684	G
54	BA	1714	U
54	BA	1730	C
54	BA	1732	C
54	BA	1758	U

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Mol	Chain	Res	Type
54	BA	1761	C
54	BA	1764	C
54	BA	1773	A
54	BA	1779	U
54	BA	1782	U
54	BA	1784	A
54	BA	1800	C
54	BA	1801	A
54	BA	1808	A
54	BA	1810	A
54	BA	1815	A
54	BA	1816	C
54	BA	1821	A
54	BA	1834	U
54	BA	1835	G
54	BA	1847	A
54	BA	1848	A
54	BA	1855	U
54	BA	1873	G
54	BA	1906	G
54	BA	1912	A
54	BA	1914	C
54	BA	1929	G
54	BA	1937	A
54	BA	1938	A
54	BA	1939	U
54	BA	1940	U
54	BA	1945	G
54	BA	1953	A
54	BA	1955	U
54	BA	1956	U
54	BA	1962	C
54	BA	1963	U
54	BA	1964	G
54	BA	1966	A
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1981	A
54	BA	1982	U
54	BA	1993	U
54	BA	1997	C

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Mol	Chain	Res	Type
54	BA	2005	A
54	BA	2021	C
54	BA	2022	U
54	BA	2023	C
54	BA	2030	A
54	BA	2031	A
54	BA	2032	G
54	BA	2035	G
54	BA	2043	C
54	BA	2052	A
54	BA	2059	A
54	BA	2060	A
54	BA	2061	G
54	BA	2069	G
54	BA	2073	C
54	BA	2076	U
54	BA	2092	U
54	BA	2095	A
54	BA	2109	U
54	BA	2112	G
54	BA	2113	U
54	BA	2114	A
54	BA	2117	A
54	BA	2118	U
54	BA	2126	A
54	BA	2127	G
54	BA	2133	G
54	BA	2155	U
54	BA	2157	G
54	BA	2159	G
54	BA	2160	C
54	BA	2169	A
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2192	U
54	BA	2194	U
54	BA	2196	C
54	BA	2197	U
54	BA	2199	A
54	BA	2213	U
54	BA	2224	G

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Mol	Chain	Res	Type
54	BA	2225	A
54	BA	2230	G
54	BA	2238	G
54	BA	2239	G
54	BA	2246	G
54	BA	2251	G
54	BA	2267	A
54	BA	2268	A
54	BA	2269	G
54	BA	2283	C
54	BA	2296	U
54	BA	2297	A
54	BA	2308	G
54	BA	2309	A
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2334	U
54	BA	2335	A
54	BA	2347	C
54	BA	2361	G
54	BA	2383	G
54	BA	2385	C
54	BA	2403	C
54	BA	2406	A
54	BA	2407	A
54	BA	2419	U
54	BA	2425	A
54	BA	2427	C
54	BA	2428	G
54	BA	2429	G
54	BA	2430	A
54	BA	2432	A
54	BA	2433	A
54	BA	2441	U
54	BA	2448	A
54	BA	2452	C
54	BA	2455	G
54	BA	2473	U
54	BA	2488	G
54	BA	2491	U

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Mol	Chain	Res	Type
54	BA	2492	U
54	BA	2496	C
54	BA	2498	C
54	BA	2499	C
54	BA	2500	U
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2504	U
54	BA	2505	G
54	BA	2518	A
54	BA	2525	G
54	BA	2531	A
54	BA	2532	G
54	BA	2540	C
54	BA	2547	A
54	BA	2553	G
54	BA	2554	U
54	BA	2556	C
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2573	C
54	BA	2576	G
54	BA	2577	A
54	BA	2602	A
54	BA	2603	G
54	BA	2606	C
54	BA	2609	U
54	BA	2614	A
54	BA	2625	G
54	BA	2626	C
54	BA	2628	C
54	BA	2660	A
54	BA	2661	G
54	BA	2669	G
54	BA	2682	A
54	BA	2683	C
54	BA	2716	C
54	BA	2726	A
54	BA	2732	G
54	BA	2751	G

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Mol	Chain	Res	Type
54	BA	2755	C
54	BA	2756	U
54	BA	2765	A
54	BA	2766	A
54	BA	2777	G
54	BA	2778	A
54	BA	2780	G
54	BA	2797	U
54	BA	2808	G
54	BA	2816	G
54	BA	2817	U
54	BA	2821	A
54	BA	2830	C
54	BA	2833	U
54	BA	2850	A
54	BA	2858	C
54	BA	2859	G
54	BA	2884	U
54	BA	2894	G
54	BA	2895	G
55	BB	9	G
55	BB	13	G
55	BB	15	A
55	BB	25	U
55	BB	35	C
55	BB	42	C
55	BB	44	G
55	BB	45	A
55	BB	53	A
55	BB	64	G
55	BB	90	C
55	BB	109	A

All (241) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	60	A
21	AA	64	G
21	AA	65	A
21	AA	66	A
21	AA	70	U

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Mol	Chain	Res	Type
21	AA	172	A
21	AA	181	A
21	AA	190	A
21	AA	238	A
21	AA	244	U
21	AA	245	U
21	AA	246	A
21	AA	251	G
21	AA	281	G
21	AA	308	C
21	AA	320	A
21	AA	328	C
21	AA	343	U
21	AA	344	A
21	AA	346	G
21	AA	354	G
21	AA	357	G
21	AA	412	A
21	AA	448	A
21	AA	451	A
21	AA	481	G
21	AA	500	G
21	AA	505	G
21	AA	509	A
21	AA	532	A
21	AA	534	U
21	AA	571	U
21	AA	574	A
21	AA	575	G
21	AA	619	U
21	AA	632	U
21	AA	653	U
21	AA	659	U
21	AA	701	U
21	AA	718	A
21	AA	734	G
21	AA	761	G
21	AA	764	C
21	AA	777	A
21	AA	793	U
21	AA	818	G
21	AA	827	U

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Mol	Chain	Res	Type
21	AA	884	U
21	AA	913	A
21	AA	933	G
21	AA	960	U
21	AA	978	A
21	AA	1043	G
21	AA	1049	U
21	AA	1053	G
21	AA	1078	U
21	AA	1101	A
21	AA	1129	C
21	AA	1159	U
21	AA	1167	A
21	AA	1190	G
21	AA	1201	A
21	AA	1211	U
21	AA	1212	U
21	AA	1222	G
21	AA	1225	A
21	AA	1280	A
21	AA	1298	U
21	AA	1308	U
21	AA	1347	G
21	AA	1430	A
21	AA	1432	G
21	AA	1445	U
21	AA	1452	C
21	AA	1493	A
21	AA	1533	C
22	A1	1	G
22	A1	10	G
22	A1	32	C
22	A1	47	U
22	A1	61	C
22	A1	75	C
23	A2	81	U
23	A2	91	A
24	A3	9	G
24	A3	31	G
24	A3	47	G
24	A3	56	PSU
24	A3	69	C

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Mol	Chain	Res	Type
24	A3	75	C
24	A3	76	C
54	BA	33	C
54	BA	62	U
54	BA	74	A
54	BA	91	A
54	BA	118	A
54	BA	125	A
54	BA	143	C
54	BA	160	A
54	BA	196	A
54	BA	199	A
54	BA	215	G
54	BA	228	C
54	BA	247	G
54	BA	249	C
54	BA	278	A
54	BA	323	C
54	BA	329	G
54	BA	330	A
54	BA	345	A
54	BA	369	U
54	BA	372	G
54	BA	386	G
54	BA	421	C
54	BA	449	A
54	BA	476	G
54	BA	481	G
54	BA	526	A
54	BA	527	C
54	BA	530	G
54	BA	531	C
54	BA	532	A
54	BA	613	A
54	BA	659	G
54	BA	670	A
54	BA	750	A
54	BA	762	U
54	BA	775	G
54	BA	791	C
54	BA	809	G
54	BA	829	A

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Mol	Chain	Res	Type
54	BA	887	U
54	BA	988	A
54	BA	1069	A
54	BA	1086	A
54	BA	1087	G
54	BA	1089	A
54	BA	1128	G
54	BA	1143	A
54	BA	1206	G
54	BA	1210	G
54	BA	1224	U
54	BA	1236	G
54	BA	1254	A
54	BA	1273	U
54	BA	1288	G
54	BA	1300	G
54	BA	1312	U
54	BA	1325	U
54	BA	1340	U
54	BA	1397	U
54	BA	1427	A
54	BA	1451	C
54	BA	1458	U
54	BA	1509	A
54	BA	1597	A
54	BA	1608	A
54	BA	1609	A
54	BA	1610	A
54	BA	1617	C
54	BA	1618	A
54	BA	1674	G
54	BA	1713	A
54	BA	1731	G
54	BA	1800	C
54	BA	1834	U
54	BA	1847	A
54	BA	1857	G
54	BA	1913	A
54	BA	1936	A
54	BA	1937	A
54	BA	1945	G
54	BA	1952	A

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Mol	Chain	Res	Type
54	BA	1955	U
54	BA	1963	U
54	BA	1970	A
54	BA	1971	U
54	BA	1980	G
54	BA	1981	A
54	BA	2020	A
54	BA	2021	C
54	BA	2035	G
54	BA	2060	A
54	BA	2076	U
54	BA	2086	U
54	BA	2112	G
54	BA	2113	U
54	BA	2117	A
54	BA	2118	U
54	BA	2157	G
54	BA	2163	A
54	BA	2172	U
54	BA	2180	U
54	BA	2191	A
54	BA	2197	U
54	BA	2213	U
54	BA	2225	A
54	BA	2229	U
54	BA	2245	U
54	BA	2250	G
54	BA	2267	A
54	BA	2282	G
54	BA	2286	G
54	BA	2296	U
54	BA	2307	G
54	BA	2308	G
54	BA	2360	G
54	BA	2389	G
54	BA	2391	G
54	BA	2406	A
54	BA	2418	A
54	BA	2427	C
54	BA	2429	G
54	BA	2487	G
54	BA	2498	C

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Mol	Chain	Res	Type
54	BA	2500	U
54	BA	2503	A
54	BA	2504	U
54	BA	2531	A
54	BA	2553	G
54	BA	2563	U
54	BA	2565	A
54	BA	2576	G
54	BA	2581	G
54	BA	2585	U
54	BA	2602	A
54	BA	2605	U
54	BA	2625	G
54	BA	2668	G
54	BA	2681	C
54	BA	2682	A
54	BA	2689	U
54	BA	2751	G
54	BA	2755	C
54	BA	2780	G
54	BA	2858	C
54	BA	2887	A
55	BB	12	C
55	BB	15	A
55	BB	63	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	4SU	A1	7	22	18,21,22	1.45	2 (11%)	26,30,33	1.05	1 (3%)
22	5MU	A1	54	22	19,22,23	0.85	0	28,32,35	1.53	4 (14%)

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	5.20	1 (4%)	29,39,42	1.48	2 (6%)
24	PSU	A3	56	24	18,21,22	1.12	2 (11%)	22,30,33	1.44	3 (13%)
22	PSU	A1	55	22	18,21,22	1.02	1 (5%)	22,30,33	1.08	1 (4%)
24	4SU	A3	8	24	18,21,22	1.43	1 (5%)	26,30,33	0.77	1 (3%)
24	OMC	A3	33	24	19,22,23	0.91	0	26,31,34	0.96	1 (3%)
24	5MU	A3	55	24	19,22,23	0.87	0	28,32,35	1.66	5 (17%)
22	6MZ	A1	37	22	18,25,26	1.16	2 (11%)	16,36,39	1.57	2 (12%)
22	CM0	A1	34	22,23	22,26,27	1.55	1 (4%)	28,37,40	1.14	2 (7%)
24	H2U	A3	21	24	18,21,22	1.42	3 (16%)	21,30,33	1.08	2 (9%)

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	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
22	5MU	A1	54	22	-	0/7/25/26	0/2/2/2
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2
22	PSU	A1	55	22	-	2/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/7/25/26	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	CM0	A1	34	22,23	-	2/12/30/31	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-24.09	1.32	1.46
22	A1	34	CM0	O5-C5	-5.83	1.23	1.36
24	A3	8	4SU	C5-C4	-4.94	1.36	1.42
22	A1	7	4SU	C5-C4	-4.90	1.36	1.42
24	A3	21	H2U	C2-N3	-3.69	1.31	1.38
24	A3	21	H2U	C4-N3	-3.17	1.32	1.37
24	A3	56	PSU	O4'-C1'	-2.97	1.39	1.43
24	A3	21	H2U	O4'-C4'	-2.60	1.39	1.45
22	A1	37	6MZ	C2'-C1'	-2.36	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	7	4SU	C4-S4	-2.34	1.63	1.68
22	A1	37	6MZ	C8-N7	-2.32	1.30	1.34
22	A1	55	PSU	O4'-C1'	-2.28	1.40	1.43
24	A3	56	PSU	O4'-C4'	-2.02	1.40	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	46	7MG	N9-C8-N7	6.20	112.24	103.38
22	A1	37	6MZ	C9-N6-C6	4.97	127.15	122.87
24	A3	55	5MU	C5M-C5-C6	-4.33	117.06	122.85
22	A1	54	5MU	C5M-C5-C6	-3.95	117.57	122.85
24	A3	56	PSU	C6-C5-C4	3.95	120.96	118.20
24	A3	55	5MU	C6-C5-C4	3.20	120.71	118.03
24	A3	55	5MU	C5M-C5-C4	3.14	122.23	118.77
24	A3	55	5MU	C5-C6-N1	-3.03	120.22	123.34
22	A1	54	5MU	C6-C5-C4	2.96	120.50	118.03
22	A1	54	5MU	C5M-C5-C4	2.87	121.92	118.77
22	A1	7	4SU	C6-C5-C4	2.82	122.39	119.95
24	A3	33	OMC	O2-C2-N3	-2.73	117.89	122.33
22	A1	55	PSU	C6-C5-C4	2.67	120.06	118.20
22	A1	54	5MU	C5-C6-N1	-2.66	120.60	123.34
22	A1	34	CM0	C7-O5-C5	2.58	120.95	117.58
24	A3	56	PSU	N1-C2-N3	2.53	118.00	115.13
22	A1	37	6MZ	C2-N1-C6	2.52	118.75	116.59
24	A3	21	H2U	C5-C4-N3	2.50	119.45	116.65
22	A1	34	CM0	N3-C2-N1	2.27	117.90	114.89
24	A3	56	PSU	O4'-C1'-C2'	2.25	108.32	105.14
24	A3	55	5MU	O4-C4-C5	2.25	127.51	124.90
24	A3	8	4SU	C6-C5-C4	2.22	121.87	119.95
22	A1	46	7MG	N2-C2-N3	-2.04	115.76	119.73
24	A3	21	H2U	N3-C2-N1	2.04	118.81	116.65

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	34	CM0	O5-C7-C8-O9
22	A1	34	CM0	O5-C7-C8-O8
22	A1	55	PSU	O4'-C1'-C5-C4
22	A1	55	PSU	O4'-C1'-C5-C6
22	A1	46	7MG	C3'-C4'-C5'-O5'

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	VAL	A1	101	22,58	4,6,7	0.78	0	6,7,9	1.19	1 (16%)
58	FME	BA	3001	57	8,9,10	0.49	0	7,9,11	1.29	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	VAL	A1	101	22,58	-	4/5/6/8	-
58	FME	BA	3001	57	-	0/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	A1	101	VAL	O-C-CA	-2.61	117.93	124.78
58	BA	3001	FME	C-CA-N	2.24	113.78	109.73
58	BA	3001	FME	O-C-CA	-2.13	119.20	124.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A1	101	VAL	N-CA-CB-CG2
57	A1	101	VAL	C-CA-CB-CG1
57	A1	101	VAL	C-CA-CB-CG2
57	A1	101	VAL	N-CA-CB-CG1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

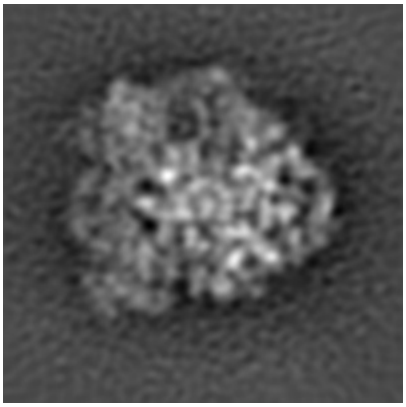
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1716. These allow visual inspection of the internal detail of the map and identification of artifacts.

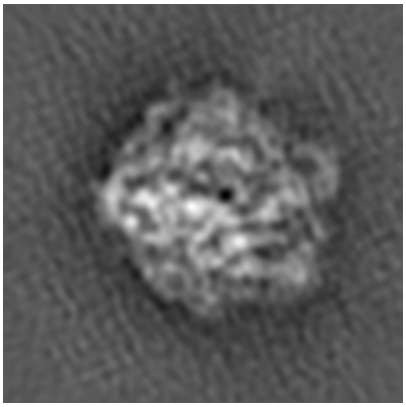
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

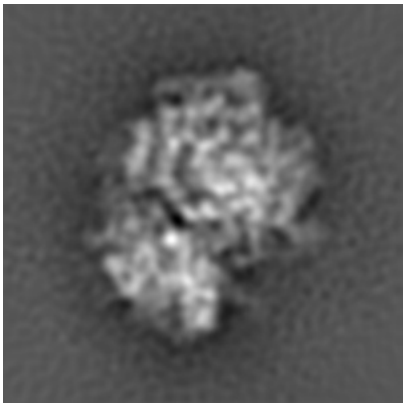
6.1.1 Primary map



X



Y

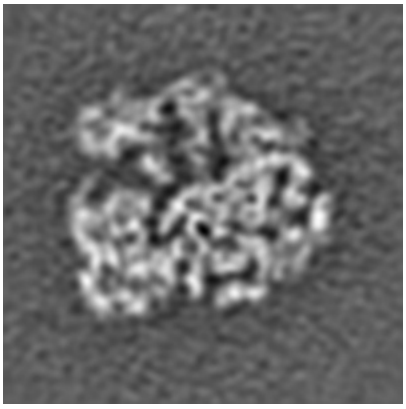


Z

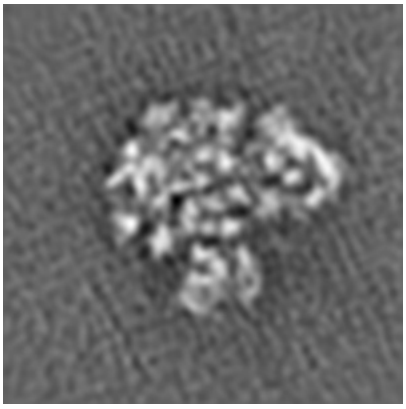
The images above show the map projected in three orthogonal directions.

6.2 Central slices

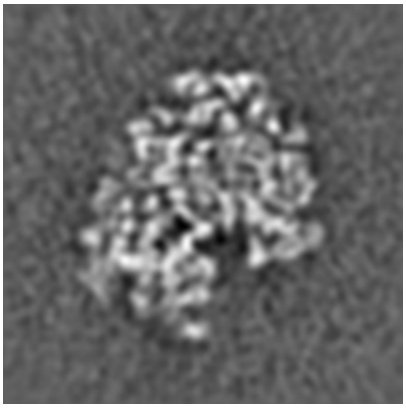
6.2.1 Primary map



X Index: 96



Y Index: 96

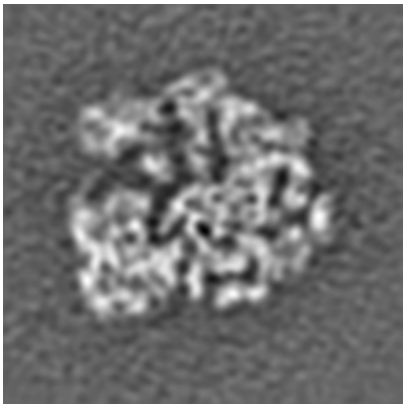


Z Index: 96

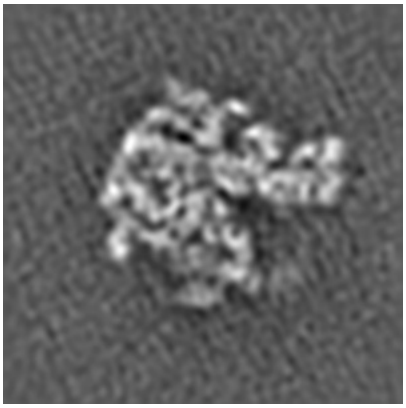
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 97



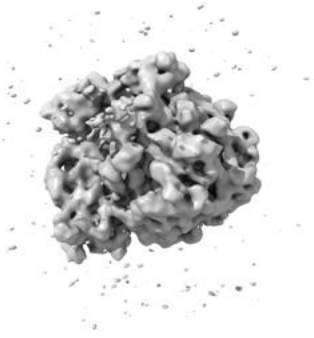
Y Index: 104

Z Index: 91

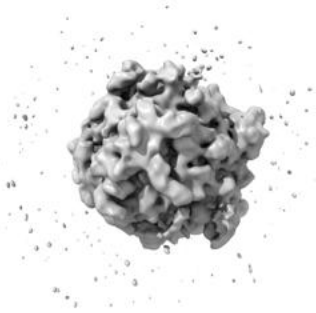
The images above show the largest variance slices of the map in three orthogonal directions.

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 30.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

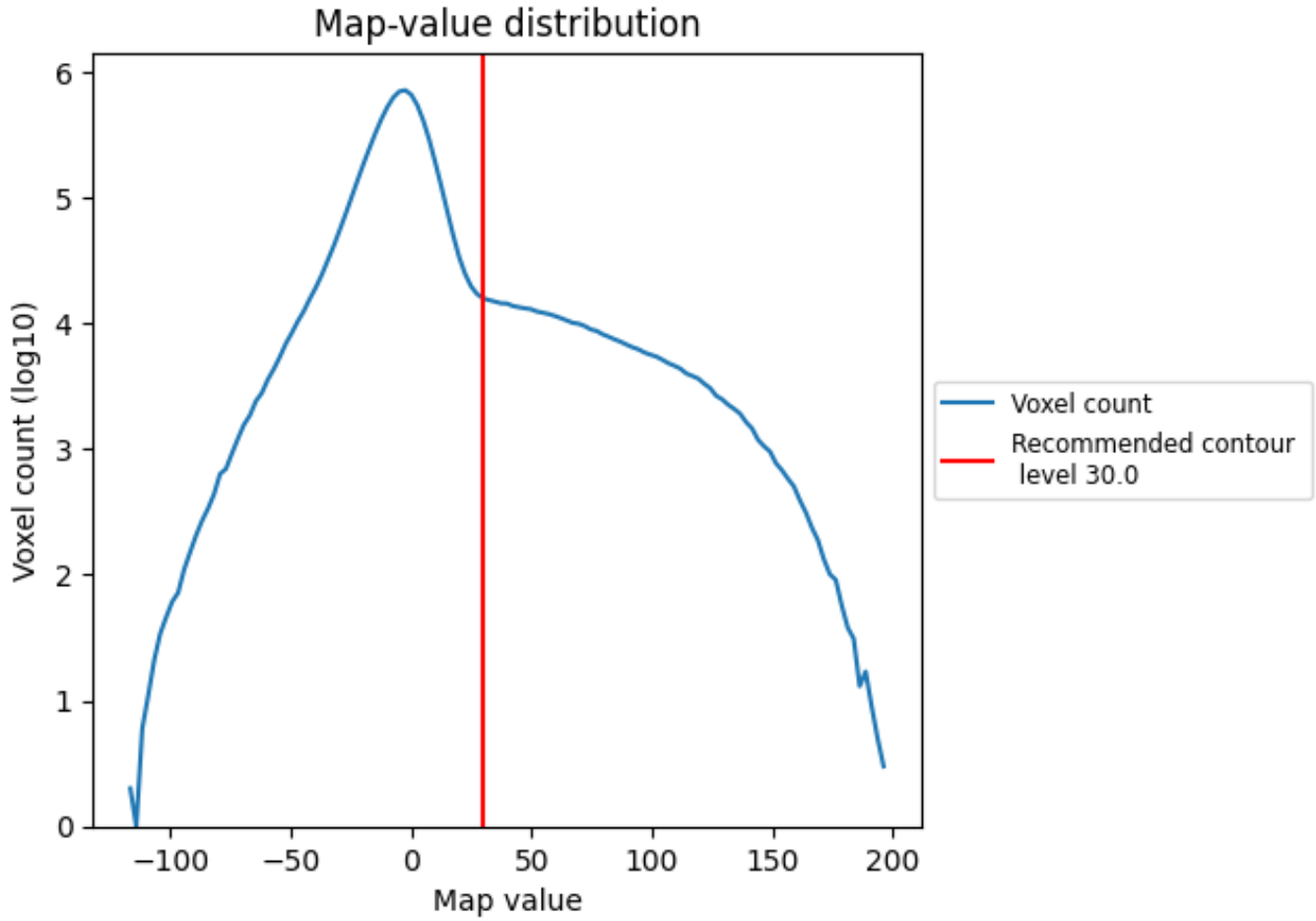
6.5 Mask visualisation (i)

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

7 Map analysis

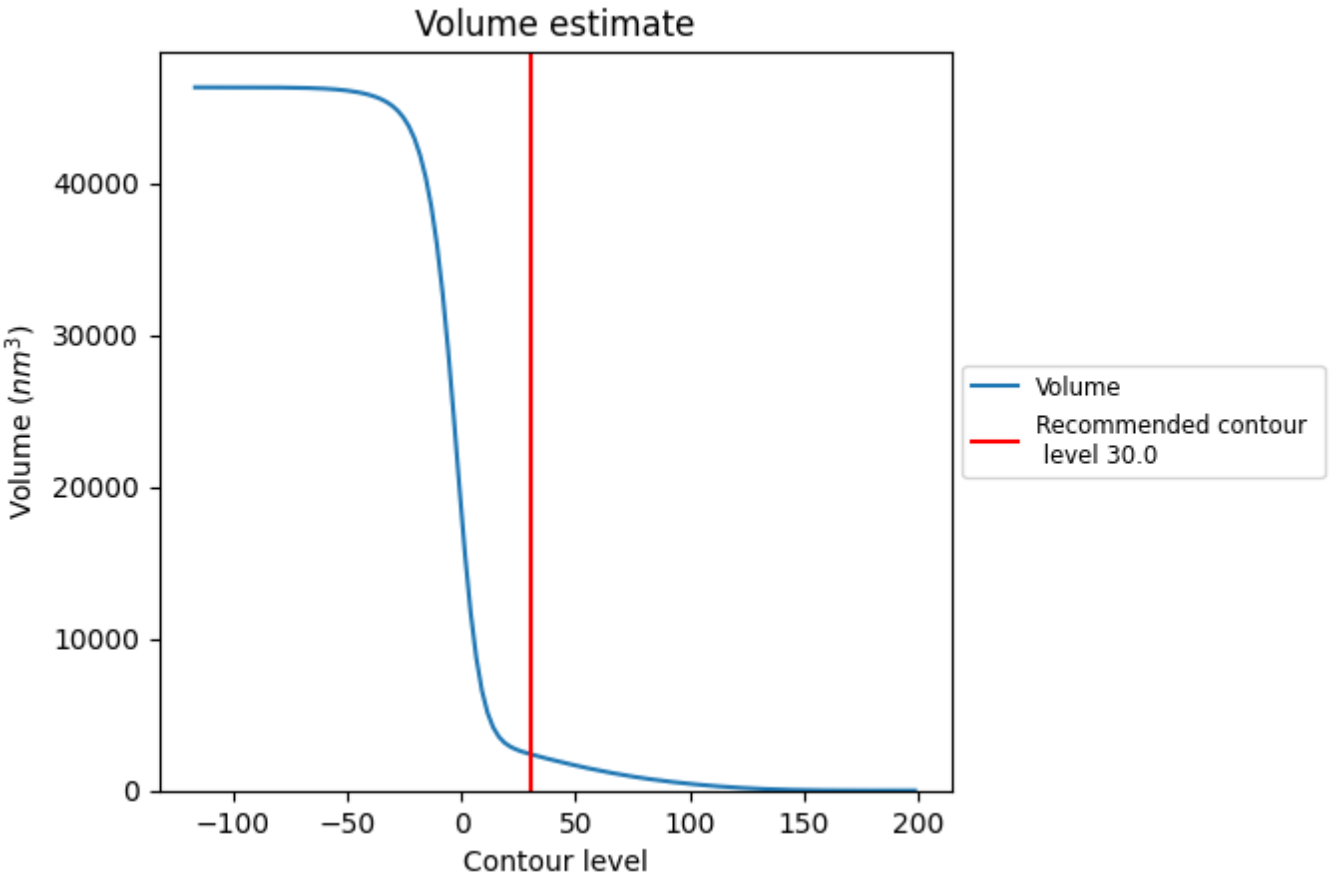
This section contains the results of statistical analysis of the map.

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.

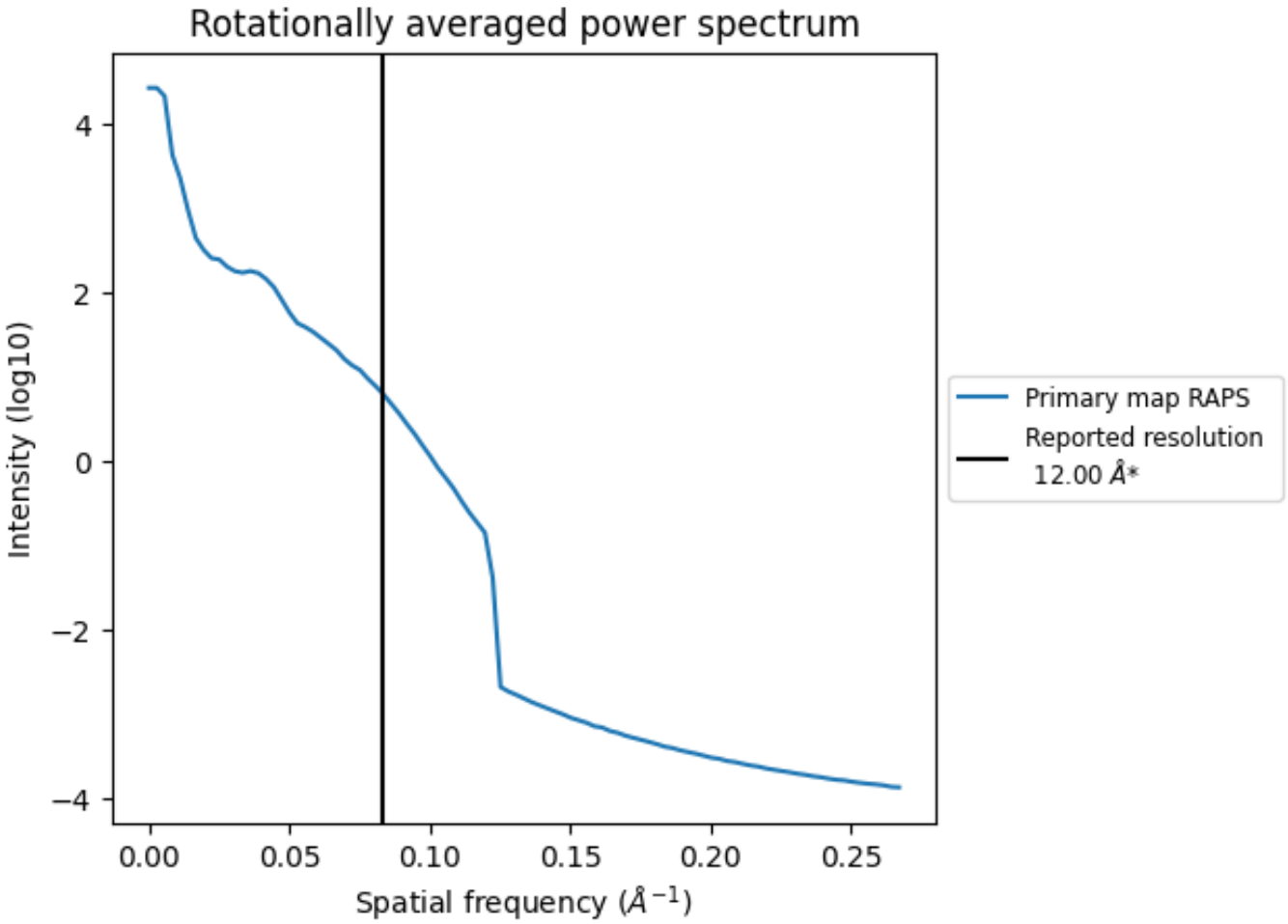
7.2 Volume estimate



The volume at the recommended contour level is 2406 nm^3; this corresponds to an approximate mass of 2173 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 0.083 Å^{-1}

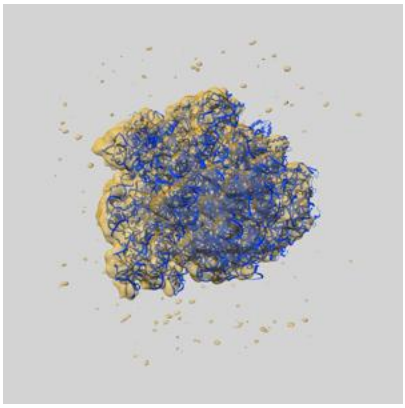
8 Fourier-Shell correlation

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

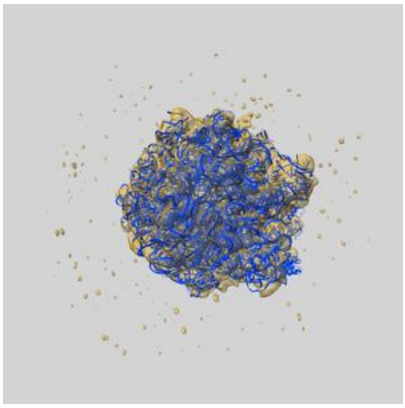
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1716 and PDB model 4V6Y. Per-residue inclusion information can be found in section 3 on page 17.

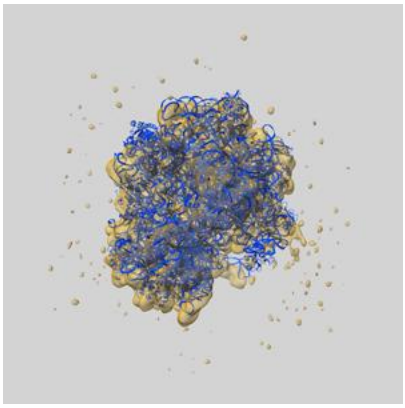
9.1 Map-model overlay



X



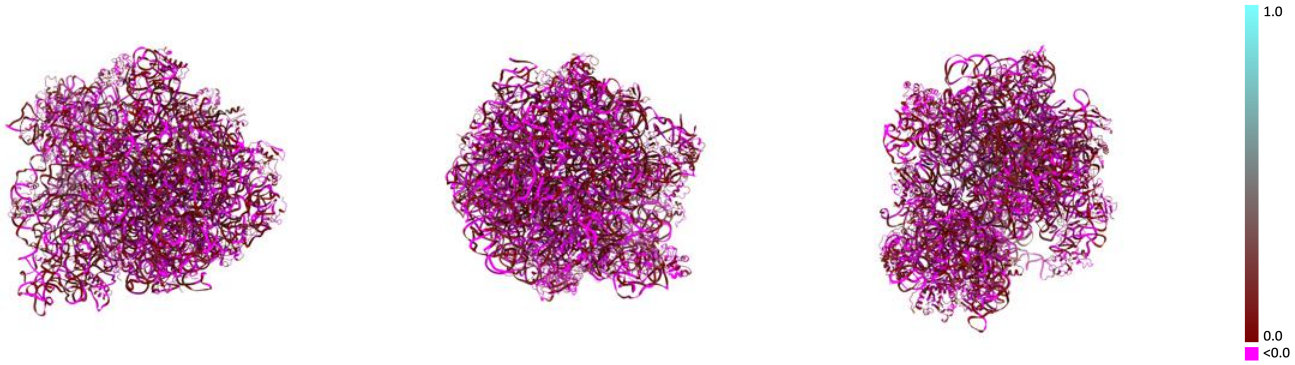
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 30.0 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.

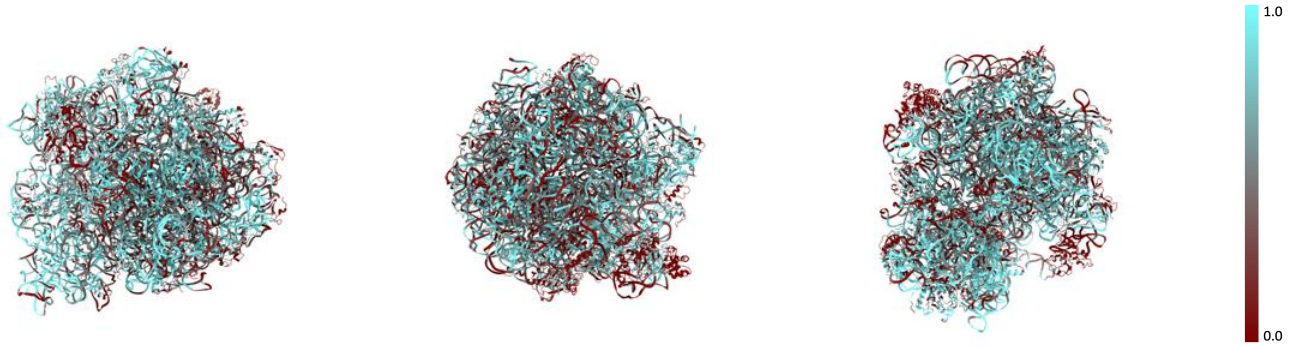
9.2 Q-score mapped to coordinate model



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.

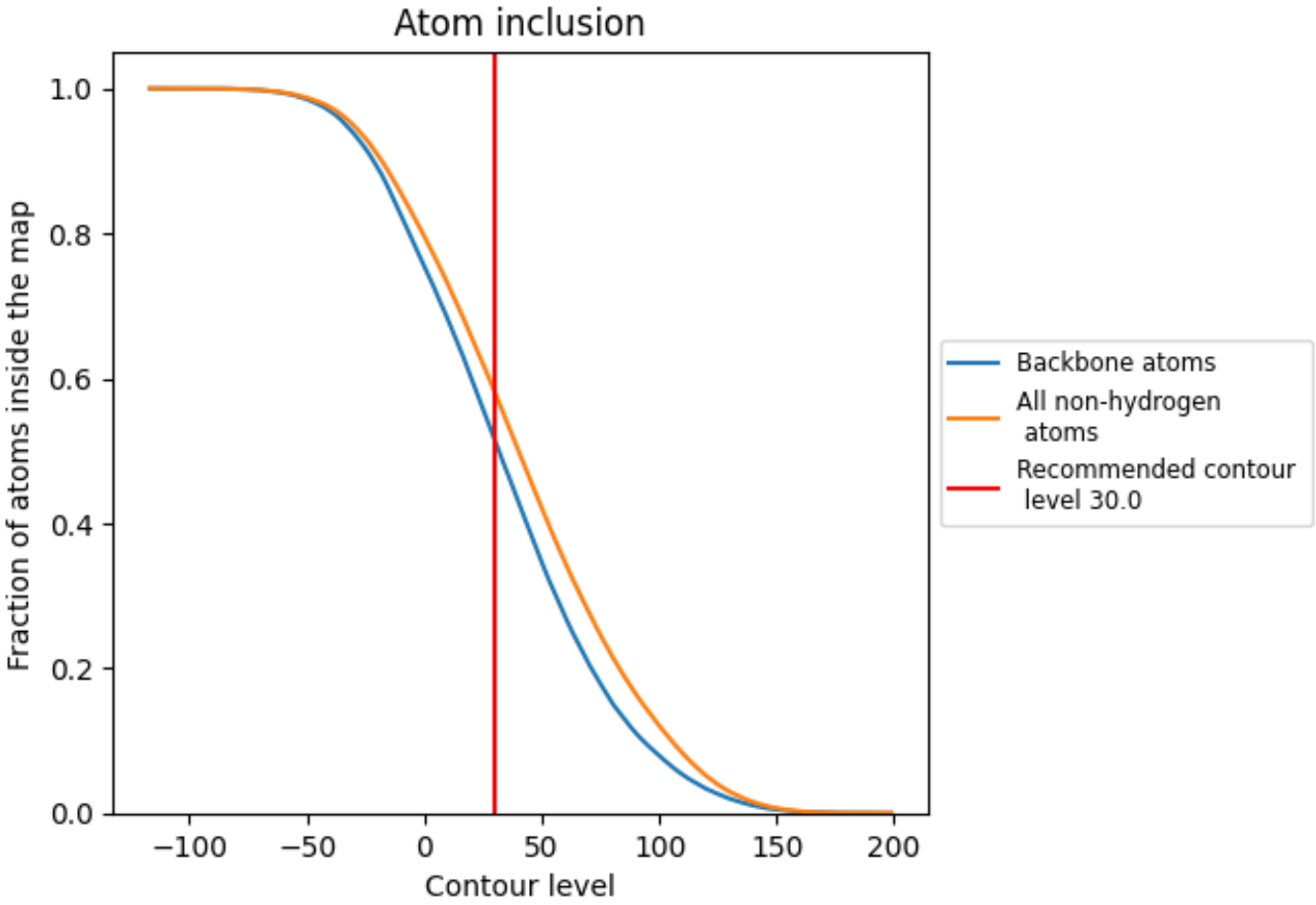
9.3 Atom inclusion mapped to coordinate model



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 (30.0).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 58% 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 (30.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5809	0.0180
A1	0.4192	-0.0110
A2	0.4078	-0.0330
A3	0.5177	0.0450
AA	0.6384	0.0190
AB	0.4785	0.0280
AC	0.6124	0.0150
AD	0.5094	-0.0070
AE	0.5488	0.0080
AF	0.3601	0.0060
AG	0.4307	0.0070
AH	0.7115	0.0430
AI	0.4730	-0.0040
AJ	0.5602	-0.0110
AK	0.5731	0.0230
AL	0.4137	-0.0070
AM	0.4438	0.0150
AN	0.6809	0.0190
AO	0.5087	0.0310
AP	0.6823	0.0440
AQ	0.5228	0.0340
AR	0.4692	0.0080
AS	0.5449	0.0160
AT	0.5951	0.0300
AU	0.6284	0.0620
B0	0.3528	-0.0110
B1	0.5891	0.0570
B2	0.3380	-0.0510
B3	0.3910	-0.0420
B4	0.5719	0.0110
B5	0.0570	-0.0090
BA	0.6258	0.0230
BB	0.6953	0.0270
BC	0.4427	-0.0250
BD	0.6047	0.0180

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Chain	Atom inclusion	Q-score
BE	0.4967	0.0200
BF	0.5647	0.0200
BG	0.4603	-0.0100
BH	0.1378	-0.0170
BI	0.0323	0.0000
BJ	0.5936	0.0040
BK	0.4420	0.0060
BL	0.3996	0.0080
BM	0.5537	0.0130
BN	0.4756	-0.0090
BO	0.6744	0.0450
BP	0.5845	0.0210
BQ	0.5551	-0.0030
BR	0.4956	0.0310
BS	0.4438	0.0030
BT	0.5173	0.0120
BU	0.4688	0.0280
BV	0.5745	0.0250
BW	0.5412	-0.0020
BX	0.2862	-0.0370
BY	0.3984	0.0120
BZ	0.6499	0.0530