Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 11:54 PM EST

PDB ID	:	4V78
EMDB ID	:	EMD-2475
Title	:	E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post3a)
Authors	:	Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on	:	2013-10-14
Resolution	:	20.00 Å(reported)
Based on initial models	:	2K4C, 2HGP, 2WRI, 3I1O

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

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

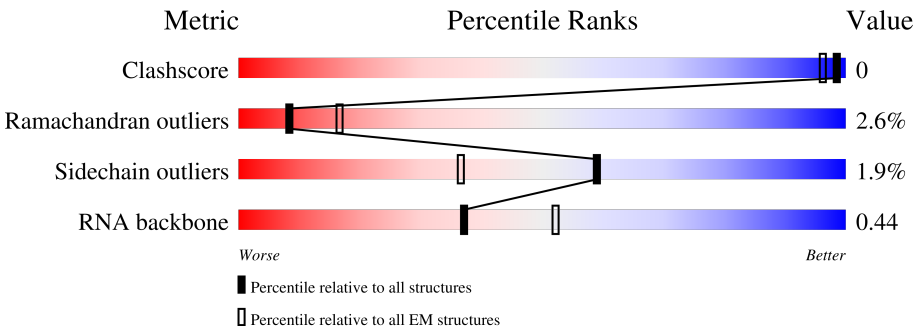
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 20.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	35%, 94%, 5% •
2	AC	208	37%, 87%, 12%
3	AD	206	22%, 86%, 12% •
4	AE	152	23%, 94%, 6%
5	AF	101	49%, 87%, 13%
6	AG	152	14%, 88%, 11% •
7	AH	130	8%, 92%, 8% •

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Mol	Chain	Length	Quality of chain
8	AI	128	5% 84% 16%
9	AJ	100	39% 86% 13%
10	AK	118	20% 92% 7%
11	AL	124	26% 85% 15%
12	AM	115	30% 90% 10%
13	AN	101	25% 87% 10%
14	AO	89	18% 88% 11%
15	AP	81	25% 78% 22%
16	AQ	82	37% 90% 9%
17	AR	57	42% 84% 16%
18	AS	81	56% 90% 9%
19	AT	86	20% 86% 13%
20	AU	53	8% 75% 25%
21	AA	1533	6% 23% 50% 22%
22	A1	76	33% 20% 46% 34%
23	A2	15	60% 27% 13%
24	A3	77	48% 23% 48% 23% 5%
25	BC	273	38% 89% 9%
26	BD	209	26% 90% 9%
27	BE	201	28% 89% 10%
28	BF	179	19% 89% 10%
29	BG	177	15% 89% 10%
30	BH	149	74% 95% 5%
31	BI	142	69% 95%
32	BJ	142	26% 90% 10%

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Mol	Chain	Length	Quality of chain
33	BK	123	40% 89% 11%
34	BL	144	40% 86% 12%
35	BM	136	22% 90% 9%
36	BN	121	25% 88% 11%
37	BO	117	21% 87% 11%
38	BP	115	25% 84% 15%
39	BQ	118	30% 85% 14%
40	BR	103	29% 92% 8%
41	BS	110	25% 92% 7%
42	BT	94	13% 91% 7%
43	BU	104	43% 88% 12%
44	BV	94	14% 95% 5%
45	BW	80	28% 89% 10%
46	BX	79	14% 86% 11%
47	BY	63	59% 92% 8%
48	BZ	59	31% 85% 12%
49	B0	57	28% 77% 21%
50	B1	52	27% 87% 13%
51	B2	46	59% 78% 22%
52	B3	65	37% 85% 14%
53	B4	38	16% 87% 13%
54	BA	2903	8% 22% 52% 22%
55	BB	118	17% 59% 19%
56	B5	234	63% 88% 7% 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

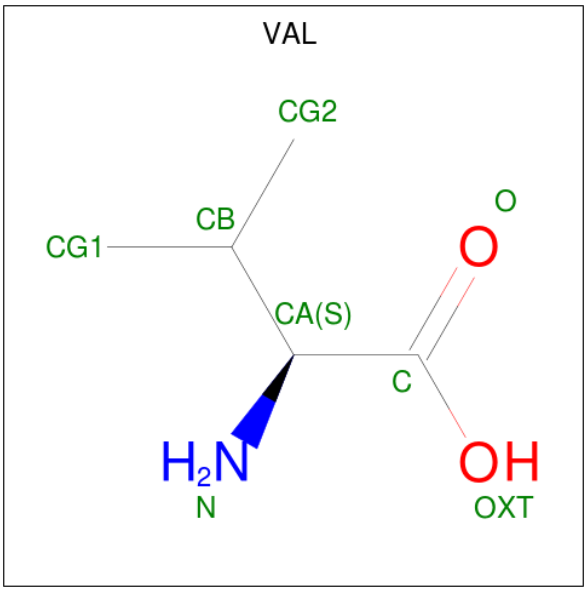
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

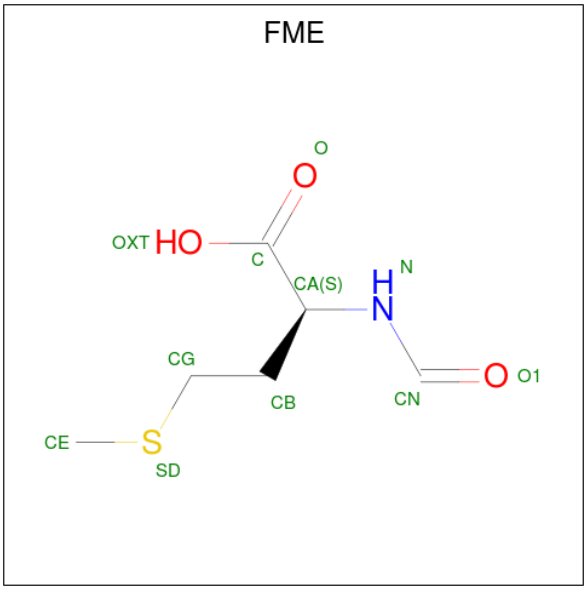
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	B5	223	1658	1038	302	312	6	0	0

- 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: $C_6H_{11}NO_3S$).



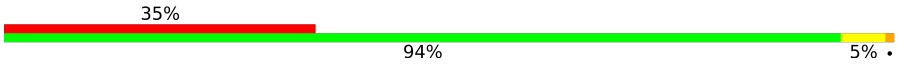
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
58	BA	1	10	6	1	2	1	0

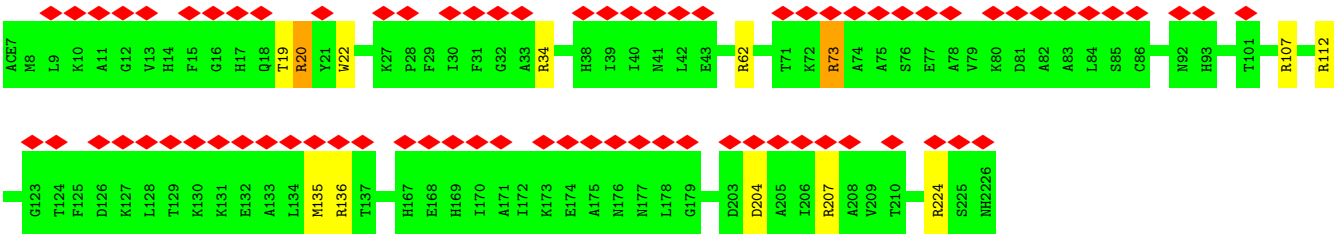
3 Residue-property plots (i)

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

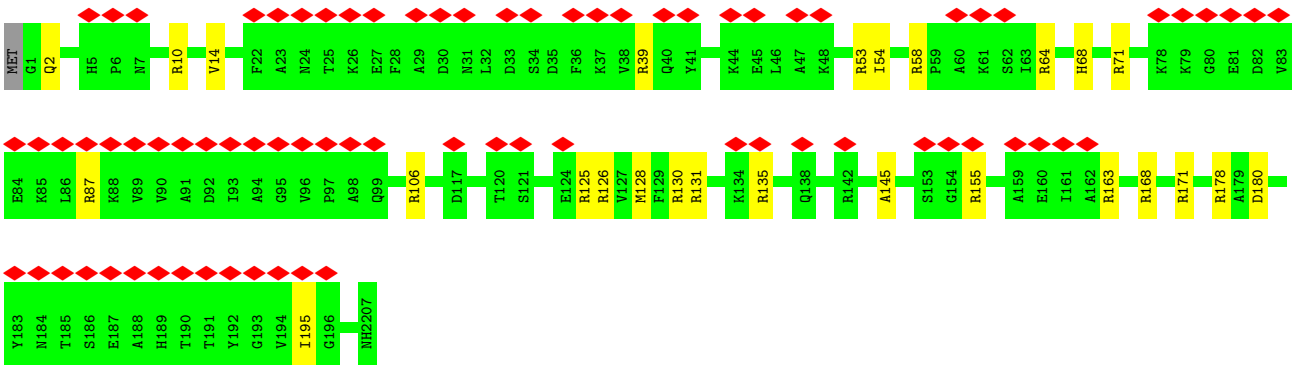
Chain AB:





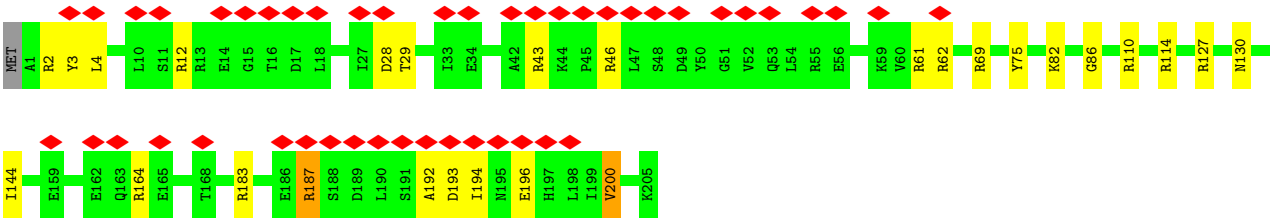
- Molecule 2: 30S ribosomal protein S3

Chain AC:



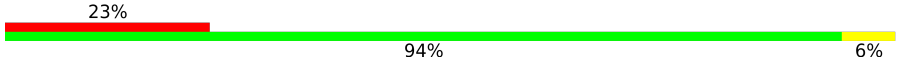
- Molecule 3: 30S ribosomal protein S4

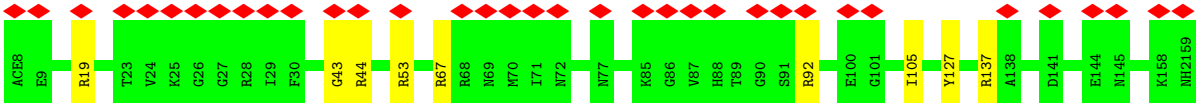
Chain AD:



• Molecule 4: 30S ribosomal protein S5

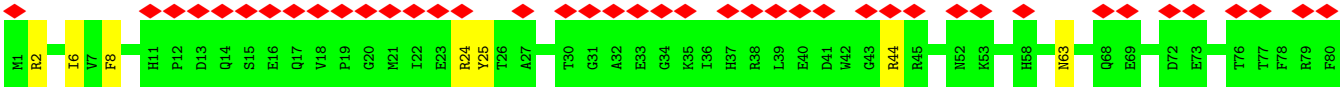
Chain AE:

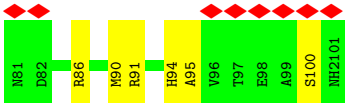




• Molecule 5: 30S ribosomal protein S6

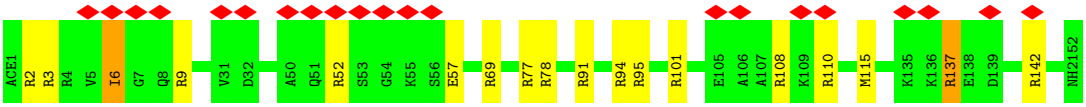
Chain AF:





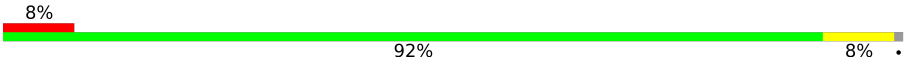
• Molecule 6: 30S ribosomal protein S7

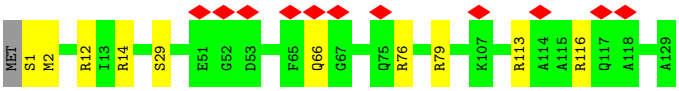
Chain AG:



• Molecule 7: 30S ribosomal protein S8

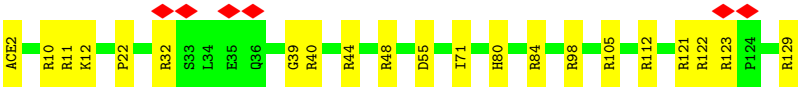
Chain AH:





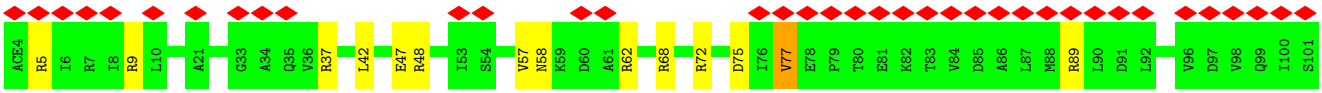
• Molecule 8: 30S ribosomal protein S9

Chain AI:



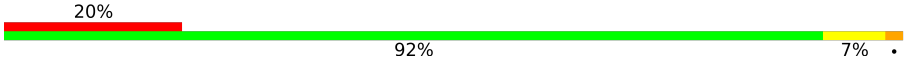
• Molecule 9: 30S ribosomal protein S10

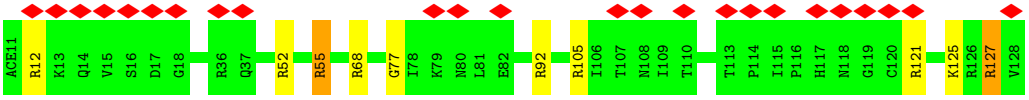
Chain AJ:



• Molecule 10: 30S ribosomal protein S11

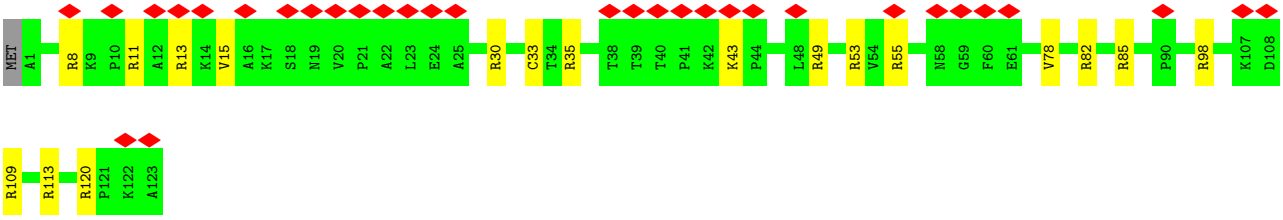
Chain AK:





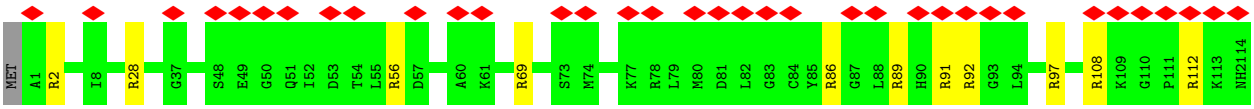
• Molecule 11: 30S ribosomal protein S12

Chain AL:



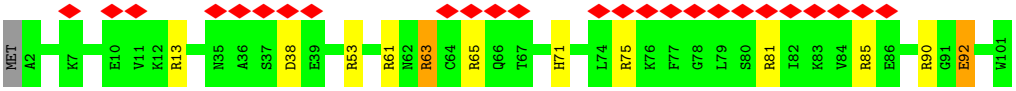
• Molecule 12: 30S ribosomal protein S13

Chain AM:



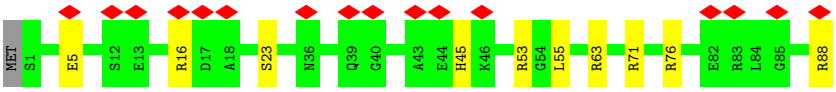
• Molecule 13: 30S ribosomal protein S14

Chain AN:



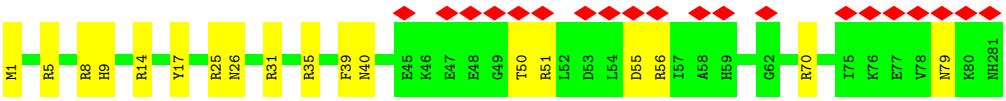
• Molecule 14: 30S ribosomal protein S15

Chain AO:



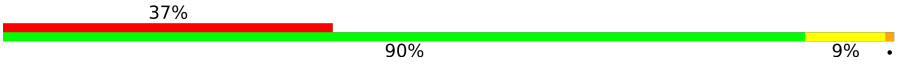
• Molecule 15: 30S ribosomal protein S16

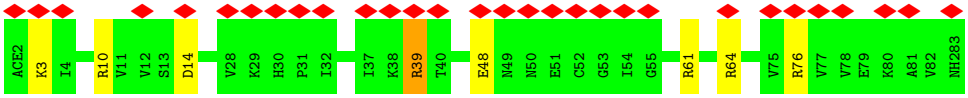
Chain AP:



• Molecule 16: 30S ribosomal protein S17

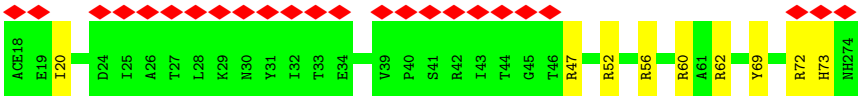
Chain AQ:





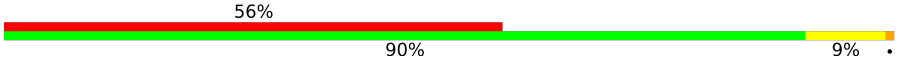
• Molecule 17: 30S ribosomal protein S18

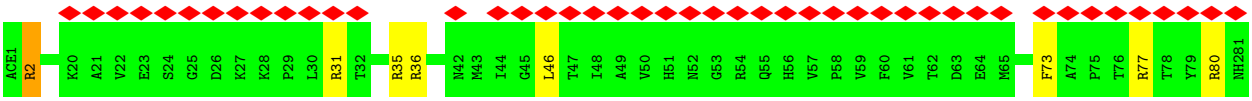
Chain AR:



• Molecule 18: 30S ribosomal protein S19

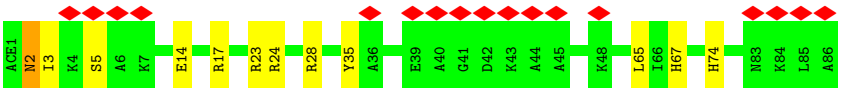
Chain AS:





• Molecule 19: 30S ribosomal protein S20

Chain AT:

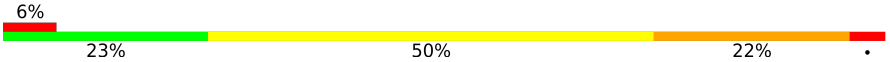


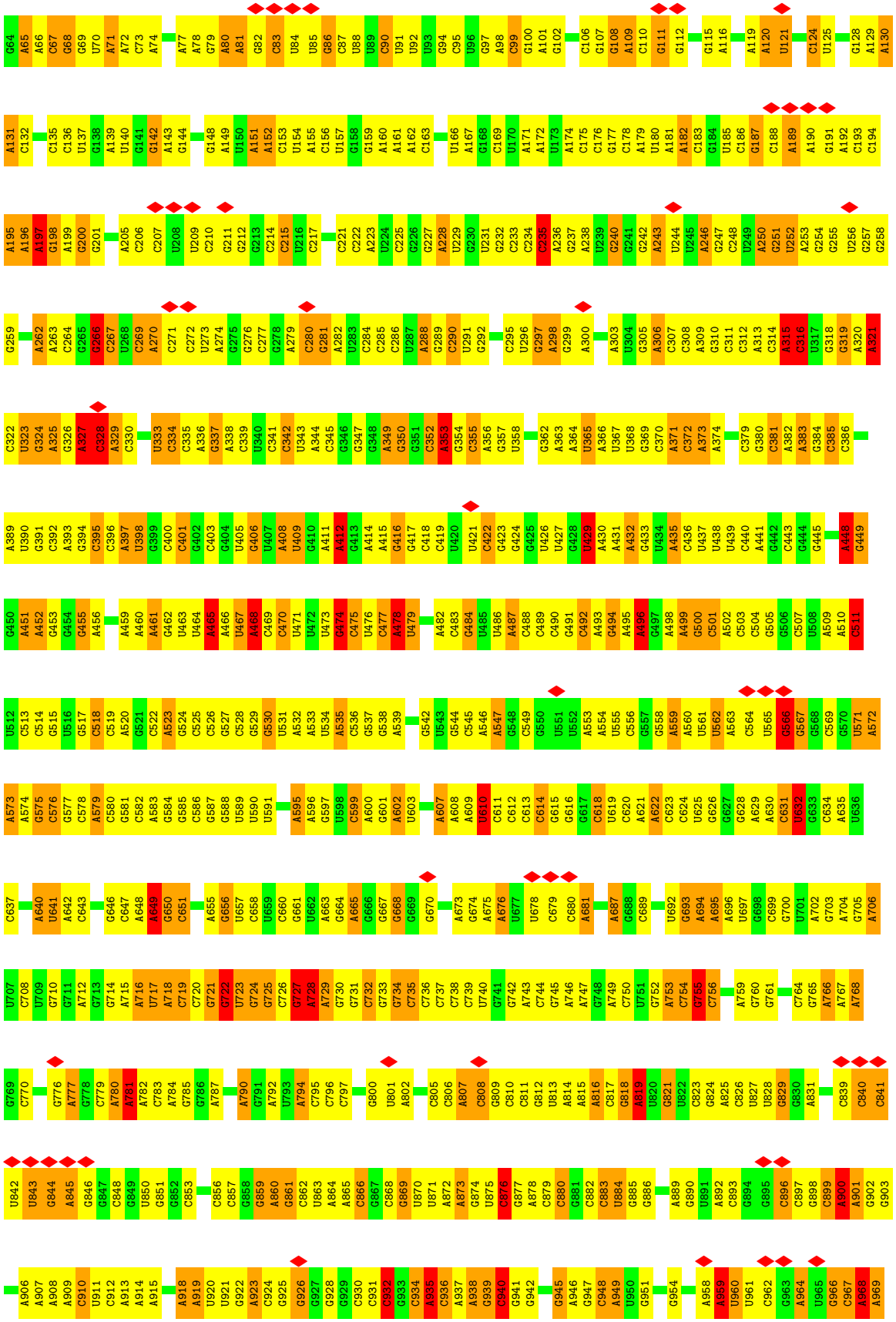
• Molecule 20: 30S ribosomal protein S21

Chain AU:

• Molecule 21: 16S ribosomal RNA

Chain AA:

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A131 C132 C135 C136 U137 G138 A139 U140 G141 G142 A143 G144 G148 A149 U150 A151 A152 C153 U154 A155 C156 U157 G158 G159 A160 A161 A162 C163 U166 A167 G168 C169 U170 A171 A172 U173 A174 C175 C176 G177 C178 A179 U180 A181 A182 C183 G184 U185 C186 G187 C188 A189 A190 G191 A192 C193 C194
A195 A196 A197 G198 A199 G200 G201 A205 C206 C207 U208 U209 C210 G211 G212 G213 C214 C215 U216 C217 C221 C222 A223 U224 C225 G226 G227 A228 U229 G230 U231 G232 C233 C234 C235 A236 G237 A238 U239 G240 G241 G242 A243 U244 U245 A246 G247 C248 U249 A250 G251 U252 A253 G254 G255 U256 G257 G258
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C322 U323 G324 A325 G326 A327 C328 A329 C330 U333 C334 C335 A336 G337 A338 C339 U340 C341 C342 U343 A344 G345 G346 G347 G348 A349 G350 G351 C352 A353 G354 C355 A356 G357 U358 G362 A363 A364 U365 A366 U367 U368 G369 C370 A371 C372 A373 A374 C379 G380 C381 A382 A383 G384 C385 C386
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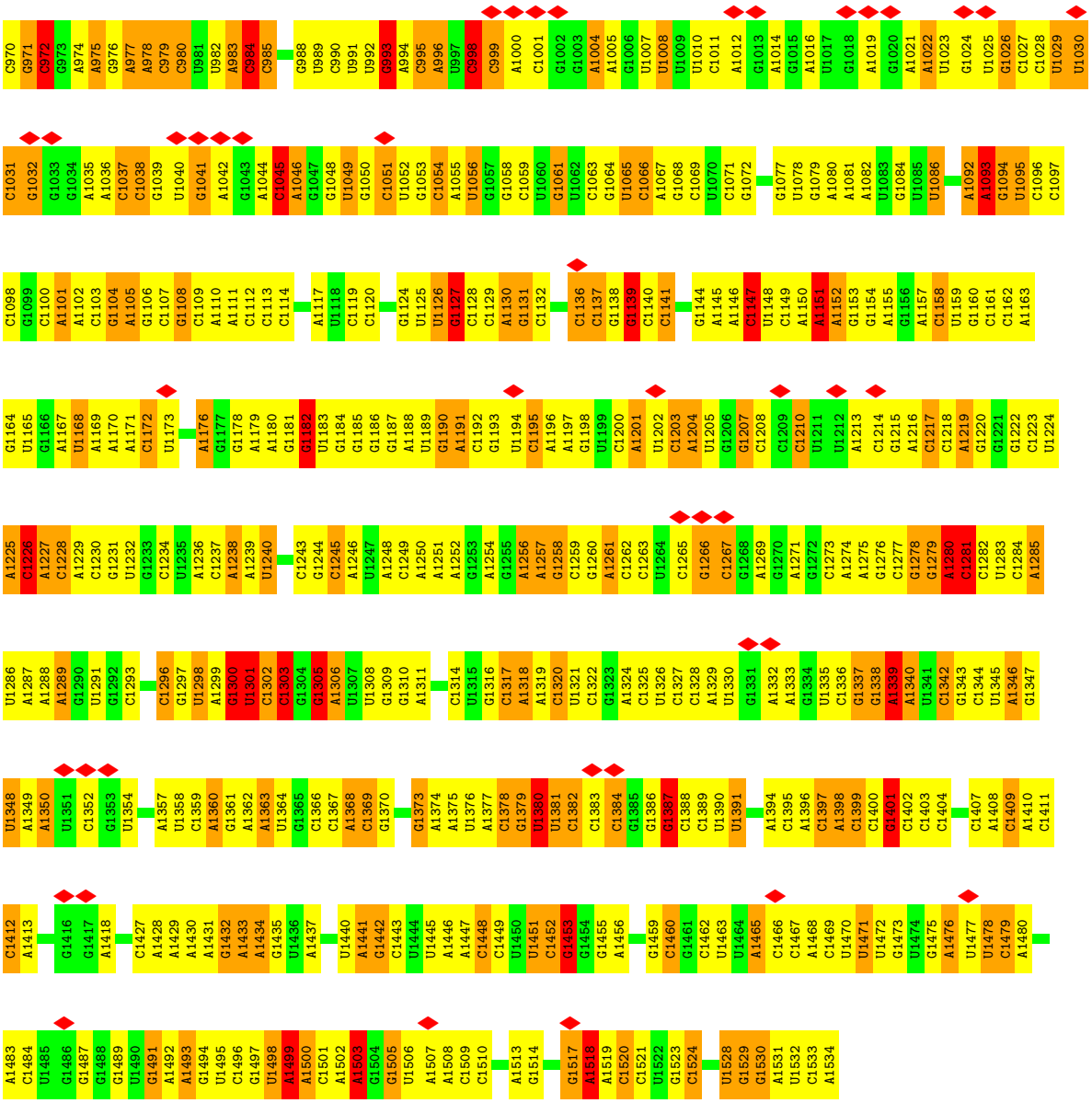
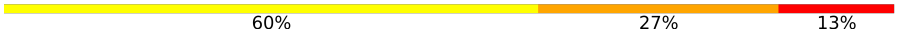


• Molecule 22: fMet-Val-tRNA-Val

Chain A1:

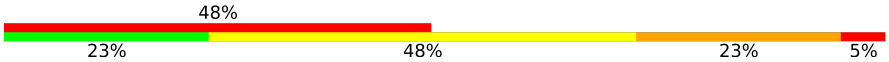
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

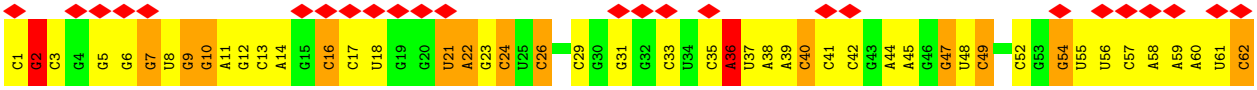
Chain A2:

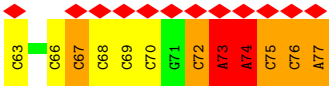


- Molecule 24: tRNA-fMet

Chain A3:

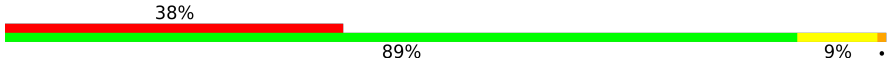


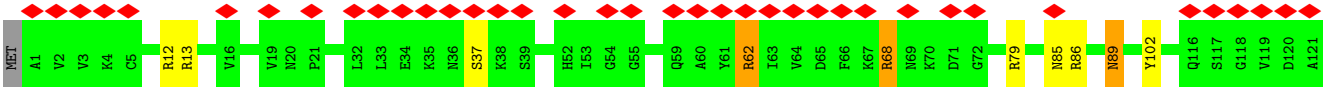


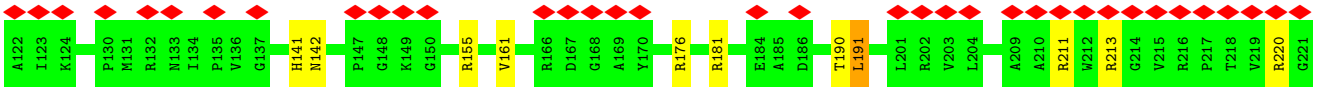


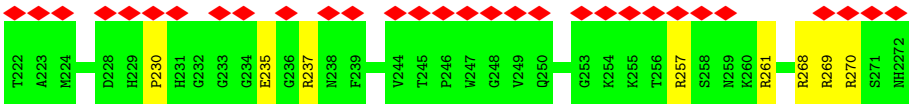
- Molecule 25: 50S ribosomal protein L2

Chain BC:



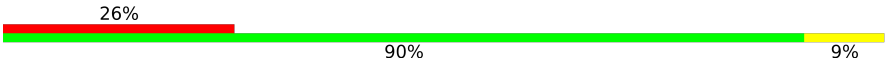


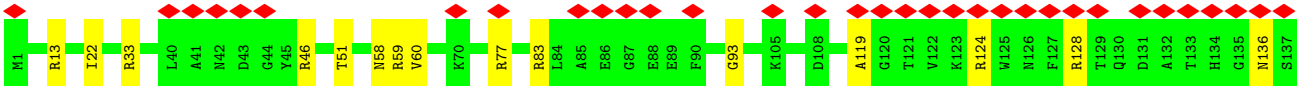


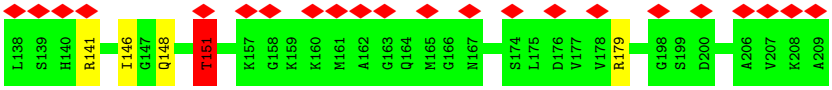


- Molecule 26: 50S ribosomal protein L3

Chain BD:

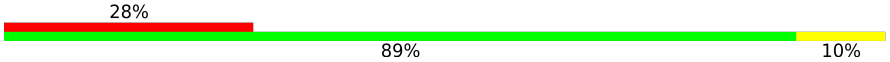


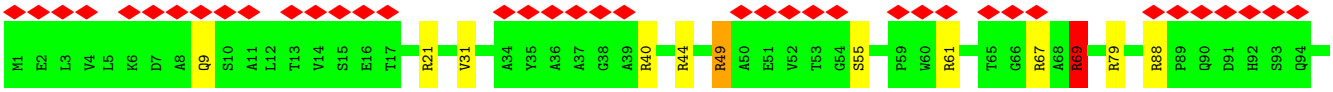


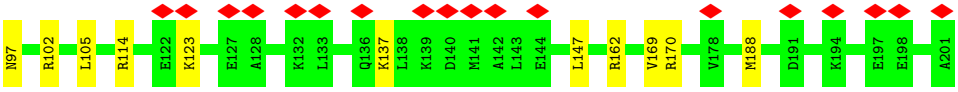


- Molecule 27: 50S ribosomal protein L4

Chain BE:

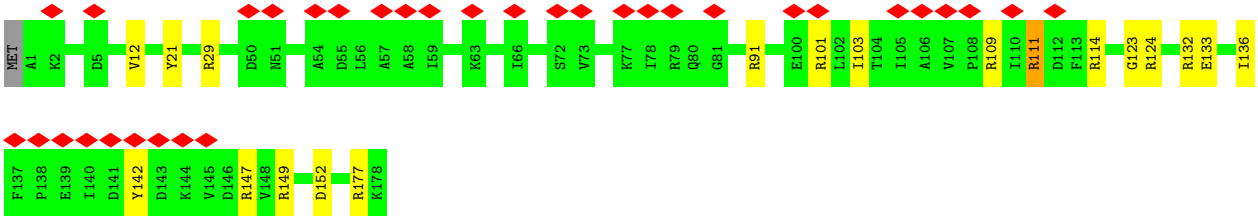






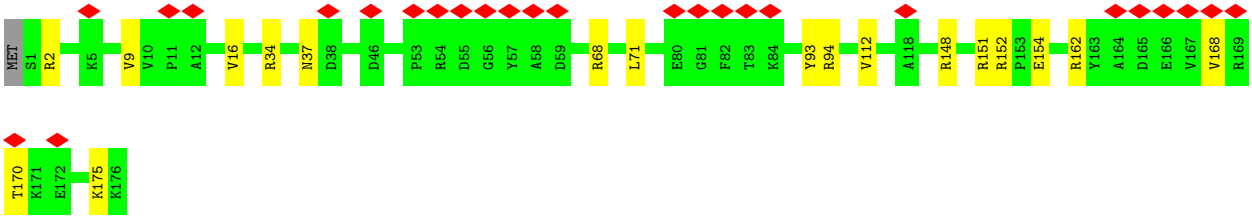
• Molecule 28: 50S ribosomal protein L5

Chain BF:



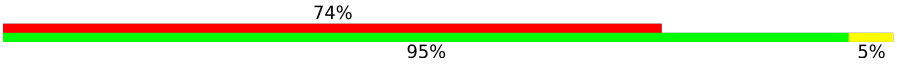
• Molecule 29: 50S ribosomal protein L6

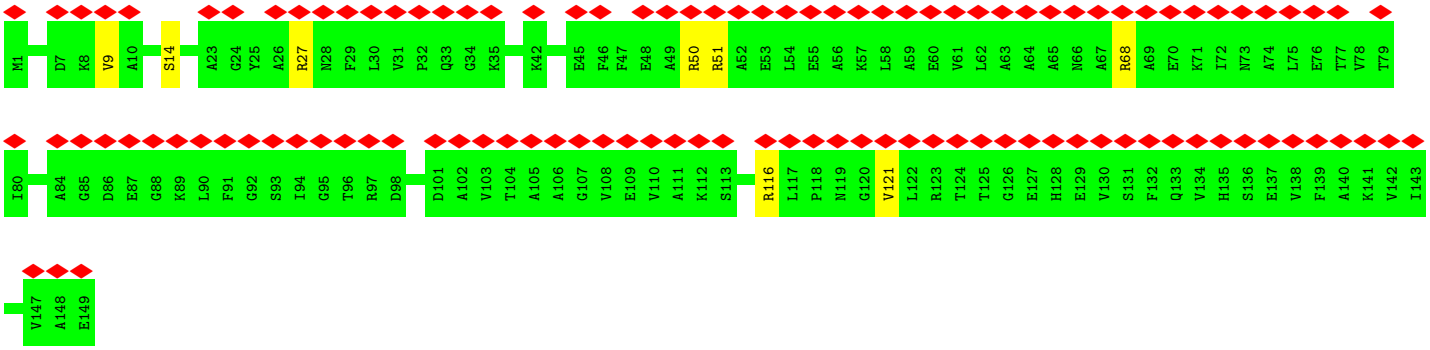
Chain BG:



• Molecule 30: 50S ribosomal protein L9

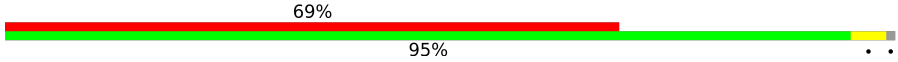
Chain BH:

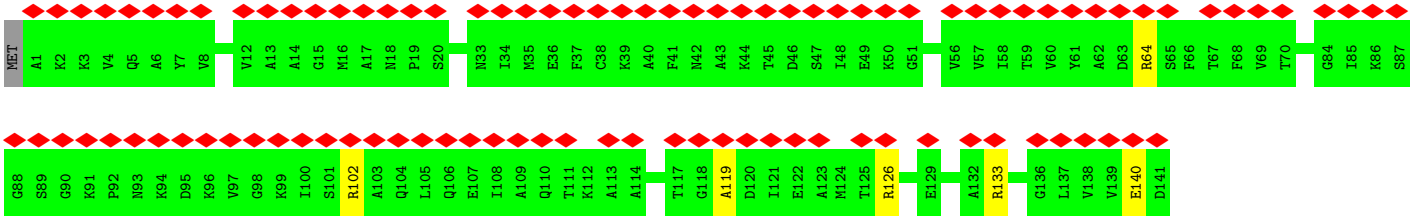




• Molecule 31: 50S ribosomal protein L11

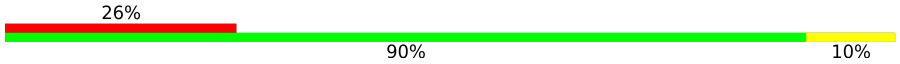
Chain BI:

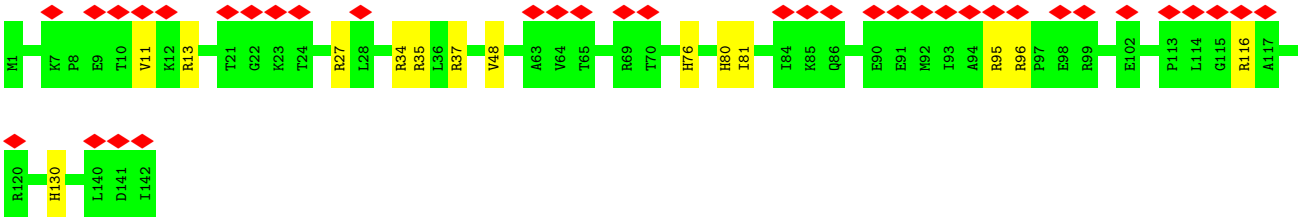




• Molecule 32: 50S ribosomal protein L13

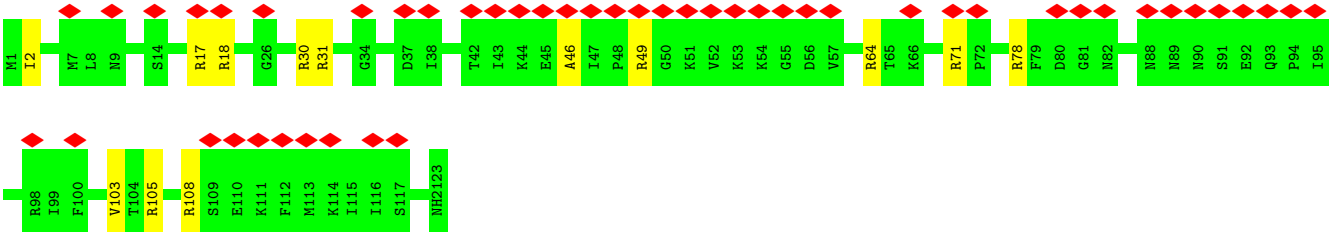
Chain BJ:





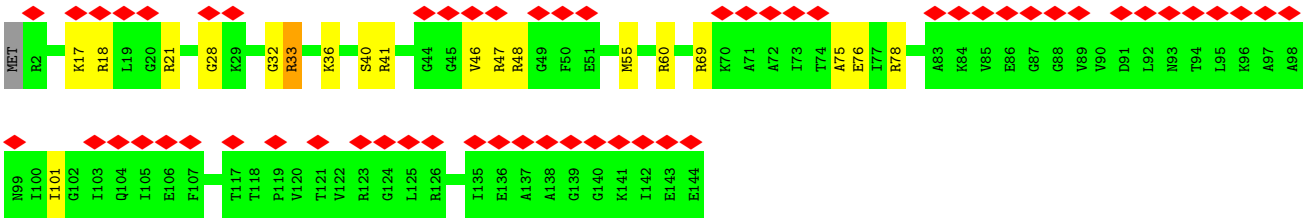
- Molecule 33: 50S ribosomal protein L14

Chain BK:



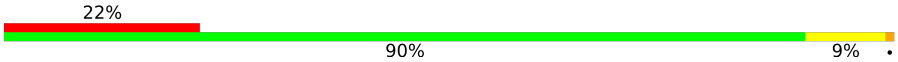
- Molecule 34: 50S ribosomal protein L15

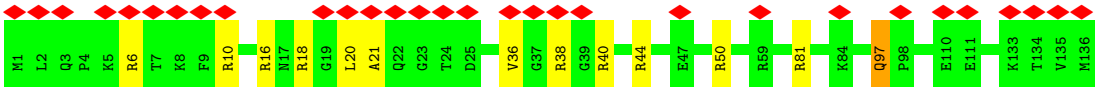
Chain BL:



- Molecule 35: 50S ribosomal protein L16

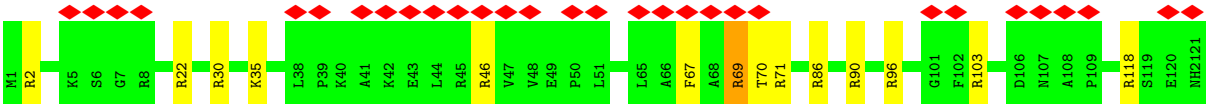
Chain BM:





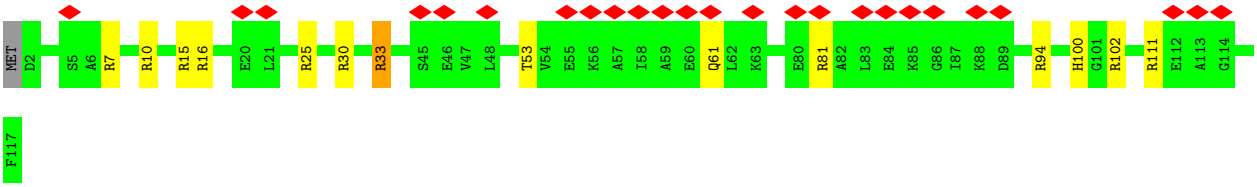
- Molecule 36: 50S ribosomal protein L17

Chain BN:



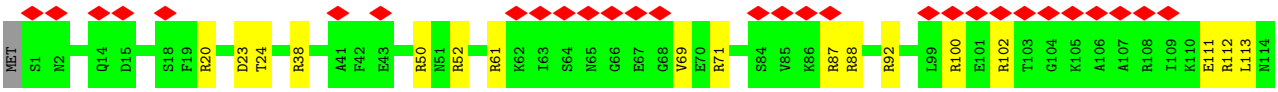
- Molecule 37: 50S ribosomal protein L18

Chain BO: 21% 87% 11%



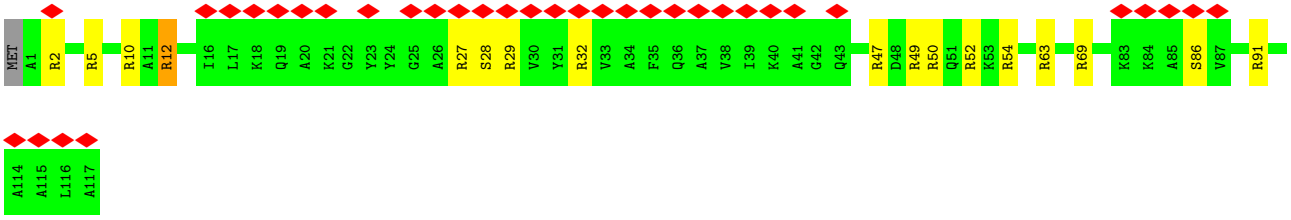
• Molecule 38: 50S ribosomal protein L19

Chain BP: 25% 84% 15%



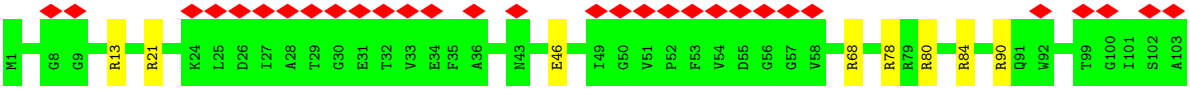
• Molecule 39: 50S ribosomal protein L20

Chain BQ: 30% 85% 14%



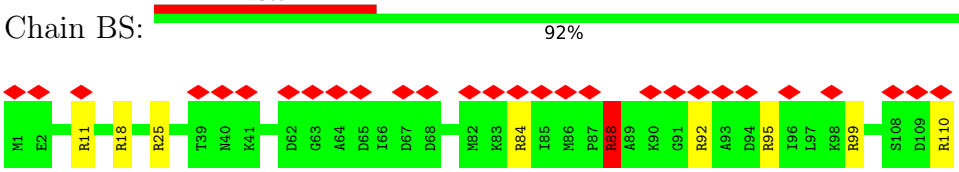
• Molecule 40: 50S ribosomal protein L21

Chain BR: 29% 92% 8%



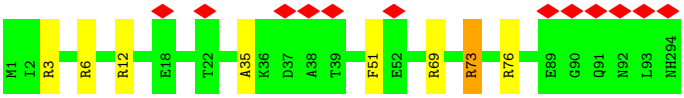
• Molecule 41: 50S ribosomal protein L22

Chain BS: 25% 92% 7%



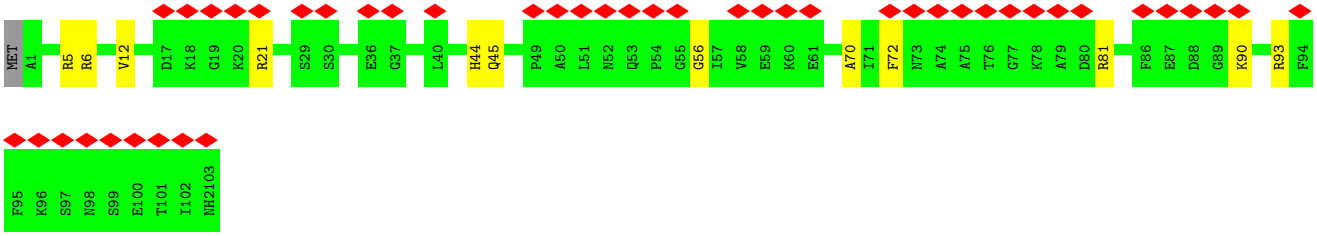
• Molecule 42: 50S ribosomal protein L23

Chain BT: 13% 91% 7%



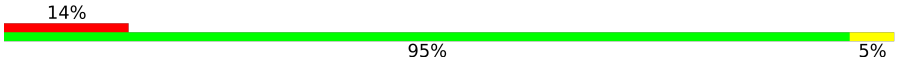
• Molecule 43: 50S ribosomal protein L24

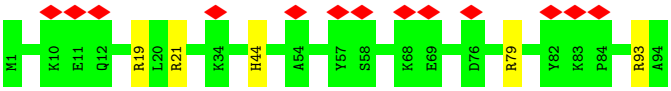
Chain BU:



• Molecule 44: 50S ribosomal protein L25

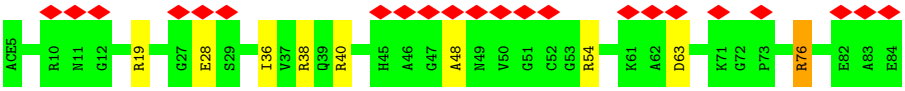
Chain BV:





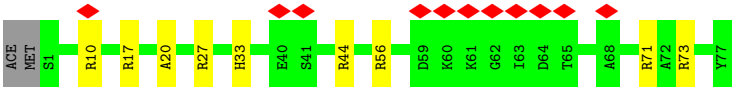
• Molecule 45: 50S ribosomal protein L27

Chain BW:



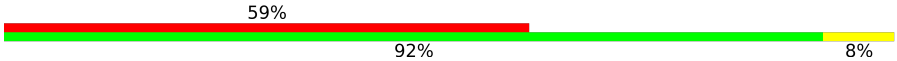
• Molecule 46: 50S ribosomal protein L28

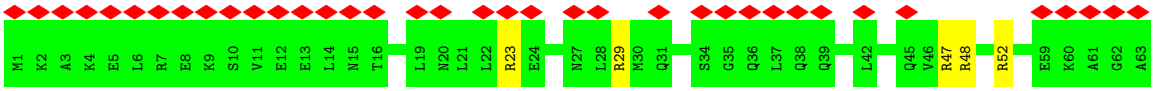
Chain BX:



• Molecule 47: 50S ribosomal protein L29

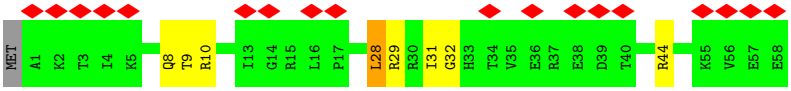
Chain BY:





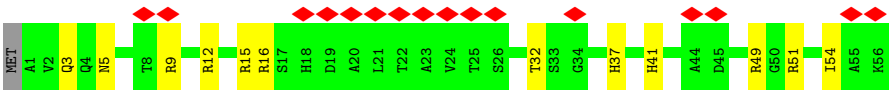
• Molecule 48: 50S ribosomal protein L30

Chain BZ:



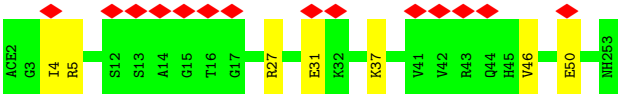
• Molecule 49: 50S ribosomal protein L32

Chain B0:



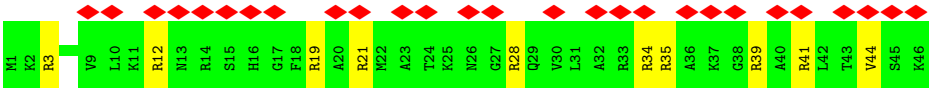
- Molecule 50: 50S ribosomal protein L33

Chain B1:



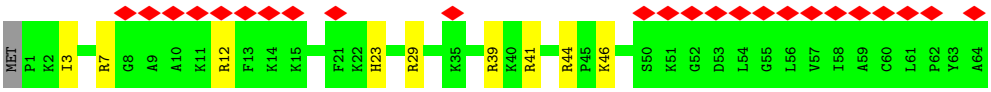
- Molecule 51: 50S ribosomal protein L34

Chain B2:



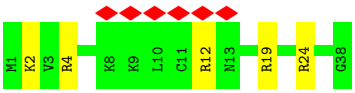
- Molecule 52: 50S ribosomal protein L35

Chain B3:



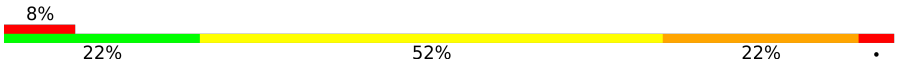
- Molecule 53: 50S ribosomal protein L36

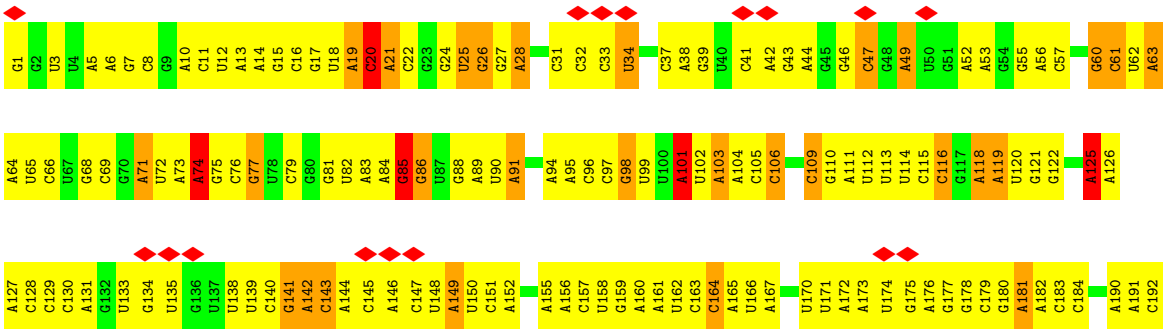
Chain B4:

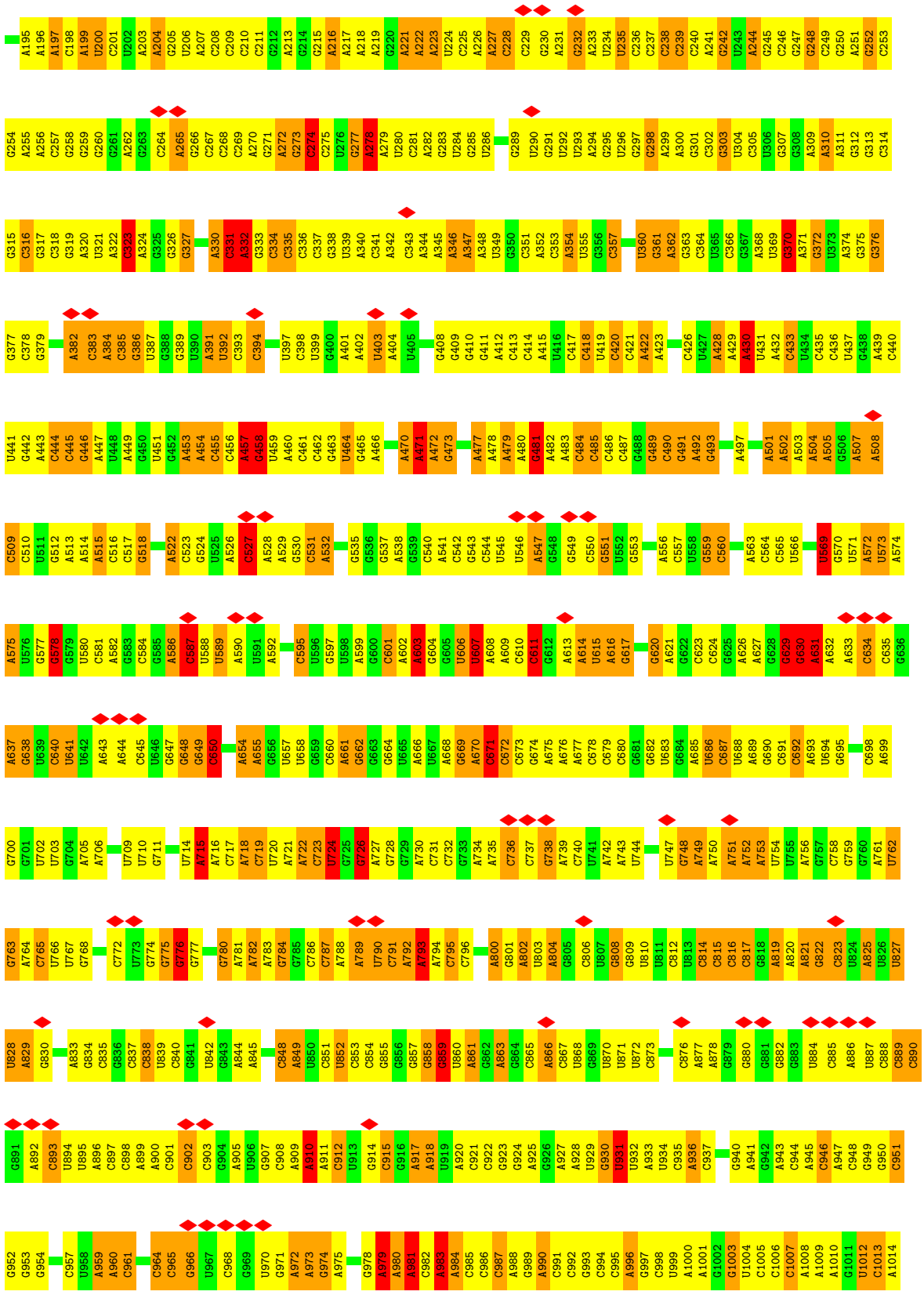


- Molecule 54: 23S ribosomal RNA

Chain BA:



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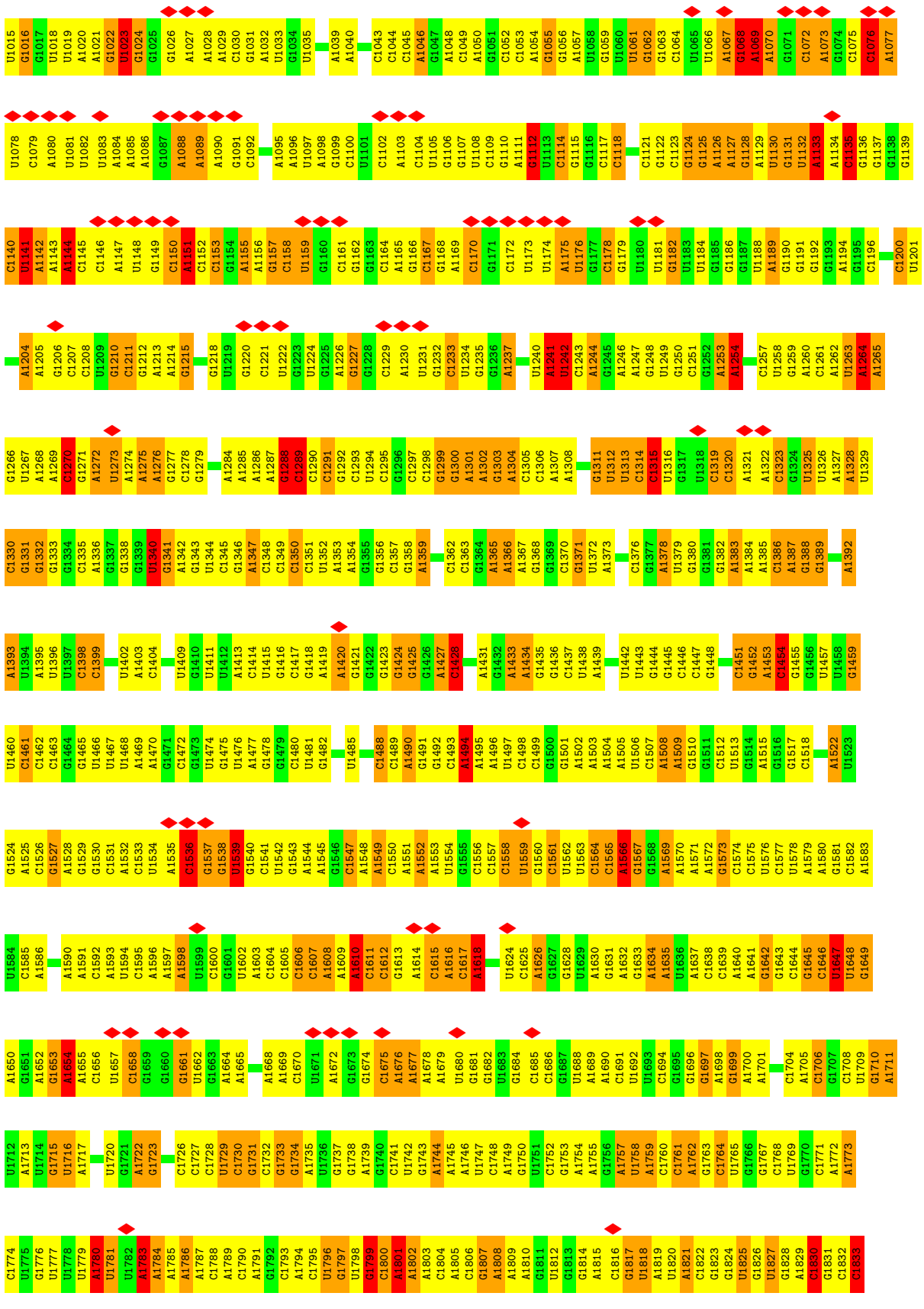
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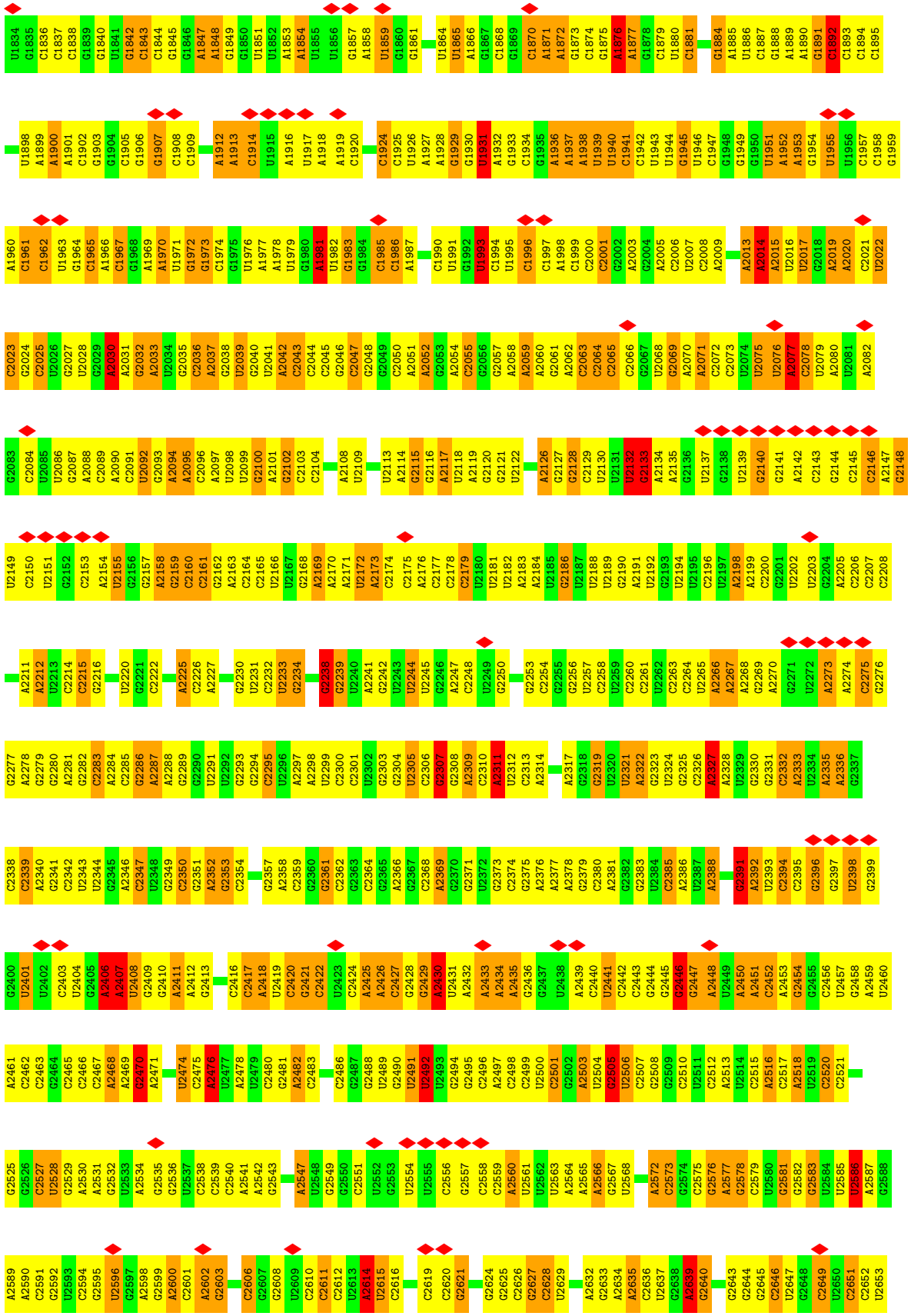
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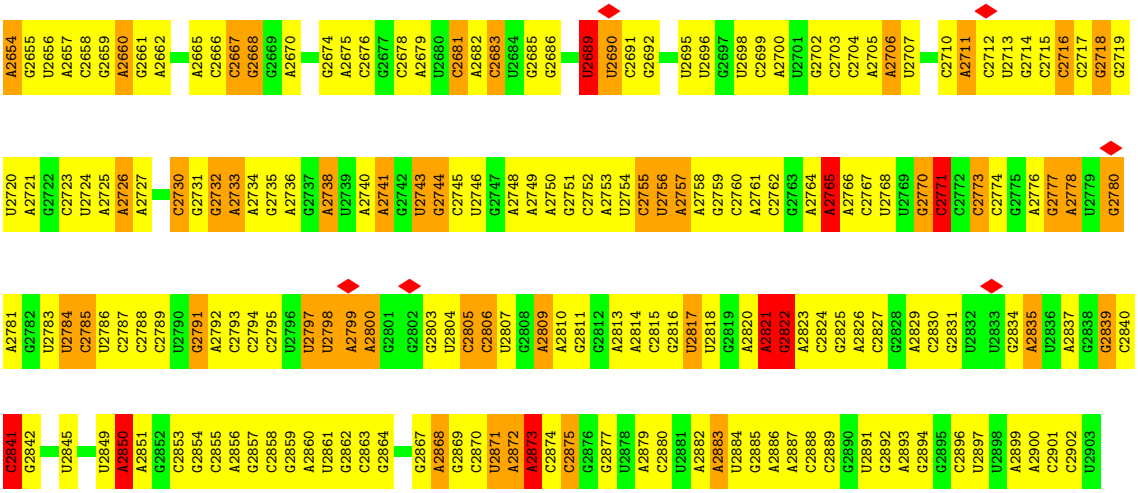
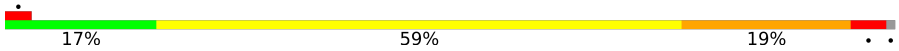
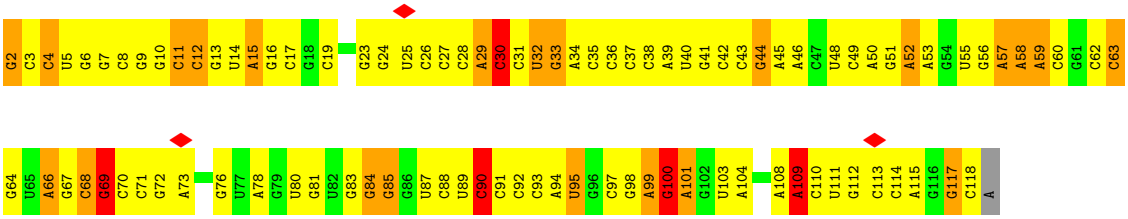


- Molecule 55: 5S ribosomal RNA

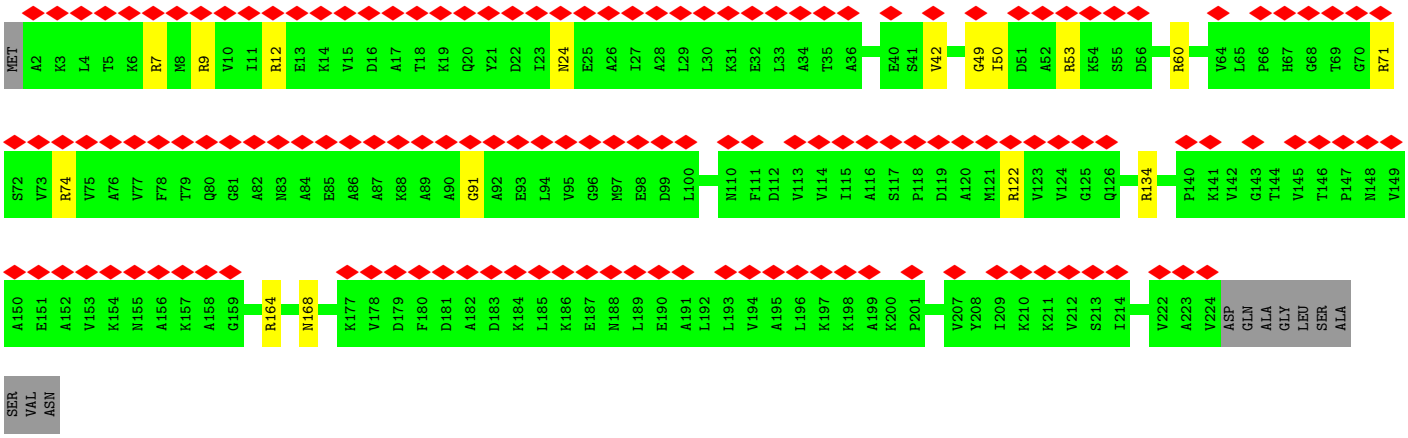
Chain BB:





- 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	5371	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
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	161000	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	222.167	Depositor
Minimum map value	-162.027	Depositor
Average map value	0.002	Depositor
Map value standard deviation	24.233	Depositor
Recommended contour level	25.0	Depositor
Map size (Å)	359.04, 359.04, 359.04	wwPDB
Map dimensions	96, 96, 96	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.74, 3.74, 3.74	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: ACE, 6MZ, FME, CM0, H2U, 5MU, PSU, 4SU, NH2, 7MG, OMC

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	0.67	0/1736	1.06	12/2340 (0.5%)
2	AC	0.70	0/1651	1.18	18/2225 (0.8%)
3	AD	0.74	0/1665	1.20	17/2227 (0.8%)
4	AE	0.66	0/1119	1.03	7/1506 (0.5%)
5	AF	0.71	0/835	1.12	7/1128 (0.6%)
6	AG	0.72	0/1188	1.27	17/1593 (1.1%)
7	AH	0.69	0/989	1.07	8/1326 (0.6%)
8	AI	0.77	0/1035	1.21	13/1377 (0.9%)
9	AJ	0.71	0/797	1.16	9/1079 (0.8%)
10	AK	0.73	0/894	1.10	8/1207 (0.7%)
11	AL	0.73	0/969	1.29	17/1300 (1.3%)
12	AM	0.72	0/884	1.36	14/1181 (1.2%)
13	AN	0.75	0/817	1.18	10/1088 (0.9%)
14	AO	0.70	0/722	1.18	7/964 (0.7%)
15	AP	0.74	0/648	1.27	11/870 (1.3%)
16	AQ	0.66	0/658	1.17	7/883 (0.8%)
17	AR	0.76	0/463	1.17	6/623 (1.0%)
18	AS	0.72	0/653	1.19	7/879 (0.8%)
19	AT	0.67	0/672	1.13	6/890 (0.7%)
20	AU	0.83	0/431	1.48	7/572 (1.2%)
21	AA	1.61	27/36759 (0.1%)	2.23	2065/57346 (3.6%)
22	A1	1.63	0/1668	2.16	80/2595 (3.1%)
23	A2	1.49	0/343	2.31	18/531 (3.4%)
24	A3	1.64	0/1722	2.26	102/2685 (3.8%)
25	BC	0.73	0/2121	1.28	21/2852 (0.7%)
26	BD	0.65	0/1586	1.19	14/2134 (0.7%)
27	BE	0.66	0/1571	1.22	14/2113 (0.7%)
28	BF	0.72	0/1444	1.18	12/1937 (0.6%)
29	BG	0.65	0/1343	1.14	9/1816 (0.5%)
30	BH	0.62	0/1122	1.08	5/1515 (0.3%)
31	BI	0.63	0/1046	1.03	4/1410 (0.3%)
32	BJ	0.71	0/1152	1.22	10/1551 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BK	0.70	0/947	1.23	10/1268 (0.8%)
34	BL	0.72	0/1054	1.29	10/1403 (0.7%)
35	BM	0.71	0/1093	1.19	9/1460 (0.6%)
36	BN	0.75	0/973	1.34	12/1301 (0.9%)
37	BO	0.71	0/902	1.27	13/1209 (1.1%)
38	BP	0.70	0/929	1.22	11/1242 (0.9%)
39	BQ	0.76	0/960	1.30	16/1278 (1.3%)
40	BR	0.68	0/829	1.18	8/1107 (0.7%)
41	BS	0.63	0/864	1.22	10/1156 (0.9%)
42	BT	0.62	0/744	1.19	7/994 (0.7%)
43	BU	0.65	0/787	1.21	6/1051 (0.6%)
44	BV	0.66	0/766	1.06	4/1025 (0.4%)
45	BW	0.71	0/604	1.26	7/799 (0.9%)
46	BX	0.72	0/635	1.28	7/848 (0.8%)
47	BY	0.65	0/510	1.24	5/677 (0.7%)
48	BZ	0.67	0/453	1.23	5/605 (0.8%)
49	B0	0.72	0/450	1.30	7/599 (1.2%)
50	B1	0.68	0/417	1.10	2/556 (0.4%)
51	B2	0.79	0/380	1.49	9/498 (1.8%)
52	B3	0.70	0/513	1.23	6/676 (0.9%)
53	B4	0.69	0/303	1.35	5/397 (1.3%)
54	BA	1.48	61/69796 (0.1%)	2.23	4183/108888 (3.8%)
55	BB	1.48	1/2800 (0.0%)	2.19	150/4367 (3.4%)
56	B5	0.62	0/1673	1.09	11/2255 (0.5%)
All	All	1.34	89/160085 (0.1%)	2.01	7075/239402 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AD	0	1
10	AK	0	1
21	AA	0	374
22	A1	0	20
23	A2	0	5
24	A3	0	13
25	BC	0	1
26	BD	0	1
31	BI	0	1
35	BM	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	BN	0	1
54	BA	0	623
55	BB	0	30
All	All	0	1072

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	2507	C	C4-N4	-5.63	1.28	1.33
21	AA	742	G	C2-N2	-5.58	1.28	1.34
21	AA	756	C	C4-N4	-5.57	1.28	1.33
54	BA	2164	C	C4-N4	-5.44	1.29	1.33
21	AA	984	C	C4-N4	-5.43	1.29	1.33
21	AA	1317	C	C4-N4	-5.41	1.29	1.33
54	BA	1507	C	C4-N4	-5.36	1.29	1.33
54	BA	635	C	C4-N4	-5.34	1.29	1.33
54	BA	1814	G	C2-N2	-5.33	1.29	1.34
54	BA	2481	G	C2-N2	-5.33	1.29	1.34
54	BA	858	G	C2-N2	-5.32	1.29	1.34
21	AA	879	C	C4-N4	-5.31	1.29	1.33
21	AA	339	C	C4-N4	-5.30	1.29	1.33
54	BA	673	C	C4-N4	-5.30	1.29	1.33
54	BA	1297	C	C4-N4	-5.30	1.29	1.33
21	AA	1096	C	C4-N4	-5.29	1.29	1.33
54	BA	1838	C	C4-N4	-5.28	1.29	1.33
54	BA	787	C	C4-N4	-5.28	1.29	1.33
21	AA	36	C	C4-N4	-5.27	1.29	1.33
54	BA	2902	C	C4-N4	-5.25	1.29	1.33
54	BA	394	C	C4-N4	-5.24	1.29	1.33
54	BA	1843	C	C4-N4	-5.23	1.29	1.33
21	AA	582	C	C4-N4	-5.22	1.29	1.33
21	AA	1266	G	C2-N2	-5.22	1.29	1.34
54	BA	298	G	C2-N2	-5.22	1.29	1.34
54	BA	1311	G	C2-N2	-5.22	1.29	1.34
54	BA	1158	C	C4-N4	-5.21	1.29	1.33
21	AA	615	G	C2-N2	-5.21	1.29	1.34
54	BA	726	G	C2-N2	-5.20	1.29	1.34
54	BA	935	C	C4-N4	-5.20	1.29	1.33
54	BA	650	C	C4-N4	-5.20	1.29	1.33
54	BA	157	C	C4-N4	-5.20	1.29	1.33
21	AA	1214	C	C4-N4	-5.20	1.29	1.33
21	AA	755	G	C2-N2	-5.19	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	1934	C	C4-N4	-5.19	1.29	1.33
54	BA	840	C	C4-N4	-5.19	1.29	1.33
54	BA	2805	C	C4-N4	-5.19	1.29	1.33
54	BA	66	C	C4-N4	-5.18	1.29	1.33
54	BA	1136	G	C2-N2	-5.17	1.29	1.34
54	BA	2463	C	C4-N4	-5.17	1.29	1.33
55	BB	28	C	C4-N4	-5.17	1.29	1.33
21	AA	1278	G	C2-N2	-5.16	1.29	1.34
21	AA	556	C	C4-N4	-5.16	1.29	1.33
54	BA	485	C	C4-N4	-5.14	1.29	1.33
21	AA	188	C	C4-N4	-5.13	1.29	1.33
54	BA	1052	C	C4-N4	-5.12	1.29	1.33
54	BA	1104	C	C4-N4	-5.12	1.29	1.33
21	AA	719	C	C4-N4	-5.12	1.29	1.33
54	BA	630	G	N1-C2	-5.12	1.33	1.37
21	AA	857	C	C4-N4	-5.12	1.29	1.33
54	BA	2610	C	C4-N4	-5.12	1.29	1.33
21	AA	599	C	C4-N4	-5.12	1.29	1.33
54	BA	456	C	C4-N4	-5.11	1.29	1.33
54	BA	1533	C	C4-N4	-5.11	1.29	1.33
54	BA	2133	G	C2-N2	-5.11	1.29	1.34
54	BA	1737	G	C2-N2	-5.11	1.29	1.34
54	BA	1962	C	C4-N4	-5.10	1.29	1.33
54	BA	318	C	C4-N4	-5.09	1.29	1.33
54	BA	660	C	C4-N4	-5.09	1.29	1.33
21	AA	326	G	C2-N2	-5.08	1.29	1.34
21	AA	1361	G	C2-N2	-5.08	1.29	1.34
54	BA	1153	C	C4-N4	-5.08	1.29	1.33
54	BA	1699	G	C2-N2	-5.08	1.29	1.34
54	BA	1837	C	C4-N4	-5.07	1.29	1.33
54	BA	1107	G	C2-N2	-5.07	1.29	1.34
21	AA	856	C	C4-N4	-5.07	1.29	1.33
54	BA	672	C	C4-N4	-5.07	1.29	1.33
54	BA	1895	C	C4-N4	-5.07	1.29	1.33
54	BA	2175	C	C4-N4	-5.06	1.29	1.33
54	BA	2527	C	C4-N4	-5.06	1.29	1.33
54	BA	1298	C	C4-N4	-5.05	1.29	1.33
54	BA	2858	C	C4-N4	-5.05	1.29	1.33
54	BA	1530	G	C2-N2	-5.04	1.29	1.34
54	BA	484	C	C4-N4	-5.04	1.29	1.33
21	AA	862	C	C4-N4	-5.03	1.29	1.33
54	BA	1585	C	C4-N4	-5.03	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	810	C	C4-N4	-5.02	1.29	1.33
54	BA	1697	G	C2-N2	-5.02	1.29	1.34
54	BA	1179	G	C2-N2	-5.02	1.29	1.34
54	BA	1531	C	C4-N4	-5.02	1.29	1.33
54	BA	2444	G	C2-N2	-5.02	1.29	1.34
21	AA	637	C	C4-N4	-5.01	1.29	1.33
21	AA	1218	C	C4-N4	-5.01	1.29	1.33
54	BA	2072	C	C4-N4	-5.01	1.29	1.33
54	BA	420	C	C4-N4	-5.01	1.29	1.33
54	BA	1007	C	C4-N4	-5.00	1.29	1.33
54	BA	1990	C	C4-N4	-5.00	1.29	1.33
54	BA	2718	G	C2-N2	-5.00	1.29	1.34
21	AA	616	G	C2-N2	-5.00	1.29	1.34

All (7075) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1617	C	N3-C2-O2	-16.02	110.69	121.90
54	BA	640	C	N3-C2-O2	-15.80	110.84	121.90
24	A3	73	A	N1-C6-N6	-13.57	110.46	118.60
54	BA	1847	A	N1-C6-N6	-13.18	110.69	118.60
54	BA	323	C	O4'-C1'-N1	12.86	118.49	108.20
21	AA	665	A	N1-C6-N6	-12.61	111.03	118.60
54	BA	2453	A	N1-C6-N6	-12.48	111.11	118.60
21	AA	977	A	N1-C6-N6	-12.36	111.19	118.60
54	BA	1668	A	N1-C6-N6	-12.18	111.30	118.60
21	AA	1319	A	N1-C6-N6	-12.16	111.30	118.60
54	BA	1352	U	O4'-C1'-N1	12.13	117.90	108.20
55	BB	99	A	N1-C6-N6	-12.12	111.33	118.60
54	BA	1854	A	N1-C6-N6	-12.11	111.33	118.60
21	AA	1288	A	N1-C6-N6	-12.07	111.36	118.60
54	BA	1434	A	N1-C6-N6	-11.81	111.51	118.60
21	AA	499	A	N1-C6-N6	-11.81	111.51	118.60
54	BA	1237	A	N1-C6-N6	-11.77	111.54	118.60
12	AM	97	ARG	NE-CZ-NH1	11.73	126.17	120.30
21	AA	573	A	N1-C6-N6	-11.70	111.58	118.60
21	AA	814	A	N1-C6-N6	-11.67	111.60	118.60
54	BA	1569	A	N1-C6-N6	-11.64	111.61	118.60
54	BA	1916	A	N1-C6-N6	-11.63	111.62	118.60
54	BA	1307	A	N1-C6-N6	-11.62	111.62	118.60
24	A3	36	A	N1-C6-N6	-11.60	111.64	118.60
54	BA	38	A	N1-C6-N6	-11.60	111.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	130	A	N1-C6-N6	-11.60	111.64	118.60
54	BA	1635	A	N1-C6-N6	-11.58	111.65	118.60
54	BA	1077	A	N1-C6-N6	-11.57	111.66	118.60
21	AA	1101	A	N1-C6-N6	-11.57	111.66	118.60
34	BL	48	ARG	NE-CZ-NH1	11.55	126.08	120.30
21	AA	1287	A	N1-C6-N6	-11.52	111.69	118.60
54	BA	2378	A	N1-C6-N6	-11.48	111.71	118.60
54	BA	1610	A	O4'-C1'-N9	11.43	117.34	108.20
21	AA	1251	A	N1-C6-N6	-11.42	111.75	118.60
21	AA	223	A	N1-C6-N6	-11.41	111.76	118.60
54	BA	346	A	N1-C6-N6	-11.40	111.76	118.60
54	BA	196	A	N1-C6-N6	-11.38	111.78	118.60
21	AA	767	A	N1-C6-N6	-11.24	111.85	118.60
21	AA	143	A	N1-C6-N6	-11.24	111.86	118.60
54	BA	2060	A	N1-C6-N6	-11.22	111.87	118.60
21	AA	673	A	N1-C6-N6	-11.22	111.87	118.60
54	BA	422	A	N1-C6-N6	-11.21	111.87	118.60
55	BB	73	A	N1-C6-N6	-11.20	111.88	118.60
54	BA	1609	A	N1-C6-N6	-11.18	111.89	118.60
54	BA	1617	C	N1-C2-O2	11.18	125.61	118.90
54	BA	2726	A	N1-C6-N6	-11.16	111.90	118.60
54	BA	1758	U	O4'-C1'-N1	11.15	117.12	108.20
54	BA	1890	A	N1-C6-N6	-11.14	111.92	118.60
54	BA	1876	A	N1-C6-N6	-11.10	111.94	118.60
54	BA	2781	A	N1-C6-N6	-11.08	111.95	118.60
54	BA	2425	A	N1-C6-N6	-11.08	111.95	118.60
21	AA	389	A	N1-C6-N6	-11.07	111.96	118.60
21	AA	1289	A	N1-C6-N6	-11.05	111.97	118.60
54	BA	886	A	N1-C6-N6	-11.05	111.97	118.60
54	BA	528	A	N1-C6-N6	-11.02	111.99	118.60
54	BA	800	A	N1-C6-N6	-11.01	111.99	118.60
54	BA	1069	A	N1-C6-N6	-11.01	111.99	118.60
21	AA	554	A	N1-C6-N6	-10.98	112.01	118.60
21	AA	1519	A	N1-C6-N6	-10.98	112.01	118.60
54	BA	1783	A	N1-C6-N6	-10.96	112.02	118.60
54	BA	501	A	N1-C6-N6	-10.95	112.03	118.60
21	AA	563	A	N1-C6-N6	-10.94	112.04	118.60
21	AA	1396	A	N1-C6-N6	-10.93	112.04	118.60
24	A3	59	A	N1-C6-N6	-10.93	112.04	118.60
54	BA	2009	A	N1-C6-N6	-10.92	112.05	118.60
21	AA	872	A	C1'-O4'-C4'	-10.91	101.17	109.90
54	BA	2750	A	N1-C6-N6	-10.91	112.05	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2547	A	N1-C6-N6	-10.91	112.05	118.60
54	BA	219	A	N1-C6-N6	-10.91	112.06	118.60
21	AA	913	A	N1-C6-N6	-10.89	112.07	118.60
54	BA	415	A	N1-C6-N6	-10.89	112.07	118.60
54	BA	207	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	2586	U	O4'-C1'-N1	10.85	116.88	108.20
54	BA	213	A	N1-C6-N6	-10.84	112.10	118.60
21	AA	609	A	N1-C6-N6	-10.84	112.10	118.60
54	BA	1126	A	N1-C6-N6	-10.83	112.10	118.60
21	AA	197	A	N1-C6-N6	-10.83	112.10	118.60
21	AA	199	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	931	U	O4'-C1'-N1	10.78	116.82	108.20
54	BA	1977	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	1808	A	N1-C6-N6	-10.77	112.14	118.60
54	BA	126	A	N1-C6-N6	-10.75	112.15	118.60
54	BA	2274	A	N1-C6-N6	-10.72	112.17	118.60
54	BA	2051	A	N1-C6-N6	-10.70	112.18	118.60
54	BA	2516	A	N1-C6-N6	-10.70	112.18	118.60
54	BA	2418	A	N1-C6-N6	-10.69	112.19	118.60
54	BA	2899	A	N1-C6-N6	-10.67	112.20	118.60
54	BA	1808	A	O4'-C1'-N9	10.66	116.72	108.20
5	AF	2	ARG	NE-CZ-NH1	10.65	125.63	120.30
54	BA	1858	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	1952	A	N1-C6-N6	-10.63	112.22	118.60
23	A2	82	A	N1-C6-N6	-10.63	112.22	118.60
21	AA	1246	A	N1-C6-N6	-10.62	112.23	118.60
54	BA	2015	A	N1-C6-N6	-10.61	112.23	118.60
21	AA	60	A	N1-C6-N6	-10.59	112.25	118.60
21	AA	510	A	N1-C6-N6	-10.57	112.26	118.60
21	AA	1216	A	N1-C6-N6	-10.55	112.27	118.60
54	BA	1998	A	N1-C6-N6	-10.52	112.29	118.60
55	BB	41	G	O4'-C1'-N9	10.51	116.61	108.20
21	AA	937	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	2135	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	2572	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	2147	A	N1-C6-N6	-10.49	112.30	118.60
54	BA	1759	A	N1-C6-N6	-10.49	112.31	118.60
21	AA	172	A	N1-C6-N6	-10.47	112.32	118.60
25	BC	235	GLU	OE1-CD-OE2	-10.45	110.76	123.30
24	A3	60	A	N1-C6-N6	-10.45	112.33	118.60
21	AA	607	A	N1-C6-N6	-10.44	112.34	118.60
55	BB	87	U	O4'-C1'-N1	10.43	116.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	766	A	N1-C6-N6	-10.42	112.35	118.60
54	BA	1755	A	N1-C6-N6	-10.42	112.35	118.60
21	AA	303	A	N1-C6-N6	-10.42	112.35	118.60
54	BA	2328	A	N1-C6-N6	-10.40	112.36	118.60
21	AA	560	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	2809	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	119	A	N1-C6-N6	-10.39	112.36	118.60
54	BA	718	A	N1-C6-N6	-10.38	112.37	118.60
54	BA	2407	A	N1-C6-N6	-10.38	112.37	118.60
54	BA	2339	C	O4'-C1'-N1	10.38	116.50	108.20
55	BB	94	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	1919	A	N1-C6-N6	-10.36	112.39	118.60
21	AA	306	A	N1-C6-N6	-10.35	112.39	118.60
55	BB	46	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	2266	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	1133	A	N1-C6-N6	-10.34	112.39	118.60
54	BA	1784	A	N1-C6-N6	-10.34	112.40	118.60
54	BA	2386	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	1046	A	O4'-C1'-N9	10.31	116.45	108.20
38	BP	61	ARG	NE-CZ-NH1	10.30	125.45	120.30
54	BA	1142	A	N1-C6-N6	-10.29	112.43	118.60
54	BA	626	A	N1-C6-N6	-10.28	112.43	118.60
21	AA	559	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	515	A	N1-C6-N6	-10.27	112.44	118.60
21	AA	968	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	981	A	N1-C6-N6	-10.24	112.46	118.60
54	BA	1591	A	N1-C6-N6	-10.23	112.46	118.60
55	BB	50	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	1197	A	N1-C6-N6	-10.21	112.48	118.60
54	BA	941	A	N1-C6-N6	-10.21	112.48	118.60
16	AQ	48	GLU	OE1-CD-OE2	-10.20	111.06	123.30
54	BA	218	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	959	A	N1-C6-N6	-10.19	112.48	118.60
54	BA	270	A	N1-C6-N6	-10.18	112.49	118.60
21	AA	1229	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	849	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	1265	A	N1-C6-N6	-10.17	112.50	118.60
54	BA	2814	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	1496	A	N1-C6-N6	-10.15	112.51	118.60
54	BA	1070	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	152	A	N1-C6-N6	-10.14	112.52	118.60
12	AM	56	ARG	NE-CZ-NH1	10.13	125.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	441	A	N1-C6-N6	-10.13	112.52	118.60
21	AA	1311	A	N1-C6-N6	-10.12	112.53	118.60
54	BA	1495	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	2654	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	1717	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	371	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	2736	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	844	A	N1-C6-N6	-10.07	112.56	118.60
21	AA	448	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	655	A	O4'-C1'-N9	10.06	116.25	108.20
21	AA	313	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	1586	A	N1-C6-N6	-10.03	112.58	118.60
23	A2	90	U	C1'-O4'-C4'	-10.03	101.88	109.90
54	BA	282	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	2634	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	1384	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	2058	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	2679	A	N1-C6-N6	-10.00	112.60	118.60
21	AA	696	A	N1-C6-N6	-9.99	112.61	118.60
21	AA	1022	A	N1-C6-N6	-9.97	112.61	118.60
21	AA	1333	A	N1-C6-N6	-9.97	112.62	118.60
24	A3	38	A	N1-C6-N6	-9.97	112.62	118.60
21	AA	338	A	N1-C6-N6	-9.96	112.62	118.60
54	BA	2433	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	1304	A	N1-C6-N6	-9.96	112.62	118.60
54	BA	2163	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	1377	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	1004	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	1000	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	982	C	N3-C2-O2	-9.93	114.95	121.90
54	BA	1679	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	608	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	947	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	1301	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	633	A	N1-C6-N6	-9.89	112.67	118.60
54	BA	722	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	2900	A	N1-C6-N6	-9.86	112.68	118.60
21	AA	482	A	N1-C6-N6	-9.86	112.68	118.60
54	BA	1169	A	N1-C6-N6	-9.86	112.68	118.60
21	AA	253	A	N1-C6-N6	-9.86	112.69	118.60
54	BA	592	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	1885	A	N1-C6-N6	-9.84	112.70	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AC	53	ARG	NE-CZ-NH1	9.83	125.22	120.30
21	AA	363	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	2879	A	N1-C6-N6	-9.83	112.70	118.60
21	AA	190	A	N1-C6-N6	-9.82	112.71	118.60
21	AA	1204	A	N1-C6-N6	-9.82	112.71	118.60
21	AA	1363	A	N1-C6-N6	-9.82	112.71	118.60
3	AD	61	ARG	NE-CZ-NH1	9.81	125.21	120.30
25	BC	261	ARG	NE-CZ-NH1	9.81	125.21	120.30
54	BA	1272	A	N1-C6-N6	-9.81	112.71	118.60
40	BR	84	ARG	NE-CZ-NH1	9.81	125.20	120.30
21	AA	974	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	1156	A	N1-C6-N6	-9.81	112.72	118.60
54	BA	1260	A	N1-C6-N6	-9.80	112.72	118.60
36	BN	96	ARG	NE-CZ-NH1	9.80	125.20	120.30
54	BA	311	A	N1-C6-N6	-9.79	112.73	118.60
54	BA	146	A	N1-C6-N6	-9.79	112.73	118.60
21	AA	53	A	N1-C6-N6	-9.78	112.73	118.60
21	AA	1431	A	N1-C6-N6	-9.77	112.73	118.60
54	BA	1275	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	298	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	228	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	336	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	632	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	752	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	2430	A	N1-C6-N6	-9.77	112.74	118.60
21	AA	1413	A	N1-C6-N6	-9.75	112.75	118.60
25	BC	68	ARG	NE-CZ-NH1	9.75	125.18	120.30
21	AA	807	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	1672	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	900	A	N1-C6-N6	-9.74	112.76	118.60
21	AA	195	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	1785	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2352	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	103	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1080	A	N1-C6-N6	-9.73	112.76	118.60
21	AA	179	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1515	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1937	A	N1-C6-N6	-9.73	112.76	118.60
21	AA	246	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	2176	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	1805	A	N1-C6-N6	-9.72	112.77	118.60
21	AA	777	A	N1-C6-N6	-9.72	112.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	960	A	N1-C6-N6	-9.72	112.77	118.60
53	B4	24	ARG	NE-CZ-NH1	9.71	125.16	120.30
21	AA	171	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	1913	A	N1-C6-N6	-9.71	112.78	118.60
21	AA	825	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1522	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1095	A	N1-C6-N6	-9.69	112.78	118.60
54	BA	2020	A	N1-C6-N6	-9.69	112.78	118.60
54	BA	1749	A	N1-C6-N6	-9.69	112.79	118.60
54	BA	101	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	734	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	1067	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	2665	A	N1-C6-N6	-9.66	112.81	118.60
54	BA	982	C	O4'-C1'-N1	9.65	115.92	108.20
55	BB	109	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	1429	A	N1-C6-N6	-9.65	112.81	118.60
22	A1	35	A	N1-C6-N6	-9.64	112.82	118.60
54	BA	1774	C	N3-C2-O2	-9.64	115.16	121.90
54	BA	2070	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2564	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	99	U	O4'-C1'-N1	9.62	115.90	108.20
27	BE	102	ARG	NE-CZ-NH1	9.62	125.11	120.30
54	BA	861	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1978	A	N1-C6-N6	-9.62	112.83	118.60
21	AA	1227	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1353	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	2013	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	282	A	N1-C6-N6	-9.61	112.84	118.60
21	AA	675	A	N1-C6-N6	-9.61	112.84	118.60
54	BA	125	A	N1-C6-N6	-9.61	112.84	118.60
39	BQ	91	ARG	NE-CZ-NH1	9.60	125.10	120.30
54	BA	1583	A	N1-C6-N6	-9.60	112.84	118.60
21	AA	749	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	2281	A	N1-C6-N6	-9.60	112.84	118.60
24	A3	77	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	1552	A	O4'-C1'-N9	9.59	115.87	108.20
54	BA	2887	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	1544	A	N1-C6-N6	-9.59	112.85	118.60
21	AA	1130	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1701	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	2610	C	N3-C2-O2	-9.57	115.20	121.90
55	BB	34	A	N1-C6-N6	-9.57	112.86	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	227	A	N1-C6-N6	-9.56	112.86	118.60
54	BA	63	A	N1-C6-N6	-9.56	112.87	118.60
54	BA	943	A	N1-C6-N6	-9.56	112.87	118.60
54	BA	2518	A	N1-C6-N6	-9.56	112.86	118.60
21	AA	831	A	N1-C6-N6	-9.55	112.87	118.60
3	AD	12	ARG	NE-CZ-NH1	9.55	125.07	120.30
54	BA	637	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	751	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	2497	A	N1-C6-N6	-9.54	112.87	118.60
21	AA	74	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	199	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	2307	G	O4'-C1'-N9	9.54	115.83	108.20
51	B2	21	ARG	NE-CZ-NH1	9.54	125.07	120.30
54	BA	2287	A	N1-C6-N6	-9.53	112.88	118.60
14	AO	16	ARG	NE-CZ-NH1	9.53	125.06	120.30
54	BA	1213	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2171	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2435	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	1014	A	N1-C6-N6	-9.53	112.89	118.60
54	BA	1652	A	N1-C6-N6	-9.53	112.89	118.60
54	BA	750	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2142	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	2635	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	1508	A	N1-C6-N6	-9.51	112.89	118.60
55	BB	39	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	1434	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	1145	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	241	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	280	U	O4'-C1'-N1	9.50	115.80	108.20
54	BA	1532	A	N1-C6-N6	-9.50	112.90	118.60
24	A3	22	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	2126	A	N1-C6-N6	-9.49	112.90	118.60
54	BA	2879	A	C5-C6-N1	9.49	122.45	117.70
54	BA	1084	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	181	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	397	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	493	A	N1-C6-N6	-9.49	112.91	118.60
16	AQ	39	ARG	NE-CZ-NH1	9.48	125.04	120.30
54	BA	654	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	1936	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	1889	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	1014	A	N1-C6-N6	-9.47	112.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	26	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1871	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1943	U	O4'-C1'-N1	9.46	115.77	108.20
54	BA	2590	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	482	A	N1-C6-N6	-9.46	112.92	118.60
21	AA	1368	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1744	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	262	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	1143	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	1637	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	784	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	1256	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	454	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	142	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	279	A	N1-C6-N6	-9.43	112.94	118.60
12	AM	28	ARG	NE-CZ-NH1	9.43	125.01	120.30
21	AA	1225	A	N1-C6-N6	-9.42	112.95	118.60
26	BD	77	ARG	NE-CZ-NH1	9.42	125.01	120.30
54	BA	1420	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1722	A	N1-C6-N6	-9.42	112.95	118.60
22	A1	21	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1009	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	1151	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	192	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	1068	G	O4'-C1'-N9	9.41	115.73	108.20
54	BA	1819	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	1250	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	919	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	2587	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	782	A	N1-C6-N6	-9.39	112.96	118.60
54	BA	983	A	N1-C6-N6	-9.39	112.96	118.60
9	AJ	5	ARG	NE-CZ-NH1	9.39	124.99	120.30
54	BA	479	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	2108	A	N1-C6-N6	-9.39	112.97	118.60
4	AE	53	ARG	NE-CZ-NH1	9.38	124.99	120.30
21	AA	98	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	1610	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	1082	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	1046	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	443	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	1302	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1593	A	N1-C6-N6	-9.37	112.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	466	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	503	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1932	A	N1-C6-N6	-9.37	112.98	118.60
23	A2	79	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	412	A	N1-C6-N6	-9.36	112.98	118.60
21	AA	792	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	203	A	N1-C6-N6	-9.36	112.98	118.60
54	BA	1789	A	N1-C6-N6	-9.36	112.99	118.60
54	BA	909	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	2602	A	O4'-C1'-N9	9.34	115.67	108.20
37	BO	102	ARG	NE-CZ-NH1	9.34	124.97	120.30
54	BA	160	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1525	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	1010	A	N1-C6-N6	-9.34	113.00	118.60
54	BA	802	A	N1-C6-N6	-9.32	113.00	118.60
54	BA	1535	A	N1-C6-N6	-9.32	113.01	118.60
55	BB	66	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	2376	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	2478	A	N1-C6-N6	-9.32	113.01	118.60
22	A1	9	A	N1-C6-N6	-9.31	113.01	118.60
46	BX	44	ARG	NE-CZ-NH1	9.31	124.96	120.30
54	BA	979	A	O4'-C1'-N9	9.31	115.65	108.20
54	BA	2820	A	N1-C6-N6	-9.31	113.02	118.60
21	AA	743	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	2581	G	O4'-C1'-N9	9.30	115.64	108.20
21	AA	1394	A	N1-C6-N6	-9.30	113.02	118.60
15	AP	25	ARG	NE-CZ-NH1	9.29	124.95	120.30
54	BA	2725	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	933	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	1320	C	O4'-C1'-N1	9.29	115.64	108.20
54	BA	2792	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	635	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	1408	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	408	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	1468	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	2037	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	896	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	344	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2711	A	N1-C6-N6	-9.28	113.03	118.60
21	AA	1239	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2835	A	N1-C6-N6	-9.28	113.03	118.60
24	A3	11	A	N1-C6-N6	-9.27	113.04	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	547	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	2560	A	N1-C6-N6	-9.27	113.04	118.60
3	AD	127	ARG	NE-CZ-NH1	9.27	124.93	120.30
21	AA	1433	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	676	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	2381	A	N1-C6-N6	-9.26	113.04	118.60
21	AA	572	A	N1-C6-N6	-9.26	113.05	118.60
21	AA	1430	A	N1-C6-N6	-9.26	113.05	118.60
26	BD	59	ARG	NE-CZ-NH1	9.26	124.93	120.30
54	BA	322	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	1428	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	155	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	932	U	O4'-C1'-N1	9.24	115.59	108.20
54	BA	2706	A	N1-C6-N6	-9.24	113.06	118.60
21	AA	702	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	2101	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	111	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	265	A	N1-C6-N6	-9.23	113.06	118.60
1	AB	34	ARG	NE-CZ-NH1	9.23	124.91	120.30
27	BE	162	ARG	NE-CZ-NH1	9.23	124.91	120.30
54	BA	1027	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	131	A	N1-C6-N6	-9.22	113.06	118.60
54	BA	344	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1815	A	N1-C6-N6	-9.22	113.06	118.60
14	AO	53	ARG	NE-CZ-NH1	9.22	124.91	120.30
21	AA	465	A	N1-C6-N6	-9.21	113.07	118.60
21	AA	780	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	2614	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	804	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	195	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	1340	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	753	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	2541	A	N1-C6-N6	-9.19	113.08	118.60
21	AA	718	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	176	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	2825	G	O4'-C1'-N9	9.18	115.55	108.20
54	BA	1067	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	348	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1791	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	522	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	468	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	1398	A	N1-C6-N6	-9.17	113.10	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	864	A	N1-C6-N6	-9.17	113.10	118.60
21	AA	676	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	309	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	2542	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	1274	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	1395	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	1194	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	456	C	N3-C2-O2	-9.15	115.49	121.90
54	BA	572	A	C5-C6-N1	9.15	122.28	117.70
54	BA	1147	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	196	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	1005	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1274	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2030	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2268	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	915	A	N1-C6-N6	-9.14	113.11	118.60
54	BA	458	G	O4'-C1'-N9	9.14	115.51	108.20
54	BA	644	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	787	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	608	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	2675	A	N1-C6-N6	-9.14	113.12	118.60
55	BB	52	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	748	G	O4'-C1'-N9	9.14	115.51	108.20
21	AA	1021	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	975	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	250	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	1213	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	637	A	C5-C6-N1	9.12	122.26	117.70
54	BA	2212	A	O4'-C1'-N9	9.12	115.50	108.20
21	AA	996	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2868	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	72	A	C5-C6-N1	9.12	122.26	117.70
54	BA	352	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	2469	A	N1-C6-N6	-9.11	113.13	118.60
25	BC	237	ARG	NE-CZ-NH1	9.11	124.86	120.30
54	BA	127	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	1580	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	1509	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	2273	A	N1-C6-N6	-9.11	113.14	118.60
37	BO	94	ARG	NE-CZ-NH1	9.10	124.85	120.30
21	AA	1339	A	C5-C6-N1	9.10	122.25	117.70
54	BA	1419	A	N1-C6-N6	-9.10	113.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1953	A	N1-C6-N6	-9.10	113.14	118.60
7	AH	79	ARG	NE-CZ-NH1	9.09	124.85	120.30
2	AC	58	ARG	NE-CZ-NH1	9.09	124.84	120.30
54	BA	655	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	1029	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	2670	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	1630	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	1853	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	1654	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	151	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1155	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1342	C	P-O3'-C3'	9.07	130.59	119.70
54	BA	1439	A	O4'-C1'-N9	9.07	115.46	108.20
54	BA	1566	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	2335	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	523	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	1329	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	825	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	2657	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	471	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	243	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	1380	U	N3-C2-O2	-9.06	115.86	122.20
54	BA	191	A	N1-C6-N6	-9.06	113.16	118.60
21	AA	196	A	C5-C6-N1	9.06	122.23	117.70
21	AA	649	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	783	A	N1-C6-N6	-9.06	113.17	118.60
54	BA	1382	G	O4'-C1'-N9	9.05	115.44	108.20
54	BA	661	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1308	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	1367	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	2850	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	460	A	N1-C6-N6	-9.04	113.17	118.60
21	AA	983	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	2531	A	N1-C6-N6	-9.04	113.18	118.60
21	AA	553	A	N1-C6-N6	-9.03	113.18	118.60
24	A3	39	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1739	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	643	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1608	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	1042	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	181	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	262	A	N1-C6-N6	-9.01	113.19	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1238	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	1054	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	95	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1301	A	C5-C6-N1	9.00	122.20	117.70
21	AA	279	A	C5-C6-N1	9.00	122.20	117.70
54	BA	1453	A	N1-C6-N6	-9.00	113.20	118.60
32	BJ	116	ARG	NE-CZ-NH1	9.00	124.80	120.30
54	BA	1960	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	342	A	N1-C6-N6	-8.99	113.20	118.60
21	AA	19	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	231	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	497	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	1046	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	2314	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	1700	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	914	A	N1-C6-N6	-8.98	113.21	118.60
26	BD	46	ARG	NE-CZ-NH1	8.98	124.79	120.30
54	BA	1618	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	1480	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	300	A	N1-C6-N6	-8.96	113.22	118.60
21	AA	80	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1268	A	N1-C6-N6	-8.96	113.22	118.60
27	BE	114	ARG	NE-CZ-NH1	8.95	124.78	120.30
54	BA	508	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	925	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	2450	A	N1-C6-N6	-8.95	113.23	118.60
10	AK	92	ARG	NE-CZ-NH1	8.95	124.77	120.30
54	BA	1549	A	N1-C6-N6	-8.95	113.23	118.60
38	BP	38	ARG	NE-CZ-NH1	8.95	124.77	120.30
21	AA	152	A	C5-C6-N1	8.94	122.17	117.70
21	AA	729	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	1048	A	N1-C6-N6	-8.93	113.24	118.60
3	AD	62	ARG	NE-CZ-NH1	8.93	124.77	120.30
54	BA	2632	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	2628	C	N3-C2-O2	-8.93	115.65	121.90
21	AA	167	A	N1-C6-N6	-8.92	113.25	118.60
6	AG	108	ARG	NE-CZ-NH1	8.92	124.76	120.30
21	AA	461	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	53	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	716	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	892	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	2327	A	N1-C6-N6	-8.91	113.25	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1616	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1129	A	N1-C6-N6	-8.91	113.26	118.60
54	BA	432	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1606	C	N3-C2-O2	-8.90	115.67	121.90
54	BA	905	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	622	A	N1-C6-N6	-8.90	113.26	118.60
33	BK	17	ARG	NE-CZ-NH1	8.90	124.75	120.30
21	AA	1179	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	1476	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	689	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1966	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2660	A	N1-C6-N6	-8.90	113.26	118.60
47	BY	47	ARG	NE-CZ-NH1	8.89	124.75	120.30
54	BA	613	A	N1-C6-N6	-8.89	113.27	118.60
54	BA	1241	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	602	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	996	A	C1'-O4'-C4'	-8.89	102.79	109.90
21	AA	1188	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	277	G	O4'-C1'-N9	8.88	115.31	108.20
54	BA	449	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	706	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	670	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	330	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1773	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	2821	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1322	A	N1-C6-N6	-8.87	113.28	118.60
55	BB	103	U	O4'-C1'-N1	8.87	115.30	108.20
21	AA	579	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	1163	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	2406	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	1377	A	C5-C6-N1	8.86	122.13	117.70
21	AA	197	A	C5-C6-N1	8.85	122.13	117.70
54	BA	1276	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	2426	A	N1-C6-N6	-8.84	113.29	118.60
21	AA	913	A	C5-C6-N1	8.84	122.12	117.70
22	A1	59	U	O4'-C1'-N1	8.84	115.27	108.20
21	AA	205	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	1392	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	144	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	687	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	1456	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	547	A	N1-C6-N6	-8.82	113.31	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	AM	89	ARG	NE-CZ-NH1	8.82	124.71	120.30
22	A1	23	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	1089	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	648	A	N1-C6-N6	-8.79	113.32	118.60
24	A3	76	C	N3-C2-O2	-8.79	115.74	121.90
54	BA	161	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1570	A	N1-C6-N6	-8.79	113.33	118.60
24	A3	45	A	N1-C6-N6	-8.78	113.33	118.60
42	BT	12	ARG	NE-CZ-NH1	8.79	124.69	120.30
54	BA	2727	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	1848	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2094	A	N1-C6-N6	-8.78	113.33	118.60
20	AU	44	ARG	NE-CZ-NH1	8.78	124.69	120.30
54	BA	2033	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	1134	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2059	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2598	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	311	A	C5-C6-N1	8.76	122.08	117.70
54	BA	1069	A	C5-C6-N1	8.76	122.08	117.70
54	BA	1320	C	N3-C2-O2	-8.75	115.77	121.90
54	BA	2534	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	451	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	44	A	N1-C6-N6	-8.75	113.35	118.60
54	BA	255	A	N1-C6-N6	-8.74	113.35	118.60
54	BA	749	A	N1-C6-N6	-8.74	113.35	118.60
54	BA	945	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	988	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1597	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1877	A	N1-C6-N6	-8.74	113.36	118.60
21	AA	958	A	N1-C6-N6	-8.74	113.36	118.60
23	A2	91	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	817	C	N3-C2-O2	-8.73	115.79	121.90
21	AA	900	A	N1-C6-N6	-8.73	113.36	118.60
27	BE	170	ARG	NE-CZ-NH1	8.73	124.66	120.30
12	AM	69	ARG	NE-CZ-NH1	8.72	124.66	120.30
21	AA	495	A	N1-C6-N6	-8.72	113.37	118.60
21	AA	621	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	2090	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	2893	A	N1-C6-N6	-8.72	113.37	118.60
55	BB	15	A	N1-C6-N6	-8.72	113.37	118.60
41	BS	18	ARG	NE-CZ-NH1	8.72	124.66	120.30
21	AA	1271	A	N1-C6-N6	-8.71	113.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1073	A	O4'-C1'-N9	8.71	115.17	108.20
21	AA	236	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	1534	U	O4'-C1'-N1	8.71	115.16	108.20
54	BA	2071	A	N1-C6-N6	-8.71	113.38	118.60
21	AA	1152	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	1731	G	O4'-C1'-N9	8.70	115.16	108.20
2	AC	178	ARG	NE-CZ-NH1	8.70	124.65	120.30
21	AA	889	A	N1-C6-N6	-8.69	113.38	118.60
54	BA	56	A	N1-C6-N6	-8.69	113.38	118.60
54	BA	362	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	228	C	N3-C2-O2	-8.68	115.82	121.90
54	BA	28	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	788	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1885	A	C5-C6-N1	8.68	122.04	117.70
54	BA	927	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	274	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	1446	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	118	A	C5-C6-N1	8.68	122.04	117.70
21	AA	969	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1365	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	665	A	C5-C6-N1	8.67	122.03	117.70
54	BA	275	C	N3-C2-O2	-8.66	115.84	121.90
54	BA	2725	A	C5-C6-N1	8.66	122.03	117.70
21	AA	1503	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	346	A	C5-C6-N1	8.66	122.03	117.70
54	BA	1641	A	N1-C6-N6	-8.66	113.41	118.60
54	BA	2071	A	C5-C6-N1	8.66	122.03	117.70
54	BA	483	A	N1-C6-N6	-8.66	113.41	118.60
21	AA	1219	A	N1-C6-N6	-8.66	113.41	118.60
6	AG	77	ARG	NE-CZ-NH1	8.65	124.63	120.30
54	BA	2459	A	C5-C6-N1	8.65	122.03	117.70
21	AA	498	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	1092	A	N1-C6-N6	-8.65	113.41	118.60
49	B0	9	ARG	NE-CZ-NH1	8.65	124.62	120.30
54	BA	86	G	O4'-C1'-N9	8.65	115.12	108.20
54	BA	320	A	N1-C6-N6	-8.65	113.41	118.60
22	A1	41	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	371	A	C5-C6-N1	8.64	122.02	117.70
54	BA	2077	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	535	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	648	A	C5-C6-N1	8.63	122.02	117.70
54	BA	844	A	C5-C6-N1	8.63	122.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2173	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	371	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	51	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	1044	C	N3-C2-O2	-8.62	115.87	121.90
54	BA	466	A	N1-C6-N6	-8.62	113.43	118.60
30	BH	68	ARG	NE-CZ-NH1	8.61	124.61	120.30
54	BA	526	A	C5-C6-N1	8.61	122.01	117.70
54	BA	2565	A	N1-C6-N6	-8.61	113.43	118.60
21	AA	1381	U	C5'-C4'-O4'	8.61	119.43	109.10
54	BA	507	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	1981	A	O4'-C1'-N9	8.61	115.09	108.20
54	BA	2388	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	819	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	2377	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	401	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1096	A	N1-C6-N6	-8.59	113.44	118.60
21	AA	1280	A	N1-C6-N6	-8.59	113.44	118.60
21	AA	65	A	N1-C6-N6	-8.59	113.45	118.60
40	BR	13	ARG	NE-CZ-NH1	8.59	124.60	120.30
54	BA	84	A	N1-C6-N6	-8.59	113.45	118.60
21	AA	6	G	O4'-C1'-N9	8.59	115.07	108.20
54	BA	706	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	1360	A	C5-C6-N1	8.57	121.99	117.70
54	BA	1890	A	C5-C6-N1	8.57	121.99	117.70
54	BA	2005	A	N1-C6-N6	-8.57	113.46	118.60
21	AA	1269	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	490	C	N3-C2-O2	-8.57	115.90	121.90
54	BA	2171	A	C5-C6-N1	8.57	121.98	117.70
54	BA	789	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	2689	U	O4'-C1'-N1	8.57	115.05	108.20
54	BA	2461	A	N1-C6-N6	-8.56	113.46	118.60
21	AA	694	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	91	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	1127	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	1226	A	N1-C6-N6	-8.56	113.46	118.60
54	BA	2705	A	N1-C6-N6	-8.56	113.47	118.60
54	BA	2482	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	161	A	N1-C6-N6	-8.55	113.47	118.60
55	BB	78	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	13	A	N1-C6-N6	-8.55	113.47	118.60
45	BW	38	ARG	NE-CZ-NH1	8.54	124.57	120.30
54	BA	226	A	N1-C6-N6	-8.54	113.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1981	A	C5-C6-N1	8.54	121.97	117.70
21	AA	353	A	C5-C6-N1	8.54	121.97	117.70
21	AA	994	A	N1-C6-N6	-8.54	113.48	118.60
54	BA	820	A	C5-C6-N1	8.54	121.97	117.70
54	BA	1262	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	814	A	C5-C6-N1	8.53	121.97	117.70
21	AA	353	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	2080	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	865	A	N1-C6-N6	-8.52	113.48	118.60
21	AA	907	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	1189	A	N1-C6-N6	-8.52	113.49	118.60
19	AT	23	ARG	NE-CZ-NH1	8.52	124.56	120.30
54	BA	819	A	C5-C6-N1	8.52	121.96	117.70
21	AA	1045	C	N3-C2-O2	-8.51	115.94	121.90
54	BA	1085	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1552	A	C5-C6-N1	8.51	121.96	117.70
21	AA	432	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	428	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	2799	A	N1-C6-N6	-8.51	113.49	118.60
21	AA	794	A	N1-C6-N6	-8.51	113.50	118.60
25	BC	12	ARG	NE-CZ-NH1	8.51	124.55	120.30
54	BA	345	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1336	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1494	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	1738	G	O4'-C1'-N9	8.51	115.01	108.20
54	BA	1755	A	C5-C6-N1	8.51	121.95	117.70
54	BA	2117	A	C5-C6-N1	8.51	121.95	117.70
54	BA	2340	A	C5-C6-N1	8.50	121.95	117.70
54	BA	391	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	845	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	1000	A	C5-C6-N1	8.50	121.95	117.70
21	AA	655	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	590	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	980	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	1665	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	2721	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	33	A	N1-C6-N6	-8.49	113.50	118.60
54	BA	1086	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	1252	A	C5-C6-N1	8.49	121.94	117.70
21	AA	767	A	C5-C6-N1	8.48	121.94	117.70
54	BA	1403	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	918	A	N1-C6-N6	-8.48	113.51	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	716	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	1318	A	N1-C6-N6	-8.48	113.51	118.60
47	BY	48	ARG	NE-CZ-NH1	8.48	124.54	120.30
54	BA	49	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	780	A	C5-C6-N1	8.48	121.94	117.70
54	BA	2211	A	C5-C6-N1	8.47	121.94	117.70
21	AA	456	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	1439	A	N1-C6-N6	-8.47	113.52	118.60
21	AA	1465	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	804	A	C5-C6-N1	8.47	121.93	117.70
21	AA	574	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	675	A	C5-C6-N1	8.46	121.93	117.70
21	AA	1117	A	N1-C6-N6	-8.46	113.52	118.60
24	A3	73	A	C4-C5-C6	-8.46	112.77	117.00
54	BA	42	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	332	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	572	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1253	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	2468	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	10	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	300	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	1794	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	845	A	N1-C6-N6	-8.45	113.53	118.60
49	B0	15	ARG	NE-CZ-NH2	8.45	124.53	120.30
21	AA	959	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	1158	C	N3-C2-O2	-8.45	115.98	121.90
54	BA	504	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	1350	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	1214	C	N3-C2-O2	-8.45	115.99	121.90
54	BA	204	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2753	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	1248	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	272	A	N1-C6-N6	-8.44	113.53	118.60
54	BA	347	A	N1-C6-N6	-8.44	113.53	118.60
7	AH	76	ARG	NE-CZ-NH1	8.44	124.52	120.30
54	BA	125	A	C5-C6-N1	8.44	121.92	117.70
54	BA	650	C	N3-C2-O2	-8.43	116.00	121.90
54	BA	1098	A	N1-C6-N6	-8.43	113.54	118.60
18	AS	36	ARG	NE-CZ-NH1	8.43	124.51	120.30
21	AA	411	A	C5-C6-N1	8.43	121.91	117.70
21	AA	1322	C	N3-C2-O2	-8.43	116.00	121.90
22	A1	66	A	N1-C6-N6	-8.43	113.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	278	A	N1-C6-N6	-8.43	113.55	118.60
54	BA	526	A	N1-C6-N6	-8.43	113.55	118.60
21	AA	1093	A	N1-C6-N6	-8.42	113.55	118.60
7	AH	12	ARG	NE-CZ-NH1	8.42	124.51	120.30
54	BA	793	A	C5-C6-N1	8.42	121.91	117.70
54	BA	2005	A	C5-C6-N1	8.42	121.91	117.70
21	AA	1362	A	N1-C6-N6	-8.42	113.55	118.60
39	BQ	52	ARG	NE-CZ-NH1	8.42	124.51	120.30
54	BA	721	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2800	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	173	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	1786	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	273	G	O4'-C1'-N9	8.41	114.93	108.20
54	BA	513	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	2596	U	O4'-C1'-N1	8.41	114.93	108.20
54	BA	1142	A	C5-C6-N1	8.41	121.90	117.70
21	AA	1035	A	N1-C6-N6	-8.40	113.56	118.60
37	BO	111	ARG	NE-CZ-NH1	8.40	124.50	120.30
54	BA	693	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	1640	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2750	A	C5-C6-N1	8.40	121.90	117.70
54	BA	73	A	C5-C6-N1	8.40	121.90	117.70
21	AA	162	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	972	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2666	C	N3-C2-O2	-8.40	116.02	121.90
27	BE	40	ARG	NE-CZ-NH1	8.40	124.50	120.30
54	BA	1433	A	C5-C6-N1	8.39	121.90	117.70
54	BA	1590	A	N1-C6-N6	-8.39	113.56	118.60
24	A3	3	C	N3-C2-O2	-8.39	116.03	121.90
54	BA	1300	G	O4'-C1'-N9	8.39	114.92	108.20
54	BA	2340	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	222	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2755	C	O4'-C1'-N1	8.39	114.91	108.20
21	AA	975	A	N1-C6-N6	-8.39	113.57	118.60
35	BM	6	ARG	NE-CZ-NH1	8.39	124.49	120.30
54	BA	1780	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	2542	A	C5-C6-N1	8.39	121.89	117.70
21	AA	1081	A	N1-C6-N6	-8.38	113.57	118.60
33	BK	108	ARG	NE-CZ-NH1	8.38	124.49	120.30
54	BA	2333	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	182	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	2064	C	N3-C2-O2	-8.38	116.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	BO	16	ARG	NE-CZ-NH1	8.37	124.49	120.30
21	AA	873	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1230	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1668	A	C5-C6-N1	8.37	121.89	117.70
54	BA	1866	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1079	C	N3-C2-O2	-8.37	116.04	121.90
21	AA	681	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	1610	A	C5-C6-N1	8.36	121.88	117.70
54	BA	156	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	933	A	C5-C6-N1	8.36	121.88	117.70
54	BA	2317	A	N1-C6-N6	-8.36	113.59	118.60
11	AL	30	ARG	NE-CZ-NH1	8.35	124.48	120.30
21	AA	1257	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	149	A	N1-C6-N6	-8.35	113.59	118.60
32	BJ	34	ARG	NE-CZ-NH1	8.35	124.47	120.30
54	BA	1626	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	182	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	802	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1100	C	N3-C2-O2	-8.35	116.06	121.90
24	A3	39	A	C5-C6-N1	8.35	121.87	117.70
54	BA	2336	A	C5-C6-N1	8.35	121.87	117.70
21	AA	452	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	886	A	C5-C6-N1	8.34	121.87	117.70
36	BN	22	ARG	NE-CZ-NH1	8.34	124.47	120.30
54	BA	1502	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	1213	A	C5-C6-N1	8.34	121.87	117.70
54	BA	1021	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	2577	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	945	A	C5-C6-N1	8.33	121.87	117.70
54	BA	460	A	C5-C6-N1	8.33	121.86	117.70
54	BA	1962	C	N3-C2-O2	-8.33	116.07	121.90
46	BX	71	ARG	NE-CZ-NH1	8.33	124.46	120.30
54	BA	743	A	N1-C6-N6	-8.33	113.61	118.60
21	AA	845	A	O4'-C1'-N9	8.32	114.86	108.20
54	BA	456	C	N1-C2-O2	8.32	123.89	118.90
54	BA	1490	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	2306	C	O4'-C1'-N1	8.32	114.86	108.20
24	A3	73	A	C5-C6-N1	8.32	121.86	117.70
54	BA	1901	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	1340	U	O4'-C1'-N1	8.31	114.85	108.20
54	BA	2042	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	77	A	N1-C6-N6	-8.31	113.61	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1180	A	N1-C6-N6	-8.31	113.61	118.60
21	AA	509	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2114	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	1872	A	N1-C6-N6	-8.31	113.62	118.60
54	BA	1928	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	21	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	2114	A	C5-C6-N1	8.30	121.85	117.70
48	BZ	44	ARG	NE-CZ-NH1	8.29	124.45	120.30
54	BA	404	A	N1-C6-N6	-8.29	113.62	118.60
21	AA	532	A	N1-C6-N6	-8.29	113.62	118.60
21	AA	1299	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	1328	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	1566	A	C5-C6-N1	8.29	121.85	117.70
54	BA	2528	U	O4'-C1'-N1	8.29	114.83	108.20
32	BJ	37	ARG	NE-CZ-NH1	8.29	124.44	120.30
21	AA	50	A	N1-C6-N6	-8.29	113.63	118.60
21	AA	71	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	793	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1918	A	N1-C6-N6	-8.28	113.63	118.60
1	AB	107	ARG	NE-CZ-NH1	8.28	124.44	120.30
21	AA	819	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	781	A	C5-C6-N1	8.28	121.84	117.70
54	BA	2792	A	C5-C6-N1	8.28	121.84	117.70
21	AA	715	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	643	A	O4'-C1'-N9	8.28	114.82	108.20
54	BA	1607	C	N3-C2-O2	-8.28	116.11	121.90
54	BA	1603	A	C5-C6-N1	8.27	121.84	117.70
54	BA	2158	A	C5-C6-N1	8.27	121.84	117.70
21	AA	1014	A	C5-C6-N1	8.27	121.83	117.70
54	BA	761	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	1808	A	C5-C6-N1	8.27	121.83	117.70
54	BA	1395	A	C5-C6-N1	8.27	121.83	117.70
18	AS	35	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	889	C	N3-C2-O2	-8.26	116.12	121.90
54	BA	481	G	O4'-C1'-N9	8.26	114.81	108.20
21	AA	397	A	C5-C6-N1	8.26	121.83	117.70
54	BA	149	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	1086	A	C5-C6-N1	8.25	121.83	117.70
55	BB	53	A	C5-C6-N1	8.25	121.82	117.70
43	BU	5	ARG	NE-CZ-NH1	8.25	124.42	120.30
21	AA	539	A	N1-C6-N6	-8.24	113.65	118.60
21	AA	1036	A	N1-C6-N6	-8.24	113.65	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1167	A	C5-C6-N1	8.24	121.82	117.70
54	BA	515	A	C5-C6-N1	8.24	121.82	117.70
54	BA	896	A	C5-C6-N1	8.24	121.82	117.70
55	BB	59	A	N1-C6-N6	-8.24	113.65	118.60
56	B5	122	ARG	NE-CZ-NH2	8.24	124.42	120.30
2	AC	131	ARG	NE-CZ-NH1	8.24	124.42	120.30
21	AA	459	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1016	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1289	A	C5-C6-N1	8.24	121.82	117.70
21	AA	1502	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	1669	A	C5-C6-N1	8.24	121.82	117.70
54	BA	2682	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1493	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	627	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2501	C	N3-C2-O2	-8.23	116.14	121.90
28	BF	149	ARG	NE-CZ-NH1	8.23	124.42	120.30
54	BA	2434	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	487	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	1264	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2134	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2147	A	C5-C6-N1	8.23	121.81	117.70
54	BA	528	A	C5-C6-N1	8.22	121.81	117.70
54	BA	2886	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	996	A	C5-C6-N1	8.21	121.81	117.70
54	BA	1919	A	C5-C6-N1	8.21	121.81	117.70
21	AA	412	A	N1-C6-N6	-8.21	113.67	118.60
37	BO	25	ARG	NE-CZ-NH1	8.21	124.41	120.30
54	BA	199	A	C5-C6-N1	8.21	121.81	117.70
54	BA	2169	A	O4'-C1'-N9	8.21	114.77	108.20
54	BA	1393	A	C5-C6-N1	8.21	121.81	117.70
21	AA	152	A	C4-C5-C6	-8.21	112.90	117.00
21	AA	676	A	C5-C6-N1	8.21	121.80	117.70
24	A3	11	A	C5-C6-N1	8.21	121.80	117.70
54	BA	2191	A	N1-C6-N6	-8.21	113.68	118.60
25	BC	257	ARG	NE-CZ-NH1	8.21	124.40	120.30
54	BA	1717	A	C5-C6-N1	8.21	121.80	117.70
54	BA	1626	A	C5-C6-N1	8.20	121.80	117.70
54	BA	2711	A	C5-C6-N1	8.20	121.80	117.70
54	BA	586	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	2117	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	2564	A	C5-C6-N1	8.20	121.80	117.70
54	BA	901	C	N3-C2-O2	-8.19	116.17	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2418	A	C5-C6-N1	8.19	121.80	117.70
21	AA	1399	C	N3-C2-O2	-8.19	116.17	121.90
21	AA	1533	C	N3-C2-O2	-8.19	116.17	121.90
54	BA	1815	A	C5-C6-N1	8.19	121.80	117.70
54	BA	541	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2199	A	N1-C6-N6	-8.19	113.69	118.60
21	AA	1360	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2170	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	984	A	N1-C6-N6	-8.18	113.69	118.60
32	BJ	35	ARG	NE-CZ-NH1	8.18	124.39	120.30
54	BA	64	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	2476	A	C5-C6-N1	8.18	121.79	117.70
54	BA	2448	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	2458	G	O4'-C1'-N9	8.18	114.74	108.20
54	BA	91	A	O4'-C1'-N9	8.17	114.74	108.20
54	BA	833	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2826	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	14	A	C5-C6-N1	8.17	121.78	117.70
8	AI	10	ARG	NE-CZ-NH1	8.17	124.38	120.30
24	A3	58	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	1040	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	429	A	N1-C6-N6	-8.17	113.70	118.60
6	AG	3	ARG	NE-CZ-NH2	8.16	124.38	120.30
21	AA	435	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1027	A	C5-C6-N1	8.16	121.78	117.70
54	BA	1914	C	N3-C2-O2	-8.16	116.19	121.90
19	AT	24	ARG	NE-CZ-NH1	8.16	124.38	120.30
54	BA	279	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1007	C	N3-C2-O2	-8.16	116.19	121.90
54	BA	2851	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	2492	U	N3-C2-O2	-8.16	116.49	122.20
21	AA	1157	A	C5-C6-N1	8.16	121.78	117.70
27	BE	69	ARG	NE-CZ-NH1	8.16	124.38	120.30
54	BA	2212	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	1147	A	C5-C6-N1	8.16	121.78	117.70
54	BA	2468	A	C5-C6-N1	8.16	121.78	117.70
54	BA	1745	A	C5-C6-N1	8.15	121.78	117.70
54	BA	1008	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1246	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	1012	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	1451	C	N3-C2-O2	-8.15	116.19	121.90
54	BA	1439	A	C5-C6-N1	8.15	121.77	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AF	86	ARG	NE-CZ-NH1	8.15	124.37	120.30
54	BA	1772	A	N1-C6-N6	-8.14	113.71	118.60
24	A3	44	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	1640	A	C5-C6-N1	8.14	121.77	117.70
54	BA	631	A	C5-C6-N1	8.13	121.77	117.70
54	BA	1678	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	2412	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	781	A	C5-C6-N1	8.13	121.77	117.70
54	BA	251	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	2054	A	N1-C6-N6	-8.13	113.72	118.60
9	AJ	9	ARG	NE-CZ-NH1	8.13	124.36	120.30
54	BA	478	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1096	A	C5-C6-N1	8.13	121.76	117.70
21	AA	167	A	C5-C6-N1	8.12	121.76	117.70
54	BA	2322	A	N1-C6-N6	-8.12	113.72	118.60
54	BA	556	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	1067	A	C4-C5-C6	-8.12	112.94	117.00
21	AA	964	A	C5-C6-N1	8.12	121.76	117.70
21	AA	1269	A	C5-C6-N1	8.12	121.76	117.70
54	BA	38	A	C4-C5-C6	-8.12	112.94	117.00
54	BA	640	C	N1-C2-O2	8.12	123.77	118.90
54	BA	928	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	1346	A	C5-C6-N1	8.11	121.76	117.70
21	AA	1452	C	N3-C2-O2	-8.11	116.22	121.90
54	BA	1175	A	C5-C6-N1	8.11	121.75	117.70
11	AL	82	ARG	NE-CZ-NH1	8.11	124.36	120.30
54	BA	219	A	C5-C6-N1	8.11	121.75	117.70
54	BA	699	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2430	A	C5-C6-N1	8.11	121.75	117.70
21	AA	101	A	N1-C6-N6	-8.11	113.74	118.60
21	AA	747	A	N1-C6-N6	-8.11	113.74	118.60
54	BA	538	A	N1-C6-N6	-8.11	113.74	118.60
21	AA	913	A	C4-C5-C6	-8.11	112.95	117.00
21	AA	1274	A	C5-C6-N1	8.11	121.75	117.70
21	AA	1150	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	1012	A	C5-C6-N1	8.10	121.75	117.70
21	AA	983	A	C5-C6-N1	8.10	121.75	117.70
55	BB	108	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	499	A	C5-C6-N1	8.09	121.75	117.70
41	BS	88	ARG	NE-CZ-NH1	8.09	124.35	120.30
25	BC	181	ARG	NE-CZ-NH1	8.09	124.35	120.30
54	BA	928	A	C5-C6-N1	8.09	121.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1385	A	N1-C6-N6	-8.09	113.74	118.60
54	BA	2749	A	N1-C6-N6	-8.09	113.74	118.60
20	AU	17	ARG	NE-CZ-NH1	8.09	124.35	120.30
54	BA	1809	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2284	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	1713	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2682	A	C5-C6-N1	8.08	121.74	117.70
21	AA	183	C	N3-C2-O2	-8.08	116.24	121.90
21	AA	915	A	C5-C6-N1	8.08	121.74	117.70
54	BA	2298	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	1110	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	83	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	723	C	N3-C2-O2	-8.08	116.25	121.90
21	AA	1285	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	1534	A	C5-C6-N1	8.07	121.74	117.70
54	BA	74	A	N1-C6-N6	-8.07	113.76	118.60
1	AB	136	ARG	NE-CZ-NH1	8.07	124.34	120.30
37	BO	7	ARG	NE-CZ-NH1	8.07	124.34	120.30
21	AA	66	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	1000	A	N1-C6-N6	-8.07	113.76	118.60
21	AA	1130	A	C5-C6-N1	8.07	121.73	117.70
54	BA	472	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	2520	C	N3-C2-O2	-8.07	116.25	121.90
21	AA	665	A	C4-C5-C6	-8.06	112.97	117.00
47	BY	52	ARG	NE-CZ-NH1	8.06	124.33	120.30
54	BA	118	A	N1-C6-N6	-8.06	113.76	118.60
25	BC	220	ARG	NE-CZ-NH1	8.06	124.33	120.30
54	BA	866	A	C5-C6-N1	8.06	121.73	117.70
54	BA	877	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	1393	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	1503	A	C5-C6-N1	8.05	121.73	117.70
54	BA	504	A	C5-C6-N1	8.05	121.73	117.70
55	BB	108	A	C5-C6-N1	8.05	121.73	117.70
21	AA	1004	A	C5-C6-N1	8.05	121.72	117.70
21	AA	1261	A	N1-C6-N6	-8.04	113.77	118.60
21	AA	109	A	C5-C6-N1	8.04	121.72	117.70
21	AA	1111	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	1508	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	514	A	C5-C6-N1	8.04	121.72	117.70
54	BA	981	A	C5-C6-N1	8.04	121.72	117.70
54	BA	2732	G	O4'-C1'-N9	8.04	114.63	108.20
21	AA	1332	A	C5-C6-N1	8.04	121.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	AN	81	ARG	NE-CZ-NH1	8.04	124.32	120.30
54	BA	996	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	1020	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	1871	A	C5-C6-N1	8.04	121.72	117.70
21	AA	270	A	C5-C6-N1	8.04	121.72	117.70
21	AA	430	A	N1-C6-N6	-8.04	113.78	118.60
45	BW	76	ARG	NE-CZ-NH1	8.03	124.32	120.30
54	BA	190	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	1987	A	N1-C6-N6	-8.03	113.78	118.60
21	AA	878	A	C5-C6-N1	8.03	121.72	117.70
21	AA	1357	A	N1-C6-N6	-8.03	113.78	118.60
55	BB	34	A	C4-C5-C6	-8.03	112.98	117.00
54	BA	735	A	C5-C6-N1	8.03	121.71	117.70
21	AA	1446	A	C5-C6-N1	8.03	121.71	117.70
54	BA	1614	A	C5-C6-N1	8.03	121.71	117.70
21	AA	969	A	C5-C6-N1	8.02	121.71	117.70
54	BA	1579	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	1754	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	1952	A	C5-C6-N1	8.02	121.71	117.70
21	AA	864	A	C5-C6-N1	8.02	121.71	117.70
54	BA	1029	A	C5-C6-N1	8.02	121.71	117.70
54	BA	1147	A	C4-C5-C6	-8.02	112.99	117.00
22	A1	73	A	N1-C6-N6	-8.01	113.79	118.60
21	AA	288	A	N1-C6-N6	-8.01	113.79	118.60
21	AA	1196	A	N1-C6-N6	-8.01	113.79	118.60
54	BA	742	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	789	A	C5-C6-N1	8.01	121.70	117.70
54	BA	2051	A	C5-C6-N1	8.01	121.70	117.70
54	BA	644	A	C5-C6-N1	8.01	121.70	117.70
54	BA	1603	A	N1-C6-N6	-8.01	113.80	118.60
3	AD	114	ARG	NE-CZ-NH1	8.00	124.30	120.30
39	BQ	12	ARG	NE-CZ-NH2	8.00	124.30	120.30
54	BA	256	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	59	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	918	A	N1-C6-N6	-8.00	113.80	118.60
35	BM	81	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	961	C	N3-C2-O2	-8.00	116.30	121.90
21	AA	1022	A	C5-C6-N1	7.99	121.70	117.70
21	AA	1519	A	C5-C6-N1	7.99	121.70	117.70
54	BA	523	C	N3-C2-O2	-7.99	116.31	121.90
54	BA	1133	A	C5-C6-N1	7.99	121.69	117.70
54	BA	2589	A	N1-C6-N6	-7.99	113.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1434	A	C5-C6-N1	7.98	121.69	117.70
11	AL	113	ARG	NE-CZ-NH1	7.98	124.29	120.30
21	AA	693	G	O4'-C1'-N9	7.98	114.58	108.20
54	BA	1247	A	N1-C6-N6	-7.98	113.81	118.60
21	AA	344	A	C5-C6-N1	7.98	121.69	117.70
54	BA	603	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	1544	A	C5-C6-N1	7.98	121.69	117.70
21	AA	1410	A	N1-C6-N6	-7.97	113.81	118.60
21	AA	1411	C	N3-C2-O2	-7.97	116.32	121.90
21	AA	60	A	C5-C6-N1	7.96	121.68	117.70
54	BA	2346	A	N1-C6-N6	-7.96	113.82	118.60
54	BA	2799	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1698	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1713	A	C4-C5-C6	-7.96	113.02	117.00
43	BU	93	ARG	NE-CZ-NH1	7.96	124.28	120.30
54	BA	2503	A	N1-C6-N6	-7.96	113.82	118.60
21	AA	130	A	C4-C5-C6	-7.96	113.02	117.00
54	BA	371	A	C4-C5-C6	-7.96	113.02	117.00
54	BA	621	A	N1-C6-N6	-7.96	113.83	118.60
54	BA	2009	A	C5-C6-N1	7.96	121.68	117.70
54	BA	505	A	N1-C6-N6	-7.96	113.83	118.60
54	BA	1583	A	C5-C6-N1	7.96	121.68	117.70
21	AA	55	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	381	C	N3-C2-O2	-7.95	116.33	121.90
54	BA	119	A	C5-C6-N1	7.95	121.67	117.70
54	BA	1669	A	N1-C6-N6	-7.95	113.83	118.60
29	BG	152	ARG	NE-CZ-NH1	7.95	124.27	120.30
21	AA	321	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1677	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	1080	A	C5-C6-N1	7.94	121.67	117.70
54	BA	1129	A	O4'-C1'-N9	7.94	114.55	108.20
54	BA	1505	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	2274	A	C5-C6-N1	7.94	121.67	117.70
54	BA	2394	C	N3-C2-O2	-7.94	116.34	121.90
21	AA	640	A	C5-C6-N1	7.93	121.67	117.70
24	A3	58	A	C5-C6-N1	7.93	121.67	117.70
54	BA	2471	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1265	A	C5-C6-N1	7.93	121.66	117.70
21	AA	738	C	N3-C2-O2	-7.93	116.35	121.90
21	AA	1346	A	N1-C6-N6	-7.93	113.84	118.60
51	B2	35	ARG	NE-CZ-NH1	7.93	124.26	120.30
54	BA	1899	A	C5-C6-N1	7.93	121.66	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	729	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1876	A	C5-C6-N1	7.92	121.66	117.70
54	BA	2417	C	N3-C2-O2	-7.92	116.35	121.90
55	BB	11	C	N3-C2-O2	-7.92	116.35	121.90
54	BA	240	C	N3-C2-O2	-7.92	116.35	121.90
54	BA	415	A	C4-C5-C6	-7.92	113.04	117.00
14	AO	88	ARG	NE-CZ-NH1	7.92	124.26	120.30
21	AA	329	A	C5-C6-N1	7.92	121.66	117.70
54	BA	689	A	C5-C6-N1	7.92	121.66	117.70
54	BA	508	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1103	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	2119	A	C5-C6-N1	7.92	121.66	117.70
54	BA	2765	A	N1-C6-N6	-7.92	113.85	118.60
55	BB	45	A	N1-C6-N6	-7.91	113.85	118.60
21	AA	72	A	N1-C6-N6	-7.91	113.85	118.60
21	AA	1499	A	N1-C6-N6	-7.91	113.85	118.60
54	BA	2815	C	N3-C2-O2	-7.91	116.36	121.90
21	AA	28	A	N1-C6-N6	-7.91	113.86	118.60
21	AA	931	C	N3-C2-O2	-7.91	116.36	121.90
21	AA	1151	A	N1-C6-N6	-7.91	113.86	118.60
39	BQ	63	ARG	NE-CZ-NH1	7.91	124.25	120.30
54	BA	453	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	402	A	C5-C6-N1	7.91	121.65	117.70
54	BA	2734	A	N1-C6-N6	-7.91	113.86	118.60
22	A1	6	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	614	A	C5-C6-N1	7.90	121.65	117.70
43	BU	6	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	1384	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2142	A	C4-C5-C6	-7.90	113.05	117.00
21	AA	320	A	N1-C6-N6	-7.90	113.86	118.60
51	B2	39	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	614	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	322	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2873	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	366	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1394	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2740	A	C5-C6-N1	7.90	121.65	117.70
54	BA	262	A	C5-C6-N1	7.89	121.65	117.70
22	A1	66	A	C5-C6-N1	7.89	121.65	117.70
55	BB	88	C	N3-C2-O2	-7.89	116.38	121.90
21	AA	949	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	982	C	N1-C2-O2	7.89	123.63	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	191	A	C5-C6-N1	7.89	121.64	117.70
54	BA	910	A	C5-C6-N1	7.89	121.64	117.70
54	BA	2309	A	N1-C6-N6	-7.89	113.87	118.60
1	AB	207	ARG	NE-CZ-NH1	7.88	124.24	120.30
12	AM	91	ARG	NE-CZ-NH1	7.88	124.24	120.30
21	AA	65	A	O4'-C1'-N9	7.88	114.50	108.20
21	AA	1105	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	2047	C	N3-C2-O2	-7.88	116.38	121.90
54	BA	582	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	2675	A	C5-C6-N1	7.88	121.64	117.70
54	BA	384	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	706	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1040	A	C5-C6-N1	7.88	121.64	117.70
54	BA	2425	A	C4-C5-C6	-7.88	113.06	117.00
54	BA	221	A	C5-C6-N1	7.88	121.64	117.70
54	BA	152	A	C5-C6-N1	7.87	121.64	117.70
54	BA	705	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	1648	U	O4'-C1'-N1	7.87	114.50	108.20
21	AA	1214	C	N1-C2-O2	7.87	123.62	118.90
54	BA	782	A	N1-C6-N6	-7.87	113.88	118.60
13	AN	75	ARG	NE-CZ-NH1	7.87	124.23	120.30
22	A1	69	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	502	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	1453	A	C5-C6-N1	7.87	121.63	117.70
21	AA	309	A	C5-C6-N1	7.87	121.63	117.70
54	BA	655	A	C5-C6-N1	7.87	121.63	117.70
54	BA	1288	G	O4'-C1'-N9	7.87	114.49	108.20
21	AA	393	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	615	U	O4'-C1'-N1	7.86	114.49	108.20
21	AA	1283	U	O4'-C1'-N1	7.86	114.49	108.20
21	AA	1437	A	C5-C6-N1	7.86	121.63	117.70
54	BA	715	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	2019	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	2602	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	2758	A	C5-C6-N1	7.86	121.63	117.70
21	AA	1170	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1508	A	C5-C6-N1	7.86	121.63	117.70
54	BA	207	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2062	A	C5-C6-N1	7.85	121.63	117.70
21	AA	160	A	C5-C6-N1	7.85	121.63	117.70
21	AA	563	A	C5-C6-N1	7.85	121.62	117.70
54	BA	975	A	C5-C6-N1	7.85	121.62	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1677	A	C5-C6-N1	7.84	121.62	117.70
21	AA	1157	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	1678	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2288	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	1028	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	1608	A	C5-C6-N1	7.84	121.62	117.70
54	BA	28	A	C5-C6-N1	7.84	121.62	117.70
54	BA	1953	A	C5-C6-N1	7.84	121.62	117.70
54	BA	2601	C	N3-C2-O2	-7.84	116.41	121.90
54	BA	1676	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	2606	C	N3-C2-O2	-7.83	116.42	121.90
21	AA	466	A	C5-C6-N1	7.83	121.62	117.70
54	BA	752	A	C5-C6-N1	7.83	121.62	117.70
54	BA	1965	C	N3-C2-O2	-7.83	116.42	121.90
54	BA	172	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	324	A	C5-C6-N1	7.83	121.62	117.70
54	BA	2765	A	C5-C6-N1	7.83	121.62	117.70
21	AA	1044	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1032	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	1288	A	C5-C6-N1	7.83	121.61	117.70
2	AC	130	ARG	NE-CZ-NH2	7.83	124.21	120.30
47	BY	29	ARG	NE-CZ-NH1	7.82	124.21	120.30
54	BA	1522	A	C5-C6-N1	7.82	121.61	117.70
21	AA	306	A	C4-C5-C6	-7.82	113.09	117.00
21	AA	1111	A	C5-C6-N1	7.82	121.61	117.70
54	BA	241	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1155	A	N1-C6-N6	-7.82	113.91	118.60
21	AA	1176	A	N1-C6-N6	-7.81	113.91	118.60
54	BA	877	A	C5-C6-N1	7.81	121.61	117.70
21	AA	1246	A	C4-C5-C6	-7.81	113.09	117.00
54	BA	1938	A	C5-C6-N1	7.81	121.61	117.70
54	BA	2725	A	C4-C5-C6	-7.81	113.09	117.00
54	BA	2781	A	C5-C6-N1	7.81	121.61	117.70
54	BA	1559	U	O4'-C1'-N1	7.81	114.45	108.20
54	BA	2309	A	C5-C6-N1	7.81	121.60	117.70
54	BA	1616	A	C5-C6-N1	7.81	121.60	117.70
21	AA	596	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	777	A	C5-C6-N1	7.80	121.60	117.70
21	AA	374	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	1067	A	C5-C6-N1	7.80	121.60	117.70
54	BA	786	C	N3-C2-O2	-7.80	116.44	121.90
21	AA	77	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	899	C	N3-C2-O2	-7.80	116.44	121.90
22	A1	74	C	N1-C2-O2	7.80	123.58	118.90
20	AU	32	ARG	NE-CZ-NH2	7.80	124.20	120.30
21	AA	1257	A	C5-C6-N1	7.80	121.60	117.70
24	A3	35	C	N3-C2-O2	-7.80	116.44	121.90
54	BA	1070	A	C5-C6-N1	7.79	121.60	117.70
54	BA	1565	C	N3-C2-O2	-7.79	116.44	121.90
21	AA	262	A	C4-C5-C6	-7.79	113.11	117.00
54	BA	44	A	C5-C6-N1	7.79	121.60	117.70
54	BA	2015	A	C5-C6-N1	7.79	121.60	117.70
54	BA	1598	A	N1-C6-N6	-7.79	113.93	118.60
55	BB	118	C	N3-C2-O2	-7.79	116.45	121.90
21	AA	129	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	2264	C	O4'-C1'-N1	7.79	114.43	108.20
21	AA	1283	U	N3-C2-O2	-7.79	116.75	122.20
54	BA	699	A	C5-C6-N1	7.79	121.59	117.70
54	BA	896	A	C4-C5-C6	-7.79	113.11	117.00
54	BA	1007	C	N1-C2-O2	7.78	123.57	118.90
54	BA	1169	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1447	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	97	C	O4'-C1'-N1	7.78	114.43	108.20
54	BA	2776	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	264	C	N3-C2-O2	-7.78	116.45	121.90
54	BA	219	A	C4-C5-C6	-7.78	113.11	117.00
54	BA	792	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	1320	C	N1-C2-O2	7.78	123.57	118.90
54	BA	1746	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	2551	C	N3-C2-O2	-7.78	116.45	121.90
54	BA	2712	C	N3-C2-O2	-7.78	116.45	121.90
54	BA	344	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1236	A	C5-C6-N1	7.78	121.59	117.70
54	BA	532	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	920	A	N1-C6-N6	-7.78	113.94	118.60
54	BA	1354	A	N1-C6-N6	-7.78	113.93	118.60
24	A3	60	A	C5-C6-N1	7.77	121.59	117.70
54	BA	196	A	C5-C6-N1	7.77	121.59	117.70
54	BA	1175	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	630	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	160	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1244	A	N1-C6-N6	-7.77	113.94	118.60
1	AB	62	ARG	NE-CZ-NH1	7.77	124.18	120.30
54	BA	1353	A	C5-C6-N1	7.77	121.58	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1496	A	C5-C6-N1	7.77	121.58	117.70
55	BB	39	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1705	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	197	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1572	A	C5-C6-N1	7.76	121.58	117.70
55	BB	52	A	C5-C6-N1	7.76	121.58	117.70
21	AA	306	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2740	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	78	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1676	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2314	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2565	A	C5-C6-N1	7.76	121.58	117.70
54	BA	1829	A	C5-C6-N1	7.76	121.58	117.70
54	BA	2154	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	1672	A	C5-C6-N1	7.75	121.58	117.70
54	BA	323	C	N3-C2-O2	-7.75	116.47	121.90
54	BA	2755	C	N3-C2-O2	-7.75	116.47	121.90
36	BN	86	ARG	NE-CZ-NH1	7.75	124.18	120.30
36	BN	96	ARG	NE-CZ-NH2	-7.75	116.42	120.30
21	AA	382	A	N1-C6-N6	-7.75	113.95	118.60
21	AA	974	A	C5-C6-N1	7.75	121.57	117.70
54	BA	666	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1359	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1786	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2530	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	1383	A	C5-C6-N1	7.75	121.57	117.70
54	BA	1076	C	N3-C2-O2	-7.74	116.48	121.90
54	BA	1077	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1241	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2492	U	O4'-C1'-N1	7.74	114.40	108.20
21	AA	393	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1042	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2758	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	1701	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2267	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	1048	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1912	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1965	C	O4'-C1'-N1	7.74	114.39	108.20
54	BA	144	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2860	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	815	A	N1-C6-N6	-7.74	113.96	118.60
21	AA	1299	A	C5-C6-N1	7.73	121.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1126	A	C5-C6-N1	7.73	121.57	117.70
54	BA	1762	A	N1-C6-N6	-7.73	113.96	118.60
21	AA	60	A	C4-C5-C6	-7.73	113.14	117.00
54	BA	176	A	C5-C6-N1	7.73	121.56	117.70
54	BA	574	A	C5-C6-N1	7.73	121.56	117.70
54	BA	685	A	C5-C6-N1	7.73	121.56	117.70
21	AA	1146	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	2052	A	C5-C6-N1	7.73	121.56	117.70
21	AA	66	A	C5-C6-N1	7.72	121.56	117.70
21	AA	909	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1580	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1650	A	N1-C6-N6	-7.72	113.97	118.60
11	AL	109	ARG	NE-CZ-NH1	7.72	124.16	120.30
21	AA	436	C	N3-C2-O2	-7.72	116.50	121.90
54	BA	6	A	C5-C6-N1	7.72	121.56	117.70
21	AA	787	A	C5-C6-N1	7.71	121.56	117.70
54	BA	640	C	C2-N3-C4	-7.71	116.05	119.90
21	AA	183	C	O4'-C1'-N1	7.71	114.37	108.20
54	BA	1755	A	C4-C5-C6	-7.71	113.14	117.00
21	AA	728	A	C5-C6-N1	7.71	121.55	117.70
54	BA	394	C	N3-C2-O2	-7.71	116.50	121.90
54	BA	1757	A	C5-C6-N1	7.71	121.55	117.70
21	AA	695	A	N1-C6-N6	-7.71	113.98	118.60
21	AA	1158	C	N1-C2-O2	7.71	123.52	118.90
2	AC	135	ARG	NE-CZ-NH1	7.71	124.15	120.30
54	BA	2088	A	N1-C6-N6	-7.71	113.98	118.60
21	AA	131	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2176	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2541	A	C5-C6-N1	7.70	121.55	117.70
21	AA	768	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	1102	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	906	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1570	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	706	A	C5-C6-N1	7.69	121.55	117.70
21	AA	732	C	N3-C2-O2	-7.69	116.52	121.90
54	BA	2060	A	C5-C6-N1	7.69	121.55	117.70
54	BA	2610	C	N1-C2-O2	7.69	123.52	118.90
27	BE	21	ARG	NE-CZ-NH1	7.69	124.14	120.30
21	AA	493	A	C5-C6-N1	7.69	121.54	117.70
21	AA	747	A	C5-C6-N1	7.68	121.54	117.70
21	AA	1246	A	C5-C6-N1	7.68	121.54	117.70
21	AA	1531	A	C5-C6-N1	7.68	121.54	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1927	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2858	C	N3-C2-O2	-7.68	116.52	121.90
21	AA	819	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1650	A	C5-C6-N1	7.68	121.54	117.70
21	AA	573	A	C5-C6-N1	7.68	121.54	117.70
54	BA	941	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1829	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	792	A	C5-C6-N1	7.68	121.54	117.70
21	AA	1096	C	N3-C2-O2	-7.68	116.52	121.90
21	AA	1167	A	N1-C6-N6	-7.68	113.99	118.60
33	BK	64	ARG	NE-CZ-NH1	7.68	124.14	120.30
21	AA	1082	A	C5-C6-N1	7.67	121.54	117.70
54	BA	718	A	O4'-C1'-N9	7.67	114.34	108.20
54	BA	2247	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	196	A	C4-C5-C6	-7.67	113.17	117.00
22	A1	74	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	668	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	1625	C	N3-C2-O2	-7.67	116.53	121.90
21	AA	1191	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1398	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1204	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	303	A	C4-C5-C6	-7.67	113.17	117.00
54	BA	19	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1349	A	C5-C6-N1	7.67	121.53	117.70
54	BA	1548	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	621	A	C5-C6-N1	7.66	121.53	117.70
54	BA	513	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2611	C	N3-C2-O2	-7.66	116.54	121.90
21	AA	520	A	N1-C6-N6	-7.66	114.00	118.60
54	BA	582	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2700	A	N1-C6-N6	-7.66	114.00	118.60
31	BI	64	ARG	NE-CZ-NH1	7.66	124.13	120.30
54	BA	2425	A	C5-C6-N1	7.66	121.53	117.70
21	AA	907	A	C5-C6-N1	7.66	121.53	117.70
21	AA	1306	A	C5-C6-N1	7.66	121.53	117.70
21	AA	1433	A	C5-C6-N1	7.66	121.53	117.70
54	BA	911	A	N1-C6-N6	-7.66	114.00	118.60
54	BA	1169	A	C4-C5-C6	-7.65	113.17	117.00
54	BA	1937	A	C5-C6-N1	7.65	121.53	117.70
54	BA	2274	A	C4-C5-C6	-7.65	113.17	117.00
21	AA	174	A	C4-C5-C6	-7.65	113.17	117.00
22	A1	41	A	C5-C6-N1	7.65	121.53	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	990	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	1321	A	N1-C6-N6	-7.65	114.01	118.60
17	AR	62	ARG	NE-CZ-NH1	7.65	124.12	120.30
21	AA	73	C	N3-C2-O2	-7.65	116.55	121.90
21	AA	329	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	1545	A	N1-C6-N6	-7.65	114.01	118.60
55	BB	73	A	C5-C6-N1	7.65	121.53	117.70
21	AA	327	A	N1-C6-N6	-7.65	114.01	118.60
54	BA	2417	C	O4'-C1'-N1	7.65	114.32	108.20
21	AA	1163	A	C5-C6-N1	7.64	121.52	117.70
24	A3	59	A	C5-C6-N1	7.64	121.52	117.70
21	AA	364	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	705	A	C5-C6-N1	7.64	121.52	117.70
2	AC	10	ARG	NE-CZ-NH1	7.64	124.12	120.30
3	AD	187	ARG	NE-CZ-NH1	7.64	124.12	120.30
21	AA	576	C	C1'-O4'-C4'	-7.64	103.79	109.90
54	BA	800	A	C5-C6-N1	7.64	121.52	117.70
54	BA	878	A	N1-C6-N6	-7.64	114.02	118.60
54	BA	2422	C	O4'-C1'-N1	7.64	114.31	108.20
54	BA	845	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2169	A	C5-C6-N1	7.64	121.52	117.70
3	AD	183	ARG	NE-CZ-NH1	7.63	124.12	120.30
54	BA	1347	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	2311	A	C5-C6-N1	7.63	121.52	117.70
54	BA	1603	A	C4-C5-C6	-7.63	113.18	117.00
21	AA	98	A	C5-C6-N1	7.63	121.52	117.70
21	AA	363	A	C5-C6-N1	7.63	121.52	117.70
21	AA	583	A	C5-C6-N1	7.63	121.52	117.70
21	AA	767	A	C4-C5-C6	-7.63	113.18	117.00
21	AA	787	A	C4-C5-C6	-7.63	113.18	117.00
54	BA	936	A	C4-C5-C6	-7.63	113.19	117.00
54	BA	470	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	1304	A	C4-C5-C6	-7.63	113.19	117.00
21	AA	50	A	C5-C6-N1	7.63	121.51	117.70
54	BA	753	A	C5-C6-N1	7.63	121.51	117.70
54	BA	1936	A	C5-C6-N1	7.63	121.51	117.70
54	BA	979	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	673	A	C4-C5-C6	-7.62	113.19	117.00
21	AA	1223	C	N3-C2-O2	-7.62	116.56	121.90
24	A3	22	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	89	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	531	C	N3-C2-O2	-7.62	116.56	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1156	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1536	C	N3-C2-O2	-7.62	116.56	121.90
54	BA	1635	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1670	C	N3-C2-O2	-7.62	116.56	121.90
54	BA	2792	A	C4-C5-C6	-7.62	113.19	117.00
54	BA	1211	C	N3-C2-O2	-7.62	116.57	121.90
21	AA	1019	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	863	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1009	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2359	C	N3-C2-O2	-7.62	116.57	121.90
21	AA	197	A	C4-C5-C6	-7.62	113.19	117.00
21	AA	1518	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1780	A	C5-C6-N1	7.62	121.51	117.70
54	BA	466	A	C5-C6-N1	7.62	121.51	117.70
54	BA	751	A	C5-C6-N1	7.62	121.51	117.70
54	BA	223	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	2377	A	C5-C6-N1	7.61	121.51	117.70
54	BA	2432	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	947	A	C4-C5-C6	-7.61	113.19	117.00
21	AA	363	A	C4-C5-C6	-7.61	113.19	117.00
21	AA	1229	A	C5-C6-N1	7.61	121.50	117.70
54	BA	310	A	N1-C6-N6	-7.61	114.03	118.60
21	AA	892	A	N1-C6-N6	-7.61	114.04	118.60
21	AA	1171	A	N1-C6-N6	-7.61	114.04	118.60
54	BA	2306	C	N3-C2-O2	-7.61	116.58	121.90
54	BA	1001	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	356	A	C5-C6-N1	7.60	121.50	117.70
54	BA	104	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	932	C	N3-C2-O2	-7.60	116.58	121.90
21	AA	214	C	N3-C2-O2	-7.60	116.58	121.90
21	AA	1403	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	382	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	1067	A	C5-C6-N1	7.60	121.50	117.70
21	AA	54	C	O4'-C1'-N1	7.60	114.28	108.20
54	BA	637	A	C4-C5-C6	-7.59	113.20	117.00
54	BA	2097	A	N1-C6-N6	-7.59	114.04	118.60
21	AA	977	A	C5-C6-N1	7.59	121.50	117.70
54	BA	1885	A	C4-C5-C6	-7.59	113.20	117.00
54	BA	2241	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	127	A	C5-C6-N1	7.59	121.50	117.70
54	BA	2518	A	O4'-C1'-N9	7.59	114.27	108.20
21	AA	499	A	C4-C5-C6	-7.59	113.21	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	889	A	C5-C6-N1	7.59	121.49	117.70
54	BA	2600	A	N1-C6-N6	-7.59	114.05	118.60
15	AP	14	ARG	NE-CZ-NH1	7.58	124.09	120.30
54	BA	936	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	1023	U	O4'-C1'-N1	7.58	114.27	108.20
54	BA	1962	C	P-O3'-C3'	7.58	128.80	119.70
21	AA	238	A	C5-C6-N1	7.58	121.49	117.70
21	AA	487	A	C5-C6-N1	7.58	121.49	117.70
21	AA	1285	A	C5-C6-N1	7.58	121.49	117.70
8	AI	112	ARG	NE-CZ-NH1	7.58	124.09	120.30
23	A2	82	A	C5-C6-N1	7.58	121.49	117.70
52	B3	44	ARG	NE-CZ-NH1	7.58	124.09	120.30
54	BA	602	A	N1-C6-N6	-7.58	114.06	118.60
54	BA	2628	C	N1-C2-O2	7.58	123.44	118.90
21	AA	1080	A	C5-C6-N1	7.57	121.49	117.70
54	BA	877	A	C4-C5-C6	-7.57	113.21	117.00
55	BB	73	A	C4-C5-C6	-7.57	113.21	117.00
45	BW	40	ARG	NE-CZ-NH1	7.57	124.09	120.30
6	AG	95	ARG	NE-CZ-NH1	7.57	124.08	120.30
54	BA	1713	A	C5-C6-N1	7.57	121.48	117.70
21	AA	996	A	C4-C5-C6	-7.57	113.22	117.00
21	AA	1105	A	C5-C6-N1	7.57	121.48	117.70
21	AA	8	A	C5-C6-N1	7.57	121.48	117.70
24	A3	40	C	N3-C2-O2	-7.57	116.60	121.90
54	BA	1746	A	C5-C6-N1	7.57	121.48	117.70
21	AA	431	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	362	A	C5-C6-N1	7.57	121.48	117.70
54	BA	1757	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	435	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	627	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2778	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	1609	A	C5-C6-N1	7.56	121.48	117.70
54	BA	502	A	N1-C6-N6	-7.56	114.07	118.60
54	BA	2273	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2534	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2706	A	C5-C6-N1	7.55	121.48	117.70
54	BA	217	A	C5-C6-N1	7.55	121.48	117.70
21	AA	946	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	465	A	C5-C6-N1	7.55	121.47	117.70
21	AA	640	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1784	A	C4-C5-C6	-7.55	113.23	117.00
2	AC	64	ARG	NE-CZ-NH1	7.55	124.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AD	114	ARG	NE-CZ-NH2	-7.55	116.53	120.30
21	AA	1510	C	N3-C2-O2	-7.54	116.62	121.90
54	BA	1080	A	C4-C5-C6	-7.54	113.23	117.00
54	BA	640	C	N1-C2-N3	7.54	124.48	119.20
21	AA	270	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	728	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	908	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	1349	A	N1-C6-N6	-7.54	114.08	118.60
43	BU	81	ARG	NE-CZ-NH1	7.54	124.07	120.30
54	BA	1328	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1664	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	599	A	N1-C6-N6	-7.54	114.08	118.60
2	AC	163	ARG	NE-CZ-NH1	7.54	124.07	120.30
21	AA	746	A	N1-C6-N6	-7.54	114.08	118.60
21	AA	1531	A	N1-C6-N6	-7.54	114.08	118.60
55	BB	58	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	675	A	C5-C6-N1	7.53	121.47	117.70
54	BA	1489	C	N3-C2-O2	-7.53	116.63	121.90
22	A1	76	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	1637	A	C5-C6-N1	7.53	121.47	117.70
54	BA	1133	A	C4-C5-C6	-7.53	113.23	117.00
21	AA	1169	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	791	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	2422	C	N3-C2-O2	-7.53	116.63	121.90
55	BB	27	C	N3-C2-O2	-7.53	116.63	121.90
21	AA	26	A	C5-C6-N1	7.53	121.46	117.70
21	AA	704	A	C5-C6-N1	7.53	121.46	117.70
21	AA	1333	A	C5-C6-N1	7.53	121.46	117.70
21	AA	994	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1483	A	N1-C6-N6	-7.52	114.09	118.60
24	A3	3	C	N1-C2-O2	7.52	123.41	118.90
54	BA	497	A	C5-C6-N1	7.52	121.46	117.70
54	BA	886	A	C4-C5-C6	-7.52	113.24	117.00
54	BA	1580	A	C4-C5-C6	-7.52	113.24	117.00
25	BC	268	ARG	NE-CZ-NH1	7.52	124.06	120.30
54	BA	2450	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1431	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2872	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	10	A	C5-C6-N1	7.52	121.46	117.70
21	AA	718	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1046	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1260	A	C4-C5-C6	-7.52	113.24	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2095	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2835	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1201	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	526	A	C4-C5-C6	-7.51	113.24	117.00
54	BA	213	A	C5-C6-N1	7.51	121.46	117.70
54	BA	599	A	C5-C6-N1	7.51	121.46	117.70
21	AA	1513	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	1947	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	1918	A	C5-C6-N1	7.51	121.45	117.70
54	BA	2476	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	1493	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	1899	A	N1-C6-N6	-7.51	114.10	118.60
54	BA	2483	C	N3-C2-O2	-7.51	116.64	121.90
21	AA	300	A	C5-C6-N1	7.50	121.45	117.70
54	BA	544	C	N3-C2-O2	-7.50	116.65	121.90
54	BA	2614	A	C5-C6-N1	7.50	121.45	117.70
54	BA	920	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1419	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1548	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	1854	A	C5-C6-N1	7.50	121.45	117.70
21	AA	482	A	C5-C6-N1	7.50	121.45	117.70
21	AA	938	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	541	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	800	A	C4-C5-C6	-7.50	113.25	117.00
54	BA	1392	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2288	A	C5-C6-N1	7.50	121.45	117.70
21	AA	968	A	C5-C6-N1	7.50	121.45	117.70
54	BA	784	G	O4'-C1'-N9	7.50	114.20	108.20
29	BG	162	ARG	NE-CZ-NH1	7.50	124.05	120.30
40	BR	68	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	203	A	C5-C6-N1	7.50	121.45	117.70
54	BA	608	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2406	A	C5-C6-N1	7.50	121.45	117.70
21	AA	1188	A	C5-C6-N1	7.49	121.45	117.70
42	BT	69	ARG	NE-CZ-NH1	7.49	124.05	120.30
54	BA	1783	A	C5-C6-N1	7.49	121.45	117.70
39	BQ	69	ARG	NE-CZ-NH1	7.49	124.05	120.30
54	BA	1451	C	O4'-C1'-N1	7.49	114.19	108.20
54	BA	1551	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	2439	A	N1-C6-N6	-7.49	114.11	118.60
21	AA	120	A	C5-C6-N1	7.49	121.44	117.70
21	AA	383	A	N1-C6-N6	-7.49	114.11	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1340	A	C4-C5-C6	-7.49	113.26	117.00
36	BN	46	ARG	NE-CZ-NH1	7.49	124.04	120.30
6	AG	69	ARG	NE-CZ-NH1	7.49	124.04	120.30
21	AA	687	A	C4-C5-C6	-7.49	113.26	117.00
54	BA	2411	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	1953	A	C4-C5-C6	-7.49	113.26	117.00
54	BA	2031	A	N1-C6-N6	-7.49	114.11	118.60
55	BB	99	A	C5-C6-N1	7.49	121.44	117.70
21	AA	906	A	N1-C6-N6	-7.48	114.11	118.60
21	AA	1429	A	C4-C5-C6	-7.48	113.26	117.00
24	A3	77	A	C5-C6-N1	7.48	121.44	117.70
35	BM	40	ARG	NE-CZ-NH1	7.48	124.04	120.30
56	B5	164	ARG	NE-CZ-NH1	7.48	124.04	120.30
7	AH	14	ARG	NE-CZ-NH1	7.48	124.04	120.30
54	BA	1140	C	O4'-C1'-N1	7.48	114.19	108.20
54	BA	603	A	O4'-C1'-N9	7.48	114.18	108.20
21	AA	282	A	C5-C6-N1	7.48	121.44	117.70
21	AA	845	A	C5-C6-N1	7.47	121.44	117.70
54	BA	477	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	1048	A	C4-C5-C6	-7.47	113.26	117.00
54	BA	2082	A	N1-C6-N6	-7.47	114.12	118.60
21	AA	461	A	C5-C6-N1	7.47	121.44	117.70
21	AA	576	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	1698	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	218	A	C5-C6-N1	7.47	121.43	117.70
54	BA	821	A	C5-C6-N1	7.47	121.43	117.70
54	BA	1810	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	2733	A	N1-C6-N6	-7.47	114.12	118.60
54	BA	37	C	N3-C2-O2	-7.46	116.67	121.90
54	BA	890	C	N3-C2-O2	-7.46	116.67	121.90
54	BA	2388	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1847	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1180	A	C5-C6-N1	7.46	121.43	117.70
40	BR	90	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	1069	A	O4'-C1'-N9	7.46	114.17	108.20
21	AA	642	A	C5-C6-N1	7.46	121.43	117.70
26	BD	124	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	163	C	N3-C2-O2	-7.46	116.68	121.90
55	BB	36	C	N3-C2-O2	-7.46	116.68	121.90
54	BA	505	A	C5-C6-N1	7.46	121.43	117.70
26	BD	128	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	1706	C	N3-C2-O2	-7.46	116.68	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	299	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	1227	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1268	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1503	A	N1-C6-N6	-7.45	114.13	118.60
49	B0	16	ARG	NE-CZ-NH2	7.45	124.02	120.30
54	BA	2070	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1095	A	C5-C6-N1	7.45	121.42	117.70
19	AT	28	ARG	NE-CZ-NH1	7.45	124.02	120.30
21	AA	109	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	321	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1848	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2883	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	1977	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	1332	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	2632	A	C5-C6-N1	7.44	121.42	117.70
8	AI	84	ARG	NE-CZ-NH1	7.44	124.02	120.30
21	AA	131	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	696	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	935	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	131	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1254	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	1646	C	N3-C2-O2	-7.44	116.69	121.90
11	AL	11	ARG	NE-CZ-NH1	7.44	124.02	120.30
54	BA	1431	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1579	A	C5-C6-N1	7.44	121.42	117.70
21	AA	389	A	C5-C6-N1	7.43	121.42	117.70
54	BA	990	A	C5-C6-N1	7.43	121.42	117.70
21	AA	547	A	C5-C6-N1	7.43	121.42	117.70
21	AA	65	A	C5-C6-N1	7.43	121.41	117.70
21	AA	78	A	C5-C6-N1	7.43	121.42	117.70
21	AA	84	U	O4'-C1'-N1	7.43	114.14	108.20
21	AA	36	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	816	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	94	A	N1-C6-N6	-7.42	114.14	118.60
21	AA	1399	C	N1-C2-O2	7.42	123.35	118.90
21	AA	80	A	C5-C6-N1	7.42	121.41	117.70
54	BA	631	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	523	A	C5-C6-N1	7.42	121.41	117.70
54	BA	401	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1730	C	N3-C2-O2	-7.42	116.71	121.90
54	BA	2824	C	N3-C2-O2	-7.42	116.71	121.90
22	A1	69	A	C5-C6-N1	7.42	121.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	616	A	C5-C6-N1	7.42	121.41	117.70
54	BA	980	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1552	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	278	A	C5-C6-N1	7.42	121.41	117.70
54	BA	730	A	N1-C6-N6	-7.42	114.15	118.60
24	A3	76	C	P-O3'-C3'	7.42	128.60	119.70
54	BA	223	A	C5-C6-N1	7.41	121.41	117.70
21	AA	1339	A	N1-C6-N6	-7.41	114.15	118.60
21	AA	54	C	N3-C4-N4	-7.41	112.81	118.00
21	AA	608	A	C5-C6-N1	7.41	121.40	117.70
54	BA	1091	G	O4'-C1'-N9	7.41	114.13	108.20
54	BA	1286	A	C5-C6-N1	7.41	121.40	117.70
54	BA	1618	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2478	A	C5-C6-N1	7.41	121.40	117.70
54	BA	722	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2311	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	1298	U	O4'-C1'-N1	7.40	114.12	108.20
54	BA	1084	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2798	U	O4'-C1'-N1	7.40	114.12	108.20
6	AG	2	ARG	NE-CZ-NH1	7.40	124.00	120.30
54	BA	5	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	345	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1532	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	1548	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2275	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	1229	A	C4-C5-C6	-7.40	113.30	117.00
21	AA	366	A	C5-C6-N1	7.40	121.40	117.70
21	AA	912	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	1597	A	O4'-C1'-N9	7.40	114.12	108.20
54	BA	2225	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	2670	A	C5-C6-N1	7.40	121.40	117.70
21	AA	964	A	N1-C6-N6	-7.39	114.16	118.60
29	BG	68	ARG	NE-CZ-NH1	7.39	124.00	120.30
54	BA	1536	C	O4'-C1'-N1	7.39	114.11	108.20
21	AA	908	A	C5-C6-N1	7.39	121.40	117.70
3	AD	46	ARG	NE-CZ-NH1	7.39	124.00	120.30
21	AA	1476	A	C5-C6-N1	7.39	121.39	117.70
54	BA	528	A	C4-C5-C6	-7.39	113.31	117.00
35	BM	18	ARG	NE-CZ-NH1	7.39	123.99	120.30
54	BA	2147	A	C4-C5-C6	-7.39	113.31	117.00
21	AA	81	A	N1-C6-N6	-7.39	114.17	118.60
21	AA	909	A	N1-C6-N6	-7.39	114.17	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	788	A	C5-C6-N1	7.39	121.39	117.70
54	BA	2598	A	C5-C6-N1	7.39	121.39	117.70
54	BA	613	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	2278	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	2448	A	C5-C6-N1	7.38	121.39	117.70
21	AA	1093	A	C5-C6-N1	7.38	121.39	117.70
54	BA	79	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	2268	A	C5-C6-N1	7.38	121.39	117.70
21	AA	320	A	C5-C6-N1	7.38	121.39	117.70
54	BA	267	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	229	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	2738	A	N1-C6-N6	-7.38	114.17	118.60
6	AG	52	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	67	C	N3-C2-O2	-7.38	116.73	121.90
21	AA	629	A	C5-C6-N1	7.38	121.39	117.70
21	AA	915	A	C4-C5-C6	-7.38	113.31	117.00
21	AA	1465	A	C5-C6-N1	7.38	121.39	117.70
21	AA	412	A	C5-C6-N1	7.38	121.39	117.70
54	BA	661	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	1304	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1615	C	N3-C2-O2	-7.37	116.74	121.90
21	AA	151	A	C5-C6-N1	7.37	121.39	117.70
21	AA	759	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	13	A	C5-C6-N1	7.37	121.39	117.70
54	BA	71	A	C5-C6-N1	7.37	121.39	117.70
54	BA	101	A	O4'-C1'-N9	7.37	114.10	108.20
54	BA	2126	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2665	A	C5-C6-N1	7.37	121.39	117.70
54	BA	53	A	C5-C6-N1	7.37	121.38	117.70
54	BA	1451	C	N1-C2-O2	7.37	123.32	118.90
54	BA	2899	A	C5-C6-N1	7.37	121.38	117.70
21	AA	889	A	C4-C5-C6	-7.37	113.32	117.00
21	AA	1418	A	C5-C6-N1	7.37	121.38	117.70
54	BA	1050	A	C5-C6-N1	7.37	121.38	117.70
54	BA	2741	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	781	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	1342	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2703	C	N3-C2-O2	-7.36	116.75	121.90
6	AG	110	ARG	NE-CZ-NH1	7.36	123.98	120.30
39	BQ	47	ARG	NE-CZ-NH1	7.36	123.98	120.30
21	AA	349	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	176	A	C4-C5-C6	-7.36	113.32	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	947	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2711	A	C4-C5-C6	-7.36	113.32	117.00
21	AA	189	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	821	A	C4-C5-C6	-7.36	113.32	117.00
54	BA	1088	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2062	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	103	A	C5-C6-N1	7.36	121.38	117.70
54	BA	715	A	C5-C6-N1	7.36	121.38	117.70
54	BA	677	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	746	A	C5-C6-N1	7.35	121.38	117.70
54	BA	892	A	C4-C5-C6	-7.35	113.33	117.00
54	BA	1787	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	1055	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	1155	A	C5-C6-N1	7.35	121.37	117.70
21	AA	1287	A	C5-C6-N1	7.35	121.37	117.70
54	BA	1469	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1735	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	2547	A	C5-C6-N1	7.35	121.37	117.70
21	AA	238	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	2392	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1008	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2077	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	2660	A	O4'-C1'-N9	7.34	114.08	108.20
21	AA	1369	C	N3-C2-O2	-7.34	116.76	121.90
21	AA	1378	C	N3-C2-O2	-7.34	116.76	121.90
21	AA	16	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	2868	A	C5-C6-N1	7.34	121.37	117.70
21	AA	817	C	N3-C2-O2	-7.34	116.76	121.90
28	BF	132	ARG	NE-CZ-NH1	7.34	123.97	120.30
4	AE	92	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	1913	A	C5-C6-N1	7.33	121.37	117.70
21	AA	163	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	447	A	C5-C6-N1	7.33	121.36	117.70
54	BA	718	A	C5-C6-N1	7.33	121.37	117.70
21	AA	535	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2287	A	O4'-C1'-N9	7.33	114.06	108.20
54	BA	449	A	C5-C6-N1	7.33	121.36	117.70
54	BA	634	C	N3-C2-O2	-7.33	116.77	121.90
21	AA	313	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2757	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	325	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2634	A	C4-C5-C6	-7.32	113.34	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	352	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2063	C	N3-C2-O2	-7.32	116.77	121.90
21	AA	1278	G	P-O3'-C3'	7.32	128.48	119.70
54	BA	152	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	812	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	1285	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	2184	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	2893	A	C5-C6-N1	7.32	121.36	117.70
21	AA	574	A	C5-C6-N1	7.32	121.36	117.70
54	BA	103	A	C4-C5-C6	-7.32	113.34	117.00
21	AA	496	A	C5-C6-N1	7.32	121.36	117.70
21	AA	975	A	O4'-C1'-N9	7.32	114.05	108.20
54	BA	126	A	C5-C6-N1	7.32	121.36	117.70
54	BA	829	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2517	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	1784	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2856	A	N1-C6-N6	-7.31	114.21	118.60
21	AA	53	A	C4-C5-C6	-7.31	113.34	117.00
54	BA	1502	A	C4-C5-C6	-7.31	113.34	117.00
14	AO	71	ARG	NE-CZ-NH1	7.31	123.95	120.30
21	AA	1413	A	C4-C5-C6	-7.31	113.35	117.00
24	A3	59	A	C4-C5-C6	-7.31	113.35	117.00
54	BA	74	A	C5-C6-N1	7.31	121.35	117.70
54	BA	472	A	C5-C6-N1	7.31	121.35	117.70
54	BA	671	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	2800	A	C5-C6-N1	7.31	121.35	117.70
21	AA	781	A	N1-C6-N6	-7.31	114.22	118.60
21	AA	177	G	O4'-C1'-N9	7.30	114.04	108.20
54	BA	2266	A	C5-C6-N1	7.30	121.35	117.70
21	AA	969	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	1634	A	N1-C6-N6	-7.30	114.22	118.60
22	A1	35	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2169	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	399	U	O4'-C1'-N1	7.30	114.04	108.20
54	BA	899	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2376	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1109	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	1593	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	575	A	C5-C6-N1	7.29	121.35	117.70
54	BA	820	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	765	G	O4'-C1'-N9	7.29	114.03	108.20
54	BA	973	A	N1-C6-N6	-7.29	114.22	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1803	A	N1-C6-N6	-7.29	114.22	118.60
21	AA	630	A	C5-C6-N1	7.29	121.35	117.70
23	A2	79	A	C5-C6-N1	7.29	121.35	117.70
54	BA	38	A	C5-C6-N1	7.29	121.35	117.70
54	BA	2450	A	C4-C5-C6	-7.29	113.36	117.00
21	AA	371	A	C5-C6-N1	7.29	121.34	117.70
21	AA	749	A	C4-C5-C6	-7.29	113.36	117.00
54	BA	1630	A	C4-C5-C6	-7.29	113.36	117.00
24	A3	75	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	439	A	N1-C6-N6	-7.29	114.23	118.60
54	BA	1378	A	C5-C6-N1	7.29	121.34	117.70
54	BA	1938	A	N1-C6-N6	-7.29	114.23	118.60
21	AA	949	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1566	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	560	A	C5-C6-N1	7.28	121.34	117.70
54	BA	382	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1420	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1490	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1806	C	N3-C2-O2	-7.28	116.80	121.90
54	BA	2513	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	1293	C	N3-C2-O2	-7.28	116.81	121.90
21	AA	1377	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	574	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	1395	A	C4-C5-C6	-7.28	113.36	117.00
21	AA	1507	A	C5-C6-N1	7.28	121.34	117.70
54	BA	532	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1165	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1433	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	1655	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	1899	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	2757	A	C5-C6-N1	7.28	121.34	117.70
21	AA	373	A	N1-C6-N6	-7.27	114.24	118.60
21	AA	860	A	N1-C6-N6	-7.27	114.24	118.60
54	BA	2191	A	C5-C6-N1	7.27	121.34	117.70
54	BA	2565	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	768	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1264	A	C5-C6-N1	7.27	121.34	117.70
54	BA	2059	A	C5-C6-N1	7.27	121.34	117.70
21	AA	808	C	N3-C2-O2	-7.27	116.81	121.90
54	BA	2346	A	C5-C6-N1	7.27	121.33	117.70
54	BA	613	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1144	A	N1-C6-N6	-7.27	114.24	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	988	A	C5-C6-N1	7.27	121.33	117.70
21	AA	136	C	N3-C2-O2	-7.26	116.82	121.90
21	AA	554	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1308	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2646	C	N3-C2-O2	-7.26	116.81	121.90
24	A3	1	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	1062	G	O4'-C1'-N9	7.26	114.01	108.20
54	BA	959	A	O4'-C1'-N9	7.26	114.01	108.20
54	BA	1469	A	C5-C6-N1	7.26	121.33	117.70
21	AA	74	A	C5-C6-N1	7.26	121.33	117.70
21	AA	566	G	P-O3'-C3'	7.26	128.41	119.70
54	BA	603	A	C5-C6-N1	7.26	121.33	117.70
54	BA	995	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	1668	A	C4-C5-C6	-7.26	113.37	117.00
21	AA	1374	A	N1-C6-N6	-7.26	114.25	118.60
55	BB	29	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1785	A	C5-C6-N1	7.25	121.33	117.70
54	BA	1427	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	1794	A	C5-C6-N1	7.25	121.33	117.70
2	AC	39	ARG	NE-CZ-NH1	7.25	123.93	120.30
21	AA	250	A	C5-C6-N1	7.25	121.33	117.70
54	BA	449	A	C4-C5-C6	-7.25	113.37	117.00
54	BA	507	A	C5-C6-N1	7.25	121.33	117.70
21	AA	186	C	N3-C2-O2	-7.25	116.83	121.90
21	AA	280	C	N3-C2-O2	-7.25	116.83	121.90
54	BA	1759	A	C4-C5-C6	-7.25	113.38	117.00
55	BB	94	A	C5-C6-N1	7.25	121.32	117.70
54	BA	1649	G	O4'-C1'-N9	7.25	114.00	108.20
54	BA	2297	A	N1-C6-N6	-7.25	114.25	118.60
22	A1	26	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2278	A	C5-C6-N1	7.24	121.32	117.70
21	AA	1352	C	N3-C2-O2	-7.24	116.83	121.90
21	AA	1395	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	556	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2164	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	2198	A	C5-C6-N1	7.24	121.32	117.70
55	BB	15	A	C5-C6-N1	7.24	121.32	117.70
21	AA	205	A	C5-C6-N1	7.24	121.32	117.70
21	AA	288	A	C4-C5-C6	-7.24	113.38	117.00
21	AA	199	A	C5-C6-N1	7.24	121.32	117.70
21	AA	1508	A	C5-C6-N1	7.24	121.32	117.70
41	BS	25	ARG	NE-CZ-NH1	7.24	123.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2761	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	480	A	C5-C6-N1	7.23	121.32	117.70
54	BA	1644	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	2434	A	C5-C6-N1	7.23	121.32	117.70
21	AA	192	A	C4-C5-C6	-7.23	113.38	117.00
54	BA	1759	A	C5-C6-N1	7.23	121.32	117.70
12	AM	112	ARG	NE-CZ-NH1	7.23	123.92	120.30
21	AA	414	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	2820	A	C5-C6-N1	7.23	121.31	117.70
55	BB	97	C	N3-C2-O2	-7.23	116.84	121.90
21	AA	336	A	C4-C5-C6	-7.23	113.39	117.00
54	BA	547	A	C5-C6-N1	7.23	121.31	117.70
54	BA	626	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2386	A	C4-C5-C6	-7.23	113.39	117.00
21	AA	631	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	2094	A	C5-C6-N1	7.23	121.31	117.70
21	AA	949	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	2327	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2666	C	N1-C2-O2	7.22	123.23	118.90
54	BA	2721	A	C5-C6-N1	7.22	121.31	117.70
55	BB	99	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	265	A	C5-C6-N1	7.22	121.31	117.70
54	BA	347	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2515	C	N3-C2-O2	-7.22	116.84	121.90
54	BA	2749	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2886	A	C5-C6-N1	7.22	121.31	117.70
21	AA	328	C	P-O3'-C3'	7.22	128.37	119.70
28	BF	114	ARG	NE-CZ-NH1	7.22	123.91	120.30
54	BA	1650	A	C4-C5-C6	-7.22	113.39	117.00
21	AA	607	A	C5-C6-N1	7.22	121.31	117.70
54	BA	33	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	1553	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2163	A	C5-C6-N1	7.22	121.31	117.70
21	AA	274	A	C5-C6-N1	7.22	121.31	117.70
21	AA	807	A	C5-C6-N1	7.22	121.31	117.70
54	BA	94	A	C5-C6-N1	7.22	121.31	117.70
54	BA	514	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	787	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	1821	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	2183	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2322	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2227	A	N1-C6-N6	-7.21	114.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	622	A	C5-C6-N1	7.21	121.31	117.70
21	AA	44	A	N1-C6-N6	-7.21	114.27	118.60
53	B4	19	ARG	NE-CZ-NH1	7.21	123.91	120.30
54	BA	352	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	1942	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	2635	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	2761	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1569	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2435	A	C4-C5-C6	-7.21	113.39	117.00
21	AA	371	A	C4-C5-C6	-7.21	113.39	117.00
21	AA	509	A	C5-C6-N1	7.21	121.30	117.70
21	AA	1325	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	1978	A	C5-C6-N1	7.21	121.30	117.70
21	AA	1239	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2748	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	1378	A	N1-C6-N6	-7.20	114.28	118.60
39	BQ	29	ARG	NE-CZ-NH2	7.20	123.90	120.30
54	BA	323	C	N1-C2-O2	7.20	123.22	118.90
54	BA	761	A	C5-C6-N1	7.20	121.30	117.70
54	BA	632	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1287	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	2882	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	223	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	2385	C	O4'-C1'-N1	7.20	113.96	108.20
54	BA	2586	U	N3-C2-O2	-7.20	117.16	122.20
54	BA	2587	A	C5-C6-N1	7.20	121.30	117.70
55	BB	115	A	N1-C6-N6	-7.19	114.28	118.60
21	AA	856	C	N3-C2-O2	-7.19	116.86	121.90
54	BA	944	C	O4'-C1'-N1	7.19	113.95	108.20
54	BA	2628	C	O4'-C1'-N1	7.19	113.95	108.20
54	BA	1278	C	O4'-C1'-N1	7.19	113.95	108.20
14	AO	76	ARG	NE-CZ-NH1	7.19	123.89	120.30
54	BA	2101	A	C5-C6-N1	7.19	121.30	117.70
21	AA	726	C	N3-C2-O2	-7.19	116.87	121.90
54	BA	226	A	C5-C6-N1	7.19	121.29	117.70
54	BA	1046	A	C5-C6-N1	7.19	121.29	117.70
21	AA	572	A	C5-C6-N1	7.19	121.29	117.70
54	BA	340	A	C5-C6-N1	7.19	121.29	117.70
21	AA	171	A	C5-C6-N1	7.18	121.29	117.70
54	BA	182	A	C4-C5-C6	-7.18	113.41	117.00
54	BA	1322	A	C5-C6-N1	7.18	121.29	117.70
16	AQ	61	ARG	NE-CZ-NH1	7.18	123.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1470	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1591	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2033	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2534	A	C4-C5-C6	-7.18	113.41	117.00
21	AA	372	C	C1'-O4'-C4'	-7.17	104.16	109.90
21	AA	502	A	C5-C6-N1	7.17	121.29	117.70
21	AA	1499	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1970	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2103	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	642	A	N1-C6-N6	-7.17	114.30	118.60
24	A3	22	A	C5-C6-N1	7.17	121.29	117.70
25	BC	79	ARG	NE-CZ-NH1	7.17	123.89	120.30
54	BA	1655	A	C5-C6-N1	7.17	121.28	117.70
54	BA	1912	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2281	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	2426	A	C4-C5-C6	-7.17	113.41	117.00
21	AA	110	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	313	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	1073	A	N1-C6-N6	-7.17	114.30	118.60
46	BX	56	ARG	NE-CZ-NH1	7.17	123.88	120.30
54	BA	414	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	1802	A	N1-C6-N6	-7.17	114.30	118.60
55	BB	24	G	O4'-C1'-N9	7.17	113.93	108.20
21	AA	796	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	391	A	C5-C6-N1	7.16	121.28	117.70
54	BA	586	A	C5-C6-N1	7.16	121.28	117.70
11	AL	30	ARG	NE-CZ-NH2	-7.16	116.72	120.30
21	AA	129	A	C5-C6-N1	7.16	121.28	117.70
21	AA	919	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	1311	A	C5-C6-N1	7.16	121.28	117.70
51	B2	34	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	216	A	N1-C6-N6	-7.16	114.30	118.60
21	AA	498	A	C5-C6-N1	7.16	121.28	117.70
22	A1	66	A	C4-C5-C6	-7.16	113.42	117.00
54	BA	621	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2374	C	N3-C2-O2	-7.16	116.89	121.90
22	A1	76	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2082	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2823	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	227	A	O4'-C1'-N9	7.15	113.92	108.20
54	BA	2426	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1253	A	C5-C6-N1	7.15	121.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	205	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	849	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1029	A	C4-C5-C6	-7.15	113.42	117.00
22	A1	48	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	1414	C	N3-C2-O2	-7.15	116.89	121.90
54	BA	2020	A	C5-C6-N1	7.15	121.27	117.70
21	AA	195	A	C5-C6-N1	7.15	121.27	117.70
21	AA	356	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	309	A	C4-C5-C6	-7.15	113.43	117.00
21	AA	182	A	C5-C6-N1	7.14	121.27	117.70
21	AA	415	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1284	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	1780	A	O4'-C1'-N9	7.14	113.92	108.20
21	AA	559	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1112	C	N3-C2-O2	-7.14	116.90	121.90
24	A3	36	A	C5-C6-N1	7.14	121.27	117.70
54	BA	482	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1571	A	N1-C6-N6	-7.14	114.31	118.60
54	BA	1802	A	C5-C6-N1	7.14	121.27	117.70
21	AA	546	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1360	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	923	A	C5-C6-N1	7.14	121.27	117.70
54	BA	829	A	N1-C6-N6	-7.14	114.32	118.60
54	BA	1006	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1569	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	2468	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	872	A	N1-C6-N6	-7.14	114.32	118.60
21	AA	1319	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1000	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	893	C	N3-C2-O2	-7.14	116.91	121.90
2	AC	171	ARG	NE-CZ-NH2	7.13	123.87	120.30
54	BA	167	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	77	A	C4-C5-C6	-7.13	113.43	117.00
21	AA	1333	A	C4-C5-C6	-7.13	113.43	117.00
31	BI	133	ARG	NE-CZ-NH1	7.13	123.87	120.30
54	BA	845	A	C4-C5-C6	-7.13	113.43	117.00
21	AA	1350	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1551	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2248	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	936	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1085	A	C5-C6-N1	7.13	121.27	117.70
21	AA	564	C	N3-C2-O2	-7.13	116.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1275	A	N1-C6-N6	-7.13	114.32	118.60
21	AA	1467	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	404	A	C5-C6-N1	7.13	121.26	117.70
54	BA	2077	A	C5-C6-N1	7.13	121.26	117.70
21	AA	143	A	C5-C6-N1	7.12	121.26	117.70
21	AA	298	A	C5-C6-N1	7.12	121.26	117.70
21	AA	934	C	N3-C2-O2	-7.12	116.91	121.90
21	AA	1063	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	1090	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2840	C	N3-C2-O2	-7.12	116.91	121.90
54	BA	331	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	841	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	328	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	1252	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2657	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1031	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	22	C	N3-C2-O2	-7.12	116.92	121.90
54	BA	2572	A	C5-C6-N1	7.12	121.26	117.70
56	B5	9	ARG	NE-CZ-NH1	7.12	123.86	120.30
11	AL	98	ARG	NE-CZ-NH1	7.11	123.86	120.30
21	AA	1136	C	N3-C2-O2	-7.11	116.92	121.90
32	BJ	13	ARG	NE-CZ-NH1	7.11	123.86	120.30
21	AA	959	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2377	A	C4-C5-C6	-7.11	113.44	117.00
21	AA	139	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	609	A	C5-C6-N1	7.11	121.25	117.70
54	BA	173	A	C5-C6-N1	7.11	121.25	117.70
21	AA	549	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	994	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	2146	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	2358	A	C5-C6-N1	7.11	121.25	117.70
21	AA	98	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	1226	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2339	C	N3-C2-O2	-7.11	116.93	121.90
21	AA	1019	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1550	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	2145	C	N3-C2-O2	-7.10	116.93	121.90
21	AA	411	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	1549	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1449	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	844	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	1028	A	C5-C6-N1	7.10	121.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2872	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1493	A	C5-C6-N1	7.09	121.25	117.70
22	A1	58	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1327	A	N1-C6-N6	-7.09	114.34	118.60
54	BA	2170	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2883	A	C5-C6-N1	7.09	121.25	117.70
21	AA	478	A	N1-C6-N6	-7.09	114.34	118.60
54	BA	2726	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2823	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2850	A	C5-C6-N1	7.09	121.25	117.70
54	BA	878	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1454	C	O4'-C1'-N1	7.09	113.87	108.20
21	AA	1363	A	C5-C6-N1	7.09	121.24	117.70
21	AA	217	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	338	A	C5-C6-N1	7.09	121.24	117.70
54	BA	1359	A	C5-C6-N1	7.09	121.24	117.70
55	BB	109	A	C4-C5-C6	-7.09	113.46	117.00
21	AA	1176	A	C5-C6-N1	7.08	121.24	117.70
21	AA	1196	A	C5-C6-N1	7.08	121.24	117.70
54	BA	385	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	1020	A	C5-C6-N1	7.08	121.24	117.70
21	AA	984	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	1314	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	2211	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	1365	A	C5-C6-N1	7.08	121.24	117.70
54	BA	233	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1598	A	C5-C6-N1	7.08	121.24	117.70
22	A1	16	C	N3-C2-O2	-7.08	116.95	121.90
42	BT	3	ARG	NE-CZ-NH1	7.08	123.84	120.30
54	BA	222	A	C5-C6-N1	7.08	121.24	117.70
54	BA	670	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2212	A	C5-C6-N1	7.08	121.24	117.70
11	AL	8	ARG	NE-CZ-NH1	7.07	123.84	120.30
21	AA	1200	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	899	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	1901	A	C5-C6-N1	7.07	121.24	117.70
54	BA	2378	A	C4-C5-C6	-7.07	113.46	117.00
21	AA	63	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	192	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1532	A	C5-C6-N1	7.07	121.24	117.70
21	AA	1092	A	C5-C6-N1	7.07	121.23	117.70
54	BA	457	A	N1-C6-N6	-7.07	114.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	960	A	C5-C6-N1	7.07	121.23	117.70
21	AA	124	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1073	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2503	A	C5-C6-N1	7.07	121.23	117.70
1	AB	224	ARG	NE-CZ-NH1	7.07	123.83	120.30
21	AA	794	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	2829	A	C4-C5-C6	-7.07	113.47	117.00
21	AA	339	C	N3-C2-O2	-7.06	116.95	121.90
21	AA	520	A	C5-C6-N1	7.06	121.23	117.70
55	BB	35	C	N3-C2-O2	-7.06	116.95	121.90
21	AA	189	A	C5-C6-N1	7.06	121.23	117.70
21	AA	441	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	10	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	483	A	C5-C6-N1	7.06	121.23	117.70
54	BA	730	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2433	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2752	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	2058	A	C5-C6-N1	7.06	121.23	117.70
22	A1	6	A	C5-C6-N1	7.06	121.23	117.70
54	BA	503	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2850	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2336	A	N1-C6-N6	-7.06	114.37	118.60
6	AG	137	ARG	NE-CZ-NH1	7.05	123.83	120.30
54	BA	197	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1415	U	O4'-C1'-N1	7.05	113.84	108.20
54	BA	2009	A	C4-C5-C6	-7.05	113.47	117.00
8	AI	48	ARG	NE-CZ-NH1	7.05	123.83	120.30
29	BG	148	ARG	NE-CZ-NH1	7.05	123.83	120.30
54	BA	357	C	N3-C2-O2	-7.05	116.97	121.90
21	AA	74	A	C4-C5-C6	-7.05	113.48	117.00
21	AA	620	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	430	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	901	C	O4'-C1'-N1	7.05	113.84	108.20
54	BA	927	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1541	C	N3-C2-O2	-7.05	116.97	121.90
54	BA	1728	C	N3-C2-O2	-7.05	116.97	121.90
55	BB	101	A	N1-C6-N6	-7.04	114.37	118.60
21	AA	702	A	C5-C6-N1	7.04	121.22	117.70
54	BA	42	A	C5-C6-N1	7.04	121.22	117.70
54	BA	764	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1044	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	265	A	O4'-C1'-N9	7.04	113.83	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	515	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	685	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	2439	A	C5-C6-N1	7.04	121.22	117.70
21	AA	32	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	900	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1388	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	1161	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	2733	A	C5-C6-N1	7.04	121.22	117.70
21	AA	938	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1050	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	1089	A	C5-C6-N1	7.04	121.22	117.70
54	BA	182	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2518	A	C5-C6-N1	7.03	121.22	117.70
21	AA	262	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2682	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	147	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1010	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1167	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	2856	A	C5-C6-N1	7.03	121.22	117.70
48	BZ	10	ARG	NE-CZ-NH1	7.03	123.81	120.30
54	BA	1347	A	C5-C6-N1	7.03	121.21	117.70
55	BB	46	A	C5-C6-N1	7.03	121.22	117.70
21	AA	336	A	C5-C6-N1	7.03	121.21	117.70
21	AA	526	C	N3-C2-O2	-7.03	116.98	121.90
21	AA	704	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	428	A	C5-C6-N1	7.03	121.21	117.70
54	BA	2465	C	O4'-C1'-N1	7.03	113.82	108.20
21	AA	1434	A	C5-C6-N1	7.03	121.21	117.70
54	BA	668	A	C5-C6-N1	7.03	121.21	117.70
54	BA	1937	A	C4-C5-C6	-7.03	113.49	117.00
55	BB	99	A	O4'-C1'-N9	7.03	113.82	108.20
21	AA	303	A	C5-C6-N1	7.02	121.21	117.70
21	AA	937	A	C4-C5-C6	-7.02	113.49	117.00
48	BZ	29	ARG	NE-CZ-NH1	7.02	123.81	120.30
54	BA	1151	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1101	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1021	A	C5-C6-N1	7.02	121.21	117.70
54	BA	151	C	N3-C2-O2	-7.02	116.99	121.90
54	BA	1096	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	654	A	C5-C6-N1	7.02	121.21	117.70
54	BA	925	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1791	A	C5-C6-N1	7.02	121.21	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	45	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1571	A	C5-C6-N1	7.02	121.21	117.70
21	AA	595	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	1146	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	2738	A	C5-C6-N1	7.01	121.21	117.70
55	BB	115	A	C5-C6-N1	7.01	121.21	117.70
55	BB	39	A	C4-C5-C6	-7.01	113.50	117.00
21	AA	1468	A	C5-C6-N1	7.01	121.20	117.70
54	BA	91	A	C5-C6-N1	7.01	121.20	117.70
54	BA	609	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	641	U	O4'-C1'-N1	7.01	113.81	108.20
54	BA	1291	C	N3-C2-O2	-7.01	116.99	121.90
21	AA	647	C	N3-C2-O2	-7.01	117.00	121.90
21	AA	1278	G	N3-C2-N2	-7.01	115.00	119.90
21	AA	1469	C	N3-C2-O2	-7.01	117.00	121.90
54	BA	52	A	N1-C6-N6	-7.01	114.40	118.60
54	BA	1039	A	C5-C6-N1	7.01	121.20	117.70
21	AA	325	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	901	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1635	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1076	C	N1-C2-O2	7.00	123.10	118.90
54	BA	1504	A	C5-C6-N1	7.00	121.20	117.70
21	AA	496	A	N1-C6-N6	-7.00	114.40	118.60
21	AA	1441	A	N1-C6-N6	-7.00	114.40	118.60
55	BB	57	A	C5-C6-N1	7.00	121.20	117.70
21	AA	547	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	2507	C	N3-C2-O2	-7.00	117.00	121.90
21	AA	223	A	C5-C6-N1	7.00	121.20	117.70
24	A3	74	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2432	A	C5-C6-N1	7.00	121.20	117.70
21	AA	522	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	1066	U	O4'-C1'-N1	7.00	113.80	108.20
54	BA	1088	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	1495	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1688	U	O4'-C1'-N1	7.00	113.80	108.20
54	BA	1936	A	C4-C5-C6	-7.00	113.50	117.00
21	AA	1100	C	N1-C2-O2	6.99	123.10	118.90
35	BM	10	ARG	NE-CZ-NH1	6.99	123.80	120.30
54	BA	1434	A	O4'-C1'-N9	6.99	113.80	108.20
54	BA	221	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	1387	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	2358	A	N1-C6-N6	-6.99	114.41	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	448	A	C5-C6-N1	6.99	121.19	117.70
21	AA	695	A	C4-C5-C6	-6.99	113.50	117.00
21	AA	1055	A	C5-C6-N1	6.99	121.20	117.70
54	BA	213	A	C4-C5-C6	-6.99	113.50	117.00
21	AA	389	A	C4-C5-C6	-6.99	113.50	117.00
54	BA	1939	U	O4'-C1'-N1	6.99	113.79	108.20
54	BA	2270	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2298	A	C5-C6-N1	6.99	121.19	117.70
54	BA	384	A	C5-C6-N1	6.99	121.19	117.70
21	AA	19	A	C5-C6-N1	6.98	121.19	117.70
21	AA	207	C	N3-C2-O2	-6.98	117.01	121.90
22	A1	38	A	C5-C6-N1	6.98	121.19	117.70
54	BA	155	A	C5-C6-N1	6.98	121.19	117.70
54	BA	179	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	480	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	2378	A	C5-C6-N1	6.98	121.19	117.70
21	AA	696	A	C5-C6-N1	6.98	121.19	117.70
54	BA	204	A	C5-C6-N1	6.98	121.19	117.70
54	BA	249	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	1596	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2482	A	C5-C6-N1	6.98	121.19	117.70
44	BV	19	ARG	NE-CZ-NH1	6.98	123.79	120.30
54	BA	2814	A	C5-C6-N1	6.98	121.19	117.70
21	AA	501	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	216	A	C5-C6-N1	6.98	121.19	117.70
54	BA	279	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1086	A	O4'-C1'-N9	6.98	113.78	108.20
21	AA	546	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	1141	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	130	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1609	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	1827	U	O4'-C1'-N1	6.97	113.78	108.20
21	AA	1400	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2129	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2547	A	C4-C5-C6	-6.97	113.51	117.00
54	BA	2900	A	C5-C6-N1	6.97	121.19	117.70
21	AA	174	A	C5-C6-N1	6.97	121.18	117.70
21	AA	179	A	C4-C5-C6	-6.97	113.52	117.00
21	AA	1306	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	961	C	N1-C2-O2	6.97	123.08	118.90
54	BA	1117	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	1352	U	N3-C2-O2	-6.97	117.32	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1999	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2726	A	C5-C6-N1	6.97	121.18	117.70
24	A3	39	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	1027	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	1596	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	1705	A	C5-C6-N1	6.97	121.18	117.70
24	A3	42	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	426	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	2042	A	C5-C6-N1	6.96	121.18	117.70
24	A3	16	C	N1-C2-O2	6.96	123.08	118.90
54	BA	479	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1204	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1502	A	C5-C6-N1	6.96	121.18	117.70
28	BF	147	ARG	NE-CZ-NH1	6.96	123.78	120.30
21	AA	194	C	N3-C2-O2	-6.96	117.03	121.90
22	A1	26	A	C4-C5-C6	-6.96	113.52	117.00
24	A3	69	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	959	A	C5-C6-N1	6.96	121.18	117.70
54	BA	227	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1606	C	N1-C2-O2	6.96	123.07	118.90
54	BA	1815	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	2366	A	N1-C6-N6	-6.96	114.43	118.60
21	AA	1507	A	N1-C6-N6	-6.96	114.43	118.60
22	A1	71	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	627	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	643	A	C5-C6-N1	6.96	121.18	117.70
54	BA	756	A	C5-C6-N1	6.96	121.18	117.70
21	AA	865	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	1213	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	1247	A	C5-C6-N1	6.95	121.18	117.70
54	BA	2561	U	O4'-C1'-N1	6.95	113.76	108.20
55	BB	108	A	C4-C5-C6	-6.95	113.52	117.00
21	AA	161	A	C5-C6-N1	6.95	121.18	117.70
54	BA	635	C	N3-C2-O2	-6.95	117.03	121.90
21	AA	206	C	N3-C2-O2	-6.95	117.03	121.90
50	B1	27	ARG	NE-CZ-NH1	6.95	123.78	120.30
54	BA	119	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	348	A	C5-C6-N1	6.95	121.17	117.70
54	BA	529	A	C5-C6-N1	6.95	121.18	117.70
54	BA	743	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2352	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	825	A	C4-C5-C6	-6.95	113.53	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	992	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	1496	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	2030	A	C5-C6-N1	6.95	121.17	117.70
21	AA	155	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	286	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	1155	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	1544	A	C4-C5-C6	-6.95	113.53	117.00
54	BA	1739	A	C5-C6-N1	6.95	121.17	117.70
21	AA	431	A	C5-C6-N1	6.94	121.17	117.70
21	AA	478	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1801	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1957	C	O4'-C1'-N1	6.94	113.76	108.20
54	BA	2813	A	C5-C6-N1	6.94	121.17	117.70
21	AA	1130	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	550	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	1145	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	2600	A	C5-C6-N1	6.94	121.17	117.70
54	BA	143	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	1632	A	N1-C6-N6	-6.94	114.44	118.60
21	AA	695	A	C5-C6-N1	6.94	121.17	117.70
17	AR	60	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	2639	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	295	C	N3-C2-O2	-6.93	117.05	121.90
21	AA	658	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	984	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1847	A	C4-C5-C6	-6.93	113.53	117.00
55	BB	52	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	432	A	C5-C6-N1	6.93	121.17	117.70
54	BA	460	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	602	A	C5-C6-N1	6.93	121.16	117.70
21	AA	780	A	C4-C5-C6	-6.93	113.54	117.00
21	AA	937	A	C5-C6-N1	6.93	121.16	117.70
21	AA	1413	A	C5-C6-N1	6.93	121.16	117.70
54	BA	666	A	C5-C6-N1	6.93	121.16	117.70
21	AA	73	C	N1-C2-O2	6.92	123.05	118.90
21	AA	716	A	C5-C6-N1	6.92	121.16	117.70
21	AA	878	A	N1-C6-N6	-6.92	114.44	118.60
21	AA	1245	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	829	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1833	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	2902	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	1585	C	N3-C2-O2	-6.92	117.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	188	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	228	A	C5-C6-N1	6.92	121.16	117.70
21	AA	970	C	N3-C2-O2	-6.92	117.05	121.90
11	AL	55	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	422	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1275	A	C4-C5-C6	-6.92	113.54	117.00
19	AT	17	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	677	A	C5-C6-N1	6.92	121.16	117.70
54	BA	6	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	149	A	C5-C6-N1	6.92	121.16	117.70
54	BA	740	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	474	G	N3-C2-N2	-6.92	115.06	119.90
54	BA	346	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	233	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	675	A	C4-C5-C6	-6.91	113.54	117.00
54	BA	1354	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1507	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	1762	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1908	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	911	A	C5-C6-N1	6.91	121.16	117.70
54	BA	972	A	C5-C6-N1	6.91	121.16	117.70
21	AA	364	A	C5-C6-N1	6.91	121.16	117.70
21	AA	872	A	C5-C6-N1	6.91	121.16	117.70
54	BA	146	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1111	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	1205	A	N1-C6-N6	-6.91	114.45	118.60
21	AA	1203	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	1238	A	C5-C6-N1	6.91	121.15	117.70
54	BA	1919	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2706	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	2873	A	C5-C6-N1	6.91	121.15	117.70
21	AA	341	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	1150	A	C5-C6-N1	6.91	121.15	117.70
54	BA	332	A	O4'-C1'-N9	6.91	113.72	108.20
54	BA	492	A	C5-C6-N1	6.91	121.15	117.70
54	BA	2827	C	N3-C2-O2	-6.91	117.07	121.90
55	BB	34	A	C5-C6-N1	6.91	121.15	117.70
54	BA	2003	A	N1-C6-N6	-6.90	114.46	118.60
21	AA	794	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1500	A	N1-C6-N6	-6.90	114.46	118.60
35	BM	50	ARG	NE-CZ-NH1	6.90	123.75	120.30
21	AA	190	A	C5-C6-N1	6.90	121.15	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	734	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2463	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	414	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1502	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1143	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2734	A	C5-C6-N1	6.90	121.15	117.70
55	BB	53	A	C4-C5-C6	-6.90	113.55	117.00
12	AM	2	ARG	NE-CZ-NH2	6.90	123.75	120.30
21	AA	54	C	C1'-O4'-C4'	-6.90	104.38	109.90
21	AA	1329	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	1336	A	C5-C6-N1	6.90	121.15	117.70
55	BB	60	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	1205	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1796	U	O4'-C1'-N1	6.89	113.72	108.20
12	AM	92	ARG	NE-CZ-NH2	-6.89	116.85	120.30
21	AA	1483	A	C5-C6-N1	6.89	121.15	117.70
54	BA	354	A	N1-C6-N6	-6.89	114.47	118.60
54	BA	912	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	583	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	330	A	C4-C5-C6	-6.89	113.55	117.00
21	AA	1251	A	C5-C6-N1	6.89	121.14	117.70
54	BA	873	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	2261	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	1396	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	603	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	1104	C	N3-C2-O2	-6.89	117.08	121.90
56	B5	74	ARG	NE-CZ-NH1	6.89	123.74	120.30
21	AA	689	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	282	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	455	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	457	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2516	A	C5-C6-N1	6.88	121.14	117.70
54	BA	722	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	1597	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1746	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2411	A	C5-C6-N1	6.88	121.14	117.70
54	BA	183	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	228	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2381	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1055	A	C4-C5-C6	-6.88	113.56	117.00
26	BD	141	ARG	NE-CZ-NH2	6.88	123.74	120.30
54	BA	2268	A	C4-C5-C6	-6.88	113.56	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1321	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1615	C	O4'-C1'-N1	6.87	113.70	108.20
54	BA	2134	A	C5-C6-N1	6.87	121.14	117.70
21	AA	183	C	N1-C2-O2	6.87	123.02	118.90
21	AA	468	A	C5-C6-N1	6.87	121.14	117.70
21	AA	600	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	1332	G	O4'-C1'-N9	6.87	113.70	108.20
54	BA	2527	C	N3-C2-O2	-6.87	117.09	121.90
24	A3	14	A	N1-C6-N6	-6.87	114.48	118.60
21	AA	737	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	1230	C	N3-C2-O2	-6.87	117.09	121.90
24	A3	11	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	1129	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1722	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1735	A	C5-C6-N1	6.87	121.13	117.70
54	BA	2809	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1383	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	2705	A	C5-C6-N1	6.86	121.13	117.70
54	BA	330	A	C5-C6-N1	6.86	121.13	117.70
54	BA	803	U	O4'-C1'-N1	6.86	113.69	108.20
54	BA	2826	A	C5-C6-N1	6.86	121.13	117.70
54	BA	324	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	1504	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	443	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2014	A	N1-C6-N6	-6.86	114.49	118.60
54	BA	195	A	C5-C6-N1	6.86	121.13	117.70
34	BL	21	ARG	NE-CZ-NH1	6.85	123.73	120.30
54	BA	477	A	C5-C6-N1	6.85	121.13	117.70
54	BA	825	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	998	C	O4'-C1'-N1	6.85	113.68	108.20
54	BA	1978	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	2416	C	N3-C2-O2	-6.85	117.10	121.90
54	BA	177	G	O4'-C1'-N9	6.85	113.68	108.20
54	BA	2412	A	C5-C6-N1	6.85	121.12	117.70
54	BA	608	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	167	A	C5-C6-N1	6.85	121.12	117.70
54	BA	804	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1403	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1590	A	C5-C6-N1	6.84	121.12	117.70
54	BA	351	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	732	C	O4'-C1'-N1	6.84	113.67	108.20
38	BP	52	ARG	NE-CZ-NH1	6.84	123.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2335	A	C5-C6-N1	6.84	121.12	117.70
21	AA	16	A	C5-C6-N1	6.84	121.12	117.70
21	AA	290	C	N3-C2-O2	-6.84	117.11	121.90
34	BL	69	ARG	NE-CZ-NH1	6.84	123.72	120.30
54	BA	1638	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1789	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2566	A	N1-C6-N6	-6.84	114.50	118.60
55	BB	42	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	974	A	C4-C5-C6	-6.84	113.58	117.00
24	A3	60	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1675	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	576	C	N1-C2-O2	6.84	123.00	118.90
54	BA	316	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1866	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2013	A	C5-C6-N1	6.84	121.12	117.70
54	BA	892	A	C5-C6-N1	6.83	121.12	117.70
21	AA	470	C	N3-C2-O2	-6.83	117.12	121.90
22	A1	25	C	N3-C2-O2	-6.83	117.12	121.90
34	BL	41	ARG	NE-CZ-NH1	6.83	123.72	120.30
54	BA	164	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	1254	A	C5-C6-N1	6.83	121.12	117.70
54	BA	1366	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	1816	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	101	A	C5-C6-N1	6.83	121.12	117.70
54	BA	1966	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2015	A	C4-C5-C6	-6.83	113.58	117.00
21	AA	694	A	C5-C6-N1	6.83	121.11	117.70
21	AA	1059	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	1346	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	1342	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	2196	C	N3-C2-O2	-6.83	117.12	121.90
21	AA	119	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	715	A	C5-C6-N1	6.83	121.11	117.70
22	A1	26	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	1143	A	C4-C5-C6	-6.83	113.59	117.00
54	BA	1289	C	N3-C2-O2	-6.83	117.12	121.90
23	A2	91	A	C5-C6-N1	6.82	121.11	117.70
54	BA	125	A	O4'-C1'-N9	6.82	113.66	108.20
54	BA	1494	A	C5-C6-N1	6.82	121.11	117.70
21	AA	744	C	N3-C2-O2	-6.82	117.12	121.90
44	BV	93	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	1314	C	O4'-C1'-N1	6.82	113.66	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2418	A	C4-C5-C6	-6.82	113.59	117.00
36	BN	103	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	2748	A	C5-C6-N1	6.82	121.11	117.70
21	AA	338	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	2328	A	C4-C5-C6	-6.82	113.59	117.00
32	BJ	96	ARG	NE-CZ-NH1	6.82	123.71	120.30
35	BM	44	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	1204	A	O4'-C1'-N9	6.82	113.65	108.20
54	BA	1398	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	1969	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2154	A	C5-C6-N1	6.82	121.11	117.70
54	BA	165	A	N1-C6-N6	-6.81	114.51	118.60
54	BA	1592	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	243	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	294	A	C5-C6-N1	6.81	121.11	117.70
54	BA	347	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	2516	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	2612	C	N3-C2-O2	-6.81	117.13	121.90
54	BA	693	A	C5-C6-N1	6.81	121.11	117.70
54	BA	749	A	C5-C6-N1	6.81	121.11	117.70
54	BA	501	A	C5-C6-N1	6.81	121.11	117.70
54	BA	1269	A	N1-C6-N6	-6.81	114.52	118.60
21	AA	253	A	C4-C5-C6	-6.81	113.60	117.00
54	BA	1632	A	C5-C6-N1	6.81	121.10	117.70
21	AA	400	C	N3-C2-O2	-6.81	117.14	121.90
21	AA	452	A	O4'-C1'-N9	6.81	113.64	108.20
54	BA	2333	A	C5-C6-N1	6.81	121.10	117.70
55	BB	94	A	C4-C5-C6	-6.81	113.60	117.00
21	AA	528	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	1409	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	1207	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	1276	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	2681	C	N3-C2-O2	-6.80	117.14	121.90
55	BB	78	A	C5-C6-N1	6.80	121.10	117.70
22	A1	73	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1985	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	251	G	P-O3'-C3'	6.80	127.86	119.70
21	AA	1110	A	C5-C6-N1	6.80	121.10	117.70
54	BA	192	C	O4'-C1'-N1	6.80	113.64	108.20
54	BA	582	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	1616	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	1793	C	N3-C2-O2	-6.80	117.14	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1327	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	673	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1111	A	C4-C5-C6	-6.80	113.60	117.00
24	A3	73	A	C6-C5-N7	6.80	137.06	132.30
54	BA	412	A	C5-C6-N1	6.80	121.10	117.70
54	BA	453	A	C5-C6-N1	6.80	121.10	117.70
54	BA	170	U	O4'-C1'-N1	6.79	113.64	108.20
54	BA	920	A	C4-C5-C6	-6.79	113.60	117.00
21	AA	288	A	C5-C6-N1	6.79	121.10	117.70
21	AA	327	A	C5-C6-N1	6.79	121.10	117.70
21	AA	876	C	P-O3'-C3'	6.79	127.85	119.70
21	AA	1216	A	C5-C6-N1	6.79	121.10	117.70
54	BA	1574	C	N3-C2-O2	-6.79	117.14	121.90
21	AA	1216	A	C4-C5-C6	-6.79	113.61	117.00
24	A3	72	C	N3-C2-O2	-6.79	117.14	121.90
27	BE	40	ARG	NE-CZ-NH2	-6.79	116.90	120.30
54	BA	236	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	2158	A	N1-C6-N6	-6.79	114.53	118.60
21	AA	935	A	C5-C6-N1	6.79	121.09	117.70
21	AA	1281	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	1443	C	N3-C2-O2	-6.79	117.15	121.90
52	B3	41	ARG	NE-CZ-NH1	6.79	123.69	120.30
21	AA	1110	A	C4-C5-C6	-6.79	113.61	117.00
39	BQ	32	ARG	NE-CZ-NH1	6.79	123.69	120.30
54	BA	217	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	676	A	C5-C6-N1	6.79	121.09	117.70
55	BB	46	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	1380	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	569	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	748	G	C1'-O4'-C4'	-6.79	104.47	109.90
54	BA	1325	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	2352	A	C5-C6-N1	6.79	121.09	117.70
21	AA	172	A	C5-C6-N1	6.78	121.09	117.70
22	A1	21	A	C5-C6-N1	6.78	121.09	117.70
49	B0	51	ARG	NE-CZ-NH1	6.78	123.69	120.30
54	BA	522	A	C5-C6-N1	6.78	121.09	117.70
54	BA	968	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	739	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	1427	C	N3-C2-O2	-6.78	117.15	121.90
54	BA	1940	U	O4'-C1'-N1	6.78	113.62	108.20
21	AA	985	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	1456	A	C5-C6-N1	6.78	121.09	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	951	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	1237	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1272	A	C5-C6-N1	6.78	121.09	117.70
44	BV	21	ARG	NE-CZ-NH1	6.78	123.69	120.30
54	BA	2448	A	C4-C5-C6	-6.78	113.61	117.00
55	BB	68	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	795	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	505	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	1057	A	N1-C6-N6	-6.77	114.53	118.60
21	AA	120	A	N1-C6-N6	-6.77	114.54	118.60
21	AA	554	A	C4-C5-C6	-6.77	113.61	117.00
54	BA	239	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	1366	A	C5-C6-N1	6.77	121.09	117.70
54	BA	1916	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2369	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2670	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	162	A	C5-C6-N1	6.77	121.09	117.70
54	BA	2328	A	C5-C6-N1	6.77	121.08	117.70
55	BB	3	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	1431	A	C5-C6-N1	6.77	121.08	117.70
54	BA	812	C	O4'-C1'-N1	6.77	113.62	108.20
54	BA	861	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1100	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	1302	A	C5-C6-N1	6.77	121.08	117.70
21	AA	282	A	C4-C5-C6	-6.77	113.62	117.00
54	BA	1591	A	C4-C5-C6	-6.77	113.62	117.00
21	AA	414	A	C4-C5-C6	-6.76	113.62	117.00
53	B4	4	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	1656	C	N3-C2-O2	-6.76	117.16	121.90
54	BA	492	A	N1-C6-N6	-6.76	114.54	118.60
21	AA	430	A	C5-C6-N1	6.76	121.08	117.70
21	AA	924	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	575	A	N1-C6-N6	-6.76	114.54	118.60
54	BA	1480	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2129	C	O4'-C1'-N1	6.76	113.61	108.20
54	BA	2160	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2453	A	C5-C6-N1	6.76	121.08	117.70
54	BA	2675	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	66	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	729	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1045	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1152	C	N3-C2-O2	-6.76	117.17	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2590	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	142	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1230	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1275	A	C5-C6-N1	6.76	121.08	117.70
54	BA	1998	A	C5-C6-N1	6.76	121.08	117.70
21	AA	174	A	N1-C6-N6	-6.75	114.55	118.60
21	AA	451	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1328	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	321	U	O4'-C1'-N1	6.75	113.60	108.20
54	BA	2094	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	1428	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	1430	A	C5-C6-N1	6.75	121.08	117.70
22	A1	36	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	1858	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1213	A	C5-C6-N1	6.75	121.08	117.70
54	BA	861	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	1533	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	2386	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1077	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	1889	A	C5-C6-N1	6.75	121.08	117.70
54	BA	2366	A	C5-C6-N1	6.75	121.08	117.70
21	AA	1170	A	N1-C6-N6	-6.75	114.55	118.60
21	AA	1274	A	C4-C5-C6	-6.75	113.63	117.00
28	BF	177	ARG	NE-CZ-NH1	6.75	123.67	120.30
54	BA	207	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	654	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	672	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	2014	A	C5-C6-N1	6.75	121.07	117.70
54	BA	2442	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	1081	A	C5-C6-N1	6.74	121.07	117.70
38	BP	88	ARG	NE-CZ-NH1	6.74	123.67	120.30
51	B2	3	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	2829	A	N1-C6-N6	-6.74	114.55	118.60
21	AA	1534	A	N1-C6-N6	-6.74	114.56	118.60
39	BQ	49	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	1214	A	C5-C6-N1	6.74	121.07	117.70
54	BA	1287	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2198	A	N1-C6-N6	-6.74	114.56	118.60
21	AA	768	A	C4-C5-C6	-6.74	113.63	117.00
41	BS	92	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	909	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	965	C	N3-C2-O2	-6.74	117.18	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1049	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	272	A	C5-C6-N1	6.74	121.07	117.70
21	AA	1357	A	C5-C6-N1	6.74	121.07	117.70
54	BA	244	A	N1-C6-N6	-6.74	114.56	118.60
54	BA	311	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	854	C	N3-C2-O2	-6.74	117.19	121.90
54	BA	930	G	O4'-C1'-N9	6.74	113.59	108.20
21	AA	624	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2741	A	C5-C6-N1	6.73	121.07	117.70
21	AA	511	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	648	A	C4-C5-C6	-6.73	113.63	117.00
21	AA	978	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	1732	C	N3-C2-O2	-6.73	117.19	121.90
20	AU	16	ARG	NE-CZ-NH1	6.73	123.67	120.30
21	AA	345	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	857	G	N3-C2-N2	-6.73	115.19	119.90
54	BA	2434	A	C4-C5-C6	-6.73	113.64	117.00
21	AA	108	G	O4'-C1'-N9	6.73	113.58	108.20
21	AA	1056	U	O4'-C1'-N1	6.73	113.58	108.20
54	BA	611	C	N3-C2-O2	-6.73	117.19	121.90
1	AB	73	ARG	NE-CZ-NH1	6.73	123.66	120.30
54	BA	454	A	C5-C6-N1	6.73	121.06	117.70
54	BA	1039	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	1557	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1799	G	P-O3'-C3'	6.73	127.77	119.70
1	AB	112	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	274	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	2283	C	O4'-C1'-N1	6.72	113.58	108.20
51	B2	41	ARG	NE-CZ-NH2	6.72	123.66	120.30
54	BA	2054	A	C5-C6-N1	6.72	121.06	117.70
54	BA	2759	G	O4'-C1'-N9	6.72	113.58	108.20
21	AA	649	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	1451	U	P-O3'-C3'	6.72	127.77	119.70
54	BA	461	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	675	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	1535	A	C5-C6-N1	6.72	121.06	117.70
21	AA	1069	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	1699	G	O4'-C1'-N9	6.72	113.58	108.20
21	AA	143	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	1362	A	C5-C6-N1	6.72	121.06	117.70
21	AA	1492	A	C5-C6-N1	6.72	121.06	117.70
6	AG	101	ARG	NE-CZ-NH1	6.71	123.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	622	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	601	C	N3-C2-O2	-6.71	117.20	121.90
55	BB	104	A	C5-C6-N1	6.71	121.06	117.70
21	AA	487	A	C4-C5-C6	-6.71	113.64	117.00
43	BU	21	ARG	NE-CZ-NH1	6.71	123.66	120.30
54	BA	217	A	N1-C6-N6	-6.71	114.57	118.60
54	BA	1370	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	495	A	C5-C6-N1	6.71	121.06	117.70
21	AA	1501	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	106	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1515	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1170	C	O4'-C1'-N1	6.71	113.56	108.20
54	BA	2660	A	C5-C6-N1	6.71	121.05	117.70
55	BB	28	C	N3-C2-O2	-6.71	117.20	121.90
55	BB	59	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1769	U	O4'-C1'-N1	6.71	113.56	108.20
55	BB	88	C	N1-C2-O2	6.71	122.92	118.90
54	BA	31	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	599	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	717	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1165	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2407	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2462	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2634	A	C5-C6-N1	6.70	121.05	117.70
54	BA	173	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	199	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	501	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1127	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1689	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1970	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2117	A	O4'-C1'-N9	6.70	113.56	108.20
54	BA	2461	A	C5-C6-N1	6.70	121.05	117.70
24	A3	26	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	1298	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	546	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	958	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1669	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2175	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	452	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2861	U	O4'-C1'-N1	6.70	113.56	108.20
21	AA	452	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1565	C	O4'-C1'-N1	6.69	113.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1678	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	1363	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	1275	A	C5-C6-N1	6.69	121.05	117.70
54	BA	471	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1634	A	C5-C6-N1	6.69	121.05	117.70
54	BA	1952	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	2868	A	C4-C5-C6	-6.69	113.66	117.00
9	AJ	72	ARG	NE-CZ-NH1	6.69	123.64	120.30
21	AA	879	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	1145	A	C5-C6-N1	6.69	121.04	117.70
21	AA	1146	A	C5-C6-N1	6.69	121.04	117.70
54	BA	838	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	1496	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	119	A	C5-C6-N1	6.68	121.04	117.70
21	AA	663	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	794	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1176	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	14	A	C4-C5-C6	-6.68	113.66	117.00
55	BB	114	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	523	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	423	A	C5-C6-N1	6.68	121.04	117.70
54	BA	888	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1297	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1905	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	1524	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	990	C	N3-C2-O2	-6.68	117.23	121.90
54	BA	43	G	O4'-C1'-N9	6.68	113.54	108.20
54	BA	251	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1260	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2764	A	N1-C6-N6	-6.68	114.59	118.60
21	AA	1480	A	C5-C6-N1	6.67	121.04	117.70
42	BT	73	ARG	NE-CZ-NH1	6.67	123.64	120.30
54	BA	61	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1096	A	O4'-C1'-N9	6.67	113.54	108.20
54	BA	1285	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1735	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	2050	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2391	G	O4'-C1'-N9	6.67	113.54	108.20
54	BA	165	A	C5-C6-N1	6.67	121.04	117.70
21	AA	373	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1737	G	O4'-C1'-N9	6.67	113.54	108.20
54	BA	1760	C	N3-C2-O2	-6.67	117.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2059	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	1961	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2090	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2566	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2889	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	608	A	C4-C5-C6	-6.67	113.67	117.00
50	B1	5	ARG	NE-CZ-NH1	6.67	123.63	120.30
54	BA	63	A	C5-C6-N1	6.67	121.03	117.70
54	BA	2285	C	N3-C2-O2	-6.67	117.23	121.90
3	AD	2	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	1019	A	C4-C5-C6	-6.66	113.67	117.00
25	BC	270	ARG	NE-CZ-NH1	6.66	123.63	120.30
54	BA	231	A	C4-C5-C6	-6.66	113.67	117.00
13	AN	85	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	649	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1419	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1708	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	10	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	1168	U	O4'-C1'-N1	6.66	113.53	108.20
54	BA	294	A	N1-C6-N6	-6.66	114.60	118.60
21	AA	1389	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	385	C	O4'-C1'-N1	6.66	113.53	108.20
54	BA	590	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	590	A	C5-C6-N1	6.66	121.03	117.70
54	BA	602	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2727	A	C5-C6-N1	6.66	121.03	117.70
54	BA	309	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2635	A	C5-C6-N1	6.66	121.03	117.70
21	AA	436	C	O4'-C1'-N1	6.65	113.52	108.20
54	BA	863	A	C5-C6-N1	6.65	121.03	117.70
21	AA	16	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	663	A	C5-C6-N1	6.65	121.03	117.70
39	BQ	27	ARG	NE-CZ-NH1	6.65	123.63	120.30
54	BA	632	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	902	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	1262	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	629	A	N1-C6-N6	-6.65	114.61	118.60
54	BA	20	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1134	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	1502	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	563	A	N1-C6-N6	-6.65	114.61	118.60
21	AA	892	A	C5-C6-N1	6.64	121.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	975	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1686	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	816	A	C1'-O4'-C4'	-6.64	104.59	109.90
21	AA	1016	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2639	A	C5-C6-N1	6.64	121.02	117.70
38	BP	71	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	957	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1690	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1072	C	O4'-C1'-N1	6.64	113.51	108.20
54	BA	1155	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1717	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2019	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2088	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2336	A	O4'-C1'-N9	6.64	113.51	108.20
54	BA	5	A	C5-C6-N1	6.64	121.02	117.70
54	BA	820	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	909	A	C5-C6-N1	6.64	121.02	117.70
11	AL	120	ARG	NE-CZ-NH1	6.64	123.62	120.30
21	AA	936	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	482	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	975	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1315	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2214	C	N3-C2-O2	-6.64	117.25	121.90
55	BB	109	A	C5-C6-N1	6.64	121.02	117.70
21	AA	580	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	906	A	C4-C5-C6	-6.63	113.68	117.00
54	BA	231	A	C5-C6-N1	6.63	121.02	117.70
54	BA	393	C	O4'-C1'-N1	6.63	113.51	108.20
54	BA	1134	A	C5-C6-N1	6.63	121.02	117.70
25	BC	269	ARG	NE-CZ-NH1	6.63	123.62	120.30
54	BA	157	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	310	A	C5-C6-N1	6.63	121.02	117.70
21	AA	1381	U	C1'-O4'-C4'	-6.63	104.60	109.90
54	BA	510	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	739	A	C5-C6-N1	6.63	121.01	117.70
54	BA	1092	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1395	A	C1'-O4'-C4'	-6.63	104.60	109.90
54	BA	2632	A	C4-C5-C6	-6.63	113.69	117.00
21	AA	635	A	C5-C6-N1	6.63	121.01	117.70
21	AA	825	A	C5-C6-N1	6.63	121.01	117.70
22	A1	14	A	N1-C6-N6	-6.63	114.62	118.60
22	A1	21	A	C4-C5-C6	-6.63	113.69	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	16	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	502	A	C5-C6-N1	6.63	121.01	117.70
54	BA	1040	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	285	G	O4'-C1'-N9	6.62	113.50	108.20
54	BA	1477	A	N1-C6-N6	-6.62	114.62	118.60
54	BA	2538	C	N3-C2-O2	-6.62	117.26	121.90
10	AK	121	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	155	A	C5-C6-N1	6.62	121.01	117.70
21	AA	1155	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	172	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1630	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2720	U	O4'-C1'-N1	6.62	113.50	108.20
54	BA	2723	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	81	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	712	A	N1-C6-N6	-6.62	114.63	118.60
21	AA	797	C	N3-C2-O2	-6.62	117.27	121.90
32	BJ	27	ARG	NE-CZ-NH1	6.62	123.61	120.30
52	B3	12	ARG	NE-CZ-NH1	6.62	123.61	120.30
54	BA	1821	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	489	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	239	C	O4'-C1'-N1	6.62	113.49	108.20
54	BA	2715	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	99	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	1303	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1069	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1508	A	O4'-C1'-N9	6.62	113.49	108.20
21	AA	215	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	578	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	84	A	C5-C6-N1	6.61	121.01	117.70
54	BA	2284	A	C5-C6-N1	6.61	121.01	117.70
21	AA	1149	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	1280	A	C5-C6-N1	6.61	121.01	117.70
54	BA	1757	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	344	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	462	C	O4'-C1'-N1	6.61	113.49	108.20
21	AA	1230	C	N1-C2-O2	6.61	122.86	118.90
54	BA	281	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1413	A	N1-C6-N6	-6.61	114.64	118.60
55	BB	43	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	354	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1783	A	C4-C5-C6	-6.61	113.70	117.00
54	BA	1795	C	N3-C2-O2	-6.61	117.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1836	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	2761	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	1000	A	C5-C6-N1	6.61	121.00	117.70
54	BA	929	U	O4'-C1'-N1	6.61	113.48	108.20
54	BA	2781	A	C4-C5-C6	-6.60	113.70	117.00
4	AE	19	ARG	NE-CZ-NH1	6.60	123.60	120.30
21	AA	334	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	1096	C	N1-C2-O2	6.60	122.86	118.90
54	BA	181	A	C5-C6-N1	6.60	121.00	117.70
54	BA	572	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	1254	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	983	A	C5-C6-N1	6.60	121.00	117.70
21	AA	1520	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	865	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	932	U	N3-C2-O2	-6.60	117.58	122.20
54	BA	1872	A	C5-C6-N1	6.60	121.00	117.70
21	AA	914	A	C5-C6-N1	6.60	121.00	117.70
21	AA	1368	A	C5-C6-N1	6.60	121.00	117.70
22	A1	38	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	2342	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	815	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1803	A	C5-C6-N1	6.60	121.00	117.70
21	AA	1492	A	N1-C6-N6	-6.59	114.64	118.60
54	BA	1967	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	2135	A	C5-C6-N1	6.59	121.00	117.70
54	BA	2598	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1805	A	C5-C6-N1	6.59	121.00	117.70
54	BA	2158	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	120	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	574	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	919	A	C5-C6-N1	6.59	121.00	117.70
25	BC	62	ARG	NE-CZ-NH1	6.59	123.60	120.30
54	BA	1522	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1773	A	C5-C6-N1	6.59	121.00	117.70
54	BA	1912	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	2736	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	2809	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	979	C	N3-C2-O2	-6.59	117.29	121.90
21	AA	1404	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1221	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	2860	A	C5-C6-N1	6.59	120.99	117.70
12	AM	92	ARG	NE-CZ-NH1	6.59	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	AM	108	ARG	NE-CZ-NH1	6.59	123.59	120.30
21	AA	1394	A	C4-C5-C6	-6.59	113.71	117.00
21	AA	1226	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	680	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1608	A	C4-C5-C6	-6.59	113.71	117.00
54	BA	2469	A	C5-C6-N1	6.59	120.99	117.70
54	BA	2829	A	C5-C6-N1	6.59	120.99	117.70
9	AJ	89	ARG	NE-CZ-NH1	6.58	123.59	120.30
21	AA	749	A	C5-C6-N1	6.58	120.99	117.70
24	A3	57	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	1367	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2433	A	C5-C6-N1	6.58	120.99	117.70
54	BA	633	A	C5-C6-N1	6.58	120.99	117.70
54	BA	983	A	C4-C5-C6	-6.58	113.71	117.00
33	BK	49	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	2072	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	2691	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	623	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	415	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	13	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	56	A	C5-C6-N1	6.58	120.99	117.70
54	BA	532	A	O4'-C1'-N9	6.58	113.46	108.20
54	BA	802	A	C5-C6-N1	6.58	120.99	117.70
54	BA	972	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1004	U	O4'-C1'-N1	6.58	113.46	108.20
54	BA	1900	A	N1-C6-N6	-6.58	114.65	118.60
54	BA	2771	C	N3-C2-O2	-6.58	117.30	121.90
21	AA	269	C	N3-C2-O2	-6.58	117.30	121.90
41	BS	110	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	2420	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1340	U	N3-C2-O2	-6.57	117.60	122.20
21	AA	53	A	C5-C6-N1	6.57	120.98	117.70
21	AA	1480	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	69	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	71	A	N1-C6-N6	-6.57	114.66	118.60
54	BA	97	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1272	A	C4-C5-C6	-6.57	113.72	117.00
21	AA	279	A	C4-C5-C6	-6.57	113.72	117.00
21	AA	1103	C	N3-C2-O2	-6.57	117.30	121.90
34	BL	60	ARG	NE-CZ-NH1	6.57	123.58	120.30
54	BA	1105	U	O4'-C1'-N1	6.57	113.45	108.20
21	AA	681	A	C4-C5-C6	-6.57	113.72	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1810	A	C5-C6-N1	6.57	120.98	117.70
24	A3	36	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	368	A	C5-C6-N1	6.57	120.98	117.70
54	BA	422	A	C5-C6-N1	6.57	120.98	117.70
55	BB	57	A	N1-C6-N6	-6.57	114.66	118.60
21	AA	85	U	N3-C2-O2	-6.56	117.61	122.20
54	BA	821	A	N1-C6-N6	-6.56	114.66	118.60
54	BA	1874	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	355	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	366	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	25	U	O4'-C1'-N1	6.56	113.45	108.20
54	BA	257	C	O4'-C1'-N1	6.56	113.45	108.20
54	BA	423	A	N1-C6-N6	-6.56	114.66	118.60
20	AU	20	ARG	NE-CZ-NH1	6.56	123.58	120.30
21	AA	78	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	630	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2101	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2882	A	C5-C6-N1	6.56	120.98	117.70
55	BB	66	A	C5-C6-N1	6.56	120.98	117.70
8	AI	44	ARG	NE-CZ-NH1	6.56	123.58	120.30
21	AA	200	G	N1-C6-O6	-6.56	115.97	119.90
21	AA	679	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	1447	A	C5-C6-N1	6.56	120.98	117.70
22	A1	59	U	N3-C2-O2	-6.56	117.61	122.20
37	BO	7	ARG	NE-CZ-NH2	-6.56	117.02	120.30
54	BA	1118	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2602	A	C5-C6-N1	6.56	120.98	117.70
21	AA	1108	G	N1-C6-O6	-6.56	115.97	119.90
21	AA	1428	A	C5-C6-N1	6.56	120.98	117.70
54	BA	666	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	1114	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1531	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	2589	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	973	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	2776	A	C5-C6-N1	6.55	120.98	117.70
21	AA	171	A	C4-C5-C6	-6.55	113.72	117.00
24	A3	63	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	89	A	C5-C6-N1	6.55	120.98	117.70
54	BA	95	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1092	C	O4'-C1'-N1	6.55	113.44	108.20
54	BA	1373	A	N1-C6-N6	-6.55	114.67	118.60
21	AA	1319	A	C4-C5-C6	-6.55	113.73	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	971	G	N1-C6-O6	-6.55	115.97	119.90
21	AA	1375	A	C5-C6-N1	6.55	120.97	117.70
54	BA	2267	A	C5-C6-N1	6.55	120.97	117.70
21	AA	1204	A	C4-C5-C6	-6.55	113.73	117.00
22	A1	30	C	N3-C2-O2	-6.55	117.32	121.90
24	A3	74	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	454	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	943	A	C5-C6-N1	6.55	120.97	117.70
54	BA	2211	A	C4-C5-C6	-6.55	113.73	117.00
54	BA	2247	A	C5-C6-N1	6.55	120.97	117.70
54	BA	2851	A	C5-C6-N1	6.55	120.97	117.70
21	AA	1097	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	1120	C	N3-C2-O2	-6.54	117.32	121.90
24	A3	38	A	C5-C6-N1	6.54	120.97	117.70
24	A3	49	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	32	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	1169	A	C5-C6-N1	6.54	120.97	117.70
21	AA	1289	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	1476	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2008	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	2173	A	C5-C6-N1	6.54	120.97	117.70
54	BA	2003	A	C5-C6-N1	6.54	120.97	117.70
21	AA	1519	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	660	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	1990	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	2471	A	C4-C5-C6	-6.54	113.73	117.00
4	AE	53	ARG	NE-CZ-NH2	-6.53	117.03	120.30
21	AA	862	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1397	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	233	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	415	A	C5-C6-N1	6.53	120.97	117.70
54	BA	484	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	795	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	853	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	2368	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1128	G	O4'-C1'-N9	6.53	113.42	108.20
21	AA	618	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	1162	C	N3-C2-O2	-6.53	117.33	121.90
45	BW	19	ARG	NE-CZ-NH1	6.53	123.56	120.30
54	BA	2573	C	N3-C2-O2	-6.53	117.33	121.90
25	BC	269	ARG	NE-CZ-NH2	-6.53	117.04	120.30
21	AA	316	C	N3-C2-O2	-6.53	117.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1256	A	C5-C6-N1	6.53	120.96	117.70
54	BA	1135	C	N3-C4-C5	6.53	124.51	121.90
54	BA	1469	A	C4-C5-C6	-6.53	113.74	117.00
21	AA	756	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1509	A	C5-C6-N1	6.53	120.96	117.70
54	BA	2058	A	C4-C5-C6	-6.53	113.74	117.00
39	BQ	50	ARG	NE-CZ-NH1	6.52	123.56	120.30
21	AA	868	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	8	C	O4'-C1'-N1	6.52	113.42	108.20
54	BA	275	C	N1-C2-O2	6.52	122.81	118.90
54	BA	749	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2440	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	957	C	O4'-C1'-N1	6.52	113.42	108.20
2	AC	168	ARG	NE-CZ-NH1	6.52	123.56	120.30
21	AA	312	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	1022	A	C4-C5-C6	-6.52	113.74	117.00
28	BF	29	ARG	NE-CZ-NH1	6.52	123.56	120.30
54	BA	1593	A	C5-C6-N1	6.52	120.96	117.70
21	AA	181	A	C5-C6-N1	6.52	120.96	117.70
21	AA	507	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	720	C	N3-C2-O2	-6.52	117.34	121.90
22	A1	75	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	727	A	N1-C6-N6	-6.52	114.69	118.60
54	BA	2542	A	C4-C5-C6	-6.52	113.74	117.00
56	B5	60	ARG	NE-CZ-NH1	6.52	123.56	120.30
21	AA	735	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	1324	A	N1-C6-N6	-6.52	114.69	118.60
21	AA	374	A	C5-C6-N1	6.51	120.96	117.70
21	AA	1251	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	868	U	O4'-C1'-N1	6.51	113.41	108.20
54	BA	1005	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	1434	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	15	G	O4'-C1'-N9	6.51	113.41	108.20
54	BA	973	A	C5-C6-N1	6.51	120.96	117.70
30	BH	50	ARG	NE-CZ-NH1	6.51	123.56	120.30
21	AA	1066	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	7	A	C5-C6-N1	6.51	120.95	117.70
42	BT	6	ARG	NE-CZ-NH2	6.51	123.55	120.30
54	BA	792	A	C5-C6-N1	6.51	120.95	117.70
54	BA	987	C	N3-C2-O2	-6.51	117.35	121.90
54	BA	1809	A	O4'-C1'-N9	6.51	113.41	108.20
54	BA	2177	C	N3-C2-O2	-6.51	117.35	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	54	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	607	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	540	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	26	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	966	G	N3-C4-C5	-6.50	125.35	128.60
54	BA	155	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	2424	C	N3-C2-O2	-6.50	117.35	121.90
17	AR	47	ARG	NE-CZ-NH2	6.50	123.55	120.30
21	AA	156	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	308	C	N3-C2-O2	-6.50	117.35	121.90
22	A1	23	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1928	A	C5-C6-N1	6.50	120.95	117.70
21	AA	411	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	142	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1286	A	N1-C6-N6	-6.50	114.70	118.60
54	BA	1289	C	C3'-C2'-C1'	6.50	106.70	101.50
54	BA	2498	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	270	A	C5-C6-N1	6.50	120.95	117.70
54	BA	524	G	N1-C6-O6	-6.50	116.00	119.90
54	BA	833	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1809	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2153	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	460	A	N1-C6-N6	-6.49	114.70	118.60
54	BA	197	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1276	A	C5-C6-N1	6.49	120.95	117.70
21	AA	7	A	N1-C6-N6	-6.49	114.70	118.60
21	AA	441	A	C5-C6-N1	6.49	120.95	117.70
54	BA	439	A	C5-C6-N1	6.49	120.95	117.70
54	BA	2456	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	210	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	1344	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	146	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	1918	A	C4-C5-C6	-6.49	113.75	117.00
21	AA	530	G	N3-C4-C5	-6.49	125.36	128.60
21	AA	321	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	703	U	O4'-C1'-N1	6.49	113.39	108.20
21	AA	782	A	C5-C6-N1	6.49	120.94	117.70
54	BA	432	A	C5-C6-N1	6.49	120.94	117.70
54	BA	490	C	N1-C2-O2	6.48	122.79	118.90
54	BA	716	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1727	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	681	A	C5-C6-N1	6.48	120.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1916	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	583	A	N1-C6-N6	-6.48	114.71	118.60
54	BA	2095	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2657	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2712	C	N1-C2-O2	6.48	122.79	118.90
21	AA	1236	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	569	U	C1'-O4'-C4'	-6.48	104.72	109.90
54	BA	2614	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	139	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1037	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	1201	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1225	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1505	A	C5-C6-N1	6.48	120.94	117.70
24	A3	68	C	N3-C2-O2	-6.48	117.37	121.90
54	BA	2108	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1054	A	C5-C6-N1	6.47	120.94	117.70
21	AA	32	A	C5-C6-N1	6.47	120.94	117.70
54	BA	392	U	O4'-C1'-N1	6.47	113.38	108.20
54	BA	927	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1165	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	1335	C	O4'-C1'-N1	6.47	113.38	108.20
21	AA	634	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	708	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	1234	C	N3-C2-O2	-6.47	117.37	121.90
22	A1	58	A	N1-C6-N6	-6.47	114.72	118.60
54	BA	210	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	485	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1175	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1362	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2163	A	C4-C5-C6	-6.47	113.77	117.00
55	BB	8	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	436	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	721	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1610	A	C1'-O4'-C4'	-6.46	104.73	109.90
21	AA	510	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	517	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1246	A	C5-C6-N1	6.46	120.93	117.70
54	BA	1639	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2132	U	O4'-C1'-N1	6.46	113.37	108.20
8	AI	32	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	382	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1296	C	N3-C2-O2	-6.46	117.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	BT	76	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	184	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2590	A	C5-C6-N1	6.46	120.93	117.70
54	BA	789	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1600	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1612	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2654	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2765	A	O4'-C1'-N9	6.46	113.37	108.20
16	AQ	10	ARG	NE-CZ-NH1	6.46	123.53	120.30
21	AA	977	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1014	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1437	A	N1-C6-N6	-6.46	114.73	118.60
54	BA	624	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2254	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	2317	A	C5-C6-N1	6.46	120.93	117.70
21	AA	579	A	C5-C6-N1	6.46	120.93	117.70
54	BA	2738	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	190	A	C5-C6-N1	6.45	120.93	117.70
54	BA	772	C	N3-C2-O2	-6.45	117.38	121.90
54	BA	2513	A	C5-C6-N1	6.45	120.93	117.70
21	AA	1132	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	764	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	1101	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	1287	A	C4-C5-C6	-6.45	113.78	117.00
23	A2	90	U	O4'-C1'-N1	6.45	113.36	108.20
54	BA	917	A	C5-C6-N1	6.45	120.93	117.70
54	BA	997	G	N3-C2-N2	-6.45	115.39	119.90
54	BA	2150	C	N3-C2-O2	-6.45	117.39	121.90
8	AI	11	ARG	NE-CZ-NH1	6.45	123.52	120.30
21	AA	816	A	C5-C6-N1	6.45	120.92	117.70
21	AA	900	A	C4-C5-C6	-6.45	113.78	117.00
23	A2	83	U	N3-C2-O2	-6.45	117.69	122.20
35	BM	16	ARG	NE-CZ-NH1	6.45	123.52	120.30
54	BA	2700	A	C5-C6-N1	6.45	120.92	117.70
54	BA	565	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1962	C	N1-C2-O2	6.45	122.77	118.90
21	AA	816	A	N1-C6-N6	-6.45	114.73	118.60
43	BU	21	ARG	NE-CZ-NH2	-6.45	117.08	120.30
54	BA	446	G	O4'-C1'-N9	6.45	113.36	108.20
54	BA	563	A	C5-C6-N1	6.45	120.92	117.70
54	BA	1127	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1853	A	C5-C6-N1	6.44	120.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2313	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2467	C	N3-C2-O2	-6.44	117.39	121.90
3	AD	43	ARG	NE-CZ-NH1	6.44	123.52	120.30
21	AA	235	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	1324	A	C5-C6-N1	6.44	120.92	117.70
54	BA	825	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1503	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	1081	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2340	A	C4-C5-C6	-6.44	113.78	117.00
22	A1	62	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	160	A	N1-C6-N6	-6.44	114.74	118.60
26	BD	33	ARG	NE-CZ-NH1	6.44	123.52	120.30
54	BA	126	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1679	A	C5-C6-N1	6.44	120.92	117.70
21	AA	790	A	N1-C6-N6	-6.44	114.74	118.60
21	AA	1430	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1144	A	C5-C6-N1	6.44	120.92	117.70
54	BA	2407	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	177	G	N3-C4-C5	-6.43	125.38	128.60
21	AA	267	C	N3-C2-O2	-6.43	117.39	121.90
21	AA	621	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	784	A	C5-C6-N1	6.43	120.92	117.70
21	AA	1082	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1030	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1749	A	C5-C6-N1	6.43	120.92	117.70
21	AA	872	A	O4'-C1'-N9	6.43	113.34	108.20
21	AA	1129	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	1163	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1742	U	O4'-C1'-N1	6.43	113.35	108.20
54	BA	1854	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	831	A	C4-C5-C6	-6.43	113.78	117.00
21	AA	28	A	C5-C6-N1	6.43	120.92	117.70
21	AA	860	A	C5-C6-N1	6.43	120.91	117.70
54	BA	866	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	2183	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	1614	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	1819	A	C5-C6-N1	6.43	120.91	117.70
54	BA	616	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	742	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1103	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1402	U	O4'-C1'-N1	6.42	113.34	108.20
54	BA	1508	A	C4-C5-C6	-6.42	113.79	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	845	A	C1'-O4'-C4'	-6.42	104.76	109.90
21	AA	83	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	325	A	C4-C5-C6	-6.42	113.79	117.00
26	BD	124	ARG	NE-CZ-NH2	-6.42	117.09	120.30
54	BA	676	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2721	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	236	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1339	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	368	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	941	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1009	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1774	C	N1-C2-O2	6.42	122.75	118.90
21	AA	754	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	910	C	N3-C2-O2	-6.42	117.41	121.90
29	BG	34	ARG	NE-CZ-NH1	6.42	123.51	120.30
54	BA	739	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	815	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1274	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2805	C	N3-C2-O2	-6.42	117.41	121.90
21	AA	1238	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1170	A	C4-C5-C6	-6.41	113.79	117.00
21	AA	1350	A	C4-C5-C6	-6.41	113.79	117.00
36	BN	2	ARG	NE-CZ-NH1	6.41	123.51	120.30
41	BS	99	ARG	NE-CZ-NH1	6.41	123.51	120.30
54	BA	394	C	O4'-C1'-N1	6.41	113.33	108.20
54	BA	2398	U	O4'-C1'-N1	6.41	113.33	108.20
55	BB	62	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	451	A	P-O3'-C3'	6.41	127.39	119.70
54	BA	447	A	N1-C6-N6	-6.41	114.75	118.60
54	BA	1319	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1525	A	C5-C6-N1	6.41	120.91	117.70
21	AA	47	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	364	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	897	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1909	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	2088	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2142	A	C5-C6-N1	6.41	120.91	117.70
15	AP	31	ARG	NE-CZ-NH1	6.41	123.50	120.30
54	BA	1237	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	510	A	C5-C6-N1	6.41	120.90	117.70
21	AA	1219	A	C5-C6-N1	6.41	120.90	117.70
54	BA	49	A	C5-C6-N1	6.41	120.90	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1075	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	1114	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	1288	G	N1-C6-O6	-6.41	116.06	119.90
54	BA	1399	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	1941	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	2019	A	C5-C6-N1	6.41	120.90	117.70
54	BA	2900	A	C4-C5-C6	-6.41	113.80	117.00
55	BB	31	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	607	U	O4'-C1'-N1	6.40	113.32	108.20
9	AJ	62	ARG	NE-CZ-NH1	6.40	123.50	120.30
21	AA	1035	A	C5-C6-N1	6.40	120.90	117.70
23	A2	80	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	11	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	95	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2564	A	C4-C5-C6	-6.40	113.80	117.00
55	BB	50	A	C5-C6-N1	6.40	120.90	117.70
10	AK	105	ARG	NE-CZ-NH1	6.40	123.50	120.30
21	AA	886	G	N1-C6-O6	-6.40	116.06	119.90
54	BA	2232	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2403	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1345	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1490	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	19	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	1210	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	1250	A	C5-C6-N1	6.39	120.90	117.70
54	BA	900	A	C5-C6-N1	6.39	120.90	117.70
54	BA	1694	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	2813	A	C4-C5-C6	-6.39	113.80	117.00
11	AL	35	ARG	NE-CZ-NH1	6.39	123.50	120.30
54	BA	626	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	782	A	C5-C6-N1	6.39	120.90	117.70
54	BA	979	A	C5-C6-N1	6.39	120.90	117.70
21	AA	859	G	N3-C2-N2	-6.39	115.43	119.90
25	BC	213	ARG	NE-CZ-NH1	6.39	123.50	120.30
54	BA	408	G	N1-C6-O6	-6.39	116.07	119.90
54	BA	421	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	945	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1230	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1414	C	O4'-C1'-N1	6.39	113.31	108.20
54	BA	1677	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	2497	A	C5-C6-N1	6.39	120.89	117.70
15	AP	56	ARG	NE-CZ-NH1	6.39	123.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1392	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1859	U	O4'-C1'-N1	6.39	113.31	108.20
54	BA	2332	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	66	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	952	G	N1-C6-O6	-6.39	116.07	119.90
54	BA	1373	A	C5-C6-N1	6.39	120.89	117.70
54	BA	2025	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2899	A	C4-C5-C6	-6.39	113.81	117.00
21	AA	397	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1938	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	1364	U	N3-C2-O2	-6.38	117.73	122.20
54	BA	788	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1726	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	1441	A	C5-C6-N1	6.38	120.89	117.70
54	BA	1111	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2222	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2314	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2452	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2521	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	791	C	N3-C4-N4	-6.38	113.53	118.00
54	BA	1979	U	O4'-C1'-N1	6.38	113.30	108.20
54	BA	2753	A	C5-C6-N1	6.38	120.89	117.70
54	BA	645	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	2837	A	N1-C6-N6	-6.38	114.77	118.60
3	AD	164	ARG	NE-CZ-NH1	6.38	123.49	120.30
21	AA	32	A	C4-C5-C6	-6.38	113.81	117.00
24	A3	45	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1088	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2241	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2753	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2813	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	1353	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2260	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	918	A	C5-C6-N1	6.37	120.89	117.70
54	BA	2054	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2324	U	O4'-C1'-N1	6.37	113.30	108.20
54	BA	1977	A	C5-C6-N1	6.37	120.89	117.70
54	BA	2064	C	N1-C2-O2	6.37	122.72	118.90
15	AP	8	ARG	NE-CZ-NH1	6.37	123.48	120.30
54	BA	1307	A	C5-C6-N1	6.37	120.88	117.70
54	BA	1387	A	C5-C6-N1	6.37	120.89	117.70
54	BA	1637	A	C4-C5-C6	-6.37	113.82	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2764	A	C5-C6-N1	6.37	120.88	117.70
54	BA	430	A	C5-C6-N1	6.37	120.88	117.70
21	AA	221	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	365	U	O4'-C1'-N1	6.37	113.29	108.20
33	BK	31	ARG	NE-CZ-NH1	6.37	123.48	120.30
54	BA	885	C	O4'-C1'-N1	6.37	113.29	108.20
54	BA	2707	U	O4'-C1'-N1	6.37	113.29	108.20
2	AC	106	ARG	NE-CZ-NH1	6.36	123.48	120.30
11	AL	53	ARG	NE-CZ-NH1	6.36	123.48	120.30
13	AN	65	ARG	NE-CZ-NH1	6.36	123.48	120.30
21	AA	1318	A	C5-C6-N1	6.36	120.88	117.70
22	A1	76	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1262	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1614	A	C4-C5-C6	-6.36	113.82	117.00
55	BB	104	A	N1-C6-N6	-6.36	114.78	118.60
22	A1	9	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1233	C	O4'-C1'-N1	6.36	113.29	108.20
54	BA	302	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	2037	A	C5-C6-N1	6.36	120.88	117.70
21	AA	680	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	1396	A	C5-C6-N1	6.36	120.88	117.70
54	BA	57	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	298	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	794	A	N1-C6-N6	-6.36	114.78	118.60
54	BA	1268	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1567	G	O4'-C1'-N9	6.36	113.29	108.20
21	AA	1239	A	C4-C5-C6	-6.36	113.82	117.00
55	BB	45	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1564	C	N3-C2-O2	-6.35	117.45	121.90
2	AC	155	ARG	NE-CZ-NH1	6.35	123.48	120.30
21	AA	802	A	C4-C5-C6	-6.35	113.82	117.00
22	A1	56	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	497	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	1993	U	O4'-C1'-N1	6.35	113.28	108.20
54	BA	2206	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	2870	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	59	A	C5-C6-N1	6.35	120.88	117.70
21	AA	563	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	1045	C	N1-C2-O2	6.35	122.71	118.90
21	AA	436	C	N1-C2-O2	6.35	122.71	118.90
54	BA	1032	A	C5-C6-N1	6.35	120.88	117.70
54	BA	1287	A	C4-C5-C6	-6.35	113.83	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2651	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	2766	A	C5-C6-N1	6.35	120.88	117.70
21	AA	401	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	393	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	420	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	966	G	N1-C6-O6	-6.35	116.09	119.90
54	BA	1494	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	2225	A	C5-C6-N1	6.35	120.87	117.70
54	BA	2326	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	2451	A	C4-C5-C6	-6.35	113.83	117.00
21	AA	1507	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	1699	G	O4'-C1'-C2'	-6.35	99.45	105.80
21	AA	55	A	C5-C6-N1	6.34	120.87	117.70
21	AA	72	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	167	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	544	C	N1-C2-O2	6.34	122.71	118.90
54	BA	1084	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	1151	A	C5-C6-N1	6.34	120.87	117.70
54	BA	2362	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	167	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1528	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1934	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	368	U	C1'-O4'-C4'	-6.34	104.83	109.90
21	AA	179	A	C5-C6-N1	6.34	120.87	117.70
21	AA	826	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	1563	U	O4'-C1'-N1	6.34	113.27	108.20
21	AA	443	C	N3-C2-O2	-6.33	117.47	121.90
25	BC	176	ARG	NE-CZ-NH1	6.33	123.47	120.30
26	BD	13	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	238	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	362	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	2392	A	C5-C6-N1	6.33	120.87	117.70
21	AA	408	A	C4-C5-C6	-6.33	113.83	117.00
21	AA	807	A	C4-C5-C6	-6.33	113.83	117.00
34	BL	78	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	271	G	O4'-C1'-N9	6.33	113.27	108.20
54	BA	673	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1477	A	C5-C6-N1	6.33	120.87	117.70
54	BA	2531	A	C5-C6-N1	6.33	120.87	117.70
54	BA	2745	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	753	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	23	C	N3-C2-O2	-6.33	117.47	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1172	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1282	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1079	C	N1-C2-O2	6.33	122.70	118.90
21	AA	815	A	C5-C6-N1	6.33	120.86	117.70
54	BA	183	C	O4'-C1'-N1	6.33	113.26	108.20
54	BA	885	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1738	G	N3-C4-C5	-6.33	125.44	128.60
54	BA	2889	C	O4'-C1'-N1	6.33	113.26	108.20
21	AA	643	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1679	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	1706	C	N1-C2-O2	6.33	122.69	118.90
54	BA	1768	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	564	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	1222	U	O4'-C1'-N1	6.32	113.26	108.20
54	BA	2164	C	N1-C2-O2	6.32	122.69	118.90
54	BA	2658	C	N3-C2-O2	-6.32	117.47	121.90
21	AA	276	G	N3-C2-N2	-6.32	115.47	119.90
54	BA	1890	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	1491	G	N1-C6-O6	-6.32	116.11	119.90
54	BA	20	C	O4'-C1'-N1	6.32	113.25	108.20
54	BA	2589	A	C5-C6-N1	6.32	120.86	117.70
21	AA	488	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	609	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1088	A	O4'-C1'-N9	6.32	113.25	108.20
54	BA	1570	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1597	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	2875	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	1219	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	814	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2778	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2887	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	299	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	981	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	2146	C	N1-C2-O2	6.31	122.69	118.90
21	AA	431	A	C4-C5-C6	-6.31	113.84	117.00
38	BP	87	ARG	NE-CZ-NH1	6.31	123.45	120.30
54	BA	299	A	C5-C6-N1	6.31	120.86	117.70
54	BA	1665	A	C5-C6-N1	6.31	120.86	117.70
55	BB	4	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	466	A	C4-C5-C6	-6.31	113.85	117.00
24	A3	66	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	750	C	N3-C2-O2	-6.31	117.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	581	C	N3-C2-O2	-6.31	117.49	121.90
54	BA	1794	A	C4-C5-C6	-6.31	113.85	117.00
21	AA	25	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	81	A	C5-C6-N1	6.30	120.85	117.70
21	AA	483	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1997	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2699	C	N3-C2-O2	-6.30	117.49	121.90
55	BB	111	U	O4'-C1'-N1	6.30	113.24	108.20
21	AA	1117	A	C5-C6-N1	6.30	120.85	117.70
21	AA	1263	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1347	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2887	A	C5-C6-N1	6.30	120.85	117.70
21	AA	946	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	1105	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	750	A	C5-C6-N1	6.30	120.85	117.70
54	BA	2021	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	311	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1279	G	O4'-C1'-N9	6.30	113.24	108.20
54	BA	203	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1553	A	N1-C6-N6	-6.30	114.82	118.60
54	BA	2679	A	C5-C6-N1	6.30	120.85	117.70
55	BB	38	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	346	A	O4'-C1'-N9	6.29	113.24	108.20
21	AA	482	A	C4-C5-C6	-6.29	113.85	117.00
8	AI	48	ARG	NE-CZ-NH2	-6.29	117.15	120.30
21	AA	71	A	C5-C6-N1	6.29	120.85	117.70
21	AA	236	A	C5-C6-N1	6.29	120.85	117.70
21	AA	1012	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	379	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	256	A	C5-C6-N1	6.29	120.84	117.70
54	BA	1121	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1431	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1773	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	596	A	C5-C6-N1	6.29	120.84	117.70
21	AA	1005	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	893	C	N3-C2-O2	-6.29	117.50	121.90
3	AD	3	TYR	CB-CG-CD2	-6.28	117.23	121.00
5	AF	91	ARG	NE-CZ-NH1	6.28	123.44	120.30
21	AA	18	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	200	G	O4'-C1'-N9	6.28	113.23	108.20
54	BA	264	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2750	A	C4-C5-C6	-6.28	113.86	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	132	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	631	C	C1'-O4'-C4'	-6.28	104.87	109.90
21	AA	1446	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1879	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2284	A	C4-C5-C6	-6.28	113.86	117.00
18	AS	77	ARG	NE-CZ-NH2	6.28	123.44	120.30
54	BA	479	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	762	U	P-O3'-C3'	6.28	127.23	119.70
54	BA	1809	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	33	A	C5-C6-N1	6.28	120.84	117.70
21	AA	1092	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	538	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1413	A	C5-C6-N1	6.28	120.84	117.70
14	AO	53	ARG	NE-CZ-NH2	-6.28	117.16	120.30
54	BA	650	C	N1-C2-O2	6.28	122.67	118.90
54	BA	1393	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1764	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	2022	U	O4'-C1'-N1	6.28	113.22	108.20
21	AA	48	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1408	A	C5-C6-N1	6.27	120.84	117.70
54	BA	693	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	865	A	C5-C6-N1	6.27	120.84	117.70
21	AA	1000	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	1196	A	O4'-C1'-N9	6.27	113.22	108.20
21	AA	1340	A	C5-C6-N1	6.27	120.84	117.70
6	AG	78	ARG	NE-CZ-NH1	6.27	123.44	120.30
54	BA	1126	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	1876	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	1004	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	10	A	C5-C6-N1	6.27	120.83	117.70
54	BA	234	U	O4'-C1'-N1	6.27	113.22	108.20
54	BA	1685	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1715	G	O4'-C1'-N9	6.27	113.22	108.20
54	BA	1754	A	C5-C6-N1	6.27	120.83	117.70
54	BA	1960	A	C5-C6-N1	6.27	120.83	117.70
21	AA	1465	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	2858	C	N1-C2-O2	6.27	122.66	118.90
54	BA	332	A	C5-C6-N1	6.27	120.83	117.70
54	BA	796	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2347	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	329	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	978	A	C5-C6-N1	6.26	120.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	BK	78	ARG	NE-CZ-NH1	6.26	123.43	120.30
38	BP	20	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	196	A	O4'-C1'-N9	6.26	113.21	108.20
54	BA	1974	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2710	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	507	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	823	C	O4'-C1'-N1	6.26	113.21	108.20
21	AA	1374	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2281	A	C5-C6-N1	6.26	120.83	117.70
54	BA	900	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2703	C	N1-C2-O2	6.26	122.66	118.90
8	AI	121	ARG	NE-CZ-NH1	6.26	123.43	120.30
21	AA	1201	A	P-O3'-C3'	6.26	127.21	119.70
37	BO	81	ARG	NE-CZ-NH1	6.26	123.43	120.30
54	BA	2047	C	O4'-C1'-N1	6.26	113.21	108.20
54	BA	26	G	O4'-C1'-N9	6.25	113.20	108.20
54	BA	497	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	1556	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	2287	A	C5-C6-N1	6.25	120.83	117.70
54	BA	130	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	560	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	1901	A	C4-C5-C6	-6.25	113.87	117.00
22	A1	68	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	2196	C	O4'-C1'-N1	6.25	113.20	108.20
21	AA	323	U	O4'-C1'-N1	6.25	113.20	108.20
21	AA	1180	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	19	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	160	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	840	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1327	A	C5-C6-N1	6.25	120.82	117.70
54	BA	2060	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2886	A	O4'-C1'-N9	6.25	113.20	108.20
54	BA	1987	A	C5-C6-N1	6.25	120.82	117.70
54	BA	2369	A	C4-C5-C6	-6.25	113.88	117.00
2	AC	125	ARG	NE-CZ-NH1	6.24	123.42	120.30
54	BA	817	C	N1-C2-O2	6.24	122.65	118.90
54	BA	1089	A	C4-C5-C6	-6.24	113.88	117.00
22	A1	38	A	N1-C6-N6	-6.24	114.86	118.60
54	BA	127	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	865	C	O4'-C1'-N1	6.24	113.19	108.20
54	BA	2364	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	676	A	C4-C5-C6	-6.24	113.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	60	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	111	A	C5-C6-N1	6.24	120.82	117.70
54	BA	698	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1583	A	C4-C5-C6	-6.24	113.88	117.00
24	A3	58	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	823	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1433	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	2451	A	C5-C6-N1	6.24	120.82	117.70
21	AA	1250	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1513	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1465	G	N1-C6-O6	-6.24	116.16	119.90
54	BA	2073	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2736	A	C5-C6-N1	6.24	120.82	117.70
21	AA	238	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1402	C	N3-C2-O2	-6.24	117.53	121.90
22	A1	73	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	44	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	758	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2166	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	2600	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	1418	A	N1-C6-N6	-6.23	114.86	118.60
54	BA	1064	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1745	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2810	A	C5-C6-N1	6.23	120.82	117.70
21	AA	611	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1320	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	1513	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	332	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	1772	A	C5-C6-N1	6.23	120.82	117.70
54	BA	2020	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	2785	C	N3-C2-O2	-6.23	117.54	121.90
15	AP	51	ARG	NE-CZ-NH1	6.23	123.42	120.30
21	AA	612	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	369	U	O4'-C1'-N1	6.23	113.18	108.20
54	BA	2385	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	392	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1582	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2821	A	C5-C6-N1	6.23	120.81	117.70
54	BA	2457	U	O4'-C1'-N1	6.23	113.18	108.20
54	BA	440	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	775	G	O4'-C1'-N9	6.23	113.18	108.20
54	BA	2568	U	O4'-C1'-N1	6.23	113.18	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2760	C	O4'-C1'-N1	6.23	113.18	108.20
21	AA	87	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	517	C	O4'-C1'-N1	6.22	113.18	108.20
54	BA	2411	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	532	A	C5-C6-N1	6.22	120.81	117.70
21	AA	873	A	C5-C6-N1	6.22	120.81	117.70
21	AA	883	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	249	C	N1-C2-O2	6.22	122.63	118.90
54	BA	1166	G	N1-C6-O6	-6.22	116.17	119.90
54	BA	2577	A	C5-C6-N1	6.22	120.81	117.70
54	BA	910	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	2451	A	N1-C6-N6	-6.22	114.87	118.60
21	AA	178	C	N3-C2-O2	-6.22	117.55	121.90
55	BB	118	C	N1-C2-O2	6.22	122.63	118.90
21	AA	901	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	756	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	781	A	C4-C5-C6	-6.22	113.89	117.00
25	BC	155	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	1229	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	2690	U	O4'-C1'-N1	6.22	113.17	108.20
54	BA	2826	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	33	A	C4-C5-C6	-6.21	113.89	117.00
53	B4	24	ARG	NE-CZ-NH2	-6.21	117.19	120.30
21	AA	753	A	C5-C6-N1	6.21	120.81	117.70
21	AA	827	U	O4'-C1'-N1	6.21	113.17	108.20
54	BA	756	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	828	U	N3-C2-O2	-6.21	117.85	122.20
54	BA	1730	C	N1-C2-O2	6.21	122.63	118.90
21	AA	1429	A	C5-C6-N1	6.21	120.81	117.70
54	BA	2095	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1644	C	O4'-C1'-N1	6.21	113.17	108.20
54	BA	1998	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	2416	C	O4'-C1'-N1	6.21	113.17	108.20
54	BA	2453	A	C4-C5-C6	-6.21	113.89	117.00
21	AA	315	A	C5-C6-N1	6.21	120.80	117.70
22	A1	14	A	C5-C6-N1	6.21	120.80	117.70
46	BX	73	ARG	NE-CZ-NH1	6.21	123.40	120.30
54	BA	38	A	C6-C5-N7	6.21	136.65	132.30
54	BA	1610	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1900	A	C5-C6-N1	6.21	120.80	117.70
55	BB	95	U	O4'-C1'-N1	6.21	113.17	108.20
54	BA	125	A	C4-C5-C6	-6.21	113.90	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2183	A	C4-C5-C6	-6.21	113.90	117.00
21	AA	545	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	725	G	N1-C6-O6	-6.20	116.18	119.90
54	BA	2800	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	151	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1410	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2231	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1551	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2901	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	153	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	419	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	770	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1049	U	C1'-O4'-C4'	-6.20	104.94	109.90
54	BA	140	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2265	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1097	U	O4'-C1'-N1	6.20	113.16	108.20
40	BR	78	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	AA	800	G	N1-C6-O6	-6.19	116.18	119.90
21	AA	403	C	N3-C2-O2	-6.19	117.56	121.90
21	AA	864	A	C4-C5-C6	-6.19	113.90	117.00
21	AA	1011	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	670	A	C4-C5-C6	-6.19	113.90	117.00
54	BA	692	C	N3-C2-O2	-6.19	117.56	121.90
54	BA	1887	C	N3-C2-O2	-6.19	117.56	121.90
55	BB	66	A	C4-C5-C6	-6.19	113.90	117.00
21	AA	264	C	N1-C2-O2	6.19	122.61	118.90
21	AA	386	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	237	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	55	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	1021	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	2754	U	O4'-C1'-N1	6.19	113.15	108.20
55	BB	85	G	O4'-C1'-N9	6.19	113.15	108.20
21	AA	866	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1288	G	C3'-C2'-C1'	6.19	106.45	101.50
54	BA	2031	A	C5-C6-N1	6.19	120.79	117.70
21	AA	1311	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	1462	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	661	A	C5-C6-N1	6.18	120.79	117.70
54	BA	908	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	994	C	O4'-C1'-N1	6.18	113.15	108.20
54	BA	1894	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	802	A	C5-C6-N1	6.18	120.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	897	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	909	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	980	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	1188	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	905	A	C5-C6-N1	6.18	120.79	117.70
54	BA	1018	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	2585	U	O4'-C1'-N1	6.18	113.15	108.20
21	AA	1431	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	115	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1208	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	1545	A	C5-C6-N1	6.18	120.79	117.70
54	BA	1818	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2317	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	244	A	C5-C6-N1	6.18	120.79	117.70
54	BA	1258	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	1947	C	N1-C2-O2	6.18	122.61	118.90
21	AA	271	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	857	C	N3-C2-O2	-6.18	117.58	121.90
21	AA	1364	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2214	C	O4'-C1'-N1	6.18	113.14	108.20
54	BA	2587	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	1342	C	O4'-C1'-N1	6.17	113.14	108.20
54	BA	2572	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	2896	C	N3-C2-O2	-6.17	117.58	121.90
55	BB	101	A	C5-C6-N1	6.17	120.79	117.70
21	AA	1051	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1665	A	C4-C5-C6	-6.17	113.91	117.00
18	AS	2	ARG	NE-CZ-NH2	6.17	123.39	120.30
21	AA	502	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	268	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	412	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	2122	U	O4'-C1'-N1	6.17	113.14	108.20
54	BA	2560	A	C5-C6-N1	6.17	120.78	117.70
21	AA	582	C	N3-C2-O2	-6.17	117.58	121.90
24	A3	17	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1284	A	C5-C6-N1	6.17	120.78	117.70
54	BA	1385	A	C5-C6-N1	6.17	120.78	117.70
54	BA	2030	A	O4'-C1'-N9	6.17	113.13	108.20
21	AA	477	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	993	G	N3-C4-C5	-6.16	125.52	128.60
54	BA	83	A	C5-C6-N1	6.16	120.78	117.70
54	BA	228	C	N1-C2-O2	6.16	122.60	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2198	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	250	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1153	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2452	C	O4'-C1'-N1	6.16	113.13	108.20
21	AA	1248	A	C4-C5-C6	-6.16	113.92	117.00
22	A1	70	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	453	A	C5'-C4'-O4'	6.16	116.49	109.10
54	BA	1008	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1641	A	C4-C5-C6	-6.16	113.92	117.00
55	BB	12	C	N3-C2-O2	-6.16	117.59	121.90
55	BB	58	A	C5-C6-N1	6.16	120.78	117.70
55	BB	73	A	O4'-C1'-N9	6.16	113.13	108.20
21	AA	370	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	525	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	983	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	716	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1929	G	N3-C2-N2	-6.16	115.59	119.90
21	AA	518	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	614	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	56	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	398	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1654	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1843	C	N3-C2-O2	-6.16	117.59	121.90
21	AA	589	U	O4'-C1'-N1	6.15	113.12	108.20
21	AA	1259	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	595	A	C5-C6-N1	6.15	120.78	117.70
21	AA	805	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	918	A	C5-C6-N1	6.15	120.78	117.70
21	AA	1049	U	P-O3'-C3'	6.15	127.08	119.70
21	AA	1285	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	201	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1164	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2225	A	O4'-C1'-N9	6.15	113.12	108.20
21	AA	1254	A	N1-C6-N6	-6.15	114.91	118.60
54	BA	281	C	O4'-C1'-N1	6.15	113.12	108.20
54	BA	1858	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	2179	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	320	A	C4-C5-C6	-6.15	113.92	117.00
22	A1	20	G	N3-C4-C5	-6.15	125.53	128.60
54	BA	404	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	2205	A	C5-C6-N1	6.15	120.78	117.70
2	AC	126	ARG	NE-CZ-NH1	6.15	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1461	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	1779	U	O4'-C1'-N1	6.15	113.12	108.20
54	BA	2746	U	O4'-C1'-N1	6.15	113.12	108.20
40	BR	21	ARG	NE-CZ-NH1	6.15	123.37	120.30
54	BA	2636	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	2837	A	C4-C5-C6	-6.15	113.93	117.00
6	AG	142	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	152	A	N1-C6-N6	-6.14	114.91	118.60
54	BA	1509	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1338	G	N3-C2-N2	-6.14	115.60	119.90
54	BA	1503	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1654	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1877	A	C5-C6-N1	6.14	120.77	117.70
21	AA	192	A	C5-C6-N1	6.14	120.77	117.70
27	BE	88	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	1267	U	O4'-C1'-N1	6.14	113.11	108.20
54	BA	247	G	N1-C6-O6	-6.14	116.22	119.90
21	AA	1277	C	N3-C2-O2	-6.14	117.61	121.90
24	A3	67	C	N3-C2-O2	-6.14	117.60	121.90
52	B3	7	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	767	U	O4'-C1'-N1	6.14	113.11	108.20
54	BA	1868	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2435	A	C5-C6-N1	6.14	120.77	117.70
54	BA	2789	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	1521	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	218	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	1561	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2530	A	C5-C6-N1	6.13	120.77	117.70
21	AA	52	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2104	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	182	A	O4'-C1'-N9	6.13	113.11	108.20
21	AA	635	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	1705	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	2161	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1832	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2013	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2652	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	1314	C	N3-C2-O2	-6.13	117.61	121.90
22	A1	20	G	O4'-C1'-N9	6.13	113.10	108.20
44	BV	79	ARG	NE-CZ-NH1	6.13	123.36	120.30
51	B2	12	ARG	NE-CZ-NH2	6.13	123.36	120.30
53	B4	12	ARG	NE-CZ-NH1	6.13	123.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	64	A	C5-C6-N1	6.13	120.76	117.70
54	BA	835	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	925	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	60	G	N3-C2-N2	-6.13	115.61	119.90
54	BA	2432	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2823	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	1005	A	C5-C6-N1	6.12	120.76	117.70
54	BA	144	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	211	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	776	G	O4'-C1'-N9	6.12	113.10	108.20
21	AA	623	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	704	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	878	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1328	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1332	G	N3-C4-C5	-6.12	125.54	128.60
54	BA	1837	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	2301	C	N3-C2-O2	-6.12	117.61	121.90
24	A3	52	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1420	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1698	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2476	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2837	A	C5-C6-N1	6.12	120.76	117.70
54	BA	946	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1378	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2717	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2835	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1689	A	N1-C6-N6	-6.12	114.93	118.60
21	AA	324	G	N1-C6-O6	-6.12	116.23	119.90
21	AA	456	A	C5-C6-N1	6.12	120.76	117.70
21	AA	646	G	N1-C6-O6	-6.12	116.23	119.90
21	AA	792	A	O4'-C1'-N9	6.12	113.09	108.20
21	AA	1433	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	52	A	C5-C6-N1	6.12	120.76	117.70
54	BA	314	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1780	A	C4-C5-C6	-6.11	113.94	117.00
6	AG	91	ARG	NE-CZ-NH1	6.11	123.36	120.30
21	AA	1113	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1515	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	541	A	C5-C6-N1	6.11	120.75	117.70
54	BA	1744	A	C5-C6-N1	6.11	120.75	117.70
54	BA	2176	A	C4-C5-C6	-6.11	113.94	117.00
55	BB	29	A	N1-C6-N6	-6.11	114.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	51	A	C5-C6-N1	6.11	120.75	117.70
21	AA	1533	C	N1-C2-O2	6.11	122.56	118.90
22	A1	72	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	526	A	C1'-O4'-C4'	-6.11	105.01	109.90
54	BA	1437	C	O4'-C1'-N1	6.11	113.09	108.20
54	BA	2108	A	C4-C5-C6	-6.11	113.95	117.00
21	AA	40	C	N3-C2-O2	-6.11	117.63	121.90
21	AA	1157	A	C4-C5-C6	-6.11	113.95	117.00
31	BI	102	ARG	NE-CZ-NH1	6.11	123.35	120.30
54	BA	787	C	N1-C2-O2	6.11	122.56	118.90
54	BA	2035	G	O4'-C1'-N9	6.11	113.08	108.20
54	BA	2084	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	1739	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	314	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	759	A	C5-C6-N1	6.10	120.75	117.70
54	BA	161	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	706	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1313	U	N3-C2-O2	-6.10	117.93	122.20
54	BA	1417	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1866	A	C4-C5-C6	-6.10	113.95	117.00
55	BB	92	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	777	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	823	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1411	C	N1-C2-O2	6.10	122.56	118.90
54	BA	592	A	C5-C6-N1	6.10	120.75	117.70
21	AA	663	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	1252	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	15	G	N3-C2-N2	-6.10	115.63	119.90
54	BA	1512	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1933	G	O4'-C1'-N9	6.10	113.08	108.20
54	BA	2381	A	C5-C6-N1	6.10	120.75	117.70
21	AA	1317	C	N3-C2-O2	-6.10	117.63	121.90
24	A3	41	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	432	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	849	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1528	A	N1-C6-N6	-6.10	114.94	118.60
54	BA	731	C	N3-C2-O2	-6.09	117.63	121.90
54	BA	764	A	N1-C6-N6	-6.09	114.94	118.60
54	BA	1351	C	N3-C2-O2	-6.09	117.63	121.90
55	BB	113	C	N3-C2-O2	-6.09	117.63	121.90
21	AA	349	A	C5-C6-N1	6.09	120.75	117.70
21	AA	382	A	C4-C5-C6	-6.09	113.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	553	A	C5-C6-N1	6.09	120.75	117.70
54	BA	1741	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2154	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	2520	C	O4'-C1'-N1	6.09	113.07	108.20
21	AA	251	G	O4'-C1'-N9	6.09	113.07	108.20
21	AA	1236	A	N1-C6-N6	-6.09	114.95	118.60
51	B2	19	ARG	NE-CZ-NH1	6.09	123.34	120.30
54	BA	16	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2767	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	948	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2700	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	106	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	406	G	C5'-C4'-C3'	-6.09	106.26	116.00
54	BA	810	U	O4'-C1'-N1	6.09	113.07	108.20
21	AA	80	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1870	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	130	A	C6-C5-N7	6.08	136.56	132.30
21	AA	831	A	C5-C6-N1	6.08	120.74	117.70
21	AA	914	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	1217	C	N3-C2-O2	-6.08	117.64	121.90
41	BS	95	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	1196	C	O4'-C1'-N1	6.08	113.07	108.20
54	BA	2591	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2794	C	N3-C2-O2	-6.08	117.64	121.90
41	BS	11	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	442	G	N1-C6-O6	-6.08	116.25	119.90
54	BA	2376	A	C4-C5-C6	-6.08	113.96	117.00
55	BB	50	A	C4-C5-C6	-6.08	113.96	117.00
56	B5	53	ARG	NE-CZ-NH1	6.08	123.34	120.30
21	AA	493	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	322	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	984	A	O4'-C1'-N9	6.08	113.06	108.20
54	BA	2565	A	O4'-C1'-N9	6.08	113.06	108.20
5	AF	25	TYR	CB-CG-CD2	-6.08	117.35	121.00
54	BA	819	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	1117	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	1336	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	1308	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2858	C	O4'-C1'-N1	6.08	113.06	108.20
21	AA	36	C	N1-C2-O2	6.08	122.55	118.90
54	BA	602	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1404	C	N3-C2-O2	-6.08	117.65	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	222	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	433	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	101	A	C5-C6-N1	6.07	120.74	117.70
54	BA	1424	G	O4'-C1'-N9	6.07	113.06	108.20
54	BA	1640	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	2332	C	O4'-C1'-N1	6.07	113.06	108.20
54	BA	1944	U	O4'-C1'-N1	6.07	113.06	108.20
22	A1	32	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2241	A	C4-C5-C6	-6.07	113.97	117.00
7	AH	1	SER	C-N-CA	6.07	136.87	121.70
21	AA	231	U	O4'-C1'-N1	6.07	113.05	108.20
21	AA	784	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	255	A	C5-C6-N1	6.07	120.73	117.70
54	BA	630	G	N1-C6-O6	-6.07	116.26	119.90
54	BA	1178	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1302	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	1700	A	C5-C6-N1	6.07	120.73	117.70
54	BA	2051	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	2080	A	C5-C6-N1	6.07	120.73	117.70
54	BA	2853	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	179	C	O4'-C1'-N1	6.06	113.05	108.20
9	AJ	48	ARG	NE-CZ-NH2	6.06	123.33	120.30
21	AA	116	A	C5-C6-N1	6.06	120.73	117.70
21	AA	243	A	C5-C6-N1	6.06	120.73	117.70
54	BA	246	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1243	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2052	A	C4-C5-C6	-6.06	113.97	117.00
35	BM	38	ARG	NE-CZ-NH1	6.06	123.33	120.30
54	BA	320	A	C5-C6-N1	6.06	120.73	117.70
54	BA	1123	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	58	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	1112	C	N1-C2-O2	6.06	122.54	118.90
54	BA	10	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1273	U	O4'-C1'-N1	6.06	113.05	108.20
54	BA	1819	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	600	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1014	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1053	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2751	G	O4'-C1'-N9	6.06	113.05	108.20
21	AA	460	A	C5-C6-N1	6.05	120.73	117.70
54	BA	338	G	O4'-C1'-N9	6.05	113.04	108.20
54	BA	1212	G	N3-C2-N2	-6.05	115.66	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	687	A	C5-C6-N1	6.05	120.73	117.70
19	AT	2	ASN	C-N-CA	6.05	136.83	121.70
21	AA	8	A	N1-C6-N6	-6.05	114.97	118.60
21	AA	234	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	747	A	C4-C5-C6	-6.05	113.98	117.00
22	A1	69	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1189	A	C5-C6-N1	6.05	120.72	117.70
54	BA	1611	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	523	C	N1-C2-O2	6.05	122.53	118.90
54	BA	2704	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	41	G	N1-C6-O6	-6.05	116.27	119.90
21	AA	533	A	C5-C6-N1	6.05	120.72	117.70
21	AA	1273	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1307	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1571	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	262	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1413	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2480	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	509	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1288	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	300	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	318	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	657	U	O4'-C1'-N1	6.04	113.03	108.20
54	BA	1857	G	O4'-C1'-N9	6.04	113.03	108.20
54	BA	2270	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2338	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	105	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	330	A	O4'-C1'-N9	6.04	113.03	108.20
54	BA	1700	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	241	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1920	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2814	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	274	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1969	A	N1-C6-N6	-6.04	114.98	118.60
54	BA	2616	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	958	A	C5-C6-N1	6.04	120.72	117.70
12	AM	89	ARG	NE-CZ-NH2	-6.04	117.28	120.30
54	BA	374	A	N1-C6-N6	-6.04	114.98	118.60
54	BA	1314	C	C3'-C2'-C1'	6.04	106.33	101.50
54	BA	1462	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	2184	A	C5-C6-N1	6.04	120.72	117.70
21	AA	160	A	C4-C5-C6	-6.03	113.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	714	G	N3-C2-N2	-6.03	115.68	119.90
21	AA	876	C	C5'-C4'-O4'	6.03	116.34	109.10
54	BA	12	U	O4'-C1'-N1	6.03	113.03	108.20
54	BA	161	A	C5-C6-N1	6.03	120.72	117.70
54	BA	527	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1039	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	2540	C	N3-C2-O2	-6.03	117.68	121.90
55	BB	42	C	N1-C2-O2	6.03	122.52	118.90
21	AA	535	A	C4-C5-C6	-6.03	113.98	117.00
25	BC	211	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	592	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	415	A	O4'-C1'-N9	6.03	113.02	108.20
21	AA	539	A	C5-C6-N1	6.03	120.71	117.70
21	AA	1167	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	1479	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	1508	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	513	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	730	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	1960	A	C4-C5-C6	-6.03	113.99	117.00
21	AA	309	A	N1-C6-N6	-6.03	114.98	118.60
21	AA	712	A	C4-C5-C6	-6.03	113.99	117.00
29	BG	94	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	1801	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	2045	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	41	C	N3-C2-O2	-6.02	117.68	121.90
21	AA	135	C	N3-C2-O2	-6.02	117.68	121.90
21	AA	998	C	N3-C2-O2	-6.02	117.68	121.90
54	BA	911	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1626	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2406	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2818	U	O4'-C1'-N1	6.02	113.02	108.20
54	BA	318	C	O4'-C1'-N1	6.02	113.02	108.20
3	AD	69	ARG	NE-CZ-NH1	6.02	123.31	120.30
21	AA	137	U	O4'-C1'-N1	6.02	113.02	108.20
21	AA	459	A	C5-C6-N1	6.02	120.71	117.70
21	AA	553	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	575	G	P-O3'-C3'	6.02	126.92	119.70
24	A3	73	A	P-O3'-C3'	6.02	126.92	119.70
54	BA	1672	A	C4-C5-C6	-6.02	113.99	117.00
55	BB	29	A	C4-C5-C6	-6.02	113.99	117.00
14	AO	63	ARG	NE-CZ-NH1	6.02	123.31	120.30
21	AA	718	A	C4-C5-C6	-6.02	113.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1086	U	O4'-C1'-N1	6.02	113.02	108.20
21	AA	1131	G	N3-C2-N2	-6.02	115.69	119.90
54	BA	509	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	851	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	1676	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	806	C	N3-C2-O2	-6.02	117.69	121.90
22	A1	51	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	182	A	O4'-C1'-N9	6.02	113.01	108.20
54	BA	233	A	C4-C5-C6	-6.02	113.99	117.00
21	AA	44	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	999	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	1271	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	104	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	678	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	2266	A	C4-C5-C6	-6.01	113.99	117.00
21	AA	335	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	432	A	C4-C5-C6	-6.01	113.99	117.00
24	A3	76	C	N1-C2-O2	6.01	122.51	118.90
54	BA	1526	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1805	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2447	G	O4'-C1'-N9	6.01	113.01	108.20
21	AA	408	A	C5-C6-N1	6.01	120.70	117.70
54	BA	269	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	453	A	O4'-C1'-N9	6.01	113.01	108.20
55	BB	117	G	O4'-C1'-N9	6.01	113.01	108.20
54	BA	2062	A	C4-C5-C6	-6.01	114.00	117.00
17	AR	56	ARG	NE-CZ-NH1	6.01	123.30	120.30
54	BA	94	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2263	C	N3-C2-O2	-6.00	117.70	121.90
36	BN	30	ARG	NE-CZ-NH1	6.00	123.30	120.30
39	BQ	2	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	83	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	118	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2579	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1119	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	478	A	C5-C6-N1	6.00	120.70	117.70
54	BA	752	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2468	A	C3'-C2'-C1'	6.00	106.30	101.50
21	AA	448	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	456	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	876	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	73	A	N1-C6-N6	-6.00	115.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	149	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	675	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1836	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	2043	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2134	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2542	A	O4'-C1'-N9	6.00	113.00	108.20
21	AA	1036	A	C5-C6-N1	6.00	120.70	117.70
55	BB	32	U	O4'-C1'-N1	6.00	113.00	108.20
21	AA	285	C	N3-C2-O2	-5.99	117.70	121.90
21	AA	1137	C	N3-C2-O2	-5.99	117.70	121.90
21	AA	1161	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	1294	U	O4'-C1'-N1	5.99	113.00	108.20
54	BA	2005	A	C4-C5-C6	-5.99	114.00	117.00
55	BB	26	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	694	U	O4'-C1'-N1	5.99	112.99	108.20
21	AA	1208	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	1500	A	C5-C6-N1	5.99	120.69	117.70
54	BA	660	C	N1-C2-O2	5.99	122.49	118.90
54	BA	2716	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	422	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1231	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	2612	C	N1-C2-O2	5.99	122.49	118.90
21	AA	129	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	1509	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	504	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1499	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2643	G	N1-C6-O6	-5.99	116.31	119.90
21	AA	1456	A	C4-C5-C6	-5.98	114.01	117.00
52	B3	39	ARG	NE-CZ-NH1	5.98	123.29	120.30
54	BA	1032	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2705	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1150	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1213	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1284	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	436	C	O4'-C1'-N1	5.98	112.98	108.20
54	BA	1098	A	C5-C6-N1	5.98	120.69	117.70
11	AL	49	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	315	A	N1-C6-N6	-5.98	115.01	118.60
54	BA	1590	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1617	C	C6-N1-C2	-5.98	117.91	120.30
54	BA	2270	A	N1-C6-N6	-5.98	115.01	118.60
21	AA	655	A	C5-C6-N1	5.98	120.69	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1305	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	2140	G	O4'-C1'-N9	5.98	112.98	108.20
21	AA	504	C	N3-C2-O2	-5.98	117.72	121.90
23	A2	93	U	N3-C2-O2	-5.98	118.02	122.20
54	BA	402	A	N1-C6-N6	-5.98	115.01	118.60
54	BA	1749	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2732	G	N3-C4-C5	-5.98	125.61	128.60
21	AA	573	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	679	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1194	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	2247	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	28	A	C4-C5-C6	-5.97	114.01	117.00
24	A3	74	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	8	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1170	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1241	A	C4-C5-C6	-5.97	114.01	117.00
21	AA	1168	U	N3-C2-O2	-5.97	118.02	122.20
54	BA	685	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	952	G	C5-C6-N1	5.97	114.48	111.50
54	BA	1768	C	O4'-C1'-N1	5.97	112.98	108.20
54	BA	2841	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2856	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	396	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	172	A	C4-C5-C6	-5.97	114.02	117.00
32	BJ	95	ARG	NE-CZ-NH1	5.97	123.28	120.30
54	BA	444	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2165	C	N3-C2-O2	-5.97	117.72	121.90
55	BB	115	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	1460	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	2359	C	N1-C2-O2	5.96	122.48	118.90
54	BA	2430	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1306	C	O4'-C1'-N1	5.96	112.97	108.20
21	AA	43	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	613	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	1044	A	C5-C6-N1	5.96	120.68	117.70
21	AA	1195	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	821	A	O4'-C1'-N9	5.96	112.97	108.20
21	AA	560	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	1107	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1533	C	N1-C2-O2	5.96	122.48	118.90
54	BA	1618	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2208	C	N3-C2-O2	-5.96	117.73	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2730	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	882	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	866	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1150	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	435	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	63	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1135	C	C2-N3-C4	-5.96	116.92	119.90
54	BA	1428	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2000	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2139	U	O4'-C1'-N1	5.96	112.96	108.20
21	AA	738	C	N1-C2-O2	5.95	122.47	118.90
21	AA	742	G	N1-C6-O6	-5.95	116.33	119.90
21	AA	766	A	C5-C6-N1	5.95	120.68	117.70
54	BA	2459	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	328	C	N1-C2-O2	5.95	122.47	118.90
21	AA	496	A	O4'-C1'-N9	5.95	112.96	108.20
21	AA	814	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	1038	C	N3-C2-O2	-5.95	117.73	121.90
21	AA	1136	C	N1-C2-O2	5.95	122.47	118.90
54	BA	19	A	C5-C6-N1	5.95	120.67	117.70
21	AA	161	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	74	A	O4'-C1'-N9	5.95	112.96	108.20
54	BA	512	G	N1-C6-O6	-5.95	116.33	119.90
54	BA	2199	A	C5-C6-N1	5.95	120.67	117.70
54	BA	227	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	640	C	C6-N1-C2	-5.95	117.92	120.30
54	BA	1711	A	C5-C6-N1	5.95	120.67	117.70
36	BN	69	ARG	NE-CZ-NH1	5.95	123.27	120.30
54	BA	948	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	2879	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	801	G	N1-C6-O6	-5.94	116.33	119.90
21	AA	1347	G	N1-C6-O6	-5.94	116.33	119.90
54	BA	47	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	557	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1284	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1967	C	O4'-C1'-N1	5.94	112.95	108.20
21	AA	1035	A	O4'-C1'-N9	5.94	112.95	108.20
54	BA	791	C	O4'-C1'-N1	5.94	112.95	108.20
54	BA	889	C	N1-C2-O2	5.94	122.46	118.90
54	BA	216	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	959	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	810	C	N3-C2-O2	-5.94	117.75	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2070	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1472	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	879	C	N1-C2-O2	5.93	122.46	118.90
48	BZ	10	ARG	NE-CZ-NH2	5.93	123.27	120.30
54	BA	21	A	C5-C6-N1	5.93	120.67	117.70
54	BA	1331	G	N1-C6-O6	-5.93	116.34	119.90
54	BA	1403	A	O4'-C1'-N9	5.93	112.94	108.20
21	AA	263	A	C5-C6-N1	5.93	120.67	117.70
21	AA	637	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1228	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	104	A	C5-C6-N1	5.93	120.67	117.70
54	BA	1798	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	2459	A	N1-C6-N6	-5.93	115.04	118.60
55	BB	51	G	C5-C6-N1	5.93	114.47	111.50
54	BA	895	U	O4'-C1'-N1	5.93	112.94	108.20
54	BA	1013	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	1111	A	C4-C5-C6	-5.93	114.04	117.00
54	BA	1801	A	N1-C6-N6	-5.93	115.04	118.60
21	AA	469	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	556	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1098	C	N3-C2-O2	-5.93	117.75	121.90
23	A2	91	A	C4-C5-C6	-5.93	114.04	117.00
54	BA	2003	A	C4-C5-C6	-5.93	114.04	117.00
21	AA	765	G	N3-C4-C5	-5.92	125.64	128.60
21	AA	967	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	1152	A	C5-C6-N1	5.92	120.66	117.70
54	BA	156	A	C5-C6-N1	5.92	120.66	117.70
54	BA	782	A	O4'-C1'-N9	5.92	112.94	108.20
54	BA	1447	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	1586	A	C5-C6-N1	5.92	120.66	117.70
55	BB	59	A	C4-C5-C6	-5.92	114.04	117.00
55	BB	70	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	1382	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	1194	U	O4'-C1'-N1	5.92	112.94	108.20
54	BA	1628	G	C5'-C4'-O4'	5.92	116.21	109.10
54	BA	1916	A	O4'-C1'-N9	5.92	112.94	108.20
54	BA	1348	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	1446	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	418	C	N3-C2-O2	-5.92	117.76	121.90
21	AA	712	A	C5-C6-N1	5.92	120.66	117.70
24	A3	76	C	C2'-C3'-O3'	5.92	123.17	113.70
54	BA	382	A	C4-C5-C6	-5.92	114.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	661	A	P-O3'-C3'	5.92	126.80	119.70
54	BA	994	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	1653	G	O4'-C1'-N9	5.92	112.94	108.20
54	BA	2727	A	C4-C5-C6	-5.92	114.04	117.00
55	BB	78	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2175	C	O4'-C1'-N1	5.92	112.93	108.20
21	AA	465	A	C4-C5-C6	-5.92	114.04	117.00
30	BH	116	ARG	NE-CZ-NH1	5.92	123.26	120.30
55	BB	91	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	33	C	N1-C2-O2	5.91	122.45	118.90
54	BA	1888	G	O4'-C1'-N9	5.91	112.93	108.20
21	AA	756	C	N3-C4-C5	5.91	124.27	121.90
54	BA	609	A	C5-C6-N1	5.91	120.66	117.70
54	BA	1386	C	N3-C2-O2	-5.91	117.76	121.90
29	BG	93	TYR	CB-CG-CD2	-5.91	117.45	121.00
48	BZ	10	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
54	BA	1142	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	1257	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2339	C	C1'-O4'-C4'	-5.91	105.17	109.90
21	AA	307	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1012	U	O4'-C1'-N1	5.91	112.93	108.20
25	BC	237	ARG	NE-CZ-NH2	-5.91	117.35	120.30
21	AA	1093	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	2787	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1104	G	N1-C6-O6	-5.90	116.36	119.90
21	AA	1171	A	C5-C6-N1	5.90	120.65	117.70
24	A3	29	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	1288	G	N3-C4-C5	-5.90	125.65	128.60
21	AA	946	A	C5-C6-N1	5.90	120.65	117.70
54	BA	466	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	393	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	1145	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1711	A	N1-C6-N6	-5.90	115.06	118.60
21	AA	665	A	C6-C5-N7	5.90	136.43	132.30
24	A3	38	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1489	C	N1-C2-O2	5.90	122.44	118.90
54	BA	2841	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	418	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1032	G	O4'-C1'-N9	5.89	112.92	108.20
54	BA	196	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	750	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	905	A	C4-C5-C6	-5.89	114.05	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1384	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	1821	A	C5-C6-N1	5.89	120.65	117.70
15	AP	70	ARG	NE-CZ-NH1	5.89	123.25	120.30
54	BA	209	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1945	G	N1-C6-O6	-5.89	116.36	119.90
54	BA	2137	U	N3-C2-O2	-5.89	118.08	122.20
54	BA	2874	C	N3-C2-O2	-5.89	117.78	121.90
55	BB	63	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	128	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	383	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1046	A	C4-C5-C6	-5.89	114.05	117.00
21	AA	326	G	N1-C6-O6	-5.89	116.37	119.90
54	BA	931	U	N3-C2-O2	-5.89	118.08	122.20
21	AA	309	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	1067	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	2311	A	C4-C5-C6	-5.89	114.06	117.00
3	AD	110	ARG	NE-CZ-NH1	5.88	123.24	120.30
21	AA	610	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	2001	C	N3-C2-O2	-5.88	117.78	121.90
28	BF	124	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	403	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	1385	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1785	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1952	A	O4'-C1'-N9	5.88	112.91	108.20
54	BA	1121	C	O4'-C1'-N1	5.88	112.90	108.20
21	AA	67	C	N1-C2-O2	5.88	122.43	118.90
21	AA	723	U	O4'-C1'-N1	5.88	112.90	108.20
21	AA	1517	G	N1-C6-O6	-5.88	116.37	119.90
21	AA	495	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1787	A	C5-C6-N1	5.88	120.64	117.70
54	BA	2454	G	N1-C6-O6	-5.88	116.37	119.90
55	BB	19	C	N3-C2-O2	-5.88	117.79	121.90
21	AA	345	C	C1'-O4'-C4'	-5.88	105.20	109.90
21	AA	1254	A	C5-C6-N1	5.88	120.64	117.70
21	AA	817	C	O4'-C1'-N1	5.87	112.90	108.20
54	BA	978	G	N1-C6-O6	-5.87	116.38	119.90
54	BA	1495	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	1080	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	1595	C	O4'-C1'-N1	5.87	112.90	108.20
54	BA	2065	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2178	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2869	G	N3-C2-N2	-5.87	115.79	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	270	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	99	U	N3-C2-O2	-5.87	118.09	122.20
21	AA	1518	A	C5-C6-N1	5.87	120.63	117.70
54	BA	255	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	1470	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	44	A	C5-C6-N1	5.87	120.63	117.70
21	AA	756	C	N1-C2-O2	5.87	122.42	118.90
21	AA	960	U	N3-C2-O2	-5.87	118.09	122.20
54	BA	439	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	1638	C	N1-C2-O2	5.87	122.42	118.90
21	AA	492	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	890	G	O4'-C1'-N9	5.86	112.89	108.20
54	BA	2678	C	N3-C2-O2	-5.86	117.80	121.90
55	BB	15	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1652	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1732	C	N1-C2-O2	5.86	122.42	118.90
54	BA	1987	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	328	C	O4'-C1'-N1	5.86	112.89	108.20
54	BA	1057	A	C5-C6-N1	5.86	120.63	117.70
54	BA	2052	A	N1-C6-N6	-5.86	115.08	118.60
21	AA	263	A	N1-C6-N6	-5.86	115.09	118.60
21	AA	381	C	N1-C2-O2	5.86	122.41	118.90
54	BA	2354	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2556	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	356	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	1016	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	337	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	894	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2558	C	N3-C2-O2	-5.85	117.80	121.90
21	AA	624	C	O4'-C1'-N1	5.85	112.88	108.20
21	AA	1534	A	C4-C5-C6	-5.85	114.07	117.00
23	A2	79	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	2507	C	N1-C2-O2	5.85	122.41	118.90
21	AA	1197	A	C5-C6-N1	5.85	120.63	117.70
54	BA	348	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	1531	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1354	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1781	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	2425	A	O4'-C1'-N9	5.85	112.88	108.20
54	BA	2870	C	O4'-C1'-N1	5.85	112.88	108.20
55	BB	30	C	N3-C2-O2	-5.85	117.81	121.90
29	BG	2	ARG	NE-CZ-NH1	5.85	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1244	A	C5-C6-N1	5.85	120.62	117.70
54	BA	2036	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	2458	G	N3-C4-C5	-5.85	125.68	128.60
54	BA	2527	C	N1-C2-O2	5.85	122.41	118.90
22	A1	11	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	253	C	O4'-C1'-N1	5.85	112.88	108.20
54	BA	998	C	N3-C2-O2	-5.85	117.81	121.90
55	BB	56	G	O4'-C1'-N9	5.85	112.88	108.20
21	AA	175	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2007	U	O4'-C1'-N1	5.84	112.88	108.20
55	BB	31	C	O4'-C1'-N1	5.84	112.88	108.20
21	AA	1261	A	C5-C6-N1	5.84	120.62	117.70
54	BA	353	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	853	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	1761	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2874	C	N1-C2-O2	5.84	122.41	118.90
54	BA	470	A	C5-C6-N1	5.84	120.62	117.70
21	AA	272	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	503	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	498	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	2207	C	N3-C2-O2	-5.84	117.81	121.90
12	AM	86	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	AA	811	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	111	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1054	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1877	A	C4-C5-C6	-5.84	114.08	117.00
55	BB	17	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	1248	A	C5-C6-N1	5.83	120.62	117.70
54	BA	222	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	181	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	1407	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1624	U	O4'-C1'-N1	5.83	112.87	108.20
54	BA	2422	C	N1-C2-O2	5.83	122.40	118.90
54	BA	2582	G	N3-C4-C5	-5.83	125.68	128.60
54	BA	2667	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	374	A	C5-C6-N1	5.83	120.62	117.70
54	BA	2090	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	2893	A	C4-C5-C6	-5.83	114.08	117.00
15	AP	51	ARG	NE-CZ-NH2	-5.83	117.39	120.30
21	AA	610	U	N3-C2-O2	-5.83	118.12	122.20
54	BA	172	A	C5-C6-N1	5.83	120.61	117.70
54	BA	2784	U	O4'-C1'-N1	5.83	112.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	BD	58	ASN	C-N-CA	5.83	136.27	121.70
54	BA	2820	A	C4-C5-C6	-5.83	114.09	117.00
38	BP	88	ARG	NE-CZ-NH2	-5.83	117.39	120.30
54	BA	898	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1001	A	C4-C5-C6	-5.83	114.09	117.00
54	BA	1001	A	C5-C6-N1	5.83	120.61	117.70
21	AA	975	A	C1'-O4'-C4'	-5.82	105.24	109.90
54	BA	1311	G	N3-C4-C5	-5.82	125.69	128.60
54	BA	2330	G	C4'-C3'-C2'	-5.82	96.78	102.60
55	BB	87	U	N3-C2-O2	-5.82	118.12	122.20
21	AA	385	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1145	A	C3'-C2'-C1'	5.82	106.16	101.50
21	AA	1374	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1399	C	O4'-C1'-N1	5.82	112.86	108.20
3	AD	61	ARG	NE-CZ-NH2	-5.82	117.39	120.30
21	AA	629	A	C4-C5-C6	-5.82	114.09	117.00
23	A2	82	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1172	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	1857	G	N1-C6-O6	-5.82	116.41	119.90
54	BA	2399	G	N1-C6-O6	-5.82	116.41	119.90
21	AA	631	C	O4'-C1'-N1	5.82	112.86	108.20
54	BA	119	A	O4'-C1'-N9	5.82	112.86	108.20
54	BA	1312	U	P-O3'-C3'	5.82	126.68	119.70
54	BA	1565	C	N1-C2-O2	5.82	122.39	118.90
21	AA	586	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1452	C	N1-C2-O2	5.82	122.39	118.90
54	BA	2258	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	1171	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2330	G	O4'-C1'-N9	5.82	112.85	108.20
54	BA	2733	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	1237	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1994	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2468	A	O4'-C4'-C3'	5.81	110.75	106.10
54	BA	1052	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1916	A	C6-C5-N7	5.81	136.37	132.30
54	BA	324	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2194	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	2500	U	N3-C2-O2	-5.81	118.13	122.20
8	AI	98	ARG	NE-CZ-NH1	5.81	123.20	120.30
54	BA	2091	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2135	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2458	G	N1-C6-O6	-5.81	116.41	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1265	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	270	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	1652	A	C5-C6-N1	5.81	120.60	117.70
54	BA	2264	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2888	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	198	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2031	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	2478	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	694	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1191	A	C5-C6-N1	5.80	120.60	117.70
54	BA	1156	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1278	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1990	C	N1-C2-O2	5.80	122.38	118.90
54	BA	2175	C	N3-C4-C5	5.80	124.22	121.90
21	AA	101	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1499	A	C4-C5-C6	-5.80	114.10	117.00
24	A3	44	A	C5-C6-N1	5.80	120.60	117.70
54	BA	415	A	C6-C5-N7	5.80	136.36	132.30
54	BA	960	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2807	U	O4'-C1'-N1	5.80	112.84	108.20
21	AA	1095	U	C5-C6-N1	-5.80	119.80	122.70
54	BA	485	C	N1-C2-O2	5.80	122.38	118.90
54	BA	1363	C	O4'-C1'-N1	5.80	112.84	108.20
54	BA	2117	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	209	U	C3'-C2'-C1'	5.80	106.14	101.50
21	AA	880	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	903	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1424	G	N1-C6-O6	-5.80	116.42	119.90
56	B5	7	ARG	NE-CZ-NH1	5.80	123.20	120.30
16	AQ	61	ARG	NE-CZ-NH2	-5.80	117.40	120.30
21	AA	1035	A	C4-C5-C6	-5.80	114.10	117.00
25	BC	86	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	79	C	N1-C2-O2	5.80	122.38	118.90
54	BA	226	A	O4'-C1'-N9	5.80	112.84	108.20
54	BA	487	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	635	C	N1-C2-O2	5.80	122.38	118.90
54	BA	764	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1290	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	2305	U	C5'-C4'-C3'	-5.79	106.73	116.00
20	AU	33	ARG	NE-CZ-NH2	5.79	123.20	120.30
21	AA	1301	U	N3-C2-O2	-5.79	118.14	122.20
54	BA	413	C	N3-C2-O2	-5.79	117.84	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	683	U	C5'-C4'-O4'	5.79	116.05	109.10
54	BA	2041	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2806	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	740	C	N1-C2-O2	5.79	122.37	118.90
54	BA	1893	C	O4'-C1'-N1	5.79	112.83	108.20
21	AA	1080	A	N1-C6-N6	-5.79	115.13	118.60
21	AA	1318	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	1339	A	C5'-C4'-O4'	5.79	116.05	109.10
27	BE	61	ARG	NE-CZ-NH1	5.79	123.19	120.30
54	BA	876	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	991	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1147	A	O4'-C1'-N9	5.79	112.83	108.20
54	BA	1383	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2119	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2520	C	N1-C2-O2	5.79	122.37	118.90
54	BA	2849	U	N3-C2-O2	-5.79	118.15	122.20
55	BB	11	C	N1-C2-O2	5.79	122.37	118.90
21	AA	853	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1233	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	1246	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2513	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2766	A	N1-C6-N6	-5.79	115.13	118.60
21	AA	176	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	520	A	C4-C5-C6	-5.79	114.11	117.00
28	BF	91	ARG	NE-CZ-NH1	5.79	123.19	120.30
54	BA	1605	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2364	C	O4'-C1'-N1	5.78	112.83	108.20
54	BA	2583	G	N1-C6-O6	-5.78	116.43	119.90
22	A1	6	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1299	G	N7-C8-N9	5.78	115.99	113.10
15	AP	5	ARG	NE-CZ-NH1	5.78	123.19	120.30
32	BJ	37	ARG	NE-CZ-NH2	-5.78	117.41	120.30
54	BA	158	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	335	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	702	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	793	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1938	A	O4'-C1'-N9	5.78	112.82	108.20
54	BA	1990	C	O4'-C1'-N1	5.78	112.82	108.20
54	BA	2184	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	935	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	178	G	N1-C6-O6	-5.78	116.43	119.90
54	BA	1357	C	N3-C2-O2	-5.78	117.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1711	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	993	G	C5-C6-N1	5.78	114.39	111.50
21	AA	1244	G	N1-C6-O6	-5.78	116.43	119.90
21	AA	1342	C	N3-C2-O2	-5.78	117.86	121.90
54	BA	394	C	N1-C2-O2	5.78	122.37	118.90
54	BA	1266	G	N1-C6-O6	-5.78	116.43	119.90
54	BA	1326	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	1367	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	322	C	N3-C2-O2	-5.78	117.86	121.90
21	AA	860	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1336	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2205	A	N1-C6-N6	-5.78	115.13	118.60
54	BA	2765	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1043	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1232	G	C5-C6-N1	5.77	114.39	111.50
54	BA	2503	A	O4'-C1'-N9	5.77	112.82	108.20
22	A1	18	G	O4'-C1'-N9	5.77	112.82	108.20
24	A3	42	C	N1-C2-O2	5.77	122.36	118.90
54	BA	109	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	2309	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	2788	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1095	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	2603	G	O4'-C1'-N9	5.77	112.82	108.20
54	BA	2830	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	2880	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	166	U	O4'-C1'-N1	5.77	112.81	108.20
54	BA	257	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1378	A	C1'-O4'-C4'	-5.77	105.28	109.90
21	AA	876	C	O4'-C4'-C3'	-5.77	98.23	104.00
54	BA	1536	C	N1-C2-O2	5.77	122.36	118.90
54	BA	1550	C	N1-C2-O2	5.77	122.36	118.90
54	BA	2226	C	O4'-C1'-N1	5.77	112.81	108.20
21	AA	658	C	N1-C2-O2	5.77	122.36	118.90
21	AA	99	C	N1-C2-O2	5.76	122.36	118.90
21	AA	119	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	209	U	O4'-C1'-N1	5.76	112.81	108.20
21	AA	503	C	N3-C2-O2	-5.76	117.86	121.90
22	A1	48	C	N1-C2-O2	5.76	122.36	118.90
54	BA	634	C	N1-C2-O2	5.76	122.36	118.90
54	BA	1595	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	1797	G	N7-C8-N9	5.76	115.98	113.10
21	AA	631	C	N1-C2-O2	5.76	122.36	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1549	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	1145	A	O4'-C1'-N9	5.76	112.81	108.20
21	AA	1408	A	C4-C5-C6	-5.76	114.12	117.00
36	BN	71	ARG	NE-CZ-NH1	5.76	123.18	120.30
37	BO	33	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	226	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1518	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	1690	A	N1-C6-N6	-5.76	115.14	118.60
54	BA	2528	U	C5-C6-N1	-5.76	119.82	122.70
55	BB	49	C	C3'-C2'-C1'	5.76	106.11	101.50
21	AA	722	G	N1-C6-O6	-5.76	116.44	119.90
21	AA	1375	A	N1-C6-N6	-5.76	115.14	118.60
21	AA	1403	C	N1-C2-O2	5.76	122.36	118.90
21	AA	1503	A	C4-C5-C6	-5.76	114.12	117.00
24	A3	14	A	C5-C6-N1	5.76	120.58	117.70
28	BF	101	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	928	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1085	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1090	A	C5-C6-N1	5.76	120.58	117.70
54	BA	1168	G	N1-C6-O6	-5.76	116.44	119.90
54	BA	1575	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	2114	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2404	U	O4'-C1'-N1	5.76	112.81	108.20
10	AK	55	ARG	NE-CZ-NH1	5.76	123.18	120.30
21	AA	808	C	N1-C2-O2	5.76	122.36	118.90
21	AA	1354	U	N3-C2-O2	-5.76	118.17	122.20
54	BA	947	A	C6-C5-N7	5.76	136.33	132.30
54	BA	1914	C	N1-C2-O2	5.76	122.36	118.90
54	BA	1986	C	N3-C2-O2	-5.76	117.87	121.90
21	AA	923	A	C4-C5-C6	-5.76	114.12	117.00
39	BQ	5	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	786	C	N1-C2-O2	5.76	122.35	118.90
54	BA	1259	G	O4'-C1'-N9	5.76	112.81	108.20
54	BA	2050	C	N1-C2-O2	5.76	122.35	118.90
54	BA	2698	U	O4'-C1'-N1	5.76	112.81	108.20
4	AE	44	ARG	NE-CZ-NH1	5.75	123.18	120.30
21	AA	743	A	C5-C6-N1	5.75	120.58	117.70
21	AA	1203	C	O4'-C1'-N1	5.75	112.80	108.20
24	A3	24	C	N3-C2-O2	-5.75	117.87	121.90
24	A3	69	C	N1-C2-O2	5.75	122.35	118.90
54	BA	2486	C	N3-C2-O2	-5.75	117.87	121.90
7	AH	113	ARG	NE-CZ-NH1	5.75	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	373	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	1226	C	N1-C2-O2	5.75	122.35	118.90
54	BA	42	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2559	C	N3-C2-O2	-5.75	117.87	121.90
55	BB	110	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	926	G	C8-N9-C4	-5.75	104.10	106.40
21	AA	1518	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2491	U	O4'-C1'-N1	5.75	112.80	108.20
21	AA	207	C	N1-C2-O2	5.75	122.35	118.90
34	BL	18	ARG	NE-CZ-NH1	5.75	123.17	120.30
54	BA	342	A	C5-C6-N1	5.75	120.57	117.70
21	AA	421	U	O4'-C1'-N1	5.75	112.80	108.20
21	AA	600	A	C5-C6-N1	5.75	120.57	117.70
32	BJ	35	ARG	NH1-CZ-NH2	-5.75	113.08	119.40
54	BA	1539	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2460	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2611	C	N1-C2-O2	5.75	122.35	118.90
54	BA	2715	C	O4'-C1'-N1	5.75	112.80	108.20
18	AS	80	ARG	NE-CZ-NH2	-5.75	117.43	120.30
54	BA	1393	A	O4'-C4'-C3'	5.75	110.70	106.10
21	AA	190	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	350	G	C1'-O4'-C4'	-5.74	105.31	109.90
54	BA	225	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	107	G	N1-C6-O6	-5.74	116.45	119.90
21	AA	211	G	N3-C4-C5	-5.74	125.73	128.60
21	AA	571	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	1254	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1664	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2055	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	2443	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	818	G	O4'-C1'-N9	5.74	112.79	108.20
54	BA	2741	A	C4-C5-C6	-5.74	114.13	117.00
24	A3	59	A	C6-C5-N7	5.73	136.31	132.30
34	BL	47	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	1927	A	C5-C6-N1	5.73	120.57	117.70
21	AA	95	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	486	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	753	A	C4-C5-C6	-5.73	114.13	117.00
54	BA	1752	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1755	A	C6-C5-N7	5.73	136.31	132.30
13	AN	90	ARG	NE-CZ-NH2	5.73	123.17	120.30
21	AA	689	C	O4'-C1'-N1	5.73	112.78	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	715	A	C4-C5-C6	-5.73	114.14	117.00
33	BK	105	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	2295	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2679	A	C4-C5-C6	-5.73	114.14	117.00
41	BS	84	ARG	NE-CZ-NH1	5.73	123.17	120.30
21	AA	78	A	C1'-O4'-C4'	-5.73	105.32	109.90
21	AA	1383	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	301	G	O4'-C1'-N9	5.73	112.78	108.20
54	BA	471	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	2396	G	N1-C6-O6	-5.73	116.46	119.90
54	BA	964	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	1301	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	82	U	O4'-C1'-N1	5.72	112.78	108.20
54	BA	672	C	N1-C2-O2	5.72	122.33	118.90
54	BA	2277	G	N1-C6-O6	-5.72	116.47	119.90
21	AA	1026	G	N3-C2-N2	-5.72	115.89	119.90
54	BA	1264	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2361	G	O4'-C1'-N9	5.72	112.78	108.20
54	BA	2557	G	C5-C6-N1	5.72	114.36	111.50
55	BB	35	C	N1-C2-O2	5.72	122.33	118.90
21	AA	471	U	O4'-C1'-N1	5.72	112.78	108.20
21	AA	599	C	N3-C2-O2	-5.72	117.89	121.90
21	AA	1192	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	2023	C	N3-C2-O2	-5.72	117.89	121.90
21	AA	1140	C	N3-C2-O2	-5.72	117.90	121.90
49	B0	49	ARG	NE-CZ-NH1	5.72	123.16	120.30
54	BA	857	G	O4'-C1'-N9	5.72	112.78	108.20
54	BA	1772	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	303	G	C3'-C2'-C1'	5.72	106.07	101.50
21	AA	112	G	N1-C6-O6	-5.72	116.47	119.90
54	BA	644	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2273	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2465	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	519	C	N3-C2-O2	-5.71	117.90	121.90
21	AA	1271	A	C5-C6-N1	5.71	120.56	117.70
54	BA	253	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	734	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	1979	U	C4'-C3'-C2'	-5.71	96.89	102.60
54	BA	2755	C	N1-C2-O2	5.71	122.33	118.90
55	BB	71	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	2133	G	C8-N9-C4	-5.71	104.11	106.40
54	BA	112	U	O4'-C1'-N1	5.71	112.77	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	334	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	606	U	O4'-C1'-N1	5.71	112.77	108.20
54	BA	649	G	C3'-C2'-C1'	5.71	106.07	101.50
54	BA	1534	U	N3-C2-O2	-5.71	118.20	122.20
55	BB	46	A	C6-C5-N7	5.71	136.30	132.30
54	BA	2030	A	C4-C5-C6	-5.71	114.14	117.00
21	AA	530	G	O4'-C1'-N9	5.71	112.77	108.20
21	AA	1396	A	C6-C5-N7	5.71	136.30	132.30
54	BA	26	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	2774	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	2350	C	N3-C2-O2	-5.71	117.91	121.90
54	BA	1104	C	N1-C2-O2	5.70	122.32	118.90
54	BA	1218	G	C5-C6-N1	5.70	114.35	111.50
54	BA	2096	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	761	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	985	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	1547	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	2181	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	943	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1848	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2225	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2227	A	C5-C6-N1	5.70	120.55	117.70
21	AA	749	A	C6-C5-N7	5.69	136.28	132.30
21	AA	1404	C	N3-C4-N4	-5.69	114.01	118.00
21	AA	1483	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	195	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2649	C	N3-C2-O2	-5.69	117.91	121.90
21	AA	743	A	C4-C5-C6	-5.69	114.15	117.00
39	BQ	10	ARG	NE-CZ-NH1	5.69	123.15	120.30
54	BA	1141	U	N3-C2-O2	-5.69	118.22	122.20
54	BA	2369	A	N1-C6-N6	-5.69	115.19	118.60
54	BA	2430	A	C2-N3-C4	5.69	113.45	110.60
21	AA	1257	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1159	U	O4'-C1'-N1	5.69	112.75	108.20
54	BA	2460	U	C4'-C3'-C2'	-5.69	96.91	102.60
54	BA	705	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1890	A	O4'-C1'-N9	5.69	112.75	108.20
21	AA	1102	A	C5-C6-N1	5.69	120.54	117.70
21	AA	1251	A	C6-C5-N7	5.69	136.28	132.30
21	AA	1310	G	N1-C6-O6	-5.69	116.49	119.90
54	BA	873	C	N1-C2-O2	5.69	122.31	118.90
54	BA	1475	G	N1-C6-O6	-5.69	116.49	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1269	A	C5-C6-N1	5.69	120.54	117.70
54	BA	1902	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	2297	A	C5-C6-N1	5.69	120.54	117.70
21	AA	364	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	706	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	670	A	P-O3'-C3'	5.68	126.52	119.70
54	BA	974	G	N3-C2-N2	-5.68	115.92	119.90
54	BA	1365	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	1330	U	N1-C2-N3	5.68	118.31	114.90
54	BA	1576	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1701	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1765	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1808	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	2480	C	O4'-C1'-N1	5.68	112.75	108.20
6	AG	94	ARG	NE-CZ-NH1	5.68	123.14	120.30
16	AQ	64	ARG	NE-CZ-NH1	5.68	123.14	120.30
18	AS	31	ARG	NE-CZ-NH1	5.68	123.14	120.30
21	AA	163	C	N1-C2-O2	5.68	122.31	118.90
54	BA	429	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	1477	U	O4'-C1'-N1	5.68	112.74	108.20
21	AA	489	C	O4'-C1'-N1	5.68	112.74	108.20
21	AA	984	C	N1-C2-O2	5.68	122.31	118.90
54	BA	242	G	O4'-C1'-N9	5.68	112.74	108.20
54	BA	2330	G	N9-C4-C5	5.68	107.67	105.40
21	AA	422	C	N3-C4-C5	5.67	124.17	121.90
21	AA	839	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	1190	G	P-O3'-C3'	5.67	126.51	119.70
54	BA	2374	C	N1-C2-O2	5.67	122.31	118.90
54	BA	2507	C	N3-C4-C5	5.67	124.17	121.90
21	AA	248	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	615	U	C1'-O4'-C4'	-5.67	105.36	109.90
54	BA	1771	C	N3-C2-O2	-5.67	117.93	121.90
17	AR	72	ARG	NE-CZ-NH1	5.67	123.14	120.30
24	A3	44	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	1115	G	N1-C6-O6	-5.67	116.50	119.90
54	BA	1795	C	N1-C2-O2	5.67	122.30	118.90
54	BA	1843	C	N1-C2-O2	5.67	122.30	118.90
54	BA	2071	A	C4-C5-C6	-5.67	114.17	117.00
16	AQ	76	ARG	NE-CZ-NH1	5.67	123.14	120.30
21	AA	1200	C	N3-C4-C5	5.67	124.17	121.90
45	BW	54	ARG	NE-CZ-NH2	5.67	123.14	120.30
54	BA	208	C	N3-C2-O2	-5.67	117.93	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	870	U	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2447	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	870	U	N3-C2-O2	-5.67	118.23	122.20
21	AA	912	C	N1-C2-O2	5.67	122.30	118.90
54	BA	338	G	N3-C4-C5	-5.67	125.77	128.60
54	BA	574	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	890	C	N1-C2-O2	5.67	122.30	118.90
54	BA	2510	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	746	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	320	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	1789	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2353	G	O4'-C1'-N9	5.66	112.73	108.20
21	AA	345	C	N1-C2-O2	5.66	122.30	118.90
21	AA	1028	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1126	U	C3'-C2'-C1'	5.66	106.03	101.50
21	AA	1404	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	638	G	N3-C4-C5	-5.66	125.77	128.60
21	AA	1027	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1223	C	N1-C2-O2	5.66	122.29	118.90
54	BA	191	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	267	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	2289	G	C5-C6-N1	5.66	114.33	111.50
18	AS	80	ARG	NE-CZ-NH1	5.66	123.13	120.30
21	AA	533	A	N1-C6-N6	-5.66	115.21	118.60
21	AA	1322	C	N1-C2-O2	5.66	122.29	118.90
54	BA	884	U	O4'-C1'-N1	5.66	112.72	108.20
54	BA	1262	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2321	U	N3-C2-O2	-5.66	118.24	122.20
54	BA	2793	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	1410	A	C4-C5-C6	-5.65	114.17	117.00
22	A1	27	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	305	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	291	U	O4'-C1'-N1	5.65	112.72	108.20
54	BA	671	C	N1-C2-O2	5.65	122.29	118.90
54	BA	2286	G	C5-C6-N1	5.65	114.33	111.50
55	BB	49	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	532	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	938	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	518	G	N1-C6-O6	-5.65	116.51	119.90
54	BA	664	G	N1-C6-O6	-5.65	116.51	119.90
21	AA	253	A	C5-C6-N1	5.65	120.52	117.70
54	BA	157	C	O4'-C1'-N1	5.65	112.72	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1913	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	2128	G	O4'-C1'-N9	5.65	112.72	108.20
54	BA	2428	G	N1-C6-O6	-5.65	116.51	119.90
21	AA	559	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	721	G	N3-C4-C5	-5.64	125.78	128.60
22	A1	31	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	116	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	529	A	N1-C6-N6	-5.64	115.21	118.60
54	BA	1089	A	O4'-C1'-N9	5.64	112.72	108.20
54	BA	1109	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1140	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	2097	A	C5-C6-N1	5.64	120.52	117.70
21	AA	233	C	N1-C2-O2	5.64	122.29	118.90
21	AA	536	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	648	A	C1'-O4'-C4'	-5.64	105.39	109.90
31	BI	126	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	814	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	915	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1157	G	N1-C6-O6	-5.64	116.51	119.90
54	BA	2388	A	C4-C5-C6	-5.64	114.18	117.00
2	AC	87	ARG	NE-CZ-NH1	5.64	123.12	120.30
21	AA	567	G	C5-C6-N1	5.64	114.32	111.50
54	BA	28	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	163	C	N1-C2-O2	5.64	122.28	118.90
54	BA	1737	G	N1-C6-O6	-5.64	116.52	119.90
54	BA	1891	G	O4'-C1'-N9	5.64	112.71	108.20
54	BA	2310	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	1367	C	N3-C2-O2	-5.64	117.95	121.90
34	BL	33	ARG	NE-CZ-NH1	5.64	123.12	120.30
21	AA	582	C	N3-C4-C5	5.64	124.16	121.90
21	AA	1362	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	417	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	870	U	C5-C6-N1	-5.64	119.88	122.70
54	BA	2335	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	422	A	C6-C5-N7	5.63	136.24	132.30
55	BB	55	U	O4'-C1'-N1	5.63	112.71	108.20
11	AL	8	ARG	NE-CZ-NH2	-5.63	117.48	120.30
21	AA	227	G	N1-C6-O6	-5.63	116.52	119.90
21	AA	1152	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	272	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	584	C	O4'-C1'-N1	5.63	112.71	108.20
54	BA	2205	A	C4-C5-C6	-5.63	114.18	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	514	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	1497	G	N1-C6-O6	-5.63	116.52	119.90
54	BA	389	G	N3-C2-N2	-5.63	115.96	119.90
54	BA	1427	A	P-O3'-C3'	5.63	126.46	119.70
54	BA	1211	C	N1-C2-O2	5.63	122.28	118.90
54	BA	1892	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	2037	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	36	C	N3-C4-N4	-5.63	114.06	118.00
54	BA	1015	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	1991	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	2171	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	2202	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	2322	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	719	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	1699	G	N3-C2-N2	-5.63	115.96	119.90
54	BA	2044	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	277	C	N3-C2-O2	-5.62	117.96	121.90
21	AA	779	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	1151	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1226	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	511	C	O4'-C1'-N1	5.62	112.70	108.20
21	AA	576	C	O4'-C1'-N1	5.62	112.70	108.20
21	AA	728	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1288	A	C6-C5-N7	5.62	136.24	132.30
54	BA	417	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	735	A	N1-C6-N6	-5.62	115.23	118.60
54	BA	737	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	783	A	C5-C6-N1	5.62	120.51	117.70
54	BA	980	A	P-O3'-C3'	5.62	126.45	119.70
54	BA	1194	A	C5-C6-N1	5.62	120.51	117.70
54	BA	2291	U	O4'-C1'-N1	5.62	112.70	108.20
54	BA	2777	G	N1-C6-O6	-5.62	116.53	119.90
21	AA	47	C	N1-C2-O2	5.62	122.27	118.90
54	BA	129	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1366	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1823	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	1774	C	O4'-C1'-N1	5.62	112.70	108.20
1	AB	20	ARG	NE-CZ-NH2	-5.62	117.49	120.30
54	BA	860	U	O4'-C1'-N1	5.62	112.69	108.20
54	BA	1118	C	N1-C2-O2	5.62	122.27	118.90
54	BA	1505	A	C5'-C4'-O4'	5.62	115.84	109.10
21	AA	1223	C	N3-C4-N4	-5.62	114.07	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1412	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	315	G	O4'-C1'-N9	5.62	112.69	108.20
24	A3	40	C	N1-C2-O2	5.62	122.27	118.90
54	BA	354	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	758	C	O4'-C1'-N1	5.62	112.69	108.20
54	BA	910	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1014	A	C5-C6-N1	5.62	120.51	117.70
54	BA	1204	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2087	G	C5-C6-N1	5.62	114.31	111.50
54	BA	2151	U	O4'-C1'-N1	5.62	112.69	108.20
21	AA	513	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	884	U	C1'-O4'-C4'	-5.61	105.41	109.90
54	BA	2475	C	N3-C2-O2	-5.61	117.97	121.90
21	AA	206	C	N1-C2-O2	5.61	122.27	118.90
54	BA	629	G	P-O3'-C3'	5.61	126.43	119.70
54	BA	959	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	2592	G	O4'-C1'-N9	5.61	112.69	108.20
54	BA	1376	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	1847	A	O4'-C1'-N9	5.61	112.69	108.20
54	BA	1934	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2886	A	C4-C5-C6	-5.61	114.19	117.00
21	AA	848	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	105	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1617	C	N1-C2-N3	5.61	123.13	119.20
54	BA	1865	U	C5-C6-N1	-5.61	119.90	122.70
54	BA	2466	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	2731	G	N1-C6-O6	-5.61	116.53	119.90
55	BB	58	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	344	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	554	A	C6-C5-N7	5.61	136.22	132.30
54	BA	282	A	C5-C6-N1	5.61	120.50	117.70
54	BA	815	C	P-O3'-C3'	5.61	126.43	119.70
54	BA	1875	G	N1-C6-O6	-5.61	116.54	119.90
54	BA	1981	A	N1-C6-N6	-5.61	115.24	118.60
54	BA	2386	A	C6-C5-N7	5.61	136.22	132.30
54	BA	2686	G	N1-C6-O6	-5.60	116.54	119.90
54	BA	556	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1016	G	O4'-C1'-N9	5.60	112.68	108.20
54	BA	1023	U	C3'-C2'-C1'	5.60	105.98	101.50
54	BA	1437	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1872	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	2676	C	N3-C2-O2	-5.60	117.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2842	G	O4'-C1'-N9	5.60	112.68	108.20
54	BA	2510	C	O4'-C1'-N1	5.60	112.68	108.20
54	BA	2620	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	2655	G	C3'-C2'-C1'	-5.60	97.02	101.50
55	BB	51	G	N1-C6-O6	-5.60	116.54	119.90
20	AU	34	ARG	NE-CZ-NH1	5.60	123.10	120.30
21	AA	1466	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	610	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1102	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1704	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	2280	G	N1-C6-O6	-5.60	116.54	119.90
21	AA	533	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	816	A	C4-C5-C6	-5.59	114.20	117.00
26	BD	179	ARG	NE-CZ-NH1	5.59	123.10	120.30
54	BA	1822	C	N3-C2-O2	-5.59	117.98	121.90
54	BA	2749	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	912	C	N3-C4-N4	-5.59	114.08	118.00
22	A1	65	C	N3-C2-O2	-5.59	117.99	121.90
24	A3	47	G	C3'-C2'-C1'	5.59	105.97	101.50
54	BA	996	A	C5-C6-N1	5.59	120.50	117.70
55	BB	110	C	O4'-C1'-N1	5.59	112.67	108.20
21	AA	819	A	C4-C5-C6	-5.59	114.20	117.00
24	A3	77	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	18	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	633	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	1825	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	2175	C	N1-C2-O2	5.59	122.25	118.90
11	AL	85	ARG	NE-CZ-NH1	5.59	123.09	120.30
21	AA	194	C	N1-C2-O2	5.59	122.25	118.90
54	BA	300	A	C5-C6-N1	5.59	120.49	117.70
54	BA	2373	G	N3-C2-N2	-5.59	115.99	119.90
54	BA	918	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	2396	G	O4'-C1'-N9	5.59	112.67	108.20
54	BA	2578	G	C5-C6-N1	5.59	114.29	111.50
54	BA	2821	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	1258	G	N3-C4-C5	-5.58	125.81	128.60
54	BA	429	A	C5-C6-N1	5.58	120.49	117.70
54	BA	1244	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2283	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	193	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	86	G	C1'-O4'-C4'	-5.58	105.43	109.90
54	BA	336	C	N3-C2-O2	-5.58	117.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	472	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2516	A	C6-C5-N7	5.58	136.21	132.30
21	AA	187	G	N3-C2-N2	-5.58	115.99	119.90
21	AA	441	A	C6-C5-N7	5.58	136.21	132.30
21	AA	1328	C	N1-C2-O2	5.58	122.25	118.90
55	BB	53	A	N1-C6-N6	-5.58	115.25	118.60
21	AA	417	G	C5-C6-N1	5.58	114.29	111.50
54	BA	1786	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2637	U	O4'-C1'-N1	5.58	112.66	108.20
21	AA	470	C	N1-C2-O2	5.58	122.25	118.90
54	BA	718	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1020	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1691	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	2144	G	N1-C6-O6	-5.58	116.56	119.90
12	AM	108	ARG	NE-CZ-NH2	-5.57	117.51	120.30
54	BA	343	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1019	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	2149	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	2621	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	2715	C	N1-C2-O2	5.57	122.24	118.90
54	BA	2758	A	C4-C5-C6	-5.57	114.21	117.00
54	BA	531	C	N1-C2-O2	5.57	122.24	118.90
54	BA	1075	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	456	C	N3-C4-C5	5.57	124.13	121.90
21	AA	781	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	265	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	340	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	1221	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	1802	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	254	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	479	A	C6-C5-N7	5.57	136.20	132.30
54	BA	1135	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1924	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	922	C	N3-C2-O2	-5.56	118.00	121.90
54	BA	2505	G	C5-C6-N1	5.56	114.28	111.50
21	AA	243	A	P-O3'-C3'	5.56	126.38	119.70
22	A1	23	A	C4-C5-C6	-5.56	114.22	117.00
37	BO	30	ARG	NE-CZ-NH1	5.56	123.08	120.30
54	BA	739	A	N1-C6-N6	-5.56	115.26	118.60
54	BA	2170	A	C4-C5-C6	-5.56	114.22	117.00
5	AF	86	ARG	NE-CZ-NH2	-5.56	117.52	120.30
21	AA	154	U	O4'-C1'-N1	5.56	112.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	BN	118	ARG	NE-CZ-NH2	-5.56	117.52	120.30
54	BA	79	C	C3'-C2'-C1'	5.56	105.95	101.50
2	AC	71	ARG	NE-CZ-NH1	5.56	123.08	120.30
21	AA	569	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	1129	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1147	A	C6-C5-N7	5.56	136.19	132.30
21	AA	53	A	C6-C5-N7	5.56	136.19	132.30
21	AA	223	A	C6-C5-N7	5.56	136.19	132.30
21	AA	934	C	N3-C4-N4	-5.56	114.11	118.00
21	AA	1243	C	N3-C2-O2	-5.56	118.01	121.90
21	AA	1401	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	238	C	N1-C2-O2	5.56	122.23	118.90
54	BA	341	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	668	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1646	C	N1-C2-O2	5.56	122.23	118.90
54	BA	578	G	N1-C6-O6	-5.56	116.57	119.90
54	BA	686	U	O4'-C1'-N1	5.56	112.64	108.20
54	BA	1525	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	344	A	O4'-C1'-N9	5.55	112.64	108.20
21	AA	829	G	O4'-C1'-N9	5.55	112.64	108.20
22	A1	9	A	C4-C5-C6	-5.55	114.22	117.00
22	A1	33	U	N3-C2-O2	-5.55	118.31	122.20
54	BA	1128	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	1728	C	N1-C2-O2	5.55	122.23	118.90
54	BA	1729	U	N3-C2-O2	-5.55	118.31	122.20
54	BA	2174	C	N3-C2-O2	-5.55	118.01	121.90
21	AA	1203	C	P-O3'-C3'	5.55	126.36	119.70
46	BX	27	ARG	NE-CZ-NH1	5.55	123.08	120.30
54	BA	131	A	N1-C6-N6	-5.55	115.27	118.60
54	BA	441	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	840	C	N1-C2-O2	5.55	122.23	118.90
54	BA	1625	C	N1-C2-O2	5.55	122.23	118.90
54	BA	1747	U	O4'-C1'-N1	5.55	112.64	108.20
21	AA	195	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1784	A	C6-C5-N7	5.55	136.19	132.30
54	BA	2575	C	N3-C4-C5	5.55	124.12	121.90
21	AA	246	A	C5-C6-N1	5.55	120.47	117.70
21	AA	597	G	N3-C4-C5	-5.55	125.83	128.60
21	AA	889	A	C6-C5-N7	5.55	136.18	132.30
21	AA	1448	C	N3-C2-O2	-5.55	118.02	121.90
21	AA	873	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	341	C	O4'-C1'-N1	5.54	112.64	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1110	G	O4'-C1'-N9	5.54	112.64	108.20
54	BA	2091	C	O4'-C1'-N1	5.54	112.64	108.20
21	AA	1061	G	N3-C2-N2	-5.54	116.02	119.90
22	A1	36	C	N1-C2-O2	5.54	122.23	118.90
54	BA	89	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1298	C	N1-C2-O2	5.54	122.23	118.90
54	BA	1322	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2743	U	O4'-C1'-N1	5.54	112.64	108.20
17	AR	52	ARG	NE-CZ-NH1	5.54	123.07	120.30
21	AA	719	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	1151	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2456	C	O4'-C1'-N1	5.54	112.63	108.20
21	AA	990	C	N1-C2-O2	5.54	122.22	118.90
54	BA	76	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2425	A	P-O3'-C3'	5.54	126.35	119.70
21	AA	186	C	N1-C2-O2	5.54	122.22	118.90
21	AA	1059	C	N1-C2-O2	5.54	122.22	118.90
21	AA	1179	A	C5-C6-N1	5.54	120.47	117.70
54	BA	899	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2755	C	C3'-C2'-C1'	5.54	105.93	101.50
22	A1	18	G	N1-C6-O6	-5.54	116.58	119.90
54	BA	863	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2206	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	2860	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	152	A	C6-C5-N7	5.54	136.18	132.30
54	BA	806	C	N3-C2-O2	-5.54	118.03	121.90
54	BA	1868	C	O4'-C1'-N1	5.54	112.63	108.20
21	AA	1437	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	1468	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	876	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2633	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	37	C	C5'-C4'-O4'	5.53	115.74	109.10
54	BA	1528	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	1853	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	730	G	N1-C6-O6	-5.53	116.58	119.90
21	AA	1296	C	N1-C2-O2	5.53	122.22	118.90
21	AA	1359	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	477	A	C4-C5-C6	-5.53	114.24	117.00
21	AA	81	A	C1'-O4'-C4'	-5.53	105.48	109.90
21	AA	465	A	O4'-C1'-N9	5.53	112.62	108.20
21	AA	1128	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	37	C	O4'-C1'-N1	5.53	112.62	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	692	C	N1-C2-O2	5.53	122.22	118.90
54	BA	1962	C	N3-C4-C5	5.53	124.11	121.90
54	BA	2015	A	C6-C5-N7	5.53	136.17	132.30
54	BA	2073	C	C4'-C3'-C2'	-5.53	97.07	102.60
54	BA	2342	C	N1-C2-O2	5.53	122.22	118.90
27	BE	79	ARG	NE-CZ-NH1	5.52	123.06	120.30
54	BA	37	C	N1-C2-O2	5.52	122.22	118.90
54	BA	1567	G	N3-C2-N2	-5.52	116.03	119.90
54	BA	1981	A	C6-N1-C2	-5.52	115.29	118.60
21	AA	423	G	N3-C4-C5	-5.52	125.84	128.60
38	BP	92	ARG	NE-CZ-NH1	5.52	123.06	120.30
54	BA	698	C	N1-C2-O2	5.52	122.21	118.90
54	BA	1403	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	876	C	C3'-C2'-C1'	-5.52	97.08	101.50
21	AA	1011	C	N1-C2-O2	5.52	122.21	118.90
54	BA	310	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2471	A	C5-C6-N1	5.52	120.46	117.70
54	BA	2853	C	O4'-C1'-N1	5.52	112.62	108.20
21	AA	579	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	673	A	C6-C5-N7	5.52	136.16	132.30
54	BA	690	G	N1-C6-O6	-5.52	116.59	119.90
21	AA	919	A	O4'-C1'-N9	5.52	112.61	108.20
21	AA	1169	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1710	G	O4'-C1'-N9	5.52	112.61	108.20
54	BA	1791	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1958	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	2349	G	O4'-C1'-N9	5.52	112.61	108.20
54	BA	2654	A	C4-C5-C6	-5.52	114.24	117.00
55	BB	80	U	O4'-C1'-N1	5.52	112.61	108.20
21	AA	1267	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	412	A	O4'-C1'-N9	5.51	112.61	108.20
54	BA	1439	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	1858	A	O4'-C1'-N9	5.51	112.61	108.20
21	AA	87	C	N1-C2-O2	5.51	122.21	118.90
21	AA	248	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	430	A	C4-C5-C6	-5.51	114.24	117.00
21	AA	790	A	C5-C6-N1	5.51	120.46	117.70
21	AA	1266	G	N1-C6-O6	-5.51	116.59	119.90
21	AA	1402	C	N1-C2-O2	5.51	122.21	118.90
54	BA	689	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	1828	G	O4'-C1'-N9	5.51	112.61	108.20
21	AA	300	A	C4-C5-C6	-5.51	114.25	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	429	U	C5-C6-N1	-5.51	119.94	122.70
21	AA	660	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	615	U	N3-C2-O2	-5.51	118.34	122.20
54	BA	1463	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	2200	C	N3-C2-O2	-5.51	118.04	121.90
27	BE	69	ARG	NH1-CZ-NH2	-5.51	113.34	119.40
54	BA	14	A	N1-C6-N6	-5.51	115.30	118.60
54	BA	2427	C	N3-C2-O2	-5.51	118.04	121.90
21	AA	383	A	C4-C5-C6	-5.51	114.25	117.00
21	AA	1357	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	351	C	N1-C2-O2	5.51	122.20	118.90
54	BA	1977	A	C6-C5-N7	5.51	136.16	132.30
55	BB	99	A	C6-C5-N7	5.51	136.16	132.30
54	BA	929	U	C5-C6-N1	-5.50	119.95	122.70
54	BA	1668	A	C6-C5-N7	5.50	136.15	132.30
54	BA	1824	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	435	A	C5-C6-N1	5.50	120.45	117.70
54	BA	611	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	823	C	N1-C2-O2	5.50	122.20	118.90
54	BA	991	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1240	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1594	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1745	A	N1-C6-N6	-5.50	115.30	118.60
54	BA	2575	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	452	A	C6-C5-N7	5.50	136.15	132.30
54	BA	714	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	2506	U	N3-C2-O2	-5.50	118.35	122.20
54	BA	2740	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	51	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	352	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	972	C	N3-C2-O2	-5.50	118.05	121.90
22	A1	50	G	N1-C6-O6	-5.50	116.60	119.90
5	AF	44	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	AA	580	C	O4'-C1'-N1	5.50	112.60	108.20
27	BE	44	ARG	NE-CZ-NH1	5.50	123.05	120.30
54	BA	378	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1577	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1976	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	2463	C	N1-C2-O2	5.50	122.20	118.90
54	BA	2809	A	C4'-C3'-C2'	-5.50	97.10	102.60
21	AA	374	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	427	U	N3-C2-O2	-5.50	118.35	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1344	C	N1-C2-O2	5.50	122.20	118.90
54	BA	366	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1453	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1928	A	C4-C5-C6	-5.50	114.25	117.00
21	AA	336	A	C6-C5-N7	5.50	136.15	132.30
54	BA	980	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	11	C	O4'-C1'-N1	5.49	112.59	108.20
54	BA	1829	A	C4-C5-C6	-5.49	114.25	117.00
21	AA	398	U	O4'-C1'-N1	5.49	112.59	108.20
55	BB	93	C	N3-C2-O2	-5.49	118.06	121.90
21	AA	1506	U	O4'-C1'-N1	5.49	112.59	108.20
24	A3	10	G	N1-C6-O6	-5.49	116.61	119.90
54	BA	728	G	C5-C6-N1	5.49	114.25	111.50
54	BA	2469	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	2840	C	N1-C2-O2	5.49	122.19	118.90
54	BA	522	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	2006	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	1641	A	C5-C6-N1	5.48	120.44	117.70
21	AA	490	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	996	A	C6-C5-N7	5.48	136.14	132.30
54	BA	1259	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	1615	C	N1-C2-O2	5.48	122.19	118.90
54	BA	2560	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	510	A	O4'-C1'-N9	5.48	112.58	108.20
21	AA	716	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	726	C	N1-C2-O2	5.48	122.19	118.90
21	AA	1251	A	O4'-C1'-N9	5.48	112.58	108.20
54	BA	421	C	N1-C2-O2	5.48	122.19	118.90
54	BA	1269	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1286	A	O4'-C1'-N9	5.48	112.58	108.20
54	BA	1323	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	732	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	1139	G	N1-C6-O6	-5.48	116.61	119.90
52	B3	29	ARG	NE-CZ-NH1	5.48	123.04	120.30
54	BA	1578	U	N1-C2-N3	5.48	118.19	114.90
54	BA	2551	C	N1-C2-O2	5.48	122.19	118.90
54	BA	2653	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	2785	C	O4'-C1'-N1	5.48	112.58	108.20
54	BA	990	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	303	A	C6-C5-N7	5.47	136.13	132.30
21	AA	856	C	N1-C2-O2	5.47	122.18	118.90
54	BA	179	C	N1-C2-O2	5.47	122.18	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	292	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	1830	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	1368	A	C3'-C2'-C1'	5.47	105.88	101.50
54	BA	1295	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	461	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	878	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	1646	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	2662	A	C5-C6-N1	5.47	120.44	117.70
54	BA	2719	G	C5-C6-N1	5.47	114.23	111.50
54	BA	2770	G	C3'-C2'-C1'	5.47	105.88	101.50
8	AI	123	ARG	NE-CZ-NH1	5.47	123.03	120.30
21	AA	251	G	N3-C4-C5	-5.47	125.87	128.60
54	BA	457	A	O4'-C1'-N9	5.47	112.57	108.20
54	BA	1964	G	N3-C4-C5	-5.47	125.87	128.60
21	AA	94	G	N3-C2-N2	-5.47	116.07	119.90
54	BA	464	U	C3'-C2'-C1'	5.47	105.87	101.50
54	BA	723	C	N1-C2-O2	5.47	122.18	118.90
54	BA	727	A	C5-C6-N1	5.47	120.43	117.70
54	BA	766	U	O4'-C1'-N1	5.47	112.57	108.20
54	BA	2734	A	C4-C5-C6	-5.47	114.27	117.00
21	AA	65	A	C1'-O4'-C4'	-5.46	105.53	109.90
21	AA	500	G	O4'-C1'-N9	5.46	112.57	108.20
21	AA	1049	U	N3-C2-O2	-5.46	118.38	122.20
21	AA	1505	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	219	A	C6-C5-N7	5.46	136.13	132.30
21	AA	169	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	1484	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	8	C	N1-C2-O2	5.46	122.18	118.90
54	BA	357	C	N1-C2-O2	5.46	122.18	118.90
54	BA	894	U	N3-C2-O2	-5.46	118.38	122.20
54	BA	2080	A	C4-C5-C6	-5.46	114.27	117.00
11	AL	13	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	1396	U	N3-C2-O2	-5.46	118.38	122.20
54	BA	2191	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2512	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	34	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	136	C	N1-C2-O2	5.46	122.17	118.90
21	AA	1493	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	264	C	N1-C2-O2	5.46	122.18	118.90
55	BB	28	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	795	C	N1-C2-O2	5.46	122.17	118.90
49	B0	12	ARG	NE-CZ-NH2	5.46	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	384	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	720	U	O4'-C1'-N1	5.46	112.56	108.20
54	BA	937	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	2119	A	N1-C6-N6	-5.46	115.33	118.60
54	BA	2539	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	467	U	N3-C2-O2	-5.45	118.38	122.20
21	AA	1046	A	C4-C5-C6	-5.45	114.27	117.00
21	AA	1300	G	N3-C2-N2	-5.45	116.08	119.90
54	BA	1633	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	2275	C	O4'-C1'-N1	5.45	112.56	108.20
54	BA	1973	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	2055	C	N1-C2-O2	5.45	122.17	118.90
21	AA	569	C	N3-C4-C5	5.45	124.08	121.90
54	BA	221	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	2303	G	N1-C6-O6	-5.45	116.63	119.90
21	AA	892	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	1078	U	O4'-C1'-N1	5.45	112.56	108.20
21	AA	1347	G	O4'-C1'-N9	5.45	112.56	108.20
21	AA	1469	C	N1-C2-O2	5.45	122.17	118.90
54	BA	765	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	1340	U	P-O3'-C3'	5.45	126.24	119.70
54	BA	2046	G	O4'-C1'-N9	5.45	112.56	108.20
54	BA	2566	A	C4-C5-C6	-5.45	114.28	117.00
24	A3	70	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	631	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2226	C	N3-C2-O2	-5.45	118.09	121.90
21	AA	810	C	N1-C2-O2	5.45	122.17	118.90
21	AA	962	C	N3-C2-O2	-5.45	118.09	121.90
21	AA	1319	A	C6-C5-N7	5.45	136.11	132.30
30	BH	27	ARG	NE-CZ-NH1	5.45	123.02	120.30
54	BA	660	C	C5'-C4'-O4'	5.45	115.63	109.10
54	BA	2576	G	C3'-C2'-C1'	5.45	105.86	101.50
21	AA	478	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	782	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	648	G	C5-C6-N1	5.44	114.22	111.50
54	BA	1799	G	C8-N9-C4	-5.44	104.22	106.40
21	AA	1230	C	C3'-C2'-C1'	5.44	105.85	101.50
54	BA	610	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	800	A	C6-C5-N7	5.44	136.11	132.30
54	BA	857	G	C8-N9-C4	-5.44	104.22	106.40
54	BA	1554	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	1754	A	O4'-C1'-N9	5.44	112.56	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	199	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	1391	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	654	A	C6-C5-N7	5.44	136.11	132.30
54	BA	2070	A	O4'-C1'-N9	5.44	112.55	108.20
54	BA	2619	C	N3-C2-O2	-5.44	118.09	121.90
4	AE	67	ARG	NE-CZ-NH1	5.44	123.02	120.30
54	BA	1681	G	O4'-C1'-N9	5.44	112.55	108.20
21	AA	262	A	C6-C5-N7	5.44	136.11	132.30
21	AA	699	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	192	C	N1-C2-O2	5.44	122.16	118.90
54	BA	240	C	N1-C2-O2	5.44	122.16	118.90
54	BA	570	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	1059	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	1403	A	C4'-C3'-C2'	-5.44	97.16	102.60
54	BA	2274	A	C6-C5-N7	5.44	136.11	132.30
54	BA	2506	U	O4'-C1'-N1	5.44	112.55	108.20
54	BA	6	A	O4'-C1'-N9	5.44	112.55	108.20
54	BA	443	A	C4-C5-C6	-5.44	114.28	117.00
21	AA	108	G	N3-C4-C5	-5.43	125.88	128.60
21	AA	475	C	N3-C2-O2	-5.43	118.09	121.90
21	AA	1120	C	N1-C2-O2	5.43	122.16	118.90
54	BA	1125	G	C8-N9-C4	-5.43	104.23	106.40
54	BA	342	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	1265	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	1507	C	N1-C2-O2	5.43	122.16	118.90
54	BA	2087	G	N1-C6-O6	-5.43	116.64	119.90
1	AB	73	ARG	NE-CZ-NH2	-5.43	117.58	120.30
21	AA	139	A	C4-C5-C6	-5.43	114.28	117.00
21	AA	995	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	1160	G	N3-C2-N2	-5.43	116.10	119.90
22	A1	44	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1332	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1788	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	1932	A	C5-C6-N1	5.43	120.42	117.70
54	BA	2417	C	N1-C2-O2	5.43	122.16	118.90
54	BA	2532	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	2885	G	O4'-C1'-N9	5.43	112.54	108.20
54	BA	112	U	C5-C6-N1	-5.43	119.99	122.70
54	BA	542	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	986	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	992	C	O4'-C1'-N1	5.43	112.54	108.20
10	AK	68	ARG	NE-CZ-NH1	5.43	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	196	A	C6-C5-N7	5.43	136.10	132.30
21	AA	727	G	N1-C6-O6	-5.43	116.64	119.90
21	AA	739	C	N1-C2-O2	5.43	122.16	118.90
21	AA	766	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	993	G	N1-C6-O6	-5.43	116.64	119.90
47	BY	23	ARG	NE-CZ-NH1	5.43	123.01	120.30
54	BA	430	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	1022	G	O4'-C1'-N9	5.43	112.54	108.20
54	BA	1050	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	372	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	1117	C	N1-C2-O2	5.42	122.16	118.90
21	AA	436	C	C1'-O4'-C4'	-5.42	105.56	109.90
21	AA	970	C	N1-C2-O2	5.42	122.15	118.90
54	BA	2643	G	O4'-C1'-N9	5.42	112.54	108.20
54	BA	1045	C	N1-C2-O2	5.42	122.15	118.90
54	BA	1907	G	N1-C6-O6	-5.42	116.65	119.90
21	AA	142	G	N1-C6-O6	-5.42	116.65	119.90
21	AA	228	A	C6-C5-N7	5.42	136.09	132.30
21	AA	1390	U	O4'-C1'-N1	5.42	112.54	108.20
54	BA	1261	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	2577	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	462	C	N3-C2-O2	-5.42	118.11	121.90
54	BA	1434	A	C4-C5-C6	-5.42	114.29	117.00
7	AH	116	ARG	NE-CZ-NH1	5.42	123.01	120.30
21	AA	1086	U	C1'-O4'-C4'	-5.42	105.57	109.90
54	BA	238	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	688	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1466	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2169	A	C4-C5-C6	-5.41	114.29	117.00
21	AA	908	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	145	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	833	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	1313	U	C2-N1-C1'	5.41	124.19	117.70
21	AA	969	A	C6-C5-N7	5.41	136.09	132.30
54	BA	621	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1108	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1558	C	N3-C2-O2	-5.41	118.11	121.90
56	B5	12	ARG	NE-CZ-NH1	5.41	123.01	120.30
8	AI	40	ARG	NE-CZ-NH1	5.41	123.00	120.30
13	AN	61	ARG	NE-CZ-NH1	5.41	123.00	120.30
21	AA	1129	C	N1-C2-O2	5.41	122.14	118.90
21	AA	1377	A	C6-C5-N7	5.41	136.09	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1760	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2339	C	N1-C2-O2	5.41	122.15	118.90
54	BA	1176	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1188	U	N3-C2-O2	-5.41	118.42	122.20
21	AA	353	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	396	C	N3-C4-C5	5.40	124.06	121.90
23	A2	83	U	O4'-C1'-N1	5.40	112.52	108.20
45	BW	38	ARG	NE-CZ-NH2	-5.40	117.60	120.30
54	BA	180	G	C5-C6-N1	5.40	114.20	111.50
54	BA	294	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	673	C	N3-C4-C5	5.40	124.06	121.90
21	AA	615	G	O4'-C1'-N9	5.40	112.52	108.20
24	A3	49	C	N3-C4-C5	5.40	124.06	121.90
54	BA	69	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	141	G	N3-C4-C5	-5.40	125.90	128.60
54	BA	721	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	968	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	1647	U	O4'-C1'-N1	5.40	112.52	108.20
21	AA	885	G	N9-C4-C5	5.40	107.56	105.40
51	B2	28	ARG	NE-CZ-NH1	5.40	123.00	120.30
21	AA	1041	G	N1-C6-O6	-5.40	116.66	119.90
21	AA	1246	A	C6-C5-N7	5.40	136.08	132.30
54	BA	244	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	1477	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	426	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	858	G	O4'-C1'-N9	5.40	112.52	108.20
54	BA	970	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2606	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	1058	G	N3-C2-N2	-5.39	116.12	119.90
33	BK	17	ARG	NE-CZ-NH2	-5.39	117.60	120.30
54	BA	179	C	C4'-C3'-C2'	-5.39	97.21	102.60
54	BA	1270	C	N3-C2-O2	-5.39	118.12	121.90
54	BA	2535	G	N1-C6-O6	-5.39	116.66	119.90
21	AA	930	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	531	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1010	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	2873	A	O4'-C1'-N9	5.39	112.52	108.20
21	AA	716	A	O4'-C1'-N9	5.39	112.51	108.20
21	AA	783	C	N3-C2-O2	-5.39	118.13	121.90
39	BQ	54	ARG	NE-CZ-NH1	5.39	123.00	120.30
54	BA	1832	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	2792	A	C6-C5-N7	5.39	136.07	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2425	A	C6-C5-N7	5.39	136.07	132.30
54	BA	2470	G	O4'-C1'-N9	5.39	112.51	108.20
54	BA	269	C	N1-C2-O2	5.39	122.13	118.90
54	BA	372	G	C3'-C2'-C1'	-5.39	97.19	101.50
54	BA	49	A	C4-C5-C6	-5.39	114.31	117.00
54	BA	106	C	C5'-C4'-O4'	5.39	115.56	109.10
54	BA	229	C	N1-C2-O2	5.39	122.13	118.90
54	BA	285	G	C3'-C2'-C1'	-5.39	97.19	101.50
3	AD	192	ALA	C-N-CA	5.38	135.16	121.70
54	BA	743	A	O4'-C1'-N9	5.38	112.51	108.20
54	BA	1474	U	C5-C6-N1	-5.38	120.01	122.70
54	BA	2845	U	O4'-C1'-N1	5.38	112.51	108.20
54	BA	340	A	N1-C6-N6	-5.38	115.37	118.60
54	BA	1427	A	C5-C6-N1	5.38	120.39	117.70
21	AA	1147	C	O4'-C1'-N1	5.38	112.50	108.20
26	BD	83	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BA	43	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	419	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	694	U	N3-C2-O2	-5.38	118.43	122.20
54	BA	935	C	N3-C2-O2	-5.38	118.13	121.90
54	BA	1452	G	O4'-C1'-N9	5.38	112.50	108.20
54	BA	1634	A	P-O3'-C3'	5.38	126.16	119.70
54	BA	1699	G	N3-C4-C5	-5.38	125.91	128.60
54	BA	2346	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	271	C	N1-C2-O2	5.38	122.13	118.90
21	AA	526	C	N1-C2-O2	5.38	122.13	118.90
21	AA	829	G	N1-C6-O6	-5.38	116.67	119.90
21	AA	1302	C	N3-C2-O2	-5.38	118.14	121.90
54	BA	1086	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	125	U	O4'-C1'-N1	5.38	112.50	108.20
21	AA	333	U	O4'-C1'-N1	5.38	112.50	108.20
21	AA	767	A	C6-C5-N7	5.38	136.06	132.30
21	AA	1214	C	C1'-O4'-C4'	-5.38	105.60	109.90
54	BA	641	U	N3-C2-O2	-5.38	118.44	122.20
54	BA	699	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	988	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	2089	C	N3-C2-O2	-5.38	118.14	121.90
21	AA	13	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	528	A	O4'-C1'-N9	5.38	112.50	108.20
54	BA	2461	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	412	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	478	A	C4-C5-C6	-5.37	114.31	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1196	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1762	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	2685	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	229	U	N3-C2-O2	-5.37	118.44	122.20
46	BX	17	ARG	NE-CZ-NH2	5.37	122.98	120.30
54	BA	293	U	O4'-C1'-N1	5.37	112.50	108.20
54	BA	1061	U	O4'-C4'-C3'	5.37	110.40	106.10
54	BA	1658	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	2257	U	O4'-C1'-N1	5.37	112.50	108.20
54	BA	2300	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	2824	C	N1-C2-O2	5.37	122.12	118.90
21	AA	396	C	N1-C2-O2	5.37	122.12	118.90
21	AA	726	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	834	G	O4'-C1'-N9	5.37	112.50	108.20
21	AA	1303	C	N1-C2-O2	5.37	122.12	118.90
54	BA	595	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	607	U	C5'-C4'-O4'	5.37	115.54	109.10
54	BA	693	A	C4'-C3'-C2'	-5.37	97.23	102.60
54	BA	1169	A	C6-C5-N7	5.37	136.06	132.30
54	BA	1467	U	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2719	G	N1-C6-O6	-5.37	116.68	119.90
21	AA	169	C	N3-C2-O2	-5.37	118.14	121.90
21	AA	1335	U	N1-C2-N3	5.37	118.12	114.90
54	BA	542	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	2215	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	2518	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	755	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	6	A	C4-C5-C6	-5.37	114.32	117.00
54	BA	383	C	P-O3'-C3'	5.37	126.14	119.70
54	BA	796	C	N3-C4-C5	5.37	124.05	121.90
54	BA	2503	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	869	G	N3-C2-N2	-5.36	116.15	119.90
24	A3	23	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	457	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1129	A	C1'-O4'-C4'	-5.36	105.61	109.90
54	BA	1664	A	C5-C6-N1	5.36	120.38	117.70
54	BA	2397	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	2744	G	N1-C6-O6	-5.36	116.68	119.90
54	BA	882	G	N1-C6-O6	-5.36	116.68	119.90
54	BA	1102	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1854	A	C6-C5-N7	5.36	136.05	132.30
21	AA	1164	G	N1-C6-O6	-5.36	116.68	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	442	G	C5-C6-N1	5.36	114.18	111.50
54	BA	1889	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2155	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	1274	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	1720	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1880	U	O4'-C1'-N1	5.36	112.49	108.20
54	BA	1925	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	2576	G	C5-C6-N1	5.36	114.18	111.50
54	BA	2874	C	O4'-C1'-N1	5.36	112.49	108.20
21	AA	98	A	C6-C5-N7	5.36	136.05	132.30
21	AA	1349	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	1532	U	N3-C2-O2	-5.36	118.45	122.20
54	BA	957	C	N3-C4-C5	5.36	124.04	121.90
26	BD	141	ARG	NE-CZ-NH1	-5.36	117.62	120.30
54	BA	355	U	O4'-C1'-N1	5.36	112.48	108.20
54	BA	835	C	O4'-C1'-N1	5.36	112.48	108.20
54	BA	933	A	C4-C5-C6	-5.36	114.32	117.00
54	BA	2072	C	N1-C2-O2	5.36	122.11	118.90
54	BA	2902	C	N1-C2-O2	5.36	122.11	118.90
21	AA	851	G	N3-C4-C5	-5.35	125.92	128.60
54	BA	2468	A	O4'-C1'-N9	5.35	112.48	108.20
10	AK	52	ARG	NE-CZ-NH1	5.35	122.98	120.30
21	AA	1198	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	1327	A	C4-C5-C6	-5.35	114.32	117.00
54	BA	2883	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	467	U	O4'-C1'-N1	5.35	112.48	108.20
21	AA	1094	G	C5-C6-N1	5.35	114.17	111.50
21	AA	1100	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	516	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	543	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	691	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	848	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	2652	C	N1-C2-O2	5.35	122.11	118.90
55	BB	90	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	225	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	964	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	1609	A	C6-C5-N7	5.35	136.04	132.30
54	BA	2398	U	C5-C6-N1	-5.35	120.03	122.70
21	AA	1373	G	N3-C2-N2	-5.35	116.16	119.90
54	BA	2795	C	N3-C2-O2	-5.35	118.16	121.90
55	BB	71	C	O4'-C1'-N1	5.35	112.48	108.20
55	BB	73	A	C6-C5-N7	5.35	136.04	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	363	A	C6-C5-N7	5.34	136.04	132.30
21	AA	813	U	N3-C2-O2	-5.34	118.46	122.20
21	AA	1333	A	C6-C5-N7	5.34	136.04	132.30
21	AA	1382	C	N3-C4-C5	5.34	124.04	121.90
46	BX	10	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BA	114	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	235	U	C5'-C4'-O4'	5.34	115.51	109.10
54	BA	2059	A	C6-C5-N7	5.34	136.04	132.30
54	BA	2872	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	312	C	N1-C2-O2	5.34	122.11	118.90
54	BA	2133	G	N9-C4-C5	5.34	107.54	105.40
21	AA	759	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	918	A	C4-C5-C6	-5.34	114.33	117.00
21	AA	1071	C	N3-C2-O2	-5.34	118.16	121.90
21	AA	1453	G	N3-C4-C5	-5.34	125.93	128.60
36	BN	118	ARG	NE-CZ-NH1	5.34	122.97	120.30
54	BA	812	C	N1-C2-O2	5.34	122.11	118.90
54	BA	834	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	1606	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2042	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2393	U	O4'-C1'-N1	5.34	112.47	108.20
21	AA	840	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	318	C	N3-C4-C5	5.34	124.03	121.90
54	BA	611	C	N1-C2-O2	5.34	122.10	118.90
54	BA	1021	A	C5-C6-N1	5.34	120.37	117.70
54	BA	415	A	O4'-C1'-N9	5.34	112.47	108.20
54	BA	497	A	C6-C5-N7	5.34	136.04	132.30
54	BA	743	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	1585	C	N1-C2-O2	5.34	122.10	118.90
21	AA	755	G	N3-C2-N2	-5.34	116.17	119.90
54	BA	530	G	N3-C2-N2	-5.34	116.16	119.90
54	BA	589	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	742	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2875	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	2825	G	N3-C4-C5	-5.33	125.93	128.60
21	AA	100	G	N1-C6-O6	-5.33	116.70	119.90
21	AA	290	C	N1-C2-O2	5.33	122.10	118.90
21	AA	985	C	N1-C2-O2	5.33	122.10	118.90
24	A3	31	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	867	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	339	C	N1-C2-O2	5.33	122.10	118.90
54	BA	782	A	C4-C5-C6	-5.33	114.33	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	814	C	N1-C2-O2	5.33	122.10	118.90
54	BA	1957	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	2799	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	1110	A	O4'-C1'-N9	5.33	112.46	108.20
54	BA	995	C	N1-C2-O2	5.33	122.10	118.90
21	AA	188	C	N1-C2-O2	5.33	122.10	118.90
21	AA	455	G	C8-N9-C4	-5.33	104.27	106.40
21	AA	890	G	C8-N9-C4	-5.33	104.27	106.40
38	BP	88	ARG	CD-NE-CZ	5.33	131.06	123.60
54	BA	96	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	119	A	C6-C5-N7	5.33	136.03	132.30
54	BA	763	G	C5'-C4'-C3'	-5.33	107.48	116.00
54	BA	859	G	C5-C6-N1	5.33	114.17	111.50
54	BA	1095	A	C3'-C2'-C1'	5.33	105.76	101.50
54	BA	1335	C	N3-C2-O2	-5.33	118.17	121.90
21	AA	657	U	N3-C2-O2	-5.33	118.47	122.20
21	AA	1249	C	N3-C2-O2	-5.33	118.17	121.90
24	A3	13	C	O4'-C1'-N1	5.33	112.46	108.20
54	BA	792	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	2639	A	C4-C5-C6	-5.33	114.34	117.00
24	A3	75	C	N1-C2-O2	5.33	122.10	118.90
54	BA	235	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	584	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	1389	G	N3-C4-C5	-5.33	125.94	128.60
54	BA	1515	A	C6-C5-N7	5.33	136.03	132.30
54	BA	1535	A	C4-C5-C6	-5.33	114.34	117.00
54	BA	1927	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	111	G	N1-C6-O6	-5.32	116.70	119.90
21	AA	1141	C	N1-C2-O2	5.32	122.09	118.90
54	BA	156	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	808	G	N3-C4-C5	-5.32	125.94	128.60
54	BA	1670	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1812	U	O4'-C1'-N1	5.32	112.46	108.20
21	AA	1447	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	337	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	366	C	N3-C2-O2	-5.32	118.17	121.90
13	AN	75	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
21	AA	745	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	1197	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	2045	C	O4'-C1'-N1	5.32	112.46	108.20
21	AA	140	U	O4'-C1'-N1	5.32	112.45	108.20
21	AA	879	C	N3-C4-C5	5.32	124.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1191	G	C5-C6-N1	5.32	114.16	111.50
6	AG	3	ARG	NE-CZ-NH1	-5.32	117.64	120.30
28	BF	111	ARG	NE-CZ-NH1	5.32	122.96	120.30
54	BA	809	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	858	G	C3'-C2'-C1'	5.32	105.75	101.50
54	BA	2126	A	O4'-C1'-N9	5.32	112.45	108.20
21	AA	225	C	N3-C2-O2	-5.32	118.18	121.90
21	AA	1432	G	O4'-C1'-N9	5.32	112.45	108.20
54	BA	871	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	1137	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	2536	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	2662	A	N1-C6-N6	-5.32	115.41	118.60
54	BA	2725	A	O4'-C1'-N9	5.32	112.45	108.20
21	AA	910	C	C5'-C4'-C3'	-5.31	107.50	116.00
54	BA	1985	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	817	C	C1'-O4'-C4'	-5.31	105.65	109.90
54	BA	284	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1022	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	2040	G	O4'-C1'-N9	5.31	112.45	108.20
54	BA	2227	A	O4'-C1'-N9	5.31	112.45	108.20
54	BA	2634	A	C6-C5-N7	5.31	136.02	132.30
21	AA	306	A	C6-C5-N7	5.31	136.02	132.30
21	AA	661	G	N1-C6-O6	-5.31	116.71	119.90
21	AA	1332	A	C4-C5-C6	-5.31	114.34	117.00
24	A3	2	G	C6-C5-N7	5.31	133.59	130.40
54	BA	232	G	C5-C6-N1	5.31	114.16	111.50
54	BA	1181	U	O4'-C1'-N1	5.31	112.45	108.20
21	AA	575	G	O4'-C1'-N9	5.31	112.45	108.20
21	AA	971	G	C1'-O4'-C4'	-5.31	105.65	109.90
22	A1	10	G	N3-C4-C5	-5.31	125.95	128.60
54	BA	737	C	O4'-C1'-N1	5.31	112.45	108.20
21	AA	539	A	C4-C5-C6	-5.31	114.35	117.00
22	A1	8	U	N3-C2-O2	-5.31	118.48	122.20
55	BB	83	G	O4'-C1'-N9	5.31	112.44	108.20
21	AA	1232	U	O4'-C1'-N1	5.31	112.44	108.20
54	BA	614	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	1068	G	N3-C4-C5	-5.31	125.95	128.60
54	BA	2814	A	C6-C5-N7	5.31	136.01	132.30
54	BA	2896	C	O4'-C1'-N1	5.31	112.44	108.20
21	AA	349	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	326	G	C4'-C3'-C2'	-5.30	97.30	102.60
54	BA	1099	G	O4'-C1'-N9	5.30	112.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1130	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2096	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2103	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2601	C	N1-C2-O2	5.30	122.08	118.90
21	AA	1234	C	N1-C2-O2	5.30	122.08	118.90
54	BA	1070	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	2188	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	132	C	N1-C2-O2	5.30	122.08	118.90
21	AA	727	G	C5-C6-N1	5.30	114.15	111.50
21	AA	1523	G	O4'-C4'-C3'	5.30	110.34	106.10
54	BA	102	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	587	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	1003	G	N1-C6-O6	-5.30	116.72	119.90
9	AJ	68	ARG	NE-CZ-NH1	5.30	122.95	120.30
21	AA	736	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	2606	C	N1-C2-O2	5.30	122.08	118.90
21	AA	1071	C	O4'-C1'-N1	5.30	112.44	108.20
21	AA	440	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	524	G	O4'-C1'-N9	5.30	112.44	108.20
54	BA	1003	G	N3-C2-N2	-5.30	116.19	119.90
54	BA	1537	G	N3-C4-C5	-5.30	125.95	128.60
54	BA	2404	U	C5-C6-N1	-5.30	120.05	122.70
21	AA	1078	U	N3-C2-O2	-5.29	118.49	122.20
54	BA	2244	U	C5-C6-N1	-5.29	120.05	122.70
21	AA	214	C	N1-C2-O2	5.29	122.08	118.90
21	AA	1165	U	O4'-C1'-N1	5.29	112.44	108.20
54	BA	1242	U	O4'-C1'-N1	5.29	112.44	108.20
54	BA	1596	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	1727	C	C5'-C4'-O4'	5.29	115.45	109.10
54	BA	1929	G	C8-N9-C4	-5.29	104.28	106.40
9	AJ	9	ARG	NE-CZ-NH2	-5.29	117.65	120.30
21	AA	932	C	N1-C2-O2	5.29	122.08	118.90
21	AA	988	G	O4'-C1'-N9	5.29	112.43	108.20
21	AA	1449	C	N1-C2-O2	5.29	122.08	118.90
21	AA	1528	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	428	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	1481	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	1518	C	N3-C4-C5	5.29	124.02	121.90
54	BA	1634	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	2528	U	P-O3'-C3'	5.29	126.05	119.70
54	BA	345	A	C4-C5-C6	-5.29	114.36	117.00
21	AA	1173	U	O4'-C1'-N1	5.29	112.43	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	68	C	N1-C2-O2	5.29	122.07	118.90
54	BA	177	G	N3-C4-C5	-5.29	125.96	128.60
54	BA	658	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	731	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2670	A	C4'-C3'-C2'	-5.29	97.31	102.60
21	AA	876	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2066	C	N3-C2-O2	-5.29	118.20	121.90
21	AA	297	G	C5-C6-N1	5.29	114.14	111.50
21	AA	1227	A	O4'-C1'-N9	5.29	112.43	108.20
21	AA	1510	C	N1-C2-O2	5.29	122.07	118.90
30	BH	51	ARG	NE-CZ-NH1	5.29	122.94	120.30
34	BL	32	GLY	C-N-CA	5.29	134.91	121.70
54	BA	317	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	1983	G	N1-C6-O6	-5.29	116.73	119.90
54	BA	2109	U	O4'-C1'-N1	5.29	112.43	108.20
21	AA	742	G	O4'-C1'-N9	5.28	112.43	108.20
21	AA	1463	U	C5-C6-N1	-5.28	120.06	122.70
54	BA	582	A	O4'-C1'-N9	5.28	112.43	108.20
54	BA	897	C	O4'-C1'-N1	5.28	112.43	108.20
54	BA	1066	U	N1-C2-N3	5.28	118.07	114.90
54	BA	1795	C	O4'-C1'-N1	5.28	112.43	108.20
54	BA	2791	G	O4'-C1'-N9	5.28	112.43	108.20
21	AA	792	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1184	U	O4'-C1'-N1	5.28	112.43	108.20
54	BA	2278	A	C4-C5-C6	-5.28	114.36	117.00
4	AE	137	ARG	NE-CZ-NH1	5.28	122.94	120.30
21	AA	1102	A	C4-C5-C6	-5.28	114.36	117.00
24	A3	10	G	C5-C6-N1	5.28	114.14	111.50
54	BA	181	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	254	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	538	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	979	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1279	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	1459	G	N3-C4-C5	-5.28	125.96	128.60
21	AA	54	C	C5'-C4'-O4'	5.28	115.43	109.10
54	BA	273	G	C1'-O4'-C4'	-5.28	105.68	109.90
54	BA	399	U	C5-C6-N1	-5.28	120.06	122.70
54	BA	435	C	N1-C2-O2	5.28	122.07	118.90
54	BA	1200	C	N3-C2-O2	-5.28	118.21	121.90
54	BA	1552	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	549	C	N1-C2-O2	5.28	122.06	118.90
21	AA	641	U	N3-C2-O2	-5.28	118.51	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1042	A	C4-C5-C6	-5.28	114.36	117.00
24	A3	12	G	C5-C6-N1	5.28	114.14	111.50
54	BA	1574	C	N1-C2-O2	5.28	122.06	118.90
54	BA	1727	C	O4'-C1'-N1	5.28	112.42	108.20
21	AA	968	A	C2-N3-C4	5.27	113.24	110.60
21	AA	1532	U	C1'-O4'-C4'	-5.27	105.68	109.90
21	AA	861	G	C5-C6-N1	5.27	114.14	111.50
21	AA	934	C	N1-C2-O2	5.27	122.06	118.90
21	AA	1398	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	724	U	N3-C2-O2	-5.27	118.51	122.20
54	BA	987	C	N1-C2-O2	5.27	122.06	118.90
54	BA	2474	U	C3'-C2'-C1'	5.27	105.72	101.50
21	AA	177	G	N3-C2-N2	-5.27	116.21	119.90
33	BK	30	ARG	NE-CZ-NH1	5.27	122.94	120.30
54	BA	1540	G	O4'-C1'-N9	5.27	112.42	108.20
21	AA	209	U	N1-C2-N3	5.27	118.06	114.90
21	AA	572	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	1327	A	O4'-C1'-N9	5.27	112.42	108.20
54	BA	2336	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	1388	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	1442	U	O4'-C1'-N1	5.27	112.41	108.20
54	BA	1573	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	1810	A	C4-C5-C6	-5.27	114.37	117.00
54	BA	1876	A	C2-N3-C4	5.27	113.23	110.60
54	BA	1996	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	2082	A	O4'-C1'-N9	5.27	112.41	108.20
54	BA	2321	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2462	C	O4'-C1'-N1	5.27	112.41	108.20
56	B5	71	ARG	NE-CZ-NH1	5.27	122.93	120.30
6	AG	6	ILE	CA-C-N	5.27	126.73	116.20
21	AA	264	C	N3-C4-N4	-5.27	114.31	118.00
54	BA	2378	A	C6-C5-N7	5.27	135.99	132.30
54	BA	2773	C	N3-C2-O2	-5.27	118.21	121.90
55	BB	2	G	N3-C2-N2	-5.27	116.21	119.90
24	A3	47	G	N3-C2-N2	-5.26	116.22	119.90
54	BA	259	G	C5'-C4'-O4'	5.26	115.42	109.10
54	BA	623	C	N1-C2-O2	5.26	122.06	118.90
54	BA	1606	C	C3'-C2'-C1'	5.26	105.71	101.50
54	BA	2102	G	N1-C6-O6	-5.26	116.74	119.90
55	BB	37	C	N3-C2-O2	-5.26	118.22	121.90
55	BB	81	G	C5-C6-N1	5.26	114.13	111.50
21	AA	796	C	N1-C2-O2	5.26	122.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1329	A	C5-C6-N1	5.26	120.33	117.70
21	AA	284	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	327	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1273	C	N1-C2-O2	5.26	122.06	118.90
54	BA	545	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	1247	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	1297	C	N1-C2-O2	5.26	122.06	118.90
54	BA	1537	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	2554	U	O4'-C1'-N1	5.26	112.41	108.20
54	BA	2568	U	C5-C6-N1	-5.26	120.07	122.70
54	BA	2766	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	379	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	98	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	1881	C	N3-C2-O2	-5.26	118.22	121.90
21	AA	565	U	C1'-O4'-C4'	-5.26	105.69	109.90
21	AA	1179	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1194	U	N3-C2-O2	-5.26	118.52	122.20
54	BA	296	U	C5'-C4'-O4'	5.26	115.41	109.10
54	BA	1260	A	C6-C5-N7	5.26	135.98	132.30
54	BA	2674	G	N1-C6-O6	-5.26	116.75	119.90
21	AA	1453	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	510	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2103	C	N1-C2-O2	5.25	122.05	118.90
21	AA	1487	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	629	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	2214	C	N3-C4-C5	5.25	124.00	121.90
54	BA	2647	U	O4'-C1'-N1	5.25	112.40	108.20
55	BB	100	G	O4'-C1'-N9	5.25	112.40	108.20
54	BA	102	U	N3-C2-O2	-5.25	118.53	122.20
54	BA	922	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1007	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1303	G	C5-C6-N1	5.25	114.12	111.50
21	AA	313	A	C6-C5-N7	5.25	135.97	132.30
54	BA	163	C	N3-C4-C5	5.25	124.00	121.90
54	BA	1291	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1313	U	N1-C1'-C2'	5.25	120.83	114.00
1	AB	20	ARG	NE-CZ-NH1	5.25	122.92	120.30
21	AA	556	C	N1-C2-O2	5.25	122.05	118.90
21	AA	792	A	C1'-O4'-C4'	-5.25	105.70	109.90
54	BA	1559	U	N3-C2-O2	-5.25	118.53	122.20
54	BA	1844	C	N3-C2-O2	-5.25	118.23	121.90
54	BA	2494	G	N3-C4-C5	-5.25	125.98	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	989	U	C5-C6-N1	-5.25	120.08	122.70
54	BA	166	U	C4'-C3'-C2'	-5.25	97.35	102.60
54	BA	1895	C	N3-C2-O2	-5.25	118.23	121.90
54	BA	2757	A	C4-C5-C6	-5.25	114.38	117.00
55	BB	97	C	N1-C2-O2	5.25	122.05	118.90
54	BA	440	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	787	C	N3-C4-C5	5.25	124.00	121.90
54	BA	2760	C	N3-C2-O2	-5.25	118.23	121.90
9	AJ	37	ARG	NE-CZ-NH1	5.24	122.92	120.30
21	AA	438	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	640	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	1029	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	141	G	C5-C6-N1	5.24	114.12	111.50
54	BA	633	A	O4'-C1'-N9	5.24	112.39	108.20
54	BA	1653	G	N1-C6-O6	-5.24	116.75	119.90
54	BA	2822	G	N3-C4-C5	-5.24	125.98	128.60
21	AA	149	A	C5-C6-N1	5.24	120.32	117.70
21	AA	754	C	N1-C2-O2	5.24	122.05	118.90
21	AA	1218	C	N3-C2-O2	-5.24	118.23	121.90
54	BA	944	C	N3-C2-O2	-5.24	118.23	121.90
54	BA	1898	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2173	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	2238	G	C5-C6-N1	5.24	114.12	111.50
21	AA	517	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	2319	G	O4'-C1'-N9	5.24	112.39	108.20
54	BA	2385	C	C5'-C4'-O4'	5.24	115.39	109.10
15	AP	31	ARG	NE-CZ-NH2	-5.24	117.68	120.30
21	AA	1052	U	C5-C6-N1	-5.24	120.08	122.70
54	BA	993	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	1073	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1965	C	N1-C2-O2	5.24	122.04	118.90
54	BA	2380	C	N3-C2-O2	-5.24	118.23	121.90
21	AA	280	C	N1-C2-O2	5.24	122.04	118.90
54	BA	1359	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	2433	A	C1'-O4'-C4'	-5.24	105.71	109.90
10	AK	12	ARG	NE-CZ-NH1	5.24	122.92	120.30
21	AA	1336	C	N1-C2-O2	5.24	122.04	118.90
54	BA	370	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	717	C	N1-C2-O2	5.24	122.04	118.90
54	BA	751	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	2000	C	N1-C2-O2	5.24	122.04	118.90
55	BB	12	C	N1-C2-O2	5.24	122.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	341	C	N1-C2-O2	5.23	122.04	118.90
22	A1	20	G	C8-N9-C4	-5.23	104.31	106.40
21	AA	899	C	N1-C2-O2	5.23	122.04	118.90
21	AA	1478	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	85	G	C5-C6-N1	5.23	114.12	111.50
54	BA	1004	U	C5-C6-N1	-5.23	120.08	122.70
54	BA	1044	C	N1-C2-O2	5.23	122.04	118.90
54	BA	2481	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	372	C	N3-C2-O2	-5.23	118.24	121.90
21	AA	655	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	1604	C	C4'-C3'-C2'	-5.23	97.37	102.60
54	BA	2093	G	N1-C6-O6	-5.23	116.76	119.90
54	BA	2245	U	C5-C6-N1	-5.23	120.08	122.70
55	BB	5	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	1936	A	C6-C5-N7	5.23	135.96	132.30
21	AA	29	U	O4'-C1'-N1	5.23	112.38	108.20
21	AA	250	A	O4'-C1'-N9	5.23	112.38	108.20
21	AA	296	U	N3-C2-O2	-5.23	118.54	122.20
21	AA	1498	U	C3'-C2'-C1'	5.23	105.68	101.50
54	BA	226	A	C3'-C2'-C1'	5.23	105.68	101.50
54	BA	1350	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	1512	C	C5'-C4'-O4'	5.23	115.37	109.10
54	BA	1616	A	C3'-C2'-C1'	-5.23	97.32	101.50
21	AA	455	G	N7-C8-N9	5.22	115.71	113.10
54	BA	147	C	N1-C2-O2	5.22	122.03	118.90
21	AA	603	U	C5-C6-N1	-5.22	120.09	122.70
21	AA	1523	G	C3'-C2'-C1'	5.22	105.68	101.50
54	BA	1874	C	O4'-C1'-N1	5.22	112.38	108.20
54	BA	2873	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	124	C	N1-C2-O2	5.22	122.03	118.90
21	AA	311	C	N1-C2-O2	5.22	122.03	118.90
21	AA	665	A	C2-N3-C4	5.22	113.21	110.60
54	BA	445	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	2239	G	N3-C4-C5	-5.22	125.99	128.60
22	A1	29	U	C5-C6-N1	-5.22	120.09	122.70
54	BA	1871	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	845	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	1069	C	N1-C2-O2	5.22	122.03	118.90
21	AA	1218	C	C1'-O4'-C4'	-5.22	105.73	109.90
54	BA	1045	C	O4'-C1'-N1	5.22	112.37	108.20
54	BA	1675	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2097	A	C4-C5-C6	-5.22	114.39	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2515	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2579	C	O4'-C1'-N1	5.22	112.37	108.20
21	AA	189	A	C4-C5-C6	-5.21	114.39	117.00
21	AA	1470	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	101	A	C4-C5-C6	-5.21	114.39	117.00
54	BA	560	C	N1-C2-O2	5.21	122.03	118.90
54	BA	959	A	C1'-O4'-C4'	-5.21	105.73	109.90
54	BA	1465	G	O4'-C1'-N9	5.21	112.37	108.20
54	BA	2797	U	O4'-C1'-N1	5.21	112.37	108.20
21	AA	979	C	N1-C2-O2	5.21	122.03	118.90
54	BA	177	G	C5-C6-N1	5.21	114.11	111.50
54	BA	1293	C	N3-C2-O2	-5.21	118.25	121.90
55	BB	103	U	N1-C2-N3	5.21	118.03	114.90
22	A1	13	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	1172	C	O4'-C1'-N1	5.21	112.37	108.20
21	AA	1261	A	C4-C5-C6	-5.21	114.40	117.00
24	A3	5	G	C5'-C4'-C3'	-5.21	107.67	116.00
27	BE	49	ARG	NE-CZ-NH1	5.21	122.90	120.30
54	BA	1498	C	N3-C2-O2	-5.21	118.25	121.90
54	BA	624	C	N1-C2-O2	5.21	122.02	118.90
54	BA	687	C	N3-C2-O2	-5.21	118.26	121.90
54	BA	892	A	C6-C5-N7	5.21	135.94	132.30
54	BA	2496	C	O4'-C1'-N1	5.21	112.36	108.20
21	AA	513	C	N1-C2-O2	5.20	122.02	118.90
21	AA	1413	A	C6-C5-N7	5.20	135.94	132.30
21	AA	1521	C	N1-C2-O2	5.20	122.02	118.90
54	BA	838	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1079	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1708	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2254	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	715	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2441	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2699	C	N1-C2-O2	5.20	122.02	118.90
21	AA	542	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	865	C	N1-C2-O2	5.20	122.02	118.90
54	BA	1773	A	C4'-C3'-C2'	-5.20	97.40	102.60
54	BA	1936	A	P-O3'-C3'	5.20	125.94	119.70
54	BA	2092	U	N3-C2-O2	-5.20	118.56	122.20
55	BB	38	C	C4'-C3'-C2'	-5.20	97.40	102.60
21	AA	1467	C	N1-C2-O2	5.20	122.02	118.90
54	BA	34	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	170	U	C5-C6-N1	-5.20	120.10	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	368	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	2762	C	N3-C2-O2	-5.20	118.26	121.90
21	AA	281	G	C3'-C2'-C1'	5.20	105.66	101.50
54	BA	280	U	N3-C2-O2	-5.20	118.56	122.20
54	BA	2590	A	C6-C5-N7	5.20	135.94	132.30
23	A2	90	U	P-O3'-C3'	5.20	125.93	119.70
54	BA	2499	C	N3-C2-O2	-5.20	118.26	121.90
21	AA	401	C	O4'-C1'-N1	5.19	112.36	108.20
24	A3	1	C	N1-C2-O2	5.19	122.02	118.90
28	BF	109	ARG	NE-CZ-NH1	5.19	122.90	120.30
54	BA	1886	U	O4'-C1'-N1	5.19	112.36	108.20
54	BA	260	G	O4'-C1'-N9	5.19	112.35	108.20
54	BA	921	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	1173	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	691	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	1072	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	2214	C	N1-C2-O2	5.19	122.02	118.90
54	BA	2506	U	N1-C2-N3	5.19	118.02	114.90
54	BA	2656	U	O4'-C1'-N1	5.19	112.35	108.20
21	AA	501	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1423	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	2837	A	C4'-C3'-C2'	-5.19	97.41	102.60
21	AA	437	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	837	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	1506	U	N3-C2-O2	-5.19	118.57	122.20
54	BA	2076	U	O4'-C1'-N1	5.19	112.35	108.20
21	AA	254	G	C1'-O4'-C4'	-5.19	105.75	109.90
21	AA	697	U	O4'-C1'-N1	5.19	112.35	108.20
29	BG	162	ARG	NE-CZ-NH2	-5.19	117.71	120.30
54	BA	2129	C	N1-C2-O2	5.19	122.01	118.90
54	BA	2358	A	C4-C5-C6	-5.19	114.41	117.00
21	AA	26	A	C3'-C2'-C1'	5.18	105.65	101.50
21	AA	1139	G	C5-C6-N1	5.18	114.09	111.50
21	AA	1200	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1384	C	N3-C2-O2	-5.18	118.27	121.90
21	AA	1441	A	C1'-O4'-C4'	-5.18	105.75	109.90
54	BA	374	A	C5'-C4'-O4'	5.18	115.32	109.10
54	BA	1488	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	1905	C	O4'-C1'-N1	5.18	112.35	108.20
24	A3	49	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	1249	U	C5-C6-N1	-5.18	120.11	122.70
21	AA	1119	C	N3-C2-O2	-5.18	118.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	327	G	N3-C2-N2	-5.18	116.27	119.90
54	BA	917	A	N1-C6-N6	-5.18	115.49	118.60
54	BA	2098	U	O4'-C1'-N1	5.18	112.34	108.20
54	BA	2186	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	2232	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	2248	C	N1-C2-O2	5.18	122.01	118.90
54	BA	2786	U	O4'-C1'-N1	5.18	112.34	108.20
21	AA	257	G	C5-C6-N1	5.18	114.09	111.50
21	AA	668	G	N1-C6-O6	-5.18	116.79	119.90
21	AA	1497	G	N9-C4-C5	5.18	107.47	105.40
54	BA	723	C	N3-C4-N4	-5.18	114.38	118.00
54	BA	1806	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1401	G	N3-C4-C5	-5.17	126.01	128.60
24	A3	73	A	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	620	G	N3-C4-C5	-5.17	126.01	128.60
54	BA	2075	U	N3-C2-O2	-5.17	118.58	122.20
54	BA	2702	G	N3-C2-N2	-5.17	116.28	119.90
21	AA	1475	G	C5-C6-N1	5.17	114.09	111.50
54	BA	484	C	N1-C2-O2	5.17	122.00	118.90
21	AA	1278	G	N9-C4-C5	5.17	107.47	105.40
21	AA	1308	U	C1'-O4'-C4'	-5.17	105.76	109.90
24	A3	9	G	C1'-O4'-C4'	-5.17	105.76	109.90
19	AT	35	TYR	CB-CG-CD2	-5.17	117.90	121.00
21	AA	611	C	N3-C4-C5	5.17	123.97	121.90
37	BO	10	ARG	NE-CZ-NH1	5.17	122.89	120.30
54	BA	268	C	O4'-C1'-N1	5.17	112.34	108.20
54	BA	1128	G	C5-C6-N1	5.17	114.08	111.50
54	BA	1541	C	N1-C2-O2	5.17	122.00	118.90
54	BA	2330	G	N1-C6-O6	-5.17	116.80	119.90
13	AN	13	ARG	NE-CZ-NH1	5.17	122.88	120.30
23	A2	83	U	N1-C2-N3	5.17	118.00	114.90
54	BA	237	C	N1-C2-O2	5.17	122.00	118.90
54	BA	242	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	535	G	C5-C6-N1	5.17	114.08	111.50
21	AA	121	U	N3-C2-O2	-5.17	118.58	122.20
24	A3	26	C	N1-C2-O2	5.17	122.00	118.90
40	BR	80	ARG	NE-CZ-NH1	5.17	122.88	120.30
54	BA	679	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1096	A	C6-C5-N7	5.17	135.92	132.30
54	BA	1297	C	N3-C4-C5	5.17	123.97	121.90
54	BA	2361	G	N1-C6-O6	-5.17	116.80	119.90
56	B5	134	ARG	NE-CZ-NH1	5.17	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1291	U	O4'-C1'-N1	5.17	112.33	108.20
54	BA	465	G	N3-C2-N2	-5.17	116.28	119.90
54	BA	1604	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	553	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	1301	A	C1'-O4'-C4'	-5.16	105.77	109.90
54	BA	1894	C	N1-C2-O2	5.16	122.00	118.90
54	BA	1895	C	N1-C2-O2	5.16	122.00	118.90
54	BA	2746	U	C5-C6-N1	-5.16	120.12	122.70
21	AA	22	G	C5-C6-N1	5.16	114.08	111.50
21	AA	559	A	O4'-C1'-N9	5.16	112.33	108.20
21	AA	1269	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	897	C	N1-C2-O2	5.16	122.00	118.90
21	AA	240	G	N1-C6-O6	-5.16	116.80	119.90
21	AA	282	A	C6-C5-N7	5.16	135.91	132.30
54	BA	223	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	817	C	N1-C2-O2	5.16	122.00	118.90
54	BA	12	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	526	A	C6-C5-N7	5.16	135.91	132.30
54	BA	1649	G	C1'-O4'-C4'	-5.16	105.77	109.90
56	B5	49	GLY	C-N-CA	5.16	134.60	121.70
21	AA	1194	U	C1'-O4'-C4'	-5.16	105.78	109.90
54	BA	1552	A	C2-N3-C4	5.16	113.18	110.60
54	BA	1642	G	O4'-C1'-N9	5.16	112.33	108.20
21	AA	572	A	C1'-O4'-C4'	-5.16	105.78	109.90
21	AA	1387	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	247	G	C5-C6-N1	5.16	114.08	111.50
54	BA	2133	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	2462	C	N1-C2-O2	5.16	121.99	118.90
21	AA	734	G	N3-C4-C5	-5.15	126.02	128.60
54	BA	248	G	N3-C2-N2	-5.15	116.29	119.90
54	BA	2594	C	N3-C2-O2	-5.15	118.29	121.90
54	BA	2805	C	N1-C2-O2	5.15	121.99	118.90
21	AA	994	A	C6-C5-N7	5.15	135.91	132.30
21	AA	1530	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1179	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1743	G	C5-C6-N1	5.15	114.08	111.50
54	BA	1790	C	N3-C2-O2	-5.15	118.29	121.90
54	BA	1815	A	O4'-C1'-N9	5.15	112.32	108.20
54	BA	2392	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	2902	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	493	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	682	G	C5-C6-N1	5.15	114.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1436	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1524	G	C8-N9-C4	-5.15	104.34	106.40
54	BA	2155	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2304	G	C5-C6-N1	5.15	114.08	111.50
22	A1	58	A	C4-C5-C6	-5.15	114.43	117.00
24	A3	62	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	55	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	2778	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	602	A	C4-C5-C6	-5.15	114.43	117.00
21	AA	1366	C	N3-C2-O2	-5.15	118.30	121.90
24	A3	61	U	N3-C2-O2	-5.15	118.60	122.20
54	BA	338	G	C8-N9-C4	-5.15	104.34	106.40
54	BA	744	U	N3-C2-O2	-5.15	118.60	122.20
54	BA	1972	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	1983	G	N9-C4-C5	5.15	107.46	105.40
54	BA	2735	G	N1-C6-O6	-5.15	116.81	119.90
13	AN	63	ARG	NE-CZ-NH1	5.14	122.87	120.30
21	AA	1106	G	N1-C6-O6	-5.14	116.81	119.90
54	BA	852	U	O4'-C1'-N1	5.14	112.32	108.20
54	BA	1607	C	N1-C2-O2	5.14	121.99	118.90
54	BA	2871	U	O4'-C1'-N1	5.14	112.32	108.20
21	AA	337	G	N1-C6-O6	-5.14	116.81	119.90
21	AA	368	U	N3-C2-O2	-5.14	118.60	122.20
21	AA	416	G	N1-C6-O6	-5.14	116.81	119.90
21	AA	590	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	1108	U	N1-C2-N3	5.14	117.98	114.90
54	BA	1181	U	C5-C6-N1	-5.14	120.13	122.70
54	BA	2407	A	C6-C5-N7	5.14	135.90	132.30
54	BA	2482	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2592	G	N1-C6-O6	-5.14	116.81	119.90
55	BB	9	G	C5-C6-N1	5.14	114.07	111.50
21	AA	823	C	N3-C4-C5	5.14	123.96	121.90
54	BA	566	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2100	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	2267	A	C4-C5-C6	-5.14	114.43	117.00
55	BB	113	C	N1-C2-O2	5.14	121.98	118.90
21	AA	48	C	C3'-C2'-C1'	5.14	105.61	101.50
21	AA	1214	C	N3-C4-C5	5.14	123.96	121.90
21	AA	1368	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	1485	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2024	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	2288	A	C4-C5-C6	-5.14	114.43	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2586	U	C3'-C2'-C1'	5.14	105.61	101.50
21	AA	977	A	C2-N3-C4	5.14	113.17	110.60
54	BA	135	U	O4'-C1'-N1	5.14	112.31	108.20
54	BA	515	A	C6-C5-N7	5.14	135.90	132.30
54	BA	917	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2731	G	O4'-C1'-N9	5.14	112.31	108.20
21	AA	723	U	C5-C6-N1	-5.14	120.13	122.70
21	AA	862	C	N1-C2-O2	5.14	121.98	118.90
21	AA	1318	A	O4'-C1'-N9	5.14	112.31	108.20
26	BD	77	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
54	BA	1371	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	1387	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2033	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	2087	G	O4'-C1'-N9	5.14	112.31	108.20
54	BA	2463	C	N3-C4-C5	5.14	123.95	121.90
54	BA	2707	U	N3-C2-O2	-5.14	118.60	122.20
54	BA	1	G	C5-C6-N1	5.13	114.07	111.50
54	BA	57	C	O4'-C1'-N1	5.13	112.31	108.20
54	BA	459	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	2627	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2827	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2841	C	N1-C2-O2	5.13	121.98	118.90
21	AA	201	G	C5-C6-N1	5.13	114.07	111.50
54	BA	15	G	C8-N9-C4	-5.13	104.35	106.40
54	BA	853	C	N3-C4-N4	-5.13	114.41	118.00
54	BA	1496	A	C6-C5-N7	5.13	135.89	132.30
54	BA	1561	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2394	C	N1-C2-O2	5.13	121.98	118.90
15	AP	35	ARG	NE-CZ-NH1	5.13	122.86	120.30
21	AA	651	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	870	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	1062	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1205	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	2078	C	N3-C2-O2	-5.13	118.31	121.90
21	AA	1193	G	N3-C2-N2	-5.13	116.31	119.90
21	AA	1305	G	O4'-C4'-C3'	5.13	110.20	106.10
54	BA	2504	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	2576	G	N1-C6-O6	-5.13	116.82	119.90
24	A3	31	G	O4'-C1'-N9	5.13	112.30	108.20
21	AA	1145	A	C6-C5-N7	5.13	135.89	132.30
54	BA	209	C	O4'-C1'-N1	5.13	112.30	108.20
54	BA	996	A	C4-C5-C6	-5.13	114.44	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2126	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	2806	C	N1-C2-O2	5.13	121.98	118.90
54	BA	2864	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	562	U	O4'-C1'-N1	5.12	112.30	108.20
21	AA	939	G	N3-C4-C5	-5.12	126.04	128.60
54	BA	2371	G	N3-C2-N2	-5.12	116.31	119.90
55	BB	56	G	C8-N9-C4	-5.12	104.35	106.40
21	AA	718	A	C3'-C2'-C1'	5.12	105.60	101.50
54	BA	1699	G	C1'-O4'-C4'	-5.12	105.80	109.90
54	BA	2547	A	C6-C5-N7	5.12	135.89	132.30
21	AA	383	A	C5-C6-N1	5.12	120.26	117.70
21	AA	1293	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1182	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1229	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1258	U	C5-C6-N1	-5.12	120.14	122.70
54	BA	1844	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	2189	U	O4'-C1'-N1	5.12	112.30	108.20
21	AA	342	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	274	C	N1-C2-O2	5.12	121.97	118.90
54	BA	1112	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	1943	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	2295	C	O4'-C1'-N1	5.12	112.30	108.20
21	AA	1031	C	C2-N3-C4	-5.12	117.34	119.90
54	BA	551	G	N7-C8-N9	5.12	115.66	113.10
54	BA	1421	G	C5-C6-N1	5.12	114.06	111.50
54	BA	1570	A	C6-C5-N7	5.12	135.88	132.30
54	BA	2057	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2163	A	O4'-C1'-N9	5.12	112.30	108.20
54	BA	2678	C	C5'-C4'-O4'	5.12	115.24	109.10
54	BA	2831	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	395	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	886	A	C6-C5-N7	5.12	135.88	132.30
54	BA	1434	A	C2-N3-C4	5.12	113.16	110.60
21	AA	162	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	286	C	N1-C2-O2	5.12	121.97	118.90
21	AA	295	C	N1-C2-O2	5.12	121.97	118.90
21	AA	750	C	N1-C2-O2	5.12	121.97	118.90
54	BA	423	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	473	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	842	U	O4'-C1'-N1	5.12	112.29	108.20
54	BA	1081	U	O4'-C1'-N1	5.12	112.29	108.20
54	BA	1382	G	N3-C4-C5	-5.12	126.04	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2561	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	2756	U	P-O3'-C3'	5.12	125.84	119.70
21	AA	65	A	C4-C5-C6	-5.11	114.44	117.00
21	AA	911	U	N1-C2-N3	5.11	117.97	114.90
22	A1	24	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	141	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	311	A	C6-C5-N7	5.11	135.88	132.30
54	BA	360	U	C5-C6-N1	-5.11	120.14	122.70
54	BA	984	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	1152	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	1448	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	1871	A	O4'-C1'-N9	5.11	112.29	108.20
54	BA	2453	A	C6-C5-N7	5.11	135.88	132.30
21	AA	1529	G	O4'-C1'-N9	5.11	112.29	108.20
54	BA	2521	C	O4'-C1'-N1	5.11	112.29	108.20
10	AK	127	ARG	NE-CZ-NH1	5.11	122.86	120.30
21	AA	35	G	N1-C6-O6	-5.11	116.83	119.90
21	AA	1008	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	1517	G	N3-C2-N2	-5.11	116.32	119.90
23	A2	87	U	C5'-C4'-C3'	-5.11	107.82	116.00
54	BA	709	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	2344	U	N3-C2-O2	-5.11	118.62	122.20
54	BA	2696	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	423	G	C5-C6-N1	5.11	114.06	111.50
21	AA	809	G	C5-C6-N1	5.11	114.06	111.50
21	AA	1207	G	N1-C6-O6	-5.11	116.83	119.90
21	AA	1216	A	C6-C5-N7	5.11	135.88	132.30
22	A1	41	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	483	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	1338	G	C5-C6-N1	5.11	114.06	111.50
54	BA	2453	A	C5-C6-N6	5.11	127.79	123.70
21	AA	20	U	O4'-C1'-N1	5.11	112.29	108.20
21	AA	494	G	O4'-C1'-N9	5.11	112.29	108.20
21	AA	724	G	N1-C6-O6	-5.11	116.83	119.90
21	AA	977	A	C5'-C4'-C3'	-5.11	107.83	116.00
54	BA	489	G	N3-C2-N2	-5.11	116.32	119.90
54	BA	812	C	C1'-O4'-C4'	-5.11	105.81	109.90
54	BA	1772	A	O4'-C1'-N9	5.11	112.29	108.20
54	BA	1945	G	N3-C4-C5	-5.11	126.05	128.60
54	BA	2086	U	C5-C6-N1	-5.11	120.15	122.70
54	BA	2659	G	N3-C2-N2	-5.11	116.32	119.90
55	BB	57	A	C4-C5-C6	-5.11	114.45	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	63	C	N1-C2-O2	5.11	121.96	118.90
21	AA	901	A	C4-C5-C6	-5.11	114.45	117.00
21	AA	1335	U	N3-C2-O2	-5.11	118.63	122.20
54	BA	164	C	O4'-C1'-N1	5.11	112.28	108.20
54	BA	204	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	252	G	O4'-C1'-N9	5.11	112.28	108.20
54	BA	1164	C	O4'-C1'-N1	5.11	112.28	108.20
54	BA	2366	A	C4-C5-C6	-5.11	114.45	117.00
54	BA	2541	A	C4-C5-C6	-5.11	114.45	117.00
21	AA	84	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	1217	C	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1348	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	242	G	C5-C6-N1	5.10	114.05	111.50
54	BA	2172	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	473	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	723	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	996	A	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1001	C	N3-C2-O2	-5.10	118.33	121.90
21	AA	1301	U	N1-C2-N3	5.10	117.96	114.90
54	BA	587	C	C3'-C2'-C1'	5.10	105.58	101.50
54	BA	616	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2062	A	O4'-C1'-N9	5.10	112.28	108.20
54	BA	2644	G	C5-C6-N1	5.10	114.05	111.50
21	AA	1205	U	N1-C2-N3	5.10	117.96	114.90
54	BA	1661	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	2716	C	N1-C2-O2	5.10	121.96	118.90
21	AA	483	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1418	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	640	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2579	C	N1-C2-O2	5.10	121.96	118.90
5	AF	24	ARG	NE-CZ-NH1	5.10	122.85	120.30
21	AA	406	G	N3-C4-C5	-5.10	126.05	128.60
21	AA	534	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	585	G	N3-C4-C5	-5.10	126.05	128.60
21	AA	1021	A	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1442	G	N3-C2-N2	-5.10	116.33	119.90
40	BR	13	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
54	BA	290	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	1729	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1036	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	2810	A	N1-C6-N6	-5.10	115.54	118.60
21	AA	499	A	C6-C5-N7	5.09	135.87	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	591	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	130	C	O4'-C1'-N1	5.09	112.28	108.20
54	BA	887	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1082	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1504	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	1591	A	C6-C5-N7	5.09	135.87	132.30
54	BA	2233	U	C4'-C3'-C2'	-5.09	97.50	102.60
54	BA	74	A	C1'-O4'-C4'	-5.09	105.83	109.90
54	BA	402	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	1040	A	C6-C5-N7	5.09	135.87	132.30
54	BA	1329	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1578	U	C5-C6-N1	-5.09	120.15	122.70
54	BA	1804	C	N3-C2-O2	-5.09	118.33	121.90
21	AA	11	G	N1-C6-O6	-5.09	116.85	119.90
21	AA	623	C	N1-C2-O2	5.09	121.95	118.90
54	BA	1542	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1615	C	O4'-C1'-C2'	-5.09	100.71	105.80
54	BA	1662	U	C5-C6-N1	-5.09	120.15	122.70
54	BA	1731	G	N3-C4-C5	-5.09	126.05	128.60
54	BA	2341	G	C5-C6-N1	5.09	114.05	111.50
54	BA	2494	G	C5-C6-N1	5.09	114.05	111.50
54	BA	2724	U	C5-C6-N1	-5.09	120.15	122.70
55	BB	44	G	N1-C6-O6	-5.09	116.84	119.90
21	AA	266	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	668	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	1107	C	O4'-C1'-N1	5.09	112.27	108.20
24	A3	11	A	C6-C5-N7	5.09	135.86	132.30
54	BA	64	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	507	A	O4'-C1'-N9	5.09	112.27	108.20
54	BA	550	C	N1-C2-O2	5.09	121.95	118.90
54	BA	2147	A	C6-C5-N7	5.09	135.86	132.30
1	AB	19	THR	C-N-CA	5.09	134.42	121.70
54	BA	258	G	C5-C6-N1	5.09	114.04	111.50
54	BA	304	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	772	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2421	G	O4'-C1'-N9	5.09	112.27	108.20
55	BB	41	G	N3-C4-C5	-5.09	126.06	128.60
21	AA	305	G	O4'-C1'-N9	5.09	112.27	108.20
21	AA	479	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	978	A	C4-C5-C6	-5.09	114.46	117.00
24	A3	13	C	N3-C2-O2	-5.09	118.34	121.90
54	BA	96	C	O4'-C1'-N1	5.09	112.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	223	A	O4'-C1'-N9	5.09	112.27	108.20
54	BA	518	G	O4'-C1'-N9	5.09	112.27	108.20
54	BA	1028	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	1189	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	2408	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2787	C	C5'-C4'-O4'	5.09	115.20	109.10
55	BB	104	A	C4-C5-C6	-5.09	114.46	117.00
21	AA	1259	C	N1-C2-O2	5.08	121.95	118.90
54	BA	74	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	318	C	N3-C4-N4	-5.08	114.44	118.00
54	BA	802	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	2691	C	O4'-C1'-N1	5.08	112.27	108.20
21	AA	919	A	C6-C5-N7	5.08	135.86	132.30
21	AA	1124	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	391	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	573	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	1091	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1603	A	C6-C5-N7	5.08	135.86	132.30
54	BA	1793	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2143	C	N3-C2-O2	-5.08	118.34	121.90
54	BA	2215	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2343	U	O4'-C1'-N1	5.08	112.27	108.20
21	AA	246	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	528	C	N1-C2-O2	5.08	121.95	118.90
21	AA	1146	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1569	A	C6-C5-N7	5.08	135.86	132.30
54	BA	2196	C	C5'-C4'-O4'	5.08	115.20	109.10
54	BA	2245	U	N3-C2-O2	-5.08	118.64	122.20
21	AA	702	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	1399	C	N3-C4-C5	5.08	123.93	121.90
24	A3	6	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	669	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	780	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	1632	A	C4-C5-C6	-5.08	114.46	117.00
21	AA	968	A	O4'-C1'-N9	5.08	112.26	108.20
54	BA	710	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1149	G	C5'-C4'-O4'	5.08	115.19	109.10
54	BA	1439	A	C2-N3-C4	5.08	113.14	110.60
54	BA	1716	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1933	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2626	C	N3-C2-O2	-5.08	118.34	121.90
21	AA	1386	G	N3-C4-C5	-5.08	126.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	BF	21	TYR	CB-CG-CD2	-5.08	117.95	121.00
25	BC	13	ARG	NE-CZ-NH1	5.08	122.84	120.30
54	BA	1415	U	N1-C2-N3	5.08	117.95	114.90
54	BA	1807	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	1893	C	N3-C2-O2	-5.08	118.35	121.90
54	BA	2435	A	C6-C5-N7	5.08	135.85	132.30
54	BA	1007	C	N3-C4-C5	5.07	123.93	121.90
54	BA	1647	U	C5-C6-N1	-5.07	120.16	122.70
54	BA	1820	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	1931	U	O4'-C1'-N1	5.07	112.26	108.20
24	A3	54	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	133	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	999	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	1304	A	C6-C5-N7	5.07	135.85	132.30
54	BA	1306	C	C4'-C3'-C2'	-5.07	97.53	102.60
54	BA	2115	G	C5-C6-N1	5.07	114.04	111.50
21	AA	674	G	N3-C4-C5	-5.07	126.06	128.60
21	AA	924	C	N1-C2-O2	5.07	121.94	118.90
21	AA	1324	A	C4-C5-C6	-5.07	114.47	117.00
21	AA	1505	G	C5-C6-N1	5.07	114.03	111.50
54	BA	1767	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2353	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2780	G	N3-C2-N2	-5.07	116.35	119.90
21	AA	1376	U	C5-C6-N1	-5.07	120.17	122.70
21	AA	1453	G	C8-N9-C4	-5.07	104.37	106.40
54	BA	277	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	560	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	999	U	C5-C6-N1	-5.07	120.17	122.70
54	BA	1066	U	C4'-C3'-C2'	-5.07	97.53	102.60
54	BA	1129	A	C5'-C4'-O4'	5.07	115.18	109.10
54	BA	2410	G	C5-C6-N1	5.07	114.03	111.50
54	BA	2695	U	O4'-C1'-N1	5.07	112.25	108.20
21	AA	109	A	C4-C5-C6	-5.07	114.47	117.00
21	AA	292	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	619	U	O4'-C1'-N1	5.07	112.25	108.20
21	AA	667	G	N3-C2-N2	-5.07	116.36	119.90
54	BA	106	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1100	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1804	C	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1847	A	C5-C6-N6	5.07	127.75	123.70
54	BA	2496	C	N3-C2-O2	-5.07	118.35	121.90
21	AA	155	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	400	C	N1-C2-O2	5.06	121.94	118.90
21	AA	884	U	C5-C6-N1	-5.06	120.17	122.70
21	AA	884	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	926	G	N1-C6-O6	-5.06	116.86	119.90
21	AA	1352	C	N1-C2-O2	5.06	121.94	118.90
21	AA	419	C	N1-C2-O2	5.06	121.94	118.90
21	AA	733	G	C5-C6-N1	5.06	114.03	111.50
21	AA	890	G	N3-C4-C5	-5.06	126.07	128.60
21	AA	1128	C	N1-C2-O2	5.06	121.94	118.90
21	AA	1196	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	1339	A	C1'-O4'-C4'	-5.06	105.85	109.90
24	A3	7	G	N3-C4-C5	-5.06	126.07	128.60
54	BA	441	U	N1-C2-N3	5.06	117.94	114.90
54	BA	2047	C	N1-C2-O2	5.06	121.94	118.90
54	BA	2616	C	O4'-C1'-N1	5.06	112.25	108.20
21	AA	1240	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	1401	G	N7-C8-N9	5.06	115.63	113.10
22	A1	16	C	N1-C2-O2	5.06	121.94	118.90
39	BQ	49	ARG	NE-CZ-NH2	-5.06	117.77	120.30
42	BT	51	PHE	CB-CG-CD2	-5.06	117.26	120.80
45	BW	40	ARG	NE-CZ-NH2	-5.06	117.77	120.30
54	BA	53	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	110	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	1153	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1428	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1787	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	2457	U	C5-C6-N1	-5.06	120.17	122.70
54	BA	2793	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1210	G	O4'-C1'-N9	5.06	112.25	108.20
54	BA	1692	U	N1-C2-N3	5.06	117.93	114.90
54	BA	2330	G	N3-C2-N2	-5.06	116.36	119.90
21	AA	530	G	N3-C4-N9	5.06	129.03	126.00
21	AA	705	G	N1-C6-O6	-5.06	116.87	119.90
21	AA	1500	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	616	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	1054	C	N3-C2-O2	-5.05	118.36	121.90
21	AA	1182	G	P-O3'-C3'	5.05	125.77	119.70
22	A1	61	C	N3-C2-O2	-5.05	118.36	121.90
54	BA	315	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1424	G	P-O3'-C3'	5.05	125.77	119.70
54	BA	1838	C	N3-C4-C5	5.05	123.92	121.90
54	BA	1955	U	O4'-C1'-N1	5.05	112.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2558	C	N1-C2-O2	5.05	121.93	118.90
55	BB	28	C	N1-C2-O2	5.05	121.93	118.90
8	AI	122	ARG	NE-CZ-NH1	5.05	122.83	120.30
21	AA	1127	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	291	G	N3-C2-N2	-5.05	116.36	119.90
54	BA	857	G	N7-C8-N9	5.05	115.63	113.10
54	BA	953	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	143	A	C6-C5-N7	5.05	135.84	132.30
54	BA	1125	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1613	G	C5-C6-N1	5.05	114.03	111.50
54	BA	1999	C	O4'-C1'-N1	5.05	112.24	108.20
6	AG	3	ARG	CD-NE-CZ	5.05	130.67	123.60
54	BA	1100	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	1358	G	N3-C4-C5	-5.05	126.08	128.60
54	BA	2401	U	C5'-C4'-O4'	5.05	115.16	109.10
21	AA	106	C	C5'-C4'-O4'	5.05	115.16	109.10
21	AA	940	C	N3-C2-O2	-5.05	118.37	121.90
54	BA	151	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1827	U	N3-C2-O2	-5.05	118.67	122.20
54	BA	2704	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2815	C	N1-C2-O2	5.05	121.93	118.90
54	BA	16	C	O4'-C1'-N1	5.04	112.24	108.20
54	BA	198	C	C6-N1-C2	-5.04	118.28	120.30
54	BA	774	G	O4'-C1'-N9	5.04	112.24	108.20
54	BA	1243	C	N1-C2-O2	5.04	121.93	118.90
54	BA	1685	C	N3-C4-C5	5.04	123.92	121.90
21	AA	54	C	C5-C4-N4	5.04	123.73	120.20
21	AA	1155	A	C3'-C2'-C1'	5.04	105.53	101.50
54	BA	376	G	C5-C6-N1	5.04	114.02	111.50
54	BA	1409	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	2039	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2442	C	N1-C2-O2	5.04	121.93	118.90
54	BA	90	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	559	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	738	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2099	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	626	G	N1-C6-O6	-5.04	116.88	119.90
21	AA	732	C	N1-C2-O2	5.04	121.92	118.90
21	AA	755	G	C5'-C4'-C3'	-5.04	107.94	116.00
54	BA	1148	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2155	U	N1-C2-N3	5.04	117.92	114.90
54	BA	2543	G	C5-C6-N1	5.04	114.02	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	39	A	C5'-C4'-O4'	5.04	115.15	109.10
21	AA	77	A	C6-C5-N7	5.04	135.83	132.30
21	AA	563	A	C6-C5-N7	5.04	135.83	132.30
21	AA	607	A	C6-C5-N7	5.04	135.83	132.30
21	AA	632	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	1441	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	638	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2200	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2561	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	650	C	N3-C4-C5	5.04	123.92	121.90
54	BA	859	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	1191	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	2182	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2323	G	N3-C4-C5	-5.04	126.08	128.60
21	AA	784	A	C5'-C4'-O4'	5.04	115.14	109.10
21	AA	1093	A	O4'-C1'-N9	5.04	112.23	108.20
54	BA	279	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	1864	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	2855	C	N3-C2-O2	-5.04	118.38	121.90
21	AA	333	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	353	A	O4'-C1'-N9	5.03	112.23	108.20
21	AA	1271	A	O4'-C1'-N9	5.03	112.23	108.20
54	BA	1031	G	O4'-C1'-N9	5.03	112.23	108.20
54	BA	1733	G	C5-C6-N1	5.03	114.02	111.50
54	BA	2901	C	N1-C2-O2	5.03	121.92	118.90
55	BB	76	G	C5-C6-N1	5.03	114.02	111.50
21	AA	256	U	C5-C6-N1	-5.03	120.18	122.70
54	BA	228	C	C6-N1-C2	-5.03	118.29	120.30
7	AH	76	ARG	NE-CZ-NH2	-5.03	117.78	120.30
54	BA	312	G	C5'-C4'-O4'	5.03	115.14	109.10
54	BA	508	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	1273	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	1526	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1527	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	1645	G	P-O3'-C3'	5.03	125.73	119.70
54	BA	1657	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1688	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	1805	A	C6-C5-N7	5.03	135.82	132.30
54	BA	1879	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1946	U	C5-C6-N1	-5.03	120.19	122.70
21	AA	1338	G	N1-C6-O6	-5.03	116.88	119.90
38	BP	100	ARG	NE-CZ-NH1	5.03	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1312	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	2592	G	C5-C6-N1	5.03	114.01	111.50
54	BA	2839	G	C8-N9-C4	-5.03	104.39	106.40
21	AA	628	G	N1-C6-O6	-5.03	116.88	119.90
33	BK	18	ARG	NE-CZ-NH1	5.03	122.81	120.30
49	B0	16	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
54	BA	578	G	C5-C6-N1	5.03	114.01	111.50
54	BA	1289	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2752	C	N1-C2-O2	5.03	121.92	118.90
21	AA	316	C	O4'-C1'-N1	5.03	112.22	108.20
21	AA	896	C	N3-C2-O2	-5.03	118.38	121.90
54	BA	251	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	447	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	635	C	N3-C4-C5	5.03	123.91	121.90
54	BA	979	A	C1'-O4'-C4'	-5.03	105.88	109.90
54	BA	1091	G	C4'-C3'-C2'	-5.03	97.58	102.60
54	BA	2192	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	2285	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2413	G	C5'-C4'-O4'	5.03	115.13	109.10
21	AA	140	U	C5-C6-N1	-5.02	120.19	122.70
21	AA	273	U	N3-C2-O2	-5.02	118.69	122.20
21	AA	411	A	O4'-C1'-N9	5.02	112.22	108.20
21	AA	1289	A	C6-C5-N7	5.02	135.81	132.30
37	BO	94	ARG	CD-NE-CZ	5.02	130.63	123.60
54	BA	361	G	O4'-C1'-N9	5.02	112.22	108.20
54	BA	1961	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2001	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2069	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	984	C	N3-C4-C5	5.02	123.91	121.90
55	BB	8	C	N1-C2-O2	5.02	121.91	118.90
13	AN	53	ARG	NE-CZ-NH1	5.02	122.81	120.30
54	BA	839	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1237	A	O4'-C1'-N9	5.02	112.22	108.20
54	BA	1803	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	2103	C	N3-C4-N4	-5.02	114.49	118.00
55	BB	45	A	C4-C5-C6	-5.02	114.49	117.00
11	AL	55	ARG	NE-CZ-NH2	-5.02	117.79	120.30
21	AA	851	G	C5-C6-N1	5.02	114.01	111.50
54	BA	983	A	O4'-C1'-N9	5.02	112.21	108.20
54	BA	1307	A	C6-C5-N7	5.02	135.81	132.30
54	BA	1909	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	2285	C	C4'-C3'-C2'	-5.02	97.58	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2732	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2835	A	C3'-C2'-C1'	5.02	105.52	101.50
21	AA	964	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	357	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	1890	A	C6-C5-N7	5.02	135.81	132.30
55	BB	69	G	O4'-C1'-N9	5.02	112.21	108.20
21	AA	68	G	C5-C6-N1	5.01	114.01	111.50
21	AA	850	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	1095	U	C4-C5-C6	5.01	122.71	119.70
21	AA	1378	C	N1-C2-O2	5.01	121.91	118.90
54	BA	349	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	371	A	C6-C5-N7	5.01	135.81	132.30
54	BA	795	C	O4'-C1'-N1	5.01	112.21	108.20
54	BA	888	C	N1-C2-O2	5.01	121.91	118.90
54	BA	889	C	C5'-C4'-C3'	-5.01	107.98	116.00
54	BA	1644	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1842	G	N3-C4-C5	-5.01	126.09	128.60
21	AA	256	U	N3-C2-O2	-5.01	118.69	122.20
21	AA	1297	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	1625	C	C3'-C2'-C1'	5.01	105.51	101.50
54	BA	1960	A	C6-C5-N7	5.01	135.81	132.30
21	AA	915	A	C6-C5-N7	5.01	135.81	132.30
21	AA	1326	U	N3-C2-O2	-5.01	118.69	122.20
21	AA	1501	C	N1-C2-O2	5.01	121.91	118.90
37	BO	15	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	364	C	N1-C2-O2	5.01	121.91	118.90
54	BA	470	A	C4-C5-C6	-5.01	114.49	117.00
54	BA	957	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1215	G	N3-C2-N2	-5.01	116.39	119.90
54	BA	1643	G	O4'-C1'-N9	5.01	112.21	108.20
54	BA	1656	C	N1-C2-O2	5.01	121.91	118.90
54	BA	2863	C	N3-C2-O2	-5.01	118.39	121.90
21	AA	432	A	O4'-C1'-N9	5.01	112.21	108.20
21	AA	445	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	461	A	C4-C5-C6	-5.01	114.50	117.00
21	AA	1494	G	O4'-C1'-N9	5.01	112.21	108.20
54	BA	673	C	N1-C2-O2	5.01	121.91	118.90
54	BA	1330	C	N3-C2-O2	-5.01	118.39	121.90
54	BA	1349	C	N3-C2-O2	-5.01	118.39	121.90
21	AA	656	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	454	A	C6-C5-N7	5.01	135.81	132.30
21	AA	343	U	N3-C2-O2	-5.01	118.70	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	344	A	C3'-C2'-C1'	5.01	105.51	101.50
21	AA	1427	C	N1-C2-O2	5.01	121.90	118.90
21	AA	1440	U	N3-C2-O2	-5.01	118.69	122.20
41	BS	110	ARG	NE-CZ-NH2	-5.01	117.80	120.30
54	BA	711	G	C5'-C4'-C3'	-5.01	107.99	116.00
54	BA	821	A	N9-C1'-C2'	-5.01	106.49	112.00
54	BA	1895	C	N3-C4-C5	5.01	123.90	121.90
54	BA	2619	C	N3-C4-C5	5.01	123.90	121.90
55	BB	34	A	C6-C5-N7	5.01	135.80	132.30
21	AA	544	G	O4'-C1'-N9	5.00	112.20	108.20
21	AA	932	C	O4'-C1'-N1	5.00	112.20	108.20
24	A3	2	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	1035	U	N3-C2-O2	-5.00	118.70	122.20
54	BA	1929	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	2446	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	2884	U	N3-C2-O2	-5.00	118.70	122.20
21	AA	319	G	N1-C6-O6	-5.00	116.90	119.90
21	AA	334	C	N1-C2-O2	5.00	121.90	118.90
21	AA	335	C	N1-C2-O2	5.00	121.90	118.90
21	AA	564	C	N1-C2-O2	5.00	121.90	118.90
54	BA	148	U	C5-C6-N1	-5.00	120.20	122.70
54	BA	993	G	C5-C6-N1	5.00	114.00	111.50
54	BA	1190	G	C5-C6-N1	5.00	114.00	111.50
54	BA	1501	G	C5-C6-N1	5.00	114.00	111.50
54	BA	1537	G	O4'-C1'-N9	5.00	112.20	108.20
21	AA	144	G	N3-C2-N2	-5.00	116.40	119.90
21	AA	900	A	C6-C5-N7	5.00	135.80	132.30
21	AA	1053	G	C5-C6-N1	5.00	114.00	111.50
21	AA	1098	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	1279	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	200	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	213	A	C6-C5-N7	5.00	135.80	132.30
54	BA	1015	U	C5-C6-N1	-5.00	120.20	122.70
54	BA	1597	A	C6-C5-N7	5.00	135.80	132.30
54	BA	1898	U	C5-C6-N1	-5.00	120.20	122.70
54	BA	2507	C	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (1072) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	11	C	Sidechain

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Mol	Chain	Res	Type	Group
22	A1	18	G	Sidechain
22	A1	19	G	Sidechain
22	A1	23	A	Sidechain
22	A1	24	G	Sidechain
22	A1	27	C	Sidechain
22	A1	28	C	Sidechain
22	A1	3	G	Sidechain
22	A1	44	G	Sidechain
22	A1	45	G	Sidechain
22	A1	49	G	Sidechain
22	A1	53	G	Sidechain
22	A1	58	A	Sidechain
22	A1	60	C	Sidechain
22	A1	65	C	Sidechain
22	A1	66	A	Sidechain
22	A1	67	U	Sidechain
22	A1	68	C	Sidechain
22	A1	8	U	Sidechain
22	A1	9	A	Sidechain
23	A2	84	G	Sidechain
23	A2	86	U	Sidechain
23	A2	87	U	Sidechain
23	A2	88	U	Sidechain
23	A2	90	U	Sidechain
24	A3	16	C	Sidechain
24	A3	2	G	Sidechain
24	A3	24	C	Sidechain
24	A3	26	C	Sidechain
24	A3	36	A	Sidechain
24	A3	37	U	Sidechain
24	A3	54	G	Sidechain
24	A3	62	C	Sidechain
24	A3	67	C	Sidechain
24	A3	7	G	Sidechain
24	A3	73	A	Sidechain
24	A3	74	A	Sidechain
24	A3	75	C	Sidechain
21	AA	1007	U	Sidechain
21	AA	1008	U	Sidechain
21	AA	1010	U	Sidechain
21	AA	102	G	Sidechain
21	AA	1022	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1023	U	Sidechain
21	AA	1024	G	Sidechain
21	AA	1029	U	Sidechain
21	AA	1030	U	Sidechain
21	AA	1038	C	Sidechain
21	AA	1039	G	Sidechain
21	AA	1040	U	Sidechain
21	AA	1041	G	Sidechain
21	AA	1045	C	Sidechain
21	AA	1048	G	Sidechain
21	AA	1051	C	Sidechain
21	AA	1061	G	Sidechain
21	AA	1065	U	Sidechain
21	AA	1066	C	Sidechain
21	AA	1072	G	Sidechain
21	AA	1077	G	Sidechain
21	AA	1079	G	Sidechain
21	AA	108	G	Sidechain
21	AA	1084	G	Sidechain
21	AA	1093	A	Sidechain
21	AA	1095	U	Sidechain
21	AA	1104	G	Sidechain
21	AA	1105	A	Sidechain
21	AA	1108	G	Sidechain
21	AA	111	G	Sidechain
21	AA	1127	G	Sidechain
21	AA	1131	G	Sidechain
21	AA	1136	C	Sidechain
21	AA	1137	C	Sidechain
21	AA	1139	G	Sidechain
21	AA	1141	C	Sidechain
21	AA	1144	G	Sidechain
21	AA	1147	C	Sidechain
21	AA	115	G	Sidechain
21	AA	1151	A	Sidechain
21	AA	1153	G	Sidechain
21	AA	1154	G	Sidechain
21	AA	1168	U	Sidechain
21	AA	1172	C	Sidechain
21	AA	1176	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1181	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1182	G	Sidechain
21	AA	1185	G	Sidechain
21	AA	1186	G	Sidechain
21	AA	1187	G	Sidechain
21	AA	1195	C	Sidechain
21	AA	1207	G	Sidechain
21	AA	121	U	Sidechain
21	AA	1210	C	Sidechain
21	AA	1215	G	Sidechain
21	AA	1217	C	Sidechain
21	AA	1219	A	Sidechain
21	AA	1220	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1224	U	Sidechain
21	AA	1226	C	Sidechain
21	AA	124	C	Sidechain
21	AA	1240	U	Sidechain
21	AA	1245	C	Sidechain
21	AA	1261	A	Sidechain
21	AA	1266	G	Sidechain
21	AA	1276	G	Sidechain
21	AA	128	G	Sidechain
21	AA	1280	A	Sidechain
21	AA	1281	C	Sidechain
21	AA	1285	A	Sidechain
21	AA	1289	A	Sidechain
21	AA	130	A	Sidechain
21	AA	1300	G	Sidechain
21	AA	1301	U	Sidechain
21	AA	1302	C	Sidechain
21	AA	1303	C	Sidechain
21	AA	1305	G	Sidechain
21	AA	1306	A	Sidechain
21	AA	1309	G	Sidechain
21	AA	1316	G	Sidechain
21	AA	1318	A	Sidechain
21	AA	1337	G	Sidechain
21	AA	1339	A	Sidechain
21	AA	1346	A	Sidechain
21	AA	1348	U	Sidechain
21	AA	1350	A	Sidechain
21	AA	1358	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1360	A	Sidechain
21	AA	1370	G	Sidechain
21	AA	1373	G	Sidechain
21	AA	1379	G	Sidechain
21	AA	1380	U	Sidechain
21	AA	1382	C	Sidechain
21	AA	1387	G	Sidechain
21	AA	1391	U	Sidechain
21	AA	1399	C	Sidechain
21	AA	1401	G	Sidechain
21	AA	1409	C	Sidechain
21	AA	1412	C	Sidechain
21	AA	142	G	Sidechain
21	AA	1432	G	Sidechain
21	AA	1433	A	Sidechain
21	AA	1434	A	Sidechain
21	AA	1435	G	Sidechain
21	AA	1441	A	Sidechain
21	AA	1442	G	Sidechain
21	AA	1448	C	Sidechain
21	AA	1453	G	Sidechain
21	AA	1455	G	Sidechain
21	AA	1459	G	Sidechain
21	AA	1460	C	Sidechain
21	AA	1465	A	Sidechain
21	AA	1471	U	Sidechain
21	AA	1472	U	Sidechain
21	AA	1473	G	Sidechain
21	AA	1476	A	Sidechain
21	AA	1478	U	Sidechain
21	AA	1479	C	Sidechain
21	AA	148	G	Sidechain
21	AA	1489	G	Sidechain
21	AA	1491	G	Sidechain
21	AA	1499	A	Sidechain
21	AA	1500	A	Sidechain
21	AA	1503	A	Sidechain
21	AA	1514	G	Sidechain
21	AA	1518	A	Sidechain
21	AA	152	A	Sidechain
21	AA	1528	U	Sidechain
21	AA	157	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	159	G	Sidechain
21	AA	166	U	Sidechain
21	AA	180	U	Sidechain
21	AA	187	G	Sidechain
21	AA	191	G	Sidechain
21	AA	195	A	Sidechain
21	AA	196	A	Sidechain
21	AA	197	A	Sidechain
21	AA	198	G	Sidechain
21	AA	200	G	Sidechain
21	AA	215	C	Sidechain
21	AA	228	A	Sidechain
21	AA	232	G	Sidechain
21	AA	235	C	Sidechain
21	AA	237	G	Sidechain
21	AA	242	G	Sidechain
21	AA	246	A	Sidechain
21	AA	25	C	Sidechain
21	AA	250	A	Sidechain
21	AA	252	U	Sidechain
21	AA	255	G	Sidechain
21	AA	258	G	Sidechain
21	AA	259	G	Sidechain
21	AA	26	A	Sidechain
21	AA	262	A	Sidechain
21	AA	266	G	Sidechain
21	AA	269	C	Sidechain
21	AA	270	A	Sidechain
21	AA	280	C	Sidechain
21	AA	281	G	Sidechain
21	AA	288	A	Sidechain
21	AA	29	U	Sidechain
21	AA	290	C	Sidechain
21	AA	297	G	Sidechain
21	AA	31	G	Sidechain
21	AA	310	G	Sidechain
21	AA	316	C	Sidechain
21	AA	318	G	Sidechain
21	AA	319	G	Sidechain
21	AA	321	A	Sidechain
21	AA	323	U	Sidechain
21	AA	324	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	325	A	Sidechain
21	AA	327	A	Sidechain
21	AA	328	C	Sidechain
21	AA	330	C	Sidechain
21	AA	333	U	Sidechain
21	AA	334	C	Sidechain
21	AA	337	G	Sidechain
21	AA	342	C	Sidechain
21	AA	349	A	Sidechain
21	AA	35	G	Sidechain
21	AA	353	A	Sidechain
21	AA	355	C	Sidechain
21	AA	36	C	Sidechain
21	AA	362	G	Sidechain
21	AA	365	U	Sidechain
21	AA	37	U	Sidechain
21	AA	371	A	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	383	A	Sidechain
21	AA	384	G	Sidechain
21	AA	385	C	Sidechain
21	AA	39	G	Sidechain
21	AA	391	G	Sidechain
21	AA	394	G	Sidechain
21	AA	395	C	Sidechain
21	AA	401	C	Sidechain
21	AA	405	U	Sidechain
21	AA	408	A	Sidechain
21	AA	409	U	Sidechain
21	AA	412	A	Sidechain
21	AA	416	G	Sidechain
21	AA	429	U	Sidechain
21	AA	432	A	Sidechain
21	AA	433	G	Sidechain
21	AA	435	A	Sidechain
21	AA	439	U	Sidechain
21	AA	448	A	Sidechain
21	AA	449	G	Sidechain
21	AA	455	G	Sidechain
21	AA	461	A	Sidechain
21	AA	464	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	465	A	Sidechain
21	AA	468	A	Sidechain
21	AA	470	C	Sidechain
21	AA	474	G	Sidechain
21	AA	475	C	Sidechain
21	AA	476	U	Sidechain
21	AA	478	A	Sidechain
21	AA	479	U	Sidechain
21	AA	484	G	Sidechain
21	AA	487	A	Sidechain
21	AA	491	G	Sidechain
21	AA	492	C	Sidechain
21	AA	494	G	Sidechain
21	AA	496	A	Sidechain
21	AA	5	U	Sidechain
21	AA	51	A	Sidechain
21	AA	511	C	Sidechain
21	AA	515	G	Sidechain
21	AA	518	C	Sidechain
21	AA	529	G	Sidechain
21	AA	535	A	Sidechain
21	AA	537	G	Sidechain
21	AA	538	G	Sidechain
21	AA	54	C	Sidechain
21	AA	555	U	Sidechain
21	AA	558	G	Sidechain
21	AA	561	U	Sidechain
21	AA	566	G	Sidechain
21	AA	571	U	Sidechain
21	AA	579	A	Sidechain
21	AA	581	G	Sidechain
21	AA	584	G	Sidechain
21	AA	587	G	Sidechain
21	AA	588	G	Sidechain
21	AA	595	A	Sidechain
21	AA	599	C	Sidechain
21	AA	601	G	Sidechain
21	AA	602	A	Sidechain
21	AA	61	G	Sidechain
21	AA	610	U	Sidechain
21	AA	614	C	Sidechain
21	AA	618	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	622	A	Sidechain
21	AA	625	U	Sidechain
21	AA	63	C	Sidechain
21	AA	631	C	Sidechain
21	AA	632	U	Sidechain
21	AA	640	A	Sidechain
21	AA	649	A	Sidechain
21	AA	650	G	Sidechain
21	AA	651	C	Sidechain
21	AA	656	G	Sidechain
21	AA	664	G	Sidechain
21	AA	668	G	Sidechain
21	AA	67	C	Sidechain
21	AA	670	G	Sidechain
21	AA	676	A	Sidechain
21	AA	678	U	Sidechain
21	AA	681	A	Sidechain
21	AA	687	A	Sidechain
21	AA	692	U	Sidechain
21	AA	693	G	Sidechain
21	AA	695	A	Sidechain
21	AA	706	A	Sidechain
21	AA	71	A	Sidechain
21	AA	710	G	Sidechain
21	AA	716	A	Sidechain
21	AA	717	U	Sidechain
21	AA	719	C	Sidechain
21	AA	721	G	Sidechain
21	AA	722	G	Sidechain
21	AA	723	U	Sidechain
21	AA	725	G	Sidechain
21	AA	727	G	Sidechain
21	AA	728	A	Sidechain
21	AA	731	G	Sidechain
21	AA	732	C	Sidechain
21	AA	735	C	Sidechain
21	AA	740	U	Sidechain
21	AA	752	G	Sidechain
21	AA	753	A	Sidechain
21	AA	754	C	Sidechain
21	AA	755	G	Sidechain
21	AA	760	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	761	G	Sidechain
21	AA	766	A	Sidechain
21	AA	768	A	Sidechain
21	AA	776	G	Sidechain
21	AA	780	A	Sidechain
21	AA	781	A	Sidechain
21	AA	785	G	Sidechain
21	AA	79	G	Sidechain
21	AA	790	A	Sidechain
21	AA	801	U	Sidechain
21	AA	807	A	Sidechain
21	AA	808	C	Sidechain
21	AA	816	A	Sidechain
21	AA	819	A	Sidechain
21	AA	82	G	Sidechain
21	AA	821	G	Sidechain
21	AA	824	G	Sidechain
21	AA	840	C	Sidechain
21	AA	842	U	Sidechain
21	AA	843	U	Sidechain
21	AA	844	G	Sidechain
21	AA	859	G	Sidechain
21	AA	86	G	Sidechain
21	AA	863	U	Sidechain
21	AA	866	C	Sidechain
21	AA	869	G	Sidechain
21	AA	871	U	Sidechain
21	AA	873	A	Sidechain
21	AA	874	G	Sidechain
21	AA	875	U	Sidechain
21	AA	876	C	Sidechain
21	AA	880	C	Sidechain
21	AA	883	C	Sidechain
21	AA	884	U	Sidechain
21	AA	896	C	Sidechain
21	AA	898	G	Sidechain
21	AA	90	C	Sidechain
21	AA	900	A	Sidechain
21	AA	901	A	Sidechain
21	AA	903	G	Sidechain
21	AA	91	U	Sidechain
21	AA	918	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	919	A	Sidechain
21	AA	92	U	Sidechain
21	AA	921	U	Sidechain
21	AA	922	G	Sidechain
21	AA	923	A	Sidechain
21	AA	925	G	Sidechain
21	AA	926	G	Sidechain
21	AA	928	G	Sidechain
21	AA	932	C	Sidechain
21	AA	935	A	Sidechain
21	AA	940	C	Sidechain
21	AA	941	G	Sidechain
21	AA	942	G	Sidechain
21	AA	945	G	Sidechain
21	AA	947	G	Sidechain
21	AA	948	C	Sidechain
21	AA	949	A	Sidechain
21	AA	951	G	Sidechain
21	AA	954	G	Sidechain
21	AA	959	A	Sidechain
21	AA	964	A	Sidechain
21	AA	968	A	Sidechain
21	AA	97	G	Sidechain
21	AA	972	C	Sidechain
21	AA	982	U	Sidechain
21	AA	984	C	Sidechain
21	AA	985	C	Sidechain
21	AA	99	C	Sidechain
21	AA	991	U	Sidechain
21	AA	993	G	Sidechain
21	AA	995	C	Sidechain
21	AA	998	C	Sidechain
21	AA	999	C	Sidechain
3	AD	75	TYR	Sidechain
10	AK	127	ARG	Sidechain
54	BA	1003	G	Sidechain
54	BA	1007	C	Sidechain
54	BA	101	A	Sidechain
54	BA	1016	G	Sidechain
54	BA	1023	U	Sidechain
54	BA	1024	G	Sidechain
54	BA	1055	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	106	C	Sidechain
54	BA	1062	G	Sidechain
54	BA	1072	C	Sidechain
54	BA	1076	C	Sidechain
54	BA	1078	U	Sidechain
54	BA	1083	U	Sidechain
54	BA	109	C	Sidechain
54	BA	1106	G	Sidechain
54	BA	1112	G	Sidechain
54	BA	1114	C	Sidechain
54	BA	1118	C	Sidechain
54	BA	1124	G	Sidechain
54	BA	1125	G	Sidechain
54	BA	113	U	Sidechain
54	BA	1133	A	Sidechain
54	BA	1135	C	Sidechain
54	BA	1139	G	Sidechain
54	BA	1140	C	Sidechain
54	BA	1141	U	Sidechain
54	BA	1144	A	Sidechain
54	BA	1150	C	Sidechain
54	BA	1151	A	Sidechain
54	BA	1153	C	Sidechain
54	BA	1158	C	Sidechain
54	BA	1159	U	Sidechain
54	BA	116	C	Sidechain
54	BA	1162	G	Sidechain
54	BA	1167	C	Sidechain
54	BA	1170	C	Sidechain
54	BA	1174	U	Sidechain
54	BA	1178	C	Sidechain
54	BA	1182	G	Sidechain
54	BA	1189	A	Sidechain
54	BA	1200	C	Sidechain
54	BA	1201	U	Sidechain
54	BA	1215	G	Sidechain
54	BA	1220	G	Sidechain
54	BA	1227	G	Sidechain
54	BA	1233	C	Sidechain
54	BA	1234	U	Sidechain
54	BA	1235	G	Sidechain
54	BA	1241	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1242	U	Sidechain
54	BA	1244	A	Sidechain
54	BA	1248	G	Sidechain
54	BA	125	A	Sidechain
54	BA	1250	G	Sidechain
54	BA	1251	C	Sidechain
54	BA	1254	A	Sidechain
54	BA	1263	U	Sidechain
54	BA	1264	A	Sidechain
54	BA	1270	C	Sidechain
54	BA	1275	A	Sidechain
54	BA	1277	G	Sidechain
54	BA	1288	G	Sidechain
54	BA	1289	C	Sidechain
54	BA	1291	C	Sidechain
54	BA	1299	G	Sidechain
54	BA	1303	G	Sidechain
54	BA	1304	A	Sidechain
54	BA	1311	G	Sidechain
54	BA	1315	C	Sidechain
54	BA	1316	U	Sidechain
54	BA	1319	C	Sidechain
54	BA	1320	C	Sidechain
54	BA	1323	C	Sidechain
54	BA	1328	A	Sidechain
54	BA	1330	C	Sidechain
54	BA	1331	G	Sidechain
54	BA	1333	G	Sidechain
54	BA	134	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1341	G	Sidechain
54	BA	1343	G	Sidechain
54	BA	1346	G	Sidechain
54	BA	1347	A	Sidechain
54	BA	1356	G	Sidechain
54	BA	1359	A	Sidechain
54	BA	1371	G	Sidechain
54	BA	1372	U	Sidechain
54	BA	138	U	Sidechain
54	BA	1386	C	Sidechain
54	BA	1387	A	Sidechain
54	BA	1389	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1398	C	Sidechain
54	BA	1399	C	Sidechain
54	BA	1411	U	Sidechain
54	BA	1418	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1428	C	Sidechain
54	BA	1433	A	Sidechain
54	BA	1438	U	Sidechain
54	BA	1443	U	Sidechain
54	BA	1444	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1451	C	Sidechain
54	BA	1454	C	Sidechain
54	BA	1455	G	Sidechain
54	BA	1457	U	Sidechain
54	BA	1460	U	Sidechain
54	BA	1468	U	Sidechain
54	BA	1476	U	Sidechain
54	BA	1478	G	Sidechain
54	BA	1488	C	Sidechain
54	BA	1490	A	Sidechain
54	BA	1492	G	Sidechain
54	BA	1494	A	Sidechain
54	BA	1497	U	Sidechain
54	BA	150	U	Sidechain
54	BA	1513	U	Sidechain
54	BA	1517	G	Sidechain
54	BA	1527	G	Sidechain
54	BA	1529	G	Sidechain
54	BA	1536	C	Sidechain
54	BA	1538	G	Sidechain
54	BA	1539	U	Sidechain
54	BA	1543	G	Sidechain
54	BA	1547	C	Sidechain
54	BA	1549	A	Sidechain
54	BA	1552	A	Sidechain
54	BA	1558	C	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1562	U	Sidechain
54	BA	1564	C	Sidechain
54	BA	1565	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1566	A	Sidechain
54	BA	1573	G	Sidechain
54	BA	1581	G	Sidechain
54	BA	159	G	Sidechain
54	BA	1602	U	Sidechain
54	BA	1606	C	Sidechain
54	BA	1610	A	Sidechain
54	BA	1612	C	Sidechain
54	BA	1615	C	Sidechain
54	BA	1617	C	Sidechain
54	BA	1618	A	Sidechain
54	BA	162	U	Sidechain
54	BA	1631	G	Sidechain
54	BA	164	C	Sidechain
54	BA	1642	G	Sidechain
54	BA	1647	U	Sidechain
54	BA	1649	G	Sidechain
54	BA	1653	G	Sidechain
54	BA	1654	A	Sidechain
54	BA	1658	C	Sidechain
54	BA	1676	A	Sidechain
54	BA	1677	A	Sidechain
54	BA	1680	U	Sidechain
54	BA	1682	G	Sidechain
54	BA	1684	G	Sidechain
54	BA	1697	G	Sidechain
54	BA	1699	G	Sidechain
54	BA	17	G	Sidechain
54	BA	1706	C	Sidechain
54	BA	1709	U	Sidechain
54	BA	171	U	Sidechain
54	BA	1710	G	Sidechain
54	BA	1715	G	Sidechain
54	BA	1716	U	Sidechain
54	BA	1722	A	Sidechain
54	BA	1723	G	Sidechain
54	BA	1731	G	Sidechain
54	BA	1734	G	Sidechain
54	BA	174	U	Sidechain
54	BA	1744	A	Sidechain
54	BA	1748	C	Sidechain
54	BA	175	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1750	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1759	A	Sidechain
54	BA	1761	C	Sidechain
54	BA	1762	A	Sidechain
54	BA	1763	G	Sidechain
54	BA	1777	U	Sidechain
54	BA	1780	A	Sidechain
54	BA	1781	U	Sidechain
54	BA	1783	A	Sidechain
54	BA	1786	A	Sidechain
54	BA	1796	U	Sidechain
54	BA	1797	G	Sidechain
54	BA	1799	G	Sidechain
54	BA	1800	C	Sidechain
54	BA	1807	G	Sidechain
54	BA	1817	G	Sidechain
54	BA	1818	U	Sidechain
54	BA	1821	A	Sidechain
54	BA	1825	U	Sidechain
54	BA	1826	G	Sidechain
54	BA	1827	U	Sidechain
54	BA	1830	C	Sidechain
54	BA	1831	G	Sidechain
54	BA	1833	C	Sidechain
54	BA	1840	G	Sidechain
54	BA	1842	G	Sidechain
54	BA	1843	C	Sidechain
54	BA	1845	G	Sidechain
54	BA	1848	A	Sidechain
54	BA	1849	G	Sidechain
54	BA	1851	U	Sidechain
54	BA	1854	A	Sidechain
54	BA	1859	U	Sidechain
54	BA	1861	G	Sidechain
54	BA	1865	U	Sidechain
54	BA	1876	A	Sidechain
54	BA	1881	C	Sidechain
54	BA	1884	G	Sidechain
54	BA	1892	C	Sidechain
54	BA	19	A	Sidechain
54	BA	1903	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1906	G	Sidechain
54	BA	1907	G	Sidechain
54	BA	1917	U	Sidechain
54	BA	1924	C	Sidechain
54	BA	1926	U	Sidechain
54	BA	1929	G	Sidechain
54	BA	1931	U	Sidechain
54	BA	1938	A	Sidechain
54	BA	1945	G	Sidechain
54	BA	1949	G	Sidechain
54	BA	1951	U	Sidechain
54	BA	1954	G	Sidechain
54	BA	1959	G	Sidechain
54	BA	1973	G	Sidechain
54	BA	1981	A	Sidechain
54	BA	1983	G	Sidechain
54	BA	1985	C	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	2001	C	Sidechain
54	BA	2013	A	Sidechain
54	BA	2014	A	Sidechain
54	BA	2017	U	Sidechain
54	BA	2019	A	Sidechain
54	BA	2027	G	Sidechain
54	BA	2028	U	Sidechain
54	BA	2030	A	Sidechain
54	BA	2032	G	Sidechain
54	BA	2036	C	Sidechain
54	BA	2037	A	Sidechain
54	BA	2038	G	Sidechain
54	BA	2039	U	Sidechain
54	BA	2042	A	Sidechain
54	BA	2047	C	Sidechain
54	BA	2048	G	Sidechain
54	BA	206	U	Sidechain
54	BA	2065	C	Sidechain
54	BA	2071	A	Sidechain
54	BA	2075	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2077	A	Sidechain
54	BA	2078	C	Sidechain
54	BA	2079	U	Sidechain
54	BA	2094	A	Sidechain
54	BA	2095	A	Sidechain
54	BA	21	A	Sidechain
54	BA	2100	G	Sidechain
54	BA	2102	G	Sidechain
54	BA	2120	G	Sidechain
54	BA	2121	G	Sidechain
54	BA	2128	G	Sidechain
54	BA	2130	U	Sidechain
54	BA	2132	U	Sidechain
54	BA	2133	G	Sidechain
54	BA	2140	G	Sidechain
54	BA	2141	G	Sidechain
54	BA	2146	C	Sidechain
54	BA	2148	G	Sidechain
54	BA	2159	G	Sidechain
54	BA	2161	C	Sidechain
54	BA	2162	G	Sidechain
54	BA	2168	G	Sidechain
54	BA	2179	C	Sidechain
54	BA	2186	G	Sidechain
54	BA	2190	G	Sidechain
54	BA	221	A	Sidechain
54	BA	2215	C	Sidechain
54	BA	2220	U	Sidechain
54	BA	2230	G	Sidechain
54	BA	2234	G	Sidechain
54	BA	2238	G	Sidechain
54	BA	224	U	Sidechain
54	BA	2242	G	Sidechain
54	BA	2244	U	Sidechain
54	BA	2250	G	Sidechain
54	BA	2253	G	Sidechain
54	BA	2256	G	Sidechain
54	BA	2267	A	Sidechain
54	BA	2269	G	Sidechain
54	BA	227	A	Sidechain
54	BA	2273	A	Sidechain
54	BA	2279	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	228	C	Sidechain
54	BA	2282	G	Sidechain
54	BA	2287	A	Sidechain
54	BA	2293	G	Sidechain
54	BA	2294	G	Sidechain
54	BA	2295	C	Sidechain
54	BA	2299	U	Sidechain
54	BA	2307	G	Sidechain
54	BA	2311	A	Sidechain
54	BA	2319	G	Sidechain
54	BA	232	G	Sidechain
54	BA	2327	A	Sidechain
54	BA	2331	G	Sidechain
54	BA	2332	C	Sidechain
54	BA	2336	A	Sidechain
54	BA	235	U	Sidechain
54	BA	2352	A	Sidechain
54	BA	2357	G	Sidechain
54	BA	2361	G	Sidechain
54	BA	2369	A	Sidechain
54	BA	2375	G	Sidechain
54	BA	238	C	Sidechain
54	BA	2391	G	Sidechain
54	BA	2392	A	Sidechain
54	BA	2394	C	Sidechain
54	BA	2396	G	Sidechain
54	BA	2398	U	Sidechain
54	BA	24	G	Sidechain
54	BA	2401	U	Sidechain
54	BA	2406	A	Sidechain
54	BA	2407	A	Sidechain
54	BA	2411	A	Sidechain
54	BA	2419	U	Sidechain
54	BA	2420	C	Sidechain
54	BA	2421	G	Sidechain
54	BA	2429	G	Sidechain
54	BA	2430	A	Sidechain
54	BA	2436	G	Sidechain
54	BA	244	A	Sidechain
54	BA	2445	G	Sidechain
54	BA	2446	G	Sidechain
54	BA	2450	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2451	A	Sidechain
54	BA	2452	C	Sidechain
54	BA	2454	G	Sidechain
54	BA	2468	A	Sidechain
54	BA	2470	G	Sidechain
54	BA	2476	A	Sidechain
54	BA	2482	A	Sidechain
54	BA	2488	G	Sidechain
54	BA	2489	U	Sidechain
54	BA	2490	G	Sidechain
54	BA	2492	U	Sidechain
54	BA	2495	G	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2505	G	Sidechain
54	BA	2508	G	Sidechain
54	BA	2516	A	Sidechain
54	BA	2518	A	Sidechain
54	BA	252	G	Sidechain
54	BA	2525	G	Sidechain
54	BA	2527	C	Sidechain
54	BA	2528	U	Sidechain
54	BA	2529	G	Sidechain
54	BA	2547	A	Sidechain
54	BA	2549	G	Sidechain
54	BA	2560	A	Sidechain
54	BA	2563	U	Sidechain
54	BA	2576	G	Sidechain
54	BA	2581	G	Sidechain
54	BA	2583	G	Sidechain
54	BA	2586	U	Sidechain
54	BA	2595	G	Sidechain
54	BA	2596	U	Sidechain
54	BA	26	G	Sidechain
54	BA	2600	A	Sidechain
54	BA	2606	C	Sidechain
54	BA	2608	G	Sidechain
54	BA	2614	A	Sidechain
54	BA	2615	U	Sidechain
54	BA	2621	G	Sidechain
54	BA	2624	G	Sidechain
54	BA	2625	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2627	G	Sidechain
54	BA	2628	C	Sidechain
54	BA	2635	A	Sidechain
54	BA	2639	A	Sidechain
54	BA	2640	G	Sidechain
54	BA	2645	G	Sidechain
54	BA	2649	C	Sidechain
54	BA	2651	C	Sidechain
54	BA	2661	G	Sidechain
54	BA	2668	G	Sidechain
54	BA	2683	C	Sidechain
54	BA	2689	U	Sidechain
54	BA	2692	G	Sidechain
54	BA	2711	A	Sidechain
54	BA	2713	U	Sidechain
54	BA	2716	C	Sidechain
54	BA	2718	G	Sidechain
54	BA	272	A	Sidechain
54	BA	273	G	Sidechain
54	BA	2730	C	Sidechain
54	BA	2738	A	Sidechain
54	BA	274	C	Sidechain
54	BA	2741	A	Sidechain
54	BA	2743	U	Sidechain
54	BA	2755	C	Sidechain
54	BA	2765	A	Sidechain
54	BA	2768	U	Sidechain
54	BA	277	G	Sidechain
54	BA	2771	C	Sidechain
54	BA	2773	C	Sidechain
54	BA	2777	G	Sidechain
54	BA	278	A	Sidechain
54	BA	2783	U	Sidechain
54	BA	2784	U	Sidechain
54	BA	2785	C	Sidechain
54	BA	28	A	Sidechain
54	BA	2803	G	Sidechain
54	BA	2804	U	Sidechain
54	BA	2805	C	Sidechain
54	BA	2806	C	Sidechain
54	BA	2811	G	Sidechain
54	BA	2817	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2821	A	Sidechain
54	BA	2822	G	Sidechain
54	BA	283	G	Sidechain
54	BA	2839	G	Sidechain
54	BA	2841	C	Sidechain
54	BA	2850	A	Sidechain
54	BA	2854	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2859	G	Sidechain
54	BA	2862	G	Sidechain
54	BA	2867	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	2871	U	Sidechain
54	BA	2872	A	Sidechain
54	BA	2873	A	Sidechain
54	BA	2877	G	Sidechain
54	BA	2883	A	Sidechain
54	BA	289	G	Sidechain
54	BA	2891	U	Sidechain
54	BA	2892	G	Sidechain
54	BA	2897	U	Sidechain
54	BA	297	G	Sidechain
54	BA	298	G	Sidechain
54	BA	3	U	Sidechain
54	BA	303	G	Sidechain
54	BA	307	G	Sidechain
54	BA	310	A	Sidechain
54	BA	313	G	Sidechain
54	BA	319	G	Sidechain
54	BA	323	C	Sidechain
54	BA	327	G	Sidechain
54	BA	331	C	Sidechain
54	BA	332	A	Sidechain
54	BA	333	G	Sidechain
54	BA	334	C	Sidechain
54	BA	339	U	Sidechain
54	BA	354	A	Sidechain
54	BA	357	C	Sidechain
54	BA	360	U	Sidechain
54	BA	361	G	Sidechain
54	BA	363	G	Sidechain
54	BA	370	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	375	G	Sidechain
54	BA	382	A	Sidechain
54	BA	385	C	Sidechain
54	BA	386	G	Sidechain
54	BA	39	G	Sidechain
54	BA	391	A	Sidechain
54	BA	392	U	Sidechain
54	BA	394	C	Sidechain
54	BA	397	U	Sidechain
54	BA	403	U	Sidechain
54	BA	409	G	Sidechain
54	BA	410	G	Sidechain
54	BA	418	C	Sidechain
54	BA	420	C	Sidechain
54	BA	430	A	Sidechain
54	BA	431	U	Sidechain
54	BA	433	C	Sidechain
54	BA	437	U	Sidechain
54	BA	445	C	Sidechain
54	BA	446	G	Sidechain
54	BA	457	A	Sidechain
54	BA	458	G	Sidechain
54	BA	463	G	Sidechain
54	BA	47	C	Sidechain
54	BA	471	A	Sidechain
54	BA	472	A	Sidechain
54	BA	473	G	Sidechain
54	BA	477	A	Sidechain
54	BA	479	A	Sidechain
54	BA	481	G	Sidechain
54	BA	485	C	Sidechain
54	BA	489	G	Sidechain
54	BA	49	A	Sidechain
54	BA	491	G	Sidechain
54	BA	492	A	Sidechain
54	BA	493	G	Sidechain
54	BA	502	A	Sidechain
54	BA	507	A	Sidechain
54	BA	508	A	Sidechain
54	BA	515	A	Sidechain
54	BA	518	G	Sidechain
54	BA	522	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	527	C	Sidechain
54	BA	537	G	Sidechain
54	BA	551	G	Sidechain
54	BA	559	G	Sidechain
54	BA	560	C	Sidechain
54	BA	569	U	Sidechain
54	BA	575	A	Sidechain
54	BA	578	G	Sidechain
54	BA	580	U	Sidechain
54	BA	587	C	Sidechain
54	BA	589	U	Sidechain
54	BA	595	C	Sidechain
54	BA	597	G	Sidechain
54	BA	601	C	Sidechain
54	BA	603	A	Sidechain
54	BA	606	U	Sidechain
54	BA	607	U	Sidechain
54	BA	611	C	Sidechain
54	BA	617	G	Sidechain
54	BA	629	G	Sidechain
54	BA	630	G	Sidechain
54	BA	631	A	Sidechain
54	BA	640	C	Sidechain
54	BA	641	U	Sidechain
54	BA	647	G	Sidechain
54	BA	648	G	Sidechain
54	BA	65	U	Sidechain
54	BA	650	C	Sidechain
54	BA	662	G	Sidechain
54	BA	669	G	Sidechain
54	BA	671	C	Sidechain
54	BA	674	G	Sidechain
54	BA	68	G	Sidechain
54	BA	692	C	Sidechain
54	BA	695	G	Sidechain
54	BA	7	G	Sidechain
54	BA	700	G	Sidechain
54	BA	715	A	Sidechain
54	BA	718	A	Sidechain
54	BA	72	U	Sidechain
54	BA	724	U	Sidechain
54	BA	726	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	736	C	Sidechain
54	BA	738	G	Sidechain
54	BA	74	A	Sidechain
54	BA	749	A	Sidechain
54	BA	751	A	Sidechain
54	BA	753	A	Sidechain
54	BA	754	U	Sidechain
54	BA	759	G	Sidechain
54	BA	768	G	Sidechain
54	BA	77	G	Sidechain
54	BA	776	G	Sidechain
54	BA	777	G	Sidechain
54	BA	780	G	Sidechain
54	BA	787	C	Sidechain
54	BA	789	A	Sidechain
54	BA	790	U	Sidechain
54	BA	793	A	Sidechain
54	BA	795	C	Sidechain
54	BA	802	A	Sidechain
54	BA	808	G	Sidechain
54	BA	81	G	Sidechain
54	BA	817	C	Sidechain
54	BA	819	A	Sidechain
54	BA	821	A	Sidechain
54	BA	822	G	Sidechain
54	BA	825	A	Sidechain
54	BA	827	U	Sidechain
54	BA	828	U	Sidechain
54	BA	829	A	Sidechain
54	BA	830	G	Sidechain
54	BA	838	C	Sidechain
54	BA	848	C	Sidechain
54	BA	849	A	Sidechain
54	BA	85	G	Sidechain
54	BA	852	U	Sidechain
54	BA	855	G	Sidechain
54	BA	859	G	Sidechain
54	BA	861	A	Sidechain
54	BA	863	A	Sidechain
54	BA	866	A	Sidechain
54	BA	872	U	Sidechain
54	BA	880	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	893	C	Sidechain
54	BA	902	C	Sidechain
54	BA	910	A	Sidechain
54	BA	912	C	Sidechain
54	BA	917	A	Sidechain
54	BA	918	A	Sidechain
54	BA	923	G	Sidechain
54	BA	930	G	Sidechain
54	BA	931	U	Sidechain
54	BA	936	A	Sidechain
54	BA	940	G	Sidechain
54	BA	946	C	Sidechain
54	BA	949	G	Sidechain
54	BA	951	C	Sidechain
54	BA	954	G	Sidechain
54	BA	959	A	Sidechain
54	BA	960	A	Sidechain
54	BA	964	C	Sidechain
54	BA	965	C	Sidechain
54	BA	966	G	Sidechain
54	BA	972	A	Sidechain
54	BA	979	A	Sidechain
54	BA	981	A	Sidechain
54	BA	983	A	Sidechain
54	BA	984	A	Sidechain
54	BA	987	C	Sidechain
54	BA	989	G	Sidechain
54	BA	990	A	Sidechain
55	BB	10	G	Sidechain
55	BB	100	G	Sidechain
55	BB	109	A	Sidechain
55	BB	11	C	Sidechain
55	BB	112	G	Sidechain
55	BB	117	G	Sidechain
55	BB	12	C	Sidechain
55	BB	2	G	Sidechain
55	BB	23	G	Sidechain
55	BB	30	C	Sidechain
55	BB	33	G	Sidechain
55	BB	4	C	Sidechain
55	BB	40	U	Sidechain
55	BB	48	U	Sidechain

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Mol	Chain	Res	Type	Group
55	BB	57	A	Sidechain
55	BB	58	A	Sidechain
55	BB	59	A	Sidechain
55	BB	6	G	Sidechain
55	BB	63	C	Sidechain
55	BB	64	G	Sidechain
55	BB	66	A	Sidechain
55	BB	67	G	Sidechain
55	BB	68	C	Sidechain
55	BB	69	G	Sidechain
55	BB	7	G	Sidechain
55	BB	72	G	Sidechain
55	BB	84	G	Sidechain
55	BB	90	C	Sidechain
55	BB	95	U	Sidechain
55	BB	98	G	Sidechain
25	BC	102	TYR	Sidechain
26	BD	151	THR	Peptide
31	BI	140	GLU	Mainchain
35	BM	97	GLN	Peptide
36	BN	90	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	1	0
3	AD	1643	0	1710	1	0
4	AE	1109	0	1152	0	0
5	AF	818	0	808	1	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	1	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16457	2	0
22	A1	1627	0	832	1	0
23	A2	309	0	158	0	0
24	A3	1642	0	839	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	0	0
34	BL	1045	0	1117	0	0
35	BM	1074	0	1157	0	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	1	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	31205	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BB	2504	0	1269	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	99454	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)
54:BA:1068:G:H1'	54:BA:1069:A:C6	2.45	0.51
54:BA:1131:G:C5	54:BA:2025:C:H4'	2.50	0.46
22:A1:53:G:C8	22:A1:54:5MU:H72	2.50	0.46
18:AS:46:LEU:H	18:AS:46:LEU:HD23	1.81	0.46
3:AD:86:GLY:H	3:AD:200:VAL:HG23	1.81	0.45
48:BZ:28:LEU:H	48:BZ:28:LEU:HD23	1.82	0.45
8:AI:2:ACE:H1	8:AI:22:PRO:HG2	2.00	0.44
21:AA:477:C:H2'	21:AA:478:A:C8	2.53	0.43
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.37	0.43
21:AA:315:A:HO2'	21:AA:316:C:P	2.42	0.42
54:BA:1801:A:H3'	54:BA:1802:A:C5'	2.49	0.42
54:BA:1132:U:H2'	54:BA:1133:A:C8	2.55	0.42
54:BA:2233:U:H2'	54:BA:2234:G:C8	2.55	0.42
54:BA:1891:G:H2'	54:BA:1892:C:C6	2.55	0.41
2:AC:54:ILE:HG22	2:AC:68:HIS:H	1.86	0.41
54:BA:2014:A:H2'	54:BA:2015:A:C8	2.57	0.40
54:BA:2063:C:H2'	54:BA:2064:C:C6	2.57	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%)	15 (7%)	3 (1%)	11	46
2	AC	205/208 (99%)	188 (92%)	12 (6%)	5 (2%)	6	33
3	AD	203/206 (98%)	190 (94%)	7 (3%)	6 (3%)	4	28
4	AE	150/152 (99%)	136 (91%)	11 (7%)	3 (2%)	7	38
5	AF	99/101 (98%)	83 (84%)	12 (12%)	4 (4%)	3	23
6	AG	150/152 (99%)	133 (89%)	14 (9%)	3 (2%)	7	38
7	AH	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
8	AI	126/128 (98%)	117 (93%)	6 (5%)	3 (2%)	6	33
9	AJ	98/100 (98%)	87 (89%)	6 (6%)	5 (5%)	2	19
10	AK	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9	42
11	AL	121/124 (98%)	109 (90%)	8 (7%)	4 (3%)	4	26
12	AM	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
13	AN	98/101 (97%)	86 (88%)	9 (9%)	3 (3%)	4	27
14	AO	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6	34
15	AP	79/81 (98%)	64 (81%)	9 (11%)	6 (8%)	1	13
16	AQ	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	12	48
17	AR	55/57 (96%)	51 (93%)	3 (6%)	1 (2%)	8	40
18	AS	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	12	48
19	AT	84/86 (98%)	75 (89%)	5 (6%)	4 (5%)	2	21
20	AU	51/53 (96%)	34 (67%)	13 (26%)	4 (8%)	1	13
25	BC	270/273 (99%)	241 (89%)	21 (8%)	8 (3%)	4	28
26	BD	207/209 (99%)	181 (87%)	18 (9%)	8 (4%)	3	23
27	BE	199/201 (99%)	172 (86%)	18 (9%)	9 (4%)	2	22
28	BF	176/179 (98%)	151 (86%)	20 (11%)	5 (3%)	5	30
29	BG	174/177 (98%)	151 (87%)	16 (9%)	7 (4%)	3	23
30	BH	147/149 (99%)	133 (90%)	12 (8%)	2 (1%)	11	46
31	BI	139/142 (98%)	128 (92%)	10 (7%)	1 (1%)	22	63
32	BJ	140/142 (99%)	123 (88%)	14 (10%)	3 (2%)	7	36
33	BK	121/123 (98%)	104 (86%)	13 (11%)	4 (3%)	4	26
34	BL	141/144 (98%)	110 (78%)	23 (16%)	8 (6%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BM	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	6	35
36	BN	119/121 (98%)	102 (86%)	16 (13%)	1 (1%)	19	60
37	BO	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
38	BP	112/115 (97%)	96 (86%)	12 (11%)	4 (4%)	3	25
39	BQ	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	17	57
40	BR	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
41	BS	108/110 (98%)	95 (88%)	12 (11%)	1 (1%)	17	57
42	BT	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	6	35
43	BU	101/104 (97%)	83 (82%)	13 (13%)	5 (5%)	2	20
44	BV	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
45	BW	78/80 (98%)	63 (81%)	11 (14%)	4 (5%)	2	19
46	BX	75/79 (95%)	68 (91%)	5 (7%)	2 (3%)	5	31
47	BY	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
48	BZ	56/59 (95%)	50 (89%)	3 (5%)	3 (5%)	2	19
49	B0	54/57 (95%)	48 (89%)	4 (7%)	2 (4%)	3	24
50	B1	50/52 (96%)	42 (84%)	4 (8%)	4 (8%)	1	12
51	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6	34
52	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	4	26
53	B4	36/38 (95%)	27 (75%)	8 (22%)	1 (3%)	5	30
56	B5	221/234 (94%)	207 (94%)	11 (5%)	3 (1%)	11	46
All	All	5876/6008 (98%)	5232 (89%)	490 (8%)	154 (3%)	8	31

All (154) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	73	ARG
2	AC	14	VAL
3	AD	82	LYS
9	AJ	77	VAL
15	AP	79	ASN
19	AT	3	ILE
20	AU	25	ALA
25	BC	141	HIS
32	BJ	48	VAL
32	BJ	81	ILE

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Mol	Chain	Res	Type
38	BP	113	LEU
43	BU	45	GLN
43	BU	70	ALA
45	BW	36	ILE
52	B3	3	ILE
56	B5	50	ILE
1	AB	20	ARG
2	AC	180	ASP
3	AD	194	ILE
4	AE	105	ILE
5	AF	6	ILE
5	AF	63	ASN
6	AG	6	ILE
8	AI	55	ASP
9	AJ	57	VAL
9	AJ	58	ASN
11	AL	15	VAL
13	AN	38	ASP
14	AO	45	HIS
18	AS	2	ARG
20	AU	9	GLU
20	AU	27	VAL
25	BC	68	ARG
25	BC	161	VAL
26	BD	60	VAL
26	BD	146	ILE
27	BE	9	GLN
27	BE	69	ARG
28	BF	12	VAL
28	BF	136	ILE
30	BH	9	VAL
30	BH	121	VAL
31	BI	119	ALA
33	BK	103	VAL
34	BL	33	ARG
34	BL	101	ILE
35	BM	21	ALA
43	BU	12	VAL
46	BX	20	ALA
49	B0	5	ASN
2	AC	2	GLN
3	AD	4	LEU

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Mol	Chain	Res	Type
5	AF	8	PHE
5	AF	90	MET
6	AG	115	MET
9	AJ	75	ASP
11	AL	78	VAL
14	AO	23	SER
15	AP	9	HIS
15	AP	26	ASN
15	AP	50	THR
25	BC	89	ASN
25	BC	142	ASN
26	BD	51	THR
26	BD	119	ALA
26	BD	136	ASN
26	BD	151	THR
27	BE	97	ASN
27	BE	123	LYS
29	BG	151	ARG
33	BK	46	ALA
34	BL	17	LYS
35	BM	20	LEU
35	BM	36	VAL
46	BX	33	HIS
48	BZ	9	THR
50	B1	50	GLU
53	B4	2	LYS
56	B5	91	GLY
1	AB	204	ASP
2	AC	195	ILE
3	AD	29	THR
3	AD	193	ASP
4	AE	127	TYR
8	AI	39	GLY
11	AL	33	CYS
13	AN	92	GLU
15	AP	17	TYR
16	AQ	3	LYS
19	AT	2	ASN
20	AU	52	VAL
25	BC	37	SER
26	BD	22	ILE
27	BE	31	VAL

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Mol	Chain	Res	Type
27	BE	49	ARG
28	BF	123	GLY
28	BF	133	GLU
29	BG	154	GLU
29	BG	175	LYS
34	BL	28	GLY
34	BL	46	VAL
36	BN	70	THR
38	BP	24	THR
42	BT	73	ARG
45	BW	76	ARG
52	B3	46	LYS
4	AE	43	GLY
6	AG	9	ARG
10	AK	125	LYS
11	AL	43	LYS
15	AP	40	ASN
19	AT	67	HIS
27	BE	147	LEU
27	BE	188	MET
29	BG	9	VAL
29	BG	16	VAL
33	BK	2	ILE
34	BL	75	ALA
38	BP	112	ARG
39	BQ	86	SER
41	BS	88	ARG
42	BT	35	ALA
43	BU	90	LYS
45	BW	48	ALA
48	BZ	31	ILE
56	B5	42	VAL
2	AC	145	ALA
3	AD	28	ASP
8	AI	12	LYS
13	AN	63	ARG
19	AT	65	LEU
25	BC	191	LEU
28	BF	103	ILE
34	BL	36	LYS
45	BW	63	ASP
49	B0	54	ILE

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Mol	Chain	Res	Type
50	B1	4	ILE
50	B1	37	LYS
51	B2	44	VAL
10	AK	77	GLY
25	BC	230	PRO
34	BL	55	MET
9	AJ	42	LEU
17	AR	20	ILE
29	BG	168	VAL
32	BJ	11	VAL
43	BU	56	GLY
48	BZ	32	GLY
50	B1	46	VAL
26	BD	93	GLY
29	BG	112	VAL
33	BK	71	ARG
27	BE	169	VAL
38	BP	69	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%)	178 (99%)	2 (1%)	73	84
2	AC	170/171 (99%)	169 (99%)	1 (1%)	86	92
3	AD	172/173 (99%)	167 (97%)	5 (3%)	42	64
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	86 (99%)	1 (1%)	73	84
6	AG	123/123 (100%)	121 (98%)	2 (2%)	62	79
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%)	84 (98%)	2 (2%)	50	70
10	AK	90/90 (100%)	89 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	AL	103/104 (99%)	103 (100%)	0	100	100
12	AM	91/92 (99%)	91 (100%)	0	100	100
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%)	62 (95%)	3 (5%)	27	52
16	AQ	74/74 (100%)	72 (97%)	2 (3%)	44	65
17	AR	48/48 (100%)	46 (96%)	2 (4%)	30	54
18	AS	70/70 (100%)	69 (99%)	1 (1%)	67	80
19	AT	65/65 (100%)	62 (95%)	3 (5%)	27	52
20	AU	44/44 (100%)	42 (96%)	2 (4%)	27	52
25	BC	216/217 (100%)	211 (98%)	5 (2%)	50	70
26	BD	164/164 (100%)	162 (99%)	2 (1%)	71	83
27	BE	165/165 (100%)	160 (97%)	5 (3%)	41	63
28	BF	149/150 (99%)	146 (98%)	3 (2%)	55	74
29	BG	137/138 (99%)	134 (98%)	3 (2%)	52	71
30	BH	114/114 (100%)	113 (99%)	1 (1%)	78	87
31	BI	109/110 (99%)	109 (100%)	0	100	100
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	46	66
33	BK	103/103 (100%)	103 (100%)	0	100	100
34	BL	102/103 (99%)	100 (98%)	2 (2%)	55	74
35	BM	109/109 (100%)	108 (99%)	1 (1%)	78	87
36	BN	100/100 (100%)	97 (97%)	3 (3%)	41	63
37	BO	86/87 (99%)	82 (95%)	4 (5%)	26	51
38	BP	99/100 (99%)	95 (96%)	4 (4%)	31	55
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	52	71
40	BR	84/84 (100%)	83 (99%)	1 (1%)	71	83
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%)	77 (99%)	1 (1%)	69	81
45	BW	59/59 (100%)	58 (98%)	1 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	46 (96%)	2 (4%)	30	54
49	B0	47/48 (98%)	43 (92%)	4 (8%)	10	33
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%)	50 (98%)	1 (2%)	55	74
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	171 (99%)	2 (1%)	71	83
All	All	4842/4870 (99%)	4750 (98%)	92 (2%)	59	75

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	22	TRP
1	AB	135	MET
2	AC	128	MET
3	AD	130	ASN
3	AD	144	ILE
3	AD	187	ARG
3	AD	196	GLU
3	AD	200	VAL
5	AF	100	SER
6	AG	57	GLU
6	AG	137	ARG
7	AH	2	MET
7	AH	29	SER
7	AH	66	GLN
8	AI	71	ILE
8	AI	80	HIS
8	AI	105	ARG
8	AI	129	ARG
9	AJ	47	GLU
9	AJ	77	VAL
10	AK	55	ARG
13	AN	71	HIS
13	AN	92	GLU
14	AO	5	GLU
14	AO	55	LEU

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Mol	Chain	Res	Type
15	AP	1	MET
15	AP	39	PHE
15	AP	55	ASP
16	AQ	14	ASP
16	AQ	39	ARG
17	AR	69	TYR
17	AR	73	HIS
18	AS	73	PHE
19	AT	5	SER
19	AT	14	GLU
19	AT	74	HIS
20	AU	28	LEU
20	AU	30	GLU
25	BC	62	ARG
25	BC	85	ASN
25	BC	89	ASN
25	BC	190	THR
25	BC	191	LEU
26	BD	148	GLN
26	BD	151	THR
27	BE	55	SER
27	BE	67	ARG
27	BE	69	ARG
27	BE	105	LEU
27	BE	137	LYS
28	BF	111	ARG
28	BF	142	TYR
28	BF	152	ASP
29	BG	37	ASN
29	BG	71	LEU
29	BG	170	THR
30	BH	14	SER
32	BJ	76	HIS
32	BJ	80	HIS
32	BJ	130	HIS
34	BL	40	SER
34	BL	76	GLU
35	BM	97	GLN
36	BN	35	LYS
36	BN	67	PHE
36	BN	69	ARG
37	BO	33	ARG

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Mol	Chain	Res	Type
37	BO	53	THR
37	BO	61	GLN
37	BO	100	HIS
38	BP	23	ASP
38	BP	50	ARG
38	BP	102	ARG
38	BP	111	GLU
39	BQ	12	ARG
39	BQ	28	SER
40	BR	46	GLU
41	BS	88	ARG
43	BU	44	HIS
43	BU	72	PHE
44	BV	44	HIS
45	BW	28	GLU
48	BZ	8	GLN
48	BZ	28	LEU
49	B0	3	GLN
49	B0	32	THR
49	B0	37	HIS
49	B0	41	HIS
50	B1	31	GLU
52	B3	23	HIS
56	B5	24	ASN
56	B5	168	ASN

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

Mol	Chain	Res	Type
2	AC	184	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	254 (16%)	77 (5%)
22	A1	73/76 (96%)	10 (13%)	3 (4%)
23	A2	14/15 (93%)	8 (57%)	5 (35%)
24	A3	76/77 (98%)	15 (19%)	5 (6%)
54	BA	2902/2903 (99%)	474 (16%)	117 (4%)
55	BB	116/118 (98%)	18 (15%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4710/4722 (99%)	779 (16%)	209 (4%)

All (779) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	8	A
21	AA	15	G
21	AA	16	A
21	AA	22	G
21	AA	27	G
21	AA	30	U
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	55	A
21	AA	68	G
21	AA	69	G
21	AA	70	U
21	AA	81	A
21	AA	83	C
21	AA	86	G
21	AA	90	C
21	AA	109	A
21	AA	120	A
21	AA	131	A
21	AA	151	A
21	AA	182	A
21	AA	185	U
21	AA	189	A
21	AA	197	A
21	AA	198	G
21	AA	212	G
21	AA	235	C
21	AA	240	G
21	AA	243	A
21	AA	244	U
21	AA	247	G
21	AA	251	G
21	AA	252	U
21	AA	266	G

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Mol	Chain	Res	Type
21	AA	267	C
21	AA	289	G
21	AA	299	G
21	AA	306	A
21	AA	315	A
21	AA	316	C
21	AA	321	A
21	AA	328	C
21	AA	329	A
21	AA	347	G
21	AA	350	G
21	AA	352	C
21	AA	353	A
21	AA	354	G
21	AA	358	U
21	AA	367	U
21	AA	369	G
21	AA	372	C
21	AA	373	A
21	AA	381	C
21	AA	390	U
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	409	U
21	AA	412	A
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	449	G
21	AA	452	A
21	AA	462	G
21	AA	463	U
21	AA	467	U
21	AA	468	A
21	AA	474	G
21	AA	484	G
21	AA	486	U
21	AA	496	A
21	AA	499	A
21	AA	500	G
21	AA	501	C

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Mol	Chain	Res	Type
21	AA	505	G
21	AA	511	C
21	AA	523	A
21	AA	524	G
21	AA	527	G
21	AA	530	G
21	AA	531	U
21	AA	547	A
21	AA	559	A
21	AA	562	U
21	AA	566	G
21	AA	567	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	610	U
21	AA	632	U
21	AA	649	A
21	AA	650	G
21	AA	665	A
21	AA	694	A
21	AA	700	G
21	AA	703	G
21	AA	717	U
21	AA	722	G
21	AA	724	G
21	AA	727	G
21	AA	729	A
21	AA	734	G
21	AA	755	G
21	AA	756	C
21	AA	777	A
21	AA	781	A
21	AA	794	A
21	AA	812	G
21	AA	819	A
21	AA	821	G
21	AA	828	U
21	AA	829	G

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Mol	Chain	Res	Type
21	AA	841	C
21	AA	843	U
21	AA	844	G
21	AA	845	A
21	AA	846	G
21	AA	861	G
21	AA	876	C
21	AA	877	G
21	AA	899	C
21	AA	900	A
21	AA	902	G
21	AA	910	C
21	AA	920	U
21	AA	932	C
21	AA	934	C
21	AA	935	A
21	AA	936	C
21	AA	939	G
21	AA	940	C
21	AA	945	G
21	AA	959	A
21	AA	960	U
21	AA	961	U
21	AA	966	G
21	AA	967	C
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	972	C
21	AA	975	A
21	AA	976	G
21	AA	977	A
21	AA	978	A
21	AA	979	C
21	AA	980	C
21	AA	983	A
21	AA	984	C
21	AA	993	G
21	AA	996	A
21	AA	998	C
21	AA	1004	A
21	AA	1025	U

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Mol	Chain	Res	Type
21	AA	1026	G
21	AA	1031	C
21	AA	1032	G
21	AA	1037	C
21	AA	1045	C
21	AA	1046	A
21	AA	1049	U
21	AA	1050	G
21	AA	1054	C
21	AA	1056	U
21	AA	1064	G
21	AA	1065	U
21	AA	1068	G
21	AA	1086	U
21	AA	1092	A
21	AA	1093	A
21	AA	1094	G
21	AA	1101	A
21	AA	1125	U
21	AA	1126	U
21	AA	1127	G
21	AA	1130	A
21	AA	1138	G
21	AA	1139	G
21	AA	1147	C
21	AA	1148	U
21	AA	1151	A
21	AA	1152	A
21	AA	1159	U
21	AA	1182	G
21	AA	1183	U
21	AA	1184	G
21	AA	1189	U
21	AA	1190	G
21	AA	1191	A
21	AA	1202	U
21	AA	1204	A
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1228	C
21	AA	1231	G

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Mol	Chain	Res	Type
21	AA	1238	A
21	AA	1256	A
21	AA	1257	A
21	AA	1258	G
21	AA	1260	G
21	AA	1267	C
21	AA	1279	G
21	AA	1280	A
21	AA	1281	C
21	AA	1286	U
21	AA	1298	U
21	AA	1300	G
21	AA	1301	U
21	AA	1303	C
21	AA	1317	C
21	AA	1320	C
21	AA	1321	U
21	AA	1337	G
21	AA	1338	G
21	AA	1339	A
21	AA	1340	A
21	AA	1342	C
21	AA	1343	G
21	AA	1345	U
21	AA	1363	A
21	AA	1368	A
21	AA	1369	C
21	AA	1378	C
21	AA	1379	G
21	AA	1381	U
21	AA	1384	C
21	AA	1387	G
21	AA	1397	C
21	AA	1398	A
21	AA	1401	G
21	AA	1452	C
21	AA	1453	G
21	AA	1471	U
21	AA	1493	A
21	AA	1495	U
21	AA	1499	A
21	AA	1503	A

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Mol	Chain	Res	Type
21	AA	1505	G
21	AA	1517	G
21	AA	1518	A
21	AA	1520	C
21	AA	1524	C
21	AA	1529	G
21	AA	1530	G
22	A1	16	C
22	A1	17	U
22	A1	20	G
22	A1	21	A
22	A1	33	U
22	A1	48	C
22	A1	49	G
22	A1	59	U
22	A1	74	C
22	A1	76	A
23	A2	81	U
23	A2	82	A
23	A2	84	G
23	A2	85	G
23	A2	87	U
23	A2	90	U
23	A2	91	A
23	A2	93	U
24	A3	2	G
24	A3	9	G
24	A3	10	G
24	A3	18	U
24	A3	21	H2U
24	A3	22	A
24	A3	36	A
24	A3	40	C
24	A3	48	U
24	A3	49	C
24	A3	72	C
24	A3	73	A
24	A3	74	A
24	A3	76	C
24	A3	77	A
54	BA	20	C
54	BA	27	G

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Mol	Chain	Res	Type
54	BA	34	U
54	BA	60	G
54	BA	61	C
54	BA	62	U
54	BA	63	A
54	BA	71	A
54	BA	74	A
54	BA	75	G
54	BA	77	G
54	BA	85	G
54	BA	86	G
54	BA	88	G
54	BA	91	A
54	BA	98	G
54	BA	101	A
54	BA	103	A
54	BA	118	A
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	139	U
54	BA	141	G
54	BA	142	A
54	BA	143	C
54	BA	149	A
54	BA	181	A
54	BA	197	A
54	BA	204	A
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	223	A
54	BA	230	G
54	BA	239	C
54	BA	242	G
54	BA	245	G
54	BA	248	G
54	BA	265	A
54	BA	266	G
54	BA	274	C
54	BA	278	A

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Mol	Chain	Res	Type
54	BA	286	U
54	BA	295	G
54	BA	316	C
54	BA	323	C
54	BA	330	A
54	BA	331	C
54	BA	332	A
54	BA	335	C
54	BA	346	A
54	BA	347	A
54	BA	362	A
54	BA	370	G
54	BA	372	G
54	BA	377	G
54	BA	383	C
54	BA	384	A
54	BA	386	G
54	BA	387	U
54	BA	411	G
54	BA	422	A
54	BA	428	A
54	BA	430	A
54	BA	444	C
54	BA	451	U
54	BA	453	A
54	BA	454	A
54	BA	455	C
54	BA	457	A
54	BA	458	G
54	BA	470	A
54	BA	471	A
54	BA	481	G
54	BA	484	C
54	BA	490	C
54	BA	491	G
54	BA	501	A
54	BA	504	A
54	BA	505	A
54	BA	509	C
54	BA	527	C
54	BA	531	C
54	BA	532	A

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Mol	Chain	Res	Type
54	BA	546	U
54	BA	547	A
54	BA	549	G
54	BA	571	U
54	BA	572	A
54	BA	573	U
54	BA	578	G
54	BA	586	A
54	BA	588	U
54	BA	604	G
54	BA	607	U
54	BA	611	C
54	BA	614	A
54	BA	615	U
54	BA	616	A
54	BA	617	G
54	BA	629	G
54	BA	630	G
54	BA	631	A
54	BA	634	C
54	BA	637	A
54	BA	638	G
54	BA	650	C
54	BA	654	A
54	BA	655	A
54	BA	662	G
54	BA	671	C
54	BA	672	C
54	BA	687	C
54	BA	715	A
54	BA	719	C
54	BA	722	A
54	BA	723	C
54	BA	724	U
54	BA	726	G
54	BA	736	C
54	BA	747	U
54	BA	748	G
54	BA	752	A
54	BA	763	G
54	BA	765	C
54	BA	775	G

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Mol	Chain	Res	Type
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	790	U
54	BA	791	C
54	BA	792	A
54	BA	793	A
54	BA	800	A
54	BA	804	A
54	BA	814	C
54	BA	816	C
54	BA	822	G
54	BA	823	C
54	BA	827	U
54	BA	858	G
54	BA	859	G
54	BA	889	C
54	BA	890	C
54	BA	907	G
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	924	G
54	BA	931	U
54	BA	934	U
54	BA	950	G
54	BA	961	C
54	BA	973	A
54	BA	974	G
54	BA	980	A
54	BA	981	A
54	BA	983	A
54	BA	996	A
54	BA	1012	U
54	BA	1013	C
54	BA	1022	G
54	BA	1023	U
54	BA	1024	G
54	BA	1026	G
54	BA	1033	U
54	BA	1046	A
54	BA	1055	G

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Mol	Chain	Res	Type
54	BA	1056	G
54	BA	1063	G
54	BA	1067	A
54	BA	1068	G
54	BA	1069	A
54	BA	1070	A
54	BA	1073	A
54	BA	1077	A
54	BA	1088	A
54	BA	1089	A
54	BA	1112	G
54	BA	1124	G
54	BA	1127	A
54	BA	1130	U
54	BA	1131	G
54	BA	1132	U
54	BA	1135	C
54	BA	1141	U
54	BA	1142	A
54	BA	1151	A
54	BA	1155	A
54	BA	1175	A
54	BA	1176	U
54	BA	1186	G
54	BA	1192	G
54	BA	1204	A
54	BA	1206	G
54	BA	1211	C
54	BA	1227	G
54	BA	1237	A
54	BA	1241	A
54	BA	1242	U
54	BA	1253	A
54	BA	1254	A
54	BA	1264	A
54	BA	1265	A
54	BA	1270	C
54	BA	1271	G
54	BA	1272	A
54	BA	1273	U
54	BA	1276	A
54	BA	1292	G

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Mol	Chain	Res	Type
54	BA	1300	G
54	BA	1301	A
54	BA	1302	A
54	BA	1313	U
54	BA	1314	C
54	BA	1315	C
54	BA	1325	U
54	BA	1332	G
54	BA	1341	G
54	BA	1350	C
54	BA	1365	A
54	BA	1366	A
54	BA	1368	G
54	BA	1379	U
54	BA	1380	G
54	BA	1383	A
54	BA	1388	G
54	BA	1393	A
54	BA	1416	G
54	BA	1425	G
54	BA	1427	A
54	BA	1428	C
54	BA	1434	A
54	BA	1435	G
54	BA	1452	G
54	BA	1453	A
54	BA	1454	C
54	BA	1459	G
54	BA	1461	C
54	BA	1482	G
54	BA	1491	G
54	BA	1494	A
54	BA	1509	A
54	BA	1510	G
54	BA	1522	A
54	BA	1536	C
54	BA	1537	G
54	BA	1538	G
54	BA	1539	U
54	BA	1559	U
54	BA	1566	A
54	BA	1569	A

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Mol	Chain	Res	Type
54	BA	1598	A
54	BA	1607	C
54	BA	1608	A
54	BA	1610	A
54	BA	1611	C
54	BA	1616	A
54	BA	1618	A
54	BA	1626	A
54	BA	1635	A
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1654	A
54	BA	1661	G
54	BA	1674	G
54	BA	1675	C
54	BA	1696	G
54	BA	1711	A
54	BA	1723	G
54	BA	1729	U
54	BA	1730	C
54	BA	1733	G
54	BA	1734	G
54	BA	1758	U
54	BA	1764	C
54	BA	1773	A
54	BA	1776	G
54	BA	1780	A
54	BA	1783	A
54	BA	1784	A
54	BA	1800	C
54	BA	1801	A
54	BA	1808	A
54	BA	1817	G
54	BA	1830	C
54	BA	1833	C
54	BA	1847	A
54	BA	1870	C
54	BA	1871	A
54	BA	1872	A
54	BA	1873	G
54	BA	1876	A

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Mol	Chain	Res	Type
54	BA	1877	A
54	BA	1884	G
54	BA	1900	A
54	BA	1912	A
54	BA	1914	C
54	BA	1930	G
54	BA	1931	U
54	BA	1937	A
54	BA	1939	U
54	BA	1940	U
54	BA	1941	C
54	BA	1951	U
54	BA	1952	A
54	BA	1953	A
54	BA	1955	U
54	BA	1962	C
54	BA	1963	U
54	BA	1965	C
54	BA	1967	C
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1981	A
54	BA	1982	U
54	BA	1986	C
54	BA	1993	U
54	BA	2017	U
54	BA	2020	A
54	BA	2022	U
54	BA	2023	C
54	BA	2030	A
54	BA	2032	G
54	BA	2043	C
54	BA	2052	A
54	BA	2055	C
54	BA	2059	A
54	BA	2061	G
54	BA	2068	U
54	BA	2069	G
54	BA	2076	U
54	BA	2077	A
54	BA	2092	U

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Mol	Chain	Res	Type
54	BA	2113	U
54	BA	2115	G
54	BA	2116	G
54	BA	2117	A
54	BA	2118	U
54	BA	2126	A
54	BA	2127	G
54	BA	2132	U
54	BA	2133	G
54	BA	2148	G
54	BA	2155	U
54	BA	2157	G
54	BA	2158	A
54	BA	2159	G
54	BA	2160	C
54	BA	2169	A
54	BA	2172	U
54	BA	2173	A
54	BA	2198	A
54	BA	2203	U
54	BA	2212	A
54	BA	2216	G
54	BA	2225	A
54	BA	2238	G
54	BA	2239	G
54	BA	2266	A
54	BA	2275	C
54	BA	2276	G
54	BA	2283	C
54	BA	2305	U
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2311	A
54	BA	2312	U
54	BA	2321	U
54	BA	2322	A
54	BA	2325	G
54	BA	2327	A
54	BA	2333	A
54	BA	2335	A
54	BA	2339	C

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Mol	Chain	Res	Type
54	BA	2347	C
54	BA	2350	C
54	BA	2351	G
54	BA	2353	G
54	BA	2379	G
54	BA	2383	G
54	BA	2385	C
54	BA	2388	A
54	BA	2391	G
54	BA	2395	C
54	BA	2406	A
54	BA	2407	A
54	BA	2408	U
54	BA	2409	G
54	BA	2417	C
54	BA	2418	A
54	BA	2422	C
54	BA	2425	A
54	BA	2426	A
54	BA	2427	C
54	BA	2429	G
54	BA	2430	A
54	BA	2431	U
54	BA	2433	A
54	BA	2434	A
54	BA	2435	A
54	BA	2441	U
54	BA	2446	G
54	BA	2447	G
54	BA	2448	A
54	BA	2470	G
54	BA	2474	U
54	BA	2476	A
54	BA	2491	U
54	BA	2492	U
54	BA	2501	C
54	BA	2503	A
54	BA	2505	G
54	BA	2506	U
54	BA	2520	C
54	BA	2566	A
54	BA	2567	G

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Mol	Chain	Res	Type
54	BA	2572	A
54	BA	2573	C
54	BA	2577	A
54	BA	2578	G
54	BA	2586	U
54	BA	2599	G
54	BA	2602	A
54	BA	2603	G
54	BA	2611	C
54	BA	2614	A
54	BA	2615	U
54	BA	2629	U
54	BA	2639	A
54	BA	2640	G
54	BA	2646	C
54	BA	2654	A
54	BA	2660	A
54	BA	2667	C
54	BA	2668	G
54	BA	2681	C
54	BA	2683	C
54	BA	2689	U
54	BA	2690	U
54	BA	2706	A
54	BA	2714	G
54	BA	2726	A
54	BA	2732	G
54	BA	2733	A
54	BA	2744	G
54	BA	2756	U
54	BA	2757	A
54	BA	2765	A
54	BA	2770	G
54	BA	2771	C
54	BA	2778	A
54	BA	2780	G
54	BA	2791	G
54	BA	2797	U
54	BA	2798	U
54	BA	2799	A
54	BA	2800	A
54	BA	2816	G

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Mol	Chain	Res	Type
54	BA	2817	U
54	BA	2821	A
54	BA	2822	G
54	BA	2834	G
54	BA	2835	A
54	BA	2841	C
54	BA	2850	A
54	BA	2873	A
54	BA	2875	C
54	BA	2894	G
55	BB	13	G
55	BB	14	U
55	BB	15	A
55	BB	16	G
55	BB	25	U
55	BB	29	A
55	BB	30	C
55	BB	33	G
55	BB	44	G
55	BB	69	G
55	BB	84	G
55	BB	85	G
55	BB	89	U
55	BB	90	C
55	BB	99	A
55	BB	100	G
55	BB	101	A
55	BB	109	A

All (209) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	15	G
21	AA	26	A
21	AA	31	G
21	AA	51	A
21	AA	65	A
21	AA	69	G
21	AA	80	A
21	AA	86	G
21	AA	88	U
21	AA	243	A

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Mol	Chain	Res	Type
21	AA	251	G
21	AA	298	A
21	AA	315	A
21	AA	327	A
21	AA	328	C
21	AA	353	A
21	AA	357	G
21	AA	372	C
21	AA	381	C
21	AA	448	A
21	AA	451	A
21	AA	453	G
21	AA	465	A
21	AA	496	A
21	AA	499	A
21	AA	500	G
21	AA	505	G
21	AA	523	A
21	AA	530	G
21	AA	562	U
21	AA	566	G
21	AA	575	G
21	AA	641	U
21	AA	718	A
21	AA	728	A
21	AA	734	G
21	AA	818	G
21	AA	844	G
21	AA	845	A
21	AA	860	A
21	AA	876	C
21	AA	899	C
21	AA	938	A
21	AA	959	A
21	AA	960	U
21	AA	966	G
21	AA	975	A
21	AA	977	A
21	AA	979	C
21	AA	992	U
21	AA	1025	U
21	AA	1030	U

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Mol	Chain	Res	Type
21	AA	1092	A
21	AA	1093	A
21	AA	1126	U
21	AA	1158	C
21	AA	1182	G
21	AA	1190	G
21	AA	1201	A
21	AA	1203	C
21	AA	1225	A
21	AA	1257	A
21	AA	1267	C
21	AA	1278	G
21	AA	1279	G
21	AA	1280	A
21	AA	1296	C
21	AA	1298	U
21	AA	1305	G
21	AA	1337	G
21	AA	1342	C
21	AA	1368	A
21	AA	1380	U
21	AA	1445	U
21	AA	1451	U
21	AA	1498	U
21	AA	1517	G
22	A1	19	G
22	A1	32	C
22	A1	47	U
23	A2	84	G
23	A2	87	U
23	A2	89	U
23	A2	90	U
23	A2	92	U
24	A3	9	G
24	A3	47	G
24	A3	48	U
24	A3	72	C
24	A3	76	C
54	BA	46	G
54	BA	60	G
54	BA	74	A
54	BA	121	G

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Mol	Chain	Res	Type
54	BA	125	A
54	BA	199	A
54	BA	215	G
54	BA	278	A
54	BA	346	A
54	BA	376	G
54	BA	383	C
54	BA	454	A
54	BA	464	U
54	BA	470	A
54	BA	547	A
54	BA	569	U
54	BA	571	U
54	BA	577	G
54	BA	587	C
54	BA	603	A
54	BA	615	U
54	BA	620	G
54	BA	629	G
54	BA	649	G
54	BA	661	A
54	BA	670	A
54	BA	686	U
54	BA	762	U
54	BA	790	U
54	BA	804	A
54	BA	815	C
54	BA	858	G
54	BA	979	A
54	BA	980	A
54	BA	983	A
54	BA	1012	U
54	BA	1023	U
54	BA	1055	G
54	BA	1061	U
54	BA	1068	G
54	BA	1076	C
54	BA	1122	G
54	BA	1126	A
54	BA	1128	G
54	BA	1141	U
54	BA	1144	A

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Mol	Chain	Res	Type
54	BA	1157	G
54	BA	1210	G
54	BA	1224	U
54	BA	1253	A
54	BA	1263	U
54	BA	1265	A
54	BA	1270	C
54	BA	1288	G
54	BA	1289	C
54	BA	1301	A
54	BA	1312	U
54	BA	1314	C
54	BA	1340	U
54	BA	1344	U
54	BA	1378	A
54	BA	1379	U
54	BA	1392	A
54	BA	1420	A
54	BA	1424	G
54	BA	1427	A
54	BA	1452	G
54	BA	1453	A
54	BA	1508	A
54	BA	1509	A
54	BA	1567	G
54	BA	1610	A
54	BA	1634	A
54	BA	1645	G
54	BA	1757	A
54	BA	1783	A
54	BA	1784	A
54	BA	1799	G
54	BA	1876	A
54	BA	1900	A
54	BA	1913	A
54	BA	1936	A
54	BA	1940	U
54	BA	1951	U
54	BA	1961	C
54	BA	1962	C
54	BA	1981	A
54	BA	2016	U

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Mol	Chain	Res	Type
54	BA	2033	A
54	BA	2076	U
54	BA	2115	G
54	BA	2157	G
54	BA	2275	C
54	BA	2286	G
54	BA	2307	G
54	BA	2308	G
54	BA	2312	U
54	BA	2350	C
54	BA	2407	A
54	BA	2417	C
54	BA	2425	A
54	BA	2427	C
54	BA	2429	G
54	BA	2430	A
54	BA	2433	A
54	BA	2434	A
54	BA	2474	U
54	BA	2566	A
54	BA	2572	A
54	BA	2602	A
54	BA	2615	U
54	BA	2726	A
54	BA	2732	G
54	BA	2756	U
54	BA	2770	G
54	BA	2797	U
54	BA	2809	A
55	BB	32	U
55	BB	52	A

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	$\#\|Z\| > 2$
24	5MU	A3	55	24	19,22,23	0.70	0	28,32,35	1.28	3 (10%)
22	5MU	A1	54	22	19,22,23	0.79	0	28,32,35	1.34	4 (14%)
22	4SU	A1	7	22	18,21,22	1.34	1 (5%)	26,30,33	0.88	1 (3%)
22	CM0	A1	34	22	22,26,27	1.29	1 (4%)	28,37,40	1.35	2 (7%)
24	OMC	A3	33	24	19,22,23	0.79	0	26,31,34	0.96	1 (3%)
22	6MZ	A1	37	22	18,25,26	1.06	1 (5%)	16,36,39	1.43	2 (12%)
22	PSU	A1	55	22	18,21,22	0.79	0	22,30,33	1.13	2 (9%)
24	4SU	A3	8	24	18,21,22	1.42	1 (5%)	26,30,33	0.75	1 (3%)
24	PSU	A3	56	24	18,21,22	0.93	0	22,30,33	1.27	3 (13%)
22	7MG	A1	46	22	22,26,27	5.04	1 (4%)	29,39,42	1.41	1 (3%)
24	H2U	A3	21	24	18,21,22	1.31	2 (11%)	21,30,33	1.14	3 (14%)

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-23.38	1.32	1.46
24	A3	8	4SU	C5-C4	-5.03	1.36	1.42
22	A1	7	4SU	C5-C4	-4.63	1.36	1.42
22	A1	34	CM0	O5-C5	-4.41	1.26	1.36
24	A3	21	H2U	C2-N3	-3.45	1.31	1.38
24	A3	21	H2U	C4-N3	-3.27	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	37	6MZ	C8-N7	-2.70	1.29	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	46	7MG	N9-C8-N7	5.84	111.74	103.38
22	A1	34	CM0	C7-O5-C5	4.99	124.11	117.58
22	A1	37	6MZ	C9-N6-C6	4.37	126.64	122.87
22	A1	54	5MU	C5M-C5-C6	-3.34	118.39	122.85
24	A3	55	5MU	C5M-C5-C6	-3.19	118.59	122.85
24	A3	33	OMC	O2-C2-N3	-3.07	117.34	122.33
22	A1	54	5MU	C6-C5-C4	2.99	120.53	118.03
24	A3	56	PSU	C6-C5-C4	2.95	120.26	118.20
24	A3	55	5MU	C6-C5-C4	2.94	120.49	118.03
22	A1	55	PSU	C6-C5-C4	2.80	120.16	118.20
24	A3	21	H2U	N3-C2-N1	2.72	119.53	116.65
24	A3	8	4SU	C6-C5-C4	2.66	122.25	119.95
22	A1	37	6MZ	C2-N1-C6	2.54	118.77	116.59
22	A1	54	5MU	C5-C6-N1	-2.50	120.76	123.34
24	A3	56	PSU	O4'-C1'-C2'	2.45	108.60	105.14
22	A1	7	4SU	C6-C5-C4	2.39	122.02	119.95
24	A3	55	5MU	C5-C6-N1	-2.33	120.94	123.34
22	A1	34	CM0	O8-C8-O9	-2.29	117.59	123.30
24	A3	56	PSU	N1-C2-N3	2.27	117.70	115.13
24	A3	21	H2U	C4-N3-C2	2.26	127.67	125.79
22	A1	55	PSU	O2-C2-N1	-2.20	120.37	122.79
24	A3	21	H2U	C5-C4-N3	2.14	119.06	116.65
22	A1	54	5MU	C5M-C5-C4	2.10	121.08	118.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A3	56	PSU	O4'-C1'-C5-C4
24	A3	56	PSU	O4'-C1'-C5-C6
22	A1	34	CM0	O5-C7-C8-O8
22	A1	34	CM0	O5-C7-C8-O9
22	A1	55	PSU	O4'-C1'-C5-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A1	54	5MU	1	0

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	$\#\|Z\| > 2$
58	FME	BA	3001	57	8,9,10	0.61	0	7,9,11	1.36	1 (14%)
57	VAL	A1	101	58,22	4,6,7	0.61	0	6,7,9	1.39	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	FME	BA	3001	57	-	2/7/9/11	-
57	VAL	A1	101	58,22	-	0/5/6/8	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	A1	101	VAL	O-C-CA	-3.32	116.07	124.78
58	BA	3001	FME	C-CA-N	2.58	114.38	109.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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.

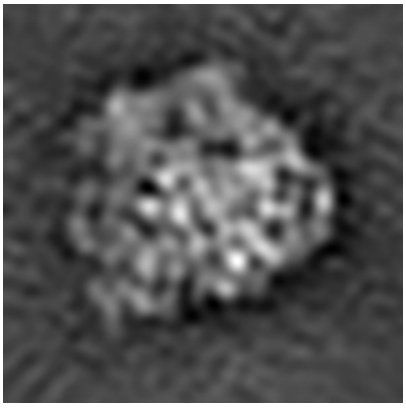
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2475. These allow visual inspection of the internal detail of the map and identification of artifacts.

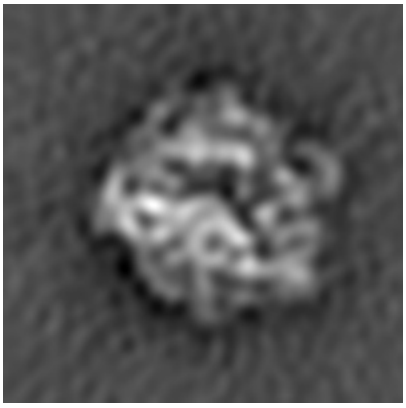
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

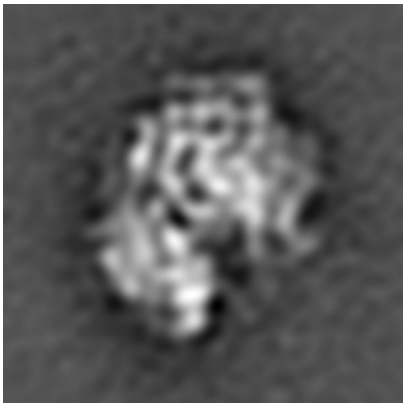
6.1.1 Primary map



X



Y



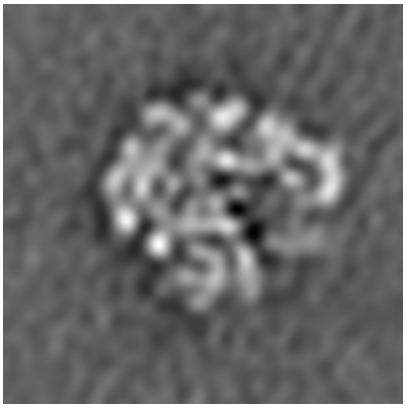
Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 48



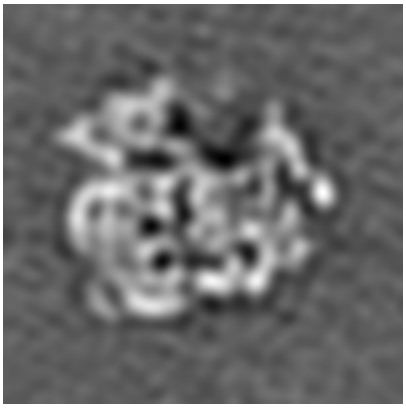
Y Index: 48

Z Index: 48

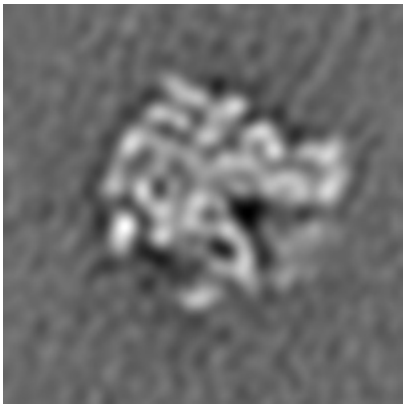
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 43



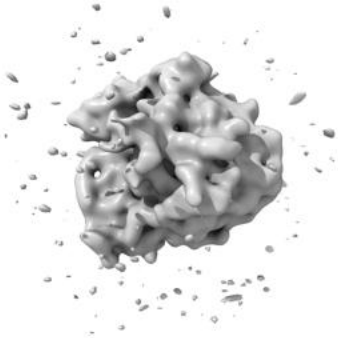
Y Index: 51

Z Index: 46

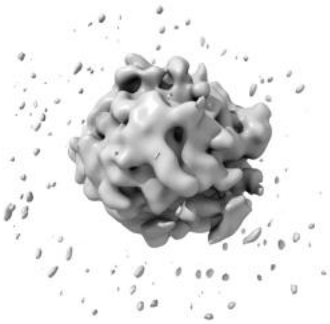
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

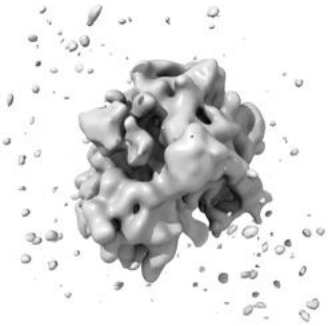
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 25.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

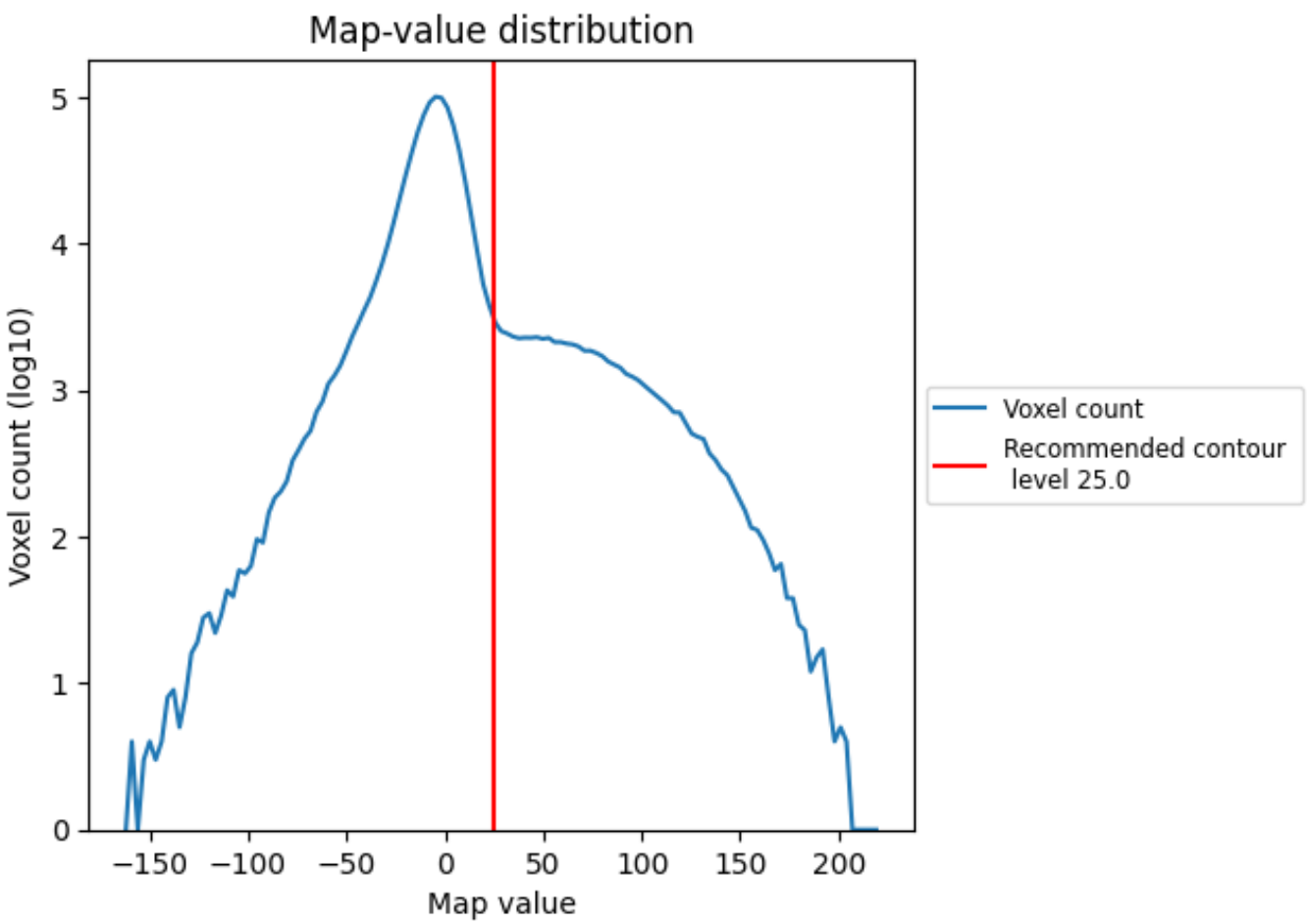
6.5 Mask visualisation (i)

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

7 Map analysis (i)

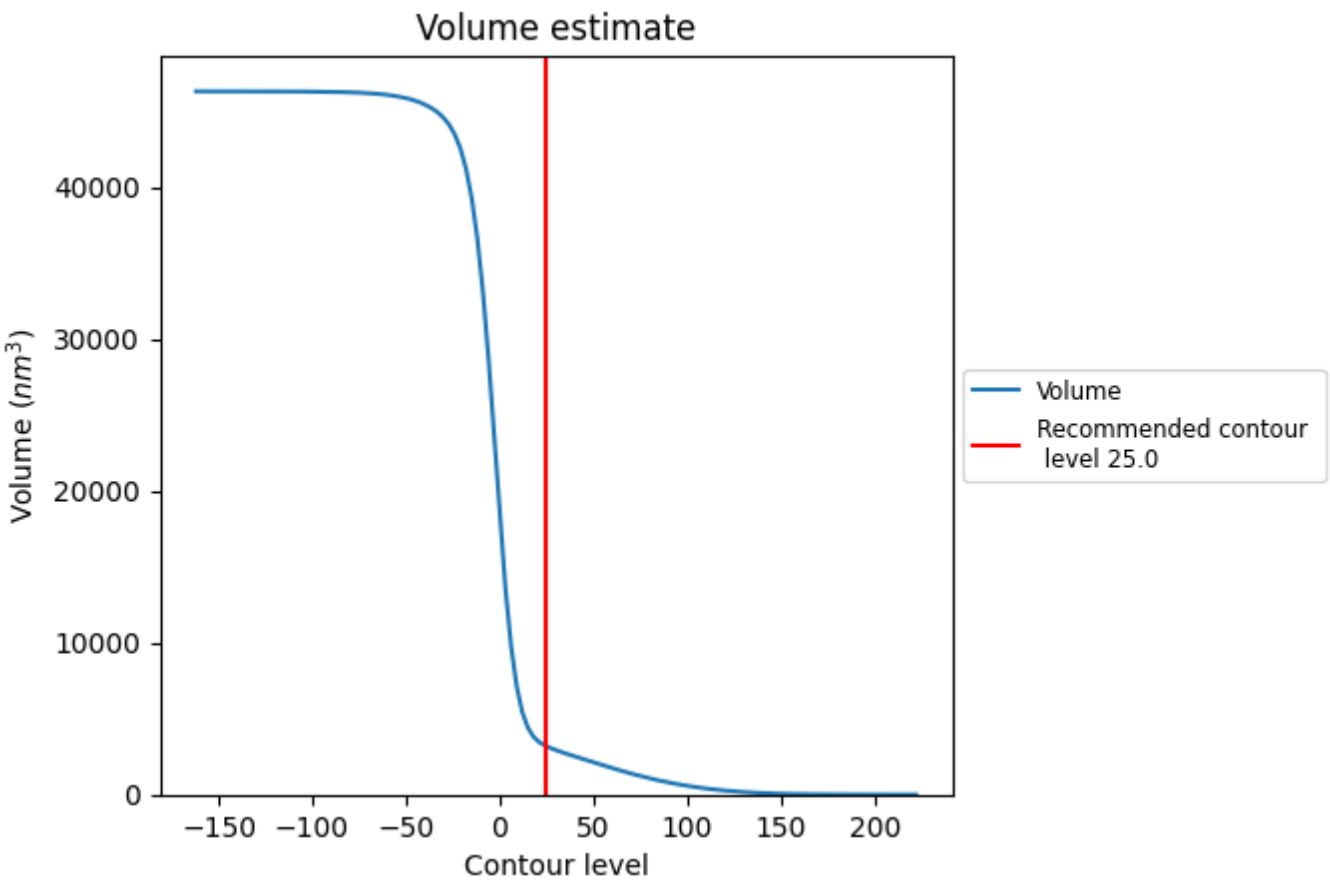
This section contains the results of statistical analysis of the map.

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.

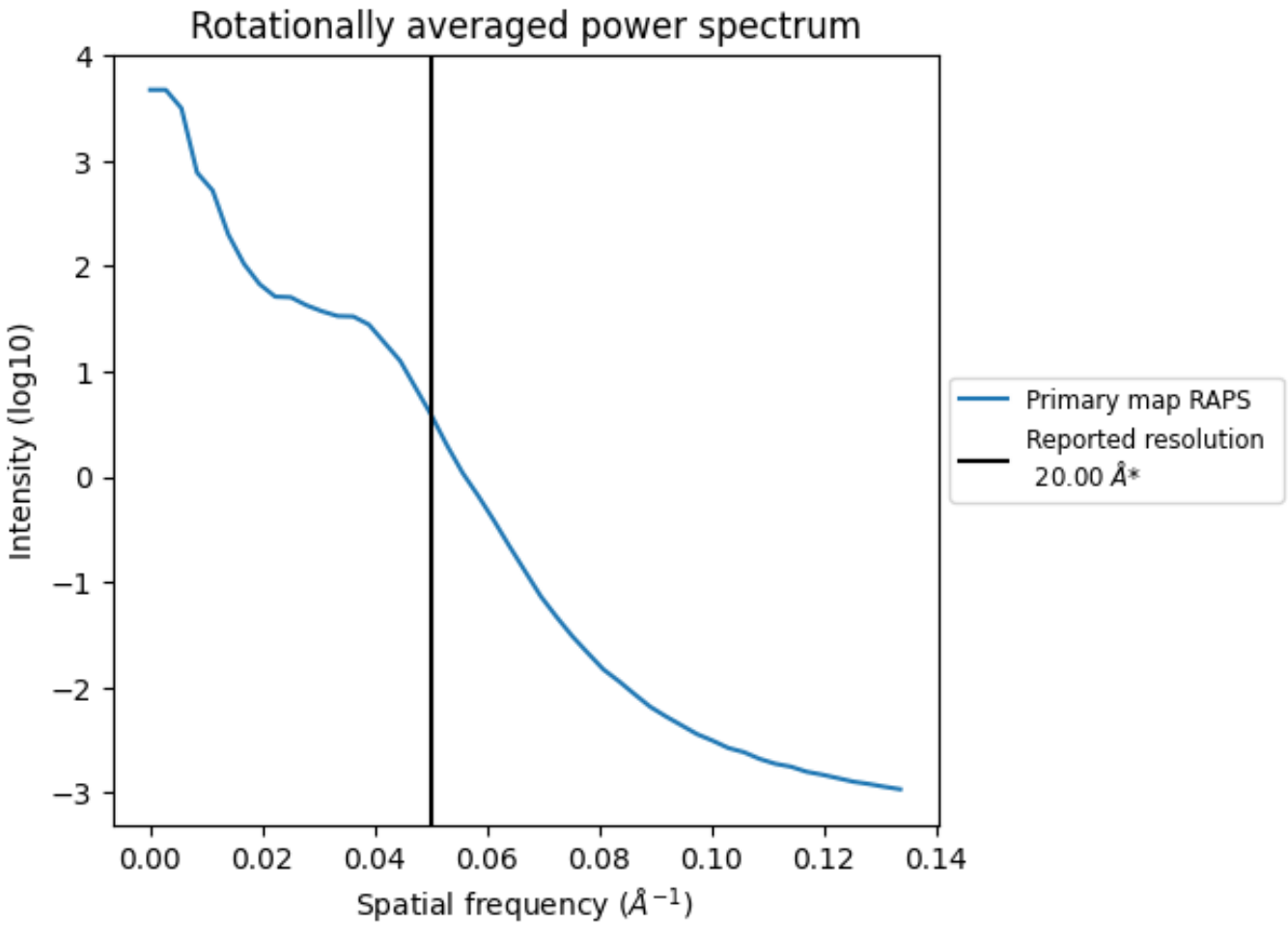
7.2 Volume estimate (i)



The volume at the recommended contour level is 3179 nm^3; this corresponds to an approximate mass of 2872 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 0.050 Å^{-1}

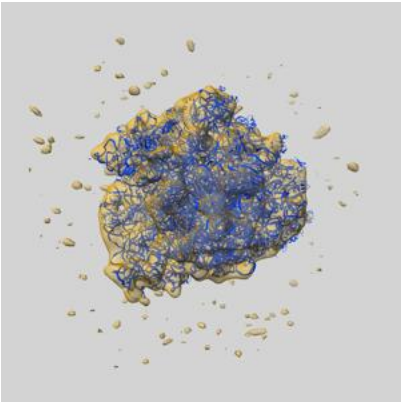
8 Fourier-Shell correlation (i)

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

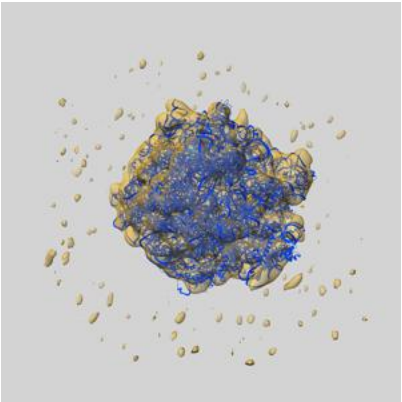
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2475 and PDB model 4V78. Per-residue inclusion information can be found in section 3 on page 17.

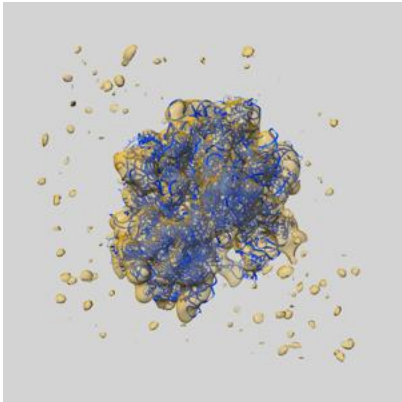
9.1 Map-model overlay (i)



X



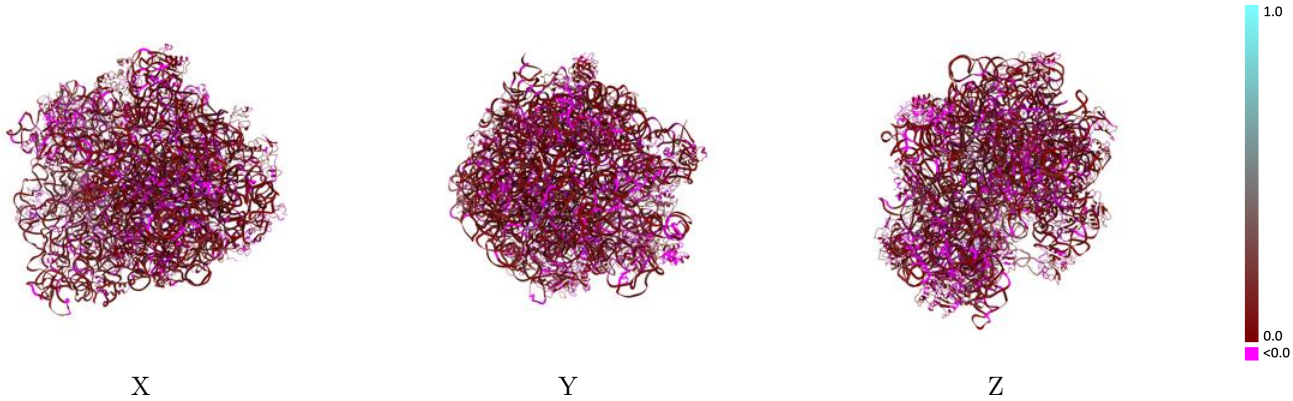
Y



Z

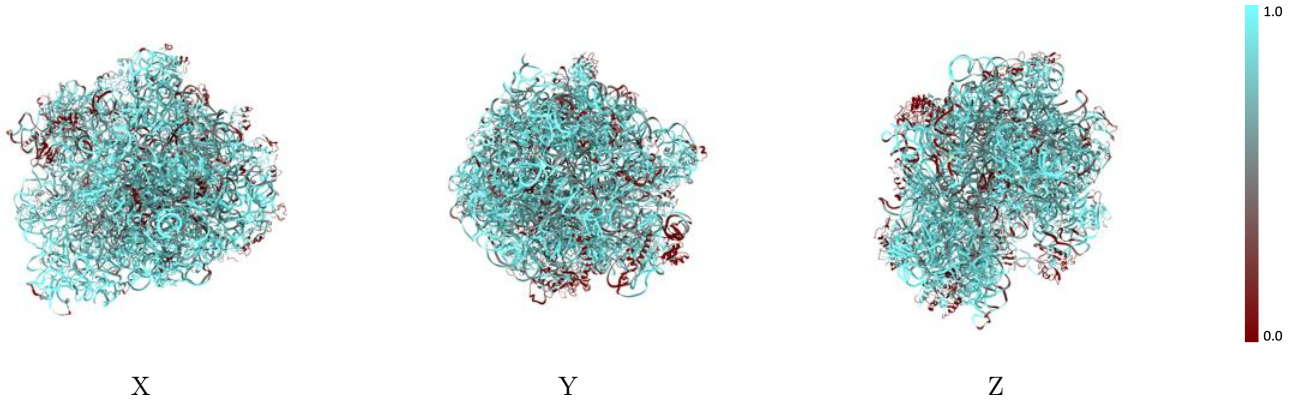
The images above show the 3D surface view of the map at the recommended contour level 25.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



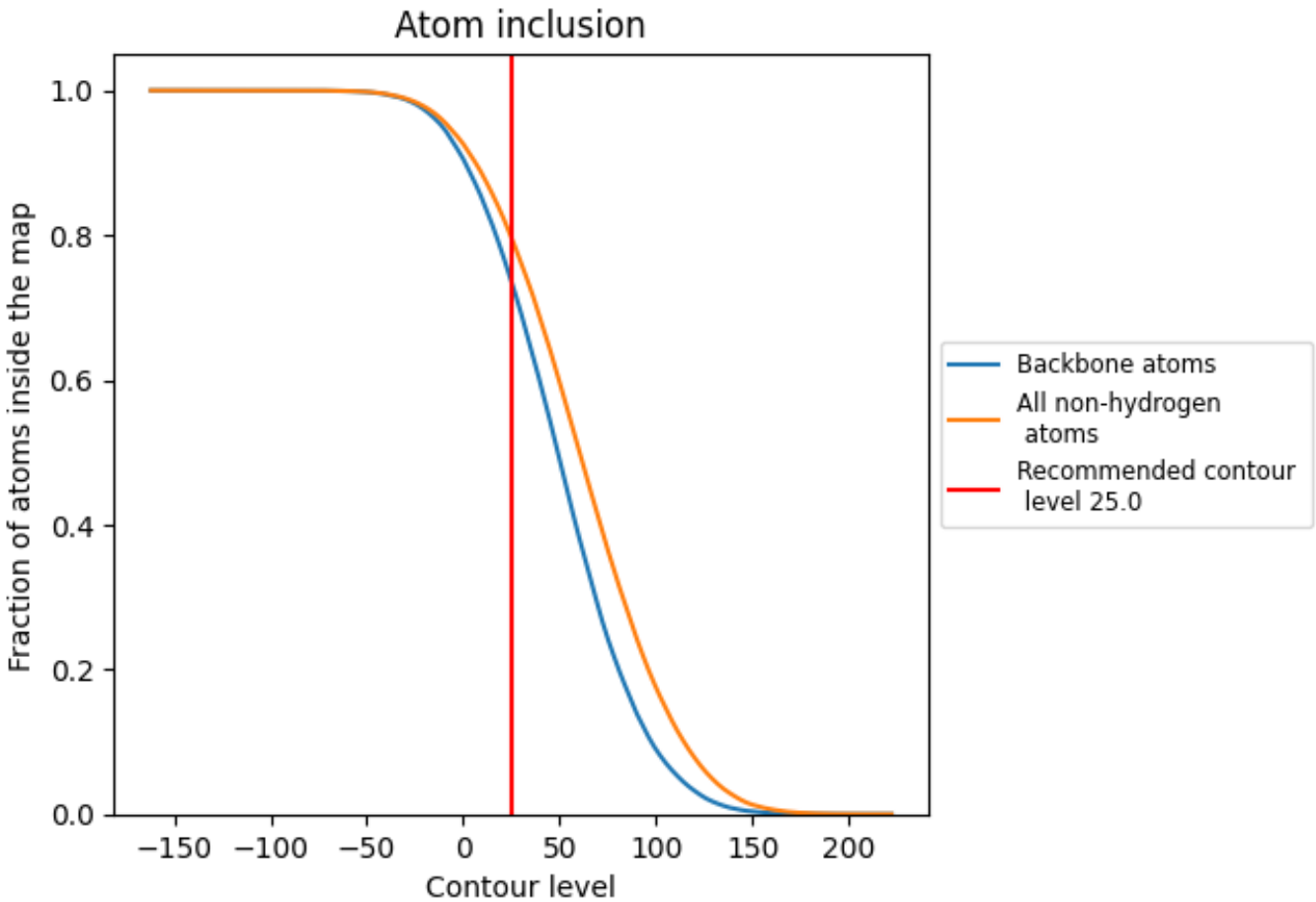
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (25.0).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 80% 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 (25.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7965	0.0510
A1	0.5153	0.0490
A2	0.9191	0.0520
A3	0.4756	0.0280
AA	0.8875	0.0630
AB	0.6055	0.0440
AC	0.6048	0.0260
AD	0.7233	0.0170
AE	0.7394	0.0430
AF	0.4906	0.0440
AG	0.8316	0.0380
AH	0.8604	0.0550
AI	0.9174	0.0200
AJ	0.6257	-0.0080
AK	0.7708	0.0520
AL	0.6992	0.0160
AM	0.6722	0.0430
AN	0.7455	0.0050
AO	0.7928	0.0410
AP	0.7391	0.0280
AQ	0.5732	0.0190
AR	0.5604	0.0150
AS	0.4375	0.0090
AT	0.8021	0.0310
AU	0.8875	0.0510
B0	0.6729	0.0180
B1	0.6733	0.0320
B2	0.3915	-0.0410
B3	0.6151	-0.0450
B4	0.7979	-0.0020
B5	0.3092	0.0100
BA	0.8619	0.0640
BB	0.8974	0.0650
BC	0.5721	-0.0060
BD	0.6983	0.0200

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Chain	Atom inclusion	Q-score
BE	0.6717	0.0260
BF	0.7650	0.0330
BG	0.7911	0.0360
BH	0.2172	0.0310
BI	0.2720	0.0380
BJ	0.6927	0.0220
BK	0.5481	0.0350
BL	0.5630	0.0080
BM	0.7380	0.0230
BN	0.7270	-0.0020
BO	0.7509	0.0270
BP	0.7466	0.0400
BQ	0.6883	-0.0030
BR	0.6826	0.0520
BS	0.6758	0.0060
BT	0.8506	0.0140
BU	0.5417	0.0130
BV	0.8293	0.0630
BW	0.7113	0.0170
BX	0.8003	0.0480
BY	0.3843	-0.0030
BZ	0.6178	0.0340