Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 06:40 PM EST

PDB ID	:	4V74
EMDB ID	:	EMD-1720
Title	:	70S-fMetVal-tRNAVal-tRNAfMet complex in hybrid pre-translocation state (pre5b)
Authors	:	Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on	:	2013-10-14
Resolution	:	17.00 Å(reported)
Based on initial models	:	3I1O, 2HGP, 2K4C, 2WRI

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

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

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

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

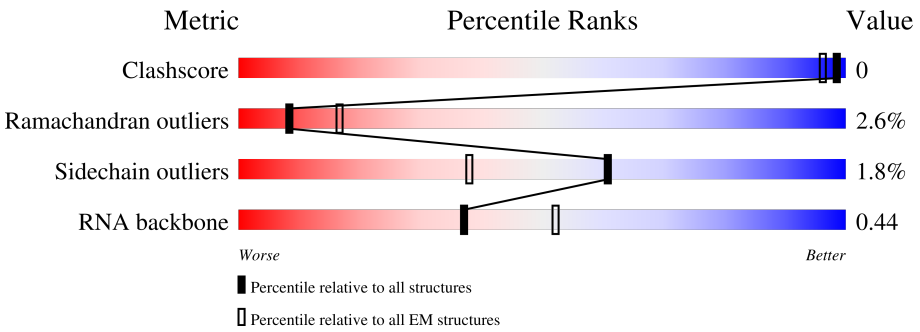
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 17.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	42% 95% 5% •
2	AC	208	51% 89% 10%
3	AD	206	41% 88% 12%
4	AE	152	42% 89% 11% •
5	AF	101	13% 90% 9% •
6	AG	152	23% 87% 12% •
7	AH	130	27% 89% 10% •

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Mol	Chain	Length	Quality of chain
8	AI	128	35% 82% 16%
9	AJ	100	21% 84% 15%
10	AK	118	23% 92% 7%
11	AL	124	31% 83% 15%
12	AM	115	28% 85% 14%
13	AN	101	40% 86% 13%
14	AO	89	6% 85% 13%
15	AP	81	43% 84% 16%
16	AQ	82	34% 91% 9%
17	AR	57	33% 79% 21%
18	AS	81	25% 88% 11%
19	AT	86	24% 93% 7%
20	AU	53	42% 79% 21%
21	AA	1533	12% 25% 49% 22%
22	A1	76	24% 17% 55% 24%
23	A2	15	7% 7% 80% 13%
24	A3	77	19% 22% 52% 25%
25	BC	273	53% 87% 12%
26	BD	209	34% 90% 9%
27	BE	201	32% 91% 9%
28	BF	179	22% 89% 11%
29	BG	177	38% 89% 11%
30	BH	149	85% 95% 5%
31	BI	142	99% 94% 5%
32	BJ	142	28% 90% 10%

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Mol	Chain	Length	Quality of chain
33	BK	123	46% 88% 11%
34	BL	144	33% 85% 13%
35	BM	136	40% 85% 15%
36	BN	121	15% 87% 12%
37	BO	117	14% 87% 11%
38	BP	115	40% 87% 12%
39	BQ	118	36% 84% 15%
40	BR	103	25% 90% 10%
41	BS	110	33% 89% 11%
42	BT	94	21% 85% 15%
43	BU	104	32% 89% 10%
44	BV	94	29% 95% 5%
45	BW	80	44% 82% 14%
46	BX	79	30% 82% 14%
47	BY	63	44% 90% 10%
48	BZ	59	31% 83% 15%
49	B0	57	30% 86% 12%
50	B1	52	25% 94% 6%
51	B2	46	52% 78% 22%
52	B3	65	54% 85% 14%
53	B4	38	34% 87% 13%
54	BA	2903	12% 23% 51% 23%
55	BB	118	6% 25% 51% 21%
56	B5	234	40% 89% 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
			Total	C	N	O	S		
5	AF	101	818	515	149	148	6	0	1

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
			Total	C	N	O	S		
6	AG	152	1178	732	227	215	4	0	1

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
			Total	C	N	O	S		
7	AH	129	979	616	173	184	6	0	0

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

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

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
			Total	C	N	O	S		
9	AJ	100	790	495	151	143	1	0	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
			Total	C	N	O	S		
10	AK	118	880	542	174	161	3	0	0

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
			Total	C	N	O	S		
11	AL	123	955	590	196	165	4	0	0

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

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

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
			Total	C	N	O	S		
13	AN	100	805	499	164	139	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AP	81	639	400	127	111	1	0	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
			Total	C	N	O	S		
16	AQ	82	652	413	122	114	3	0	1

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
			Total	C	N	O		
17	AR	57	459	290	87	82	0	1

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
			Total	C	N	O	S		
18	AS	81	641	410	121	108	2	0	1

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
			Total	C	N	O	S		
19	AT	86	668	413	137	115	3	0	0

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
			Total	C	N	O	S		
20	AU	53	429	267	87	74	1	0	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
			Total	C	N	O	P		
21	AA	1530	32828	14642	6024	10633	1529	0	0

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

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

- 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
			Total	C	N	O	P		
23	A2	15	309	140	46	109	14	0	0

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

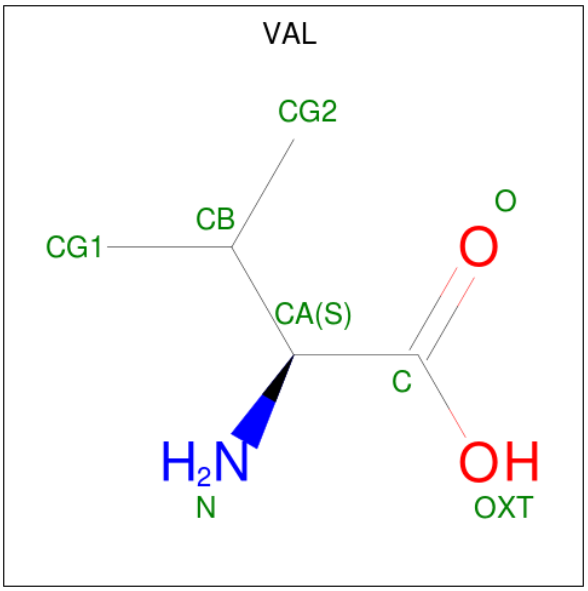
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

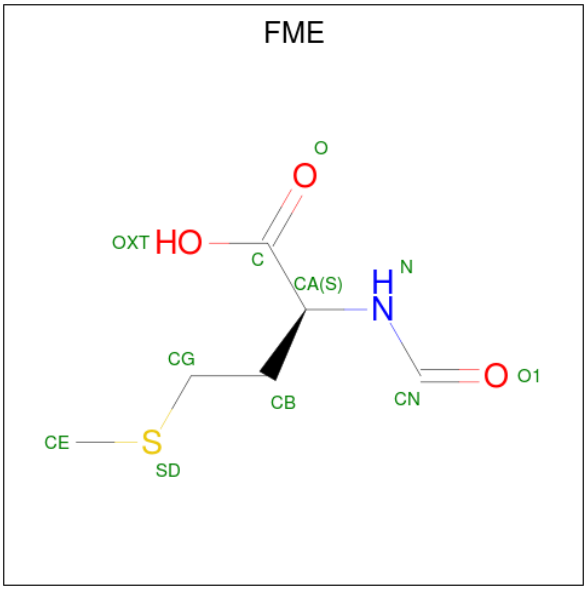
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	B5	223	1658	1038	302	312	6	0	0

- 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: $C_6H_{11}NO_3S$).



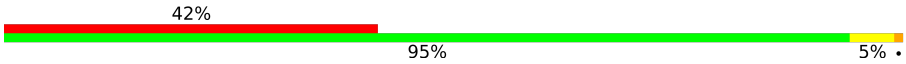
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
58	BA	1	10	6	1	2	1	0

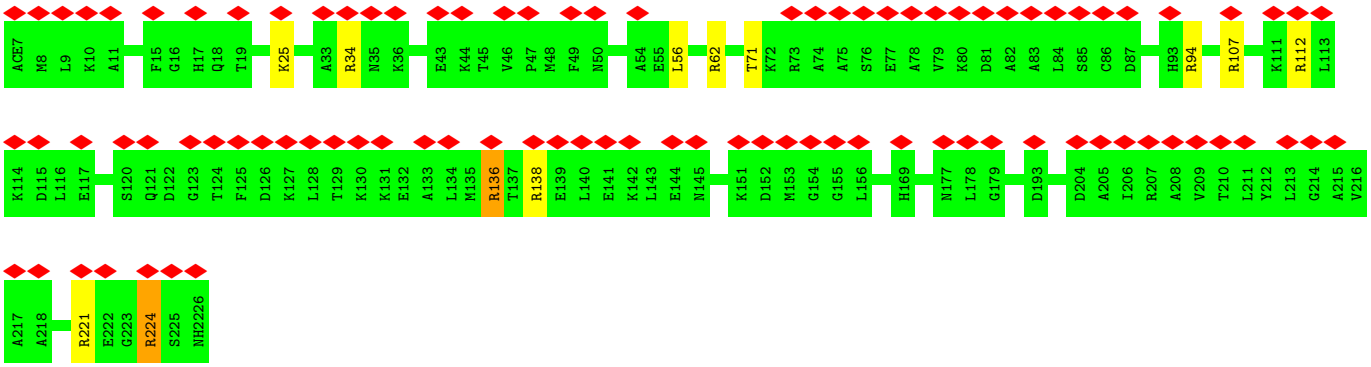
3 Residue-property plots (i)

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

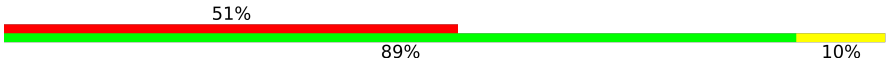
Chain AB:

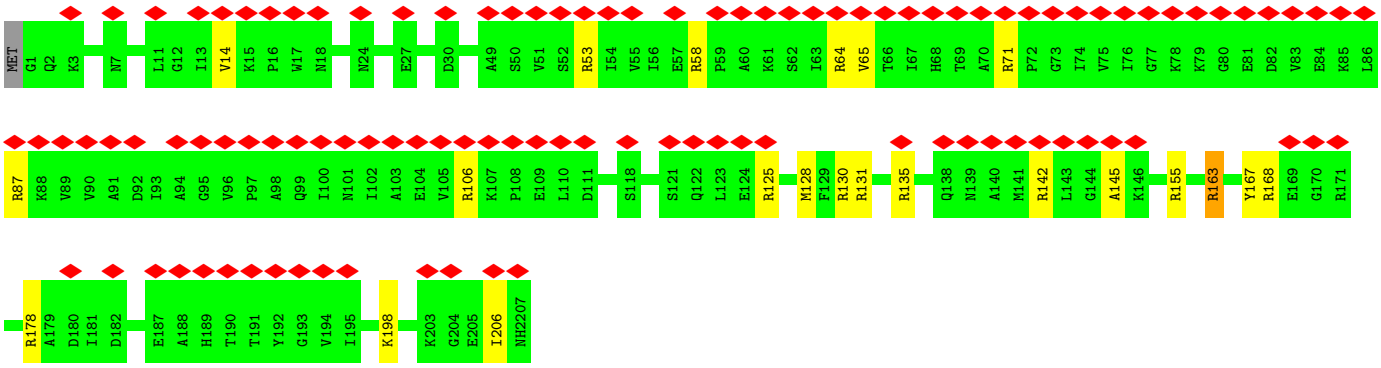




- Molecule 2: 30S ribosomal protein S3

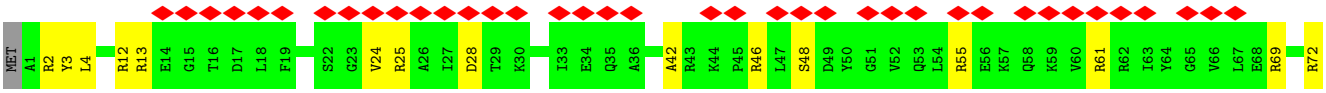
Chain AC:





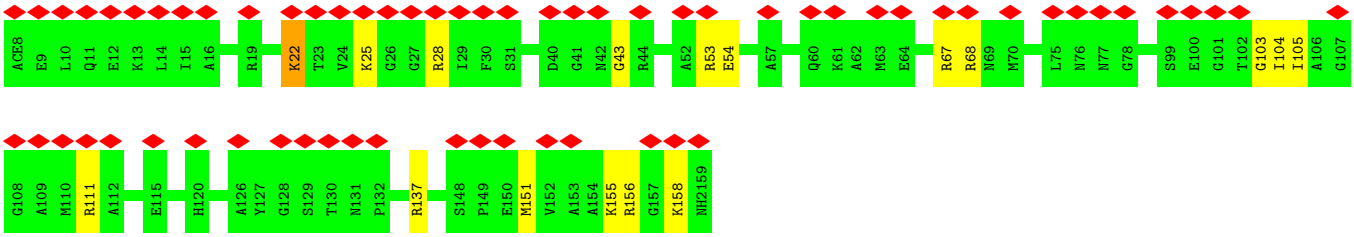
- Molecule 3: 30S ribosomal protein S4

Chain AD:



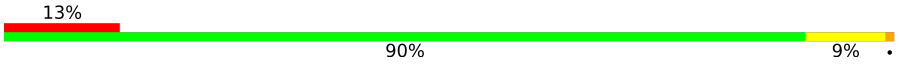
• Molecule 4: 30S ribosomal protein S5

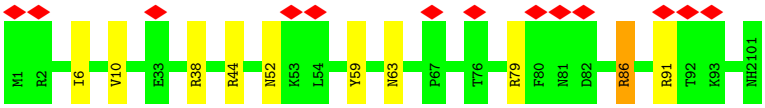
Chain AE:



• Molecule 5: 30S ribosomal protein S6

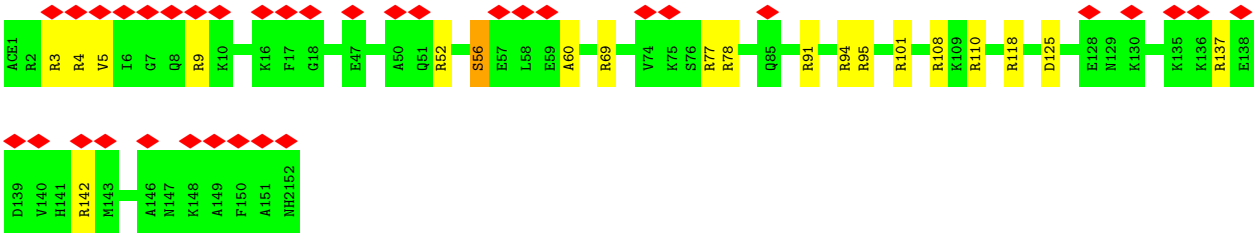
Chain AF:





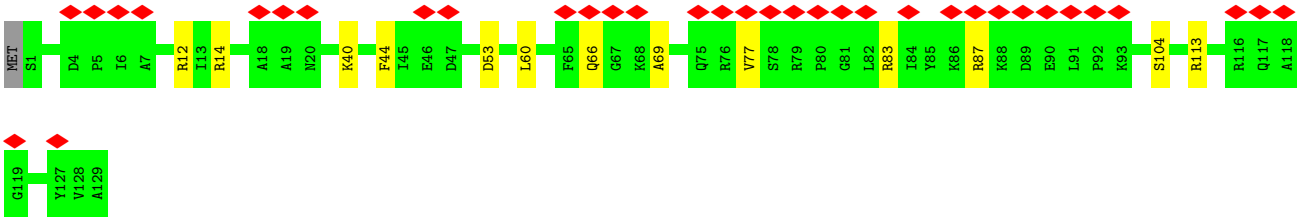
• Molecule 6: 30S ribosomal protein S7

Chain AG:



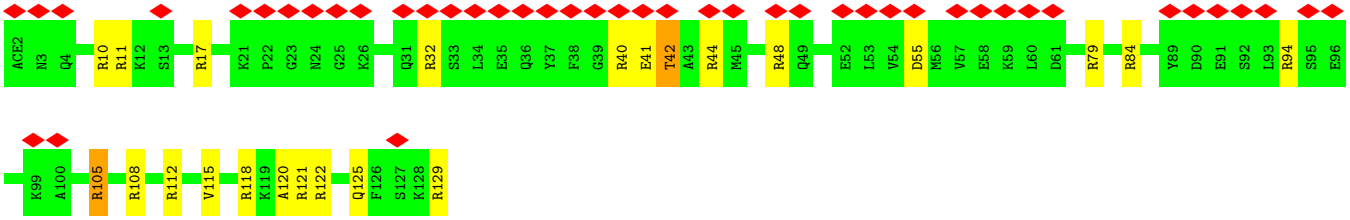
• Molecule 7: 30S ribosomal protein S8

Chain AH:



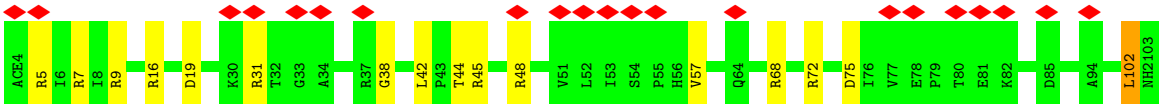
• Molecule 8: 30S ribosomal protein S9

Chain AI:



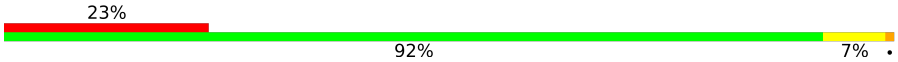
• Molecule 9: 30S ribosomal protein S10

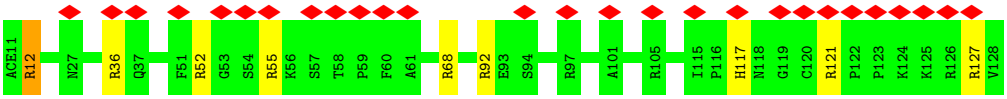
Chain AJ:



• Molecule 10: 30S ribosomal protein S11

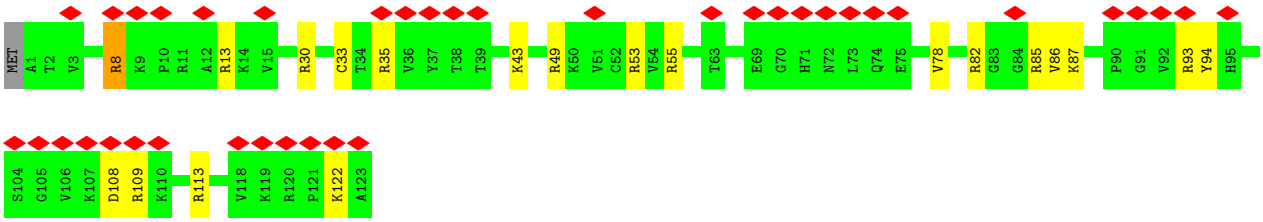
Chain AK:





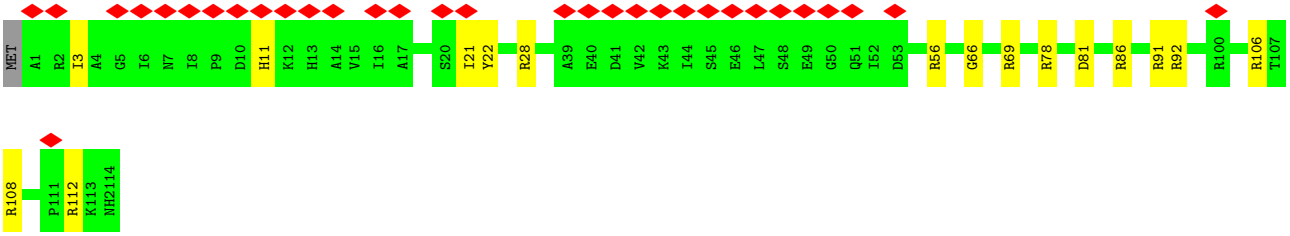
• Molecule 11: 30S ribosomal protein S12

Chain AL:



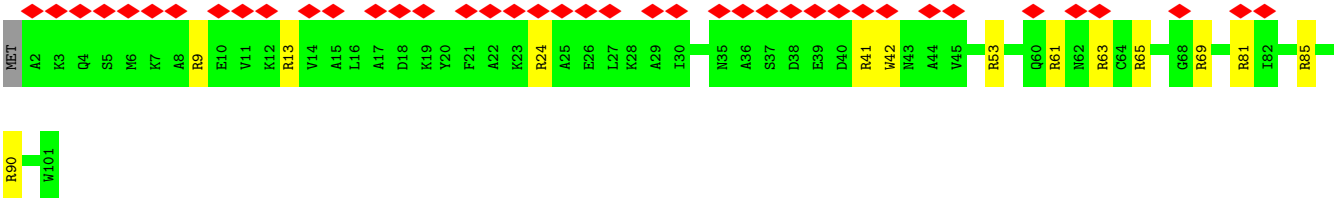
• Molecule 12: 30S ribosomal protein S13

Chain AM:



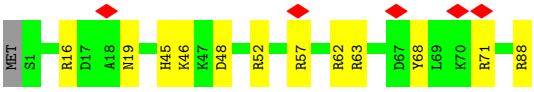
- Molecule 13: 30S ribosomal protein S14

Chain AN:



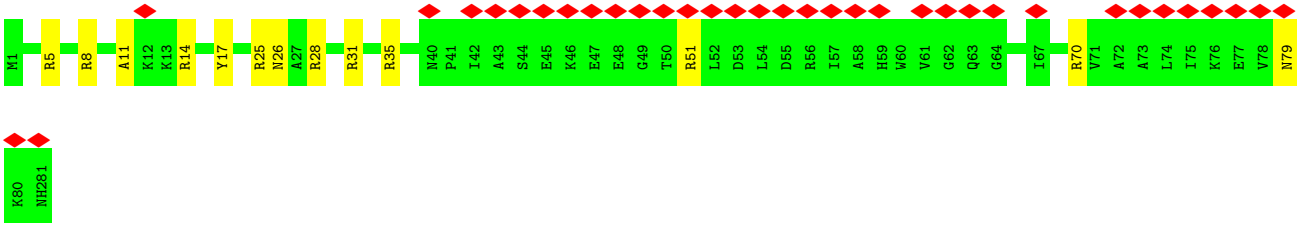
- Molecule 14: 30S ribosomal protein S15

Chain AO:



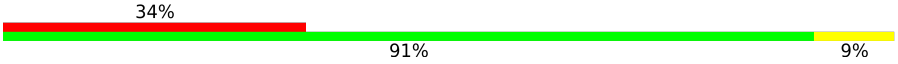
- Molecule 15: 30S ribosomal protein S16

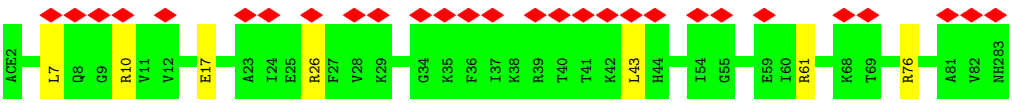
Chain AP:



- Molecule 16: 30S ribosomal protein S17

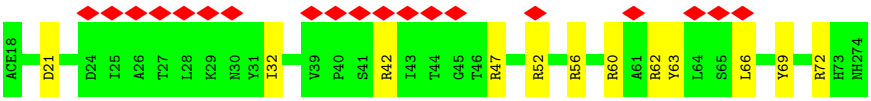
Chain AQ:





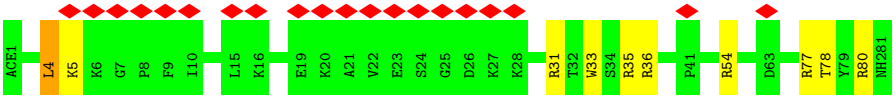
- Molecule 17: 30S ribosomal protein S18

Chain AR:



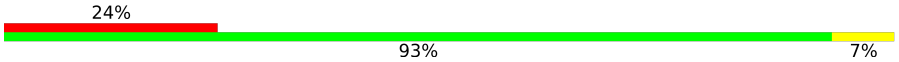
- Molecule 18: 30S ribosomal protein S19

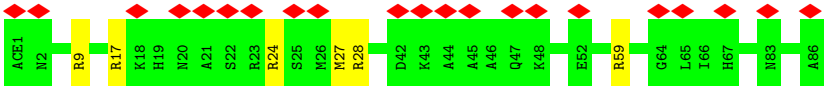
Chain AS:



• Molecule 19: 30S ribosomal protein S20

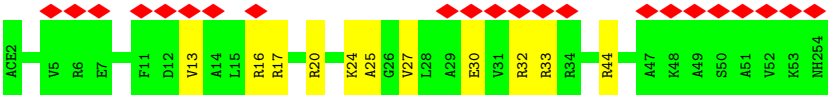
Chain AT:





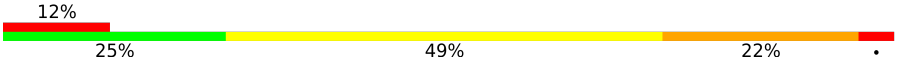
• Molecule 20: 30S ribosomal protein S21

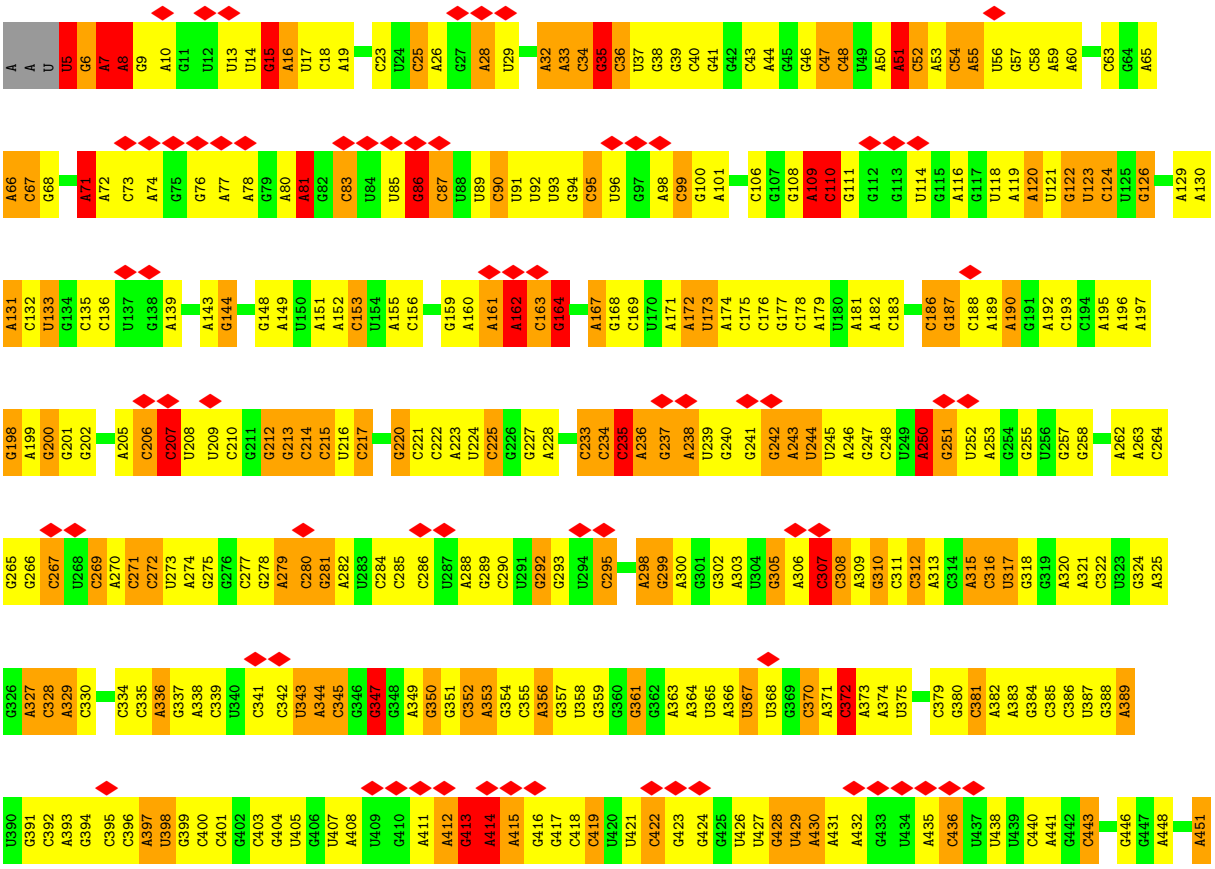
Chain AU:

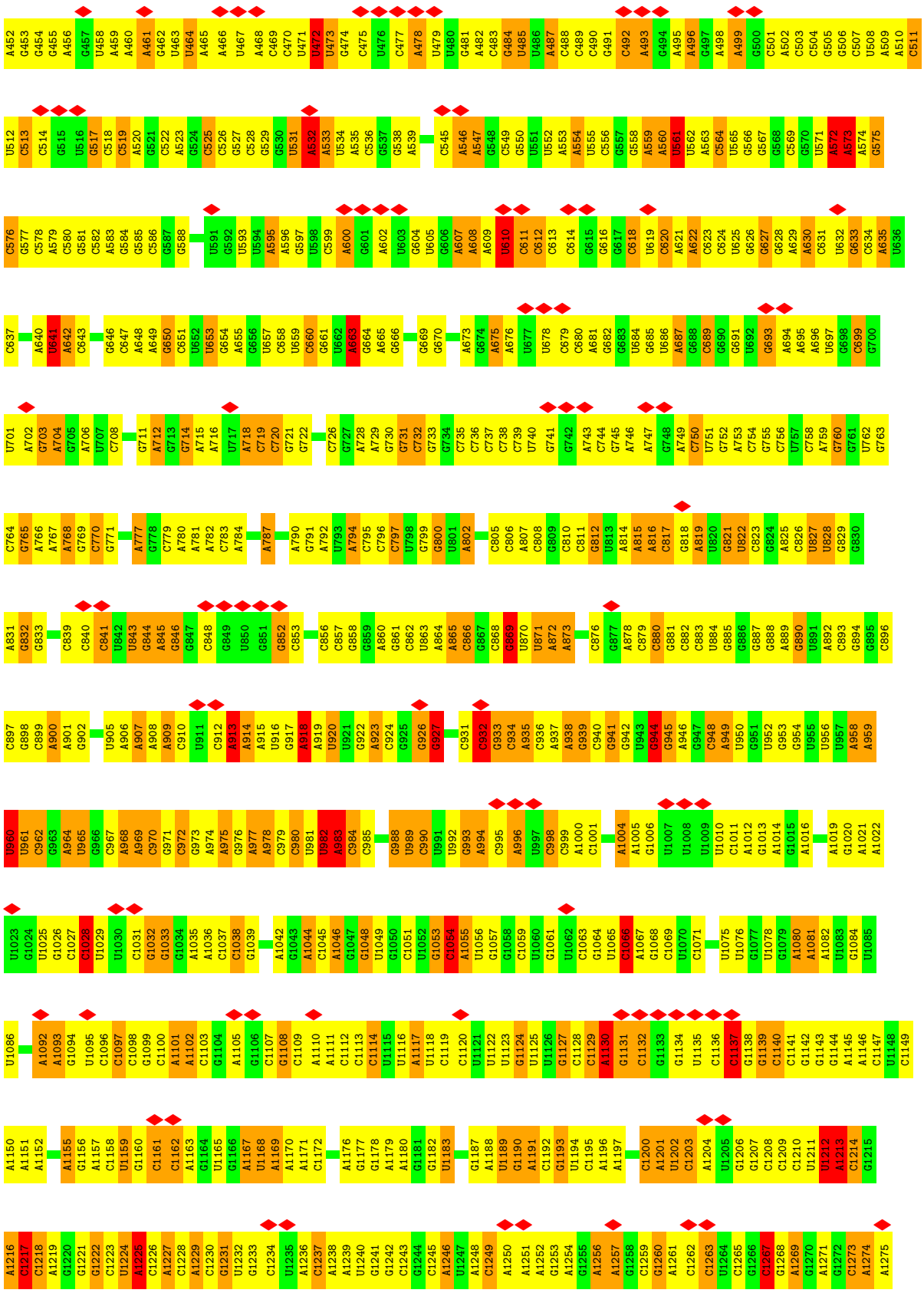


• Molecule 21: 16S ribosomal RNA

Chain AA:



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C764 G765 A766 A767 A768 G769 C770 G771 A777 G778 C779 A780 A781 A782 C783 A784 A787 A790 G791 A792 U793 A794 C795 C796 C797 U798 G799 G800 U801 A802 C805 C806 A807 C808 G809 C810 C811 G812 U813 A814 A815 A816 C817 G818 A819 U820 G821 U822 C823 G824 A825 C826 U827 U828 G829 G830
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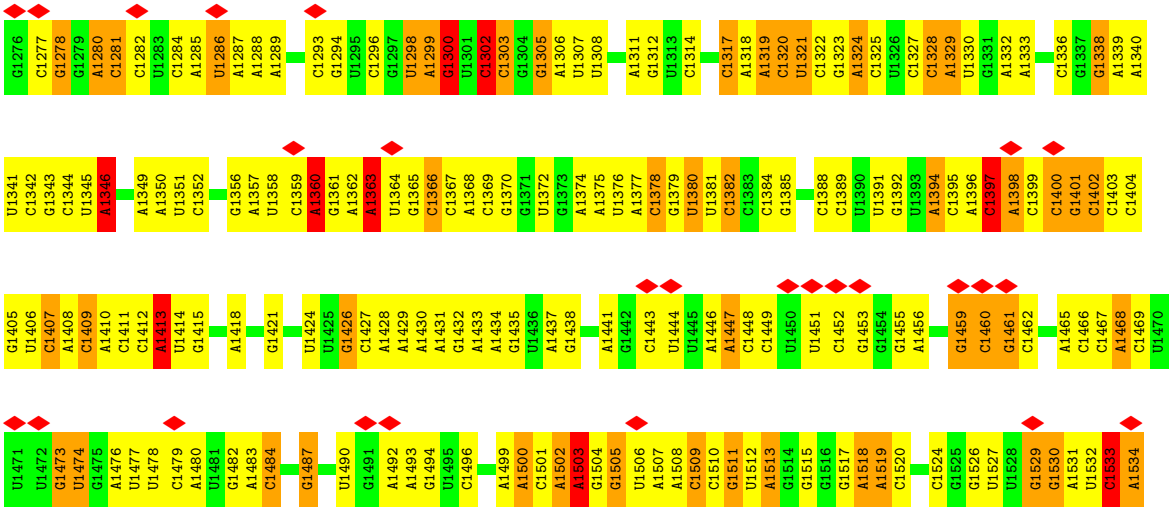
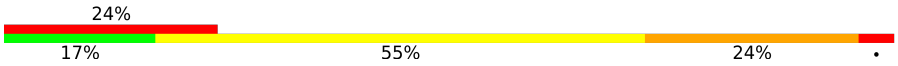
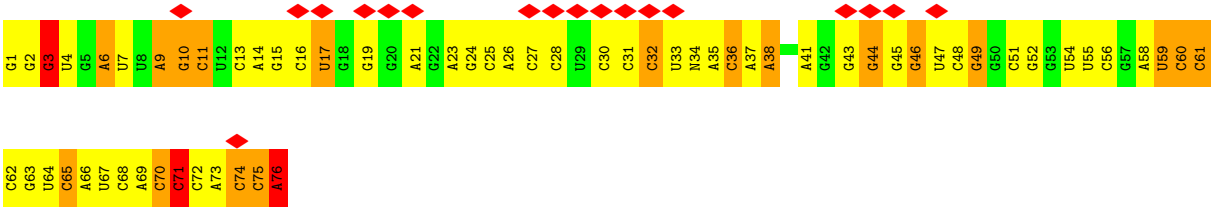
A1216 G1217 C1218 A1219 G1220 G1221 G1222 C1223 U1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 G1242 C1243 G1244 C1245 A1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 A1254 G1255 A1256 A1257 G1258 C1259 G1260 A1261 C1262 C1263 U1264 C1265 G1266 C1267 G1268 A1269 G1270 A1271 G1272 C1273 A1274 A1275



- Molecule 22: fMet-Val-tRNA-Val

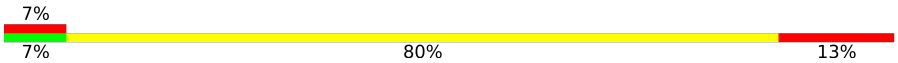
Chain A1:





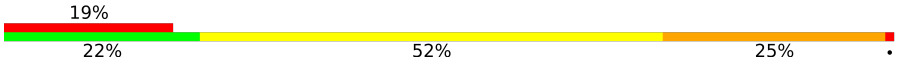
- Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

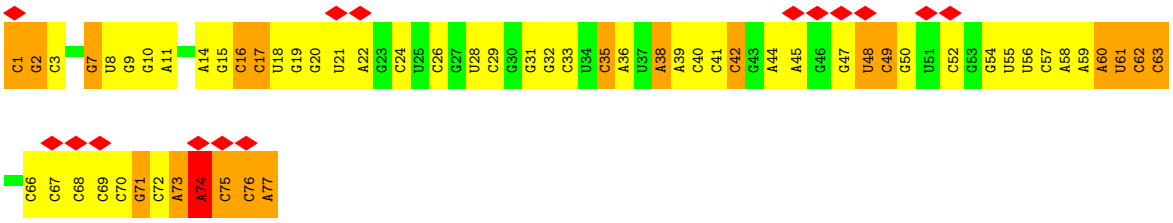
Chain A2:



- Molecule 24: tRNA-fMet

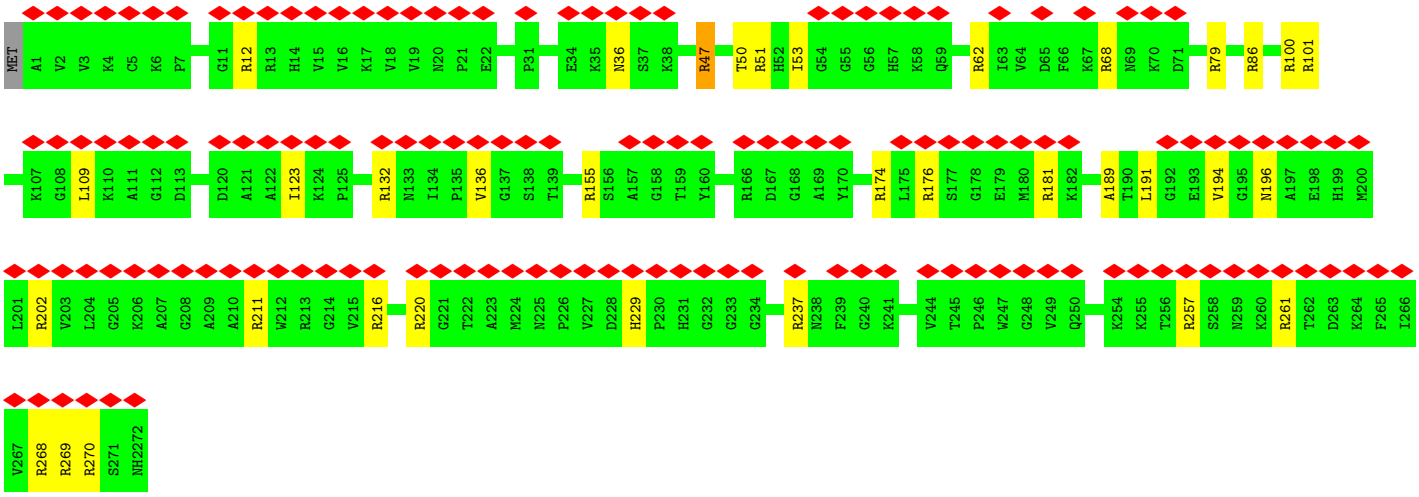
Chain A3:





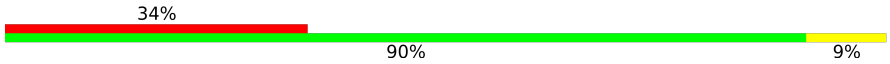
- Molecule 25: 50S ribosomal protein L2

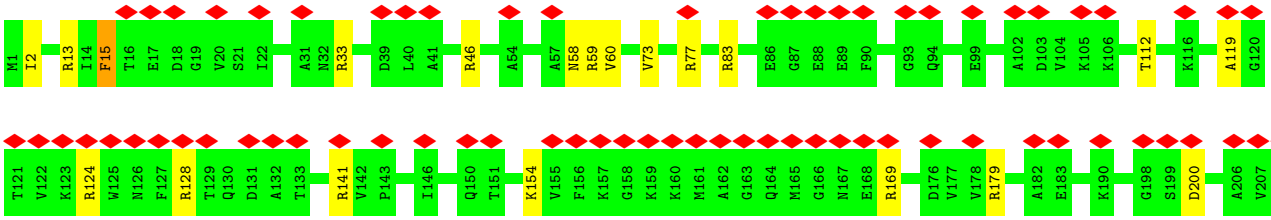
Chain BC:



- Molecule 26: 50S ribosomal protein L3

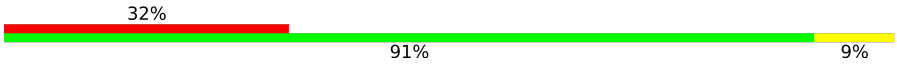
Chain BD:

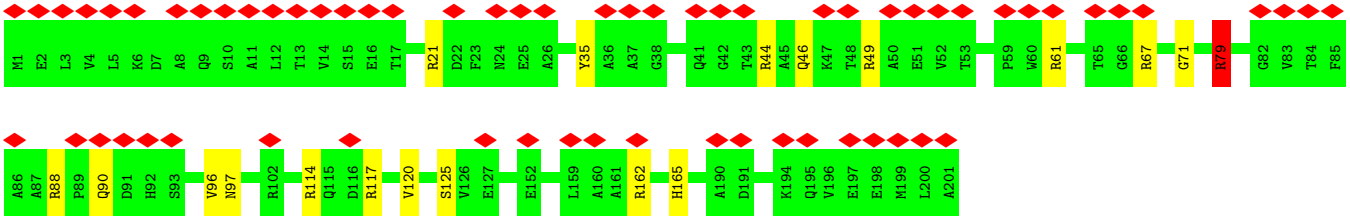




- Molecule 27: 50S ribosomal protein L4

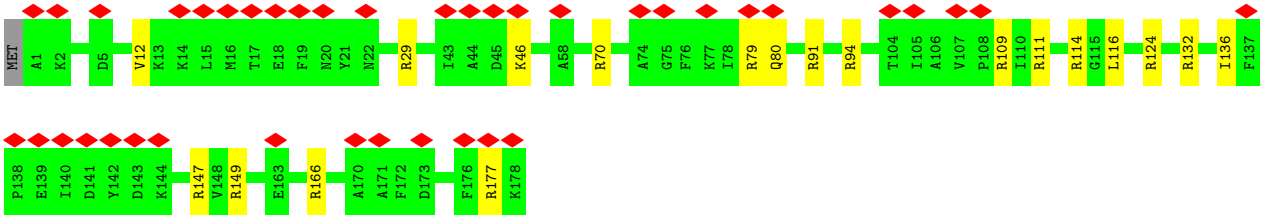
Chain BE:





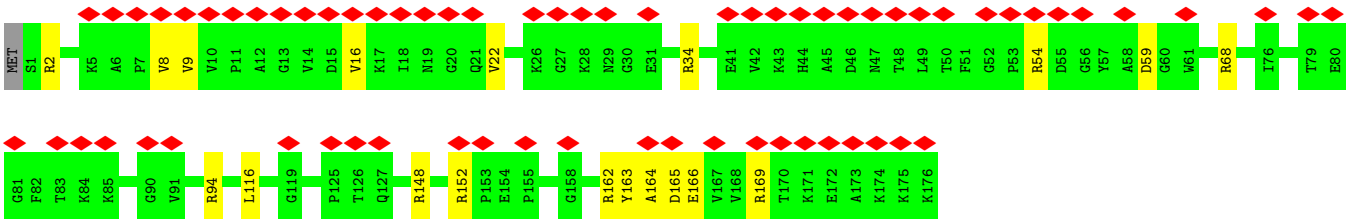
- Molecule 28: 50S ribosomal protein L5

Chain BF:



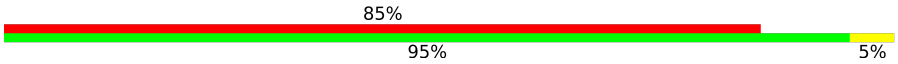
- Molecule 29: 50S ribosomal protein L6

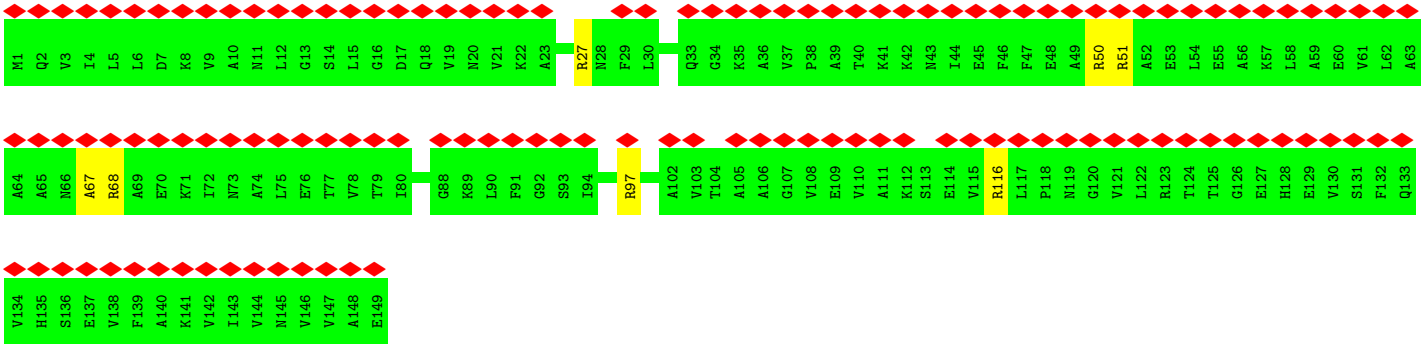
Chain BG:



- Molecule 30: 50S ribosomal protein L9

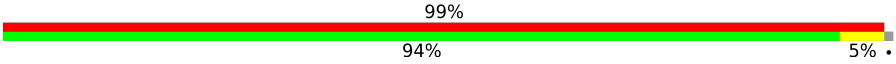
Chain BH:

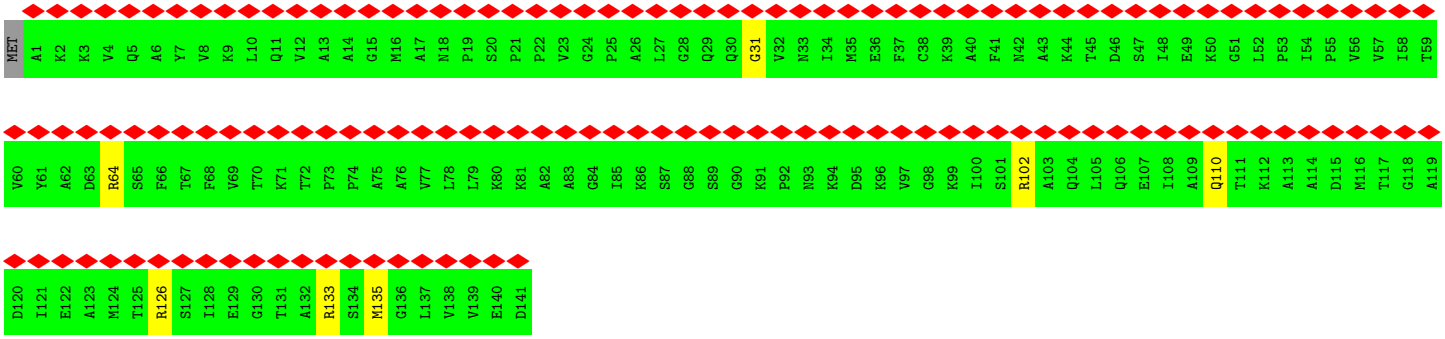




- Molecule 31: 50S ribosomal protein L11

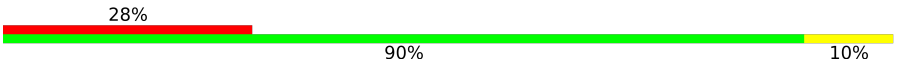
Chain BI:

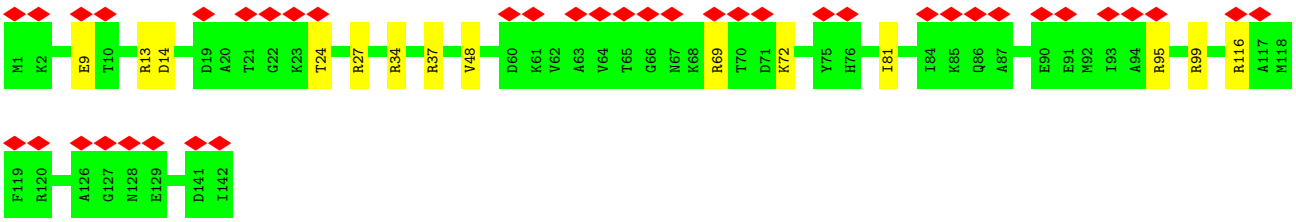




- Molecule 32: 50S ribosomal protein L13

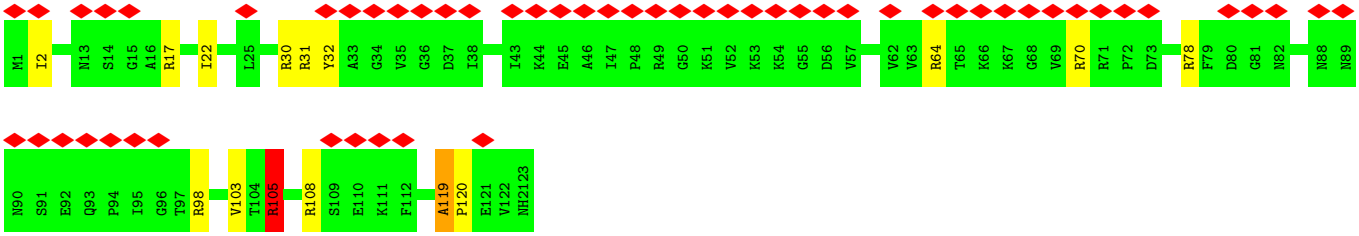
Chain BJ:





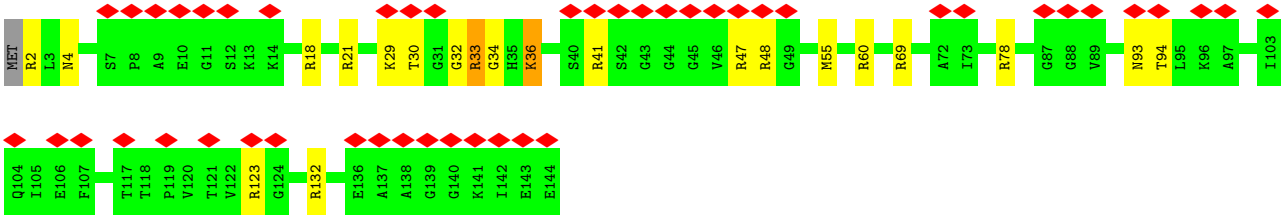
• Molecule 33: 50S ribosomal protein L14

Chain BK:



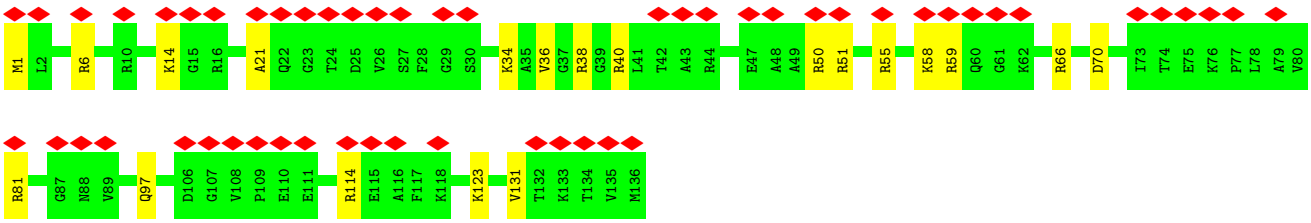
• Molecule 34: 50S ribosomal protein L15

Chain BL:



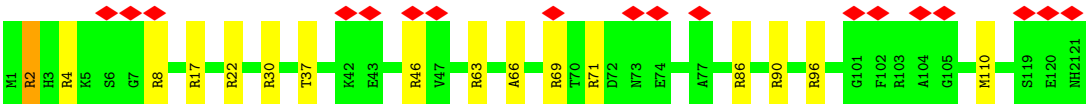
• Molecule 35: 50S ribosomal protein L16

Chain BM:



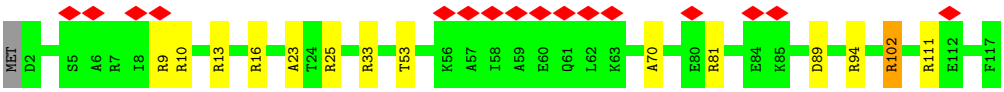
• Molecule 36: 50S ribosomal protein L17

Chain BN:



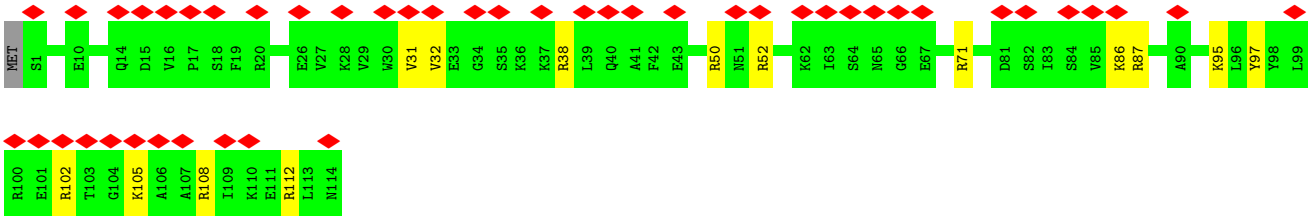
• Molecule 37: 50S ribosomal protein L18

Chain BO:



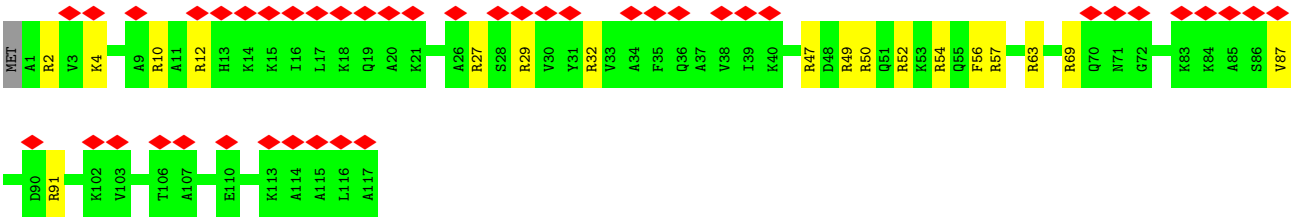
• Molecule 38: 50S ribosomal protein L19

Chain BP: 40% 87% 12%



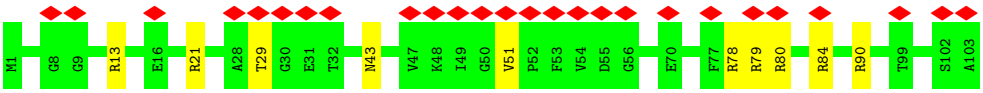
- Molecule 39: 50S ribosomal protein L20

Chain BQ: 36% 84% 15%



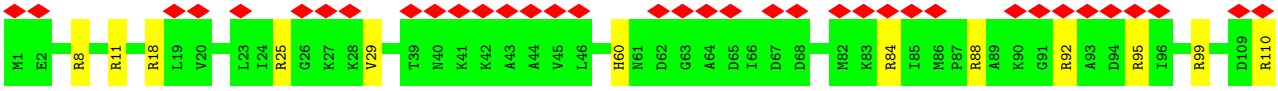
- Molecule 40: 50S ribosomal protein L21

Chain BR: 25% 90% 10%



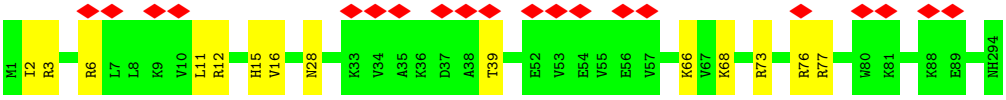
- Molecule 41: 50S ribosomal protein L22

Chain BS: 33% 89% 11%



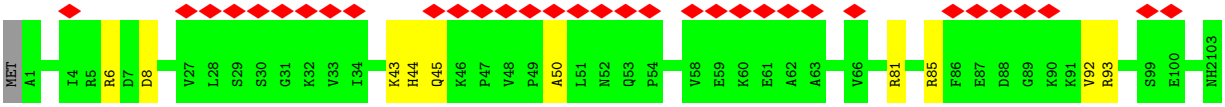
- Molecule 42: 50S ribosomal protein L23

Chain BT: 21% 85% 15%



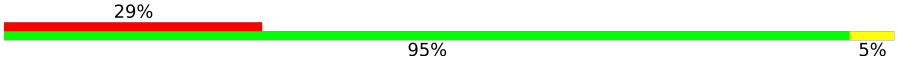
- Molecule 43: 50S ribosomal protein L24

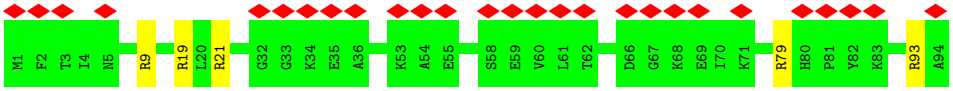
Chain BU: 32% 89% 10%



• Molecule 44: 50S ribosomal protein L25

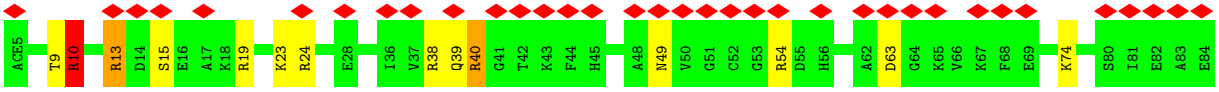
Chain BV:





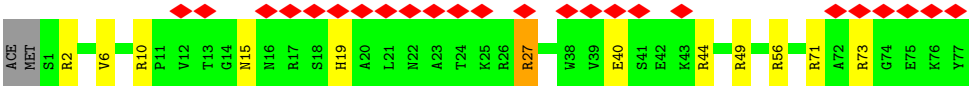
• Molecule 45: 50S ribosomal protein L27

Chain BW:



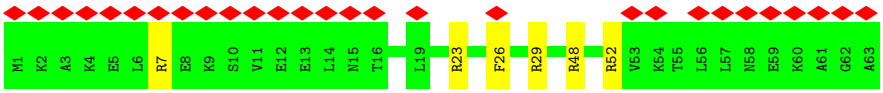
• Molecule 46: 50S ribosomal protein L28

Chain BX:



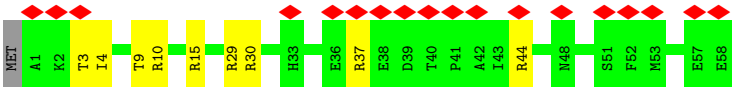
• Molecule 47: 50S ribosomal protein L29

Chain BY:



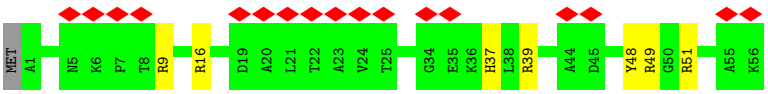
• Molecule 48: 50S ribosomal protein L30

Chain BZ:



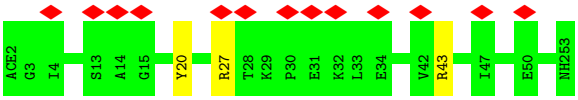
• Molecule 49: 50S ribosomal protein L32

Chain B0:



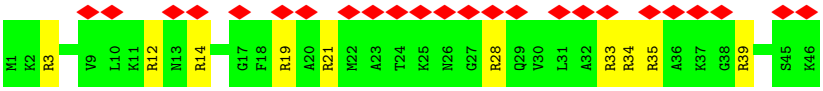
• Molecule 50: 50S ribosomal protein L33

Chain B1: 25% 94% 6%



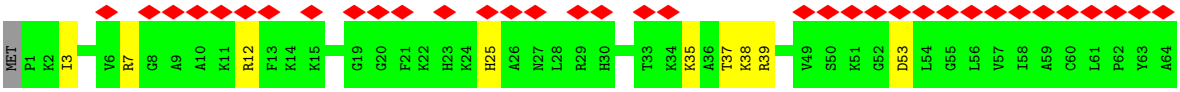
• Molecule 51: 50S ribosomal protein L34

Chain B2: 52% 78% 22%



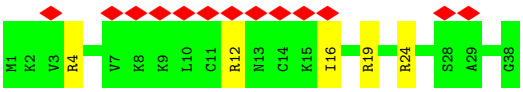
• Molecule 52: 50S ribosomal protein L35

Chain B3: 54% 85% 14%



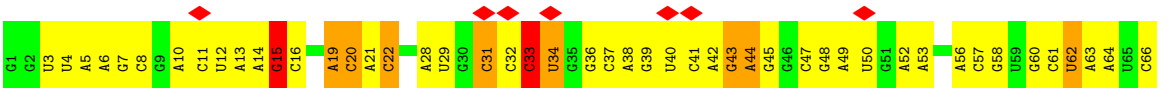
• Molecule 53: 50S ribosomal protein L36

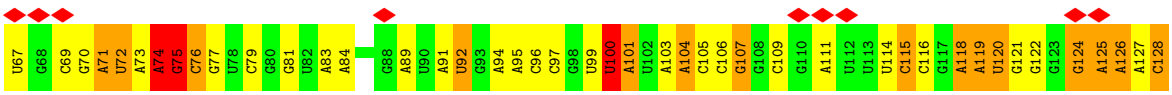
Chain B4: 34% 87% 13%

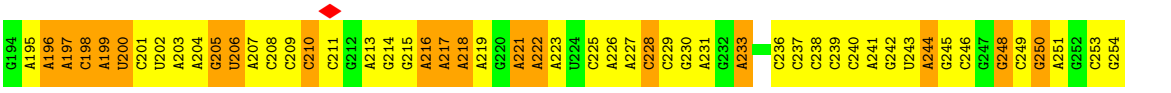


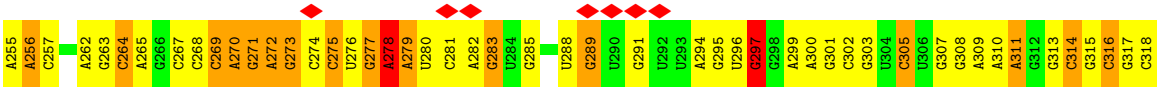
• Molecule 54: 23S ribosomal RNA

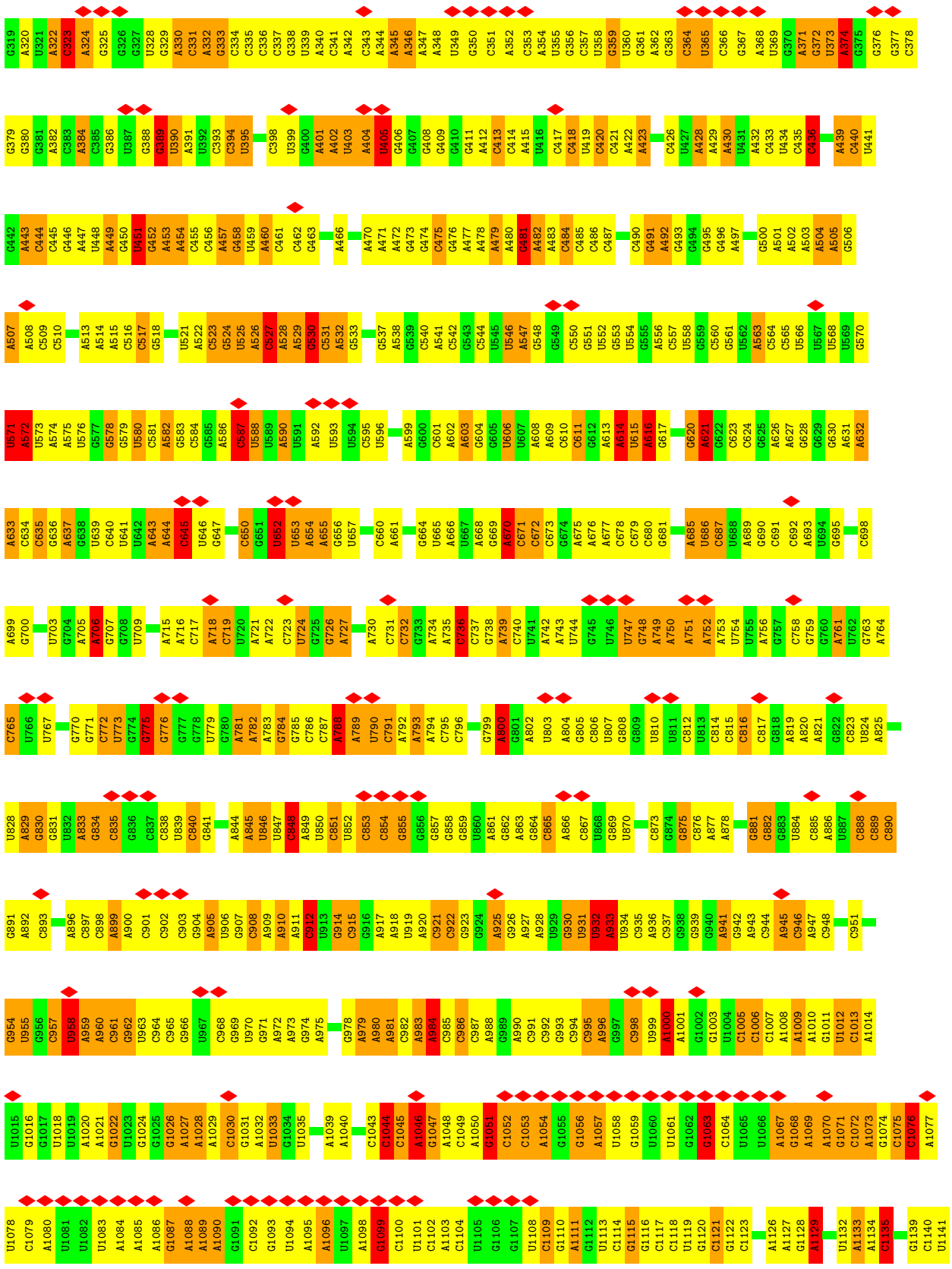
Chain BA: 12% 23% 51% 23%







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G954 U955 G956 C957 U958 A959 A960 C961 G962 U963 C964 C965 G966 U967 C968 G969 U970 G971 A972 A973 G974 A975 G978 A979 A980 A981 C982 A983 A984 C985 C986 C987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 U1004 C1005 C1006 C1007 A1008 A1009 A1010 G1011 U1012 C1013 A1014
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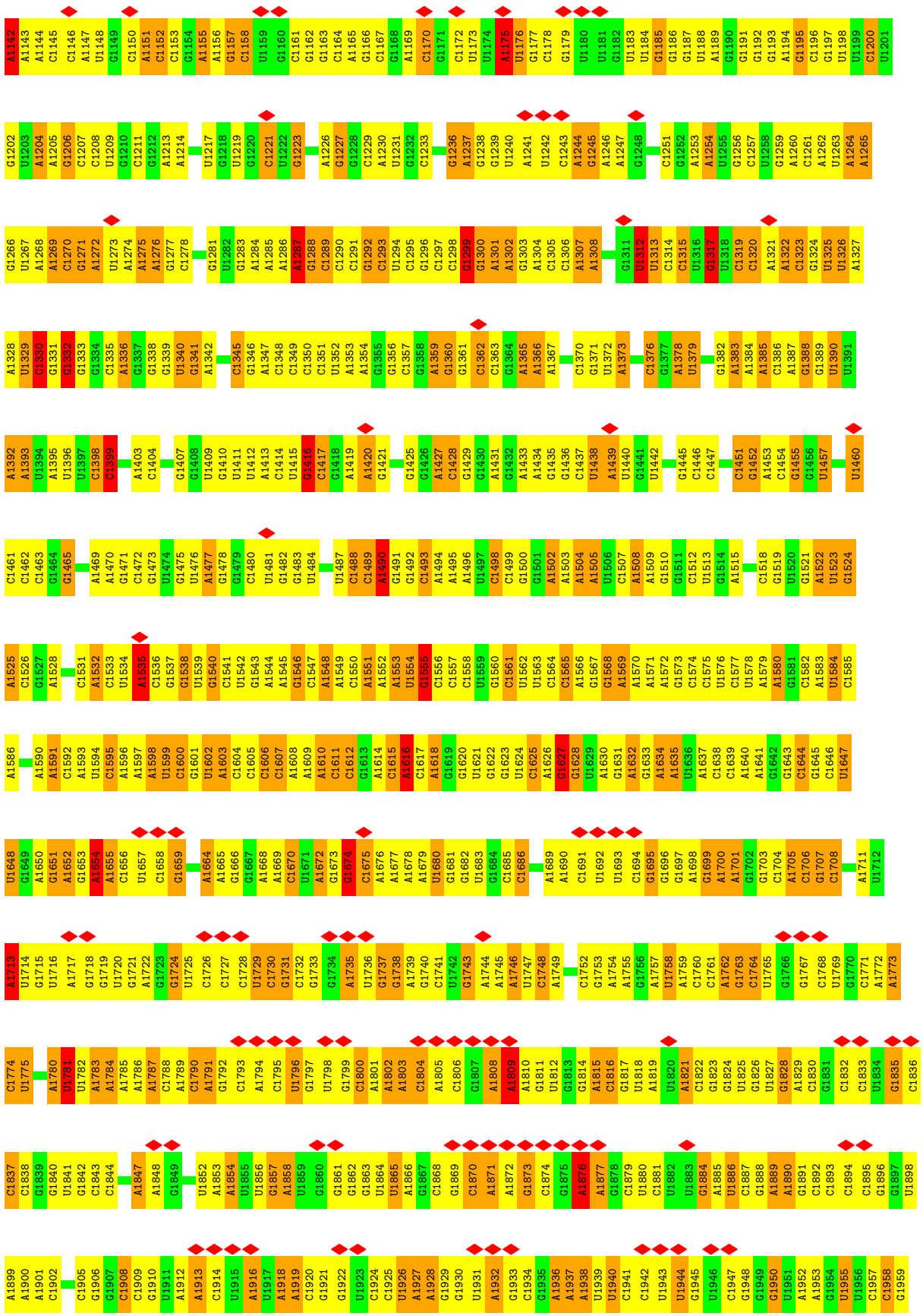
U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 G1116 C1117 C1118 U1119 G1120 C1121 G1122 C1123 A1126 A1127 G1128 A1129 U1132 A1133 A1134 C1135 G1139 C1140 U1141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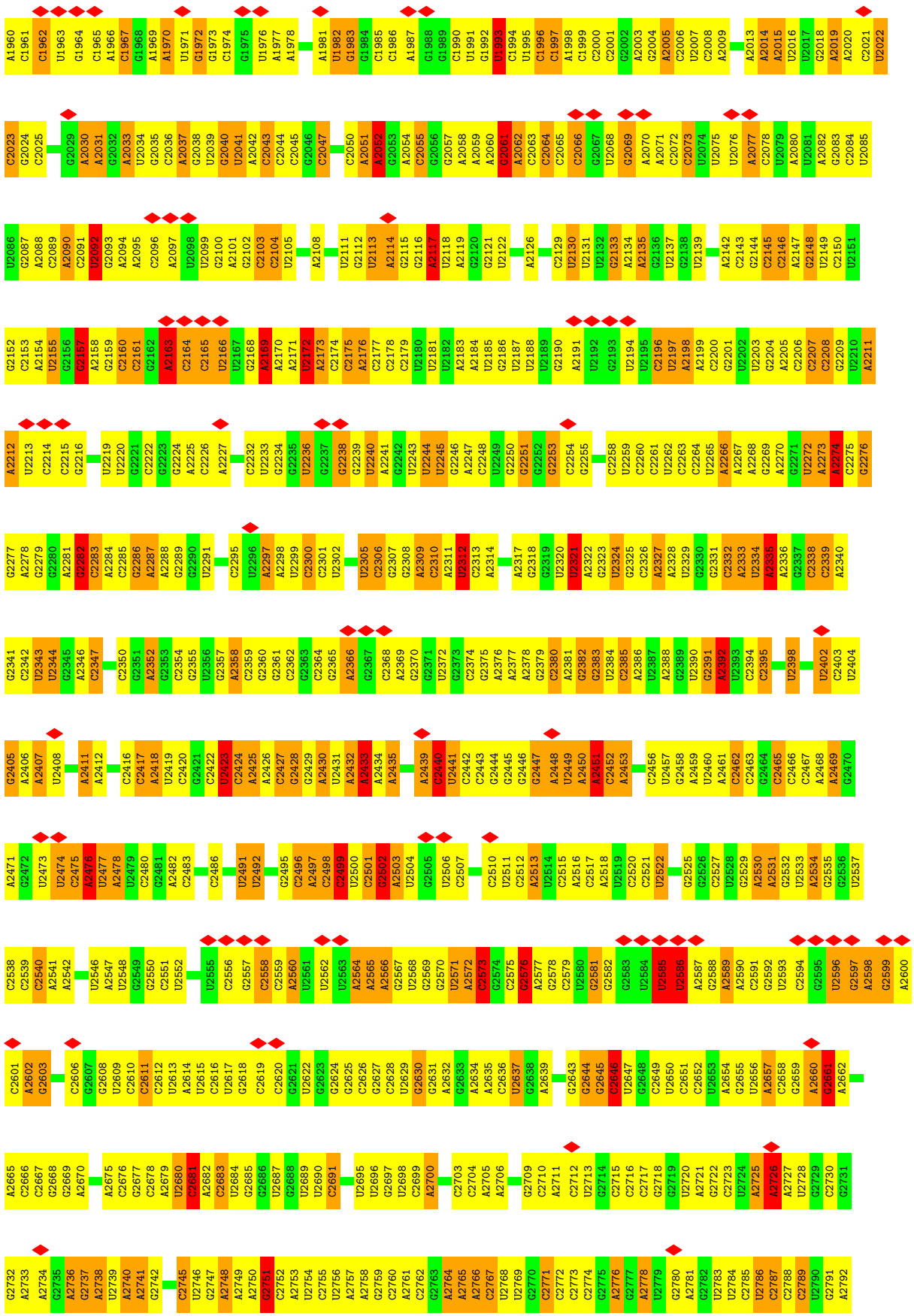
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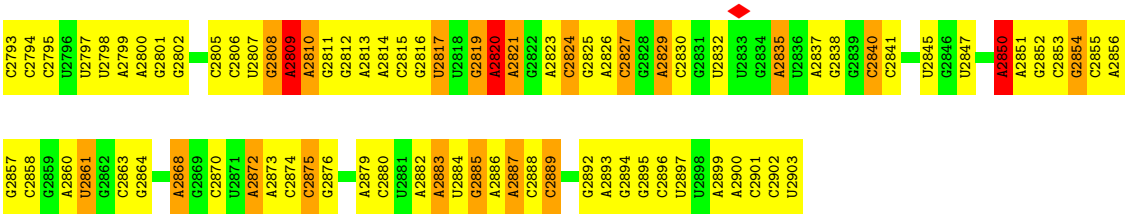
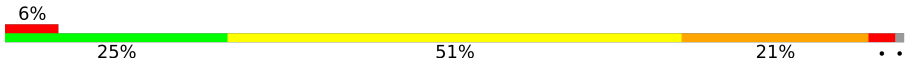
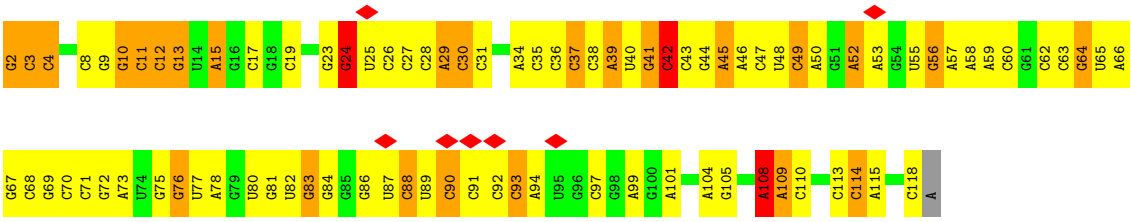


• Molecule 55: 5S ribosomal RNA

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	3052	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	162.319	Depositor
Minimum map value	-108.564	Depositor
Average map value	-1.515	Depositor
Map value standard deviation	18.464	Depositor
Recommended contour level	20.0	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.8, 2.8, 2.8	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: PSU, OMC, NH2, FME, 6MZ, CM0, 7MG, ACE, H2U, 4SU, 5MU

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	0.70	0/1736	1.07	11/2340 (0.5%)
2	AC	0.72	0/1651	1.16	16/2225 (0.7%)
3	AD	0.77	0/1665	1.23	24/2227 (1.1%)
4	AE	0.70	0/1119	1.06	10/1506 (0.7%)
5	AF	0.74	0/835	1.17	6/1128 (0.5%)
6	AG	0.74	0/1188	1.21	19/1593 (1.2%)
7	AH	0.70	0/989	1.08	5/1326 (0.4%)
8	AI	0.81	0/1035	1.34	20/1377 (1.5%)
9	AJ	0.69	0/797	1.23	13/1079 (1.2%)
10	AK	0.74	0/894	1.15	10/1207 (0.8%)
11	AL	0.76	0/969	1.23	15/1300 (1.2%)
12	AM	0.75	0/884	1.32	11/1181 (0.9%)
13	AN	0.77	0/817	1.26	12/1088 (1.1%)
14	AO	0.74	0/722	1.16	8/964 (0.8%)
15	AP	0.76	0/648	1.27	11/870 (1.3%)
16	AQ	0.70	0/658	1.06	4/883 (0.5%)
17	AR	0.81	0/463	1.29	10/623 (1.6%)
18	AS	0.76	0/653	1.13	7/879 (0.8%)
19	AT	0.68	0/672	1.05	5/890 (0.6%)
20	AU	0.83	0/431	1.44	8/572 (1.4%)
21	AA	1.53	1/36759 (0.0%)	2.22	1991/57346 (3.5%)
22	A1	1.53	0/1668	2.20	85/2595 (3.3%)
23	A2	1.47	0/343	2.25	15/531 (2.8%)
24	A3	1.53	0/1722	2.18	81/2685 (3.0%)
25	BC	0.74	0/2121	1.30	26/2852 (0.9%)
26	BD	0.68	0/1586	1.20	14/2134 (0.7%)
27	BE	0.67	0/1571	1.15	11/2113 (0.5%)
28	BF	0.74	0/1444	1.18	14/1937 (0.7%)
29	BG	0.69	0/1343	1.12	8/1816 (0.4%)
30	BH	0.65	0/1122	1.10	6/1515 (0.4%)
31	BI	0.65	0/1046	1.06	4/1410 (0.3%)
32	BJ	0.73	0/1152	1.16	8/1551 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BK	0.70	0/947	1.21	10/1268 (0.8%)
34	BL	0.73	0/1054	1.36	17/1403 (1.2%)
35	BM	0.74	0/1093	1.21	11/1460 (0.8%)
36	BN	0.77	0/973	1.36	15/1301 (1.2%)
37	BO	0.72	0/902	1.25	11/1209 (0.9%)
38	BP	0.75	0/929	1.27	8/1242 (0.6%)
39	BQ	0.80	0/960	1.32	15/1278 (1.2%)
40	BR	0.70	0/829	1.22	7/1107 (0.6%)
41	BS	0.64	0/864	1.19	10/1156 (0.9%)
42	BT	0.65	0/744	1.19	7/994 (0.7%)
43	BU	0.68	0/787	1.10	4/1051 (0.4%)
44	BV	0.71	0/766	1.16	5/1025 (0.5%)
45	BW	0.77	0/604	1.36	9/799 (1.1%)
46	BX	0.75	0/635	1.28	10/848 (1.2%)
47	BY	0.65	0/510	1.17	5/677 (0.7%)
48	BZ	0.69	0/453	1.24	6/605 (1.0%)
49	B0	0.72	0/450	1.23	5/599 (0.8%)
50	B1	0.73	0/417	1.05	2/556 (0.4%)
51	B2	0.81	0/380	1.49	11/498 (2.2%)
52	B3	0.72	0/513	1.23	5/676 (0.7%)
53	B4	0.68	0/303	1.24	4/397 (1.0%)
54	BA	1.41	2/69796 (0.0%)	2.21	4018/108888 (3.7%)
55	BB	1.42	0/2800	2.17	151/4367 (3.5%)
56	B5	0.64	0/1673	1.08	9/2255 (0.4%)
All	All	1.28	3/160085 (0.0%)	2.00	6843/239402 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	1
4	AE	0	1
14	AO	0	2
21	AA	0	368
22	A1	0	21
23	A2	0	4
24	A3	0	16
43	BU	0	1
49	B0	0	1
54	BA	0	707

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

All (3) bond length outliers are listed below:

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

All (6843) bond angle outliers are listed below:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	109	A	C4-C5-C6	-7.26	113.37	117.00
21	AA	511	C	N3-C2-O2	-7.26	116.82	121.90
21	AA	243	A	C5-C6-N1	7.26	121.33	117.70
54	BA	472	A	C5-C6-N1	7.26	121.33	117.70
54	BA	866	A	N1-C6-N6	-7.26	114.25	118.60
54	BA	83	A	C5-C6-N1	7.25	121.33	117.70
21	AA	181	A	C5-C6-N1	7.25	121.33	117.70
21	AA	411	A	C5-C6-N1	7.25	121.33	117.70
22	A1	69	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1885	A	C5-C6-N1	7.25	121.33	117.70
21	AA	510	A	C5-C6-N1	7.25	121.33	117.70
21	AA	1500	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	1472	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	1413	A	N1-C6-N6	-7.25	114.25	118.60
21	AA	650	G	N3-C2-N2	-7.25	114.83	119.90
26	BD	128	ARG	NE-CZ-NH1	7.25	123.92	120.30
54	BA	2412	A	C5-C6-N1	7.25	121.32	117.70
54	BA	2565	A	C5-C6-N1	7.25	121.32	117.70
21	AA	1021	A	C5-C6-N1	7.25	121.32	117.70
54	BA	2070	A	C4-C5-C6	-7.25	113.38	117.00
54	BA	2430	A	C5-C6-N1	7.25	121.32	117.70
10	AK	121	ARG	NE-CZ-NH1	7.24	123.92	120.30
54	BA	675	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1789	A	C5-C6-N1	7.24	121.32	117.70
25	BC	257	ARG	NE-CZ-NH1	7.24	123.92	120.30
54	BA	979	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1469	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1596	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	2660	A	C5-C6-N1	7.24	121.32	117.70
54	BA	845	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	637	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1586	A	C5-C6-N1	7.24	121.32	117.70
21	AA	161	A	C5-C6-N1	7.23	121.32	117.70
54	BA	2020	A	C1'-O4'-C4'	-7.23	104.11	109.90
54	BA	627	A	C5-C6-N1	7.23	121.31	117.70
54	BA	749	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1428	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	1549	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2893	A	N1-C6-N6	-7.23	114.26	118.60
21	AA	873	A	C5-C6-N1	7.23	121.31	117.70
54	BA	310	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	1894	C	O4'-C1'-N1	7.23	113.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2482	A	C5-C6-N1	7.23	121.31	117.70
12	AM	28	ARG	NE-CZ-NH1	7.23	123.91	120.30
21	AA	695	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1140	C	N3-C2-O2	-7.23	116.84	121.90
51	B2	28	ARG	NE-CZ-NH1	7.23	123.91	120.30
54	BA	522	A	C4-C5-C6	-7.23	113.39	117.00
21	AA	1377	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1469	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	480	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1103	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	1655	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1936	A	C5-C6-N1	7.22	121.31	117.70
21	AA	315	A	C5-C6-N1	7.22	121.31	117.70
21	AA	949	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1848	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	2434	A	C4-C5-C6	-7.22	113.39	117.00
55	BB	73	A	C5-C6-N1	7.22	121.31	117.70
21	AA	622	A	C5-C6-N1	7.22	121.31	117.70
39	BQ	10	ARG	NE-CZ-NH1	7.22	123.91	120.30
54	BA	279	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	53	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1609	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	149	A	C5-C6-N1	7.22	121.31	117.70
21	AA	780	A	C5-C6-N1	7.22	121.31	117.70
21	AA	938	A	C5-C6-N1	7.22	121.31	117.70
54	BA	311	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	1254	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2014	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2422	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	739	C	N3-C2-O2	-7.21	116.85	121.90
21	AA	1014	A	C5-C6-N1	7.21	121.31	117.70
28	BF	132	ARG	NE-CZ-NH1	7.21	123.91	120.30
54	BA	490	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	899	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	5	A	C5-C6-N1	7.21	121.31	117.70
21	AA	228	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1035	A	C5-C6-N1	7.21	121.31	117.70
54	BA	371	A	C5-C6-N1	7.21	121.31	117.70
54	BA	886	A	N1-C6-N6	-7.21	114.27	118.60
54	BA	1970	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2829	A	C5-C6-N1	7.21	121.31	117.70
21	AA	1246	A	C4-C5-C6	-7.21	113.39	117.00

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

All (1147) planarity outliers are listed below:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.2 Too-close contacts (i)

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	2	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	0	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16520	3	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	1	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0
30	BH	1111	0	1148	0	0
31	BI	1032	0	1088	0	0
32	BJ	1129	0	1162	0	0
33	BK	939	0	1012	3	0
34	BL	1045	0	1117	1	0
35	BM	1074	0	1157	2	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	1	0
38	BP	917	0	965	1	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	1	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	1	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	0	0
54	BA	62317	0	31341	4	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99659	17	0

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

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BL:30:THR:HG21	34:BL:36:LYS:H	1.72	0.54
54:BA:388:G:H2'	54:BA:389:G:H3'	1.91	0.52
42:BT:15:HIS:CG	42:BT:16:VAL:H	2.29	0.50
21:AA:1054:C:C6	23:A2:89:U:H1'	2.48	0.48
37:BO:53:THR:HG21	37:BO:70:ALA:HB1	1.98	0.46
38:BP:95:LYS:HE2	54:BA:2718:G:O3'	2.17	0.45
35:BM:34:LYS:HE3	35:BM:131:VAL:HG11	1.99	0.44
33:BK:119:ALA:H	33:BK:120:PRO:CD	2.31	0.44
21:AA:865:A:H2'	21:AA:866:C:C6	2.55	0.42
7:AH:60:LEU:H	7:AH:60:LEU:HD23	1.84	0.41
21:AA:1517:G:H2'	21:AA:1518:A:C8	2.56	0.41
4:AE:155:LYS:HE3	7:AH:44:PHE:CE1	2.56	0.41
35:BM:14:LYS:HE3	54:BA:958:U:C2	2.56	0.41
45:BW:9:THR:HB	45:BW:10:ARG:HA	2.02	0.41
54:BA:833:A:H2'	54:BA:834:G:C8	2.56	0.41
33:BK:105:ARG:H	33:BK:105:ARG:NE	2.20	0.40
33:BK:119:ALA:H	33:BK:120:PRO:HD2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (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%)	200 (92%)	17 (8%)	1 (0%)	29	69
2	AC	205/208 (99%)	184 (90%)	15 (7%)	6 (3%)	4	29
3	AD	203/206 (98%)	185 (91%)	14 (7%)	4 (2%)	7	38
4	AE	150/152 (99%)	134 (89%)	10 (7%)	6 (4%)	3	23
5	AF	99/101 (98%)	80 (81%)	13 (13%)	6 (6%)	1	17
6	AG	150/152 (99%)	136 (91%)	10 (7%)	4 (3%)	5	31
7	AH	127/130 (98%)	116 (91%)	8 (6%)	3 (2%)	6	33
8	AI	126/128 (98%)	107 (85%)	15 (12%)	4 (3%)	4	26
9	AJ	98/100 (98%)	88 (90%)	5 (5%)	5 (5%)	2	19
10	AK	116/118 (98%)	107 (92%)	7 (6%)	2 (2%)	9	42
11	AL	121/124 (98%)	107 (88%)	8 (7%)	6 (5%)	2	20
12	AM	112/115 (97%)	94 (84%)	13 (12%)	5 (4%)	2	22
13	AN	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
14	AO	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	50
15	AP	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	3	24
16	AQ	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	AR	55/57 (96%)	50 (91%)	4 (7%)	1 (2%)	8	40
18	AS	79/81 (98%)	71 (90%)	5 (6%)	3 (4%)	3	24
19	AT	84/86 (98%)	76 (90%)	8 (10%)	0	100	100
20	AU	51/53 (96%)	32 (63%)	15 (29%)	4 (8%)	1	13
25	BC	270/273 (99%)	238 (88%)	25 (9%)	7 (3%)	5	31
26	BD	207/209 (99%)	185 (89%)	17 (8%)	5 (2%)	6	33
27	BE	199/201 (99%)	171 (86%)	20 (10%)	8 (4%)	3	23
28	BF	176/179 (98%)	155 (88%)	17 (10%)	4 (2%)	6	34
29	BG	174/177 (98%)	155 (89%)	12 (7%)	7 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BH	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	22	63
31	BI	139/142 (98%)	125 (90%)	12 (9%)	2 (1%)	11	46
32	BJ	140/142 (99%)	126 (90%)	11 (8%)	3 (2%)	7	36
33	BK	121/123 (98%)	107 (88%)	10 (8%)	4 (3%)	4	26
34	BL	141/144 (98%)	124 (88%)	11 (8%)	6 (4%)	2	22
35	BM	134/136 (98%)	115 (86%)	14 (10%)	5 (4%)	3	24
36	BN	119/121 (98%)	105 (88%)	11 (9%)	3 (2%)	5	32
37	BO	114/117 (97%)	108 (95%)	3 (3%)	3 (3%)	5	31
38	BP	112/115 (97%)	92 (82%)	17 (15%)	3 (3%)	5	31
39	BQ	115/118 (98%)	108 (94%)	5 (4%)	2 (2%)	9	42
40	BR	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	4	28
41	BS	108/110 (98%)	105 (97%)	2 (2%)	1 (1%)	17	57
42	BT	92/94 (98%)	80 (87%)	6 (6%)	6 (6%)	1	16
43	BU	101/104 (97%)	83 (82%)	14 (14%)	4 (4%)	3	23
44	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
45	BW	78/80 (98%)	59 (76%)	17 (22%)	2 (3%)	5	31
46	BX	75/79 (95%)	68 (91%)	3 (4%)	4 (5%)	2	19
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	49 (88%)	4 (7%)	3 (5%)	2	19
49	B0	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
50	B1	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
51	B2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
52	B3	62/65 (95%)	54 (87%)	5 (8%)	3 (5%)	2	21
53	B4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	30
56	B5	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	29	69
All	All	5876/6008 (98%)	5245 (89%)	476 (8%)	155 (3%)	8	31

All (155) Ramachandran outliers are listed below:

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

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

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

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

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Mol	Chain	Res	Type
29	BG	164	ALA
31	BI	31	GLY
40	BR	29	THR
46	BX	19	HIS
46	BX	40	GLU
48	BZ	9	THR
4	AE	103	GLY
9	AJ	57	VAL
26	BD	73	VAL
29	BG	9	VAL
7	AH	77	VAL
25	BC	136	VAL
28	BF	136	ILE
34	BL	55	MET
46	BX	6	VAL
9	AJ	38	GLY
12	AM	66	GLY
20	AU	13	VAL
29	BG	116	LEU
53	B4	16	ILE
9	AJ	42	LEU
12	AM	3	ILE
25	BC	53	ILE
41	BS	29	VAL
11	AL	43	LYS
38	BP	32	VAL

5.3.2 Protein sidechains (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%)	168 (99%)	2 (1%)	71 83
3	AD	172/173 (99%)	171 (99%)	1 (1%)	86 92
4	AE	113/113 (100%)	112 (99%)	1 (1%)	78 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AF	87/87 (100%)	87 (100%)	0	100	100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	81	89
7	AH	104/105 (99%)	101 (97%)	3 (3%)	42	64
8	AI	105/105 (100%)	101 (96%)	4 (4%)	33	57
9	AJ	86/86 (100%)	83 (96%)	3 (4%)	36	59
10	AK	90/90 (100%)	90 (100%)	0	100	100
11	AL	103/104 (99%)	102 (99%)	1 (1%)	76	86
12	AM	91/92 (99%)	90 (99%)	1 (1%)	73	84
13	AN	83/84 (99%)	81 (98%)	2 (2%)	49	69
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%)	71 (96%)	3 (4%)	30	55
17	AR	48/48 (100%)	45 (94%)	3 (6%)	18	43
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%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	210 (97%)	6 (3%)	43	65
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%)	133 (97%)	4 (3%)	42	64
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	108 (99%)	1 (1%)	78	87
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	46	66
33	BK	103/103 (100%)	102 (99%)	1 (1%)	76	86
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%)	87 (98%)	2 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BR	84/84 (100%)	84 (100%)	0	100	100
41	BS	93/93 (100%)	92 (99%)	1 (1%)	73	84
42	BT	80/80 (100%)	80 (100%)	0	100	100
43	BU	83/84 (99%)	81 (98%)	2 (2%)	49	69
44	BV	78/78 (100%)	78 (100%)	0	100	100
45	BW	59/59 (100%)	53 (90%)	6 (10%)	7	25
46	BX	67/68 (98%)	66 (98%)	1 (2%)	65	80
47	BY	55/55 (100%)	54 (98%)	1 (2%)	59	77
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	53	72
50	B1	45/45 (100%)	44 (98%)	1 (2%)	52	71
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	48 (94%)	3 (6%)	19	45
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	169 (98%)	4 (2%)	50	70
All	All	4842/4870 (99%)	4757 (98%)	85 (2%)	61	77

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

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

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

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

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

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	248 (16%)	86 (5%)
22	A1	73/76 (96%)	15 (20%)	7 (9%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	A2	14/15 (93%)	5 (35%)	3 (21%)
24	A3	76/77 (98%)	13 (17%)	5 (6%)
54	BA	2902/2903 (99%)	464 (15%)	110 (3%)
55	BB	117/118 (99%)	15 (12%)	4 (3%)
All	All	4712/4722 (99%)	760 (16%)	215 (4%)

All (760) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G
21	AA	16	A
21	AA	28	A
21	AA	32	A
21	AA	35	G
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	52	C
21	AA	54	C
21	AA	56	U
21	AA	66	A
21	AA	67	C
21	AA	71	A
21	AA	81	A
21	AA	86	G
21	AA	90	C
21	AA	91	U
21	AA	95	C
21	AA	110	C
21	AA	121	U
21	AA	124	C
21	AA	131	A
21	AA	144	G
21	AA	163	C
21	AA	164	G
21	AA	168	G
21	AA	198	G
21	AA	207	C

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Res	Type
54	BA	1821	A
54	BA	1835	G
54	BA	1858	A
54	BA	1870	C
54	BA	1871	A
54	BA	1873	G
54	BA	1877	A
54	BA	1886	U
54	BA	1896	G
54	BA	1906	G
54	BA	1916	A
54	BA	1919	A
54	BA	1926	U
54	BA	1929	G
54	BA	1930	G
54	BA	1937	A
54	BA	1938	A
54	BA	1945	G
54	BA	1955	U
54	BA	1963	U
54	BA	1964	G
54	BA	1967	C
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1982	U
54	BA	1993	U
54	BA	1997	C
54	BA	2016	U
54	BA	2023	C
54	BA	2030	A
54	BA	2043	C
54	BA	2047	C
54	BA	2052	A
54	BA	2055	C
54	BA	2061	G
54	BA	2062	A
54	BA	2069	G
54	BA	2076	U
54	BA	2077	A
54	BA	2090	A
54	BA	2092	U

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

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

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

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

All (215) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	15	G
21	AA	32	A
21	AA	34	C
21	AA	51	A
21	AA	66	A
21	AA	71	A
21	AA	90	C
21	AA	109	A
21	AA	120	A
21	AA	123	U
21	AA	162	A
21	AA	163	C
21	AA	206	C
21	AA	212	G
21	AA	235	C
21	AA	238	A
21	AA	243	A
21	AA	251	G
21	AA	271	C
21	AA	307	C
21	AA	315	A
21	AA	316	C

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Mol	Chain	Res	Type
21	AA	327	A
21	AA	329	A
21	AA	343	U
21	AA	351	G
21	AA	354	G
21	AA	414	A
21	AA	462	G
21	AA	464	U
21	AA	472	U
21	AA	473	U
21	AA	496	A
21	AA	499	A
21	AA	531	U
21	AA	532	A
21	AA	559	A
21	AA	560	A
21	AA	575	G
21	AA	607	A
21	AA	610	U
21	AA	632	U
21	AA	641	U
21	AA	659	U
21	AA	663	A
21	AA	844	G
21	AA	869	G
21	AA	872	A
21	AA	884	U
21	AA	913	A
21	AA	926	G
21	AA	932	C
21	AA	944	G
21	AA	964	A
21	AA	982	U
21	AA	1032	G
21	AA	1054	C
21	AA	1066	C
21	AA	1080	A
21	AA	1092	A
21	AA	1101	A
21	AA	1123	U
21	AA	1124	G
21	AA	1129	C

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Mol	Chain	Res	Type
21	AA	1137	C
21	AA	1139	G
21	AA	1159	U
21	AA	1168	U
21	AA	1187	G
21	AA	1190	G
21	AA	1201	A
21	AA	1212	U
21	AA	1231	G
21	AA	1241	G
21	AA	1298	U
21	AA	1300	G
21	AA	1345	U
21	AA	1346	A
21	AA	1365	G
21	AA	1401	G
21	AA	1459	G
21	AA	1505	G
21	AA	1533	C
22	A1	10	G
22	A1	15	G
22	A1	19	G
22	A1	45	G
22	A1	46	7MG
22	A1	49	G
22	A1	70	C
23	A2	80	C
23	A2	88	U
23	A2	89	U
24	A3	16	C
24	A3	19	G
24	A3	47	G
24	A3	60	A
24	A3	62	C
54	BA	33	C
54	BA	60	G
54	BA	121	G
54	BA	125	A
54	BA	177	G
54	BA	199	A
54	BA	205	G
54	BA	221	A

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Mol	Chain	Res	Type
54	BA	222	A
54	BA	278	A
54	BA	279	A
54	BA	323	C
54	BA	332	A
54	BA	345	A
54	BA	389	G
54	BA	403	U
54	BA	448	U
54	BA	481	G
54	BA	529	A
54	BA	531	C
54	BA	546	U
54	BA	570	G
54	BA	571	U
54	BA	614	A
54	BA	615	U
54	BA	620	G
54	BA	643	A
54	BA	645	C
54	BA	652	U
54	BA	670	A
54	BA	685	A
54	BA	847	U
54	BA	853	C
54	BA	933	A
54	BA	954	G
54	BA	957	C
54	BA	978	G
54	BA	980	A
54	BA	983	A
54	BA	1005	C
54	BA	1069	A
54	BA	1070	A
54	BA	1087	G
54	BA	1099	G
54	BA	1109	C
54	BA	1185	G
54	BA	1287	A
54	BA	1288	G
54	BA	1299	G
54	BA	1300	G

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Mol	Chain	Res	Type
54	BA	1312	U
54	BA	1324	G
54	BA	1325	U
54	BA	1332	G
54	BA	1340	U
54	BA	1379	U
54	BA	1398	C
54	BA	1420	A
54	BA	1427	A
54	BA	1439	A
54	BA	1451	C
54	BA	1455	G
54	BA	1554	U
54	BA	1602	U
54	BA	1610	A
54	BA	1625	C
54	BA	1647	U
54	BA	1654	A
54	BA	1674	G
54	BA	1695	G
54	BA	1706	C
54	BA	1713	A
54	BA	1730	C
54	BA	1731	G
54	BA	1781	U
54	BA	1783	A
54	BA	1787	A
54	BA	1808	A
54	BA	1816	C
54	BA	1876	A
54	BA	1913	A
54	BA	1936	A
54	BA	1938	A
54	BA	1963	U
54	BA	1970	A
54	BA	2030	A
54	BA	2051	A
54	BA	2092	U
54	BA	2111	U
54	BA	2145	C
54	BA	2163	A
54	BA	2172	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	BA	2251	G
54	BA	2282	G
54	BA	2286	G
54	BA	2324	U
54	BA	2343	U
54	BA	2423	U
54	BA	2430	A
54	BA	2439	A
54	BA	2451	A
54	BA	2491	U
54	BA	2500	U
54	BA	2502	G
54	BA	2531	A
54	BA	2564	A
54	BA	2585	U
54	BA	2689	U
54	BA	2726	A
54	BA	2894	G
55	BB	2	G
55	BB	24	G
55	BB	56	G
55	BB	81	G

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	PSU	A1	55	22	18,21,22	0.82	0	22,30,33	1.16	1 (4%)
22	4SU	A1	7	22	18,21,22	1.46	2 (11%)	26,30,33	1.07	2 (7%)
24	5MU	A3	55	24	19,22,23	0.73	0	28,32,35	1.46	4 (14%)
22	7MG	A1	46	22	22,26,27	4.75	1 (4%)	29,39,42	1.40	1 (3%)
22	CM0	A1	34	21,22	22,26,27	1.38	2 (9%)	28,37,40	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	5MU	A1	54	22	19,22,23	0.79	0	28,32,35	1.49	5 (17%)
24	4SU	A3	8	24	18,21,22	1.39	1 (5%)	26,30,33	0.79	1 (3%)
24	OMC	A3	33	24	19,22,23	0.80	0	26,31,34	1.14	2 (7%)
24	H2U	A3	21	24	18,21,22	1.38	2 (11%)	21,30,33	1.18	2 (9%)
22	6MZ	A1	37	22	18,25,26	1.04	1 (5%)	16,36,39	1.54	2 (12%)
24	PSU	A3	56	24	18,21,22	0.94	0	22,30,33	1.16	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	PSU	A1	55	22	-	0/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/7/25/26	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
22	7MG	A1	46	22	-	1/7/37/38	0/3/3/3
22	CM0	A1	34	21,22	-	4/12/30/31	0/2/2/2
22	5MU	A1	54	22	-	0/7/25/26	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	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-22.05	1.33	1.46
22	A1	34	CM0	O5-C5	-5.02	1.25	1.36
22	A1	7	4SU	C5-C4	-5.00	1.36	1.42
24	A3	8	4SU	C5-C4	-4.78	1.36	1.42
24	A3	21	H2U	C2-N3	-3.50	1.31	1.38
24	A3	21	H2U	C4-N3	-3.34	1.31	1.37
22	A1	37	6MZ	C8-N7	-2.57	1.30	1.34
22	A1	34	CM0	O8-C8	-2.20	1.23	1.30
22	A1	7	4SU	C4-S4	-2.19	1.64	1.68

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	46	7MG	N9-C8-N7	5.85	111.75	103.38
22	A1	37	6MZ	C9-N6-C6	4.93	127.12	122.87
22	A1	54	5MU	C5M-C5-C6	-4.11	117.36	122.85
24	A3	55	5MU	C5M-C5-C6	-3.76	117.83	122.85
22	A1	54	5MU	C6-C5-C4	3.39	120.86	118.03
24	A3	55	5MU	C6-C5-C4	3.24	120.74	118.03
24	A3	33	OMC	O2-C2-N3	-3.04	117.38	122.33
22	A1	55	PSU	C6-C5-C4	3.03	120.32	118.20
24	A3	21	H2U	N3-C2-N1	2.86	119.68	116.65
22	A1	54	5MU	C5M-C5-C4	2.73	121.77	118.77
24	A3	56	PSU	O4'-C1'-C2'	2.72	108.98	105.14
24	A3	33	OMC	C2'-C1'-N1	-2.68	109.02	114.22
24	A3	55	5MU	C5-C6-N1	-2.67	120.59	123.34
24	A3	21	H2U	C4-N3-C2	2.63	127.97	125.79
24	A3	56	PSU	C6-C5-C4	2.42	119.89	118.20
24	A3	55	5MU	C5M-C5-C4	2.41	121.42	118.77
22	A1	37	6MZ	C2-N1-C6	2.33	118.58	116.59
22	A1	7	4SU	C6-C5-C4	2.31	121.95	119.95
24	A3	8	4SU	C6-C5-C4	2.27	121.92	119.95
22	A1	54	5MU	C5-C6-N1	-2.24	121.03	123.34
22	A1	7	4SU	O4'-C4'-C3'	2.18	109.43	105.11
22	A1	54	5MU	O4-C4-C5	2.00	127.22	124.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9
22	A1	46	7MG	C4'-C5'-O5'-P
22	A1	34	CM0	C6-C5-O5-C7
22	A1	34	CM0	C4-C5-O5-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
57	VAL	A1	101	58,22	4,6,7	0.76	0	6,7,9	1.52	1 (16%)
58	FME	BA	3001	57	8,9,10	0.63	0	7,9,11	1.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	VAL	A1	101	58,22	-	0/5/6/8	-
58	FME	BA	3001	57	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	A1	101	VAL	O-C-CA	-3.66	115.18	124.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

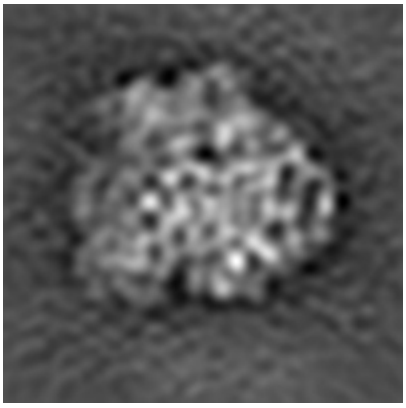
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1720. These allow visual inspection of the internal detail of the map and identification of artifacts.

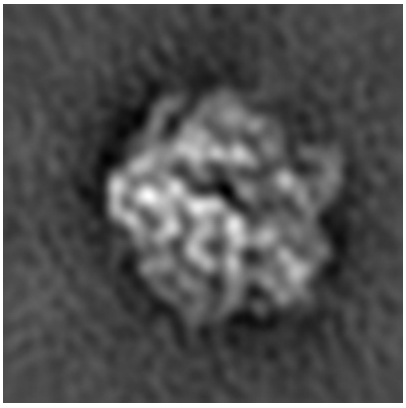
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

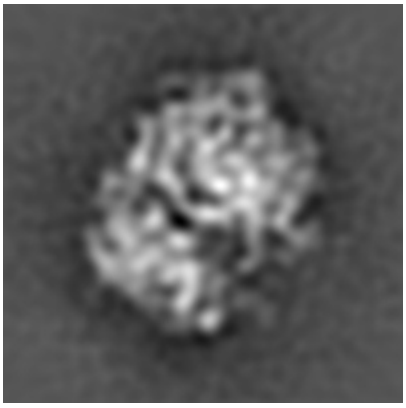
6.1.1 Primary map



X



Y



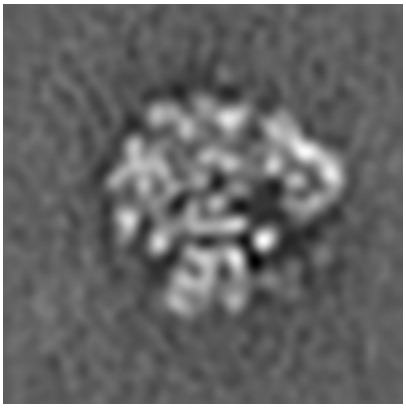
Z

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

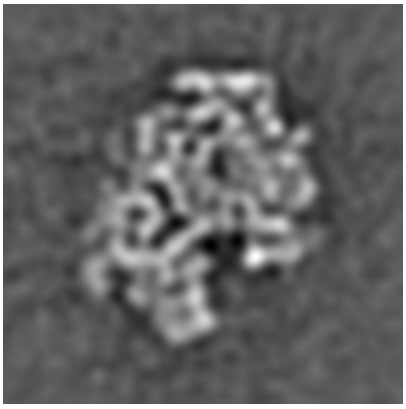
6.2 Central slices (i)

6.2.1 Primary map

X Index: 64



Y Index: 64

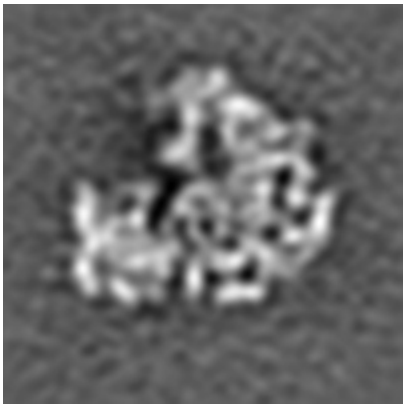


Z Index: 64

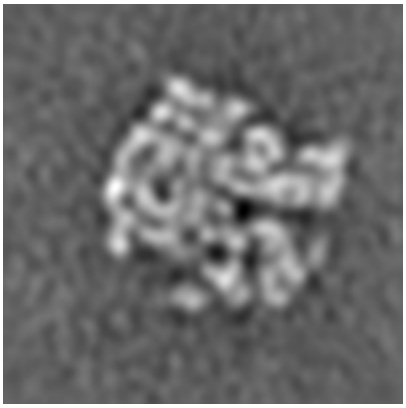
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

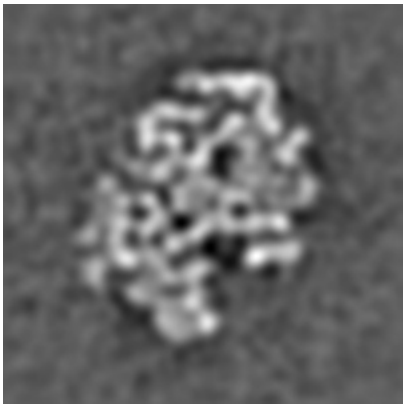
6.3.1 Primary map



X Index: 65



Y Index: 70

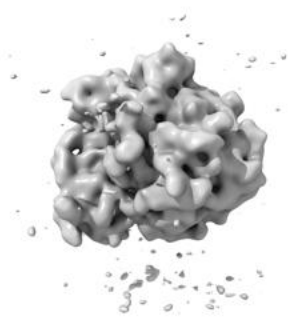


Z Index: 62

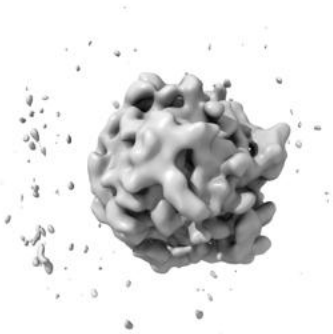
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

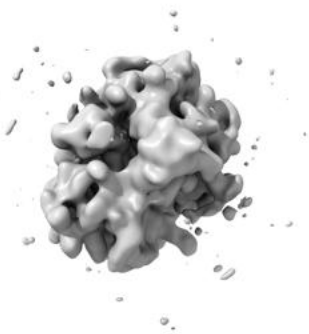
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 20.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

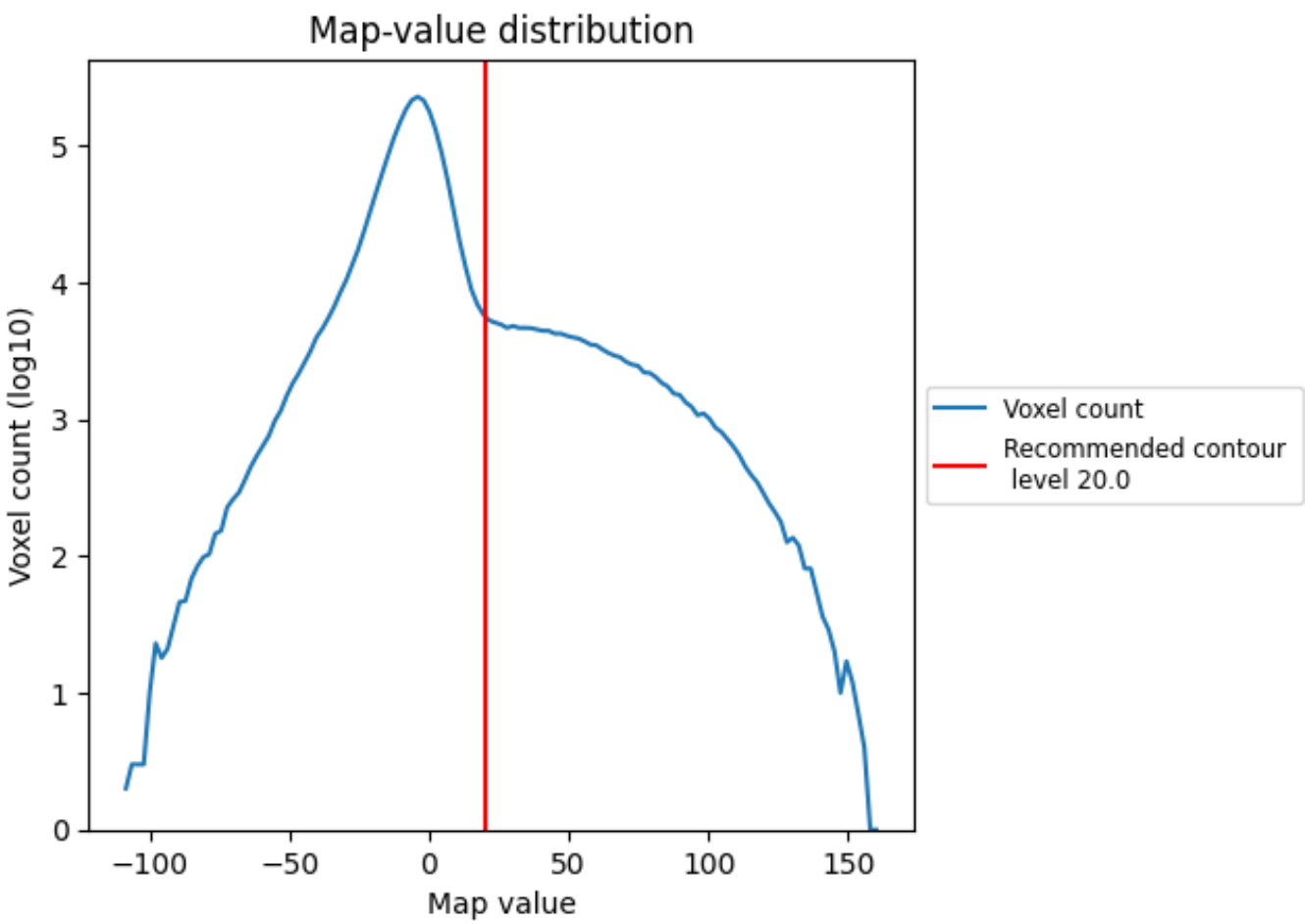
6.5 Mask visualisation (i)

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

7 Map analysis (i)

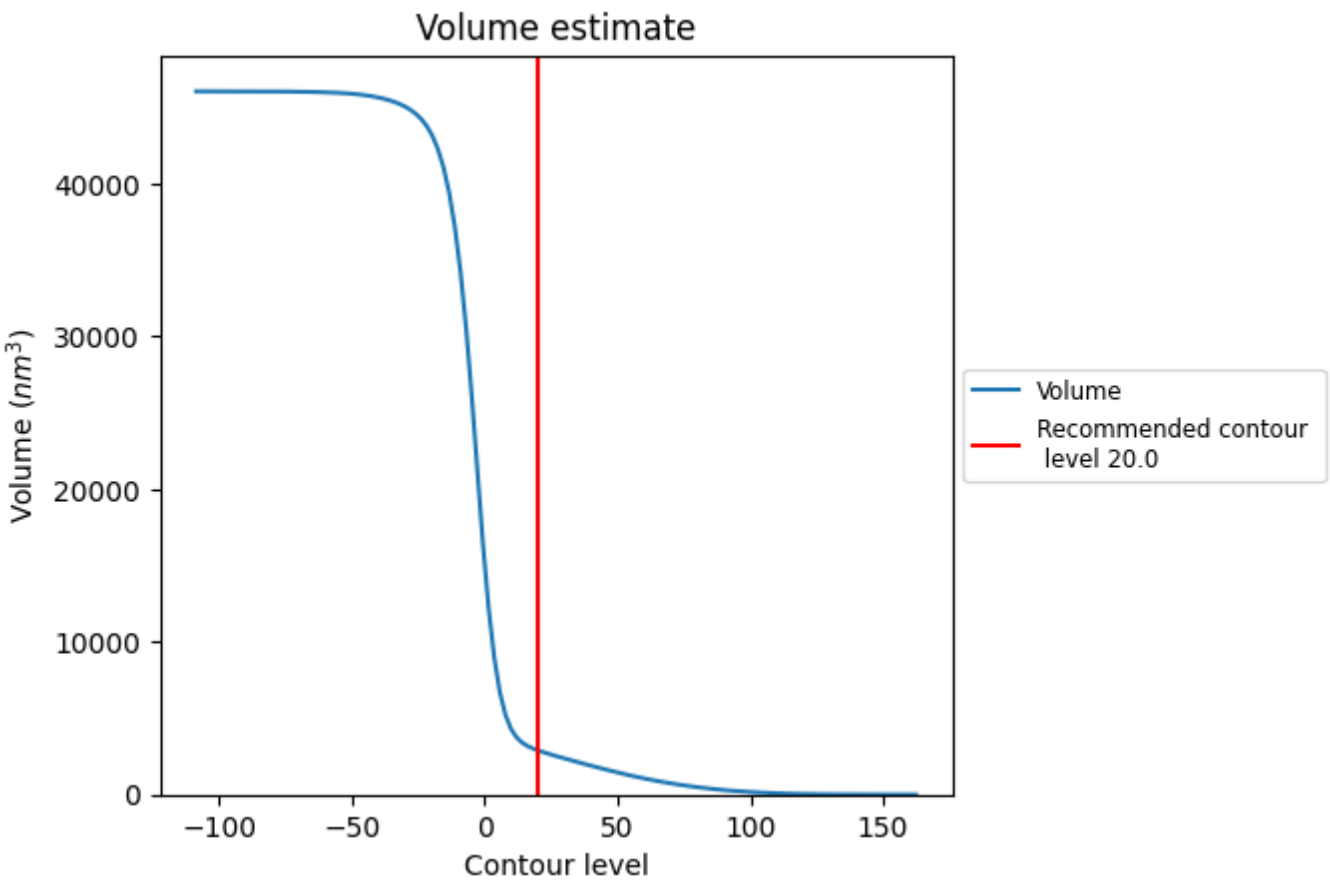
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

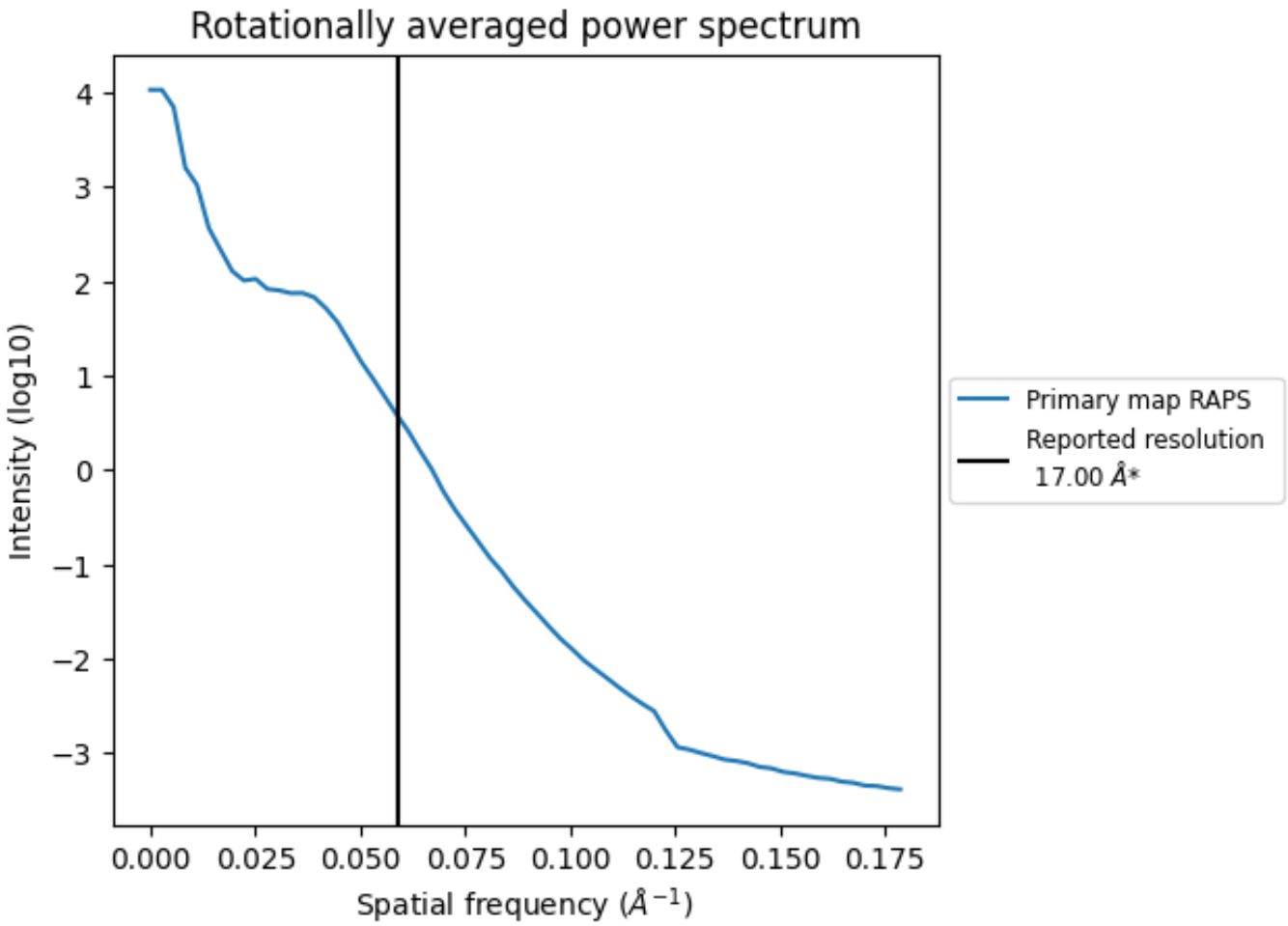
7.2 Volume estimate (i)



The volume at the recommended contour level is 2895 nm^3; this corresponds to an approximate mass of 2615 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 0.059 Å^{-1}

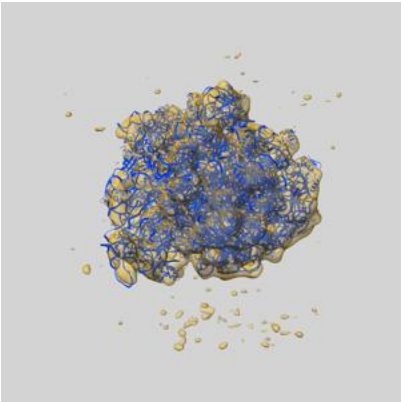
8 Fourier-Shell correlation (i)

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

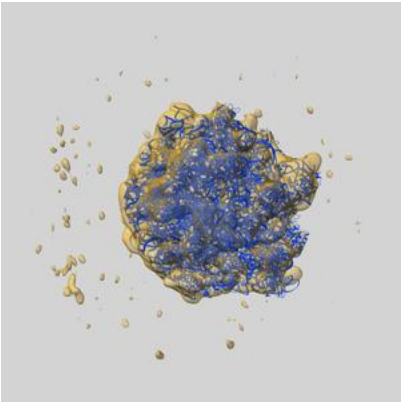
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1720 and PDB model 4V74. Per-residue inclusion information can be found in section 3 on page 17.

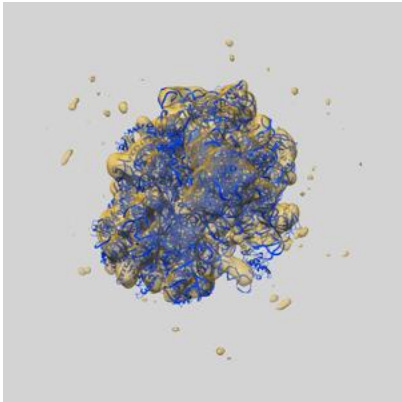
9.1 Map-model overlay (i)



X



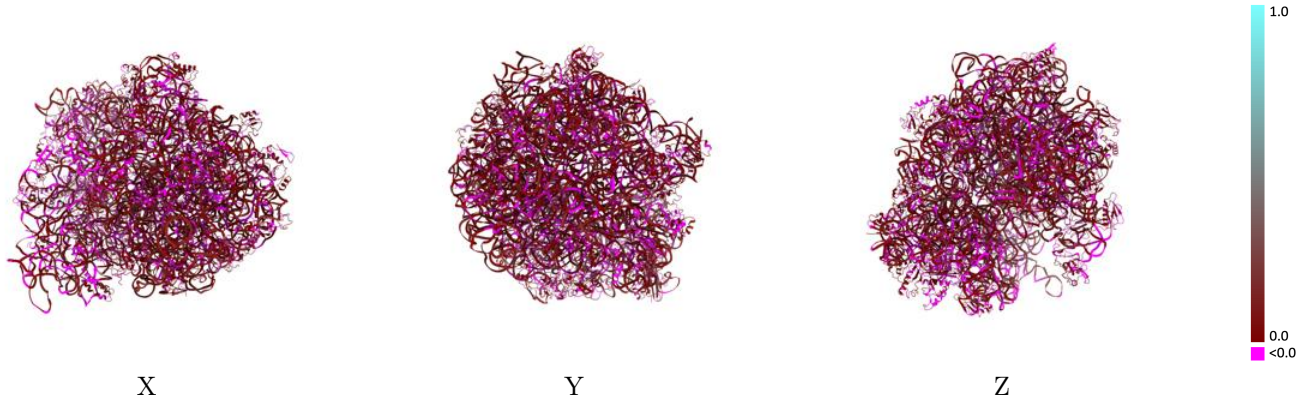
Y



Z

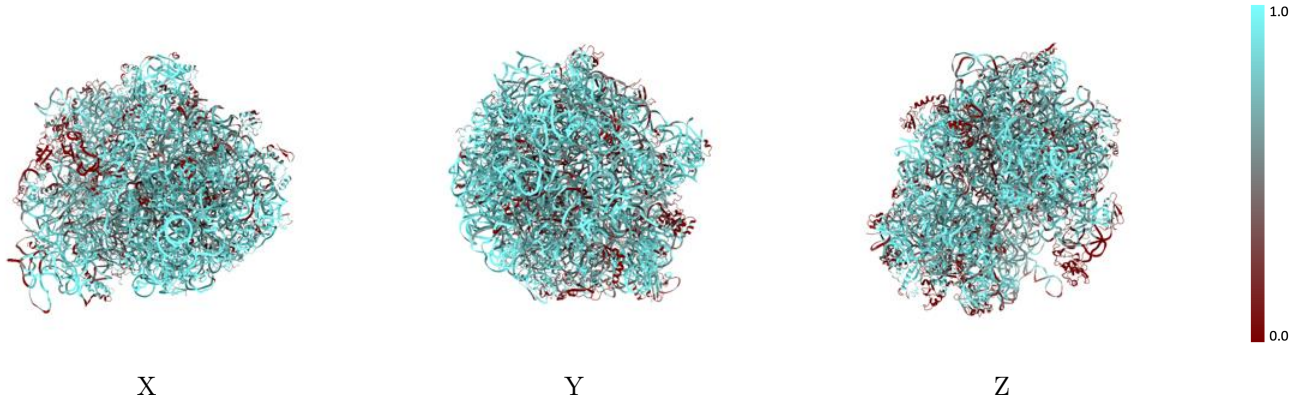
The images above show the 3D surface view of the map at the recommended contour level 20.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



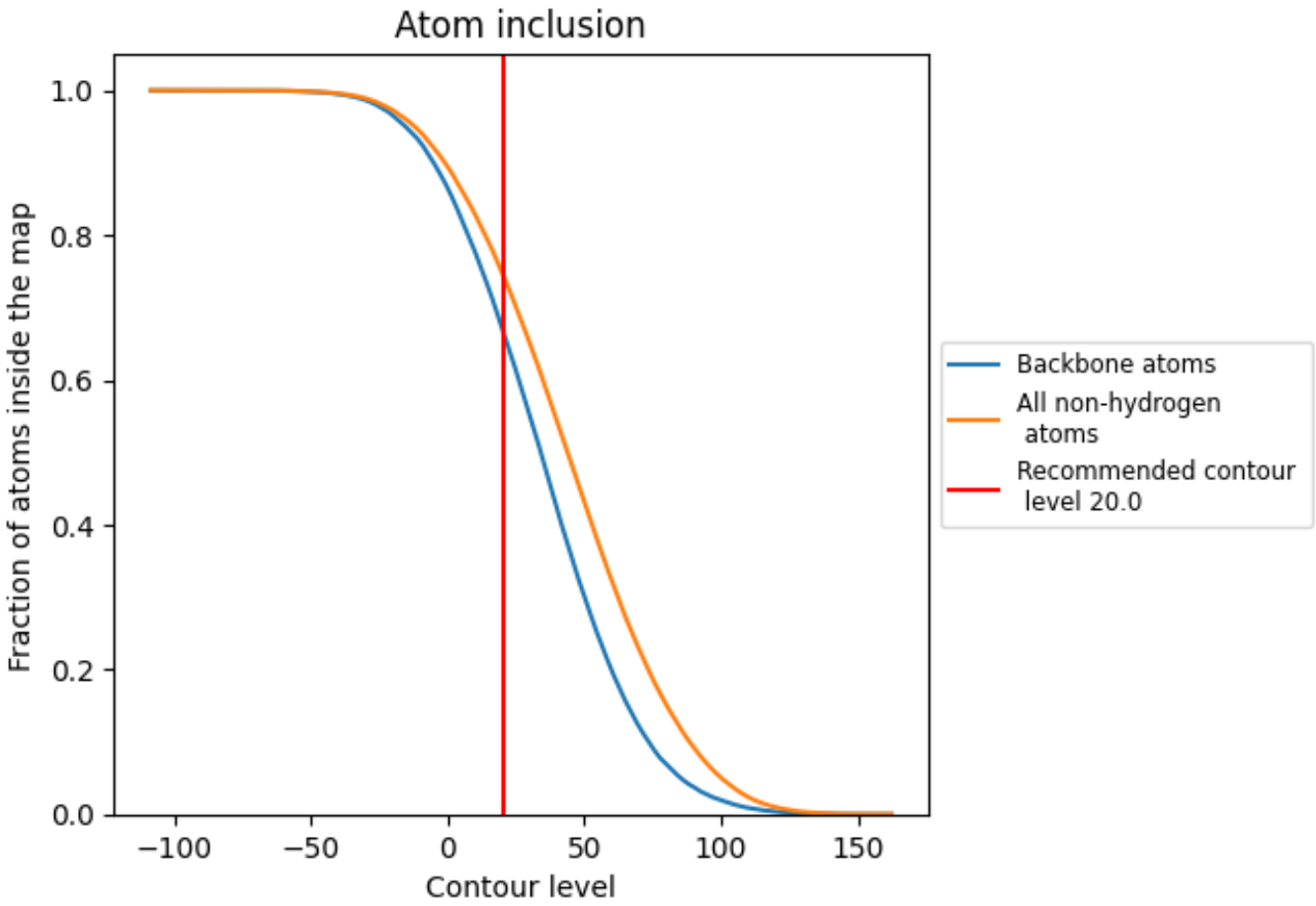
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (i)



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 (20.0).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (20.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7471	0.0520
A1	0.6958	0.0570
A2	0.7735	0.0820
A3	0.7095	0.0620
AA	0.8142	0.0590
AB	0.5495	0.0480
AC	0.4725	0.0200
AD	0.5572	0.0210
AE	0.5534	0.0290
AF	0.8130	0.0430
AG	0.7018	0.0390
AH	0.6573	0.0280
AI	0.6239	0.0300
AJ	0.7696	0.0250
AK	0.7088	0.0460
AL	0.6167	0.0240
AM	0.6734	0.0350
AN	0.5581	0.0250
AO	0.9087	0.0320
AP	0.5251	-0.0030
AQ	0.6472	0.0240
AR	0.6606	0.0150
AS	0.7276	0.0360
AT	0.7132	-0.0010
AU	0.5550	0.0350
B0	0.6822	0.0130
B1	0.7005	0.0550
B2	0.4676	0.0060
B3	0.4521	-0.0330
B4	0.6473	0.0220
B5	0.5695	0.0360
BA	0.8149	0.0680
BB	0.8850	0.0740
BC	0.4536	-0.0050
BD	0.6378	0.0320

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Chain	Atom inclusion	Q-score
BE	0.6184	0.0150
BF	0.7332	0.0500
BG	0.5775	0.0360
BH	0.1414	0.0060
BI	0.0000	-0.0000
BJ	0.6791	0.0210
BK	0.5449	0.0280
BL	0.6457	0.0230
BM	0.5873	0.0190
BN	0.8299	0.0250
BO	0.8389	0.0260
BP	0.5484	0.0270
BQ	0.5738	-0.0130
BR	0.7064	0.0470
BS	0.6316	0.0290
BT	0.7109	0.0300
BU	0.6641	0.0110
BV	0.6707	0.0320
BW	0.5344	-0.0070
BX	0.6339	0.0030
BY	0.5252	0.0260
BZ	0.6384	0.0530