Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:25 PM EST

PDB ID	:	4V70
EMDB ID	:	EMD-1718
Title	:	E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate pre-translocation state (pre3)
Authors	:	Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on	:	2013-10-14
Resolution	:	17.00 Å(reported)
Based on initial models	:	2HGP, 3I1O, 2K4C, 2WRI

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

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

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

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

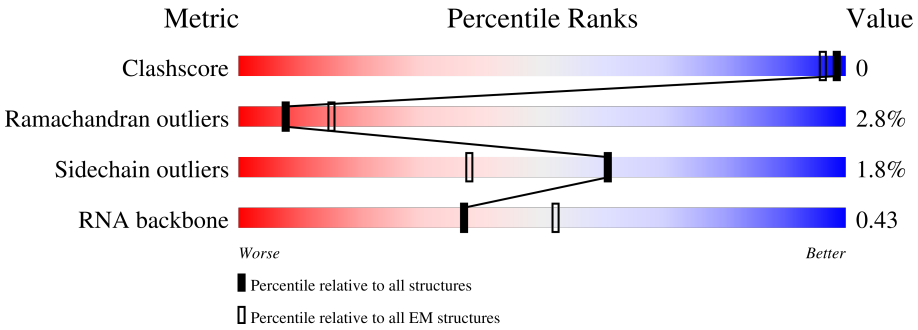
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance

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

The reported resolution of this entry is 17.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	220	42% 93% 7%
2	AC	208	46% 87% 12%
3	AD	206	50% 89% 10%
4	AE	152	24% 94% 6%
5	AF	101	20% 85% 15%
6	AG	152	39% 88% 11%
7	AH	130	21% 92% 8%

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Mol	Chain	Length	Quality of chain
8	AI	128	27% 85% 13%
9	AJ	100	35% 85% 14%
10	AK	118	23% 92% 8%
11	AL	124	23% 86% 12%
12	AM	115	26% 82% 17%
13	AN	101	23% 85% 12%
14	AO	89	26% 89% 10%
15	AP	81	33% 89% 10%
16	AQ	82	28% 89% 11%
17	AR	57	33% 89% 11%
18	AS	81	19% 89% 11%
19	AT	86	20% 87% 13%
20	AU	53	32% 75% 25%
21	AA	1533	5% 25% 49% 22%
22	A1	76	33% 26% 53% 17%
23	A2	15	27% 27% 33% 27% 13%
24	A3	77	34% 26% 48% 22%
25	BC	273	46% 87% 12%
26	BD	209	31% 87% 12%
27	BE	201	34% 92% 8%
28	BF	179	21% 89% 11%
29	BG	177	24% 93% 6%
30	BH	149	69% 93% 7%
31	BI	142	98% 94% 6%
32	BJ	142	32% 89% 11%

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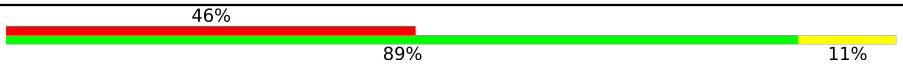
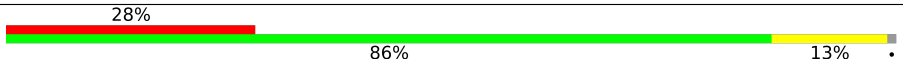
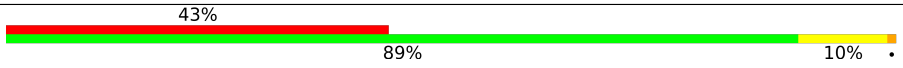
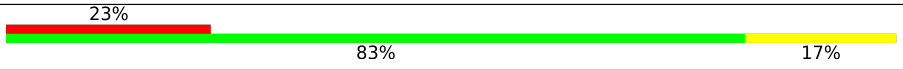
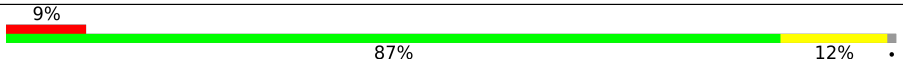
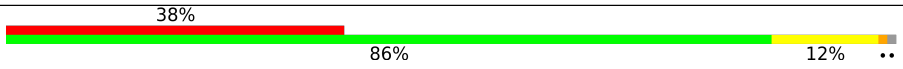
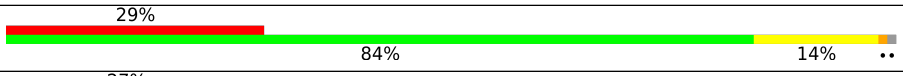
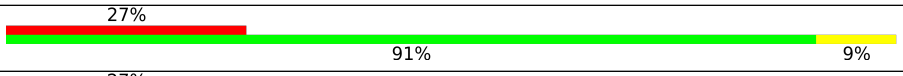
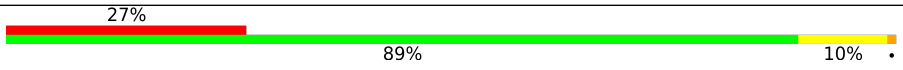
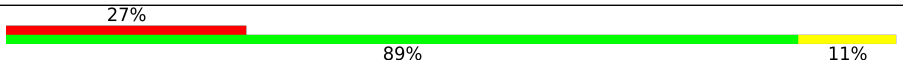
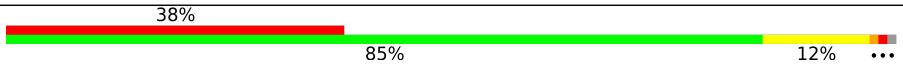
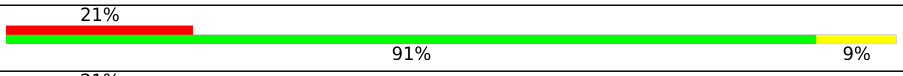
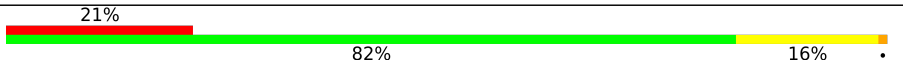
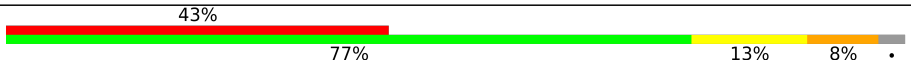
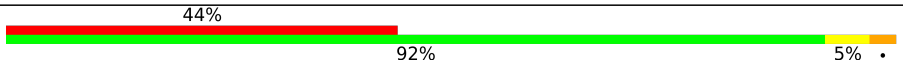
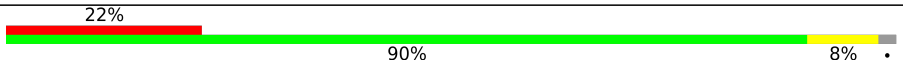
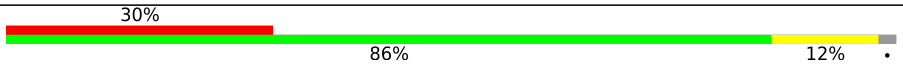
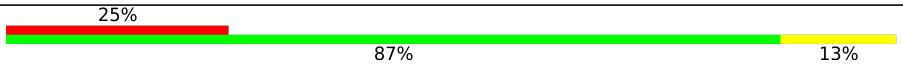
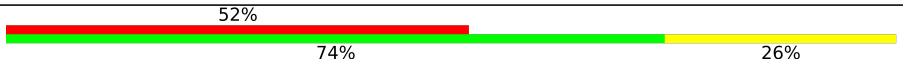
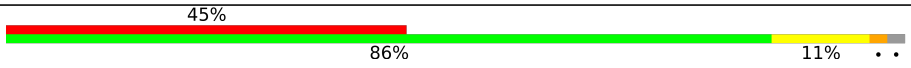
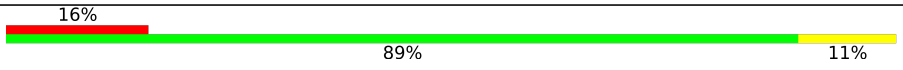
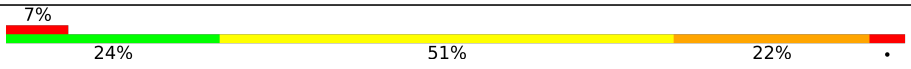
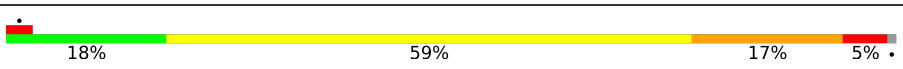
Mol	Chain	Length	Quality of chain
33	BK	123	
34	BL	144	
35	BM	136	
36	BN	121	
37	BO	117	
38	BP	115	
39	BQ	118	
40	BR	103	
41	BS	110	
42	BT	94	
43	BU	104	
44	BV	94	
45	BW	80	
46	BX	79	
47	BY	63	
48	BZ	59	
49	B0	57	
50	B1	52	
51	B2	46	
52	B3	65	
53	B4	38	
54	BA	2903	
55	BB	118	
56	B5	234	

2 Entry composition (i)

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	7	ACE	-	acetylation	UNP P0A7V0
AB	226	NH2	-	amidation	UNP P0A7V0

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	8	ACE	-	acetylation	UNP P0A7W1
AE	159	NH2	-	amidation	UNP P0A7W1

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	1	ACE	-	acetylation	UNP P02359
AG	152	NH2	-	amidation	UNP P02359

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AJ	4	ACE	-	acetylation	UNP P0A7R5
AJ	103	NH2	-	amidation	UNP P0A7R5

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AQ	2	ACE	-	acetylation	UNP P0AG63
AQ	83	NH2	-	amidation	UNP P0AG63

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

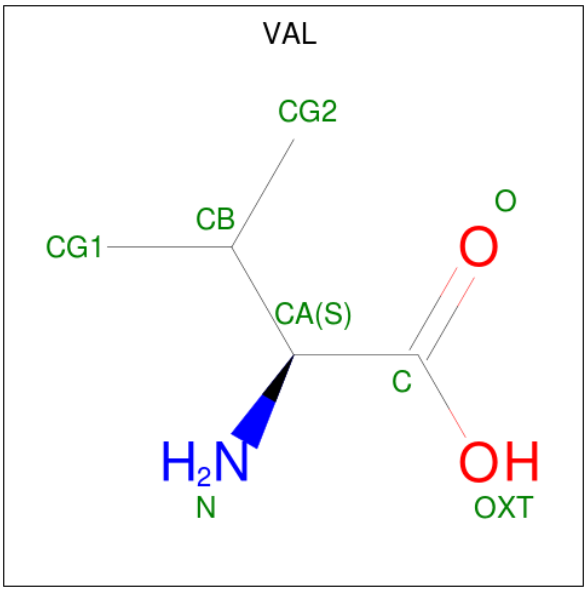
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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

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

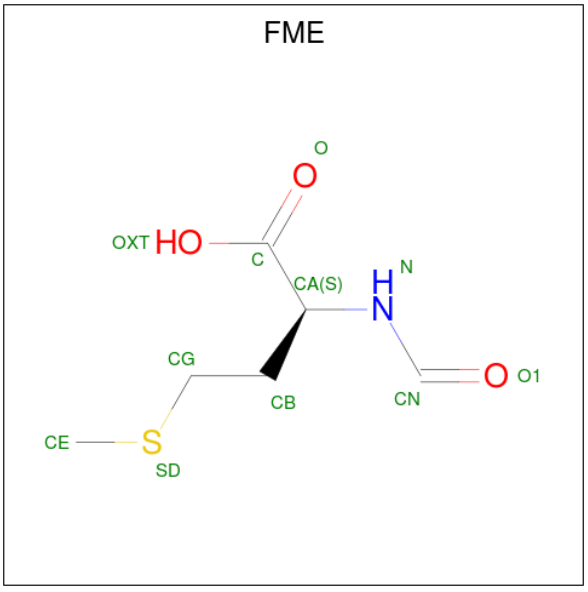
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

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



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

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



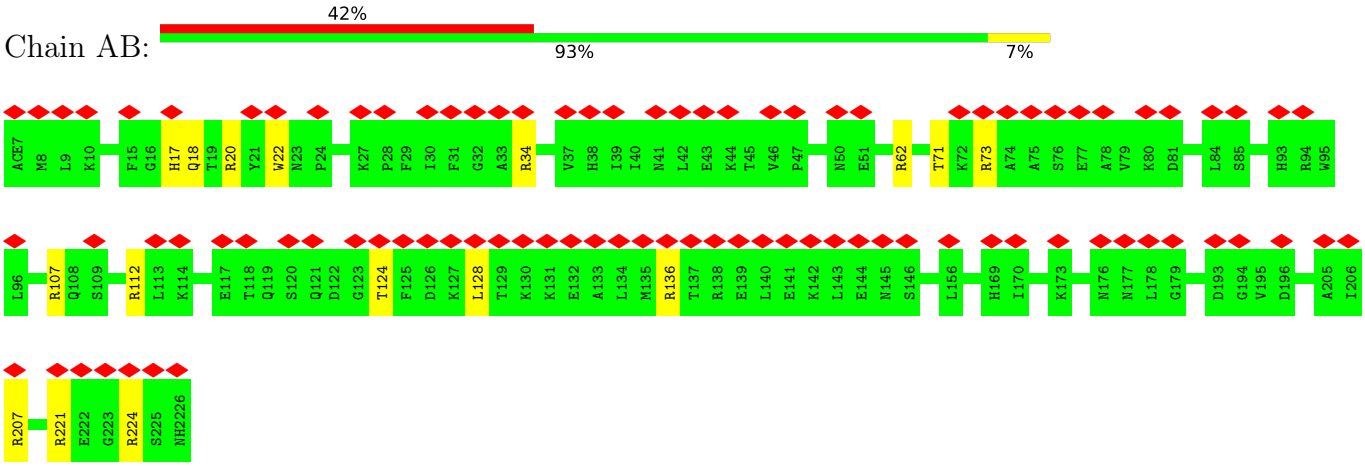
Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

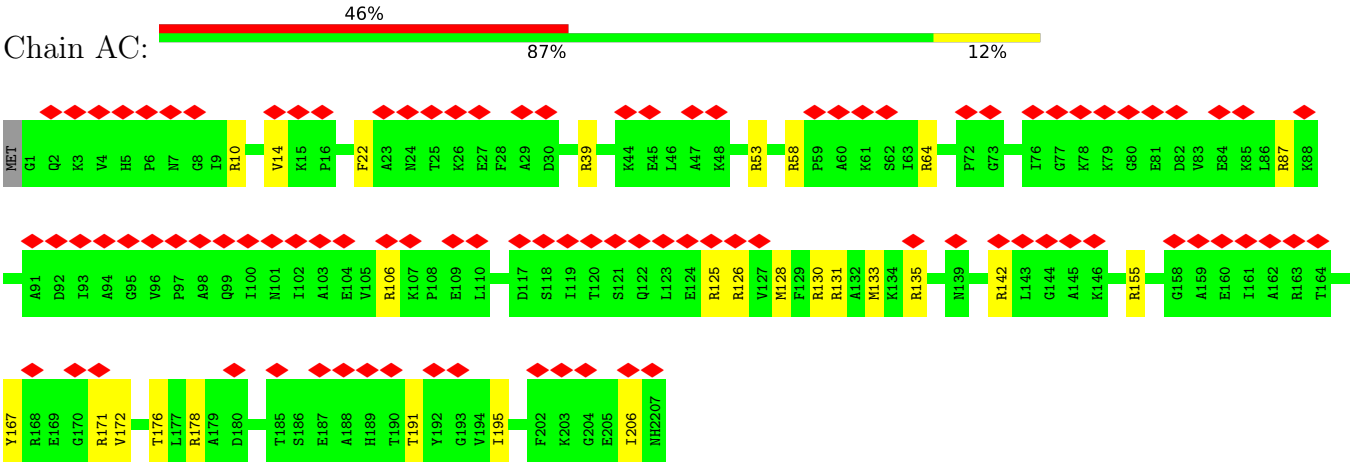
• Molecule 1: 30S ribosomal protein S2

Chain AB:



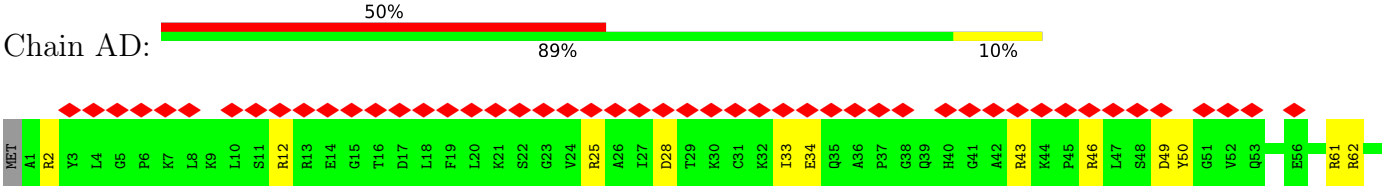
• Molecule 2: 30S ribosomal protein S3

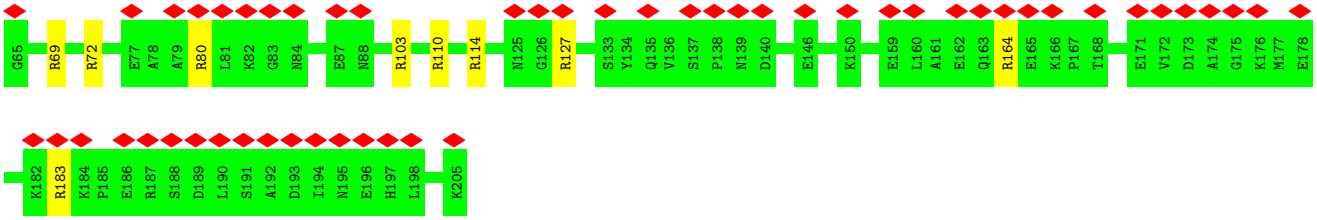
Chain AC:



• Molecule 3: 30S ribosomal protein S4

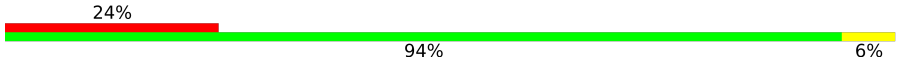
Chain AD:

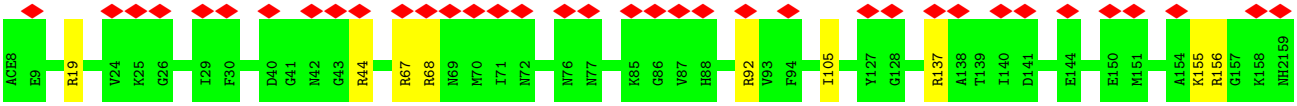




• Molecule 4: 30S ribosomal protein S5

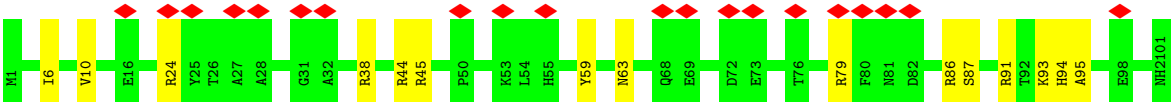
Chain AE:





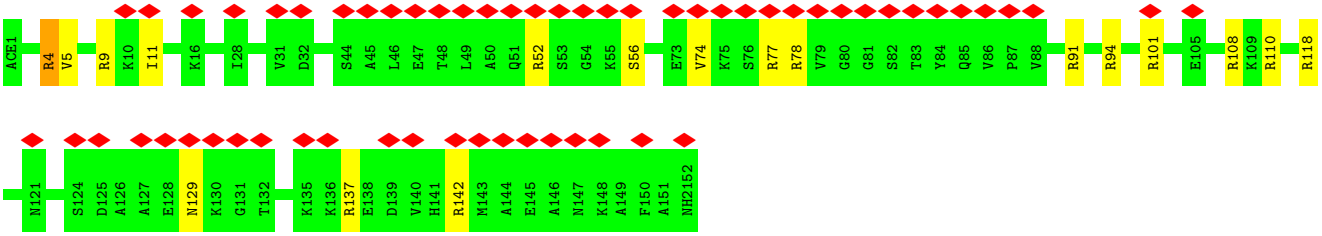
• Molecule 5: 30S ribosomal protein S6

Chain AF:



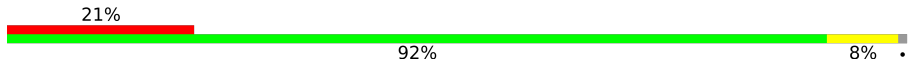
• Molecule 6: 30S ribosomal protein S7

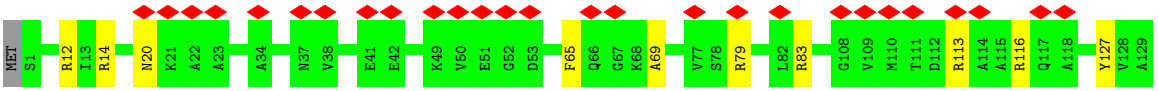
Chain AG:



• Molecule 7: 30S ribosomal protein S8

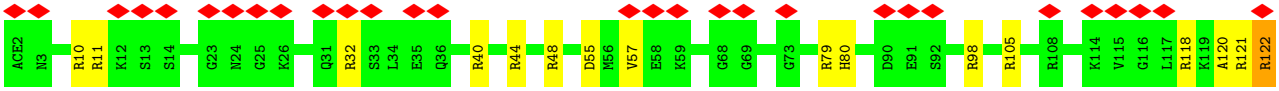
Chain AH:

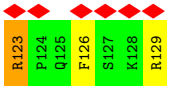




• Molecule 8: 30S ribosomal protein S9

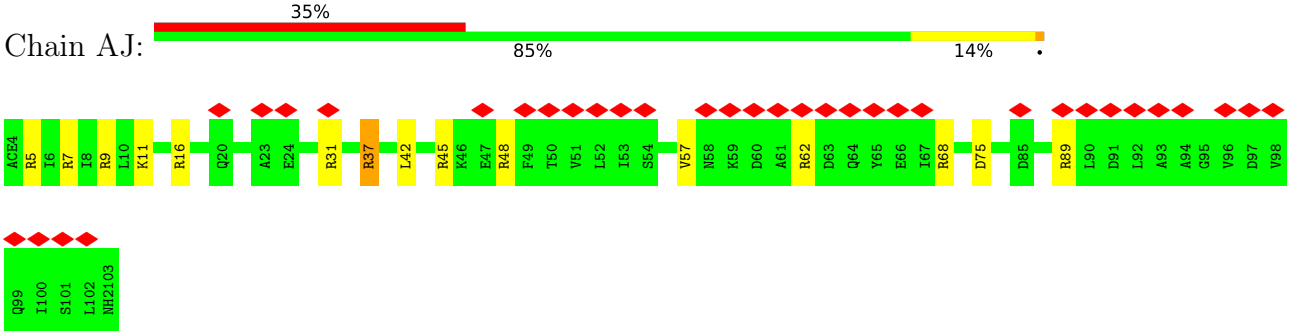
Chain AI:





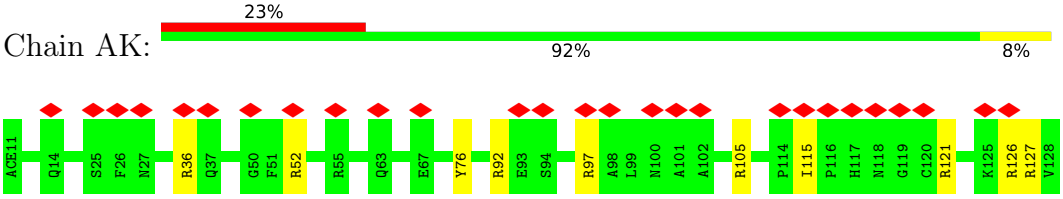
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



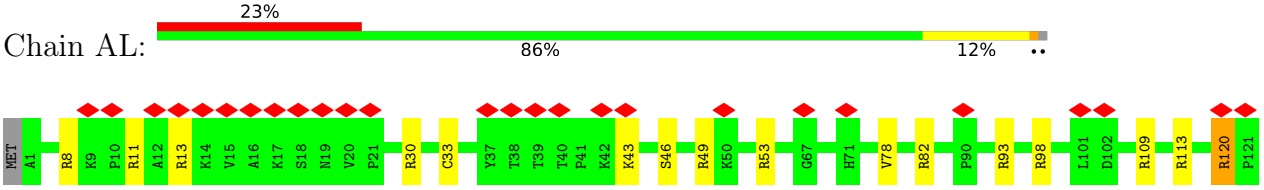
• Molecule 10: 30S ribosomal protein S11

Chain AK:



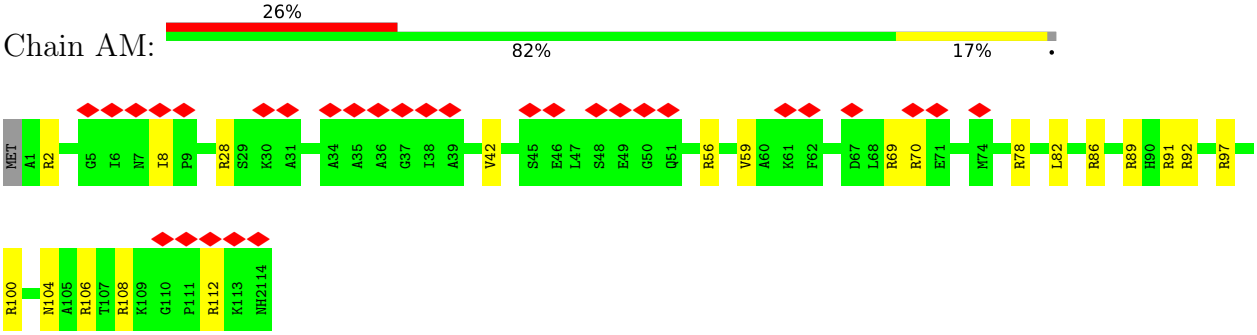
• Molecule 11: 30S ribosomal protein S12

Chain AL:



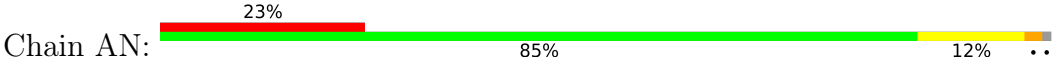
• Molecule 12: 30S ribosomal protein S13

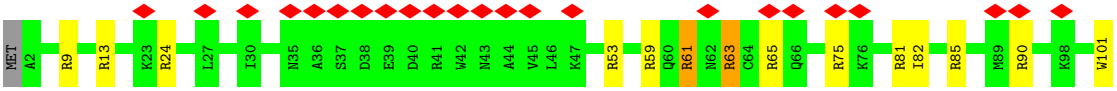
Chain AM:



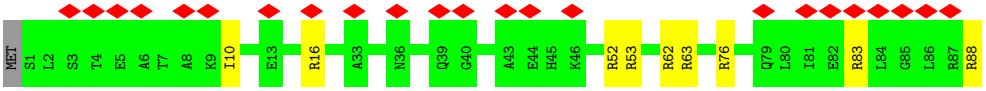
• Molecule 13: 30S ribosomal protein S14

Chain AN:

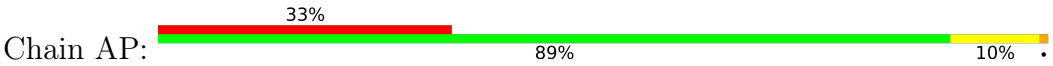


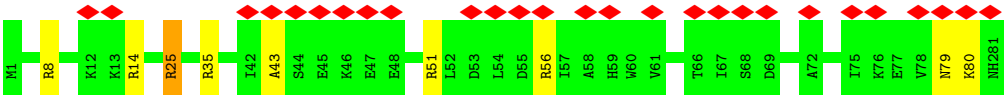


• Molecule 14: 30S ribosomal protein S15

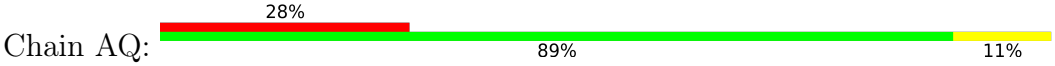


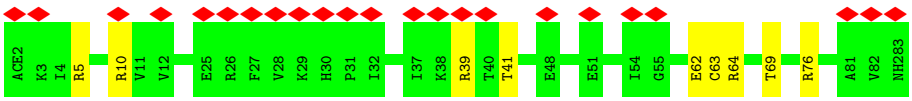
• Molecule 15: 30S ribosomal protein S16



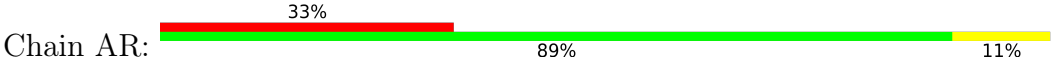


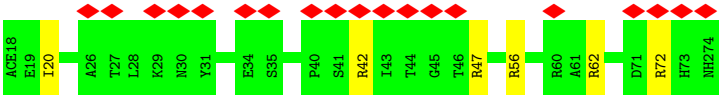
• Molecule 16: 30S ribosomal protein S17



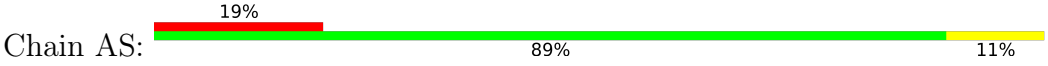


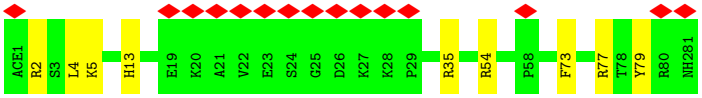
• Molecule 17: 30S ribosomal protein S18



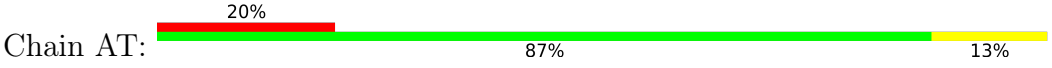


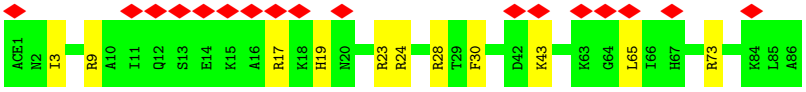
• Molecule 18: 30S ribosomal protein S19





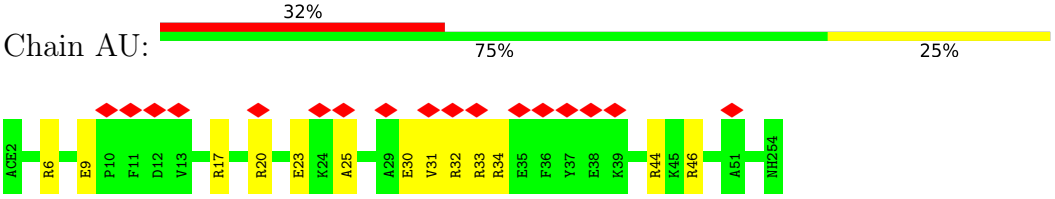
• Molecule 19: 30S ribosomal protein S20





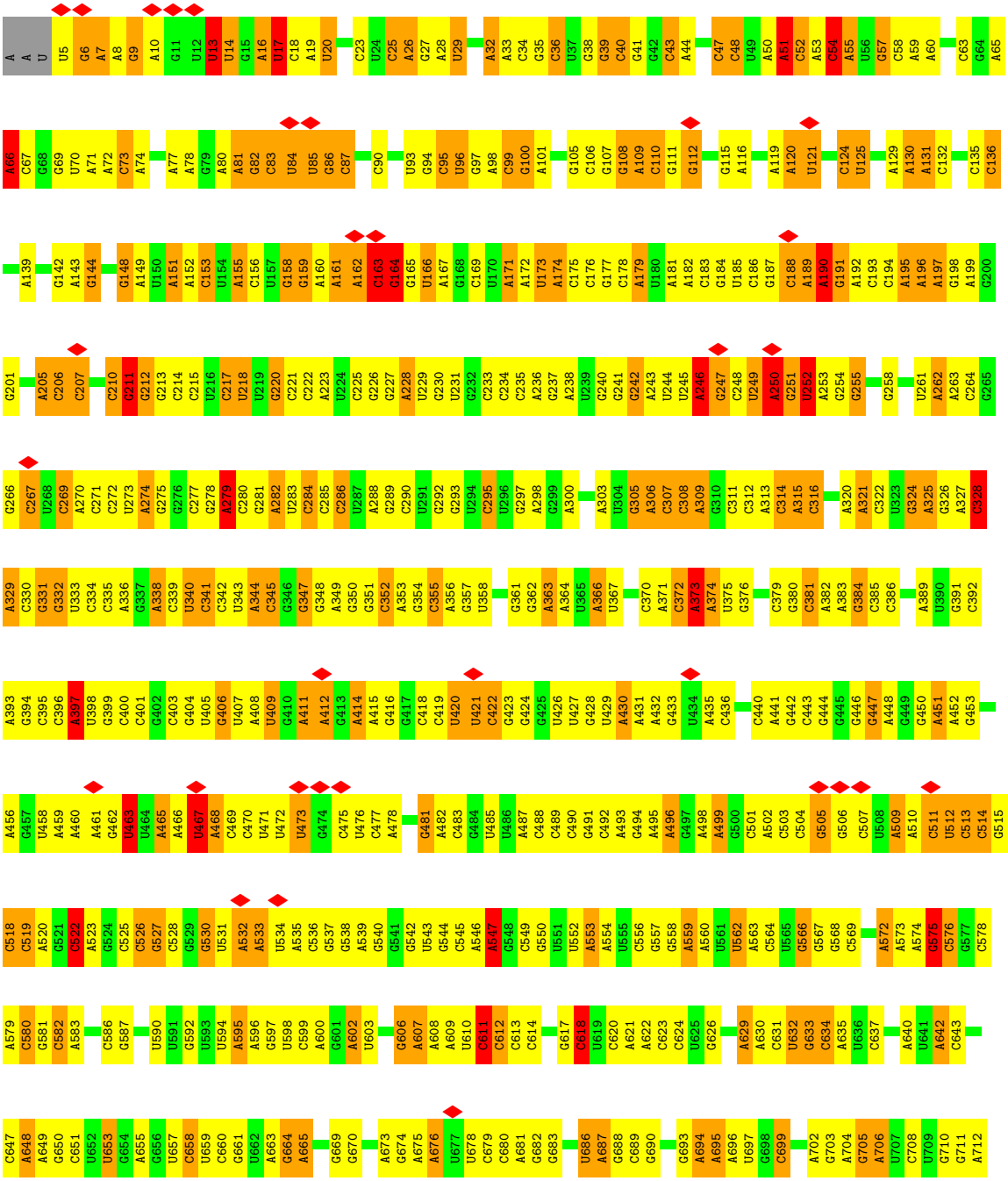
• Molecule 20: 30S ribosomal protein S21

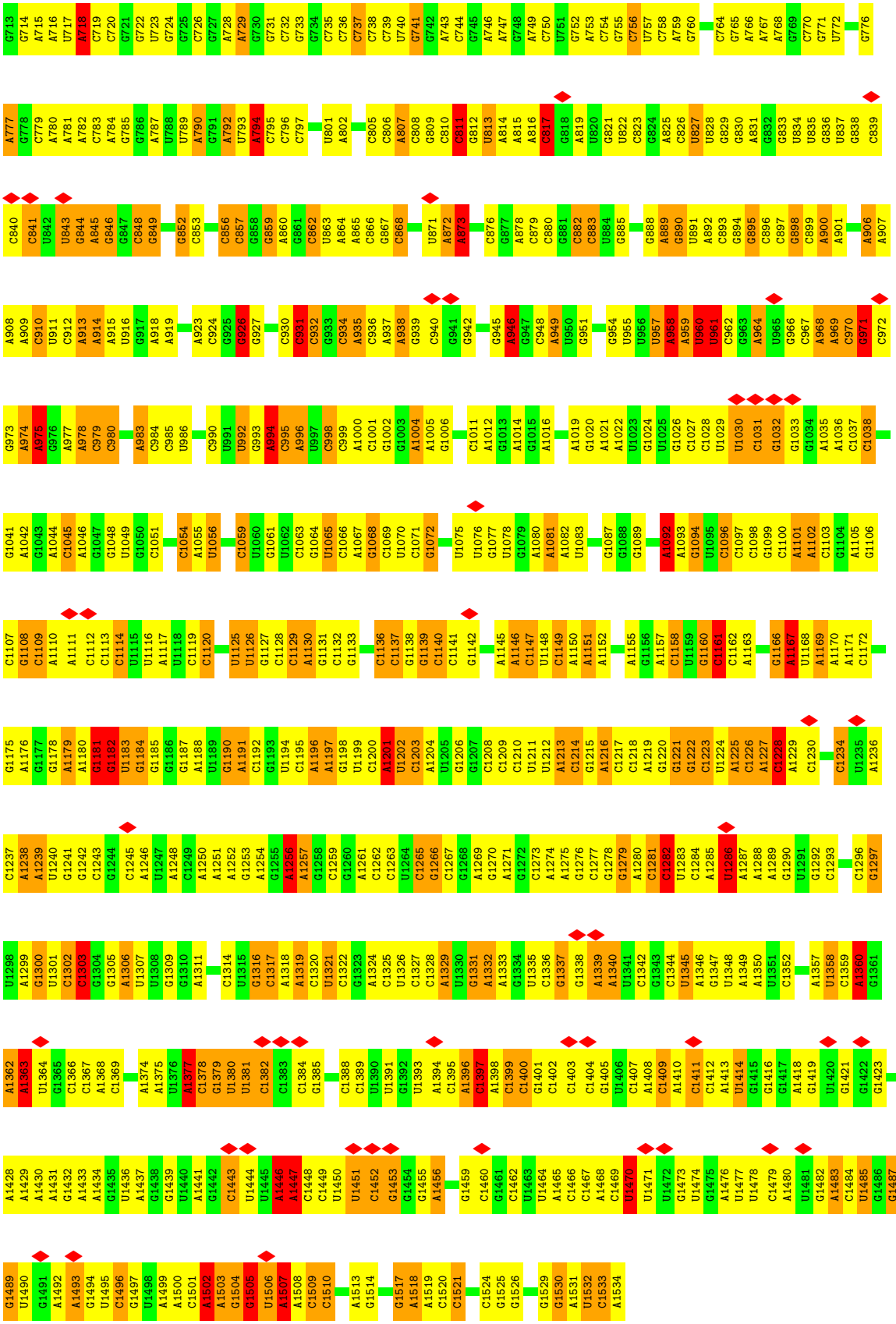
Chain AU:



• Molecule 21: 16S ribosomal RNA

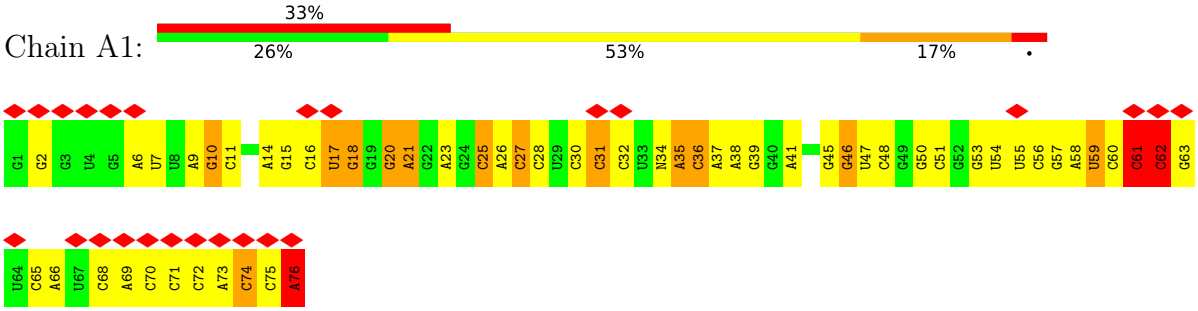
Chain AA:





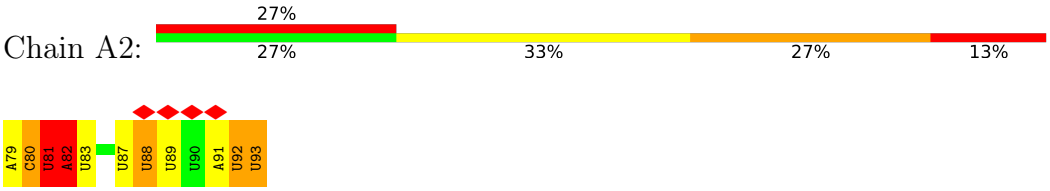
• Molecule 22: fMet-Val-tRNA-Val

Chain A1:



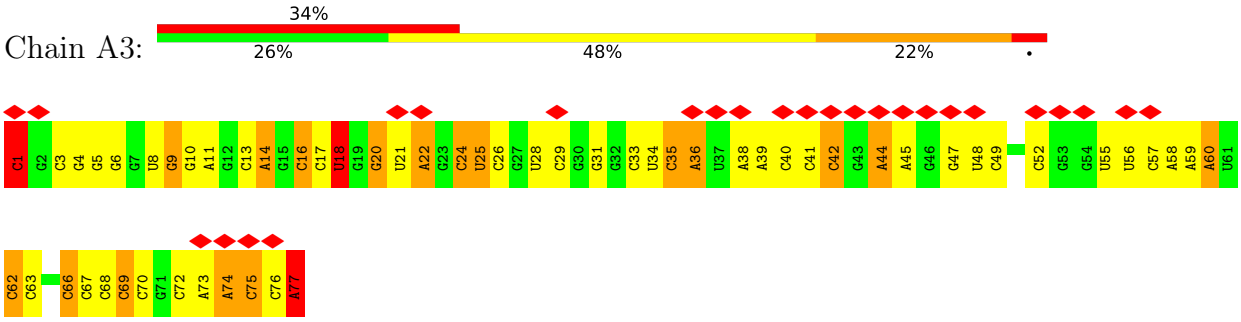
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

Chain A2:



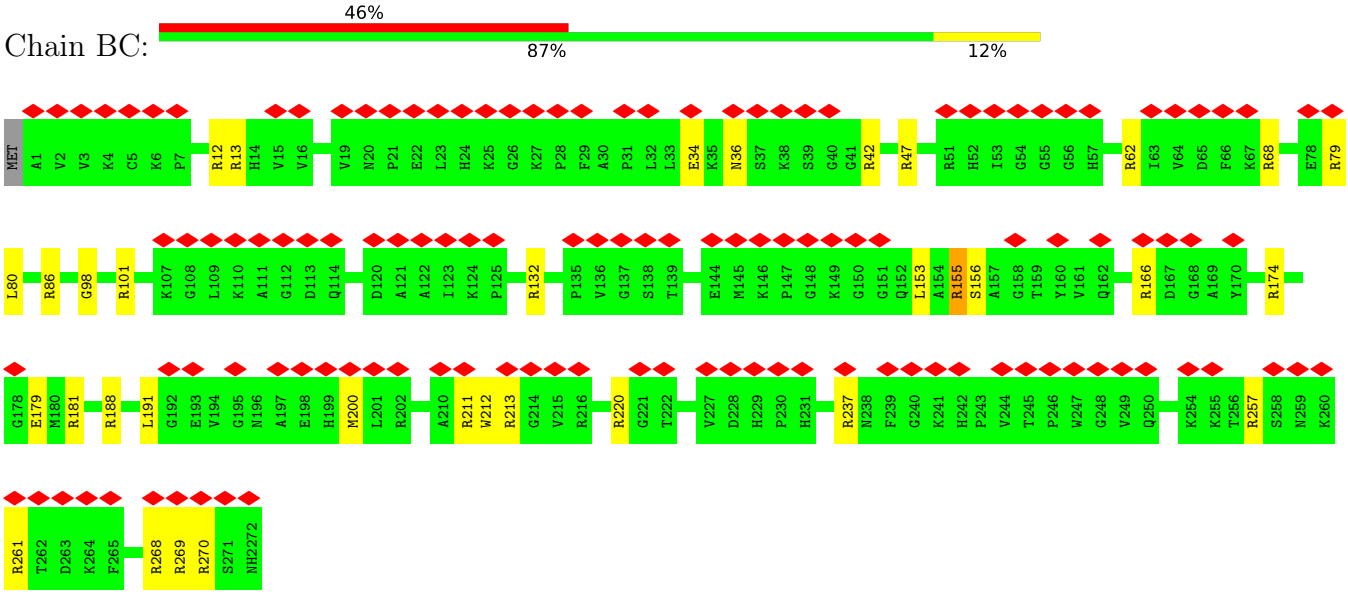
• Molecule 24: tRNA-fMet

Chain A3:



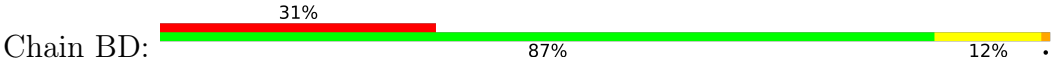
• Molecule 25: 50S ribosomal protein L2

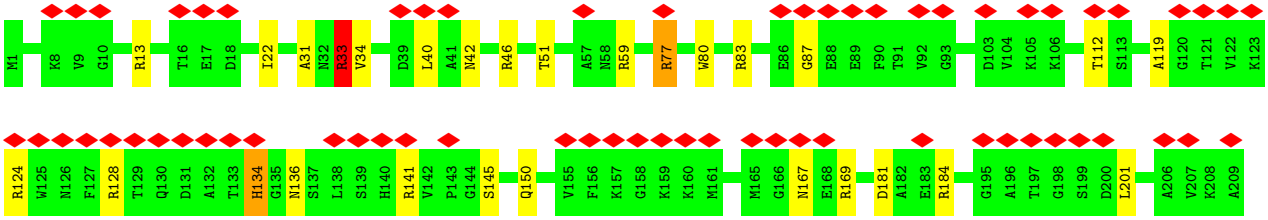
Chain BC:



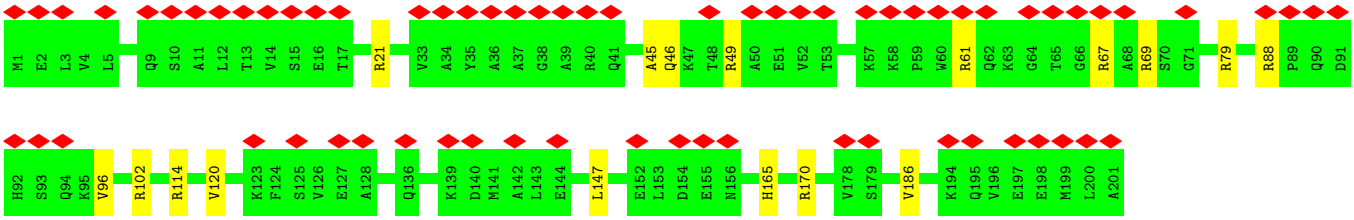
• Molecule 26: 50S ribosomal protein L3

Chain BD:

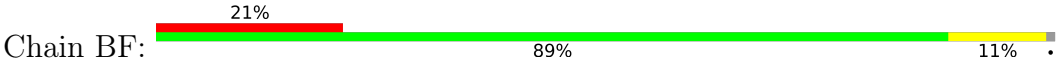


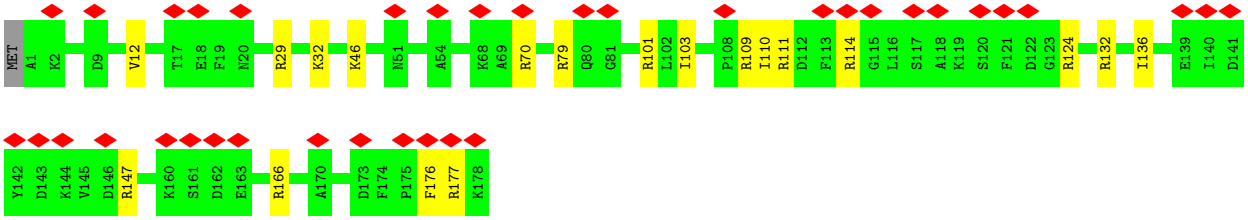


• Molecule 27: 50S ribosomal protein L4

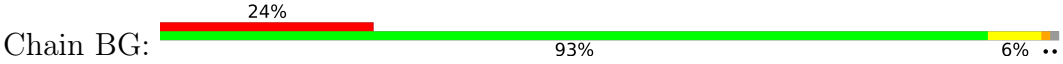


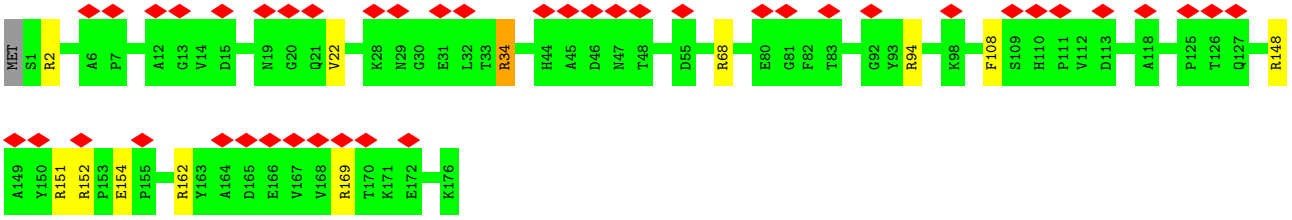
• Molecule 28: 50S ribosomal protein L5



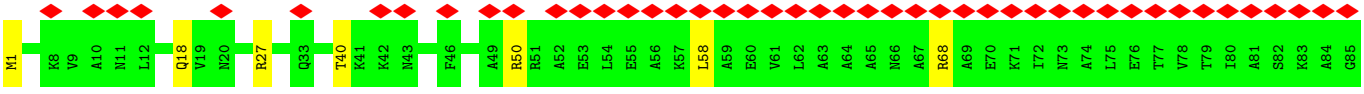


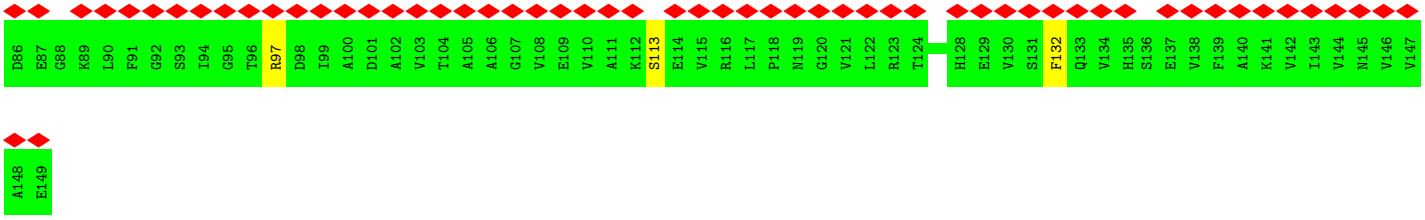
• Molecule 29: 50S ribosomal protein L6





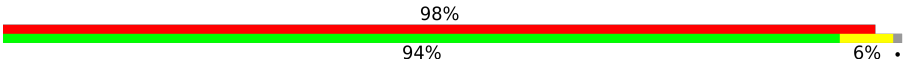
• Molecule 30: 50S ribosomal protein L9

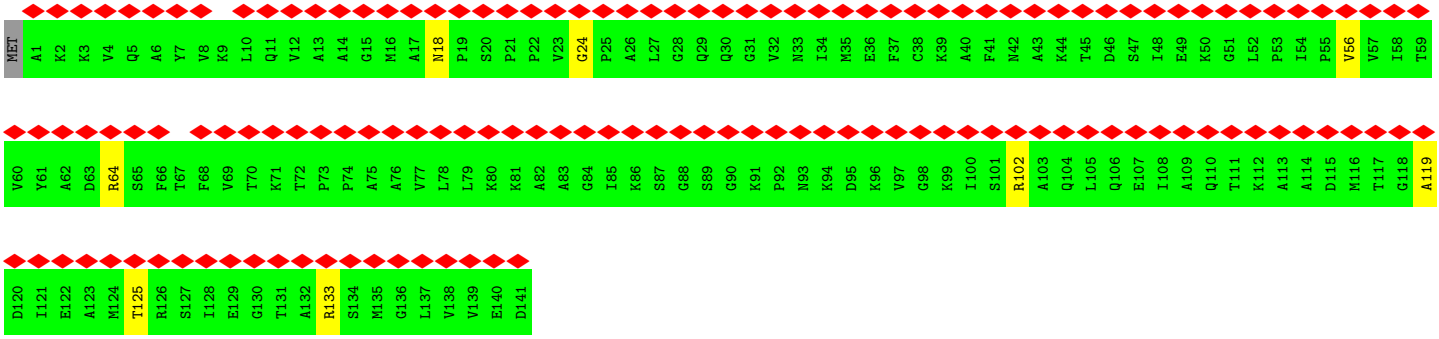




• Molecule 31: 50S ribosomal protein L11

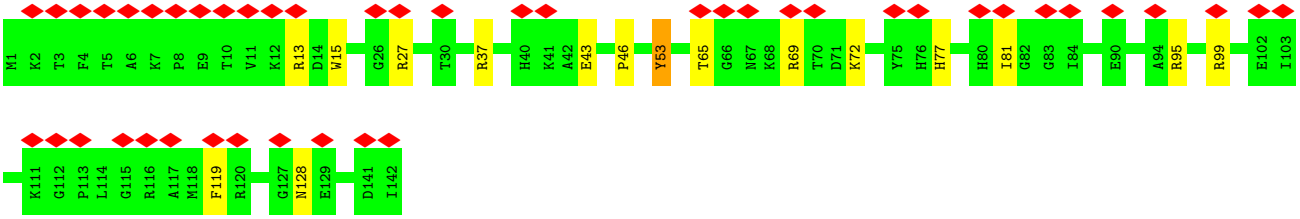
Chain BI:





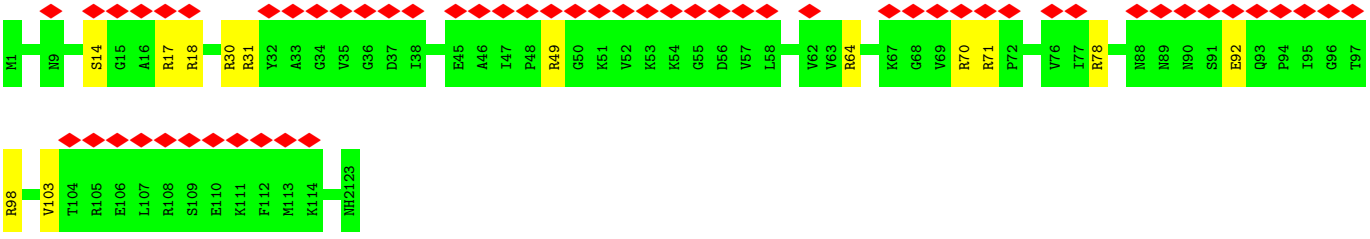
• Molecule 32: 50S ribosomal protein L13

Chain BJ:



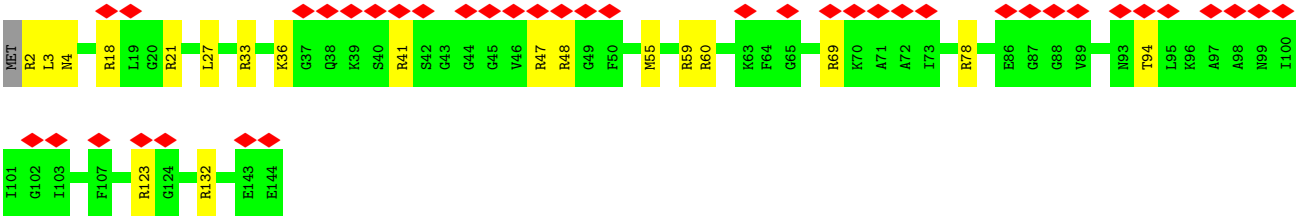
• Molecule 33: 50S ribosomal protein L14

Chain BK:



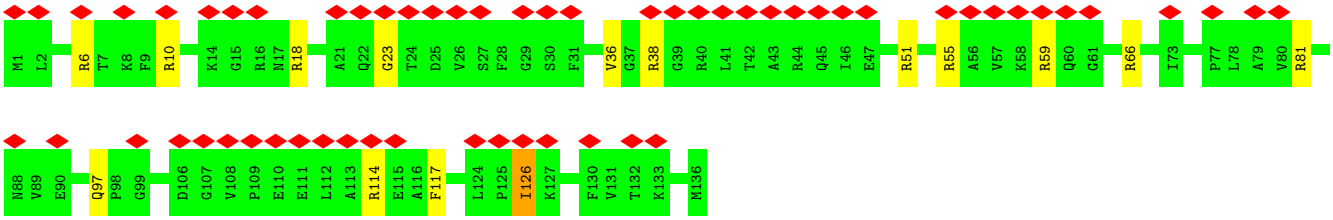
• Molecule 34: 50S ribosomal protein L15

Chain BL:



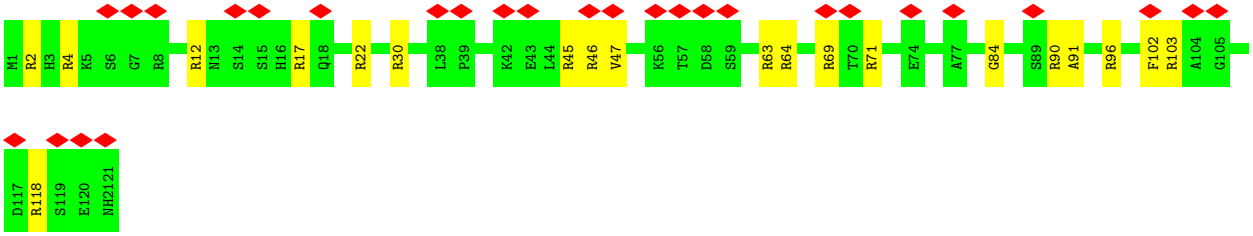
• Molecule 35: 50S ribosomal protein L16

Chain BM:



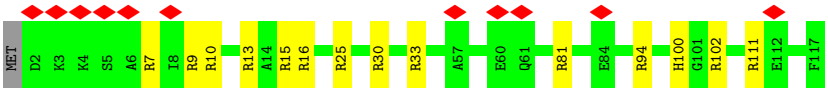
• Molecule 36: 50S ribosomal protein L17

Chain BN:



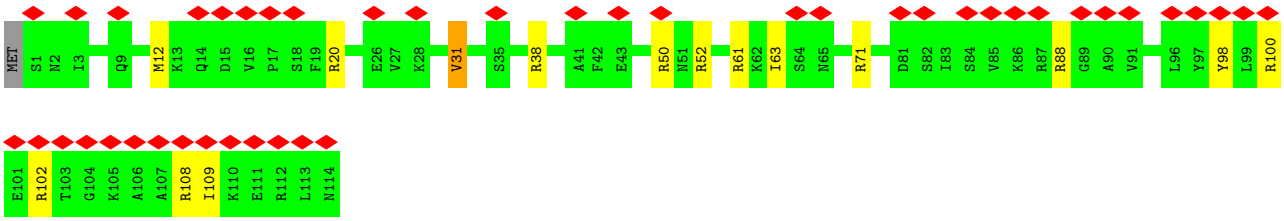
• Molecule 37: 50S ribosomal protein L18

Chain BO:



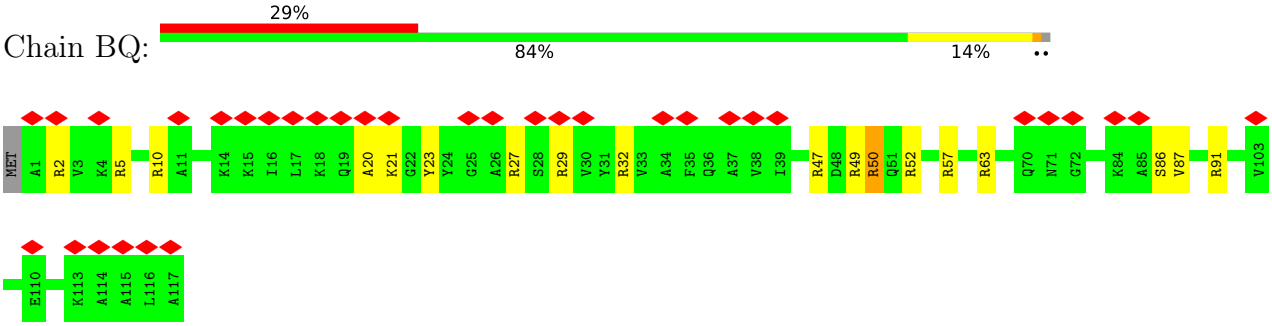
• Molecule 38: 50S ribosomal protein L19

Chain BP:



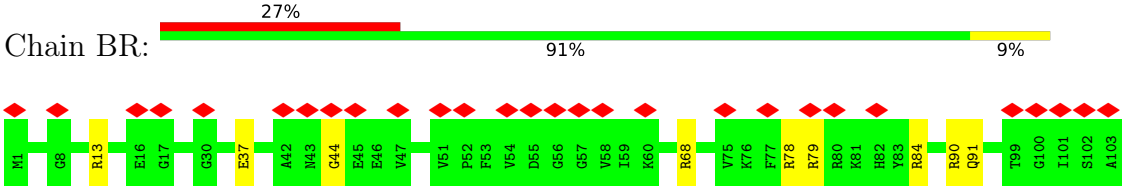
• Molecule 39: 50S ribosomal protein L20

Chain BQ:



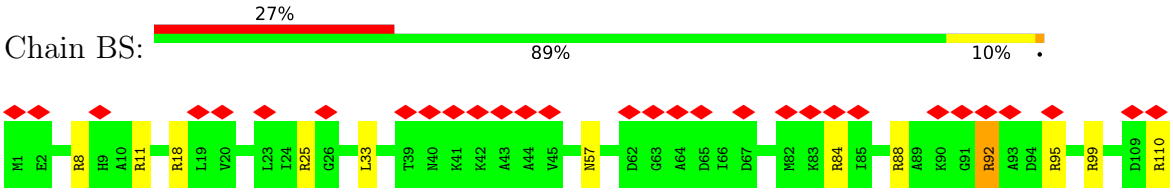
• Molecule 40: 50S ribosomal protein L21

Chain BR:



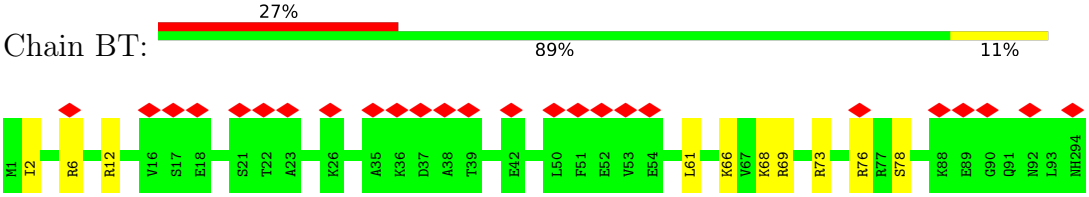
• Molecule 41: 50S ribosomal protein L22

Chain BS:



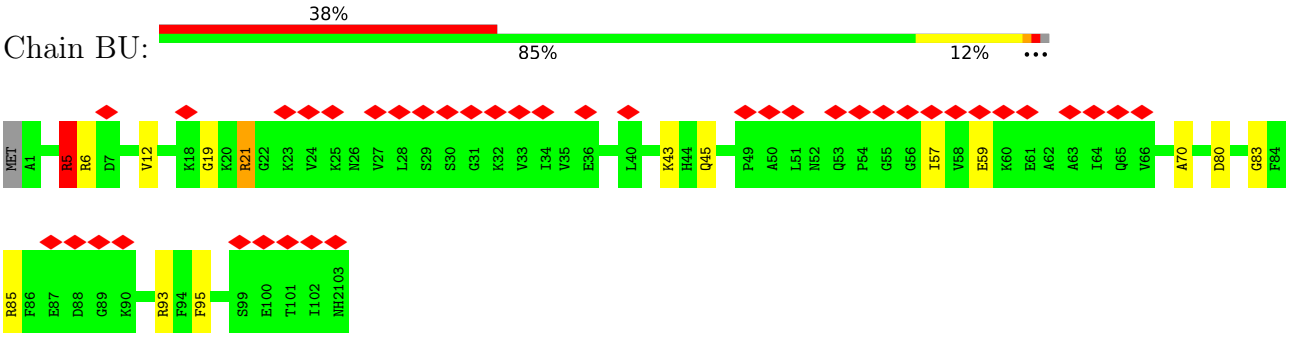
• Molecule 42: 50S ribosomal protein L23

Chain BT:



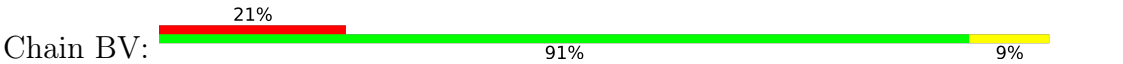
• Molecule 43: 50S ribosomal protein L24

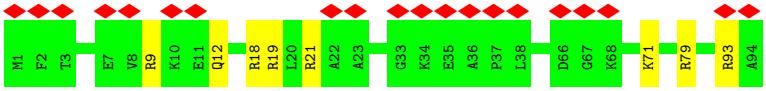
Chain BU:



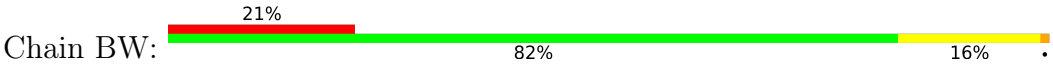
• Molecule 44: 50S ribosomal protein L25

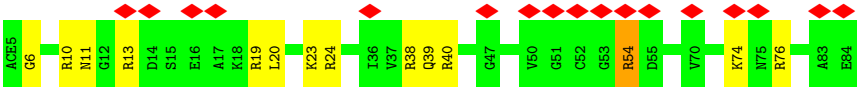
Chain BV:



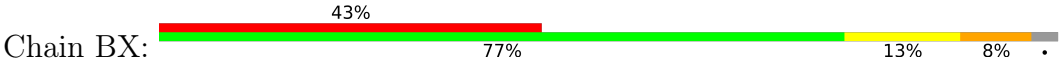


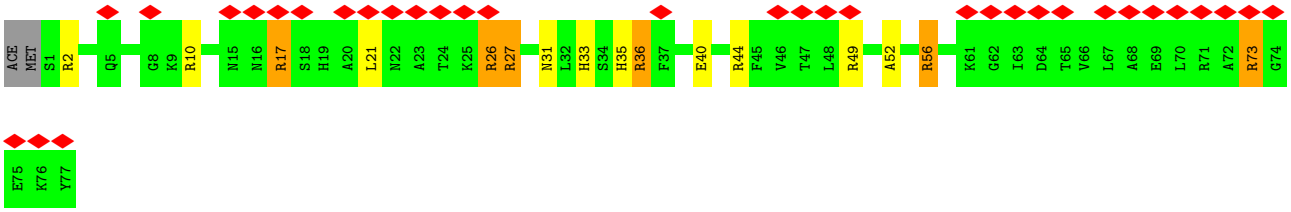
• Molecule 45: 50S ribosomal protein L27



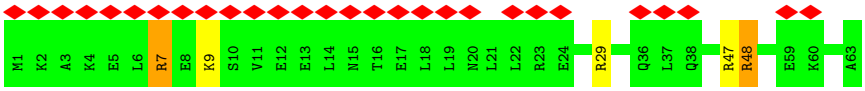


• Molecule 46: 50S ribosomal protein L28

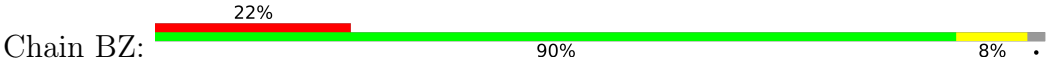


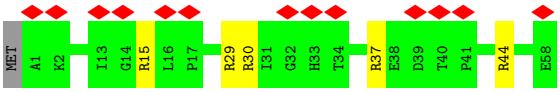


• Molecule 47: 50S ribosomal protein L29

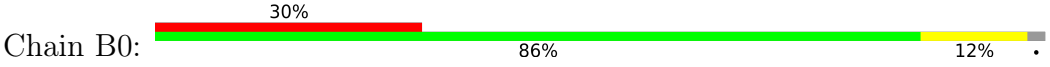


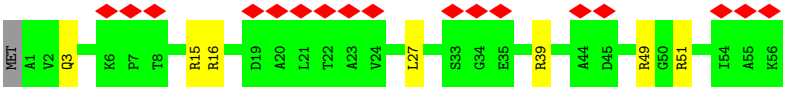
• Molecule 48: 50S ribosomal protein L30



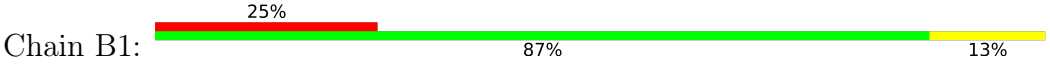


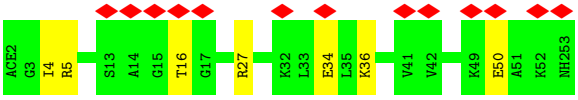
• Molecule 49: 50S ribosomal protein L32





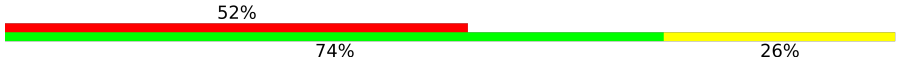
• Molecule 50: 50S ribosomal protein L33

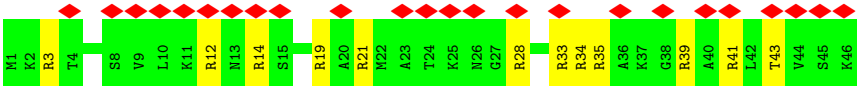




• Molecule 51: 50S ribosomal protein L34

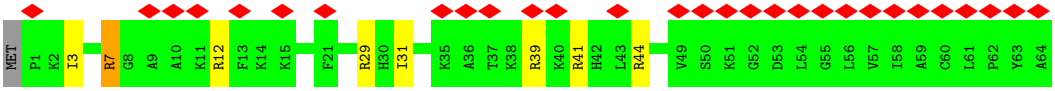
Chain B2:





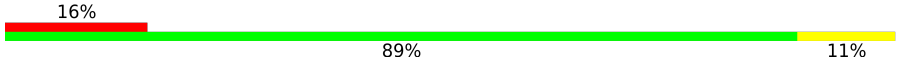
• Molecule 52: 50S ribosomal protein L35

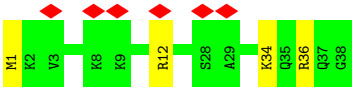
Chain B3:



• Molecule 53: 50S ribosomal protein L36

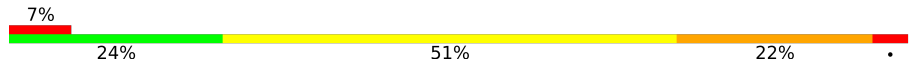
Chain B4:

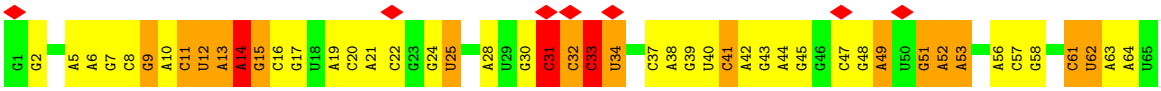


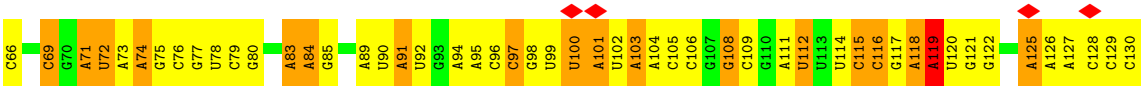


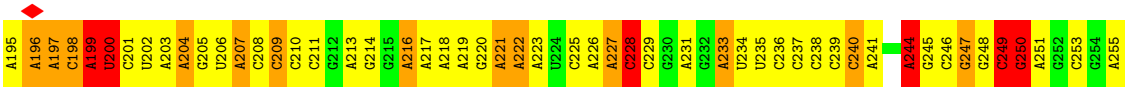
• Molecule 54: 23S ribosomal RNA

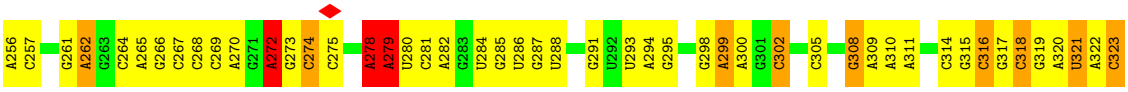
Chain BA:

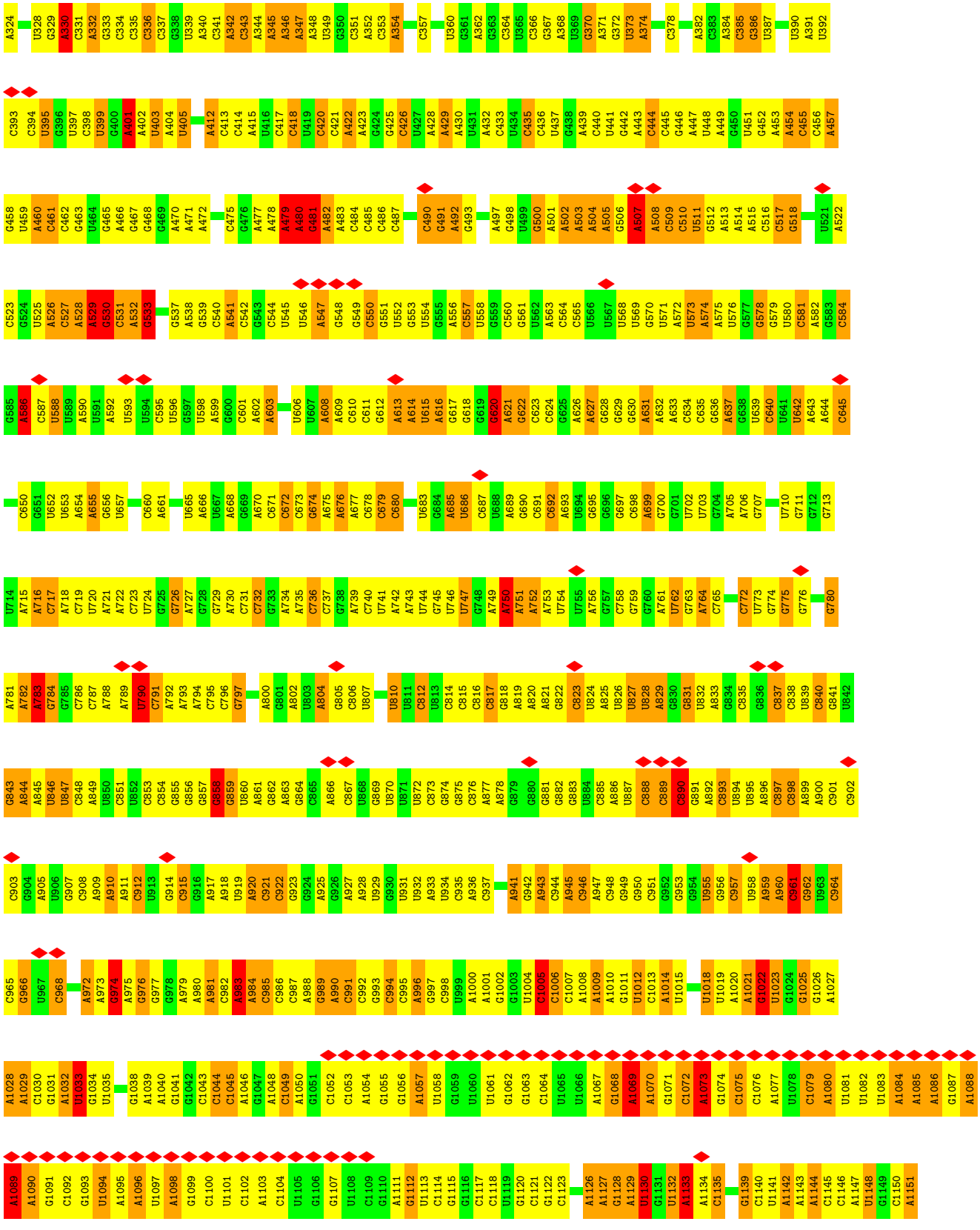


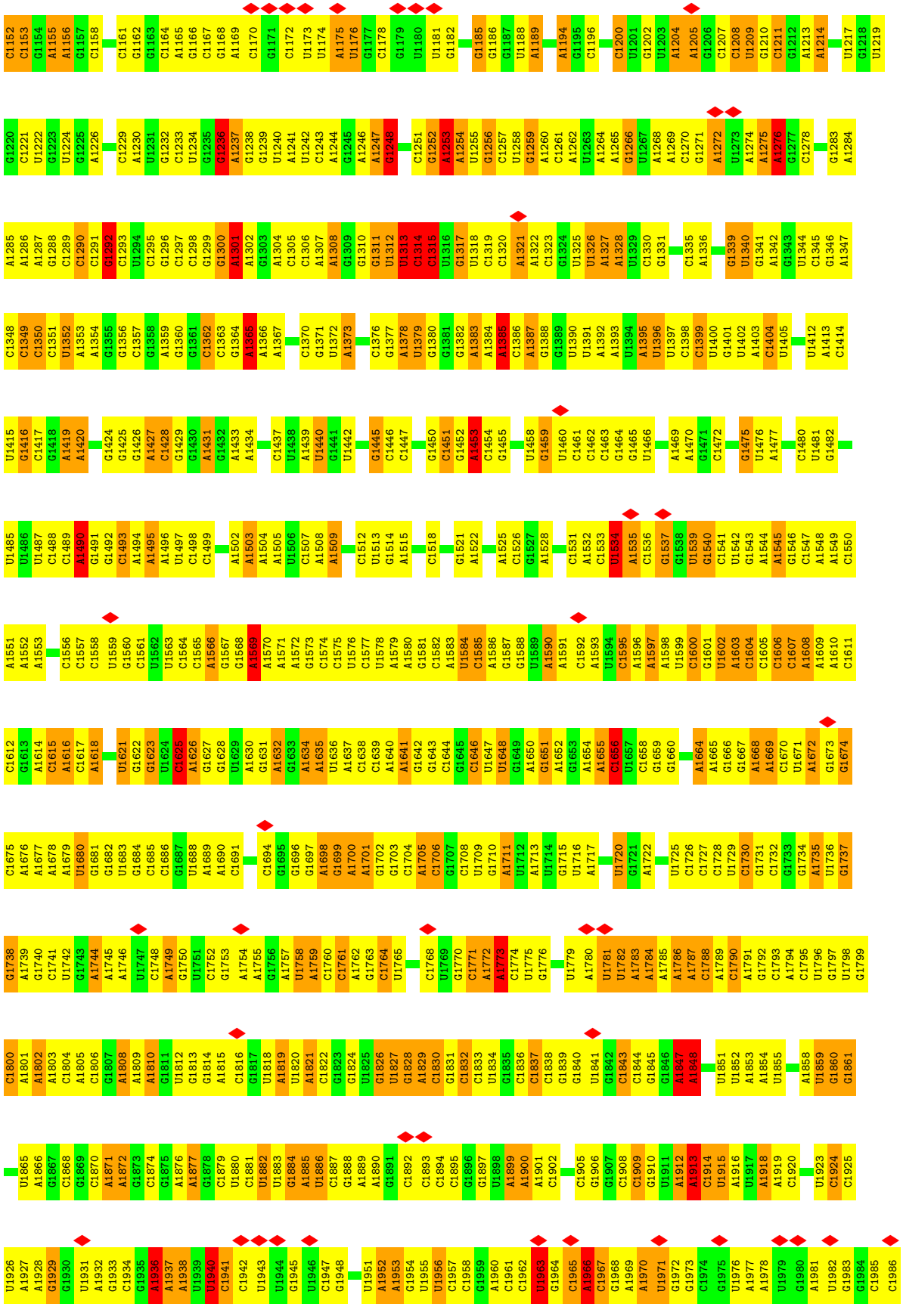


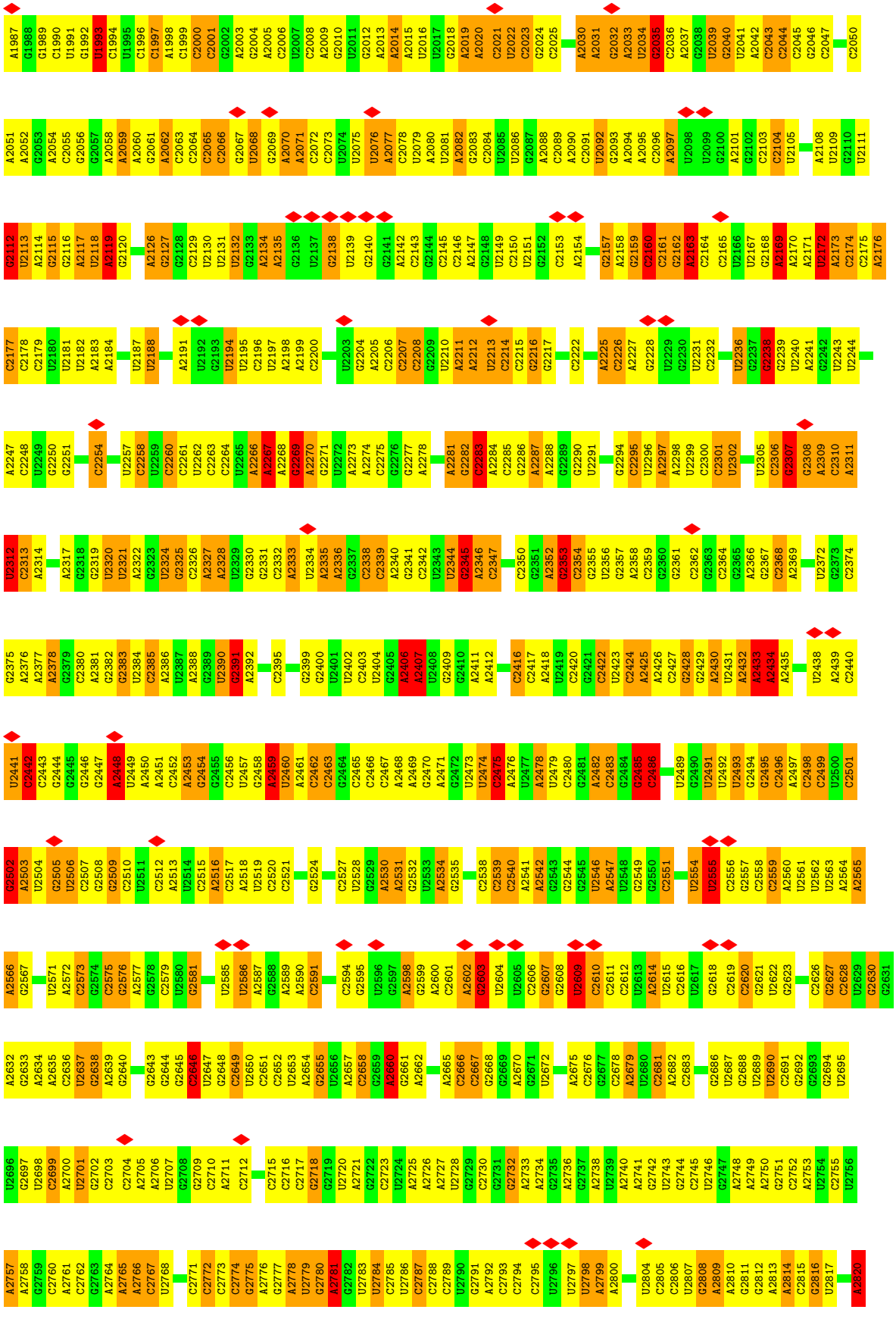


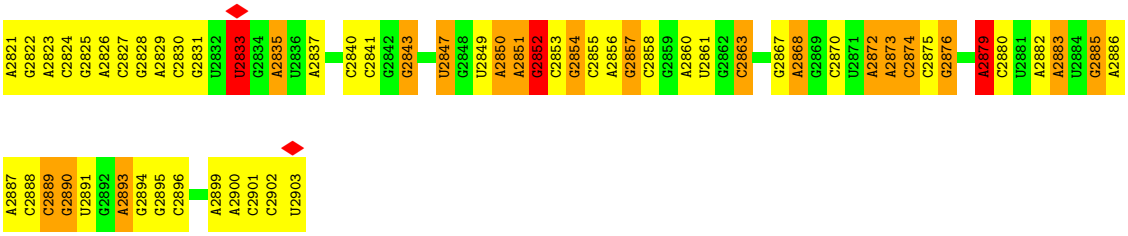






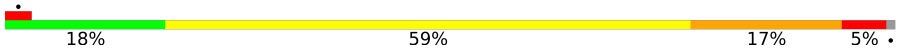


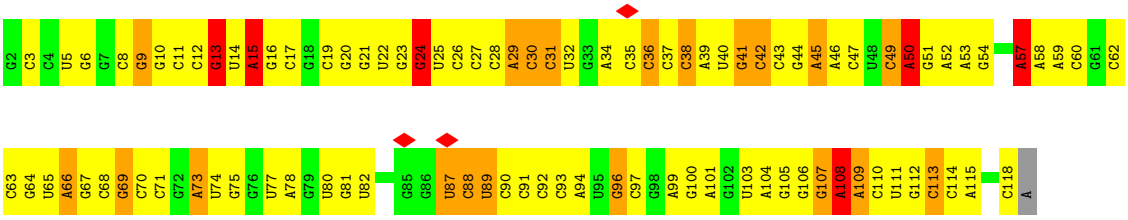




• Molecule 55: 5S ribosomal RNA

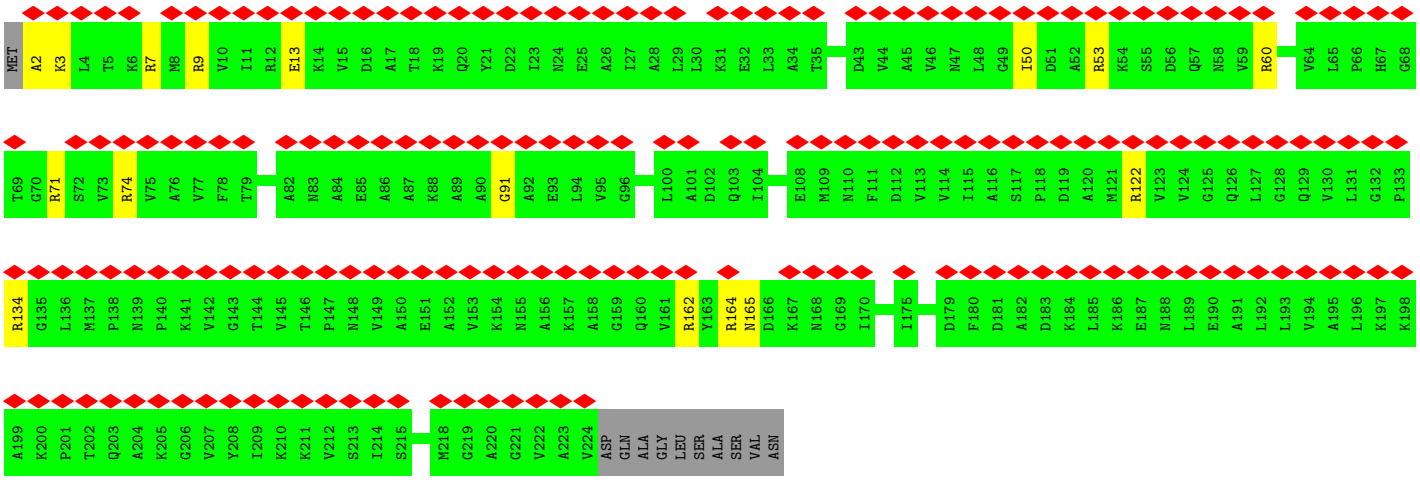
Chain BB:





• 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	2648	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	local	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	162740	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	165.351	Depositor
Minimum map value	-111.639	Depositor
Average map value	-1.339	Depositor
Map value standard deviation	17.775	Depositor
Recommended contour level	20.0	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.8, 2.8, 2.8	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AB	0.74	0/1736	1.04	11/2340 (0.5%)
2	AC	0.75	0/1651	1.19	17/2225 (0.8%)
3	AD	0.80	0/1665	1.19	16/2227 (0.7%)
4	AE	0.73	0/1119	1.04	7/1506 (0.5%)
5	AF	0.76	0/835	1.17	8/1128 (0.7%)
6	AG	0.77	0/1188	1.19	13/1593 (0.8%)
7	AH	0.71	0/989	1.03	8/1326 (0.6%)
8	AI	0.83	0/1035	1.33	19/1377 (1.4%)
9	AJ	0.75	0/797	1.24	12/1079 (1.1%)
10	AK	0.77	0/894	1.18	9/1207 (0.7%)
11	AL	0.78	0/969	1.23	14/1300 (1.1%)
12	AM	0.77	0/884	1.30	16/1181 (1.4%)
13	AN	0.80	0/817	1.35	12/1088 (1.1%)
14	AO	0.74	0/722	1.20	9/964 (0.9%)
15	AP	0.80	0/648	1.15	5/870 (0.6%)
16	AQ	0.72	0/658	1.10	7/883 (0.8%)
17	AR	0.82	0/463	1.18	5/623 (0.8%)
18	AS	0.78	0/653	1.12	6/879 (0.7%)
19	AT	0.71	0/672	1.18	8/890 (0.9%)
20	AU	0.86	0/431	1.59	9/572 (1.6%)
21	AA	1.52	0/36759	2.22	1943/57346 (3.4%)
22	A1	1.54	0/1668	2.18	94/2595 (3.6%)
23	A2	1.50	0/343	2.20	15/531 (2.8%)
24	A3	1.51	0/1722	2.19	80/2685 (3.0%)
25	BC	0.76	0/2121	1.28	25/2852 (0.9%)
26	BD	0.71	0/1586	1.19	12/2134 (0.6%)
27	BE	0.70	0/1571	1.14	9/2113 (0.4%)
28	BF	0.77	0/1444	1.16	12/1937 (0.6%)
29	BG	0.72	0/1343	1.14	9/1816 (0.5%)
30	BH	0.70	0/1122	1.11	5/1515 (0.3%)
31	BI	0.69	0/1046	1.08	4/1410 (0.3%)
32	BJ	0.76	0/1152	1.12	6/1551 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BK	0.73	0/947	1.20	10/1268 (0.8%)
34	BL	0.75	0/1054	1.29	14/1403 (1.0%)
35	BM	0.78	0/1093	1.23	12/1460 (0.8%)
36	BN	0.79	0/973	1.35	16/1301 (1.2%)
37	BO	0.76	0/902	1.29	15/1209 (1.2%)
38	BP	0.76	0/929	1.27	9/1242 (0.7%)
39	BQ	0.80	0/960	1.30	15/1278 (1.2%)
40	BR	0.75	0/829	1.12	6/1107 (0.5%)
41	BS	0.68	0/864	1.19	11/1156 (1.0%)
42	BT	0.68	0/744	1.17	5/994 (0.5%)
43	BU	0.73	0/787	1.15	7/1051 (0.7%)
44	BV	0.74	0/766	1.17	6/1025 (0.6%)
45	BW	0.78	0/604	1.34	10/799 (1.3%)
46	BX	0.78	0/635	1.35	10/848 (1.2%)
47	BY	0.71	0/510	1.22	5/677 (0.7%)
48	BZ	0.72	0/453	1.27	5/605 (0.8%)
49	B0	0.74	0/450	1.22	5/599 (0.8%)
50	B1	0.76	0/417	1.09	2/556 (0.4%)
51	B2	0.82	0/380	1.56	13/498 (2.6%)
52	B3	0.75	0/513	1.26	8/676 (1.2%)
53	B4	0.68	0/303	1.13	2/397 (0.5%)
54	BA	1.40	1/69796 (0.0%)	2.21	4048/108888 (3.7%)
55	BB	1.41	0/2800	2.18	153/4367 (3.5%)
56	B5	0.68	0/1673	1.13	11/2255 (0.5%)
All	All	1.28	1/160085 (0.0%)	1.99	6823/239402 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AC	0	1
8	AI	0	1
9	AJ	0	1
10	AK	0	1
21	AA	0	365
22	A1	0	13
23	A2	0	5
24	A3	0	17
25	BC	0	1
43	BU	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	BA	0	636
55	BB	0	20
All	All	0	1062

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	BA	945	A	N3-C4	5.58	1.38	1.34

All (6823) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	330	A	O4'-C1'-N9	12.97	118.58	108.20
54	BA	2270	A	N1-C6-N6	-12.77	110.94	118.60
54	BA	900	A	N1-C6-N6	-12.68	110.99	118.60
54	BA	1069	A	N1-C6-N6	-12.45	111.13	118.60
54	BA	1616	A	N1-C6-N6	-12.33	111.20	118.60
54	BA	2530	A	N1-C6-N6	-12.18	111.29	118.60
21	AA	573	A	N1-C6-N6	-12.12	111.33	118.60
54	BA	119	A	N1-C6-N6	-12.10	111.34	118.60
54	BA	34	U	O4'-C1'-N1	12.09	117.87	108.20
54	BA	959	A	N1-C6-N6	-12.08	111.35	118.60
54	BA	2227	A	N1-C6-N6	-12.07	111.36	118.60
54	BA	1382	G	O4'-C1'-N9	12.05	117.84	108.20
54	BA	1272	A	N1-C6-N6	-11.96	111.42	118.60
54	BA	928	A	N1-C6-N6	-11.96	111.43	118.60
54	BA	2117	A	N1-C6-N6	-11.90	111.46	118.60
21	AA	766	A	N1-C6-N6	-11.80	111.52	118.60
54	BA	2882	A	N1-C6-N6	-11.74	111.55	118.60
21	AA	320	A	N1-C6-N6	-11.72	111.57	118.60
54	BA	1046	A	O4'-C1'-N9	11.65	117.52	108.20
21	AA	600	A	N1-C6-N6	-11.59	111.65	118.60
21	AA	1394	A	N1-C6-N6	-11.54	111.68	118.60
54	BA	1847	A	N1-C6-N6	-11.54	111.68	118.60
54	BA	504	A	N1-C6-N6	-11.51	111.69	118.60
54	BA	810	U	O4'-C1'-N1	11.46	117.37	108.20
54	BA	2590	A	N1-C6-N6	-11.44	111.74	118.60
54	BA	2705	A	N1-C6-N6	-11.43	111.74	118.60
21	AA	728	A	N1-C6-N6	-11.36	111.78	118.60
21	AA	629	A	N1-C6-N6	-11.35	111.79	118.60
54	BA	2833	U	O4'-C1'-N1	11.34	117.27	108.20
54	BA	2090	A	N1-C6-N6	-11.32	111.81	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1352	U	O4'-C1'-N1	11.32	117.25	108.20
21	AA	675	A	N1-C6-N6	-11.28	111.83	118.60
54	BA	983	A	N1-C6-N6	-11.24	111.86	118.60
54	BA	753	A	N1-C6-N6	-11.23	111.86	118.60
21	AA	389	A	N1-C6-N6	-11.21	111.87	118.60
54	BA	2565	A	N1-C6-N6	-11.16	111.91	118.60
21	AA	1518	A	N1-C6-N6	-11.14	111.91	118.60
54	BA	602	A	N1-C6-N6	-11.10	111.94	118.60
54	BA	556	A	N1-C6-N6	-11.08	111.95	118.60
21	AA	371	A	N1-C6-N6	-11.05	111.97	118.60
55	BB	94	A	N1-C6-N6	-11.04	111.97	118.60
54	BA	165	A	N1-C6-N6	-10.99	112.00	118.60
54	BA	1393	A	N1-C6-N6	-10.97	112.02	118.60
54	BA	1029	A	N1-C6-N6	-10.95	112.03	118.60
54	BA	1304	A	N1-C6-N6	-10.95	112.03	118.60
54	BA	1021	A	N1-C6-N6	-10.93	112.04	118.60
54	BA	2425	A	N1-C6-N6	-10.93	112.04	118.60
54	BA	1853	A	N1-C6-N6	-10.92	112.05	118.60
54	BA	1591	A	N1-C6-N6	-10.92	112.05	118.60
54	BA	300	A	N1-C6-N6	-10.92	112.05	118.60
21	AA	681	A	N1-C6-N6	-10.90	112.06	118.60
24	A3	36	A	N1-C6-N6	-10.90	112.06	118.60
54	BA	1525	A	N1-C6-N6	-10.90	112.06	118.60
21	AA	282	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	781	A	N1-C6-N6	-10.88	112.07	118.60
54	BA	1586	A	N1-C6-N6	-10.87	112.08	118.60
54	BA	1746	A	N1-C6-N6	-10.87	112.08	118.60
21	AA	1398	A	N1-C6-N6	-10.86	112.08	118.60
24	A3	74	A	N1-C6-N6	-10.87	112.08	118.60
54	BA	10	A	N1-C6-N6	-10.85	112.09	118.60
10	AK	92	ARG	NE-CZ-NH1	10.85	125.72	120.30
54	BA	2266	A	N1-C6-N6	-10.84	112.09	118.60
21	AA	994	A	N1-C6-N6	-10.78	112.13	118.60
54	BA	384	A	N1-C6-N6	-10.77	112.14	118.60
54	BA	2900	A	N1-C6-N6	-10.77	112.14	118.60
21	AA	262	A	N1-C6-N6	-10.76	112.14	118.60
21	AA	554	A	N1-C6-N6	-10.74	112.15	118.60
21	AA	279	A	N1-C6-N6	-10.74	112.16	118.60
21	AA	1333	A	N1-C6-N6	-10.74	112.15	118.60
21	AA	1000	A	N1-C6-N6	-10.74	112.16	118.60
21	AA	171	A	N1-C6-N6	-10.70	112.18	118.60
54	BA	2114	A	N1-C6-N6	-10.70	112.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	483	A	N1-C6-N6	-10.70	112.18	118.60
54	BA	2268	A	N1-C6-N6	-10.70	112.18	118.60
54	BA	1916	A	N1-C6-N6	-10.69	112.19	118.60
21	AA	747	A	N1-C6-N6	-10.67	112.20	118.60
21	AA	1180	A	N1-C6-N6	-10.67	112.20	118.60
21	AA	468	A	N1-C6-N6	-10.67	112.20	118.60
21	AA	495	A	N1-C6-N6	-10.66	112.20	118.60
54	BA	2060	A	N1-C6-N6	-10.66	112.20	118.60
54	BA	2297	A	N1-C6-N6	-10.65	112.21	118.60
54	BA	2513	A	N1-C6-N6	-10.64	112.21	118.60
54	BA	933	A	N1-C6-N6	-10.64	112.22	118.60
54	BA	1755	A	N1-C6-N6	-10.63	112.22	118.60
54	BA	382	A	N1-C6-N6	-10.63	112.22	118.60
54	BA	878	A	N1-C6-N6	-10.63	112.22	118.60
21	AA	78	A	N1-C6-N6	-10.61	112.23	118.60
21	AA	665	A	N1-C6-N6	-10.60	112.24	118.60
21	AA	1433	A	N1-C6-N6	-10.59	112.25	118.60
54	BA	2872	A	N1-C6-N6	-10.57	112.26	118.60
21	AA	695	A	N1-C6-N6	-10.53	112.28	118.60
54	BA	142	A	N1-C6-N6	-10.53	112.28	118.60
21	AA	356	A	N1-C6-N6	-10.52	112.29	118.60
54	BA	1098	A	N1-C6-N6	-10.51	112.30	118.60
54	BA	278	A	N1-C6-N6	-10.51	112.30	118.60
54	BA	1147	A	N1-C6-N6	-10.49	112.30	118.60
21	AA	1169	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	2670	A	N1-C6-N6	-10.47	112.32	118.60
54	BA	1552	A	O4'-C1'-N9	10.47	116.58	108.20
13	AN	75	ARG	NE-CZ-NH1	10.45	125.52	120.30
54	BA	2439	A	N1-C6-N6	-10.44	112.33	118.60
54	BA	910	A	N1-C6-N6	-10.43	112.34	118.60
21	AA	1299	A	N1-C6-N6	-10.43	112.34	118.60
21	AA	1499	A	N1-C6-N6	-10.42	112.34	118.60
21	AA	825	A	N1-C6-N6	-10.41	112.35	118.60
54	BA	1434	A	N1-C6-N6	-10.41	112.35	118.60
54	BA	1635	A	N1-C6-N6	-10.39	112.36	118.60
54	BA	1265	A	N1-C6-N6	-10.39	112.36	118.60
54	BA	1545	A	N1-C6-N6	-10.39	112.37	118.60
54	BA	1614	A	N1-C6-N6	-10.38	112.37	118.60
21	AA	873	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	2886	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	368	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	1174	U	O4'-C1'-N1	10.36	116.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1932	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	1090	A	N1-C6-N6	-10.34	112.40	118.60
54	BA	371	A	N1-C6-N6	-10.33	112.41	118.60
21	AA	622	A	N1-C6-N6	-10.32	112.41	118.60
21	AA	1349	A	N1-C6-N6	-10.31	112.41	118.60
54	BA	1534	U	O4'-C1'-N1	10.29	116.44	108.20
54	BA	1805	A	N1-C6-N6	-10.29	112.43	118.60
21	AA	1146	A	N1-C6-N6	-10.29	112.43	118.60
54	BA	2274	A	N1-C6-N6	-10.28	112.43	118.60
54	BA	727	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	199	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	1086	A	N1-C6-N6	-10.26	112.44	118.60
21	AA	53	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	819	A	N1-C6-N6	-10.25	112.45	118.60
54	BA	2518	A	N1-C6-N6	-10.22	112.47	118.60
54	BA	2810	A	N1-C6-N6	-10.22	112.47	118.60
54	BA	344	A	N1-C6-N6	-10.21	112.47	118.60
54	BA	1490	A	N1-C6-N6	-10.20	112.48	118.60
19	AT	17	ARG	NE-CZ-NH1	10.19	125.39	120.30
54	BA	2814	A	N1-C6-N6	-10.17	112.50	118.60
54	BA	2741	A	N1-C6-N6	-10.17	112.50	118.60
21	AA	1036	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	1000	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	1067	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	1428	A	N1-C6-N6	-10.15	112.51	118.60
21	AA	1397	C	N3-C2-O2	-10.13	114.81	121.90
54	BA	63	A	N1-C6-N6	-10.13	112.52	118.60
54	BA	1085	A	N1-C6-N6	-10.13	112.52	118.60
54	BA	126	A	N1-C6-N6	-10.12	112.53	118.60
25	BC	79	ARG	NE-CZ-NH1	10.12	125.36	120.30
54	BA	280	U	O4'-C1'-N1	10.12	116.29	108.20
21	AA	1014	A	N1-C6-N6	-10.11	112.53	118.60
54	BA	2163	A	N1-C6-N6	-10.11	112.53	118.60
21	AA	119	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	2126	A	O4'-C1'-N9	10.11	116.28	108.20
54	BA	2646	C	N3-C2-O2	-10.10	114.83	121.90
54	BA	2497	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	1496	A	N1-C6-N6	-10.09	112.54	118.60
21	AA	782	A	N1-C6-N6	-10.08	112.55	118.60
21	AA	465	A	N1-C6-N6	-10.08	112.55	118.60
54	BA	592	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	627	A	N1-C6-N6	-10.07	112.56	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2170	A	N1-C6-N6	-10.07	112.56	118.60
39	BQ	52	ARG	NE-CZ-NH1	10.07	125.33	120.30
21	AA	1377	A	N1-C6-N6	-10.06	112.56	118.60
21	AA	152	A	N1-C6-N6	-10.05	112.57	118.60
54	BA	1384	A	N1-C6-N6	-10.05	112.57	118.60
24	A3	45	A	N1-C6-N6	-10.04	112.58	118.60
21	AA	81	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	1046	A	N1-C6-N6	-10.03	112.58	118.60
54	BA	1285	A	N1-C6-N6	-10.03	112.58	118.60
21	AA	72	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	923	A	N1-C6-N6	-10.02	112.59	118.60
54	BA	1772	A	N1-C6-N6	-10.01	112.59	118.60
54	BA	1175	A	N1-C6-N6	-10.01	112.59	118.60
21	AA	510	A	N1-C6-N6	-10.01	112.60	118.60
21	AA	630	A	N1-C6-N6	-10.01	112.60	118.60
54	BA	64	A	N1-C6-N6	-10.01	112.60	118.60
54	BA	1634	A	N1-C6-N6	-10.01	112.60	118.60
9	AJ	31	ARG	NE-CZ-NH1	10.00	125.30	120.30
54	BA	196	A	O4'-C1'-N9	9.99	116.19	108.20
54	BA	1580	A	N1-C6-N6	-9.99	112.61	118.60
54	BA	1809	A	N1-C6-N6	-9.99	112.61	118.60
54	BA	1789	A	N1-C6-N6	-9.99	112.61	118.60
54	BA	626	A	N1-C6-N6	-9.98	112.61	118.60
55	BB	46	A	N1-C6-N6	-9.97	112.62	118.60
11	AL	93	ARG	NE-CZ-NH1	9.95	125.28	120.30
54	BA	2547	A	N1-C6-N6	-9.95	112.63	118.60
39	BQ	63	ARG	NE-CZ-NH1	9.95	125.27	120.30
21	AA	958	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	219	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	1188	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	780	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	861	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	1057	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	532	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	1502	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	764	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	547	A	N1-C6-N6	-9.91	112.65	118.60
54	BA	1584	U	O4'-C1'-N1	9.90	116.12	108.20
21	AA	151	A	N1-C6-N6	-9.90	112.66	118.60
21	AA	1447	A	N1-C6-N6	-9.90	112.66	118.60
54	BA	2309	A	N1-C6-N6	-9.89	112.66	118.60
21	AA	315	A	N1-C6-N6	-9.89	112.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1410	A	N1-C6-N6	-9.89	112.67	118.60
21	AA	8	A	N1-C6-N6	-9.88	112.67	118.60
21	AA	1285	A	N1-C6-N6	-9.88	112.67	118.60
21	AA	968	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	821	A	N1-C6-N6	-9.86	112.68	118.60
54	BA	2358	A	N1-C6-N6	-9.86	112.68	118.60
54	BA	699	A	N1-C6-N6	-9.86	112.68	118.60
54	BA	1264	A	N1-C6-N6	-9.86	112.69	118.60
21	AA	363	A	N1-C6-N6	-9.85	112.69	118.60
36	BN	30	ARG	NE-CZ-NH1	9.85	125.22	120.30
54	BA	160	A	N1-C6-N6	-9.85	112.69	118.60
54	BA	1569	A	N1-C6-N6	-9.85	112.69	118.60
24	A3	59	A	N1-C6-N6	-9.83	112.70	118.60
45	BW	24	ARG	NE-CZ-NH1	9.83	125.21	120.30
54	BA	1937	A	N1-C6-N6	-9.82	112.70	118.60
21	AA	1054	C	O4'-C1'-N1	9.81	116.05	108.20
21	AA	520	A	N1-C6-N6	-9.80	112.72	118.60
3	AD	164	ARG	NE-CZ-NH1	9.80	125.20	120.30
21	AA	192	A	N1-C6-N6	-9.80	112.72	118.60
54	BA	354	A	N1-C6-N6	-9.80	112.72	118.60
21	AA	1476	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	1532	A	N1-C6-N6	-9.76	112.75	118.60
54	BA	2632	A	N1-C6-N6	-9.76	112.75	118.60
54	BA	1009	A	N1-C6-N6	-9.75	112.75	118.60
21	AA	1216	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	981	A	N1-C6-N6	-9.75	112.75	118.60
21	AA	274	A	N1-C6-N6	-9.74	112.75	118.60
21	AA	583	A	N1-C6-N6	-9.74	112.75	118.60
54	BA	204	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2426	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1088	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1749	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2679	A	N1-C6-N6	-9.73	112.76	118.60
24	A3	22	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	1494	A	N1-C6-N6	-9.72	112.77	118.60
21	AA	969	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	569	U	O4'-C1'-N1	9.71	115.97	108.20
54	BA	2213	U	O4'-C1'-N1	9.71	115.96	108.20
21	AA	704	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1678	A	N1-C6-N6	-9.69	112.78	118.60
55	BB	15	A	N1-C6-N6	-9.69	112.78	118.60
54	BA	2482	A	N1-C6-N6	-9.69	112.79	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	715	A	N1-C6-N6	-9.68	112.79	118.60
21	AA	635	A	N1-C6-N6	-9.68	112.80	118.60
21	AA	1021	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	1253	A	N1-C6-N6	-9.68	112.80	118.60
54	BA	1387	A	N1-C6-N6	-9.67	112.80	118.60
21	AA	1042	A	N1-C6-N6	-9.67	112.80	118.60
24	A3	77	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	1205	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	2706	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	2212	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	328	C	N3-C2-O2	-9.64	115.15	121.90
54	BA	1871	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	2158	A	N1-C6-N6	-9.63	112.82	118.60
13	AN	65	ARG	NE-CZ-NH1	9.63	125.11	120.30
54	BA	1938	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	49	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	677	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	945	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	53	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	943	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	2820	A	N1-C6-N6	-9.61	112.83	118.60
21	AA	414	A	N1-C6-N6	-9.61	112.83	118.60
54	BA	2474	U	O4'-C1'-N1	9.60	115.88	108.20
21	AA	1311	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	1204	A	N1-C6-N6	-9.60	112.84	118.60
21	AA	959	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	322	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	1143	A	N1-C6-N6	-9.59	112.85	118.60
54	BA	1757	A	N1-C6-N6	-9.59	112.85	118.60
21	AA	167	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	872	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	144	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	1427	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	1758	U	O4'-C1'-N1	9.58	115.86	108.20
21	AA	246	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	866	A	N1-C6-N6	-9.58	112.85	118.60
54	BA	241	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1156	A	N1-C6-N6	-9.57	112.86	118.60
21	AA	1502	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	886	A	N1-C6-N6	-9.56	112.86	118.60
55	BB	89	U	O4'-C1'-N1	9.56	115.85	108.20
54	BA	1783	A	N1-C6-N6	-9.56	112.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1535	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	2094	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	546	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	2564	A	N1-C6-N6	-9.54	112.88	118.60
55	BB	52	A	N1-C6-N6	-9.54	112.88	118.60
21	AA	243	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	590	A	N1-C6-N6	-9.54	112.88	118.60
54	BA	1365	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	2104	C	O4'-C1'-N1	9.52	115.81	108.20
27	BE	114	ARG	NE-CZ-NH1	9.51	125.05	120.30
22	A1	38	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	1672	A	N1-C6-N6	-9.50	112.90	118.60
21	AA	1346	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	2071	A	N1-C6-N6	-9.49	112.90	118.60
54	BA	1301	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	788	A	N1-C6-N6	-9.49	112.91	118.60
54	BA	2169	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	502	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	767	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	441	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	1362	A	N1-C6-N6	-9.48	112.91	118.60
54	BA	2346	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	1534	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	608	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	877	A	N1-C6-N6	-9.47	112.92	118.60
51	B2	14	ARG	NE-CZ-NH1	9.47	125.03	120.30
54	BA	941	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	218	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	265	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	975	A	N1-C6-N6	-9.46	112.92	118.60
54	BA	1762	A	N1-C6-N6	-9.46	112.92	118.60
27	BE	88	ARG	NE-CZ-NH1	9.46	125.03	120.30
21	AA	749	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	787	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	1711	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	480	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	1111	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	931	U	O4'-C1'-N1	9.44	115.75	108.20
54	BA	1848	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	111	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	2879	A	N1-C6-N6	-9.44	112.94	118.60
22	A1	41	A	N1-C6-N6	-9.44	112.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1073	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	401	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	2119	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	2247	A	N1-C6-N6	-9.43	112.94	118.60
9	AJ	48	ARG	NE-CZ-NH1	9.42	125.01	120.30
54	BA	309	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	411	A	N1-C6-N6	-9.42	112.95	118.60
54	BA	661	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	1735	A	N1-C6-N6	-9.41	112.96	118.60
54	BA	670	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	330	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	1854	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	1342	A	N1-C6-N6	-9.39	112.96	118.60
54	BA	2809	A	N1-C6-N6	-9.39	112.96	118.60
21	AA	914	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	1117	A	N1-C6-N6	-9.39	112.97	118.60
24	A3	1	C	N3-C2-O2	-9.39	115.33	121.90
54	BA	1566	A	N1-C6-N6	-9.39	112.97	118.60
21	AA	1081	A	N1-C6-N6	-9.38	112.97	118.60
21	AA	189	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	1699	G	O4'-C1'-N9	9.37	115.69	108.20
54	BA	2531	A	N1-C6-N6	-9.37	112.98	118.60
55	BB	78	A	N1-C6-N6	-9.37	112.98	118.60
8	AI	79	ARG	NE-CZ-NH1	9.36	124.98	120.30
54	BA	2199	A	N1-C6-N6	-9.36	112.99	118.60
21	AA	706	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	2035	G	O4'-C1'-N9	9.35	115.68	108.20
54	BA	936	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	1953	A	N1-C6-N6	-9.35	112.99	118.60
6	AG	118	ARG	NE-CZ-NH1	9.35	124.97	120.30
21	AA	1225	A	N1-C6-N6	-9.34	113.00	118.60
22	A1	76	A	N1-C6-N6	-9.34	113.00	118.60
29	BG	151	ARG	NE-CZ-NH1	9.34	124.97	120.30
21	AA	1171	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	181	A	N1-C6-N6	-9.32	113.00	118.60
21	AA	609	A	N1-C6-N6	-9.32	113.00	118.60
54	BA	73	A	N1-C6-N6	-9.32	113.01	118.60
30	BH	50	ARG	NE-CZ-NH1	9.32	124.96	120.30
54	BA	2690	U	O4'-C1'-N1	9.32	115.66	108.20
54	BA	990	A	N1-C6-N6	-9.31	113.01	118.60
6	AG	78	ARG	NE-CZ-NH1	9.31	124.96	120.30
21	AA	1446	A	N1-C6-N6	-9.31	113.01	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1969	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	1102	A	N1-C6-N6	-9.31	113.01	118.60
21	AA	1336	C	N3-C2-O2	-9.31	115.39	121.90
34	BL	123	ARG	NE-CZ-NH1	9.31	124.95	120.30
21	AA	253	A	N1-C6-N6	-9.30	113.02	118.60
21	AA	1465	A	N1-C6-N6	-9.30	113.02	118.60
5	AF	24	ARG	NE-CZ-NH1	9.29	124.95	120.30
54	BA	1936	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	2328	A	N1-C6-N6	-9.29	113.02	118.60
54	BA	173	A	N1-C6-N6	-9.29	113.03	118.60
21	AA	130	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	1668	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2758	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2288	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	1353	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1759	A	N1-C6-N6	-9.27	113.04	118.60
21	AA	935	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1503	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	2740	A	N1-C6-N6	-9.27	113.04	118.60
20	AU	17	ARG	NE-CZ-NH1	9.26	124.93	120.30
54	BA	2147	A	N1-C6-N6	-9.26	113.05	118.60
54	BA	1230	A	N1-C6-N6	-9.25	113.05	118.60
54	BA	1385	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	1092	A	N1-C6-N6	-9.25	113.05	118.60
22	A1	6	A	N1-C6-N6	-9.24	113.06	118.60
22	A1	69	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	1157	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	607	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	553	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	1287	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	649	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	294	A	N1-C6-N6	-9.22	113.06	118.60
54	BA	453	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1641	A	N1-C6-N6	-9.22	113.07	118.60
21	AA	1306	A	N1-C6-N6	-9.21	113.07	118.60
21	AA	1363	A	N1-C6-N6	-9.21	113.07	118.60
31	BI	133	ARG	NE-CZ-NH1	9.21	124.91	120.30
54	BA	2765	A	N1-C6-N6	-9.21	113.07	118.60
21	AA	696	A	N1-C6-N6	-9.21	113.07	118.60
21	AA	794	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	2799	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	1241	A	N1-C6-N6	-9.21	113.07	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	816	A	N1-C6-N6	-9.21	113.08	118.60
21	AA	865	A	N1-C6-N6	-9.19	113.08	118.60
15	AP	51	ARG	NE-CZ-NH1	9.19	124.89	120.30
21	AA	499	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	1130	A	N1-C6-N6	-9.19	113.09	118.60
21	AA	1319	A	N1-C6-N6	-9.19	113.09	118.60
3	AD	69	ARG	NE-CZ-NH1	9.18	124.89	120.30
54	BA	609	A	N1-C6-N6	-9.18	113.09	118.60
20	AU	6	ARG	NE-CZ-NH1	9.17	124.89	120.30
21	AA	1492	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	2142	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1821	A	N1-C6-N6	-9.16	113.10	118.60
54	BA	478	A	N1-C6-N6	-9.16	113.10	118.60
21	AA	663	A	N1-C6-N6	-9.16	113.11	118.60
21	AA	1429	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1395	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	1288	A	N1-C6-N6	-9.15	113.11	118.60
34	BL	48	ARG	NE-CZ-NH1	9.14	124.87	120.30
21	AA	1155	A	N1-C6-N6	-9.14	113.11	118.60
54	BA	1819	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	918	A	N1-C6-N6	-9.14	113.12	118.60
21	AA	308	C	N3-C2-O2	-9.13	115.51	121.90
21	AA	1136	C	N3-C2-O2	-9.13	115.51	121.90
54	BA	2033	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	1610	A	N1-C6-N6	-9.13	113.12	118.60
54	BA	104	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	1055	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	477	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1918	A	N1-C6-N6	-9.12	113.13	118.60
21	AA	777	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	920	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1998	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	960	A	N1-C6-N6	-9.11	113.13	118.60
21	AA	98	A	N1-C6-N6	-9.11	113.13	118.60
21	AA	640	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	2829	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	718	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2422	C	O4'-C1'-N1	9.10	115.48	108.20
21	AA	892	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2212	A	O4'-C1'-N9	9.10	115.48	108.20
54	BA	988	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2614	A	N1-C6-N6	-9.10	113.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	448	A	N1-C6-N6	-9.10	113.14	118.60
54	BA	2030	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	1204	A	N1-C6-N6	-9.09	113.14	118.60
54	BA	482	A	N1-C6-N6	-9.09	113.14	118.60
54	BA	2478	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	1508	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	1858	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	101	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	849	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	1269	A	N1-C6-N6	-9.08	113.15	118.60
21	AA	1152	A	N1-C6-N6	-9.08	113.15	118.60
26	BD	77	ARG	NE-CZ-NH1	9.08	124.84	120.30
54	BA	996	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	782	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	833	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	1328	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	654	A	N1-C6-N6	-9.06	113.16	118.60
54	BA	909	A	N1-C6-N6	-9.06	113.16	118.60
25	BC	132	ARG	NE-CZ-NH1	9.06	124.83	120.30
54	BA	825	A	N1-C6-N6	-9.06	113.17	118.60
55	BB	39	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1650	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	44	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	197	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1095	A	N1-C6-N6	-9.05	113.17	118.60
21	AA	65	A	N1-C6-N6	-9.04	113.17	118.60
21	AA	764	C	N3-C2-O2	-9.04	115.57	121.90
54	BA	2095	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	2005	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	2076	U	O4'-C1'-N1	9.04	115.43	108.20
54	BA	1528	A	N1-C6-N6	-9.04	113.18	118.60
21	AA	1396	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	528	A	N1-C6-N6	-9.04	113.18	118.60
54	BA	505	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	2059	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	2058	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1268	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	28	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2541	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	915	A	C5-C6-N1	9.02	122.21	117.70
52	B3	12	ARG	NE-CZ-NH1	9.02	124.81	120.30
54	BA	2721	A	N1-C6-N6	-9.02	113.19	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1676	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	2298	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	38	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	1785	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	1966	A	N1-C6-N6	-9.01	113.19	118.60
21	AA	270	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	2211	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	2634	A	N1-C6-N6	-9.01	113.19	118.60
21	AA	431	A	N1-C6-N6	-9.00	113.20	118.60
21	AA	1213	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	983	A	C5-C6-N1	9.00	122.20	117.70
21	AA	7	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	10	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	1191	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	1456	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	2336	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	1126	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	2566	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	1077	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	207	A	N1-C6-N6	-8.97	113.22	118.60
24	A3	73	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	616	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	1637	A	N1-C6-N6	-8.96	113.22	118.60
56	B5	162	ARG	NE-CZ-NH1	8.96	124.78	120.30
21	AA	815	A	C5-C6-N1	8.95	122.18	117.70
54	BA	2097	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	345	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	675	A	C5-C6-N1	8.95	122.17	117.70
54	BA	1597	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	586	A	C5-C6-N1	8.94	122.17	117.70
8	AI	44	ARG	NE-CZ-NH1	8.94	124.77	120.30
2	AC	106	ARG	NE-CZ-NH1	8.94	124.77	120.30
21	AA	32	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	1350	A	N1-C6-N6	-8.94	113.24	118.60
37	BO	7	ARG	NE-CZ-NH1	8.94	124.77	120.30
10	AK	105	ARG	NE-CZ-NH1	8.94	124.77	120.30
21	AA	1201	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	573	A	C5-C6-N1	8.93	122.17	117.70
54	BA	756	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	1165	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	2627	G	N3-C2-N2	-8.93	113.65	119.90
54	BA	422	A	N1-C6-N6	-8.92	113.25	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	792	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	1269	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	1952	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	2418	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	2450	A	N1-C6-N6	-8.91	113.25	118.60
55	BB	108	A	N1-C6-N6	-8.91	113.25	118.60
21	AA	303	A	N1-C6-N6	-8.91	113.25	118.60
21	AA	918	A	N1-C6-N6	-8.91	113.25	118.60
21	AA	938	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1089	A	N1-C6-N6	-8.91	113.25	118.60
1	AB	112	ARG	NE-CZ-NH1	8.91	124.75	120.30
54	BA	1495	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	2753	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1453	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1246	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1801	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	1447	A	C5-C6-N1	8.89	122.15	117.70
40	BR	79	ARG	NE-CZ-NH1	8.89	124.75	120.30
20	AU	34	ARG	NE-CZ-NH1	8.89	124.74	120.30
21	AA	1433	A	C5-C6-N1	8.88	122.14	117.70
54	BA	643	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	2042	A	N1-C6-N6	-8.88	113.27	118.60
54	BA	1084	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	250	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	217	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	2868	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	1329	A	N1-C6-N6	-8.87	113.28	118.60
36	BN	46	ARG	NE-CZ-NH1	8.87	124.73	120.30
54	BA	2407	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	2468	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	160	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	1257	A	N1-C6-N6	-8.86	113.29	118.60
54	BA	541	A	N1-C6-N6	-8.85	113.29	118.60
21	AA	55	A	N1-C6-N6	-8.85	113.29	118.60
35	BM	55	ARG	NE-CZ-NH2	8.85	124.72	120.30
54	BA	1570	A	N1-C6-N6	-8.85	113.29	118.60
48	BZ	30	ARG	NE-CZ-NH1	8.84	124.72	120.30
21	AA	889	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	176	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	322	A	C5-C6-N1	8.84	122.12	117.70
54	BA	1247	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	1901	A	N1-C6-N6	-8.84	113.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	155	A	N1-C6-N6	-8.83	113.30	118.60
21	AA	164	G	O4'-C1'-N9	8.83	115.27	108.20
21	AA	1519	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	346	A	N1-C6-N6	-8.83	113.31	118.60
54	BA	1981	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	1664	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	195	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	915	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	190	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	352	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	321	A	N1-C6-N6	-8.81	113.32	118.60
54	BA	2092	U	O4'-C1'-N1	8.80	115.24	108.20
21	AA	74	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	429	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	196	A	N1-C6-N6	-8.79	113.32	118.60
21	AA	1531	A	N1-C6-N6	-8.79	113.32	118.60
31	BI	102	ARG	NE-CZ-NH1	8.79	124.69	120.30
54	BA	1773	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	2516	A	N1-C6-N6	-8.79	113.33	118.60
8	AI	123	ARG	NE-CZ-NH1	8.78	124.69	120.30
21	AA	784	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	146	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	244	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2062	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2184	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	263	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	1503	A	C5-C6-N1	8.78	122.09	117.70
54	BA	1276	A	N1-C6-N6	-8.78	113.33	118.60
54	BA	2893	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	143	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	608	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	149	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	514	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	613	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	1302	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	288	A	N1-C6-N6	-8.76	113.34	118.60
21	AA	574	A	N1-C6-N6	-8.76	113.34	118.60
54	BA	19	A	N1-C6-N6	-8.76	113.35	118.60
56	B5	9	ARG	NE-CZ-NH1	8.76	124.68	120.30
54	BA	689	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	182	A	N1-C6-N6	-8.75	113.35	118.60
21	AA	408	A	N1-C6-N6	-8.75	113.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	974	A	N1-C6-N6	-8.75	113.35	118.60
25	BC	188	ARG	NE-CZ-NH1	8.75	124.67	120.30
23	A2	79	A	C5-C6-N1	8.74	122.07	117.70
54	BA	1321	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	1509	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	2327	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	666	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	456	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	972	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1439	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	1274	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1262	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	382	A	N1-C6-N6	-8.73	113.36	118.60
24	A3	44	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	1280	A	N1-C6-N6	-8.72	113.37	118.60
2	AC	142	ARG	NE-CZ-NH1	8.72	124.66	120.30
21	AA	51	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	428	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	262	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	1606	C	O4'-C1'-N1	8.72	115.17	108.20
21	AA	236	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	1784	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	1433	A	N1-C6-N6	-8.71	113.38	118.60
23	A2	91	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	668	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	2154	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	2635	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	847	U	O4'-C1'-N1	8.70	115.16	108.20
54	BA	1610	A	O4'-C1'-N9	8.70	115.16	108.20
24	A3	36	A	C5-C6-N1	8.69	122.05	117.70
54	BA	1654	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	2503	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	1626	A	N1-C6-N6	-8.69	113.39	118.60
38	BP	100	ARG	NE-CZ-NH1	8.69	124.64	120.30
54	BA	2386	A	N1-C6-N6	-8.69	113.39	118.60
13	AN	63	ARG	NE-CZ-NH1	8.68	124.64	120.30
54	BA	1713	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	492	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	1046	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1927	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1504	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	1397	C	N1-C2-O2	8.67	124.10	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2135	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	430	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	1054	C	N3-C2-O2	-8.67	115.83	121.90
21	AA	13	U	C1'-O4'-C4'	-8.67	102.97	109.90
21	AA	978	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	1032	A	C5-C6-N1	8.66	122.03	117.70
54	BA	152	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	1420	A	N1-C6-N6	-8.66	113.41	118.60
21	AA	459	A	N1-C6-N6	-8.65	113.41	118.60
35	BM	51	ARG	NE-CZ-NH1	8.65	124.63	120.30
54	BA	2886	A	O4'-C1'-N9	8.65	115.12	108.20
21	AA	493	A	N1-C6-N6	-8.65	113.41	118.60
46	BX	27	ARG	NE-CZ-NH1	8.65	124.62	120.30
21	AA	509	A	N1-C6-N6	-8.65	113.41	118.60
21	AA	172	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	899	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1403	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1548	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	977	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	2082	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	231	A	N1-C6-N6	-8.63	113.42	118.60
55	BB	15	A	C5-C6-N1	8.63	122.01	117.70
54	BA	2682	A	C5-C6-N1	8.63	122.01	117.70
21	AA	139	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	718	A	O4'-C1'-N9	8.62	115.09	108.20
21	AA	1289	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	807	A	N1-C6-N6	-8.62	113.43	118.60
21	AA	1271	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	2104	C	N3-C2-O2	-8.61	115.87	121.90
21	AA	831	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	1204	A	O4'-C1'-N9	8.61	115.09	108.20
3	AD	25	ARG	NE-CZ-NH1	8.60	124.60	120.30
21	AA	1022	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1717	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	676	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	2461	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	2589	A	N1-C6-N6	-8.59	113.44	118.60
21	AA	718	A	N1-C6-N6	-8.59	113.45	118.60
54	BA	2055	C	N3-C2-O2	-8.59	115.89	121.90
21	AA	878	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	2225	A	N1-C6-N6	-8.58	113.45	118.60
2	AC	64	ARG	NE-CZ-NH1	8.58	124.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2267	A	N1-C6-N6	-8.58	113.45	118.60
21	AA	412	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	513	A	C5-C6-N1	8.56	121.98	117.70
3	AD	110	ARG	NE-CZ-NH1	8.56	124.58	120.30
21	AA	1239	A	N1-C6-N6	-8.56	113.47	118.60
54	BA	1265	A	C5-C6-N1	8.56	121.98	117.70
21	AA	374	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	1069	A	C5-C6-N1	8.55	121.97	117.70
54	BA	1027	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	507	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	789	A	N1-C6-N6	-8.55	113.47	118.60
28	BF	177	ARG	NE-CZ-NH1	8.54	124.57	120.30
54	BA	2191	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	1266	G	O4'-C1'-N9	8.54	115.03	108.20
55	BB	104	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	2238	G	O4'-C1'-N9	8.53	115.02	108.20
21	AA	860	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	1394	A	C5-C6-N1	8.53	121.96	117.70
12	AM	92	ARG	NE-CZ-NH1	8.52	124.56	120.30
25	BC	270	ARG	NE-CZ-NH1	8.52	124.56	120.30
54	BA	1971	U	O4'-C1'-N1	8.52	115.02	108.20
54	BA	2198	A	N1-C6-N6	-8.52	113.49	118.60
8	AI	98	ARG	NE-CZ-NH1	8.52	124.56	120.30
38	BP	71	ARG	NE-CZ-NH1	8.52	124.56	120.30
21	AA	1113	C	N3-C2-O2	-8.52	115.94	121.90
54	BA	1900	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	2430	A	C5-C6-N1	8.51	121.96	117.70
21	AA	1254	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	1347	A	N1-C6-N6	-8.51	113.49	118.60
54	BA	2134	A	N1-C6-N6	-8.51	113.50	118.60
39	BQ	5	ARG	NE-CZ-NH1	8.50	124.55	120.30
21	AA	843	U	O4'-C1'-N1	8.50	115.00	108.20
54	BA	2733	A	N1-C6-N6	-8.50	113.50	118.60
21	AA	262	A	C5-C6-N1	8.50	121.95	117.70
54	BA	705	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	982	C	N3-C2-O2	-8.50	115.95	121.90
21	AA	1158	C	N3-C2-O2	-8.49	115.95	121.90
54	BA	1936	A	C5-C6-N1	8.49	121.95	117.70
54	BA	532	A	O4'-C1'-N9	8.49	114.99	108.20
54	BA	961	C	N3-C2-O2	-8.49	115.96	121.90
54	BA	1056	G	O4'-C1'-N9	8.49	114.99	108.20
54	BA	1552	A	N1-C6-N6	-8.48	113.51	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	17	C	N3-C2-O2	-8.48	115.96	121.90
54	BA	973	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	1155	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	2278	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	2850	A	N1-C6-N6	-8.48	113.51	118.60
1	AB	107	ARG	NE-CZ-NH1	8.48	124.54	120.30
54	BA	2572	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	227	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	844	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	1439	A	O4'-C1'-N9	8.47	114.98	108.20
21	AA	26	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	1016	A	N1-C6-N6	-8.47	113.52	118.60
21	AA	397	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	511	C	N3-C2-O2	-8.46	115.97	121.90
54	BA	586	A	N1-C6-N6	-8.46	113.52	118.60
21	AA	642	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	515	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	1829	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	2813	A	N1-C6-N6	-8.46	113.52	118.60
54	BA	599	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	1515	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	1048	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	71	A	N1-C6-N6	-8.45	113.53	118.60
21	AA	676	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	529	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2080	A	N1-C6-N6	-8.45	113.53	118.60
36	BN	118	ARG	NE-CZ-NH1	8.45	124.53	120.30
54	BA	633	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	734	A	N1-C6-N6	-8.45	113.53	118.60
34	BL	69	ARG	NE-CZ-NH1	8.45	124.52	120.30
54	BA	644	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	685	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2682	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	861	A	C5-C6-N1	8.45	121.92	117.70
54	BA	2077	A	C5-C6-N1	8.44	121.92	117.70
54	BA	2860	A	N1-C6-N6	-8.44	113.53	118.60
55	BB	50	A	N1-C6-N6	-8.44	113.53	118.60
56	B5	60	ARG	NE-CZ-NH1	8.44	124.52	120.30
21	AA	1493	A	C5-C6-N1	8.44	121.92	117.70
21	AA	1378	C	N3-C2-O2	-8.44	115.99	121.90
42	BT	73	ARG	NE-CZ-NH1	8.44	124.52	120.30
54	BA	2700	A	N1-C6-N6	-8.44	113.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	758	C	N3-C2-O2	-8.43	116.00	121.90
21	AA	1246	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	479	A	N1-C6-N6	-8.43	113.54	118.60
20	AU	32	ARG	NE-CZ-NH1	8.43	124.52	120.30
54	BA	497	A	N1-C6-N6	-8.43	113.54	118.60
21	AA	1082	A	N1-C6-N6	-8.43	113.54	118.60
21	AA	205	A	N1-C6-N6	-8.43	113.54	118.60
21	AA	918	A	C5-C6-N1	8.43	121.91	117.70
54	BA	323	C	N3-C2-O2	-8.43	116.00	121.90
54	BA	1168	G	O4'-C1'-N9	8.43	114.94	108.20
54	BA	1404	C	N3-C2-O2	-8.43	116.00	121.90
54	BA	2412	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	979	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	172	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	1899	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2335	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	2727	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	278	A	C5-C6-N1	8.41	121.90	117.70
54	BA	749	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	802	A	C5-C6-N1	8.41	121.90	117.70
54	BA	1080	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	754	C	N3-C2-O2	-8.40	116.02	121.90
54	BA	255	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	1150	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	815	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	1970	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	393	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	1110	A	N1-C6-N6	-8.40	113.56	118.60
34	BL	21	ARG	NE-CZ-NH1	8.40	124.50	120.30
54	BA	2009	A	N1-C6-N6	-8.40	113.56	118.60
21	AA	1179	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	889	C	N3-C2-O2	-8.39	116.03	121.90
54	BA	1505	A	N1-C6-N6	-8.39	113.57	118.60
14	AO	88	ARG	NE-CZ-NH1	8.38	124.49	120.30
21	AA	498	A	N1-C6-N6	-8.38	113.57	118.60
17	AR	72	ARG	NE-CZ-NH2	8.38	124.49	120.30
4	AE	156	ARG	NE-CZ-NH1	8.38	124.49	120.30
54	BA	457	A	N1-C6-N6	-8.38	113.57	118.60
14	AO	52	ARG	NE-CZ-NH1	8.38	124.49	120.30
54	BA	631	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	460	A	N1-C6-N6	-8.38	113.57	118.60
21	AA	1469	C	N3-C2-O2	-8.38	116.04	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	603	A	N1-C6-N6	-8.38	113.58	118.60
54	BA	1096	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1885	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1677	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	1196	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1237	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	2020	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	2333	A	N1-C6-N6	-8.37	113.58	118.60
21	AA	802	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1214	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1336	A	N1-C6-N6	-8.36	113.58	118.60
4	AE	137	ARG	NE-CZ-NH1	8.36	124.48	120.30
54	BA	1962	C	N3-C2-O2	-8.36	116.05	121.90
22	A1	66	A	N1-C6-N6	-8.36	113.58	118.60
21	AA	559	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	432	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	1610	A	C5-C6-N1	8.36	121.88	117.70
2	AC	58	ARG	NE-CZ-NH1	8.36	124.48	120.30
30	BH	97	ARG	NE-CZ-NH1	8.35	124.48	120.30
54	BA	510	C	N3-C2-O2	-8.35	116.06	121.90
54	BA	2654	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	750	A	N1-C6-N6	-8.34	113.59	118.60
21	AA	1054	C	N1-C2-O2	8.34	123.91	118.90
21	AA	1340	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	1260	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	1912	A	N1-C6-N6	-8.34	113.59	118.60
54	BA	1383	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	2748	A	N1-C6-N6	-8.34	113.60	118.60
21	AA	1299	A	C5-C6-N1	8.34	121.87	117.70
54	BA	1308	A	N1-C6-N6	-8.34	113.60	118.60
54	BA	1913	A	N1-C6-N6	-8.34	113.60	118.60
25	BC	268	ARG	NE-CZ-NH1	8.33	124.47	120.30
54	BA	1812	U	O4'-C1'-N1	8.33	114.87	108.20
54	BA	2453	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1871	A	C5-C6-N1	8.33	121.86	117.70
54	BA	2432	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	2646	C	N1-C2-O2	8.33	123.90	118.90
21	AA	432	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	71	A	C5-C6-N1	8.32	121.86	117.70
21	AA	673	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	2176	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	702	A	N1-C6-N6	-8.31	113.61	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	527	C	N3-C2-O2	-8.31	116.08	121.90
21	AA	461	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	621	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	2598	A	N1-C6-N6	-8.30	113.62	118.60
26	BD	46	ARG	NE-CZ-NH1	8.30	124.45	120.30
54	BA	1213	A	N1-C6-N6	-8.30	113.62	118.60
54	BA	685	A	C5-C6-N1	8.30	121.85	117.70
21	AA	547	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	181	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	1020	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	226	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	439	A	N1-C6-N6	-8.29	113.63	118.60
54	BA	613	A	O4'-C1'-N9	8.29	114.83	108.20
55	BB	59	A	N1-C6-N6	-8.29	113.63	118.60
50	B1	27	ARG	NE-CZ-NH1	8.28	124.44	120.30
54	BA	125	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1373	A	N1-C6-N6	-8.28	113.63	118.60
7	AH	83	ARG	NE-CZ-NH1	8.28	124.44	120.30
54	BA	177	G	O4'-C1'-N9	8.28	114.82	108.20
54	BA	518	G	O4'-C1'-N9	8.28	114.82	108.20
54	BA	1151	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	1156	A	C5-C6-N1	8.28	121.84	117.70
54	BA	2054	A	N1-C6-N6	-8.28	113.63	118.60
54	BA	789	A	C5-C6-N1	8.27	121.84	117.70
36	BN	71	ARG	NE-CZ-NH1	8.27	124.44	120.30
34	BL	59	ARG	NE-CZ-NH2	8.27	124.43	120.30
54	BA	2070	A	N1-C6-N6	-8.27	113.64	118.60
21	AA	1339	A	N1-C6-N6	-8.26	113.64	118.60
54	BA	2565	A	C5-C6-N1	8.26	121.83	117.70
21	AA	1145	A	N1-C6-N6	-8.26	113.64	118.60
3	AD	103	ARG	NE-CZ-NH1	8.26	124.43	120.30
21	AA	949	A	N1-C6-N6	-8.26	113.64	118.60
21	AA	1167	A	N1-C6-N6	-8.26	113.64	118.60
21	AA	1101	A	N1-C6-N6	-8.26	113.65	118.60
54	BA	119	A	C5-C6-N1	8.26	121.83	117.70
32	BJ	95	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	2503	A	O4'-C1'-N9	8.26	114.81	108.20
21	AA	80	A	N1-C6-N6	-8.25	113.65	118.60
21	AA	560	A	C5-C6-N1	8.25	121.83	117.70
21	AA	179	A	N1-C6-N6	-8.25	113.65	118.60
21	AA	366	A	C5-C6-N1	8.25	121.83	117.70
54	BA	614	A	N1-C6-N6	-8.25	113.65	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AI	129	ARG	NE-CZ-NH1	8.25	124.42	120.30
21	AA	510	A	C5-C6-N1	8.24	121.82	117.70
21	AA	1250	A	N1-C6-N6	-8.24	113.65	118.60
46	BX	2	ARG	NE-CZ-NH1	8.24	124.42	120.30
54	BA	1194	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	2518	A	C5-C6-N1	8.24	121.82	117.70
21	AA	1105	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1382	C	N3-C2-O2	-8.24	116.13	121.90
54	BA	1913	A	C5-C6-N1	8.24	121.82	117.70
54	BA	508	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	596	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	728	A	C5-C6-N1	8.23	121.82	117.70
54	BA	761	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	452	A	N1-C6-N6	-8.23	113.66	118.60
22	A1	73	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2655	G	O4'-C1'-N9	8.23	114.78	108.20
21	AA	563	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	792	A	N1-C6-N6	-8.23	113.66	118.60
45	BW	10	ARG	NE-CZ-NH1	8.23	124.41	120.30
54	BA	2241	A	N1-C6-N6	-8.23	113.67	118.60
54	BA	752	A	N1-C6-N6	-8.22	113.67	118.60
8	AI	48	ARG	NE-CZ-NH1	8.22	124.41	120.30
18	AS	35	ARG	NE-CZ-NH1	8.22	124.41	120.30
21	AA	383	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	161	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	1381	U	N3-C2-O2	-8.22	116.45	122.20
51	B2	21	ARG	NE-CZ-NH1	8.22	124.41	120.30
54	BA	800	A	N1-C6-N6	-8.22	113.67	118.60
55	BB	58	A	N1-C6-N6	-8.22	113.67	118.60
54	BA	1987	A	N1-C6-N6	-8.21	113.67	118.60
42	BT	76	ARG	NE-CZ-NH1	8.21	124.41	120.30
54	BA	716	A	N1-C6-N6	-8.21	113.67	118.60
21	AA	129	A	N1-C6-N6	-8.21	113.67	118.60
21	AA	673	A	C5-C6-N1	8.21	121.80	117.70
54	BA	2726	A	N1-C6-N6	-8.21	113.68	118.60
22	A1	21	A	N1-C6-N6	-8.21	113.68	118.60
21	AA	602	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	1360	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1757	A	C5-C6-N1	8.20	121.80	117.70
21	AA	1493	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1127	A	O4'-C1'-N9	8.20	114.76	108.20
54	BA	2037	A	N1-C6-N6	-8.19	113.68	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1219	A	N1-C6-N6	-8.19	113.69	118.60
38	BP	88	ARG	NE-CZ-NH1	8.19	124.39	120.30
54	BA	2173	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	2879	A	O4'-C1'-N9	8.19	114.75	108.20
54	BA	2725	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	118	A	C5-C6-N1	8.18	121.79	117.70
21	AA	279	A	C5-C6-N1	8.18	121.79	117.70
54	BA	270	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1088	A	C5-C6-N1	8.18	121.79	117.70
54	BA	1461	C	N3-C2-O2	-8.18	116.18	121.90
54	BA	2434	A	N1-C6-N6	-8.18	113.69	118.60
21	AA	1437	A	N1-C6-N6	-8.17	113.69	118.60
54	BA	1264	A	C5-C6-N1	8.17	121.79	117.70
54	BA	2173	A	C5-C6-N1	8.17	121.79	117.70
54	BA	1129	A	O4'-C1'-N9	8.17	114.74	108.20
38	BP	102	ARG	NE-CZ-NH1	8.17	124.38	120.30
54	BA	645	C	N3-C2-O2	-8.17	116.18	121.90
54	BA	960	A	C5-C6-N1	8.16	121.78	117.70
54	BA	1284	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	2738	A	N1-C6-N6	-8.16	113.70	118.60
21	AA	345	C	N3-C2-O2	-8.16	116.19	121.90
54	BA	522	A	N1-C6-N6	-8.16	113.70	118.60
54	BA	2666	C	N3-C2-O2	-8.16	116.19	121.90
21	AA	523	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	532	A	C5-C6-N1	8.15	121.77	117.70
54	BA	1384	A	C5-C6-N1	8.15	121.77	117.70
24	A3	60	A	N1-C6-N6	-8.14	113.71	118.60
54	BA	6	A	N1-C6-N6	-8.14	113.71	118.60
21	AA	1093	A	N1-C6-N6	-8.14	113.72	118.60
55	BB	45	A	C5-C6-N1	8.13	121.77	117.70
21	AA	1336	C	N1-C2-O2	8.13	123.78	118.90
54	BA	197	A	N1-C6-N6	-8.12	113.72	118.60
54	BA	299	A	N1-C6-N6	-8.12	113.72	118.60
54	BA	2003	A	N1-C6-N6	-8.12	113.72	118.60
21	AA	1374	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1322	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	2014	A	C5-C6-N1	8.12	121.76	117.70
22	A1	35	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1367	A	N1-C6-N6	-8.12	113.73	118.60
34	BL	132	ARG	NE-CZ-NH1	8.12	124.36	120.30
54	BA	423	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	6	G	P-O3'-C3'	8.11	129.44	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	730	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	1008	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	223	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	1227	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	71	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	574	A	C5-C6-N1	8.11	121.75	117.70
33	BK	78	ARG	NE-CZ-NH1	8.10	124.35	120.30
54	BA	1544	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	750	A	C5-C6-N1	8.10	121.75	117.70
54	BA	2602	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	493	A	C5-C6-N1	8.10	121.75	117.70
54	BA	1226	A	N1-C6-N6	-8.10	113.74	118.60
54	BA	1854	A	C5-C6-N1	8.10	121.75	117.70
54	BA	846	U	O4'-C1'-N1	8.09	114.67	108.20
54	BA	1626	A	C5-C6-N1	8.09	121.75	117.70
54	BA	1630	A	N1-C6-N6	-8.09	113.74	118.60
54	BA	2560	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2773	C	O4'-C1'-N1	8.09	114.67	108.20
29	BG	152	ARG	NE-CZ-NH1	8.09	124.35	120.30
54	BA	1791	A	N1-C6-N6	-8.09	113.75	118.60
54	BA	2198	A	C5-C6-N1	8.09	121.74	117.70
54	BA	2158	A	C5-C6-N1	8.09	121.74	117.70
21	AA	152	A	C5-C6-N1	8.08	121.74	117.70
21	AA	364	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	1136	C	O4'-C1'-N1	8.08	114.66	108.20
54	BA	1780	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	2322	A	N1-C6-N6	-8.08	113.75	118.60
54	BA	2761	A	N1-C6-N6	-8.08	113.75	118.60
45	BW	38	ARG	NE-CZ-NH1	8.07	124.34	120.30
51	B2	28	ARG	NE-CZ-NH1	8.07	124.34	120.30
54	BA	1000	A	C5-C6-N1	8.07	121.73	117.70
54	BA	2212	A	C5-C6-N1	8.07	121.73	117.70
21	AA	1257	A	C5-C6-N1	8.07	121.73	117.70
54	BA	1593	A	N1-C6-N6	-8.07	113.76	118.60
3	AD	127	ARG	NE-CZ-NH1	8.06	124.33	120.30
13	AN	13	ARG	NE-CZ-NH1	8.06	124.33	120.30
21	AA	1346	A	C5-C6-N1	8.06	121.73	117.70
54	BA	1262	A	C5-C6-N1	8.06	121.73	117.70
54	BA	2352	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	615	U	O4'-C1'-N1	8.06	114.65	108.20
54	BA	1572	A	C5-C6-N1	8.06	121.73	117.70
54	BA	905	A	N1-C6-N6	-8.06	113.77	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2077	A	N1-C6-N6	-8.06	113.77	118.60
54	BA	2856	A	N1-C6-N6	-8.06	113.77	118.60
12	AM	56	ARG	NE-CZ-NH1	8.06	124.33	120.30
22	A1	23	A	C5-C6-N1	8.06	121.73	117.70
54	BA	1241	A	O4'-C1'-N9	8.06	114.64	108.20
21	AA	1147	C	N3-C2-O2	-8.05	116.26	121.90
13	AN	53	ARG	NE-CZ-NH1	8.05	124.33	120.30
54	BA	83	A	N1-C6-N6	-8.05	113.77	118.60
55	BB	36	C	N3-C2-O2	-8.05	116.27	121.90
54	BA	323	C	N1-C2-O2	8.05	123.73	118.90
54	BA	1914	C	N3-C2-O2	-8.05	116.27	121.90
21	AA	60	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	727	A	C5-C6-N1	8.05	121.72	117.70
54	BA	1652	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	2448	A	N1-C6-N6	-8.04	113.77	118.60
54	BA	2736	A	N1-C6-N6	-8.04	113.77	118.60
54	BA	575	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	2572	A	C5-C6-N1	8.04	121.72	117.70
54	BA	2660	A	N1-C6-N6	-8.04	113.78	118.60
21	AA	28	A	C5-C6-N1	8.04	121.72	117.70
54	BA	478	A	C5-C6-N1	8.04	121.72	117.70
54	BA	480	A	C5-C6-N1	8.04	121.72	117.70
41	BS	99	ARG	NE-CZ-NH1	8.04	124.32	120.30
54	BA	654	A	C5-C6-N1	8.04	121.72	117.70
54	BA	928	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1001	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	1815	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	1932	A	C5-C6-N1	8.03	121.72	117.70
54	BA	1785	A	C5-C6-N1	8.03	121.72	117.70
21	AA	162	A	N1-C6-N6	-8.03	113.78	118.60
22	A1	58	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	2502	G	O4'-C1'-N9	8.03	114.62	108.20
21	AA	1480	A	N1-C6-N6	-8.02	113.78	118.60
54	BA	896	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	2837	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	5	A	N1-C6-N6	-8.02	113.79	118.60
21	AA	648	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	1877	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	644	A	C5-C6-N1	8.01	121.71	117.70
54	BA	1614	A	C5-C6-N1	8.01	121.71	117.70
54	BA	2705	A	C4-C5-C6	-8.01	112.99	117.00
54	BA	2771	C	N3-C2-O2	-8.01	116.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	228	A	N1-C6-N6	-8.01	113.80	118.60
21	AA	595	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	251	A	N1-C6-N6	-8.01	113.80	118.60
54	BA	572	A	C5-C6-N1	8.01	121.70	117.70
54	BA	1073	A	C5-C6-N1	8.01	121.70	117.70
54	BA	1522	A	N1-C6-N6	-8.01	113.80	118.60
19	AT	73	ARG	NE-CZ-NH2	-8.00	116.30	120.30
21	AA	712	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	131	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2497	A	O4'-C1'-N9	8.00	114.60	108.20
21	AA	119	A	C5-C6-N1	8.00	121.70	117.70
54	BA	812	C	N3-C2-O2	-8.00	116.30	121.90
54	BA	1794	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2433	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	42	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2835	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	637	A	N1-C6-N6	-7.99	113.80	118.60
54	BA	2459	A	N1-C6-N6	-7.99	113.80	118.60
21	AA	864	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	1163	A	C5-C6-N1	7.99	121.69	117.70
54	BA	598	U	O4'-C1'-N1	7.99	114.59	108.20
54	BA	1535	A	C5-C6-N1	7.99	121.69	117.70
21	AA	109	A	N1-C6-N6	-7.99	113.81	118.60
21	AA	1467	C	N3-C2-O2	-7.99	116.31	121.90
54	BA	2317	A	N1-C6-N6	-7.99	113.81	118.60
54	BA	2376	A	N1-C6-N6	-7.98	113.81	118.60
24	A3	38	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	981	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1204	A	C5-C6-N1	7.98	121.69	117.70
21	AA	174	A	C5-C6-N1	7.98	121.69	117.70
21	AA	300	A	C5-C6-N1	7.98	121.69	117.70
21	AA	415	A	O4'-C1'-N9	7.98	114.58	108.20
21	AA	687	A	N1-C6-N6	-7.98	113.81	118.60
54	BA	2468	A	C5-C6-N1	7.98	121.69	117.70
21	AA	579	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	2800	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	790	A	N1-C6-N6	-7.97	113.82	118.60
21	AA	356	A	C5-C6-N1	7.97	121.69	117.70
54	BA	1142	A	N1-C6-N6	-7.97	113.82	118.60
55	BB	53	A	C5-C6-N1	7.97	121.69	117.70
54	BA	1428	C	N3-C2-O2	-7.96	116.33	121.90
54	BA	1783	A	C5-C6-N1	7.96	121.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	342	A	N1-C6-N6	-7.96	113.83	118.60
21	AA	344	A	C5-C6-N1	7.95	121.68	117.70
54	BA	2287	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	66	A	C5-C6-N1	7.95	121.67	117.70
54	BA	56	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	2326	C	N3-C2-O2	-7.95	116.34	121.90
21	AA	1519	A	C5-C6-N1	7.95	121.67	117.70
54	BA	142	A	C5-C6-N1	7.95	121.67	117.70
54	BA	1583	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	1508	A	N1-C6-N6	-7.95	113.83	118.60
33	BK	64	ARG	NE-CZ-NH1	7.95	124.27	120.30
54	BA	2899	A	C5-C6-N1	7.95	121.67	117.70
54	BA	432	A	C5-C6-N1	7.94	121.67	117.70
54	BA	1010	A	C5-C6-N1	7.94	121.67	117.70
54	BA	2542	A	N1-C6-N6	-7.94	113.83	118.60
21	AA	192	A	C5-C6-N1	7.94	121.67	117.70
21	AA	353	A	C5-C6-N1	7.94	121.67	117.70
21	AA	1318	A	N1-C6-N6	-7.94	113.84	118.60
24	A3	77	A	C5-C6-N1	7.94	121.67	117.70
54	BA	742	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	792	A	C5-C6-N1	7.94	121.67	117.70
21	AA	1145	A	C5-C6-N1	7.94	121.67	117.70
52	B3	7	ARG	NE-CZ-NH1	7.94	124.27	120.30
21	AA	274	A	C5-C6-N1	7.93	121.67	117.70
19	AT	28	ARG	NE-CZ-NH1	7.93	124.27	120.30
33	BK	71	ARG	NE-CZ-NH1	7.93	124.27	120.30
54	BA	2019	A	C5-C6-N1	7.93	121.66	117.70
20	AU	20	ARG	NE-CZ-NH1	7.93	124.26	120.30
21	AA	315	A	C5-C6-N1	7.93	121.66	117.70
54	BA	272	A	O4'-C1'-N9	7.93	114.54	108.20
54	BA	734	A	C5-C6-N1	7.93	121.66	117.70
54	BA	1890	A	C5-C6-N1	7.92	121.66	117.70
21	AA	300	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	1598	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	2882	A	C4-C5-C6	-7.92	113.04	117.00
54	BA	1616	A	C5-C6-N1	7.92	121.66	117.70
22	A1	61	C	N3-C2-O2	-7.92	116.36	121.90
30	BH	68	ARG	NE-CZ-NH1	7.92	124.26	120.30
54	BA	1241	A	C5-C6-N1	7.92	121.66	117.70
21	AA	412	A	C5-C6-N1	7.92	121.66	117.70
54	BA	943	A	C5-C6-N1	7.92	121.66	117.70
54	BA	1938	A	C5-C6-N1	7.92	121.66	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AL	82	ARG	NE-CZ-NH1	7.91	124.26	120.30
21	AA	559	A	C5-C6-N1	7.91	121.66	117.70
21	AA	383	A	C5-C6-N1	7.91	121.66	117.70
54	BA	2273	A	N1-C6-N6	-7.91	113.86	118.60
21	AA	1163	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	1420	A	C5-C6-N1	7.90	121.65	117.70
54	BA	1646	C	N3-C2-O2	-7.90	116.37	121.90
54	BA	2321	U	O4'-C1'-N1	7.90	114.52	108.20
54	BA	877	A	C5-C6-N1	7.90	121.65	117.70
54	BA	1912	A	C5-C6-N1	7.90	121.65	117.70
2	AC	10	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	371	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2117	A	C5-C6-N1	7.90	121.65	117.70
54	BA	2530	A	C5-C6-N1	7.90	121.65	117.70
54	BA	191	A	N1-C6-N6	-7.89	113.86	118.60
9	AJ	45	ARG	NE-CZ-NH1	7.89	124.25	120.30
54	BA	1525	A	C4-C5-C6	-7.89	113.05	117.00
54	BA	1395	A	C5-C6-N1	7.89	121.64	117.70
21	AA	889	A	C5-C6-N1	7.89	121.64	117.70
54	BA	477	A	C5-C6-N1	7.89	121.64	117.70
21	AA	205	A	C5-C6-N1	7.89	121.64	117.70
54	BA	1469	A	N1-C6-N6	-7.89	113.87	118.60
54	BA	1103	A	N1-C6-N6	-7.89	113.87	118.60
55	BB	109	A	C5-C6-N1	7.89	121.64	117.70
21	AA	181	A	C5-C6-N1	7.88	121.64	117.70
54	BA	447	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	802	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	1434	A	C5-C6-N1	7.88	121.64	117.70
55	BB	101	A	C5-C6-N1	7.88	121.64	117.70
21	AA	116	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	715	A	C5-C6-N1	7.88	121.64	117.70
8	AI	121	ARG	NE-CZ-NH1	7.88	124.24	120.30
54	BA	1307	A	N1-C6-N6	-7.88	113.87	118.60
9	AJ	37	ARG	NE-CZ-NH1	7.88	124.24	120.30
21	AA	716	A	N1-C6-N6	-7.88	113.88	118.60
21	AA	996	A	N1-C6-N6	-7.88	113.88	118.60
54	BA	2899	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	546	A	C5-C6-N1	7.87	121.64	117.70
54	BA	74	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	627	A	C5-C6-N1	7.87	121.64	117.70
55	BB	109	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	2020	A	C5-C6-N1	7.87	121.64	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1362	A	C5-C6-N1	7.87	121.63	117.70
24	A3	16	C	N3-C2-O2	-7.86	116.40	121.90
54	BA	279	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	428	A	C5-C6-N1	7.86	121.63	117.70
23	A2	82	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2814	A	C4-C5-C6	-7.86	113.07	117.00
54	BA	804	A	N1-C6-N6	-7.86	113.89	118.60
54	BA	1801	A	C5-C6-N1	7.85	121.63	117.70
21	AA	415	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2698	U	O4'-C1'-N1	7.85	114.48	108.20
21	AA	327	A	N1-C6-N6	-7.85	113.89	118.60
21	AA	1429	A	C5-C6-N1	7.84	121.62	117.70
54	BA	63	A	C5-C6-N1	7.84	121.62	117.70
54	BA	893	C	N3-C2-O2	-7.84	116.41	121.90
54	BA	2764	A	N1-C6-N6	-7.84	113.89	118.60
21	AA	768	A	C5-C6-N1	7.84	121.62	117.70
21	AA	431	A	C5-C6-N1	7.84	121.62	117.70
54	BA	160	A	C5-C6-N1	7.84	121.62	117.70
21	AA	539	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	340	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	1142	A	C5-C6-N1	7.84	121.62	117.70
21	AA	938	A	C5-C6-N1	7.84	121.62	117.70
21	AA	1413	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	787	C	N3-C2-O2	-7.84	116.41	121.90
54	BA	693	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	2657	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	938	A	O4'-C1'-N9	7.83	114.47	108.20
45	BW	13	ARG	NE-CZ-NH1	7.83	124.22	120.30
54	BA	925	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	171	A	C5-C6-N1	7.83	121.61	117.70
54	BA	905	A	C5-C6-N1	7.83	121.61	117.70
21	AA	754	C	N1-C2-O2	7.83	123.60	118.90
21	AA	1357	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	1598	A	C5-C6-N1	7.83	121.61	117.70
54	BA	626	A	C4-C5-C6	-7.83	113.09	117.00
21	AA	777	A	C5-C6-N1	7.82	121.61	117.70
54	BA	332	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	348	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	2740	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1028	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	1284	A	C5-C6-N1	7.82	121.61	117.70
54	BA	1014	A	N1-C6-N6	-7.82	113.91	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1050	A	C5-C6-N1	7.82	121.61	117.70
54	BA	2448	A	C5-C6-N1	7.82	121.61	117.70
37	BO	81	ARG	NE-CZ-NH1	7.81	124.20	120.30
54	BA	1151	A	C5-C6-N1	7.81	121.61	117.70
54	BA	1244	A	N1-C6-N6	-7.81	113.92	118.60
54	BA	504	A	C5-C6-N1	7.81	121.60	117.70
54	BA	1054	A	N1-C6-N6	-7.81	113.92	118.60
54	BA	2711	A	C5-C6-N1	7.81	121.60	117.70
54	BA	374	A	C5-C6-N1	7.80	121.60	117.70
54	BA	1359	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	1518	A	C4-C5-C6	-7.80	113.10	117.00
19	AT	9	ARG	NE-CZ-NH1	7.80	124.20	120.30
21	AA	873	A	C5-C6-N1	7.79	121.60	117.70
21	AA	1151	A	N1-C6-N6	-7.79	113.92	118.60
26	BD	169	ARG	NE-CZ-NH1	7.79	124.20	120.30
54	BA	1433	A	C5-C6-N1	7.79	121.60	117.70
21	AA	66	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	1383	A	C5-C6-N1	7.79	121.60	117.70
54	BA	1919	A	N1-C6-N6	-7.79	113.92	118.60
21	AA	523	A	C5-C6-N1	7.79	121.59	117.70
54	BA	947	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	2281	A	N1-C6-N6	-7.79	113.93	118.60
21	AA	124	C	O4'-C1'-N1	7.79	114.43	108.20
54	BA	2712	C	N3-C2-O2	-7.79	116.45	121.90
21	AA	1395	C	N3-C2-O2	-7.78	116.45	121.90
54	BA	1539	U	O4'-C1'-N1	7.78	114.43	108.20
21	AA	59	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	71	A	O4'-C1'-N9	7.78	114.43	108.20
54	BA	556	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2826	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	1095	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2015	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	384	A	C5-C6-N1	7.78	121.59	117.70
21	AA	50	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	508	A	C5-C6-N1	7.78	121.59	117.70
21	AA	1180	A	C5-C6-N1	7.77	121.59	117.70
54	BA	229	C	O4'-C1'-N1	7.77	114.42	108.20
21	AA	766	A	C5-C6-N1	7.77	121.59	117.70
54	BA	1982	U	O4'-C1'-N1	7.77	114.42	108.20
54	BA	2475	C	N3-C2-O2	-7.77	116.46	121.90
21	AA	937	A	N1-C6-N6	-7.77	113.94	118.60
25	BC	181	ARG	NE-CZ-NH1	7.77	124.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	532	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1009	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2101	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	2471	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	980	A	C5-C6-N1	7.76	121.58	117.70
54	BA	131	A	C5-C6-N1	7.76	121.58	117.70
54	BA	103	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	120	A	C5-C6-N1	7.76	121.58	117.70
43	BU	21	ARG	NE-CZ-NH1	7.76	124.18	120.30
54	BA	6	A	C5-C6-N1	7.76	121.58	117.70
54	BA	569	U	C1'-O4'-C4'	-7.76	103.69	109.90
54	BA	21	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	207	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2430	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	582	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	984	A	C5-C6-N1	7.75	121.58	117.70
54	BA	1272	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2886	A	C5-C6-N1	7.75	121.58	117.70
21	AA	373	A	N1-C6-N6	-7.75	113.95	118.60
9	AJ	9	ARG	NE-CZ-NH1	7.75	124.17	120.30
54	BA	344	A	C5-C6-N1	7.75	121.57	117.70
21	AA	77	A	N1-C6-N6	-7.74	113.95	118.60
21	AA	120	A	N1-C6-N6	-7.74	113.95	118.60
21	AA	968	A	C5-C6-N1	7.74	121.57	117.70
54	BA	94	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1981	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2778	A	C5-C6-N1	7.74	121.57	117.70
54	BA	675	A	N1-C6-N6	-7.74	113.95	118.60
54	BA	2635	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1004	A	C5-C6-N1	7.74	121.57	117.70
21	AA	1014	A	C5-C6-N1	7.74	121.57	117.70
35	BM	114	ARG	NE-CZ-NH1	7.74	124.17	120.30
21	AA	845	A	C5-C6-N1	7.74	121.57	117.70
54	BA	195	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	613	A	C5-C6-N1	7.74	121.57	117.70
54	BA	689	A	C5-C6-N1	7.74	121.57	117.70
21	AA	98	A	C5-C6-N1	7.73	121.57	117.70
54	BA	330	A	C1'-O4'-C4'	-7.73	103.72	109.90
54	BA	705	A	C5-C6-N1	7.73	121.56	117.70
54	BA	101	A	N1-C6-N6	-7.73	113.96	118.60
54	BA	125	A	C5-C6-N1	7.73	121.56	117.70
54	BA	395	U	O4'-C1'-N1	7.73	114.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	702	A	C5-C6-N1	7.72	121.56	117.70
21	AA	964	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1632	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	60	A	C5-C6-N1	7.72	121.56	117.70
54	BA	833	A	C5-C6-N1	7.72	121.56	117.70
54	BA	2268	A	C5-C6-N1	7.72	121.56	117.70
21	AA	563	A	C5-C6-N1	7.72	121.56	117.70
54	BA	89	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	1027	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1133	A	N1-C6-N6	-7.72	113.97	118.60
21	AA	246	A	C5-C6-N1	7.71	121.56	117.70
21	AA	199	A	N1-C6-N6	-7.71	113.97	118.60
49	B0	39	ARG	NE-CZ-NH1	7.71	124.16	120.30
3	AD	80	ARG	NE-CZ-NH1	7.71	124.15	120.30
21	AA	262	A	C4-C5-C6	-7.71	113.15	117.00
44	BV	93	ARG	NE-CZ-NH1	7.71	124.15	120.30
54	BA	233	A	C5-C6-N1	7.71	121.55	117.70
54	BA	1848	A	C5-C6-N1	7.71	121.55	117.70
54	BA	2531	A	C5-C6-N1	7.71	121.55	117.70
54	BA	1808	A	O4'-C1'-N9	7.71	114.36	108.20
25	BC	220	ARG	NE-CZ-NH1	7.71	124.15	120.30
22	A1	38	A	C5-C6-N1	7.70	121.55	117.70
44	BV	19	ARG	NE-CZ-NH1	7.70	124.15	120.30
54	BA	176	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1690	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1900	A	C5-C6-N1	7.70	121.55	117.70
54	BA	2851	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1101	U	O4'-C1'-N1	7.70	114.36	108.20
54	BA	1802	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	1167	A	C5-C6-N1	7.70	121.55	117.70
21	AA	913	A	C5-C6-N1	7.70	121.55	117.70
54	BA	845	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	1490	A	O4'-C1'-N9	7.70	114.36	108.20
54	BA	1129	A	C1'-O4'-C4'	-7.69	103.74	109.90
54	BA	346	A	C5-C6-N1	7.69	121.55	117.70
54	BA	1765	U	O4'-C1'-N1	7.69	114.35	108.20
54	BA	2887	A	N1-C6-N6	-7.69	113.98	118.60
21	AA	336	A	N1-C6-N6	-7.69	113.98	118.60
46	BX	10	ARG	NE-CZ-NH1	7.69	124.14	120.30
54	BA	415	A	N1-C6-N6	-7.69	113.98	118.60
54	BA	1677	A	C5-C6-N1	7.69	121.55	117.70
54	BA	2062	A	C5-C6-N1	7.69	121.55	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	BY	47	ARG	NE-CZ-NH1	7.69	124.14	120.30
54	BA	1301	A	C5-C6-N1	7.69	121.55	117.70
54	BA	1175	A	C5-C6-N1	7.69	121.54	117.70
54	BA	1787	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	104	A	C5-C6-N1	7.68	121.54	117.70
54	BA	2013	A	N1-C6-N6	-7.68	113.99	118.60
21	AA	923	A	C5-C6-N1	7.68	121.54	117.70
22	A1	26	A	C5-C6-N1	7.68	121.54	117.70
54	BA	1889	A	C5-C6-N1	7.68	121.54	117.70
25	BC	237	ARG	NE-CZ-NH1	7.68	124.14	120.30
32	BJ	37	ARG	NE-CZ-NH1	7.68	124.14	120.30
51	B2	3	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	AB	62	ARG	NE-CZ-NH1	7.68	124.14	120.30
19	AT	24	ARG	NE-CZ-NH1	7.68	124.14	120.30
21	AA	621	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	1032	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	457	A	C5-C6-N1	7.67	121.54	117.70
21	AA	1398	A	C5-C6-N1	7.67	121.54	117.70
54	BA	1614	A	C4-C5-C6	-7.67	113.16	117.00
21	AA	1500	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	1609	A	N1-C6-N6	-7.67	114.00	118.60
21	AA	1502	A	C5-C6-N1	7.67	121.53	117.70
54	BA	2411	A	N1-C6-N6	-7.67	114.00	118.60
54	BA	838	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	1144	A	N1-C6-N6	-7.66	114.00	118.60
21	AA	50	A	C5-C6-N1	7.66	121.53	117.70
54	BA	1367	A	C5-C6-N1	7.66	121.53	117.70
21	AA	158	G	P-O3'-C3'	7.66	128.89	119.70
21	AA	344	A	N1-C6-N6	-7.66	114.00	118.60
54	BA	2031	A	C5-C6-N1	7.66	121.53	117.70
54	BA	655	A	C5-C6-N1	7.66	121.53	117.70
21	AA	182	A	C5-C6-N1	7.65	121.53	117.70
21	AA	1446	A	C5-C6-N1	7.65	121.53	117.70
21	AA	556	C	N3-C2-O2	-7.65	116.54	121.90
21	AA	1289	A	C5-C6-N1	7.65	121.53	117.70
54	BA	1566	A	C5-C6-N1	7.65	121.53	117.70
21	AA	1080	A	N1-C6-N6	-7.65	114.01	118.60
21	AA	1082	A	C5-C6-N1	7.65	121.53	117.70
54	BA	91	A	N1-C6-N6	-7.65	114.01	118.60
21	AA	706	A	C5-C6-N1	7.65	121.53	117.70
21	AA	389	A	C4-C5-C6	-7.65	113.18	117.00
54	BA	443	A	C5-C6-N1	7.64	121.52	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	892	A	C5-C6-N1	7.64	121.52	117.70
54	BA	279	A	C5-C6-N1	7.64	121.52	117.70
54	BA	933	A	C5-C6-N1	7.64	121.52	117.70
54	BA	1490	A	C5-C6-N1	7.64	121.52	117.70
54	BA	1978	A	N1-C6-N6	-7.64	114.01	118.60
54	BA	2590	A	C4-C5-C6	-7.64	113.18	117.00
54	BA	2639	A	C5-C6-N1	7.64	121.52	117.70
54	BA	1453	A	C5-C6-N1	7.64	121.52	117.70
21	AA	1303	C	N3-C2-O2	-7.64	116.55	121.90
6	AG	77	ARG	NE-CZ-NH1	7.64	124.12	120.30
21	AA	1507	A	C5-C6-N1	7.64	121.52	117.70
54	BA	73	A	C5-C6-N1	7.64	121.52	117.70
54	BA	1585	C	N3-C2-O2	-7.64	116.56	121.90
16	AQ	39	ARG	NE-CZ-NH1	7.63	124.12	120.30
54	BA	262	A	C5-C6-N1	7.63	121.52	117.70
54	BA	231	A	C5-C6-N1	7.63	121.52	117.70
54	BA	1754	A	N1-C6-N6	-7.63	114.02	118.60
2	AC	178	ARG	NE-CZ-NH1	7.63	124.12	120.30
21	AA	583	A	C5-C6-N1	7.63	121.52	117.70
54	BA	241	A	C5-C6-N1	7.63	121.52	117.70
54	BA	368	A	C5-C6-N1	7.63	121.52	117.70
54	BA	422	A	C5-C6-N1	7.63	121.52	117.70
21	AA	482	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	411	A	C4-C5-C6	-7.63	113.19	117.00
21	AA	559	A	O4'-C1'-N9	7.63	114.30	108.20
54	BA	1632	A	C5-C6-N1	7.62	121.51	117.70
14	AO	53	ARG	NE-CZ-NH1	7.62	124.11	120.30
12	AM	2	ARG	NE-CZ-NH1	7.62	124.11	120.30
54	BA	1253	A	C5-C6-N1	7.62	121.51	117.70
27	BE	49	ARG	NE-CZ-NH1	7.62	124.11	120.30
54	BA	223	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1678	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2071	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1327	A	C5-C6-N1	7.62	121.51	117.70
2	AC	53	ARG	NE-CZ-NH1	7.61	124.11	120.30
21	AA	1248	A	C5-C6-N1	7.61	121.51	117.70
37	BO	25	ARG	NE-CZ-NH1	7.61	124.11	120.30
54	BA	126	A	C5-C6-N1	7.61	121.51	117.70
54	BA	1054	A	C5-C6-N1	7.61	121.51	117.70
54	BA	1378	A	C5-C6-N1	7.61	121.51	117.70
54	BA	1858	A	C5-C6-N1	7.61	121.51	117.70
54	BA	2835	A	C5-C6-N1	7.61	121.51	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	496	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	1805	A	C5-C6-N1	7.61	121.50	117.70
21	AA	197	A	C5-C6-N1	7.61	121.50	117.70
54	BA	751	A	C5-C6-N1	7.61	121.50	117.70
54	BA	10	A	C5-C6-N1	7.60	121.50	117.70
54	BA	1977	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	743	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	1004	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	706	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	961	C	N1-C2-O2	7.60	123.46	118.90
54	BA	1134	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	1143	A	C5-C6-N1	7.60	121.50	117.70
21	AA	106	C	N3-C2-O2	-7.60	116.58	121.90
54	BA	1828	G	O4'-C1'-N9	7.60	114.28	108.20
54	BA	1953	A	C4-C5-C6	-7.60	113.20	117.00
54	BA	1966	A	C5-C6-N1	7.60	121.50	117.70
21	AA	1251	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	1808	A	N1-C6-N6	-7.60	114.04	118.60
44	BV	79	ARG	NE-CZ-NH1	7.59	124.10	120.30
21	AA	325	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	1404	C	N1-C2-O2	7.59	123.45	118.90
54	BA	1786	A	N1-C6-N6	-7.59	114.05	118.60
21	AA	298	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	2433	A	C5-C6-N1	7.59	121.50	117.70
21	AA	665	A	C5-C6-N1	7.59	121.49	117.70
54	BA	1705	A	C5-C6-N1	7.59	121.49	117.70
21	AA	807	A	C5-C6-N1	7.59	121.49	117.70
21	AA	1357	A	C5-C6-N1	7.59	121.49	117.70
22	A1	9	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	1393	A	C4-C5-C6	-7.58	113.21	117.00
54	BA	199	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1504	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2766	A	C5-C6-N1	7.58	121.49	117.70
21	AA	533	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1853	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2340	A	N1-C6-N6	-7.58	114.05	118.60
54	BA	2469	A	N1-C6-N6	-7.58	114.05	118.60
21	AA	642	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2170	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1889	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	2555	U	O4'-C1'-N1	7.57	114.26	108.20
21	AA	768	A	N1-C6-N6	-7.57	114.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2311	A	N1-C6-N6	-7.57	114.06	118.60
21	AA	183	C	O4'-C1'-N1	7.57	114.26	108.20
54	BA	454	A	N1-C6-N6	-7.57	114.06	118.60
21	AA	1044	A	N1-C6-N6	-7.57	114.06	118.60
12	AM	108	ARG	NE-CZ-NH1	7.57	124.08	120.30
21	AA	696	A	C5-C6-N1	7.57	121.48	117.70
54	BA	204	A	C5-C6-N1	7.57	121.48	117.70
54	BA	603	A	C5-C6-N1	7.57	121.48	117.70
21	AA	1513	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	149	A	N1-C6-N6	-7.56	114.06	118.60
21	AA	509	A	C5-C6-N1	7.56	121.48	117.70
21	AA	1433	A	C4-C5-C6	-7.56	113.22	117.00
54	BA	1960	A	C5-C6-N1	7.56	121.48	117.70
24	A3	59	A	C4-C5-C6	-7.56	113.22	117.00
21	AA	381	C	N3-C2-O2	-7.56	116.61	121.90
21	AA	466	A	C5-C6-N1	7.56	121.48	117.70
21	AA	792	A	C5-C6-N1	7.56	121.48	117.70
51	B2	39	ARG	NE-CZ-NH1	7.56	124.08	120.30
54	BA	44	A	N1-C6-N6	-7.56	114.06	118.60
54	BA	2346	A	C5-C6-N1	7.56	121.48	117.70
21	AA	1250	A	C5-C6-N1	7.55	121.48	117.70
54	BA	449	A	C5-C6-N1	7.55	121.48	117.70
54	BA	2388	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	622	A	C5-C6-N1	7.55	121.48	117.70
54	BA	31	C	N3-C2-O2	-7.55	116.61	121.90
21	AA	533	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	52	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	182	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2275	C	N3-C2-O2	-7.55	116.61	121.90
21	AA	1136	C	N1-C2-O2	7.55	123.43	118.90
54	BA	1669	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	983	A	C5-C6-N1	7.55	121.47	117.70
22	A1	76	A	C5-C6-N1	7.55	121.47	117.70
54	BA	1780	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2711	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1585	C	O4'-C1'-N1	7.54	114.24	108.20
54	BA	1040	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1307	A	C5-C6-N1	7.54	121.47	117.70
54	BA	1327	A	N1-C6-N6	-7.54	114.07	118.60
54	BA	2089	C	O4'-C1'-N1	7.54	114.23	108.20
24	A3	76	C	N3-C2-O2	-7.54	116.62	121.90
54	BA	182	A	N1-C6-N6	-7.54	114.08	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	282	A	C5-C6-N1	7.54	121.47	117.70
24	A3	1	C	N1-C2-O2	7.54	123.42	118.90
21	AA	675	A	C5-C6-N1	7.54	121.47	117.70
54	BA	903	C	O4'-C1'-N1	7.54	114.23	108.20
54	BA	2792	A	N1-C6-N6	-7.54	114.08	118.60
8	AI	105	ARG	NE-CZ-NH1	7.54	124.07	120.30
33	BK	30	ARG	NE-CZ-NH1	7.54	124.07	120.30
54	BA	402	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	466	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	1393	A	C5-C6-N1	7.53	121.47	117.70
54	BA	2764	A	C5-C6-N1	7.53	121.47	117.70
21	AA	1096	C	N3-C2-O2	-7.53	116.63	121.90
54	BA	421	C	N3-C2-O2	-7.53	116.63	121.90
21	AA	1224	U	O4'-C1'-N1	7.53	114.22	108.20
21	AA	1408	A	N1-C6-N6	-7.53	114.08	118.60
21	AA	681	A	C4-C5-C6	-7.53	113.23	117.00
21	AA	1345	U	C1'-O4'-C4'	-7.53	103.88	109.90
54	BA	2308	G	O4'-C1'-N9	7.53	114.22	108.20
54	BA	1496	A	C5-C6-N1	7.53	121.46	117.70
54	BA	2225	A	C5-C6-N1	7.53	121.46	117.70
54	BA	2749	A	C5-C6-N1	7.53	121.46	117.70
21	AA	583	A	C4-C5-C6	-7.52	113.24	117.00
12	AM	70	ARG	NE-CZ-NH1	7.52	124.06	120.30
21	AA	1067	A	C5-C6-N1	7.52	121.46	117.70
54	BA	848	C	N3-C2-O2	-7.52	116.63	121.90
21	AA	468	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1571	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1791	A	C5-C6-N1	7.52	121.46	117.70
54	BA	282	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2406	A	C5-C6-N1	7.52	121.46	117.70
21	AA	307	C	N3-C2-O2	-7.51	116.64	121.90
54	BA	972	A	C5-C6-N1	7.51	121.46	117.70
54	BA	1987	A	C5-C6-N1	7.51	121.46	117.70
21	AA	371	A	C4-C5-C6	-7.51	113.24	117.00
54	BA	761	A	C5-C6-N1	7.51	121.46	117.70
54	BA	1928	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	2297	A	C5-C6-N1	7.51	121.46	117.70
21	AA	16	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	33	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	356	A	C4-C5-C6	-7.51	113.25	117.00
21	AA	432	A	C5-C6-N1	7.51	121.45	117.70
21	AA	648	A	C5-C6-N1	7.51	121.45	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	718	A	C5-C6-N1	7.51	121.45	117.70
54	BA	9	G	O4'-C1'-N9	7.51	114.21	108.20
54	BA	515	A	C5-C6-N1	7.51	121.45	117.70
22	A1	73	A	C5-C6-N1	7.51	121.45	117.70
54	BA	1366	A	N1-C6-N6	-7.51	114.10	118.60
54	BA	1635	A	C5-C6-N1	7.51	121.45	117.70
41	BS	18	ARG	NE-CZ-NH1	7.50	124.05	120.30
22	A1	21	A	C5-C6-N1	7.50	121.45	117.70
54	BA	756	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2031	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	974	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1427	A	C5-C6-N1	7.50	121.45	117.70
55	BB	29	A	N1-C6-N6	-7.50	114.10	118.60
55	BB	73	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	174	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	655	A	C5-C6-N1	7.50	121.45	117.70
54	BA	502	A	N1-C6-N6	-7.50	114.10	118.60
54	BA	602	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1312	U	P-O3'-C3'	7.50	128.69	119.70
54	BA	1655	A	C5-C6-N1	7.50	121.45	117.70
21	AA	238	A	N1-C6-N6	-7.49	114.10	118.60
21	AA	1109	C	N3-C2-O2	-7.49	116.65	121.90
54	BA	221	A	N1-C6-N6	-7.49	114.10	118.60
21	AA	195	A	C5-C6-N1	7.49	121.45	117.70
54	BA	1739	A	N1-C6-N6	-7.49	114.11	118.60
21	AA	1213	A	C5-C6-N1	7.49	121.44	117.70
21	AA	964	A	N1-C6-N6	-7.49	114.11	118.60
21	AA	781	A	N1-C6-N6	-7.48	114.11	118.60
21	AA	1377	A	C5-C6-N1	7.48	121.44	117.70
22	A1	32	C	N3-C2-O2	-7.48	116.66	121.90
54	BA	142	A	C1'-O4'-C4'	-7.48	103.92	109.90
54	BA	722	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	2766	A	N1-C6-N6	-7.48	114.11	118.60
54	BA	156	A	C5-C6-N1	7.48	121.44	117.70
54	BA	637	A	C5-C6-N1	7.48	121.44	117.70
54	BA	1755	A	C5-C6-N1	7.48	121.44	117.70
2	AC	171	ARG	NE-CZ-NH1	7.48	124.04	120.30
54	BA	2171	A	C5-C6-N1	7.48	121.44	117.70
54	BA	119	A	C4-C5-C6	-7.47	113.26	117.00
36	BN	64	ARG	NE-CZ-NH1	7.47	124.04	120.30
54	BA	161	A	C5-C6-N1	7.47	121.44	117.70
21	AA	81	A	C5-C6-N1	7.47	121.44	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	461	A	C5-C6-N1	7.47	121.44	117.70
54	BA	195	A	C5-C6-N1	7.47	121.43	117.70
54	BA	2005	A	C5-C6-N1	7.47	121.43	117.70
54	BA	2422	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	2825	G	O4'-C1'-N9	7.47	114.18	108.20
54	BA	1342	A	C5-C6-N1	7.47	121.43	117.70
54	BA	1759	A	C5-C6-N1	7.47	121.43	117.70
21	AA	1229	A	N1-C6-N6	-7.47	114.12	118.60
21	AA	1396	A	C5-C6-N1	7.47	121.43	117.70
21	AA	482	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1404	C	N3-C2-O2	-7.46	116.67	121.90
54	BA	2378	A	C5-C6-N1	7.46	121.43	117.70
54	BA	155	A	C5-C6-N1	7.46	121.43	117.70
21	AA	1368	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	1419	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	2082	A	C5-C6-N1	7.46	121.43	117.70
21	AA	371	A	C5-C6-N1	7.46	121.43	117.70
21	AA	914	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1029	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2288	A	C5-C6-N1	7.46	121.43	117.70
21	AA	595	A	C5-C6-N1	7.46	121.43	117.70
54	BA	626	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1640	A	N1-C6-N6	-7.46	114.13	118.60
21	AA	694	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	1019	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	877	A	C4-C5-C6	-7.45	113.27	117.00
54	BA	1413	A	N1-C6-N6	-7.45	114.13	118.60
21	AA	1203	C	N3-C2-O2	-7.45	116.68	121.90
21	AA	313	A	N1-C6-N6	-7.45	114.13	118.60
39	BQ	50	ARG	NE-CZ-NH1	7.45	124.03	120.30
54	BA	896	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1679	A	C5-C6-N1	7.45	121.43	117.70
21	AA	274	A	C4-C5-C6	-7.45	113.28	117.00
21	AA	608	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1698	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2169	A	C5-C6-N1	7.45	121.42	117.70
54	BA	2736	A	C5-C6-N1	7.45	121.42	117.70
55	BB	78	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1700	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	1789	A	C4-C5-C6	-7.45	113.28	117.00
21	AA	535	A	C5-C6-N1	7.45	121.42	117.70
48	BZ	44	ARG	NE-CZ-NH1	7.45	124.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1403	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1941	C	N3-C2-O2	-7.45	116.69	121.90
21	AA	155	A	C4-C5-C6	-7.44	113.28	117.00
21	AA	279	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	460	A	N1-C6-N6	-7.44	114.13	118.60
54	BA	503	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1287	A	N1-C6-N6	-7.44	114.13	118.60
54	BA	1508	A	C5-C6-N1	7.44	121.42	117.70
21	AA	547	A	C5-C6-N1	7.44	121.42	117.70
21	AA	1176	A	N1-C6-N6	-7.44	114.14	118.60
21	AA	1483	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	572	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	1866	A	N1-C6-N6	-7.44	114.13	118.60
20	AU	46	ARG	NE-CZ-NH1	7.44	124.02	120.30
54	BA	928	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	1806	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	2063	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	2129	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	1028	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1029	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	118	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	2091	C	N3-C2-O2	-7.44	116.69	121.90
21	AA	766	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	1953	A	C5-C6-N1	7.44	121.42	117.70
21	AA	33	A	C5-C6-N1	7.43	121.42	117.70
21	AA	959	A	C5-C6-N1	7.43	121.42	117.70
54	BA	927	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	2750	A	C5-C6-N1	7.43	121.42	117.70
54	BA	565	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	1815	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2809	A	C5-C6-N1	7.43	121.42	117.70
12	AM	86	ARG	NE-CZ-NH1	7.43	124.02	120.30
17	AR	47	ARG	NE-CZ-NH1	7.43	124.02	120.30
18	AS	54	ARG	NE-CZ-NH1	7.43	124.02	120.30
54	BA	352	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2797	U	O4'-C1'-N1	7.43	114.14	108.20
21	AA	1111	A	C5-C6-N1	7.43	121.41	117.70
54	BA	844	A	C5-C6-N1	7.43	121.42	117.70
54	BA	1522	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2406	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	161	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	1503	A	N1-C6-N6	-7.43	114.14	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1493	C	N3-C2-O2	-7.43	116.70	121.90
39	BQ	27	ARG	NE-CZ-NH1	7.42	124.01	120.30
54	BA	2333	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1251	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1353	A	C5-C6-N1	7.42	121.41	117.70
54	BA	2171	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	366	A	N1-C6-N6	-7.42	114.15	118.60
21	AA	308	C	N1-C2-O2	7.42	123.35	118.90
54	BA	538	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1274	A	C5-C6-N1	7.42	121.41	117.70
54	BA	466	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1286	A	N1-C6-N6	-7.42	114.15	118.60
6	AG	101	ARG	NE-CZ-NH1	7.41	124.01	120.30
21	AA	19	A	N1-C6-N6	-7.41	114.15	118.60
54	BA	345	A	C5-C6-N1	7.41	121.41	117.70
54	BA	1668	A	C5-C6-N1	7.41	121.41	117.70
54	BA	1961	C	N3-C2-O2	-7.41	116.71	121.90
54	BA	2163	A	O4'-C1'-N9	7.41	114.13	108.20
21	AA	906	A	C5-C6-N1	7.41	121.41	117.70
54	BA	1463	C	N3-C2-O2	-7.41	116.71	121.90
54	BA	984	A	N1-C6-N6	-7.41	114.15	118.60
21	AA	1456	A	C5-C6-N1	7.41	121.40	117.70
54	BA	1877	A	C5-C6-N1	7.41	121.40	117.70
54	BA	205	G	O4'-C1'-N9	7.41	114.12	108.20
54	BA	2426	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2561	U	O4'-C1'-N1	7.41	114.12	108.20
21	AA	600	A	C4-C5-C6	-7.41	113.30	117.00
54	BA	1890	A	N1-C6-N6	-7.41	114.16	118.60
2	AC	39	ARG	NE-CZ-NH1	7.40	124.00	120.30
54	BA	324	A	C5-C6-N1	7.40	121.40	117.70
54	BA	925	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1302	A	C5-C6-N1	7.40	121.40	117.70
22	A1	16	C	N3-C2-O2	-7.40	116.72	121.90
54	BA	2176	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2270	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2600	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1223	C	N3-C2-O2	-7.40	116.72	121.90
21	AA	1238	A	C5-C6-N1	7.40	121.40	117.70
24	A3	59	A	C5-C6-N1	7.40	121.40	117.70
24	A3	73	A	C5-C6-N1	7.40	121.40	117.70
6	AG	9	ARG	NE-CZ-NH1	7.40	124.00	120.30
21	AA	901	A	C5-C6-N1	7.40	121.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1110	A	C5-C6-N1	7.40	121.40	117.70
54	BA	430	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2534	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	189	A	C5-C6-N1	7.39	121.40	117.70
54	BA	101	A	C5-C6-N1	7.39	121.40	117.70
54	BA	490	C	N3-C2-O2	-7.39	116.72	121.90
54	BA	1672	A	C5-C6-N1	7.39	121.40	117.70
54	BA	1872	A	C5-C6-N1	7.39	121.40	117.70
54	BA	1970	A	C5-C6-N1	7.39	121.40	117.70
55	BB	34	A	N1-C6-N6	-7.39	114.16	118.60
21	AA	1238	A	N1-C6-N6	-7.39	114.17	118.60
21	AA	280	C	N3-C2-O2	-7.39	116.73	121.90
46	BX	36	ARG	NE-CZ-NH1	7.39	123.99	120.30
54	BA	804	A	C5-C6-N1	7.39	121.39	117.70
54	BA	2376	A	C5-C6-N1	7.39	121.39	117.70
54	BA	2461	A	C5-C6-N1	7.39	121.39	117.70
54	BA	1046	A	C5-C6-N1	7.39	121.39	117.70
54	BA	2366	A	N1-C6-N6	-7.39	114.17	118.60
55	BB	57	A	C5-C6-N1	7.39	121.39	117.70
21	AA	1501	C	N3-C2-O2	-7.38	116.73	121.90
54	BA	1808	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2070	A	C5-C6-N1	7.38	121.39	117.70
21	AA	435	A	N1-C6-N6	-7.38	114.17	118.60
17	AR	56	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	572	A	C5-C6-N1	7.38	121.39	117.70
24	A3	22	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1328	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1616	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	1570	A	C4-C5-C6	-7.38	113.31	117.00
54	BA	1918	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2741	A	C5-C6-N1	7.38	121.39	117.70
12	AM	106	ARG	NE-CZ-NH1	7.38	123.99	120.30
21	AA	1196	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2126	A	C5-C6-N1	7.38	121.39	117.70
54	BA	655	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	1089	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1419	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1780	A	O4'-C1'-N9	7.38	114.10	108.20
21	AA	1132	C	N3-C2-O2	-7.38	116.74	121.90
54	BA	900	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1304	A	C4-C5-C6	-7.37	113.31	117.00
56	B5	164	ARG	NE-CZ-NH2	7.37	123.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1170	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2090	A	C5-C6-N1	7.37	121.39	117.70
54	BA	2826	A	C5-C6-N1	7.37	121.39	117.70
14	AO	16	ARG	NE-CZ-NH1	7.37	123.98	120.30
54	BA	547	A	C5-C6-N1	7.37	121.38	117.70
54	BA	2887	A	C5-C6-N1	7.37	121.39	117.70
54	BA	217	A	C5-C6-N1	7.37	121.38	117.70
54	BA	1591	A	C5-C6-N1	7.36	121.38	117.70
21	AA	415	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1430	A	N1-C6-N6	-7.36	114.18	118.60
54	BA	472	A	C5-C6-N1	7.36	121.38	117.70
54	BA	590	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1226	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1469	A	C5-C6-N1	7.36	121.38	117.70
21	AA	328	C	N1-C2-O2	7.36	123.31	118.90
54	BA	740	C	N3-C2-O2	-7.36	116.75	121.90
21	AA	448	A	C5-C6-N1	7.36	121.38	117.70
21	AA	841	C	N3-C2-O2	-7.36	116.75	121.90
54	BA	155	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	920	A	C4-C5-C6	-7.36	113.32	117.00
54	BA	1502	A	C5-C6-N1	7.36	121.38	117.70
35	BM	6	ARG	NE-CZ-NH1	7.35	123.98	120.30
54	BA	2378	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	2564	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2868	A	C5-C6-N1	7.35	121.38	117.70
54	BA	324	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	1055	A	C5-C6-N1	7.35	121.38	117.70
54	BA	829	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2497	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2498	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	190	A	C5-C6-N1	7.35	121.37	117.70
21	AA	1146	A	C5-C6-N1	7.35	121.37	117.70
54	BA	1085	A	C5-C6-N1	7.35	121.37	117.70
54	BA	435	C	N3-C2-O2	-7.35	116.76	121.90
54	BA	616	A	C5-C6-N1	7.35	121.37	117.70
54	BA	1789	A	C5-C6-N1	7.35	121.37	117.70
21	AA	353	A	N1-C6-N6	-7.34	114.19	118.60
21	AA	753	A	N1-C6-N6	-7.34	114.19	118.60
54	BA	2132	U	O4'-C1'-N1	7.34	114.08	108.20
38	BP	20	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	160	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	509	C	N3-C2-O2	-7.34	116.76	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2058	A	C5-C6-N1	7.34	121.37	117.70
21	AA	728	A	C4-C5-C6	-7.34	113.33	117.00
46	BX	73	ARG	NE-CZ-NH1	7.34	123.97	120.30
54	BA	449	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	1591	A	C4-C5-C6	-7.34	113.33	117.00
54	BA	2610	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2761	A	C5-C6-N1	7.34	121.37	117.70
22	A1	9	A	C5-C6-N1	7.34	121.37	117.70
54	BA	74	A	C5-C6-N1	7.34	121.37	117.70
21	AA	602	A	C5-C6-N1	7.34	121.37	117.70
21	AA	1261	A	C5-C6-N1	7.34	121.37	117.70
54	BA	947	A	C5-C6-N1	7.34	121.37	117.70
2	AC	155	ARG	NE-CZ-NH1	7.33	123.97	120.30
54	BA	2266	A	C5-C6-N1	7.33	121.37	117.70
54	BA	2314	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	298	A	C5-C6-N1	7.33	121.37	117.70
21	AA	814	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	906	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	371	A	C4-C5-C6	-7.33	113.34	117.00
54	BA	861	A	C4-C5-C6	-7.33	113.34	117.00
54	BA	1990	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	1275	A	C5-C6-N1	7.33	121.36	117.70
21	AA	781	A	C5-C6-N1	7.33	121.36	117.70
54	BA	1596	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	1916	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2820	A	C5-C6-N1	7.33	121.36	117.70
41	BS	11	ARG	NE-CZ-NH1	7.32	123.96	120.30
54	BA	810	U	N3-C2-O2	-7.32	117.07	122.20
54	BA	900	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	1030	C	N3-C2-O2	-7.32	116.77	121.90
54	BA	2033	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2164	C	N3-C2-O2	-7.32	116.77	121.90
21	AA	339	C	N3-C2-O2	-7.32	116.78	121.90
21	AA	844	G	O4'-C1'-N9	7.32	114.06	108.20
36	BN	2	ARG	NE-CZ-NH1	7.32	123.96	120.30
47	BY	29	ARG	NE-CZ-NH1	7.32	123.96	120.30
54	BA	1784	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1899	A	C5-C6-N1	7.32	121.36	117.70
21	AA	196	A	C5-C6-N1	7.32	121.36	117.70
46	BX	26	ARG	NE-CZ-NH1	7.32	123.96	120.30
54	BA	142	A	C4-C5-C6	-7.32	113.34	117.00
54	BA	886	A	C5-C6-N1	7.32	121.36	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1515	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1810	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	2435	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	221	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2665	A	C5-C6-N1	7.31	121.36	117.70
21	AA	411	A	C5-C6-N1	7.31	121.36	117.70
22	A1	58	A	C5-C6-N1	7.31	121.36	117.70
54	BA	2778	A	N1-C6-N6	-7.31	114.21	118.60
21	AA	284	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	1676	A	C5-C6-N1	7.31	121.36	117.70
21	AA	1248	A	N1-C6-N6	-7.31	114.21	118.60
54	BA	472	A	N1-C6-N6	-7.31	114.22	118.60
54	BA	2503	A	C5-C6-N1	7.31	121.35	117.70
21	AA	1275	A	N1-C6-N6	-7.31	114.22	118.60
24	A3	11	A	C5-C6-N1	7.31	121.35	117.70
24	A3	60	A	C5-C6-N1	7.31	121.35	117.70
54	BA	715	A	N1-C6-N6	-7.31	114.22	118.60
54	BA	1086	A	C5-C6-N1	7.31	121.35	117.70
54	BA	453	A	C5-C6-N1	7.31	121.35	117.70
54	BA	1169	A	N1-C6-N6	-7.31	114.22	118.60
54	BA	1439	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2799	A	O4'-C1'-N9	7.30	114.04	108.20
21	AA	819	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	1098	A	C5-C6-N1	7.30	121.35	117.70
54	BA	173	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1634	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1739	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1749	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	2541	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2019	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	144	A	C5-C6-N1	7.30	121.35	117.70
54	BA	671	C	N3-C2-O2	-7.30	116.79	121.90
54	BA	1103	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1847	A	C5-C6-N1	7.30	121.35	117.70
54	BA	901	C	N3-C2-O2	-7.29	116.79	121.90
54	BA	2614	A	C5-C6-N1	7.29	121.35	117.70
21	AA	649	A	C5-C6-N1	7.29	121.35	117.70
21	AA	1519	A	C4-C5-C6	-7.29	113.35	117.00
54	BA	222	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	2114	A	C5-C6-N1	7.29	121.35	117.70
21	AA	327	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1396	A	C4-C5-C6	-7.29	113.36	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2799	A	C5-C6-N1	7.29	121.35	117.70
54	BA	1205	A	O4'-C1'-N9	7.29	114.03	108.20
54	BA	2450	A	C5-C6-N1	7.29	121.34	117.70
21	AA	124	C	P-O3'-C3'	7.29	128.44	119.70
21	AA	329	A	C5-C6-N1	7.29	121.34	117.70
21	AA	579	A	C5-C6-N1	7.29	121.34	117.70
21	AA	1022	A	C4-C5-C6	-7.29	113.36	117.00
54	BA	1321	A	C5-C6-N1	7.29	121.34	117.70
10	AK	36	ARG	NE-CZ-NH1	7.28	123.94	120.30
54	BA	2786	U	O4'-C1'-N1	7.28	114.03	108.20
54	BA	2134	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1216	A	C4-C5-C6	-7.28	113.36	117.00
30	BH	27	ARG	NE-CZ-NH1	7.28	123.94	120.30
54	BA	1275	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	2273	A	C5-C6-N1	7.28	121.34	117.70
21	AA	715	A	C5-C6-N1	7.28	121.34	117.70
21	AA	977	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2412	A	C5-C6-N1	7.28	121.34	117.70
54	BA	2530	A	C4-C5-C6	-7.27	113.36	117.00
21	AA	155	A	C5-C6-N1	7.27	121.34	117.70
21	AA	937	A	C5-C6-N1	7.27	121.34	117.70
21	AA	1507	A	N1-C6-N6	-7.27	114.24	118.60
22	A1	41	A	C5-C6-N1	7.27	121.34	117.70
54	BA	1194	A	C5-C6-N1	7.27	121.34	117.70
54	BA	2534	A	C5-C6-N1	7.27	121.34	117.70
54	BA	1819	A	C5-C6-N1	7.27	121.33	117.70
23	A2	91	A	C5-C6-N1	7.27	121.33	117.70
35	BM	10	ARG	NE-CZ-NH1	7.27	123.94	120.30
54	BA	501	A	N1-C6-N6	-7.27	114.24	118.60
54	BA	14	A	C5-C6-N1	7.27	121.33	117.70
54	BA	582	A	C5-C6-N1	7.27	121.33	117.70
54	BA	28	A	C5-C6-N1	7.26	121.33	117.70
54	BA	753	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1048	A	C5-C6-N1	7.26	121.33	117.70
21	AA	1369	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	294	A	C5-C6-N1	7.26	121.33	117.70
54	BA	974	G	O4'-C1'-N9	7.26	114.01	108.20
54	BA	1503	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	1872	A	N1-C6-N6	-7.26	114.24	118.60
21	AA	578	C	N3-C2-O2	-7.26	116.82	121.90
12	AM	69	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	794	A	C5-C6-N1	7.26	121.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	983	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	2632	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2733	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1144	A	C5-C6-N1	7.26	121.33	117.70
21	AA	1352	C	N3-C2-O2	-7.26	116.82	121.90
26	BD	83	ARG	NE-CZ-NH1	7.26	123.93	120.30
54	BA	800	A	C4-C5-C6	-7.26	113.37	117.00
54	BA	1735	A	C5-C6-N1	7.25	121.33	117.70
21	AA	250	A	C5-C6-N1	7.25	121.33	117.70
29	BG	94	ARG	NE-CZ-NH1	7.25	123.93	120.30
54	BA	1067	A	C5-C6-N1	7.25	121.33	117.70
54	BA	2135	A	C5-C6-N1	7.25	121.33	117.70
24	A3	39	A	C5-C6-N1	7.25	121.33	117.70
54	BA	2602	A	C5-C6-N1	7.25	121.33	117.70
54	BA	64	A	C5-C6-N1	7.25	121.33	117.70
54	BA	910	A	C5-C6-N1	7.25	121.33	117.70
54	BA	2478	A	C5-C6-N1	7.25	121.33	117.70
21	AA	1157	A	C5-C6-N1	7.25	121.32	117.70
54	BA	980	A	N1-C6-N6	-7.25	114.25	118.60
54	BA	1392	A	N1-C6-N6	-7.25	114.25	118.60
21	AA	1400	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	556	A	C4-C5-C6	-7.24	113.38	117.00
54	BA	632	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2154	A	C5-C6-N1	7.24	121.32	117.70
54	BA	331	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	1544	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1774	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	1762	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2162	G	N3-C2-N2	-7.24	114.83	119.90
55	BB	108	A	C5-C6-N1	7.24	121.32	117.70
15	AP	35	ARG	NE-CZ-NH1	7.24	123.92	120.30
21	AA	817	C	N3-C2-O2	-7.24	116.83	121.90
28	BF	111	ARG	NE-CZ-NH1	7.24	123.92	120.30
54	BA	706	A	C5-C6-N1	7.24	121.32	117.70
55	BB	115	A	N1-C6-N6	-7.24	114.26	118.60
10	AK	127	ARG	NE-CZ-NH1	7.23	123.92	120.30
21	AA	1216	A	C5-C6-N1	7.23	121.32	117.70
22	A1	35	A	C5-C6-N1	7.23	121.32	117.70
54	BA	1929	G	O4'-C1'-N9	7.23	113.99	108.20
21	AA	663	A	C5-C6-N1	7.23	121.32	117.70
21	AA	958	A	C5-C6-N1	7.23	121.32	117.70
21	AA	1256	A	N1-C6-N6	-7.23	114.26	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	BF	132	ARG	NE-CZ-NH1	7.23	123.92	120.30
54	BA	203	A	C5-C6-N1	7.23	121.32	117.70
54	BA	507	A	C5-C6-N1	7.23	121.32	117.70
54	BA	1553	A	C5-C6-N1	7.23	121.32	117.70
54	BA	1803	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	2459	A	C5-C6-N1	7.23	121.32	117.70
54	BA	227	A	C5-C6-N1	7.23	121.32	117.70
54	BA	429	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1431	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	145	C	C1'-O4'-C4'	-7.22	104.12	109.90
54	BA	1593	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1691	C	N3-C2-O2	-7.22	116.84	121.90
21	AA	969	A	C5-C6-N1	7.22	121.31	117.70
21	AA	1001	C	N3-C2-O2	-7.22	116.84	121.90
21	AA	1036	A	C5-C6-N1	7.22	121.31	117.70
54	BA	1133	A	C5-C6-N1	7.22	121.31	117.70
21	AA	285	C	N3-C2-O2	-7.22	116.85	121.90
21	AA	665	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	2734	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	1680	U	O4'-C1'-N1	7.22	113.97	108.20
54	BA	1969	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2706	A	C5-C6-N1	7.22	121.31	117.70
54	BA	384	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	1570	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1810	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2042	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2634	A	C5-C6-N1	7.21	121.31	117.70
54	BA	2257	U	O4'-C1'-N1	7.21	113.97	108.20
21	AA	1201	A	P-O3'-C3'	7.21	128.35	119.70
21	AA	1252	A	C5-C6-N1	7.21	121.31	117.70
21	AA	465	A	O4'-C1'-N9	7.21	113.97	108.20
54	BA	1378	A	N1-C6-N6	-7.21	114.28	118.60
54	BA	2870	C	O4'-C1'-N1	7.21	113.97	108.20
54	BA	2717	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	362	A	C5-C6-N1	7.20	121.30	117.70
54	BA	2439	A	C5-C6-N1	7.20	121.30	117.70
55	BB	66	A	N1-C6-N6	-7.20	114.28	118.60
55	BB	99	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	466	A	N1-C6-N6	-7.20	114.28	118.60
21	AA	1285	A	C5-C6-N1	7.20	121.30	117.70
22	A1	31	C	N3-C2-O2	-7.20	116.86	121.90
54	BA	347	A	N1-C6-N6	-7.20	114.28	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	592	A	C5-C6-N1	7.20	121.30	117.70
54	BA	602	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	2090	A	C4-C5-C6	-7.20	113.40	117.00
21	AA	72	A	C5-C6-N1	7.20	121.30	117.70
21	AA	694	A	C5-C6-N1	7.20	121.30	117.70
36	BN	17	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	1090	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	2649	C	N3-C2-O2	-7.20	116.86	121.90
26	BD	128	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	84	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	1937	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1281	C	C1'-O4'-C4'	-7.19	104.14	109.90
55	BB	104	A	C5-C6-N1	7.19	121.30	117.70
21	AA	459	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1597	A	C5-C6-N1	7.19	121.30	117.70
56	B5	74	ARG	NE-CZ-NH1	7.19	123.90	120.30
21	AA	328	C	P-O3'-C3'	7.19	128.33	119.70
54	BA	1205	A	C5-C6-N1	7.19	121.30	117.70
21	AA	199	A	C5-C6-N1	7.19	121.29	117.70
54	BA	226	A	C5-C6-N1	7.19	121.29	117.70
54	BA	866	A	C5-C6-N1	7.19	121.30	117.70
21	AA	109	A	C5-C6-N1	7.19	121.29	117.70
21	AA	495	A	C5-C6-N1	7.19	121.29	117.70
54	BA	743	A	N1-C6-N6	-7.19	114.29	118.60
54	BA	2226	C	N3-C2-O2	-7.19	116.87	121.90
54	BA	145	C	O4'-C1'-N1	7.18	113.95	108.20
54	BA	1745	A	C5-C6-N1	7.18	121.29	117.70
55	BB	34	A	C5-C6-N1	7.18	121.29	117.70
21	AA	621	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1246	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1579	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2384	U	O4'-C1'-N1	7.18	113.94	108.20
54	BA	2501	C	N3-C2-O2	-7.18	116.87	121.90
54	BA	2322	A	C5-C6-N1	7.18	121.29	117.70
54	BA	2606	C	N3-C2-O2	-7.18	116.88	121.90
21	AA	329	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	668	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1618	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	1367	A	C4-C5-C6	-7.17	113.41	117.00
54	BA	1665	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	2425	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1336	A	C5-C6-N1	7.17	121.29	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	74	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1549	A	C5-C6-N1	7.17	121.29	117.70
54	BA	2434	A	C5-C6-N1	7.17	121.29	117.70
11	AL	30	ARG	NE-CZ-NH1	7.17	123.89	120.30
21	AA	373	A	C5-C6-N1	7.17	121.28	117.70
21	AA	1281	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	759	A	N1-C6-N6	-7.17	114.30	118.60
21	AA	787	A	C5-C6-N1	7.17	121.28	117.70
54	BA	342	A	C5-C6-N1	7.17	121.28	117.70
21	AA	746	A	C5-C6-N1	7.17	121.28	117.70
21	AA	1398	A	C4-C5-C6	-7.17	113.42	117.00
54	BA	191	A	C5-C6-N1	7.17	121.28	117.70
22	A1	74	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	911	A	C5-C6-N1	7.16	121.28	117.70
54	BA	959	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2267	A	C5-C6-N1	7.16	121.28	117.70
21	AA	1480	A	C5-C6-N1	7.16	121.28	117.70
7	AH	113	ARG	NE-CZ-NH1	7.16	123.88	120.30
21	AA	573	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	596	A	C5-C6-N1	7.16	121.28	117.70
54	BA	94	A	N1-C6-N6	-7.16	114.31	118.60
21	AA	1021	A	C5-C6-N1	7.16	121.28	117.70
54	BA	233	A	N1-C6-N6	-7.16	114.31	118.60
54	BA	752	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2281	A	C5-C6-N1	7.16	121.28	117.70
49	B0	51	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	631	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2823	A	C5-C6-N1	7.15	121.28	117.70
16	AQ	63	CYS	C-N-CA	7.15	139.58	121.70
21	AA	1339	A	C5-C6-N1	7.15	121.28	117.70
21	AA	1468	A	C5-C6-N1	7.15	121.28	117.70
23	A2	79	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	899	A	C5-C6-N1	7.15	121.28	117.70
54	BA	927	A	C5-C6-N1	7.15	121.28	117.70
21	AA	510	A	C4-C5-C6	-7.15	113.42	117.00
21	AA	695	A	C5-C6-N1	7.15	121.28	117.70
21	AA	889	A	C4-C5-C6	-7.15	113.42	117.00
21	AA	975	A	N1-C6-N6	-7.15	114.31	118.60
54	BA	1020	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1213	A	C5-C6-N1	7.15	121.28	117.70
13	AN	85	ARG	NE-CZ-NH1	7.15	123.87	120.30
21	AA	1329	A	C4-C5-C6	-7.15	113.43	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	41	A	C4-C5-C6	-7.15	113.42	117.00
21	AA	498	A	C5-C6-N1	7.15	121.27	117.70
37	BO	10	ARG	NE-CZ-NH1	7.15	123.87	120.30
48	BZ	15	ARG	NE-CZ-NH1	7.15	123.87	120.30
54	BA	1152	C	N3-C2-O2	-7.15	116.90	121.90
54	BA	2851	A	C5-C6-N1	7.15	121.27	117.70
21	AA	1320	C	N3-C2-O2	-7.15	116.90	121.90
21	AA	1363	A	C5-C6-N1	7.15	121.27	117.70
21	AA	309	A	C5-C6-N1	7.14	121.27	117.70
21	AA	313	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1200	C	N3-C2-O2	-7.14	116.90	121.90
28	BF	166	ARG	NE-CZ-NH1	7.14	123.87	120.30
54	BA	1366	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1804	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	749	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1536	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	1551	A	C5-C6-N1	7.14	121.27	117.70
54	BA	2879	A	C5-C6-N1	7.14	121.27	117.70
21	AA	743	A	C5-C6-N1	7.14	121.27	117.70
21	AA	901	A	N1-C6-N6	-7.14	114.32	118.60
54	BA	897	C	O4'-C1'-N1	7.14	113.91	108.20
54	BA	19	A	C5-C6-N1	7.14	121.27	117.70
54	BA	990	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1287	A	C5-C6-N1	7.14	121.27	117.70
24	A3	36	A	C4-C5-C6	-7.14	113.43	117.00
54	BA	1630	A	C5-C6-N1	7.14	121.27	117.70
21	AA	1317	C	N3-C2-O2	-7.13	116.91	121.90
21	AA	129	A	C5-C6-N1	7.13	121.27	117.70
21	AA	609	A	C4-C5-C6	-7.13	113.43	117.00
54	BA	1387	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1773	A	C5-C6-N1	7.13	121.27	117.70
54	BA	2060	A	C5-C6-N1	7.13	121.27	117.70
21	AA	1150	A	C5-C6-N1	7.13	121.27	117.70
54	BA	125	A	O4'-C1'-N9	7.13	113.91	108.20
41	BS	110	ARG	NE-CZ-NH1	7.13	123.86	120.30
54	BA	181	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1551	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	2800	A	C5-C6-N1	7.13	121.27	117.70
21	AA	124	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	483	A	C5-C6-N1	7.13	121.26	117.70
54	BA	1470	A	C5-C6-N1	7.13	121.26	117.70
24	A3	75	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	1201	A	C5-C6-N1	7.12	121.26	117.70
54	BA	478	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	482	A	C5-C6-N1	7.12	121.26	117.70
54	BA	1652	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2758	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1180	A	C4-C5-C6	-7.12	113.44	117.00
25	BC	261	ARG	NE-CZ-NH1	7.12	123.86	120.30
54	BA	1937	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	1349	C	O4'-C1'-N1	7.12	113.89	108.20
54	BA	2738	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	635	A	C4-C5-C6	-7.11	113.44	117.00
54	BA	141	G	O4'-C1'-N9	7.11	113.89	108.20
54	BA	439	A	C5-C6-N1	7.11	121.26	117.70
54	BA	2381	A	N1-C6-N6	-7.11	114.33	118.60
54	BA	2814	A	C5-C6-N1	7.11	121.26	117.70
54	BA	2900	A	C4-C5-C6	-7.11	113.44	117.00
21	AA	183	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	946	A	C5-C6-N1	7.11	121.26	117.70
21	AA	1138	G	O4'-C1'-N9	7.11	113.89	108.20
54	BA	456	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	1096	A	C5-C6-N1	7.11	121.26	117.70
54	BA	1552	A	C5-C6-N1	7.11	121.25	117.70
54	BA	1940	U	O4'-C1'-N1	7.11	113.89	108.20
54	BA	2145	C	N3-C2-O2	-7.11	116.92	121.90
21	AA	872	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2517	C	N3-C2-O2	-7.11	116.92	121.90
24	A3	45	A	C4-C5-C6	-7.11	113.45	117.00
21	AA	729	A	N1-C6-N6	-7.11	114.34	118.60
21	AA	853	C	N3-C2-O2	-7.11	116.93	121.90
32	BJ	27	ARG	NE-CZ-NH1	7.11	123.85	120.30
37	BO	13	ARG	NE-CZ-NH1	7.11	123.85	120.30
54	BA	368	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	2411	A	C5-C6-N1	7.11	121.25	117.70
21	AA	167	A	C5-C6-N1	7.10	121.25	117.70
54	BA	911	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	2726	A	C5-C6-N1	7.10	121.25	117.70
54	BA	781	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1147	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1583	A	C5-C6-N1	7.10	121.25	117.70
54	BA	2014	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	2126	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	2205	A	C5-C6-N1	7.10	121.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	213	G	N3-C2-N2	-7.10	114.93	119.90
21	AA	687	A	C5-C6-N1	7.10	121.25	117.70
54	BA	661	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	743	A	C5-C6-N1	7.10	121.25	117.70
54	BA	751	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	1392	A	C5-C6-N1	7.10	121.25	117.70
21	AA	1329	A	C5-C6-N1	7.10	121.25	117.70
21	AA	132	C	N3-C2-O2	-7.09	116.93	121.90
54	BA	2515	C	N3-C2-O2	-7.09	116.93	121.90
54	BA	2518	A	O4'-C1'-N9	7.09	113.88	108.20
21	AA	164	G	P-O3'-C3'	7.09	128.21	119.70
54	BA	609	A	C5-C6-N1	7.09	121.25	117.70
54	BA	756	A	C4-C5-C6	-7.09	113.45	117.00
54	BA	2873	A	N1-C6-N6	-7.09	114.34	118.60
24	A3	41	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	1271	A	C5-C6-N1	7.09	121.25	117.70
54	BA	270	A	C5-C6-N1	7.09	121.24	117.70
54	BA	1211	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	2284	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2542	A	C5-C6-N1	7.09	121.24	117.70
21	AA	152	A	C4-C5-C6	-7.09	113.46	117.00
21	AA	608	A	C4-C5-C6	-7.09	113.46	117.00
21	AA	1410	A	C4-C5-C6	-7.09	113.46	117.00
54	BA	44	A	C5-C6-N1	7.09	121.24	117.70
54	BA	2060	A	C4-C5-C6	-7.09	113.46	117.00
54	BA	2587	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	2600	A	N1-C6-N6	-7.09	114.35	118.60
45	BW	24	ARG	NE-CZ-NH2	-7.08	116.76	120.30
21	AA	1022	A	C5-C6-N1	7.08	121.24	117.70
54	BA	149	A	C5-C6-N1	7.08	121.24	117.70
54	BA	988	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2103	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	490	C	O4'-C1'-N1	7.08	113.86	108.20
54	BA	1786	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2882	A	C5-C6-N1	7.08	121.24	117.70
21	AA	197	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	371	A	O4'-C1'-N9	7.08	113.86	108.20
54	BA	821	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1528	A	C5-C6-N1	7.08	121.24	117.70
10	AK	52	ARG	NE-CZ-NH1	7.08	123.84	120.30
21	AA	475	C	N3-C2-O2	-7.08	116.95	121.90
21	AA	478	A	C5-C6-N1	7.08	121.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	423	A	C5-C6-N1	7.08	121.24	117.70
54	BA	197	A	C5-C6-N1	7.07	121.24	117.70
54	BA	462	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1349	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	2635	A	C4-C5-C6	-7.07	113.46	117.00
56	B5	122	ARG	NE-CZ-NH1	7.07	123.84	120.30
21	AA	487	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	2088	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	116	A	C5-C6-N1	7.07	121.23	117.70
21	AA	228	A	C5-C6-N1	7.07	121.24	117.70
21	AA	1362	A	C4-C5-C6	-7.07	113.46	117.00
42	BT	69	ARG	NE-CZ-NH1	7.07	123.83	120.30
54	BA	574	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	51	A	C5-C6-N1	7.07	121.23	117.70
21	AA	1518	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2900	A	C5-C6-N1	7.07	121.23	117.70
21	AA	1349	A	C5-C6-N1	7.07	121.23	117.70
21	AA	1441	A	N1-C6-N6	-7.07	114.36	118.60
21	AA	101	A	C5-C6-N1	7.07	121.23	117.70
21	AA	1192	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	430	A	C4-C5-C6	-7.07	113.47	117.00
21	AA	1137	C	N3-C2-O2	-7.06	116.95	121.90
21	AA	1252	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	49	A	C5-C6-N1	7.06	121.23	117.70
54	BA	526	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	2566	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2847	U	O4'-C1'-N1	7.06	113.85	108.20
21	AA	1169	A	C5-C6-N1	7.06	121.23	117.70
54	BA	264	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	1008	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1553	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	1998	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2738	A	C5-C6-N1	7.06	121.23	117.70
21	AA	1280	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1308	A	C5-C6-N1	7.06	121.23	117.70
21	AA	32	A	C5-C6-N1	7.06	121.23	117.70
21	AA	430	A	N1-C6-N6	-7.06	114.36	118.60
21	AA	1036	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	147	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	608	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1615	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	2227	A	C5-C6-N1	7.06	121.23	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2547	A	C5-C6-N1	7.06	121.23	117.70
55	BB	110	C	O4'-C1'-N1	7.06	113.85	108.20
21	AA	47	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	1276	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2009	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	527	C	N1-C2-O2	7.05	123.13	118.90
54	BA	716	A	C5-C6-N1	7.05	121.23	117.70
54	BA	2309	A	C5-C6-N1	7.05	121.23	117.70
54	BA	223	A	C5-C6-N1	7.05	121.23	117.70
54	BA	255	A	C5-C6-N1	7.05	121.23	117.70
21	AA	802	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1010	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	1794	A	C5-C6-N1	7.05	121.23	117.70
54	BA	2425	A	C4-C5-C6	-7.05	113.47	117.00
21	AA	162	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1274	A	N1-C6-N6	-7.05	114.37	118.60
21	AA	909	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	621	A	C5-C6-N1	7.05	121.22	117.70
54	BA	749	A	C4-C5-C6	-7.05	113.48	117.00
54	BA	1525	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2358	A	C4-C5-C6	-7.05	113.48	117.00
27	BE	67	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	721	A	N1-C6-N6	-7.04	114.37	118.60
54	BA	765	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	210	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	1046	A	C5-C6-N1	7.04	121.22	117.70
22	A1	11	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	994	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1870	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	676	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1359	C	N3-C2-O2	-7.04	116.97	121.90
21	AA	59	A	C5-C6-N1	7.04	121.22	117.70
21	AA	306	A	N1-C6-N6	-7.04	114.38	118.60
21	AA	767	A	C5-C6-N1	7.04	121.22	117.70
21	AA	913	A	P-O3'-C3'	7.04	128.15	119.70
21	AA	949	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1035	A	C5-C6-N1	7.04	121.22	117.70
54	BA	262	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	739	A	C5-C6-N1	7.04	121.22	117.70
21	AA	825	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	501	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1738	G	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	1342	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	1496	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	1670	C	N3-C2-O2	-7.03	116.98	121.90
22	A1	56	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1147	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	1848	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	69	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1805	A	C4-C5-C6	-7.03	113.49	117.00
21	AA	1394	A	C4-C5-C6	-7.03	113.49	117.00
21	AA	7	A	C5-C6-N1	7.02	121.21	117.70
54	BA	204	A	C4-C5-C6	-7.02	113.49	117.00
21	AA	8	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1441	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1532	A	C5-C6-N1	7.02	121.21	117.70
54	BA	1638	C	N3-C2-O2	-7.02	116.98	121.90
54	BA	2395	C	N3-C2-O2	-7.02	116.98	121.90
54	BA	2727	A	C5-C6-N1	7.02	121.21	117.70
55	BB	50	A	C5-C6-N1	7.02	121.21	117.70
21	AA	363	A	C5-C6-N1	7.02	121.21	117.70
54	BA	143	C	N3-C2-O2	-7.02	116.99	121.90
54	BA	835	C	N3-C2-O2	-7.02	116.99	121.90
54	BA	1998	A	C5-C6-N1	7.02	121.21	117.70
54	BA	272	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1236	A	N1-C6-N6	-7.02	114.39	118.60
56	B5	134	ARG	NE-CZ-NH1	7.02	123.81	120.30
54	BA	973	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1509	A	C5-C6-N1	7.01	121.21	117.70
11	AL	113	ARG	NE-CZ-NH1	7.01	123.81	120.30
13	AN	9	ARG	NE-CZ-NH1	7.01	123.81	120.30
54	BA	1634	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	2336	A	C5-C6-N1	7.01	121.21	117.70
21	AA	496	A	C5-C6-N1	7.01	121.21	117.70
21	AA	1431	A	C5-C6-N1	7.01	121.21	117.70
54	BA	231	A	C4-C5-C6	-7.01	113.49	117.00
54	BA	492	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1829	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2810	A	C5-C6-N1	7.01	121.21	117.70
21	AA	553	A	C4-C5-C6	-7.01	113.50	117.00
39	BQ	32	ARG	NE-CZ-NH2	7.01	123.81	120.30
23	A2	91	A	C4-C5-C6	-7.01	113.50	117.00
54	BA	2366	A	C5-C6-N1	7.01	121.20	117.70
7	AH	116	ARG	NE-CZ-NH1	7.01	123.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	401	C	N3-C2-O2	-7.01	117.00	121.90
21	AA	1176	A	C5-C6-N1	7.01	121.20	117.70
33	BK	18	ARG	NE-CZ-NH1	7.01	123.80	120.30
54	BA	783	A	N1-C6-N6	-7.01	114.40	118.60
54	BA	1254	A	C5-C6-N1	7.01	121.20	117.70
54	BA	2407	A	C5-C6-N1	7.01	121.20	117.70
21	AA	553	A	C5-C6-N1	7.00	121.20	117.70
54	BA	1080	A	C5-C6-N1	7.00	121.20	117.70
51	B2	33	ARG	NE-CZ-NH1	7.00	123.80	120.30
54	BA	53	A	C5-C6-N1	7.00	121.20	117.70
54	BA	347	A	C5-C6-N1	7.00	121.20	117.70
54	BA	878	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1069	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	1427	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	2047	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2581	G	O4'-C1'-N9	7.00	113.80	108.20
54	BA	2647	U	O4'-C1'-N1	7.00	113.80	108.20
3	AD	43	ARG	NE-CZ-NH1	7.00	123.80	120.30
54	BA	1129	A	C5'-C4'-O4'	7.00	117.50	109.10
55	BB	46	A	C5-C6-N1	7.00	121.20	117.70
21	AA	172	A	C5-C6-N1	7.00	121.20	117.70
21	AA	1465	A	C5-C6-N1	7.00	121.20	117.70
54	BA	601	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	1001	A	C5-C6-N1	7.00	121.20	117.70
21	AA	386	C	N3-C2-O2	-6.99	117.00	121.90
21	AA	430	A	C5-C6-N1	6.99	121.20	117.70
54	BA	460	A	C5-C6-N1	6.99	121.20	117.70
54	BA	1039	A	C5-C6-N1	6.99	121.20	117.70
54	BA	1928	A	C5-C6-N1	6.99	121.20	117.70
54	BA	2104	C	N1-C2-O2	6.99	123.10	118.90
21	AA	1534	A	C5-C6-N1	6.99	121.20	117.70
21	AA	463	U	C1'-O4'-C4'	-6.99	104.31	109.90
21	AA	1081	A	C5-C6-N1	6.99	121.20	117.70
26	BD	13	ARG	NE-CZ-NH1	6.99	123.80	120.30
54	BA	1963	U	O4'-C1'-N1	6.99	113.79	108.20
54	BA	2467	C	O4'-C1'-N1	6.99	113.79	108.20
21	AA	792	A	O4'-C1'-N9	6.99	113.79	108.20
54	BA	1098	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	1918	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	633	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2045	C	N3-C2-O2	-6.99	117.01	121.90
55	BB	99	A	C5-C6-N1	6.99	121.19	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	391	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	1876	A	C5-C6-N1	6.99	121.19	117.70
55	BB	12	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	1101	A	C5-C6-N1	6.98	121.19	117.70
54	BA	503	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	1759	A	C4-C5-C6	-6.98	113.51	117.00
21	AA	780	A	C5-C6-N1	6.98	121.19	117.70
21	AA	998	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	13	A	C5-C6-N1	6.98	121.19	117.70
48	BZ	29	ARG	NE-CZ-NH1	6.98	123.79	120.30
54	BA	127	A	C5-C6-N1	6.98	121.19	117.70
54	BA	352	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	1211	C	O4'-C1'-N1	6.98	113.78	108.20
54	BA	1287	A	C5-C6-N1	6.98	121.19	117.70
21	AA	78	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1385	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1431	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1489	C	N3-C2-O2	-6.98	117.02	121.90
54	BA	1700	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2283	C	O4'-C1'-N1	6.98	113.78	108.20
54	BA	2757	A	C5-C6-N1	6.98	121.19	117.70
21	AA	1306	A	C5-C6-N1	6.98	121.19	117.70
51	B2	35	ARG	NE-CZ-NH1	6.98	123.79	120.30
54	BA	2805	C	N3-C2-O2	-6.98	117.02	121.90
21	AA	663	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	1130	A	C5-C6-N1	6.97	121.19	117.70
21	AA	1468	A	N1-C6-N6	-6.97	114.42	118.60
36	BN	12	ARG	NE-CZ-NH1	6.97	123.79	120.30
54	BA	91	A	C5-C6-N1	6.97	121.19	117.70
21	AA	414	A	C5-C6-N1	6.97	121.19	117.70
54	BA	151	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	975	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1579	A	N1-C6-N6	-6.97	114.42	118.60
21	AA	1430	A	C5-C6-N1	6.97	121.19	117.70
54	BA	1384	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	1698	A	N1-C6-N6	-6.97	114.42	118.60
54	BA	2059	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2336	A	C4-C5-C6	-6.97	113.52	117.00
55	BB	46	A	C4-C5-C6	-6.97	113.52	117.00
21	AA	1346	A	C4-C5-C6	-6.97	113.52	117.00
13	AN	81	ARG	NE-CZ-NH1	6.97	123.78	120.30
21	AA	1219	A	C5-C6-N1	6.97	121.18	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1368	A	C5-C6-N1	6.97	121.18	117.70
54	BA	457	A	C4-C5-C6	-6.97	113.52	117.00
21	AA	747	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1105	A	C5-C6-N1	6.96	121.18	117.70
54	BA	718	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2078	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	2873	A	C5-C6-N1	6.96	121.18	117.70
21	AA	465	A	C5-C6-N1	6.96	121.18	117.70
21	AA	784	A	C5-C6-N1	6.96	121.18	117.70
32	BJ	99	ARG	NE-CZ-NH1	6.96	123.78	120.30
54	BA	781	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	2184	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2632	A	C4-C5-C6	-6.96	113.52	117.00
22	A1	6	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	167	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	919	A	C5-C6-N1	6.96	121.18	117.70
21	AA	1428	A	C5-C6-N1	6.96	121.18	117.70
54	BA	265	A	C5-C6-N1	6.96	121.18	117.70
54	BA	634	C	N3-C2-O2	-6.96	117.03	121.90
21	AA	845	A	N1-C6-N6	-6.96	114.43	118.60
21	AA	609	A	C5-C6-N1	6.96	121.18	117.70
55	BB	39	A	C5-C6-N1	6.96	121.18	117.70
21	AA	160	A	C5-C6-N1	6.95	121.18	117.70
54	BA	1314	C	N3-C2-O2	-6.95	117.03	121.90
21	AA	1502	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	1749	A	C5-C6-N1	6.95	121.18	117.70
54	BA	1916	A	C4-C5-C6	-6.95	113.52	117.00
54	BA	2516	A	C4-C5-C6	-6.95	113.52	117.00
21	AA	1520	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	788	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1102	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	1586	A	C5-C6-N1	6.95	121.17	117.70
55	BB	42	C	N3-C2-O2	-6.95	117.03	121.90
55	BB	66	A	C5-C6-N1	6.95	121.17	117.70
21	AA	695	A	C4-C5-C6	-6.95	113.53	117.00
21	AA	756	C	N3-C2-O2	-6.95	117.04	121.90
22	A1	75	C	N3-C2-O2	-6.95	117.04	121.90
37	BO	16	ARG	NE-CZ-NH1	6.95	123.77	120.30
54	BA	1111	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2721	A	C5-C6-N1	6.95	121.17	117.70
21	AA	374	A	C5-C6-N1	6.95	121.17	117.70
21	AA	985	C	N3-C2-O2	-6.95	117.04	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	69	C	N3-C2-O2	-6.95	117.04	121.90
54	BA	320	A	C5-C6-N1	6.95	121.17	117.70
54	BA	2326	C	N1-C2-O2	6.95	123.07	118.90
21	AA	1044	A	C5-C6-N1	6.94	121.17	117.70
54	BA	190	A	N1-C6-N6	-6.94	114.43	118.60
55	BB	80	U	O4'-C1'-N1	6.94	113.75	108.20
1	AB	207	ARG	NE-CZ-NH1	6.94	123.77	120.30
21	AA	1484	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	2342	C	N3-C2-O2	-6.94	117.04	121.90
5	AF	86	ARG	NE-CZ-NH1	6.94	123.77	120.30
54	BA	2660	A	C5-C6-N1	6.94	121.17	117.70
21	AA	631	C	N3-C2-O2	-6.94	117.04	121.90
21	AA	1476	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	1046	A	C1'-O4'-C4'	-6.94	104.35	109.90
54	BA	1978	A	C5-C6-N1	6.94	121.17	117.70
55	BB	97	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	2311	A	C5-C6-N1	6.94	121.17	117.70
54	BA	2377	A	N1-C6-N6	-6.94	114.44	118.60
55	BB	73	A	C5-C6-N1	6.94	121.17	117.70
54	BA	20	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	1274	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1548	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	1603	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	2427	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	2560	A	C5-C6-N1	6.93	121.17	117.70
21	AA	282	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	349	A	N1-C6-N6	-6.93	114.44	118.60
21	AA	549	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	2142	A	C5-C6-N1	6.93	121.17	117.70
38	BP	52	ARG	NE-CZ-NH1	6.93	123.77	120.30
54	BA	943	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	1197	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	84	A	C5-C6-N1	6.93	121.16	117.70
22	A1	14	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2667	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	1611	C	N3-C2-O2	-6.92	117.05	121.90
21	AA	328	C	O4'-C1'-N1	6.92	113.74	108.20
21	AA	624	C	N3-C2-O2	-6.92	117.05	121.90
54	BA	311	A	C5-C6-N1	6.92	121.16	117.70
54	BA	715	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	1596	A	C5-C6-N1	6.92	121.16	117.70
54	BA	1640	A	C5-C6-N1	6.92	121.16	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1760	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	313	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	163	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	563	A	C5-C6-N1	6.92	121.16	117.70
54	BA	2158	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	2310	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	787	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	1021	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	517	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	1686	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	2211	A	C5-C6-N1	6.92	121.16	117.70
21	AA	335	C	N3-C2-O2	-6.92	117.06	121.90
21	AA	897	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	1225	A	C5-C6-N1	6.91	121.16	117.70
54	BA	95	A	C5-C6-N1	6.91	121.16	117.70
54	BA	1194	A	C4-C5-C6	-6.91	113.54	117.00
54	BA	1690	A	C5-C6-N1	6.91	121.16	117.70
54	BA	2435	A	C5-C6-N1	6.91	121.16	117.70
54	BA	2875	C	N3-C2-O2	-6.91	117.06	121.90
55	BB	27	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	1134	A	C5-C6-N1	6.91	121.16	117.70
4	AE	67	ARG	NE-CZ-NH1	6.91	123.75	120.30
54	BA	13	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	2314	A	C5-C6-N1	6.91	121.16	117.70
21	AA	338	A	C5-C6-N1	6.91	121.15	117.70
37	BO	30	ARG	NE-CZ-NH1	6.91	123.75	120.30
54	BA	915	C	N3-C2-O2	-6.90	117.07	121.90
54	BA	920	A	C5-C6-N1	6.90	121.15	117.70
21	AA	364	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1773	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	2054	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2327	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2381	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2559	C	O4'-C1'-N1	6.90	113.72	108.20
54	BA	693	A	C5-C6-N1	6.90	121.15	117.70
54	BA	793	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1354	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	1717	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1754	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1952	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2406	A	O4'-C1'-N9	6.90	113.72	108.20
54	BA	2587	A	C5-C6-N1	6.90	121.15	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AI	122	ARG	NE-CZ-NH2	6.90	123.75	120.30
21	AA	935	A	C5-C6-N1	6.90	121.15	117.70
54	BA	176	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	412	A	C5-C6-N1	6.90	121.15	117.70
54	BA	677	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	1182	G	O4'-C1'-N9	6.90	113.72	108.20
54	BA	2205	A	N1-C6-N6	-6.90	114.46	118.60
2	AC	135	ARG	NE-CZ-NH1	6.90	123.75	120.30
54	BA	783	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2392	A	N1-C6-N6	-6.90	114.46	118.60
21	AA	23	C	N3-C2-O2	-6.89	117.07	121.90
54	BA	103	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1713	A	C5-C6-N1	6.89	121.15	117.70
54	BA	1772	A	C5-C6-N1	6.89	121.15	117.70
21	AA	790	A	C5-C6-N1	6.89	121.14	117.70
12	AM	28	ARG	NE-CZ-NH1	6.89	123.75	120.30
21	AA	214	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	1102	A	C4-C5-C6	-6.89	113.56	117.00
21	AA	1400	C	C3'-C2'-C1'	6.89	107.01	101.50
54	BA	516	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1127	A	C5-C6-N1	6.89	121.14	117.70
54	BA	2362	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1545	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	2095	A	C4-C5-C6	-6.89	113.56	117.00
21	AA	174	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	600	A	C5-C6-N1	6.88	121.14	117.70
54	BA	362	A	N1-C6-N6	-6.88	114.47	118.60
54	BA	1385	A	O4'-C1'-N9	6.88	113.71	108.20
54	BA	2837	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1303	C	N1-C2-O2	6.88	123.03	118.90
54	BA	873	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	331	G	N1-C6-O6	-6.88	115.77	119.90
54	BA	990	A	C1'-O4'-C4'	-6.88	104.39	109.90
54	BA	2041	U	O4'-C1'-N1	6.88	113.70	108.20
21	AA	1254	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	678	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	2850	A	C5-C6-N1	6.88	121.14	117.70
21	AA	223	A	C5-C6-N1	6.88	121.14	117.70
21	AA	675	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	892	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	391	A	C5-C6-N1	6.88	121.14	117.70
54	BA	2725	A	C5-C6-N1	6.88	121.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	655	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	1296	C	N3-C2-O2	-6.88	117.09	121.90
54	BA	502	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1322	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1459	G	O4'-C1'-N9	6.88	113.70	108.20
54	BA	2374	C	N3-C2-O2	-6.88	117.09	121.90
17	AR	62	ARG	NE-CZ-NH1	6.87	123.74	120.30
21	AA	1197	A	C5-C6-N1	6.87	121.14	117.70
54	BA	918	A	C5-C6-N1	6.87	121.14	117.70
54	BA	2135	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	2266	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	2453	A	C5-C6-N1	6.87	121.14	117.70
6	AG	137	ARG	NE-CZ-NH1	6.87	123.74	120.30
21	AA	370	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	923	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	1360	A	C5-C6-N1	6.87	121.14	117.70
21	AA	1452	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	892	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1293	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	2577	A	N1-C6-N6	-6.87	114.48	118.60
19	AT	23	ARG	NE-CZ-NH1	6.87	123.73	120.30
54	BA	1246	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	2309	A	C4-C5-C6	-6.87	113.57	117.00
21	AA	794	A	C5-C6-N1	6.87	121.13	117.70
21	AA	1311	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1603	A	C5-C6-N1	6.87	121.13	117.70
55	BB	52	A	C5-C6-N1	6.87	121.13	117.70
21	AA	267	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	814	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	2067	G	O4'-C1'-N9	6.87	113.69	108.20
2	AC	131	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	157	C	N3-C2-O2	-6.86	117.09	121.90
54	BA	435	C	O4'-C1'-N1	6.86	113.69	108.20
54	BA	529	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2813	A	C5-C6-N1	6.86	121.13	117.70
21	AA	924	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	592	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	1256	A	C5-C6-N1	6.86	121.13	117.70
21	AA	1375	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	300	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	2163	A	C5-C6-N1	6.86	121.13	117.70
3	AD	114	ARG	NE-CZ-NH1	6.86	123.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1064	G	N3-C2-N2	-6.86	115.10	119.90
21	AA	1152	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1073	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	1650	A	C5-C6-N1	6.86	121.13	117.70
21	AA	309	A	N1-C6-N6	-6.86	114.48	118.60
21	AA	729	A	C5-C6-N1	6.86	121.13	117.70
54	BA	800	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1076	C	O4'-C1'-N1	6.86	113.69	108.20
21	AA	907	A	C5-C6-N1	6.86	121.13	117.70
54	BA	673	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	680	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	614	A	C5-C6-N1	6.85	121.13	117.70
54	BA	1009	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	1433	A	C4-C5-C6	-6.85	113.57	117.00
54	BA	196	A	C5-C6-N1	6.85	121.13	117.70
21	AA	640	A	C5-C6-N1	6.85	121.13	117.70
21	AA	739	C	N3-C2-O2	-6.85	117.11	121.90
54	BA	1701	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	648	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	765	G	O4'-C1'-N9	6.85	113.68	108.20
21	AA	1363	A	C4-C5-C6	-6.85	113.58	117.00
21	AA	1447	A	O4'-C1'-N9	6.85	113.68	108.20
32	BJ	69	ARG	NE-CZ-NH1	6.85	123.72	120.30
54	BA	433	C	N3-C2-O2	-6.85	117.11	121.90
9	AJ	89	ARG	NE-CZ-NH1	6.85	123.72	120.30
21	AA	236	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	382	A	C5-C6-N1	6.85	121.12	117.70
21	AA	716	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2468	A	C4-C5-C6	-6.84	113.58	117.00
21	AA	857	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	1510	C	N3-C2-O2	-6.84	117.11	121.90
24	A3	74	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	1244	A	C5-C6-N1	6.84	121.12	117.70
21	AA	65	A	C5-C6-N1	6.84	121.12	117.70
54	BA	504	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	587	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1315	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	1902	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	2328	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	2577	A	C5-C6-N1	6.84	121.12	117.70
54	BA	2628	C	N3-C2-O2	-6.84	117.11	121.90
21	AA	253	A	C4-C5-C6	-6.83	113.58	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	342	C	N3-C2-O2	-6.83	117.11	121.90
21	AA	879	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	1462	C	N3-C2-O2	-6.83	117.12	121.90
54	BA	514	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2482	A	C5-C6-N1	6.83	121.12	117.70
54	BA	2675	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	2723	C	N3-C2-O2	-6.83	117.12	121.90
14	AO	63	ARG	NE-CZ-NH1	6.83	123.72	120.30
22	A1	18	G	O4'-C1'-N9	6.83	113.66	108.20
54	BA	1689	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	971	G	N1-C6-O6	-6.83	115.80	119.90
55	BB	13	G	O4'-C1'-N9	6.83	113.66	108.20
11	AL	11	ARG	NE-CZ-NH1	6.83	123.71	120.30
54	BA	2312	U	O4'-C1'-N1	6.83	113.66	108.20
21	AA	81	A	C4-C5-C6	-6.83	113.59	117.00
21	AA	514	C	N3-C2-O2	-6.83	117.12	121.90
36	BN	90	ARG	NE-CZ-NH1	6.83	123.71	120.30
21	AA	915	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	782	A	C5-C6-N1	6.82	121.11	117.70
54	BA	988	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	1326	U	O4'-C1'-N1	6.82	113.66	108.20
54	BA	737	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	2612	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	345	C	N1-C2-O2	6.82	122.99	118.90
54	BA	222	A	C5-C6-N1	6.82	121.11	117.70
54	BA	863	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2665	A	N1-C6-N6	-6.82	114.51	118.60
54	BA	1618	A	C5-C6-N1	6.81	121.11	117.70
54	BA	2746	U	O4'-C1'-N1	6.81	113.65	108.20
18	AS	2	ARG	NE-CZ-NH1	6.81	123.71	120.30
54	BA	2146	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	1227	A	C5-C6-N1	6.81	121.11	117.70
54	BA	1590	A	N1-C6-N6	-6.81	114.51	118.60
14	AO	83	ARG	NE-CZ-NH1	6.81	123.70	120.30
21	AA	1395	C	N1-C2-O2	6.81	122.99	118.90
54	BA	207	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	1744	A	N1-C6-N6	-6.81	114.52	118.60
54	BA	2227	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	2270	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	2451	A	N1-C6-N6	-6.81	114.51	118.60
54	BA	2679	A	C5-C6-N1	6.81	121.10	117.70
5	AF	38	ARG	NE-CZ-NH1	6.81	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	BO	94	ARG	NE-CZ-NH1	6.81	123.70	120.30
54	BA	987	C	O4'-C1'-N1	6.81	113.64	108.20
21	AA	681	A	C5-C6-N1	6.80	121.10	117.70
21	AA	749	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	470	A	N1-C6-N6	-6.80	114.52	118.60
54	BA	1165	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1757	A	C4-C5-C6	-6.80	113.60	117.00
21	AA	983	A	N1-C6-N6	-6.80	114.52	118.60
54	BA	2774	C	O4'-C1'-N1	6.80	113.64	108.20
21	AA	10	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1410	A	C5-C6-N1	6.80	121.10	117.70
24	A3	58	A	N1-C6-N6	-6.80	114.52	118.60
54	BA	611	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	2222	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	1151	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	1366	A	C4-C5-C6	-6.80	113.60	117.00
15	AP	25	ARG	NE-CZ-NH1	6.80	123.70	120.30
54	BA	89	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	130	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	730	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1730	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	2369	A	N1-C6-N6	-6.80	114.52	118.60
54	BA	1398	C	N3-C2-O2	-6.79	117.14	121.90
21	AA	272	C	N3-C2-O2	-6.79	117.14	121.90
21	AA	1302	C	N3-C2-O2	-6.79	117.14	121.90
21	AA	1408	A	C5-C6-N1	6.79	121.10	117.70
54	BA	1247	A	C4-C5-C6	-6.79	113.60	117.00
54	BA	1269	A	C4-C5-C6	-6.79	113.60	117.00
6	AG	94	ARG	NE-CZ-NH1	6.79	123.69	120.30
21	AA	487	A	C5-C6-N1	6.79	121.10	117.70
21	AA	826	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	246	C	N3-C2-O2	-6.79	117.15	121.90
21	AA	918	A	C4-C5-C6	-6.79	113.61	117.00
37	BO	15	ARG	NE-CZ-NH1	6.79	123.69	120.30
54	BA	885	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	2751	G	O4'-C1'-N9	6.79	113.63	108.20
54	BA	2807	U	O4'-C1'-N1	6.79	113.63	108.20
25	BC	174	ARG	NE-CZ-NH1	6.79	123.69	120.30
54	BA	99	U	O4'-C1'-N1	6.79	113.63	108.20
54	BA	825	A	C5-C6-N1	6.79	121.09	117.70
40	BR	13	ARG	NE-CZ-NH1	6.79	123.69	120.30
54	BA	2872	A	C5-C6-N1	6.79	121.09	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	90	C	O4'-C1'-N1	6.79	113.63	108.20
21	AA	635	A	C5-C6-N1	6.78	121.09	117.70
54	BA	282	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1090	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1247	A	C5-C6-N1	6.78	121.09	117.70
54	BA	510	C	N1-C2-O2	6.78	122.97	118.90
1	AB	136	ARG	NE-CZ-NH1	6.78	123.69	120.30
21	AA	71	A	C5-C6-N1	6.78	121.09	117.70
54	BA	332	A	C5-C6-N1	6.78	121.09	117.70
54	BA	643	A	C5-C6-N1	6.78	121.09	117.70
54	BA	849	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2675	A	C5-C6-N1	6.78	121.09	117.70
54	BA	497	A	C5-C6-N1	6.78	121.09	117.70
54	BA	563	A	N1-C6-N6	-6.78	114.53	118.60
54	BA	742	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1664	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2749	A	N1-C6-N6	-6.78	114.53	118.60
21	AA	507	C	N3-C2-O2	-6.78	117.16	121.90
21	AA	996	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2575	C	C3'-C2'-C1'	6.77	106.92	101.50
21	AA	860	A	C5-C6-N1	6.77	121.09	117.70
25	BC	211	ARG	NE-CZ-NH1	6.77	123.69	120.30
54	BA	1354	A	C5-C6-N1	6.77	121.09	117.70
21	AA	696	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	72	A	C4-C5-C6	-6.77	113.62	117.00
54	BA	1637	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2376	A	C4-C5-C6	-6.77	113.61	117.00
12	AM	97	ARG	NE-CZ-NH1	6.77	123.68	120.30
21	AA	1100	C	N3-C2-O2	-6.77	117.16	121.90
54	BA	56	A	C5-C6-N1	6.77	121.08	117.70
54	BA	1365	A	C5-C6-N1	6.77	121.08	117.70
21	AA	1155	A	C4-C5-C6	-6.76	113.62	117.00
21	AA	1236	A	C5-C6-N1	6.76	121.08	117.70
54	BA	126	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	985	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1075	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1853	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	2476	A	C5-C6-N1	6.76	121.08	117.70
21	AA	753	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1531	A	C5-C6-N1	6.76	121.08	117.70
54	BA	311	A	N1-C6-N6	-6.76	114.54	118.60
54	BA	575	A	C5-C6-N1	6.76	121.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	716	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1114	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1347	A	C5-C6-N1	6.76	121.08	117.70
54	BA	2860	A	C5-C6-N1	6.76	121.08	117.70
21	AA	620	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	1375	A	C5-C6-N1	6.76	121.08	117.70
54	BA	196	A	N1-C6-N6	-6.76	114.54	118.60
54	BA	2051	A	C5-C6-N1	6.76	121.08	117.70
54	BA	635	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	810	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	219	A	C5-C6-N1	6.76	121.08	117.70
54	BA	526	A	C5-C6-N1	6.76	121.08	117.70
29	BG	169	ARG	NE-CZ-NH1	6.75	123.68	120.30
54	BA	2690	U	C1'-O4'-C4'	-6.75	104.50	109.90
21	AA	934	C	N3-C2-O2	-6.75	117.17	121.90
54	BA	1286	A	C5-C6-N1	6.75	121.08	117.70
54	BA	892	A	N1-C6-N6	-6.75	114.55	118.60
54	BA	1503	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1654	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1802	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1986	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	1821	A	C5-C6-N1	6.75	121.07	117.70
24	A3	40	C	N3-C2-O2	-6.75	117.18	121.90
54	BA	1711	A	C4-C5-C6	-6.75	113.63	117.00
54	BA	1830	C	N3-C2-O2	-6.75	117.18	121.90
21	AA	28	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	110	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1598	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2813	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2823	A	N1-C6-N6	-6.74	114.56	118.60
21	AA	1302	C	O4'-C1'-N1	6.74	113.59	108.20
54	BA	1353	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1451	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	2037	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2278	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	10	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2369	A	C5-C6-N1	6.74	121.07	117.70
55	BB	8	C	N3-C2-O2	-6.74	117.18	121.90
55	BB	94	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2129	C	O4'-C1'-N1	6.74	113.59	108.20
54	BA	146	A	C5-C6-N1	6.74	121.07	117.70
54	BA	364	C	N3-C2-O2	-6.74	117.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1013	C	N3-C2-O2	-6.74	117.19	121.90
54	BA	2147	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2199	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2590	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2824	C	N3-C2-O2	-6.74	117.19	121.90
54	BA	2893	A	C5-C6-N1	6.74	121.07	117.70
54	BA	2705	A	C5-C6-N1	6.73	121.07	117.70
54	BA	964	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	1074	G	O4'-C1'-N9	6.73	113.59	108.20
54	BA	1336	A	C4-C5-C6	-6.73	113.63	117.00
54	BA	2058	A	C4-C5-C6	-6.73	113.63	117.00
21	AA	456	A	C4-C5-C6	-6.73	113.63	117.00
54	BA	2214	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	980	C	N3-C2-O2	-6.73	117.19	121.90
24	A3	22	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	945	A	C5-C6-N1	6.73	121.06	117.70
54	BA	310	A	N1-C6-N6	-6.73	114.56	118.60
54	BA	1610	A	C4-C5-C6	-6.73	113.64	117.00
21	AA	564	C	N3-C2-O2	-6.72	117.19	121.90
36	BN	45	ARG	NE-CZ-NH1	6.72	123.66	120.30
54	BA	447	A	C5-C6-N1	6.72	121.06	117.70
54	BA	898	C	O4'-C1'-N1	6.72	113.58	108.20
21	AA	228	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	815	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	819	A	C5-C6-N1	6.72	121.06	117.70
54	BA	1070	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	1494	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1672	A	C4-C5-C6	-6.72	113.64	117.00
55	BB	26	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	251	A	C5-C6-N1	6.72	121.06	117.70
54	BA	1920	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	246	A	C4-C5-C6	-6.72	113.64	117.00
21	AA	1093	A	C5-C6-N1	6.72	121.06	117.70
24	A3	45	A	C5-C6-N1	6.72	121.06	117.70
54	BA	213	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	284	U	O4'-C1'-N1	6.72	113.58	108.20
54	BA	1007	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	2510	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	2622	U	O4'-C1'-N1	6.72	113.58	108.20
21	AA	74	A	C5-C6-N1	6.72	121.06	117.70
21	AA	177	G	O4'-C1'-N9	6.72	113.58	108.20
24	A3	60	A	C4-C5-C6	-6.72	113.64	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1895	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	340	A	C5-C6-N1	6.71	121.06	117.70
54	BA	633	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	793	A	N1-C6-N6	-6.71	114.57	118.60
54	BA	2108	A	N1-C6-N6	-6.71	114.57	118.60
55	BB	58	A	C5-C6-N1	6.71	121.06	117.70
21	AA	831	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1175	A	O4'-C1'-N9	6.71	113.57	108.20
54	BA	2779	U	O4'-C1'-N1	6.71	113.57	108.20
54	BA	2392	A	C5-C6-N1	6.71	121.05	117.70
54	BA	2703	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	316	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	1479	C	N3-C2-O2	-6.71	117.21	121.90
54	BA	853	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	2513	A	C5-C6-N1	6.71	121.05	117.70
54	BA	2861	U	O4'-C1'-N1	6.71	113.56	108.20
54	BA	1966	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	53	A	C5-C6-N1	6.70	121.05	117.70
21	AA	143	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2097	A	C5-C6-N1	6.70	121.05	117.70
21	AA	864	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	332	A	O4'-C1'-N9	6.70	113.56	108.20
2	AC	39	ARG	NE-CZ-NH2	-6.70	116.95	120.30
21	AA	263	A	C5-C6-N1	6.70	121.05	117.70
21	AA	451	A	N1-C6-N6	-6.70	114.58	118.60
24	A3	35	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	167	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1077	A	C5-C6-N1	6.70	121.05	117.70
54	BA	2755	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2762	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2025	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2499	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	607	A	C5-C6-N1	6.70	121.05	117.70
21	AA	1333	A	C5-C6-N1	6.70	121.05	117.70
54	BA	76	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	264	C	N3-C2-O2	-6.69	117.21	121.90
21	AA	1012	A	C5-C6-N1	6.69	121.05	117.70
21	AA	389	A	C5-C6-N1	6.69	121.05	117.70
54	BA	213	A	C5-C6-N1	6.69	121.05	117.70
54	BA	734	A	C4-C5-C6	-6.69	113.65	117.00
54	BA	399	U	O4'-C1'-N1	6.69	113.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1111	A	N1-C6-N6	-6.69	114.59	118.60
54	BA	1126	A	C5-C6-N1	6.69	121.05	117.70
54	BA	2055	C	N1-C2-O2	6.69	122.91	118.90
21	AA	48	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	397	U	O4'-C1'-N1	6.69	113.55	108.20
54	BA	1494	A	C5-C6-N1	6.69	121.04	117.70
21	AA	1269	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	936	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	1035	U	O4'-C1'-N1	6.69	113.55	108.20
54	BA	2065	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2520	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	532	A	N1-C6-N6	-6.69	114.59	118.60
54	BA	2527	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2753	A	C4-C5-C6	-6.69	113.66	117.00
21	AA	16	A	C5-C6-N1	6.68	121.04	117.70
54	BA	2031	A	C4-C5-C6	-6.68	113.66	117.00
21	AA	618	C	C1'-O4'-C4'	-6.68	104.55	109.90
54	BA	156	A	N1-C6-N6	-6.68	114.59	118.60
54	BA	1320	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	2167	U	O4'-C1'-N1	6.68	113.55	108.20
54	BA	2748	A	C5-C6-N1	6.68	121.04	117.70
24	A3	68	C	N3-C2-O2	-6.68	117.22	121.90
21	AA	1508	A	C5-C6-N1	6.68	121.04	117.70
54	BA	66	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	300	A	C5-C6-N1	6.68	121.04	117.70
54	BA	422	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1169	A	C5-C6-N1	6.68	121.04	117.70
55	BB	59	A	C5-C6-N1	6.68	121.04	117.70
54	BA	398	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1243	C	N3-C2-O2	-6.68	117.22	121.90
11	AL	98	ARG	NE-CZ-NH1	6.68	123.64	120.30
21	AA	336	A	C5-C6-N1	6.68	121.04	117.70
21	AA	460	A	C5-C6-N1	6.68	121.04	117.70
21	AA	750	C	N3-C2-O2	-6.68	117.23	121.90
54	BA	1237	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1641	A	C5-C6-N1	6.68	121.04	117.70
5	AF	44	ARG	NE-CZ-NH1	6.67	123.64	120.30
21	AA	1035	A	N1-C6-N6	-6.67	114.59	118.60
54	BA	936	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1200	C	N3-C2-O2	-6.67	117.23	121.90
55	BB	50	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	1033	U	O4'-C1'-N1	6.67	113.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	92	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	975	A	C5-C6-N1	6.67	121.04	117.70
54	BA	727	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	2094	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	2883	A	C5-C6-N1	6.67	121.04	117.70
21	AA	1098	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	1311	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	1625	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	55	A	C5-C6-N1	6.67	121.03	117.70
21	AA	163	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	1169	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	677	A	C5-C6-N1	6.67	121.03	117.70
54	BA	1505	A	C5-C6-N1	6.67	121.03	117.70
21	AA	1059	C	N3-C2-O2	-6.66	117.24	121.90
40	BR	68	ARG	NE-CZ-NH1	6.66	123.63	120.30
54	BA	374	A	N1-C6-N6	-6.66	114.60	118.60
54	BA	699	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1548	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1578	U	O4'-C1'-N1	6.66	113.53	108.20
21	AA	363	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	610	U	N3-C2-O2	-6.66	117.54	122.20
54	BA	655	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	1604	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	2086	U	O4'-C1'-N1	6.66	113.53	108.20
21	AA	270	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	908	A	N1-C6-N6	-6.66	114.61	118.60
21	AA	1037	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1155	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2670	A	C5-C6-N1	6.66	121.03	117.70
21	AA	1111	A	C4-C5-C6	-6.66	113.67	117.00
21	AA	173	U	C1'-O4'-C4'	-6.66	104.58	109.90
21	AA	270	A	C5-C6-N1	6.66	121.03	117.70
21	AA	382	A	C5-C6-N1	6.66	121.03	117.70
21	AA	1092	A	C5-C6-N1	6.66	121.03	117.70
24	A3	38	A	C5-C6-N1	6.66	121.03	117.70
34	BL	33	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	1155	A	C5-C6-N1	6.65	121.03	117.70
54	BA	1772	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	2388	A	C5-C6-N1	6.65	121.03	117.70
21	AA	488	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	268	C	N3-C2-O2	-6.65	117.24	121.90
54	BA	753	A	C4-C5-C6	-6.65	113.67	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	451	A	C5-C6-N1	6.65	121.02	117.70
21	AA	1213	A	C4-C5-C6	-6.65	113.68	117.00
41	BS	92	ARG	NE-CZ-NH1	6.65	123.62	120.30
54	BA	2077	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	2821	A	C5-C6-N1	6.65	121.02	117.70
54	BA	10	A	C4-C5-C6	-6.65	113.68	117.00
54	BA	378	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	175	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	461	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1070	A	C5-C6-N1	6.64	121.02	117.70
21	AA	1469	C	N1-C2-O2	6.64	122.89	118.90
54	BA	2072	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	393	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1084	A	C5-C6-N1	6.64	121.02	117.70
21	AA	1286	U	O4'-C1'-N1	6.64	113.51	108.20
54	BA	471	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1236	G	O4'-C1'-N9	6.64	113.51	108.20
54	BA	1165	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1580	A	C5-C6-N1	6.64	121.02	117.70
8	AI	32	ARG	NE-CZ-NH1	6.63	123.62	120.30
54	BA	1221	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	890	G	O4'-C1'-N9	6.63	113.51	108.20
54	BA	1602	U	O4'-C1'-N1	6.63	113.51	108.20
10	AK	121	ARG	NE-CZ-NH2	6.63	123.62	120.30
21	AA	547	A	C4-C5-C6	-6.63	113.68	117.00
54	BA	2088	A	C5-C6-N1	6.63	121.02	117.70
21	AA	1378	C	N1-C2-O2	6.63	122.88	118.90
54	BA	2781	A	C5-C6-N1	6.63	121.02	117.70
21	AA	1492	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	104	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	218	A	C5-C6-N1	6.63	121.01	117.70
54	BA	2013	A	C5-C6-N1	6.63	121.01	117.70
21	AA	1188	A	C5-C6-N1	6.63	121.01	117.70
54	BA	1732	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1745	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	2853	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	9	G	C1'-O4'-C4'	-6.62	104.60	109.90
21	AA	347	G	P-O3'-C3'	6.62	127.65	119.70
21	AA	704	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1323	C	N3-C2-O2	-6.62	117.26	121.90
54	BA	143	C	O4'-C1'-N1	6.62	113.50	108.20
54	BA	981	A	C4-C5-C6	-6.62	113.69	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1104	C	N3-C2-O2	-6.62	117.26	121.90
54	BA	2482	A	C4-C5-C6	-6.62	113.69	117.00
11	AL	109	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	519	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	2009	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2073	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	311	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1043	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	715	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	766	A	C1'-O4'-C4'	-6.62	104.61	109.90
21	AA	1319	A	C5-C6-N1	6.62	121.01	117.70
21	AA	77	A	C5-C6-N1	6.62	121.01	117.70
21	AA	1483	A	C5-C6-N1	6.61	121.01	117.70
54	BA	249	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	2095	A	C5-C6-N1	6.61	121.01	117.70
54	BA	2287	A	C5-C6-N1	6.61	121.01	117.70
54	BA	1262	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	1285	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	2055	C	O4'-C1'-N1	6.61	113.49	108.20
54	BA	2340	A	C5-C6-N1	6.61	121.01	117.70
21	AA	912	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	919	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	1081	U	O4'-C1'-N1	6.61	113.49	108.20
54	BA	1518	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1669	A	C5-C6-N1	6.61	121.01	117.70
54	BA	666	A	C5-C6-N1	6.61	121.00	117.70
54	BA	1919	A	C5-C6-N1	6.61	121.00	117.70
21	AA	186	C	N3-C2-O2	-6.61	117.28	121.90
21	AA	513	C	N3-C2-O2	-6.61	117.28	121.90
21	AA	959	A	C4-C5-C6	-6.61	113.70	117.00
21	AA	972	C	N3-C2-O2	-6.61	117.28	121.90
21	AA	990	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	1480	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	2829	A	C5-C6-N1	6.61	121.00	117.70
23	A2	80	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	2463	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	825	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1854	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	312	C	N3-C2-O2	-6.60	117.28	121.90
25	BC	269	ARG	NE-CZ-NH1	6.60	123.60	120.30
54	BA	2175	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	470	C	N3-C2-O2	-6.60	117.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1196	A	C4-C5-C6	-6.60	113.70	117.00
24	A3	14	A	C5-C6-N1	6.60	121.00	117.70
24	A3	24	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	111	A	C5-C6-N1	6.60	121.00	117.70
55	BB	63	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	404	A	C5-C6-N1	6.60	121.00	117.70
21	AA	1332	A	C5-C6-N1	6.59	121.00	117.70
55	BB	115	A	C5-C6-N1	6.59	121.00	117.70
54	BA	2089	C	N3-C2-O2	-6.59	117.28	121.90
54	BA	2662	A	C5-C6-N1	6.59	121.00	117.70
21	AA	900	A	N1-C6-N6	-6.59	114.64	118.60
54	BA	564	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	739	A	N1-C6-N6	-6.59	114.65	118.60
54	BA	2147	A	C5-C6-N1	6.59	121.00	117.70
54	BA	1590	A	C4-C5-C6	-6.59	113.70	117.00
54	BA	1590	A	C5-C6-N1	6.59	121.00	117.70
44	BV	9	ARG	NE-CZ-NH1	6.59	123.59	120.30
54	BA	56	A	C4-C5-C6	-6.59	113.71	117.00
54	BA	1798	U	O4'-C1'-N1	6.59	113.47	108.20
21	AA	1158	C	N1-C2-O2	6.59	122.85	118.90
21	AA	1172	C	N3-C2-O2	-6.59	117.29	121.90
54	BA	1298	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	44	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	708	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	1166	G	N1-C6-O6	-6.58	115.95	119.90
54	BA	1967	C	N3-C2-O2	-6.58	117.29	121.90
21	AA	1368	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1711	A	C5-C6-N1	6.58	120.99	117.70
21	AA	1000	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	661	A	C5-C6-N1	6.58	120.99	117.70
54	BA	885	C	O4'-C1'-N1	6.58	113.46	108.20
54	BA	979	A	C5-C6-N1	6.58	120.99	117.70
54	BA	1284	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1608	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2456	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	2887	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	579	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	330	A	C5-C6-N1	6.58	120.99	117.70
54	BA	689	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	730	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	2039	U	O4'-C1'-N1	6.58	113.46	108.20
21	AA	1113	C	N1-C2-O2	6.58	122.85	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	305	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1575	C	N3-C2-O2	-6.58	117.30	121.90
21	AA	878	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	475	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	62	U	C1'-O4'-C4'	-6.57	104.64	109.90
54	BA	1561	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	640	A	C4-C5-C6	-6.57	113.71	117.00
18	AS	79	TYR	CB-CG-CD2	-6.57	117.06	121.00
21	AA	772	U	C1'-O4'-C4'	-6.57	104.64	109.90
21	AA	1019	A	C5-C6-N1	6.57	120.98	117.70
54	BA	440	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	840	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2050	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2284	A	N1-C6-N6	-6.57	114.66	118.60
21	AA	908	A	C5-C6-N1	6.57	120.98	117.70
21	AA	1428	A	C4-C5-C6	-6.57	113.72	117.00
42	BT	12	ARG	NE-CZ-NH1	6.57	123.58	120.30
54	BA	241	A	C4-C5-C6	-6.57	113.72	117.00
54	BA	1809	A	C5-C6-N1	6.57	120.98	117.70
54	BA	2418	A	C5-C6-N1	6.57	120.98	117.70
21	AA	1042	A	C5-C6-N1	6.57	120.98	117.70
27	BE	79	ARG	NE-CZ-NH1	6.57	123.58	120.30
55	BB	11	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	2856	A	C5-C6-N1	6.56	120.98	117.70
21	AA	816	A	C5-C6-N1	6.56	120.98	117.70
26	BD	124	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	792	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	898	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	947	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	1574	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1785	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	325	A	C5-C6-N1	6.56	120.98	117.70
54	BA	335	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2766	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	418	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	814	A	C5-C6-N1	6.56	120.98	117.70
21	AA	839	C	N3-C2-O2	-6.56	117.31	121.90
34	BL	78	ARG	NE-CZ-NH1	6.56	123.58	120.30
36	BN	22	ARG	NE-CZ-NH1	6.56	123.58	120.30
54	BA	1313	U	O4'-C1'-N1	6.56	113.45	108.20
54	BA	1866	A	C5-C6-N1	6.56	120.98	117.70
21	AA	243	A	C4-C5-C6	-6.56	113.72	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	435	A	C5-C6-N1	6.56	120.98	117.70
21	AA	931	C	P-O3'-C3'	6.56	127.57	119.70
54	BA	541	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	2114	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	139	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2715	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	320	A	C4-C5-C6	-6.55	113.72	117.00
21	AA	910	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1259	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1261	A	N1-C6-N6	-6.55	114.67	118.60
21	AA	1492	A	C5-C6-N1	6.55	120.98	117.70
47	BY	48	ARG	NE-CZ-NH1	6.55	123.58	120.30
54	BA	927	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	1977	A	C5-C6-N1	6.55	120.98	117.70
41	BS	95	ARG	NE-CZ-NH1	6.55	123.58	120.30
54	BA	675	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	722	A	C5-C6-N1	6.55	120.98	117.70
54	BA	888	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1417	C	N3-C2-O2	-6.55	117.31	121.90
21	AA	1080	A	C5-C6-N1	6.55	120.98	117.70
21	AA	1499	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	782	A	C5-C6-N1	6.55	120.98	117.70
54	BA	1363	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1894	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	203	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	227	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	2278	A	C5-C6-N1	6.55	120.97	117.70
21	AA	251	G	P-O3'-C3'	6.55	127.56	119.70
28	BF	70	ARG	NE-CZ-NH1	6.55	123.57	120.30
54	BA	1597	A	C4-C5-C6	-6.55	113.73	117.00
21	AA	794	A	C4-C5-C6	-6.55	113.73	117.00
22	A1	23	A	N1-C6-N6	-6.55	114.67	118.60
54	BA	2416	C	N3-C2-O2	-6.55	117.32	121.90
21	AA	813	U	O4'-C1'-N1	6.54	113.44	108.20
54	BA	1292	G	O4'-C1'-N9	6.54	113.44	108.20
21	AA	1399	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	2332	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	2880	C	N3-C2-O2	-6.54	117.32	121.90
11	AL	8	ARG	NE-CZ-NH1	6.54	123.57	120.30
21	AA	938	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	1402	C	N3-C2-O2	-6.54	117.32	121.90
24	A3	44	A	C4-C5-C6	-6.54	113.73	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	BN	96	ARG	NE-CZ-NH1	6.54	123.57	120.30
54	BA	42	A	C5-C6-N1	6.54	120.97	117.70
54	BA	2591	C	N3-C2-O2	-6.54	117.32	121.90
55	BB	39	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	1299	A	C4-C5-C6	-6.54	113.73	117.00
22	A1	65	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	78	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	883	C	N3-C2-O2	-6.54	117.32	121.90
22	A1	6	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1226	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1678	A	C4-C5-C6	-6.54	113.73	117.00
13	AN	24	ARG	NE-CZ-NH1	6.54	123.57	120.30
54	BA	91	A	O4'-C1'-N9	6.54	113.43	108.20
54	BA	2465	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	290	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	878	A	C5-C6-N1	6.54	120.97	117.70
54	BA	1472	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	2471	A	C5-C6-N1	6.54	120.97	117.70
55	BB	77	U	O4'-C1'-N1	6.54	113.43	108.20
54	BA	1039	A	N1-C6-N6	-6.53	114.68	118.60
54	BA	240	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	941	A	C5-C6-N1	6.53	120.97	117.70
54	BA	1189	A	C5-C6-N1	6.53	120.97	117.70
21	AA	1499	A	C5-C6-N1	6.53	120.96	117.70
54	BA	1788	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	130	A	C5-C6-N1	6.53	120.96	117.70
21	AA	1117	A	C5-C6-N1	6.53	120.96	117.70
54	BA	812	C	N1-C2-O2	6.53	122.82	118.90
54	BA	944	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1414	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	796	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	2030	A	C5-C6-N1	6.53	120.96	117.70
55	BB	70	C	N3-C2-O2	-6.53	117.33	121.90
21	AA	723	U	O3'-P-O5'	-6.52	91.61	104.00
54	BA	726	G	O4'-C1'-N9	6.52	113.42	108.20
21	AA	44	A	C5-C6-N1	6.52	120.96	117.70
54	BA	1015	U	O4'-C1'-N1	6.52	113.42	108.20
21	AA	238	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	321	U	O4'-C1'-N1	6.52	113.41	108.20
54	BA	590	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2333	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	965	C	N3-C2-O2	-6.52	117.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2359	C	N3-C2-O2	-6.52	117.34	121.90
12	AM	91	ARG	NE-CZ-NH1	6.51	123.56	120.30
21	AA	630	A	C5-C6-N1	6.51	120.96	117.70
54	BA	233	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	1126	A	P-O3'-C3'	6.51	127.52	119.70
54	BA	1261	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1269	A	C5-C6-N1	6.51	120.96	117.70
54	BA	2369	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	685	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	83	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	1188	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	37	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	820	A	C5-C6-N1	6.51	120.96	117.70
54	BA	1701	A	C5-C6-N1	6.51	120.96	117.70
54	BA	179	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1635	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1914	C	N1-C2-O2	6.51	122.81	118.90
54	BA	2556	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	1171	A	C4-C5-C6	-6.51	113.75	117.00
22	A1	38	A	C4-C5-C6	-6.51	113.75	117.00
22	A1	69	A	C5-C6-N1	6.51	120.95	117.70
54	BA	415	A	C5-C6-N1	6.51	120.95	117.70
54	BA	429	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	523	C	N3-C2-O2	-6.51	117.34	121.90
24	A3	58	A	C5-C6-N1	6.51	120.95	117.70
54	BA	78	U	O4'-C1'-N1	6.51	113.40	108.20
54	BA	165	A	C4-C5-C6	-6.51	113.75	117.00
54	BA	1605	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1914	C	O4'-C1'-N1	6.51	113.41	108.20
25	BC	42	ARG	NE-CZ-NH1	6.50	123.55	120.30
9	AJ	7	ARG	NE-CZ-NH1	6.50	123.55	120.30
21	AA	1000	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1936	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2899	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	33	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	599	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	831	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1209	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	1271	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	145	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	819	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1096	A	C4-C5-C6	-6.50	113.75	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	217	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	374	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	1340	A	C5-C6-N1	6.50	120.95	117.70
21	AA	1513	A	C5-C6-N1	6.50	120.95	117.70
54	BA	723	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	735	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2452	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2634	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2827	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	320	A	C5-C6-N1	6.50	120.95	117.70
54	BA	541	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1612	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2328	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2441	U	O4'-C1'-N1	6.50	113.40	108.20
54	BA	1362	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1836	C	N3-C2-O2	-6.50	117.35	121.90
1	AB	221	ARG	NE-CZ-NH1	6.49	123.55	120.30
21	AA	306	A	C5-C6-N1	6.49	120.95	117.70
21	AA	856	C	N3-C2-O2	-6.49	117.36	121.90
21	AA	1012	A	N1-C6-N6	-6.49	114.70	118.60
54	BA	2274	A	C5-C6-N1	6.49	120.95	117.70
21	AA	192	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	721	A	C5-C6-N1	6.49	120.94	117.70
54	BA	845	A	C5-C6-N1	6.49	120.95	117.70
54	BA	1925	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2160	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	314	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1708	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1784	A	C4-C5-C6	-6.49	113.75	117.00
54	BA	2377	A	C5-C6-N1	6.49	120.94	117.70
56	B5	53	ARG	NE-CZ-NH1	6.49	123.54	120.30
21	AA	1324	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	167	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	2753	A	C5-C6-N1	6.49	120.94	117.70
21	AA	511	C	N1-C2-O2	6.49	122.79	118.90
21	AA	1110	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	544	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2676	C	N3-C2-O2	-6.49	117.36	121.90
53	B4	12	ARG	NE-CZ-NH1	6.48	123.54	120.30
54	BA	872	U	O4'-C1'-N1	6.48	113.39	108.20
54	BA	2710	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	1032	G	O4'-C1'-N9	6.48	113.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1288	G	O4'-C1'-N9	6.48	113.39	108.20
54	BA	1771	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	1809	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	1251	A	C4-C5-C6	-6.48	113.76	117.00
24	A3	52	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	795	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	2639	A	N1-C6-N6	-6.48	114.71	118.60
54	BA	423	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	666	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1058	U	O4'-C1'-N1	6.48	113.38	108.20
55	BB	91	C	N3-C2-O2	-6.48	117.36	121.90
21	AA	456	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1044	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1654	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1947	C	N3-C2-O2	-6.48	117.36	121.90
54	BA	2179	C	O4'-C1'-N1	6.48	113.38	108.20
21	AA	1170	A	N1-C6-N6	-6.48	114.71	118.60
54	BA	2776	A	C5-C6-N1	6.48	120.94	117.70
21	AA	784	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	420	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2215	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2761	A	C4-C5-C6	-6.47	113.76	117.00
21	AA	1102	A	C5-C6-N1	6.47	120.94	117.70
24	A3	70	C	N3-C2-O2	-6.47	117.37	121.90
36	BN	69	ARG	NE-CZ-NH1	6.47	123.54	120.30
54	BA	838	C	N1-C2-O2	6.47	122.78	118.90
54	BA	2082	A	C4-C5-C6	-6.47	113.76	117.00
55	BB	65	U	O4'-C1'-N1	6.47	113.38	108.20
21	AA	502	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1556	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2385	C	N3-C2-O2	-6.47	117.37	121.90
8	AI	121	ARG	NE-CZ-NH2	-6.47	117.07	120.30
21	AA	1434	A	C5-C6-N1	6.47	120.93	117.70
54	BA	1606	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1086	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1135	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2094	A	C5-C6-N1	6.47	120.93	117.70
54	BA	2165	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2837	A	C5-C6-N1	6.47	120.93	117.70
21	AA	18	C	N3-C2-O2	-6.46	117.37	121.90
21	AA	1248	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1357	A	C4-C5-C6	-6.46	113.77	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	772	C	N3-C2-O2	-6.46	117.37	121.90
21	AA	1500	A	C5-C6-N1	6.46	120.93	117.70
18	AS	77	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	917	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1228	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	560	A	N1-C6-N6	-6.46	114.72	118.60
54	BA	192	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1532	A	C4-C5-C6	-6.46	113.77	117.00
7	AH	127	TYR	CB-CG-CD2	-6.46	117.13	121.00
21	AA	95	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	673	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	795	C	N3-C2-O2	-6.46	117.38	121.90
28	BF	124	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	341	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1189	A	N1-C6-N6	-6.46	114.73	118.60
54	BA	432	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	976	G	N3-C4-C5	-6.45	125.37	128.60
54	BA	1230	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	2512	C	N3-C2-O2	-6.45	117.38	121.90
36	BN	103	ARG	NE-CZ-NH1	6.45	123.53	120.30
21	AA	1384	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	401	A	C5-C6-N1	6.45	120.92	117.70
54	BA	1889	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	2347	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	2418	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	2541	A	C4-C5-C6	-6.45	113.77	117.00
26	BD	184	ARG	NE-CZ-NH1	6.45	123.53	120.30
54	BA	1477	A	C5-C6-N1	6.45	120.92	117.70
7	AH	83	ARG	NE-CZ-NH2	-6.45	117.08	120.30
21	AA	19	A	C5-C6-N1	6.45	120.92	117.70
54	BA	1652	A	C4-C5-C6	-6.45	113.78	117.00
3	AD	12	ARG	NE-CZ-NH1	6.45	123.52	120.30
54	BA	61	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	353	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	1088	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1117	C	N3-C2-O2	-6.45	117.39	121.90
21	AA	574	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1103	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	1229	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2386	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	52	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	119	A	C4-C5-C6	-6.44	113.78	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1409	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	477	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1056	G	N3-C4-C5	-6.44	125.38	128.60
54	BA	2092	U	N3-C2-O2	-6.44	117.69	122.20
54	BA	2403	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	44	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	623	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	161	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1119	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	1466	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	1502	A	O4'-C1'-N9	6.44	113.35	108.20
54	BA	1595	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2119	A	C5-C6-N1	6.44	120.92	117.70
21	AA	546	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1477	A	N1-C6-N6	-6.44	114.74	118.60
54	BA	1167	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1420	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	2420	C	N3-C2-O2	-6.43	117.40	121.90
55	BB	17	C	N3-C2-O2	-6.43	117.39	121.90
21	AA	535	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	1064	C	N3-C2-O2	-6.43	117.40	121.90
41	BS	88	ARG	NE-CZ-NH1	6.43	123.52	120.30
54	BA	316	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2547	A	C4-C5-C6	-6.43	113.78	117.00
55	BB	5	U	O4'-C1'-N1	6.43	113.34	108.20
11	AL	53	ARG	NE-CZ-NH1	6.43	123.51	120.30
21	AA	253	A	C5-C6-N1	6.43	120.92	117.70
54	BA	670	A	C5-C6-N1	6.43	120.91	117.70
54	BA	1454	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	321	A	C5-C6-N1	6.43	120.91	117.70
21	AA	629	A	C5-C6-N1	6.43	120.91	117.70
54	BA	996	A	C4-C5-C6	-6.43	113.79	117.00
55	BB	62	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	441	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	1282	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	819	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	1278	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	2298	A	C5-C6-N1	6.43	120.91	117.70
54	BA	2411	A	C4-C5-C6	-6.43	113.79	117.00
35	BM	81	ARG	NE-CZ-NH1	6.42	123.51	120.30
54	BA	996	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2200	C	N3-C2-O2	-6.42	117.40	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2795	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	8	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1453	G	N3-C4-C5	-6.42	125.39	128.60
54	BA	968	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	1502	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1694	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	2001	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	482	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1387	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2198	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1507	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	219	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1722	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1814	G	C5'-C4'-O4'	6.42	116.80	109.10
54	BA	2765	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2268	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	825	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1609	A	C5-C6-N1	6.42	120.91	117.70
21	AA	1287	A	C4-C5-C6	-6.41	113.79	117.00
21	AA	1333	A	C4-C5-C6	-6.41	113.79	117.00
21	AA	1344	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	1563	U	O4'-C1'-N1	6.41	113.33	108.20
21	AA	969	A	C4-C5-C6	-6.41	113.79	117.00
25	BC	213	ARG	NE-CZ-NH1	6.41	123.51	120.30
54	BA	925	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	1793	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	315	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	1876	A	N1-C6-N6	-6.41	114.75	118.60
54	BA	2620	C	N3-C2-O2	-6.41	117.41	121.90
21	AA	900	A	C5-C6-N1	6.41	120.91	117.70
44	BV	18	ARG	NE-CZ-NH1	6.41	123.50	120.30
53	B4	36	ARG	NE-CZ-NH1	6.41	123.50	120.30
54	BA	190	A	C5-C6-N1	6.41	120.90	117.70
54	BA	354	A	C5-C6-N1	6.41	120.90	117.70
54	BA	1070	A	C3'-C2'-C1'	6.41	106.62	101.50
21	AA	522	C	N3-C2-O2	-6.41	117.42	121.90
21	AA	614	C	N3-C2-O2	-6.41	117.42	121.90
21	AA	1201	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	1349	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	903	C	N3-C2-O2	-6.41	117.42	121.90
55	BB	118	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	2015	A	C5-C6-N1	6.40	120.90	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2161	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1143	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1387	A	O4'-C1'-N9	6.40	113.32	108.20
54	BA	1905	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	2291	U	O4'-C1'-N1	6.40	113.32	108.20
54	BA	2572	A	O4'-C1'-N9	6.40	113.32	108.20
54	BA	616	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1050	A	N1-C6-N6	-6.40	114.76	118.60
54	BA	2003	A	C4-C5-C6	-6.40	113.80	117.00
55	BB	57	A	N1-C6-N6	-6.40	114.76	118.60
21	AA	1163	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	717	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	1057	A	C5-C6-N1	6.40	120.90	117.70
21	AA	726	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	909	A	C5-C6-N1	6.40	120.90	117.70
54	BA	250	G	N3-C2-N2	-6.40	115.42	119.90
54	BA	1664	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	67	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	978	A	C5-C6-N1	6.39	120.90	117.70
54	BA	1345	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	1499	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	238	A	C5-C6-N1	6.39	120.90	117.70
21	AA	490	C	N3-C2-O2	-6.39	117.42	121.90
54	BA	909	A	C5-C6-N1	6.39	120.90	117.70
54	BA	1932	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	2151	U	O4'-C1'-N1	6.39	113.31	108.20
21	AA	1412	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	1717	A	C4-C5-C6	-6.39	113.81	117.00
56	B5	71	ARG	NE-CZ-NH1	6.39	123.50	120.30
21	AA	441	A	C5-C6-N1	6.39	120.89	117.70
21	AA	499	A	C4-C5-C6	-6.39	113.81	117.00
21	AA	554	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1735	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1938	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	2883	A	N1-C6-N6	-6.39	114.77	118.60
21	AA	303	A	C5-C6-N1	6.39	120.89	117.70
54	BA	146	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	531	C	N3-C2-O2	-6.39	117.43	121.90
21	AA	139	A	C4-C5-C6	-6.39	113.81	117.00
21	AA	1146	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	1434	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	624	C	N3-C2-O2	-6.38	117.43	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1085	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2542	A	O4'-C1'-N9	6.38	113.31	108.20
54	BA	1498	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	215	C	N3-C2-O2	-6.38	117.43	121.90
21	AA	680	C	N3-C2-O2	-6.38	117.43	121.90
54	BA	639	U	O4'-C1'-N1	6.38	113.31	108.20
54	BA	1112	G	N1-C6-O6	-6.38	116.07	119.90
54	BA	1569	A	C5-C6-N1	6.38	120.89	117.70
54	BA	2091	C	N1-C2-O2	6.38	122.73	118.90
54	BA	2101	A	C5-C6-N1	6.38	120.89	117.70
21	AA	919	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	922	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	1832	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	794	A	N1-C6-N6	-6.38	114.77	118.60
54	BA	959	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1076	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	1413	A	C4-C5-C6	-6.38	113.81	117.00
55	BB	49	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	694	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2443	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	2654	A	C5-C6-N1	6.38	120.89	117.70
22	A1	66	A	C5-C6-N1	6.37	120.89	117.70
41	BS	8	ARG	NE-CZ-NH1	6.37	123.49	120.30
43	BU	85	ARG	NE-CZ-NH2	-6.37	117.11	120.30
55	BB	29	A	C5-C6-N1	6.37	120.89	117.70
54	BA	144	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	348	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	449	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	2037	A	C5-C6-N1	6.37	120.89	117.70
54	BA	2426	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	408	A	C5-C6-N1	6.37	120.89	117.70
21	AA	1063	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1107	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1357	C	N3-C2-O2	-6.37	117.44	121.90
54	BA	1744	A	C5-C6-N1	6.37	120.89	117.70
54	BA	1824	G	O4'-C1'-N9	6.37	113.30	108.20
54	BA	2042	A	C4-C5-C6	-6.37	113.81	117.00
24	A3	17	C	N1-C2-O2	6.37	122.72	118.90
54	BA	486	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	1150	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	362	A	C4-C5-C6	-6.37	113.82	117.00
55	BB	45	A	N1-C6-N6	-6.37	114.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	5	A	C5-C6-N1	6.36	120.88	117.70
54	BA	492	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	742	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1351	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	975	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1178	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	716	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	724	G	N1-C6-O6	-6.36	116.08	119.90
21	AA	816	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	1451	C	O4'-C1'-N1	6.36	113.29	108.20
54	BA	1646	C	N1-C2-O2	6.36	122.72	118.90
54	BA	1885	A	C5-C6-N1	6.36	120.88	117.70
54	BA	2070	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	1045	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	97	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	228	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1748	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	131	A	C4-C5-C6	-6.36	113.82	117.00
24	A3	44	A	C5-C6-N1	6.36	120.88	117.70
54	BA	272	A	N1-C6-N6	-6.36	114.79	118.60
54	BA	615	U	N3-C2-O2	-6.36	117.75	122.20
54	BA	1413	A	C5-C6-N1	6.36	120.88	117.70
21	AA	747	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	807	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	1071	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	1285	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	428	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	911	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	933	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	2666	C	N1-C2-O2	6.36	122.71	118.90
55	BB	110	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	452	A	C5-C6-N1	6.35	120.88	117.70
51	B2	19	ARG	NE-CZ-NH1	6.35	123.48	120.30
54	BA	490	C	N1-C2-O2	6.35	122.71	118.90
55	BB	93	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	672	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	2518	A	C4-C5-C6	-6.35	113.82	117.00
55	BB	41	G	O4'-C1'-N9	6.35	113.28	108.20
21	AA	865	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	71	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	508	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	2143	C	N3-C2-O2	-6.35	117.45	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2281	A	C4-C5-C6	-6.35	113.83	117.00
55	BB	88	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	519	C	O4'-C1'-N1	6.35	113.28	108.20
21	AA	649	A	C4-C5-C6	-6.35	113.83	117.00
24	A3	57	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	1095	A	C4-C5-C6	-6.35	113.83	117.00
54	BA	1153	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	236	A	C5-C6-N1	6.35	120.87	117.70
22	A1	71	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	298	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1577	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	176	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	1152	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	1419	G	N1-C6-O6	-6.34	116.10	119.90
34	BL	41	ARG	NE-CZ-NH1	6.34	123.47	120.30
39	BQ	49	ARG	NE-CZ-NH1	6.34	123.47	120.30
54	BA	2516	A	C5-C6-N1	6.34	120.87	117.70
21	AA	1176	A	C4-C5-C6	-6.34	113.83	117.00
22	A1	35	A	C4-C5-C6	-6.34	113.83	117.00
27	BE	102	ARG	NE-CZ-NH1	6.34	123.47	120.30
54	BA	960	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1475	G	O4'-C1'-N9	6.34	113.27	108.20
21	AA	1531	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	1129	C	N3-C2-O2	-6.34	117.46	121.90
21	AA	1306	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	1348	C	N3-C2-O2	-6.34	117.47	121.90
54	BA	1461	C	N1-C2-O2	6.34	122.70	118.90
54	BA	1997	C	N3-C2-O2	-6.34	117.47	121.90
54	BA	2264	C	N3-C2-O2	-6.34	117.47	121.90
21	AA	767	A	C4-C5-C6	-6.33	113.83	117.00
22	A1	17	U	O4'-C1'-N1	6.33	113.27	108.20
54	BA	2830	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1483	A	C4-C5-C6	-6.33	113.83	117.00
22	A1	23	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	540	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	1451	C	N1-C2-O2	6.33	122.70	118.90
54	BA	2117	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	38	A	C5-C6-N1	6.33	120.87	117.70
54	BA	1278	C	O4'-C1'-N1	6.33	113.26	108.20
21	AA	949	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	2670	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	199	A	C4-C5-C6	-6.33	113.84	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1705	A	N1-C6-N6	-6.33	114.80	118.60
54	BA	2372	U	O4'-C1'-N1	6.33	113.26	108.20
21	AA	1005	A	N1-C6-N6	-6.33	114.80	118.60
21	AA	26	A	C5-C6-N1	6.33	120.86	117.70
21	AA	1016	A	C4-C5-C6	-6.33	113.84	117.00
24	A3	77	A	O4'-C1'-N9	6.33	113.26	108.20
54	BA	52	A	C5-C6-N1	6.33	120.86	117.70
54	BA	1746	A	C5-C6-N1	6.33	120.86	117.70
54	BA	1942	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	660	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	1509	A	O4'-C1'-N9	6.32	113.26	108.20
54	BA	2153	C	N3-C2-O2	-6.32	117.47	121.90
54	BA	2764	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	470	A	C5-C6-N1	6.32	120.86	117.70
54	BA	1121	C	N3-C2-O2	-6.32	117.47	121.90
21	AA	502	A	C5-C6-N1	6.32	120.86	117.70
21	AA	1423	G	O4'-C1'-N9	6.32	113.26	108.20
21	AA	1480	A	C4-C5-C6	-6.32	113.84	117.00
44	BV	21	ARG	NE-CZ-NH2	6.32	123.46	120.30
54	BA	412	A	N1-C6-N6	-6.32	114.81	118.60
54	BA	1028	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	1268	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2540	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	679	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2619	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	1264	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	1027	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	1302	C	C1'-O4'-C4'	-6.32	104.85	109.90
22	A1	69	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	627	A	C4-C5-C6	-6.32	113.84	117.00
21	AA	1328	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	121	U	O4'-C1'-N1	6.31	113.25	108.20
21	AA	1204	A	C5-C6-N1	6.31	120.86	117.70
28	BF	114	ARG	NE-CZ-NH1	6.31	123.46	120.30
54	BA	764	A	C5-C6-N1	6.31	120.86	117.70
54	BA	788	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1505	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	2097	A	C4-C5-C6	-6.31	113.84	117.00
27	BE	69	ARG	NE-CZ-NH1	6.31	123.45	120.30
54	BA	2317	A	C5-C6-N1	6.31	120.86	117.70
21	AA	478	A	N1-C6-N6	-6.31	114.81	118.60
21	AA	1288	A	C5-C6-N1	6.31	120.85	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	11	A	N1-C6-N6	-6.31	114.81	118.60
54	BA	309	A	C5-C6-N1	6.31	120.86	117.70
54	BA	1285	A	C5-C6-N1	6.31	120.86	117.70
54	BA	1318	U	O4'-C1'-N1	6.31	113.25	108.20
54	BA	2052	A	C5-C6-N1	6.31	120.86	117.70
54	BA	2579	C	N3-C2-O2	-6.31	117.48	121.90
41	BS	25	ARG	NE-CZ-NH1	6.31	123.45	120.30
54	BA	1328	A	C4-C5-C6	-6.31	113.85	117.00
54	BA	2183	A	C5-C6-N1	6.31	120.85	117.70
54	BA	2712	C	N1-C2-O2	6.31	122.68	118.90
21	AA	1314	C	N3-C2-O2	-6.31	117.49	121.90
54	BA	41	C	N3-C2-O2	-6.31	117.49	121.90
21	AA	381	C	N1-C2-O2	6.30	122.68	118.90
54	BA	1495	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1641	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2258	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2466	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2855	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	53	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	554	U	O4'-C1'-N1	6.30	113.24	108.20
54	BA	1322	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1630	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1901	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	243	A	C5-C6-N1	6.30	120.85	117.70
21	AA	749	A	C5-C6-N1	6.30	120.85	117.70
22	A1	26	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	309	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1650	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1877	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	321	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	699	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	849	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	2335	A	C5-C6-N1	6.29	120.85	117.70
21	AA	1082	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	1413	A	C5-C6-N1	6.29	120.85	117.70
21	AA	572	A	N1-C6-N6	-6.29	114.83	118.60
21	AA	978	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	1081	A	C4-C5-C6	-6.29	113.85	117.00
38	BP	38	ARG	NE-CZ-NH1	6.29	123.45	120.30
54	BA	72	U	O4'-C1'-N1	6.29	113.23	108.20
54	BA	1265	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	2247	A	C5-C6-N1	6.29	120.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2835	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	866	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	878	A	O4'-C1'-N9	6.29	113.23	108.20
54	BA	1632	A	C4-C5-C6	-6.29	113.86	117.00
19	AT	73	ARG	NE-CZ-NH1	6.29	123.44	120.30
21	AA	130	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	935	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	958	A	C4-C5-C6	-6.29	113.86	117.00
52	B3	44	ARG	NE-CZ-NH2	6.29	123.44	120.30
54	BA	354	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	643	A	O4'-C1'-N9	6.29	113.23	108.20
54	BA	1313	U	N3-C2-O2	-6.29	117.80	122.20
54	BA	1704	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	2598	A	C5-C6-N1	6.29	120.84	117.70
21	AA	1340	A	C4-C5-C6	-6.29	113.86	117.00
24	A3	73	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	229	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	886	A	C4-C5-C6	-6.29	113.86	117.00
7	AH	79	ARG	NE-CZ-NH1	6.29	123.44	120.30
21	AA	697	U	O4'-C1'-N1	6.29	113.23	108.20
21	AA	1413	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	57	C	O4'-C1'-N1	6.29	113.23	108.20
54	BA	152	A	C5-C6-N1	6.29	120.84	117.70
54	BA	910	A	C4-C5-C6	-6.29	113.86	117.00
54	BA	1270	C	N3-C2-O2	-6.29	117.50	121.90
21	AA	936	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	606	U	O4'-C1'-N1	6.28	113.23	108.20
54	BA	744	U	O4'-C1'-N1	6.28	113.23	108.20
54	BA	1304	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1526	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2386	A	C5-C6-N1	6.28	120.84	117.70
21	AA	499	A	C5-C6-N1	6.28	120.84	117.70
54	BA	453	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1230	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1416	G	O4'-C1'-N9	6.28	113.22	108.20
54	BA	2225	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2745	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2781	A	N1-C6-N6	-6.28	114.83	118.60
21	AA	1293	C	N3-C2-O2	-6.28	117.50	121.90
22	A1	25	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1639	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2432	A	C5-C6-N1	6.28	120.84	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2773	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	89	A	C5-C6-N1	6.28	120.84	117.70
54	BA	256	A	C5-C6-N1	6.28	120.84	117.70
54	BA	584	C	O4'-C1'-N1	6.28	113.22	108.20
54	BA	719	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	932	C	N3-C2-O2	-6.28	117.51	121.90
21	AA	1288	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	1325	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	1437	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1999	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	2080	A	C5-C6-N1	6.28	120.84	117.70
54	BA	2084	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	2424	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	2589	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	300	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	1243	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	125	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	866	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1373	A	C5-C6-N1	6.28	120.84	117.70
54	BA	1770	G	O4'-C1'-N9	6.28	113.22	108.20
54	BA	2052	A	N1-C6-N6	-6.28	114.83	118.60
54	BA	1233	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2559	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	303	A	C4-C5-C6	-6.27	113.86	117.00
21	AA	1246	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	528	A	C5-C6-N1	6.27	120.84	117.70
54	BA	2682	A	C4-C5-C6	-6.27	113.86	117.00
54	BA	2716	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	987	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1291	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	848	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1151	A	C5-C6-N1	6.27	120.83	117.70
21	AA	1237	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1449	C	N3-C2-O2	-6.27	117.51	121.90
34	BL	18	ARG	NE-CZ-NH1	6.27	123.43	120.30
21	AA	54	C	C5'-C4'-C3'	-6.27	105.97	116.00
21	AA	466	A	O4'-C1'-N9	6.27	113.22	108.20
21	AA	501	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	534	U	N3-C2-O2	-6.27	117.81	122.20
21	AA	1171	A	C5-C6-N1	6.27	120.83	117.70
35	BM	38	ARG	NE-CZ-NH1	6.27	123.43	120.30
54	BA	937	C	N3-C2-O2	-6.27	117.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1057	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	1399	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2422	C	N1-C2-O2	6.27	122.66	118.90
21	AA	34	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2780	G	O4'-C1'-N9	6.27	113.21	108.20
21	AA	823	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	941	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1244	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	1533	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1803	A	C5-C6-N1	6.26	120.83	117.70
54	BA	1934	C	O4'-C1'-N1	6.26	113.21	108.20
54	BA	1952	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2734	A	C5-C6-N1	6.26	120.83	117.70
54	BA	2874	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	90	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	95	A	N1-C6-N6	-6.26	114.84	118.60
54	BA	2314	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2539	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	643	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	1229	A	C5-C6-N1	6.26	120.83	117.70
21	AA	1456	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	63	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	73	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2051	A	N1-C6-N6	-6.26	114.84	118.60
54	BA	586	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	796	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1868	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	58	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2564	A	C4-C5-C6	-6.25	113.87	117.00
55	BB	28	C	N3-C2-O2	-6.25	117.52	121.90
24	A3	3	C	N3-C2-O2	-6.25	117.52	121.90
54	BA	345	A	C4-C5-C6	-6.25	113.87	117.00
21	AA	383	A	C4-C5-C6	-6.25	113.87	117.00
21	AA	711	G	N1-C6-O6	-6.25	116.15	119.90
21	AA	1225	A	C4-C5-C6	-6.25	113.87	117.00
21	AA	1437	A	C4-C5-C6	-6.25	113.87	117.00
21	AA	1128	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	14	A	N1-C6-N6	-6.25	114.85	118.60
54	BA	479	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2071	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	1208	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	1418	A	C5-C6-N1	6.25	120.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	704	A	C5-C6-N1	6.25	120.82	117.70
22	A1	60	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	1987	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2486	C	N3-C2-O2	-6.25	117.53	121.90
21	AA	930	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	999	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1607	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2636	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1879	C	N3-C2-O2	-6.24	117.53	121.90
43	BU	6	ARG	NE-CZ-NH1	6.24	123.42	120.30
54	BA	1927	A	C5-C6-N1	6.24	120.82	117.70
54	BA	2274	A	C4-C5-C6	-6.24	113.88	117.00
55	BB	71	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	1019	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	208	C	N3-C2-O2	-6.24	117.53	121.90
56	B5	7	ARG	NE-CZ-NH1	6.24	123.42	120.30
21	AA	699	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	722	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	899	A	C4-C5-C6	-6.24	113.88	117.00
55	BB	87	U	N3-C2-O2	-6.24	117.83	122.20
3	AD	46	ARG	NE-CZ-NH1	6.24	123.42	120.30
21	AA	344	A	C4-C5-C6	-6.24	113.88	117.00
25	BC	188	ARG	NE-CZ-NH2	-6.24	117.18	120.30
54	BA	38	A	C4-C5-C6	-6.24	113.88	117.00
21	AA	777	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	1377	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	1741	C	N3-C2-O2	-6.23	117.54	121.90
13	AN	59	ARG	NE-CZ-NH1	6.23	123.42	120.30
21	AA	728	A	C6-C5-N7	6.23	136.66	132.30
21	AA	1239	A	C5-C6-N1	6.23	120.82	117.70
54	BA	94	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	1049	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1142	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	1658	C	N3-C2-O2	-6.23	117.54	121.90
24	A3	75	C	N1-C2-O2	6.23	122.64	118.90
34	BL	47	ARG	NE-CZ-NH1	6.23	123.42	120.30
54	BA	343	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	610	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	1386	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	2742	G	O4'-C1'-N9	6.23	113.18	108.20
9	AJ	68	ARG	NE-CZ-NH1	6.23	123.42	120.30
21	AA	151	A	C4-C5-C6	-6.23	113.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	374	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	642	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	751	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	1260	A	C4-C5-C6	-6.23	113.89	117.00
21	AA	1336	C	O4'-C1'-N1	6.23	113.18	108.20
21	AA	349	A	C5-C6-N1	6.22	120.81	117.70
21	AA	1179	A	C5-C6-N1	6.22	120.81	117.70
21	AA	1462	C	N3-C2-O2	-6.22	117.54	121.90
21	AA	1476	A	C5-C6-N1	6.22	120.81	117.70
54	BA	322	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	107	G	N1-C6-O6	-6.22	116.17	119.90
21	AA	182	A	C4-C5-C6	-6.22	113.89	117.00
43	BU	85	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	351	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	557	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	644	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	821	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	118	A	C4-C5-C6	-6.22	113.89	117.00
2	AC	87	ARG	NE-CZ-NH1	6.22	123.41	120.30
21	AA	1502	A	C1'-O4'-C4'	-6.22	104.92	109.90
24	A3	39	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	281	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	426	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1254	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	2820	A	C4-C5-C6	-6.22	113.89	117.00
55	BB	89	U	N3-C2-O2	-6.22	117.85	122.20
54	BA	480	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	779	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	1016	A	C5-C6-N1	6.22	120.81	117.70
54	BA	444	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1453	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1689	A	C5-C6-N1	6.22	120.81	117.70
21	AA	171	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1257	C	N3-C2-O2	-6.21	117.55	121.90
8	AI	10	ARG	NE-CZ-NH1	6.21	123.41	120.30
21	AA	177	G	N3-C4-C5	-6.21	125.49	128.60
54	BA	2451	A	C5-C6-N1	6.21	120.81	117.70
55	BB	37	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	248	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	584	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1839	G	N1-C6-O6	-6.21	116.17	119.90
54	BA	1129	A	N1-C6-N6	-6.21	114.88	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1367	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	282	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	501	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1958	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	414	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1234	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1376	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1504	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2547	A	O4'-C1'-N9	6.20	113.16	108.20
9	AJ	16	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	AA	251	G	N3-C4-C5	-6.20	125.50	128.60
21	AA	970	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2433	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1324	A	C5-C6-N1	6.20	120.80	117.70
54	BA	414	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2115	G	O4'-C1'-N9	6.20	113.16	108.20
54	BA	2706	A	C4-C5-C6	-6.20	113.90	117.00
1	AB	34	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	AA	109	A	P-O3'-C3'	6.20	127.14	119.70
40	BR	84	ARG	NE-CZ-NH1	6.20	123.40	120.30
54	BA	111	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	182	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1053	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1762	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1120	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1275	A	C5-C6-N1	6.20	120.80	117.70
54	BA	2711	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	213	G	N1-C6-O6	-6.20	116.18	119.90
21	AA	880	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1092	C	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1493	C	N1-C2-O2	6.20	122.62	118.90
54	BA	2285	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1204	A	C4-C5-C6	-6.19	113.90	117.00
3	AD	62	ARG	NE-CZ-NH1	6.19	123.40	120.30
54	BA	310	A	C5-C6-N1	6.19	120.80	117.70
54	BA	344	A	C4-C5-C6	-6.19	113.90	117.00
21	AA	1284	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	436	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1044	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1592	C	N3-C2-O2	-6.19	117.57	121.90
55	BB	3	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	2247	A	C4-C5-C6	-6.19	113.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	AK	126	ARG	NE-CZ-NH1	6.19	123.39	120.30
21	AA	379	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	576	C	N3-C2-O2	-6.19	117.57	121.90
25	BC	257	ARG	NE-CZ-NH1	6.19	123.39	120.30
54	BA	515	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	1509	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	2254	C	N3-C2-O2	-6.19	117.57	121.90
24	A3	42	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	96	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	216	A	N1-C6-N6	-6.19	114.89	118.60
54	BA	897	C	N3-C2-O2	-6.19	117.57	121.90
22	A1	68	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	731	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	921	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1403	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1573	G	N1-C6-O6	-6.18	116.19	119.90
54	BA	1833	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	1069	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1644	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1706	C	N3-C2-O2	-6.18	117.57	121.90
55	BB	104	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	469	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	744	C	N3-C2-O2	-6.18	117.58	121.90
42	BT	6	ARG	NE-CZ-NH1	6.18	123.39	120.30
54	BA	1969	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2000	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	101	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	560	A	C4-C5-C6	-6.18	113.91	117.00
21	AA	984	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	403	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	705	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1308	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	2704	C	N3-C2-O2	-6.18	117.58	121.90
54	BA	99	U	N3-C2-O2	-6.17	117.88	122.20
54	BA	487	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	83	A	C5-C6-N1	6.17	120.79	117.70
54	BA	2332	C	O4'-C1'-N1	6.17	113.14	108.20
54	BA	2600	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	162	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	419	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	845	A	C4-C5-C6	-6.17	113.91	117.00
21	AA	1092	A	C4-C5-C6	-6.17	113.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1887	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	1219	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	2604	U	O4'-C1'-N1	6.17	113.14	108.20
21	AA	60	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	440	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	770	C	N3-C2-O2	-6.17	117.58	121.90
22	A1	14	A	N1-C6-N6	-6.17	114.90	118.60
35	BM	66	ARG	NE-CZ-NH1	6.17	123.39	120.30
54	BA	1100	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1531	C	O4'-C1'-N1	6.17	113.14	108.20
54	BA	1879	C	O4'-C1'-N1	6.17	113.14	108.20
54	BA	2476	A	N1-C6-N6	-6.17	114.90	118.60
25	BC	12	ARG	NE-CZ-NH1	6.17	123.38	120.30
54	BA	42	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	1320	C	O4'-C1'-N1	6.17	113.13	108.20
54	BA	2045	C	N1-C2-O2	6.17	122.60	118.90
54	BA	2378	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	166	U	O4'-C1'-N1	6.17	113.13	108.20
54	BA	439	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	613	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	443	A	N1-C6-N6	-6.16	114.90	118.60
54	BA	802	A	C4-C5-C6	-6.16	113.92	117.00
55	BB	60	C	N3-C2-O2	-6.16	117.59	121.90
20	AU	44	ARG	NE-CZ-NH1	6.16	123.38	120.30
21	AA	653	U	O4'-C1'-N1	6.16	113.13	108.20
54	BA	2727	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	2736	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	235	C	N3-C2-O2	-6.16	117.59	121.90
35	BM	59	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	2616	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1129	A	C5-C6-N1	6.16	120.78	117.70
24	A3	67	C	N3-C2-O2	-6.16	117.59	121.90
28	BF	79	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	786	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	1566	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	1004	A	C4-C5-C6	-6.15	113.92	117.00
39	BQ	10	ARG	NE-CZ-NH1	6.15	123.38	120.30
21	AA	629	A	C4-C5-C6	-6.15	113.92	117.00
21	AA	1524	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	244	A	C5-C6-N1	6.15	120.78	117.70
54	BA	538	A	N1-C6-N6	-6.15	114.91	118.60
54	BA	1648	U	O4'-C1'-N1	6.15	113.12	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2241	A	C5-C6-N1	6.15	120.78	117.70
54	BA	2741	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	761	A	C4-C5-C6	-6.15	113.92	117.00
55	BB	96	G	O4'-C1'-N9	6.15	113.12	108.20
21	AA	1374	A	C5-C6-N1	6.15	120.77	117.70
54	BA	337	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1208	C	N3-C2-O2	-6.15	117.60	121.90
54	BA	1272	A	C4-C5-C6	-6.15	113.93	117.00
21	AA	164	G	N1-C6-O6	-6.15	116.21	119.90
21	AA	837	U	O4'-C1'-N1	6.15	113.12	108.20
54	BA	693	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	1260	A	C5-C6-N1	6.15	120.77	117.70
37	BO	111	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	31	C	N1-C2-O2	6.14	122.59	118.90
54	BA	2528	U	O4'-C1'-N1	6.14	113.12	108.20
10	AK	76	TYR	CB-CG-CD2	-6.14	117.31	121.00
21	AA	173	U	O4'-C1'-N1	6.14	113.11	108.20
21	AA	189	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	196	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	393	A	C5-C6-N1	6.14	120.77	117.70
21	AA	523	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1448	C	N3-C2-O2	-6.14	117.60	121.90
24	A3	63	C	N3-C2-O2	-6.14	117.60	121.90
39	BQ	5	ARG	NE-CZ-NH2	-6.14	117.23	120.30
54	BA	382	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2342	C	N1-C2-O2	6.14	122.58	118.90
54	BA	844	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	867	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2432	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	1011	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	257	C	O4'-C1'-N1	6.14	113.11	108.20
54	BA	1236	G	C3'-C2'-C1'	6.14	106.41	101.50
54	BA	1881	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2088	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2870	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1335	C	O4'-C1'-N1	6.14	113.11	108.20
54	BA	2469	A	C5-C6-N1	6.14	120.77	117.70
6	AG	142	ARG	NE-CZ-NH1	6.14	123.37	120.30
54	BA	346	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	143	A	C4-C5-C6	-6.13	113.93	117.00
21	AA	873	A	C4-C5-C6	-6.13	113.93	117.00
21	AA	1327	C	N3-C2-O2	-6.13	117.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BC	166	ARG	NE-CZ-NH1	6.13	123.37	120.30
54	BA	22	C	O4'-C1'-N1	6.13	113.11	108.20
54	BA	106	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	789	A	O4'-C1'-N9	6.13	113.11	108.20
54	BA	1844	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1900	A	C4-C5-C6	-6.13	113.93	117.00
21	AA	811	C	C3'-C2'-C1'	6.13	106.41	101.50
21	AA	160	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	855	G	N1-C6-O6	-6.13	116.22	119.90
54	BA	948	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	1004	U	O4'-C1'-N1	6.13	113.11	108.20
54	BA	2191	A	C5-C6-N1	6.13	120.77	117.70
54	BA	2197	U	O4'-C1'-N1	6.13	113.10	108.20
21	AA	498	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	278	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	620	G	N3-C4-C5	-6.13	125.54	128.60
54	BA	1458	U	O4'-C1'-N1	6.13	113.10	108.20
54	BA	1686	C	O4'-C1'-N1	6.13	113.10	108.20
54	BA	1740	G	N1-C6-O6	-6.13	116.22	119.90
54	BA	238	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	394	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2170	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2679	A	C4-C5-C6	-6.13	113.94	117.00
21	AA	940	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	2435	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1330	C	O4'-C1'-N1	6.12	113.10	108.20
21	AA	647	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1768	C	N3-C2-O2	-6.12	117.61	121.90
21	AA	1257	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	1302	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2339	C	O4'-C1'-N1	6.12	113.10	108.20
54	BA	2840	C	N3-C2-O2	-6.12	117.62	121.90
3	AD	72	ARG	NE-CZ-NH1	6.12	123.36	120.30
21	AA	1210	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	650	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1299	G	N3-C2-N2	-6.12	115.62	119.90
54	BA	1826	G	C2'-C3'-O3'	6.12	123.49	113.70
54	BA	2800	A	C4-C5-C6	-6.12	113.94	117.00
21	AA	222	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	1880	U	O4'-C1'-N1	6.12	113.09	108.20
54	BA	2479	U	O4'-C1'-N1	6.12	113.09	108.20
21	AA	575	G	P-O3'-C3'	6.12	127.04	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1289	C	N3-C2-O2	-6.12	117.62	121.90
54	BA	2699	C	N3-C2-O2	-6.12	117.62	121.90
21	AA	173	U	N3-C2-O2	-6.11	117.92	122.20
21	AA	178	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	226	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	1351	C	O4'-C1'-N1	6.11	113.09	108.20
54	BA	1713	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	1728	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	495	A	C4-C5-C6	-6.11	113.94	117.00
21	AA	840	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	294	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	513	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	1913	A	O4'-C1'-N9	6.11	113.09	108.20
12	AM	100	ARG	NE-CZ-NH1	6.11	123.35	120.30
21	AA	36	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	286	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	811	C	N3-C2-O2	-6.11	117.62	121.90
29	BG	68	ARG	NE-CZ-NH1	6.11	123.35	120.30
54	BA	1020	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	1901	A	C5-C6-N1	6.11	120.75	117.70
54	BA	2767	C	N3-C2-O2	-6.11	117.62	121.90
55	BB	114	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	334	C	N3-C2-O2	-6.11	117.63	121.90
21	AA	400	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	595	C	N3-C2-O2	-6.11	117.63	121.90
54	BA	1545	A	C5-C6-N1	6.11	120.75	117.70
54	BA	1781	U	O4'-C1'-N1	6.11	113.08	108.20
54	BA	2260	C	N3-C2-O2	-6.11	117.63	121.90
21	AA	1269	A	C5-C6-N1	6.10	120.75	117.70
54	BA	645	C	N1-C2-O2	6.10	122.56	118.90
21	AA	526	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	729	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	860	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	872	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	279	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	323	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	569	U	C5'-C4'-O4'	6.10	116.42	109.10
54	BA	1991	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	2261	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	2295	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	234	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	618	C	N3-C2-O2	-6.10	117.63	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1218	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	366	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	32	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	106	C	N1-C2-O2	6.10	122.56	118.90
21	AA	329	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	11	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	286	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	687	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1173	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	2174	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	2611	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	269	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	790	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	805	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	1273	C	N3-C2-O2	-6.10	117.63	121.90
21	AA	16	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	448	A	C4-C5-C6	-6.09	113.95	117.00
46	BX	49	ARG	NE-CZ-NH1	6.09	123.35	120.30
54	BA	357	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	758	C	N3-C2-O2	-6.09	117.63	121.90
54	BA	784	G	N3-C2-N2	-6.09	115.63	119.90
54	BA	1470	A	N1-C6-N6	-6.09	114.94	118.60
54	BA	1606	C	C1'-O4'-C4'	-6.09	105.02	109.90
54	BA	2212	A	C4-C5-C6	-6.09	113.95	117.00
22	A1	50	G	N1-C6-O6	-6.09	116.24	119.90
54	BA	575	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	1350	C	N3-C2-O2	-6.09	117.64	121.90
54	BA	2888	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	195	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	802	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	2637	U	O4'-C1'-N1	6.09	113.07	108.20
55	BB	52	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	914	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	574	A	O4'-C1'-N9	6.09	113.07	108.20
54	BA	2142	A	C4-C5-C6	-6.09	113.95	117.00
55	BB	30	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	1246	A	C5-C6-N1	6.09	120.74	117.70
21	AA	151	A	C5-C6-N1	6.09	120.74	117.70
54	BA	710	U	O4'-C1'-N1	6.09	113.07	108.20
54	BA	982	C	N1-C2-O2	6.09	122.55	118.90
54	BA	1437	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	1389	C	N3-C2-O2	-6.08	117.64	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	237	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	86	G	O4'-C1'-N9	6.08	113.07	108.20
40	BR	90	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	324	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1819	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2815	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2654	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	43	C	C5'-C4'-C3'	-6.08	106.27	116.00
54	BA	2231	U	O4'-C1'-N1	6.08	113.06	108.20
54	BA	2652	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2889	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	1079	C	O4'-C1'-N1	6.08	113.06	108.20
54	BA	1960	A	N1-C6-N6	-6.08	114.95	118.60
54	BA	2399	G	N1-C6-O6	-6.08	116.25	119.90
21	AA	782	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1431	A	N1-C6-N6	-6.08	114.95	118.60
54	BA	1557	C	N3-C2-O2	-6.08	117.65	121.90
21	AA	979	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	1145	A	C4-C5-C6	-6.07	113.96	117.00
40	BR	78	ARG	NE-CZ-NH1	6.07	123.34	120.30
54	BA	484	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	544	C	O4'-C1'-N1	6.07	113.06	108.20
54	BA	1359	A	C5-C6-N1	6.07	120.74	117.70
54	BA	1801	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	2829	A	C4-C5-C6	-6.07	113.96	117.00
55	BB	29	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	357	G	C3'-C2'-C1'	6.07	106.36	101.50
21	AA	994	A	C4-C5-C6	-6.07	113.96	117.00
29	BG	162	ARG	NE-CZ-NH1	6.07	123.34	120.30
54	BA	116	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	992	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1018	U	O4'-C1'-N1	6.07	113.06	108.20
54	BA	1822	C	N3-C2-O2	-6.07	117.65	121.90
21	AA	780	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	1679	A	N1-C6-N6	-6.07	114.96	118.60
21	AA	1443	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	890	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1582	C	N3-C2-O2	-6.07	117.65	121.90
41	BS	84	ARG	NE-CZ-NH1	6.07	123.33	120.30
54	BA	64	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	348	A	C5-C6-N1	6.07	120.73	117.70
54	BA	1383	A	C4-C5-C6	-6.07	113.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1528	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	703	G	O4'-C1'-N9	6.07	113.05	108.20
54	BA	2573	C	N3-C2-O2	-6.07	117.66	121.90
54	BA	1981	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	2108	A	C5-C6-N1	6.06	120.73	117.70
21	AA	131	A	C5-C6-N1	6.06	120.73	117.70
21	AA	602	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	1147	C	N1-C2-O2	6.06	122.54	118.90
54	BA	1214	A	C5-C6-N1	6.06	120.73	117.70
54	BA	1447	C	N3-C2-O2	-6.06	117.66	121.90
56	B5	122	ARG	NE-CZ-NH2	-6.06	117.27	120.30
21	AA	995	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	1141	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1347	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1821	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	233	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	251	G	O4'-C1'-N9	6.06	113.05	108.20
21	AA	386	C	N1-C2-O2	6.06	122.53	118.90
54	BA	1676	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	1924	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	634	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1569	A	C4-C5-C6	-6.06	113.97	117.00
21	AA	1038	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	1170	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1746	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2005	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2442	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	913	A	N1-C6-N6	-6.05	114.97	118.60
29	BG	2	ARG	NE-CZ-NH1	6.05	123.33	120.30
54	BA	19	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	22	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	1191	A	C5-C6-N1	6.05	120.72	117.70
21	AA	1262	C	N3-C2-O2	-6.05	117.66	121.90
21	AA	1322	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	454	A	C5-C6-N1	6.05	120.73	117.70
54	BA	2313	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	2560	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	2868	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	664	G	N1-C6-O6	-6.05	116.27	119.90
21	AA	735	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1580	A	C4-C5-C6	-6.05	113.97	117.00
54	BA	1902	C	O4'-C1'-N1	6.05	113.04	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	322	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1046	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1541	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	2750	A	N1-C6-N6	-6.05	114.97	118.60
54	BA	280	U	N3-C2-O2	-6.05	117.97	122.20
54	BA	791	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	2036	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	2572	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	2854	G	N1-C6-O6	-6.05	116.27	119.90
21	AA	712	A	C5-C6-N1	6.04	120.72	117.70
24	A3	29	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	320	A	N1-C6-N6	-6.04	114.97	118.60
54	BA	404	A	N1-C6-N6	-6.04	114.97	118.60
21	AA	1289	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2594	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	743	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1101	A	P-O3'-C3'	6.04	126.95	119.70
21	AA	1195	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	1214	C	C1'-O4'-C4'	-6.04	105.07	109.90
4	AE	19	ARG	NE-CZ-NH1	6.04	123.32	120.30
21	AA	738	C	N3-C2-O2	-6.04	117.67	121.90
33	BK	70	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	1027	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	712	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	844	G	N3-C2-N2	-6.03	115.68	119.90
54	BA	2450	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	393	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	574	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	1097	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	1521	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	986	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2358	A	C5-C6-N1	6.03	120.72	117.70
2	AC	125	ARG	NE-CZ-NH1	6.03	123.31	120.30
54	BA	16	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	21	A	C4-C5-C6	-6.03	113.98	117.00
21	AA	1418	A	N1-C6-N6	-6.03	114.98	118.60
22	A1	60	C	C1'-O4'-C4'	-6.03	105.08	109.90
54	BA	905	A	C4-C5-C6	-6.03	113.99	117.00
15	AP	14	ARG	NE-CZ-NH1	6.03	123.31	120.30
21	AA	1261	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	1871	A	O4'-C1'-N9	6.03	113.02	108.20
21	AA	468	A	C4-C5-C6	-6.02	113.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BC	101	ARG	NE-CZ-NH1	6.02	123.31	120.30
22	A1	28	C	N3-C2-O2	-6.02	117.68	121.90
54	BA	1586	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2882	A	C6-C5-N7	6.02	136.52	132.30
35	BM	18	ARG	NE-CZ-NH1	6.02	123.31	120.30
54	BA	932	U	O4'-C1'-N1	6.02	113.02	108.20
54	BA	1752	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	1274	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1054	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1321	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	1685	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	2581	G	N1-C6-O6	-6.02	116.29	119.90
21	AA	655	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	217	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2080	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	2787	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	206	C	N3-C2-O2	-6.02	117.69	121.90
25	BC	86	ARG	NE-CZ-NH1	6.02	123.31	120.30
54	BA	1379	U	O4'-C1'-N1	6.02	113.01	108.20
21	AA	1318	A	C5-C6-N1	6.01	120.71	117.70
54	BA	1549	A	N1-C6-N6	-6.01	114.99	118.60
21	AA	288	A	C5-C6-N1	6.01	120.71	117.70
54	BA	386	G	P-O3'-C3'	6.01	126.92	119.70
54	BA	1052	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	1230	C	N3-C2-O2	-6.01	117.69	121.90
22	A1	72	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1244	A	O4'-C1'-N9	6.01	113.01	108.20
54	BA	1608	A	N1-C6-N6	-6.01	114.99	118.60
21	AA	1024	G	N1-C6-O6	-6.01	116.29	119.90
46	BX	56	ARG	NE-CZ-NH1	6.01	123.31	120.30
54	BA	542	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	889	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	2184	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2480	C	O4'-C1'-N1	6.01	113.01	108.20
21	AA	98	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	198	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1874	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	996	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	1357	C	O4'-C1'-N1	6.01	113.01	108.20
54	BA	2850	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	1512	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1005	A	C5-C6-N1	6.00	120.70	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	172	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	599	A	C5-C6-N1	6.00	120.70	117.70
54	BA	620	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	806	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1847	A	O4'-C1'-N9	6.00	113.00	108.20
54	BA	2546	U	O4'-C1'-N1	6.00	113.00	108.20
21	AA	408	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	736	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1020	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	2352	A	C5-C6-N1	6.00	120.70	117.70
21	AA	172	A	C4-C5-C6	-6.00	114.00	117.00
33	BK	31	ARG	NE-CZ-NH1	6.00	123.30	120.30
54	BA	21	A	C5-C6-N1	6.00	120.70	117.70
54	BA	1395	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1547	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1727	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2248	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	152	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2081	U	O4'-C1'-N1	6.00	113.00	108.20
54	BA	2858	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1350	A	C5-C6-N1	6.00	120.70	117.70
54	BA	1933	G	N1-C6-O6	-6.00	116.30	119.90
54	BA	2788	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	364	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	630	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	1214	C	N3-C2-O2	-5.99	117.70	121.90
54	BA	205	G	N1-C6-O6	-5.99	116.31	119.90
54	BA	854	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1893	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2589	A	C5-C6-N1	5.99	120.70	117.70
8	AI	11	ARG	NE-CZ-NH1	5.99	123.30	120.30
21	AA	706	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	741	G	N1-C6-O6	-5.99	116.31	119.90
21	AA	1093	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	1157	A	C4-C5-C6	-5.99	114.00	117.00
39	BQ	2	ARG	NE-CZ-NH1	5.99	123.30	120.30
54	BA	57	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	96	C	O4'-C1'-N1	5.99	112.99	108.20
54	BA	1014	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1419	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	1117	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1045	C	N3-C2-O2	-5.99	117.71	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2507	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	2610	C	N1-C2-O2	5.99	122.49	118.90
55	BB	31	C	N3-C2-O2	-5.99	117.71	121.90
21	AA	59	A	C4-C5-C6	-5.99	114.01	117.00
3	AD	61	ARG	NE-CZ-NH1	5.99	123.29	120.30
21	AA	1429	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1574	C	O4'-C1'-N1	5.99	112.99	108.20
54	BA	2614	A	C4-C5-C6	-5.99	114.01	117.00
55	BB	66	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	757	U	N3-C2-O2	-5.98	118.01	122.20
54	BA	49	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1158	C	N3-C2-O2	-5.98	117.71	121.90
16	AQ	10	ARG	NE-CZ-NH1	5.98	123.29	120.30
21	AA	1352	C	N1-C2-O2	5.98	122.49	118.90
21	AA	1369	C	N1-C2-O2	5.98	122.49	118.90
54	BA	1427	A	P-O3'-C3'	5.98	126.88	119.70
54	BA	1522	A	C4-C5-C6	-5.98	114.01	117.00
55	BB	59	A	C4-C5-C6	-5.98	114.01	117.00
55	BB	105	G	O4'-C1'-N9	5.98	112.99	108.20
54	BA	1565	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	2023	C	N3-C2-O2	-5.98	117.71	121.90
54	BA	2101	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2288	A	C4-C5-C6	-5.98	114.01	117.00
55	BB	82	U	O4'-C1'-N1	5.98	112.98	108.20
21	AA	432	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	621	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1899	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	637	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	764	C	N1-C2-O2	5.98	122.49	118.90
54	BA	1780	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2169	A	O4'-C1'-N9	5.98	112.98	108.20
55	BB	45	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	416	G	N3-C2-N2	-5.97	115.72	119.90
54	BA	870	U	O4'-C1'-N1	5.97	112.98	108.20
54	BA	946	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2501	C	O4'-C1'-C2'	-5.97	99.83	105.80
6	AG	52	ARG	NE-CZ-NH1	5.97	123.29	120.30
54	BA	1306	C	O4'-C1'-N1	5.97	112.98	108.20
54	BA	2443	C	O4'-C1'-N1	5.97	112.98	108.20
54	BA	2480	C	N3-C2-O2	-5.97	117.72	121.90
5	AF	91	ARG	NE-CZ-NH1	5.97	123.29	120.30
21	AA	1217	C	N3-C2-O2	-5.97	117.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1014	A	C5-C6-N1	5.97	120.69	117.70
21	AA	865	A	C5-C6-N1	5.97	120.69	117.70
22	A1	32	C	N1-C2-O2	5.97	122.48	118.90
54	BA	518	G	C1'-O4'-C4'	-5.97	105.12	109.90
54	BA	2752	C	N3-C2-O2	-5.97	117.72	121.90
55	BB	63	C	O4'-C1'-N1	5.97	112.97	108.20
21	AA	1509	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	5	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2551	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	280	C	N1-C2-O2	5.97	122.48	118.90
21	AA	352	C	N3-C2-O2	-5.97	117.72	121.90
24	A3	39	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	270	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	468	G	N1-C6-O6	-5.97	116.32	119.90
54	BA	1141	U	O4'-C1'-N1	5.97	112.97	108.20
54	BA	1705	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	896	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	614	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1372	U	O4'-C1'-N1	5.96	112.97	108.20
54	BA	1579	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2179	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	2440	C	N3-C2-O2	-5.96	117.72	121.90
54	BA	998	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1050	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1123	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2022	U	O4'-C1'-N1	5.96	112.97	108.20
21	AA	436	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	878	A	C5-C6-N1	5.96	120.68	117.70
54	BA	1962	C	N1-C2-O2	5.96	122.48	118.90
54	BA	2119	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2646	C	O4'-C1'-N1	5.96	112.97	108.20
54	BA	833	A	O4'-C1'-N9	5.96	112.97	108.20
55	BB	53	A	N1-C6-N6	-5.96	115.02	118.60
54	BA	1080	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1243	C	O4'-C1'-N1	5.96	112.97	108.20
54	BA	2300	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2825	G	N1-C6-O6	-5.96	116.33	119.90
54	BA	994	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2491	U	O4'-C1'-N1	5.96	112.97	108.20
54	BA	53	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2681	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	554	A	C5-C6-N1	5.95	120.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1239	A	C4-C5-C6	-5.95	114.02	117.00
26	BD	141	ARG	NE-CZ-NH1	5.95	123.28	120.30
54	BA	522	A	C5-C6-N1	5.95	120.68	117.70
54	BA	1021	A	C5-C6-N1	5.95	120.68	117.70
54	BA	2003	A	C5-C6-N1	5.95	120.68	117.70
21	AA	397	A	C5-C6-N1	5.95	120.68	117.70
54	BA	1312	U	O4'-C1'-N1	5.95	112.96	108.20
21	AA	1014	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	340	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	1141	U	N3-C2-O2	-5.95	118.03	122.20
54	BA	1755	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	2241	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	2771	C	N1-C2-O2	5.95	122.47	118.90
21	AA	660	C	N3-C2-O2	-5.95	117.74	121.90
21	AA	1245	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	318	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	522	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	1550	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1871	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	2666	C	O4'-C1'-N1	5.95	112.96	108.20
21	AA	99	C	N3-C2-O2	-5.95	117.74	121.90
22	A1	27	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	415	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	2683	C	N3-C2-O2	-5.95	117.74	121.90
21	AA	1035	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1102	C	O4'-C1'-N1	5.94	112.95	108.20
21	AA	1404	C	N1-C2-O2	5.94	122.47	118.90
54	BA	299	A	C5-C6-N1	5.94	120.67	117.70
54	BA	513	A	N1-C6-N6	-5.94	115.03	118.60
54	BA	550	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	815	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2810	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1787	A	C4-C5-C6	-5.94	114.03	117.00
48	BZ	37	ARG	NE-CZ-NH1	5.94	123.27	120.30
21	AA	539	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1675	C	N3-C2-O2	-5.94	117.74	121.90
55	BB	19	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	1342	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1408	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	525	U	O4'-C1'-N1	5.93	112.95	108.20
54	BA	665	U	O4'-C1'-N1	5.93	112.95	108.20
54	BA	816	C	O4'-C1'-N1	5.93	112.95	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2368	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	116	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	392	C	N3-C2-O2	-5.93	117.75	121.90
22	A1	21	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1079	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	2211	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2327	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2390	U	O4'-C1'-N1	5.93	112.95	108.20
54	BA	2778	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	132	C	N1-C2-O2	5.93	122.46	118.90
54	BA	1182	G	N1-C6-O6	-5.93	116.34	119.90
54	BA	2575	C	O4'-C1'-N1	5.93	112.94	108.20
54	BA	2856	A	C4-C5-C6	-5.93	114.04	117.00
16	AQ	76	ARG	NE-CZ-NH1	5.93	123.26	120.30
23	A2	81	U	O4'-C1'-N1	5.93	112.94	108.20
51	B2	34	ARG	NE-CZ-NH1	5.93	123.26	120.30
54	BA	413	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	902	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	1786	A	C4-C5-C6	-5.93	114.04	117.00
21	AA	766	A	O4'-C1'-N9	5.92	112.94	108.20
54	BA	2269	G	N1-C6-O6	-5.92	116.35	119.90
21	AA	108	G	O4'-C1'-N9	5.92	112.94	108.20
54	BA	265	A	O4'-C1'-N9	5.92	112.94	108.20
6	AG	110	ARG	NE-CZ-NH1	5.92	123.26	120.30
21	AA	1226	C	N3-C2-O2	-5.92	117.75	121.90
21	AA	1534	A	C4-C5-C6	-5.92	114.04	117.00
26	BD	59	ARG	NE-CZ-NH1	5.92	123.26	120.30
54	BA	1236	G	O4'-C4'-C3'	5.92	110.84	106.10
21	AA	946	A	N1-C6-N6	-5.92	115.05	118.60
54	BA	216	A	C5-C6-N1	5.92	120.66	117.70
54	BA	2758	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	74	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1276	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	1434	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	136	C	N3-C2-O2	-5.92	117.76	121.90
52	B3	41	ARG	NE-CZ-NH2	5.92	123.26	120.30
54	BA	547	A	O4'-C1'-N9	5.92	112.93	108.20
54	BA	611	C	N1-C2-O2	5.92	122.45	118.90
54	BA	814	C	O4'-C1'-N1	5.92	112.93	108.20
54	BA	951	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	2243	U	O4'-C1'-N1	5.92	112.93	108.20
54	BA	2392	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	2789	C	N3-C2-O2	-5.92	117.76	121.90
55	BB	113	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	995	C	N3-C2-O2	-5.91	117.76	121.90
21	AA	900	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	2556	C	O4'-C1'-N1	5.91	112.93	108.20
21	AA	1254	A	C5-C6-N1	5.91	120.66	117.70
54	BA	183	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1826	G	P-O3'-C3'	5.91	126.79	119.70
54	BA	2483	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2809	A	C4-C5-C6	-5.91	114.05	117.00
19	AT	24	ARG	NE-CZ-NH2	-5.91	117.35	120.30
54	BA	1170	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	2860	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1205	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1637	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	2407	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	386	G	N3-C4-C5	-5.91	125.65	128.60
54	BA	1551	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1618	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1732	C	N1-C2-O2	5.91	122.44	118.90
54	BA	1815	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	2565	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	2657	A	C5-C6-N1	5.91	120.65	117.70
45	BW	19	ARG	NE-CZ-NH1	5.90	123.25	120.30
54	BA	526	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	530	G	N3-C2-N2	-5.90	115.77	119.90
21	AA	906	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	451	U	O4'-C1'-N1	5.90	112.92	108.20
54	BA	1295	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	2412	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	2361	G	O4'-C1'-N9	5.90	112.92	108.20
54	BA	1543	G	N1-C6-O6	-5.90	116.36	119.90
54	BA	2700	A	C5-C6-N1	5.90	120.65	117.70
21	AA	1430	A	C4-C5-C6	-5.89	114.05	117.00
25	BC	13	ARG	NE-CZ-NH1	5.89	123.25	120.30
54	BA	640	C	N3-C2-O2	-5.89	117.77	121.90
54	BA	1794	A	C4-C5-C6	-5.89	114.05	117.00
54	BA	1892	C	N3-C2-O2	-5.89	117.77	121.90
54	BA	1370	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2768	U	O4'-C1'-N1	5.89	112.91	108.20
55	BB	58	A	C4-C5-C6	-5.89	114.05	117.00
21	AA	330	C	N3-C2-O2	-5.89	117.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1046	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	385	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1872	A	O4'-C1'-N9	5.89	112.91	108.20
54	BA	2467	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	816	C	N3-C2-O2	-5.89	117.78	121.90
23	A2	82	A	N1-C6-N6	-5.89	115.07	118.60
54	BA	1094	U	O4'-C1'-N1	5.89	112.91	108.20
54	BA	2008	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2385	C	O4'-C1'-N1	5.89	112.91	108.20
55	BB	118	C	O4'-C1'-N1	5.88	112.91	108.20
54	BA	2021	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	879	C	N1-C2-O2	5.88	122.43	118.90
54	BA	546	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	2317	A	C4-C5-C6	-5.88	114.06	117.00
11	AL	120	ARG	NE-CZ-NH2	5.88	123.24	120.30
21	AA	679	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	71	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	131	A	N1-C6-N6	-5.88	115.07	118.60
54	BA	341	C	O4'-C1'-N1	5.88	112.90	108.20
54	BA	900	A	C6-C5-N7	5.88	136.42	132.30
54	BA	1783	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	1382	C	C1'-O4'-C4'	-5.88	105.20	109.90
54	BA	267	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1623	G	N1-C6-O6	-5.88	116.37	119.90
54	BA	2062	A	O4'-C1'-N9	5.88	112.90	108.20
54	BA	2806	C	N3-C2-O2	-5.88	117.78	121.90
21	AA	355	C	N3-C2-O2	-5.88	117.79	121.90
29	BG	34	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	1402	U	O4'-C1'-N1	5.88	112.90	108.20
21	AA	129	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1040	A	N1-C6-N6	-5.88	115.08	118.60
54	BA	1508	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2350	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	917	A	N1-C6-N6	-5.87	115.08	118.60
54	BA	1700	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2346	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	80	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	1330	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	611	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	732	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1481	U	O4'-C1'-N1	5.87	112.90	108.20
21	AA	179	A	C5-C6-N1	5.87	120.63	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	430	A	C4-C5-C6	-5.87	114.07	117.00
22	A1	58	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	507	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	1463	C	N1-C2-O2	5.87	122.42	118.90
54	BA	2006	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	528	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	876	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1350	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	1466	U	O4'-C1'-N1	5.87	112.89	108.20
21	AA	463	U	C5-C6-N1	-5.87	119.77	122.70
21	AA	882	C	N3-C2-O2	-5.87	117.79	121.90
21	AA	1407	C	N3-C2-O2	-5.87	117.80	121.90
54	BA	609	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	804	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	983	A	O4'-C1'-N9	5.87	112.89	108.20
54	BA	1246	A	O4'-C1'-N9	5.87	112.89	108.20
54	BA	2793	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2828	G	N3-C2-N2	-5.87	115.79	119.90
21	AA	603	U	O4'-C1'-N1	5.86	112.89	108.20
21	AA	759	A	C5-C6-N1	5.86	120.63	117.70
54	BA	253	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1172	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1156	A	C4-C5-C6	-5.86	114.07	117.00
21	AA	63	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	351	C	C3'-C2'-C1'	5.86	106.19	101.50
54	BA	990	A	O4'-C1'-N9	5.86	112.89	108.20
54	BA	1314	C	N1-C2-O2	5.86	122.42	118.90
54	BA	2513	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	2740	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1319	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	153	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	737	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2700	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	2774	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	993	G	O4'-C1'-N9	5.86	112.88	108.20
54	BA	485	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	1990	C	N1-C2-O2	5.85	122.41	118.90
21	AA	309	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	2033	A	C4-C5-C6	-5.85	114.07	117.00
8	AI	118	ARG	NE-CZ-NH1	5.85	123.22	120.30
54	BA	2320	U	N3-C2-O2	-5.85	118.11	122.20
21	AA	80	A	C5-C6-N1	5.85	120.62	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1184	G	N3-C4-C5	-5.85	125.68	128.60
54	BA	2776	A	N1-C6-N6	-5.85	115.09	118.60
21	AA	205	A	C4-C5-C6	-5.85	114.08	117.00
21	AA	404	G	N1-C6-O6	-5.85	116.39	119.90
21	AA	792	A	C4-C5-C6	-5.85	114.08	117.00
21	AA	1265	C	N3-C2-O2	-5.85	117.81	121.90
21	AA	1503	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	918	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1352	U	N3-C2-O2	-5.85	118.11	122.20
21	AA	25	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	2302	U	O4'-C1'-N1	5.85	112.88	108.20
21	AA	536	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	421	C	N1-C2-O2	5.84	122.41	118.90
54	BA	1144	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1335	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2380	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2695	U	O4'-C1'-N1	5.84	112.88	108.20
21	AA	689	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	721	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1150	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1480	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	2691	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	191	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	223	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	265	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1145	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1761	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2322	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	2535	G	O4'-C1'-N9	5.84	112.87	108.20
21	AA	948	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	637	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	1800	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2678	C	N3-C2-O2	-5.84	117.81	121.90
24	A3	77	A	C3'-C2'-C1'	5.84	106.17	101.50
54	BA	103	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	209	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2354	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2672	U	O4'-C1'-N1	5.84	112.87	108.20
54	BA	184	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1164	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1739	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	2821	A	N1-C6-N6	-5.84	115.10	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1460	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2385	C	C5'-C4'-O4'	5.83	116.10	109.10
54	BA	1564	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1908	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1909	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2059	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	2171	A	C4-C5-C6	-5.83	114.08	117.00
54	BA	2178	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	181	A	C4-C5-C6	-5.83	114.08	117.00
21	AA	1277	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	703	U	O4'-C1'-N1	5.83	112.87	108.20
54	BA	966	G	N1-C6-O6	-5.83	116.40	119.90
54	BA	1196	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2504	U	N3-C2-O2	-5.83	118.12	122.20
54	BA	47	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	364	C	N1-C2-O2	5.83	122.40	118.90
21	AA	916	U	O4'-C1'-N1	5.83	112.86	108.20
54	BA	2187	U	O4'-C1'-N1	5.83	112.86	108.20
54	BA	2273	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	65	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	545	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1977	A	C4-C5-C6	-5.83	114.09	117.00
21	AA	934	C	N1-C2-O2	5.83	122.39	118.90
21	AA	1300	G	C3'-C2'-C1'	5.82	106.16	101.50
54	BA	336	C	N3-C2-O2	-5.82	117.82	121.90
54	BA	991	C	N3-C2-O2	-5.82	117.82	121.90
54	BA	1021	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1301	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1571	A	N1-C6-N6	-5.82	115.11	118.60
54	BA	1960	A	C4-C5-C6	-5.82	114.09	117.00
10	AK	97	ARG	NE-CZ-NH1	5.82	123.21	120.30
54	BA	1272	A	P-O3'-C3'	5.82	126.69	119.70
27	BE	21	ARG	NE-CZ-NH1	5.82	123.21	120.30
54	BA	155	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	445	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2054	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	2649	C	O4'-C1'-N1	5.82	112.86	108.20
54	BA	491	G	N1-C6-O6	-5.82	116.41	119.90
54	BA	2022	U	C1'-O4'-C4'	-5.82	105.25	109.90
54	BA	2902	C	N3-C2-O2	-5.82	117.83	121.90
55	BB	53	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	396	C	N3-C2-O2	-5.81	117.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2590	A	C6-C5-N7	5.81	136.37	132.30
21	AA	580	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	863	A	N1-C6-N6	-5.81	115.11	118.60
54	BA	1204	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	2720	U	O4'-C1'-N1	5.81	112.85	108.20
27	BE	170	ARG	NE-CZ-NH1	5.81	123.20	120.30
21	AA	974	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	334	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2404	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	2503	A	C4-C5-C6	-5.81	114.09	117.00
21	AA	66	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	565	C	N1-C2-O2	5.81	122.38	118.90
54	BA	997	G	N1-C6-O6	-5.81	116.42	119.90
54	BA	1072	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	2164	C	N1-C2-O2	5.81	122.39	118.90
54	BA	2715	C	O4'-C1'-N1	5.81	112.85	108.20
55	BB	15	A	O4'-C1'-N9	5.81	112.85	108.20
54	BA	786	C	O4'-C1'-N1	5.81	112.84	108.20
54	BA	1312	U	C1'-O4'-C4'	-5.81	105.26	109.90
54	BA	2733	A	C4-C5-C6	-5.81	114.10	117.00
55	BB	35	C	N3-C2-O2	-5.81	117.84	121.90
5	AF	79	ARG	NE-CZ-NH2	5.80	123.20	120.30
20	AU	33	ARG	NE-CZ-NH1	5.80	123.20	120.30
22	A1	61	C	C6-N1-C2	-5.80	117.98	120.30
54	BA	142	A	O4'-C1'-N9	5.80	112.84	108.20
54	BA	213	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	1207	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	2454	G	N1-C6-O6	-5.80	116.42	119.90
21	AA	13	U	O4'-C4'-C3'	5.80	110.74	106.10
21	AA	1513	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	119	A	C6-C5-N7	5.80	136.36	132.30
54	BA	239	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1385	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	188	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	783	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	613	A	C4-C5-C6	-5.80	114.10	117.00
55	BB	94	A	C5-C6-N1	5.80	120.60	117.70
21	AA	1041	G	N1-C6-O6	-5.80	116.42	119.90
37	BO	111	ARG	NE-CZ-NH2	-5.80	117.40	120.30
54	BA	1816	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1985	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	2149	U	O4'-C1'-N1	5.80	112.84	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2364	C	O4'-C1'-N1	5.80	112.84	108.20
21	AA	895	G	N3-C2-N2	-5.79	115.84	119.90
21	AA	1465	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	900	A	O4'-C1'-N9	5.79	112.83	108.20
54	BA	1843	C	N3-C2-O2	-5.79	117.84	121.90
54	BA	2823	A	C4-C5-C6	-5.79	114.10	117.00
55	BB	108	A	C4-C5-C6	-5.79	114.10	117.00
21	AA	1359	C	N1-C2-O2	5.79	122.38	118.90
54	BA	653	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1253	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	2267	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	2649	C	N1-C2-O2	5.79	122.38	118.90
21	AA	395	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	190	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	552	U	O4'-C1'-N1	5.79	112.83	108.20
21	AA	718	A	C4-C5-C6	-5.79	114.11	117.00
38	BP	61	ARG	NE-CZ-NH1	5.79	123.19	120.30
54	BA	1459	G	N3-C4-C5	-5.79	125.71	128.60
54	BA	2639	A	C4-C5-C6	-5.79	114.11	117.00
21	AA	857	C	N1-C2-O2	5.79	122.37	118.90
54	BA	1084	A	C4-C5-C6	-5.79	114.11	117.00
54	BA	1774	C	N1-C2-O2	5.79	122.37	118.90
21	AA	960	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	2799	A	C4-C5-C6	-5.79	114.11	117.00
55	BB	43	C	N3-C2-O2	-5.79	117.85	121.90
28	BF	29	ARG	NE-CZ-NH1	5.78	123.19	120.30
54	BA	1426	G	O4'-C1'-N9	5.78	112.83	108.20
54	BA	1782	U	C3'-C2'-C1'	5.78	106.13	101.50
54	BA	2283	C	N3-C2-O2	-5.78	117.85	121.90
21	AA	51	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	66	C	N1-C2-O2	5.78	122.37	118.90
54	BA	302	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	957	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	1214	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	582	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1665	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2792	A	C5-C6-N1	5.78	120.59	117.70
21	AA	249	U	N3-C2-O2	-5.78	118.16	122.20
54	BA	161	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	654	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	864	G	C3'-C2'-C1'	5.78	106.12	101.50
54	BA	942	G	N3-C2-N2	-5.78	115.86	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1134	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2658	C	N3-C2-O2	-5.78	117.86	121.90
39	BQ	57	ARG	NE-CZ-NH1	5.77	123.19	120.30
54	BA	2901	C	N3-C2-O2	-5.77	117.86	121.90
24	A3	49	C	N3-C2-O2	-5.77	117.86	121.90
26	BD	124	ARG	NE-CZ-NH2	-5.77	117.41	120.30
54	BA	737	C	O4'-C1'-N1	5.77	112.82	108.20
21	AA	1114	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	127	A	N1-C6-N6	-5.77	115.14	118.60
54	BA	1127	A	N1-C6-N6	-5.77	115.14	118.60
54	BA	2723	C	N1-C2-O2	5.77	122.36	118.90
21	AA	325	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	505	A	C5-C6-N1	5.77	120.58	117.70
54	BA	613	A	C5'-C4'-C3'	-5.77	106.77	116.00
54	BA	657	U	O4'-C1'-N1	5.77	112.82	108.20
54	BA	2196	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	612	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	868	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	1508	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	218	A	C4-C5-C6	-5.77	114.12	117.00
54	BA	1006	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	835	U	O4'-C1'-N1	5.77	112.81	108.20
21	AA	741	G	N3-C2-N2	-5.76	115.86	119.90
21	AA	797	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	1133	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	563	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1603	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1912	A	C4-C5-C6	-5.76	114.12	117.00
11	AL	49	ARG	NE-CZ-NH1	5.76	123.18	120.30
21	AA	100	G	N1-C6-O6	-5.76	116.44	119.90
21	AA	220	G	N1-C6-O6	-5.76	116.44	119.90
21	AA	250	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1851	U	O4'-C1'-N1	5.76	112.81	108.20
21	AA	509	A	C4-C5-C6	-5.76	114.12	117.00
22	A1	9	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	165	A	C5-C6-N1	5.76	120.58	117.70
54	BA	909	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1768	C	O4'-C1'-N1	5.76	112.81	108.20
54	BA	2785	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	881	G	C5-C6-N1	5.76	114.38	111.50
21	AA	183	C	C1'-O4'-C4'	-5.76	105.29	109.90
54	BA	1258	U	O4'-C1'-N1	5.76	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	722	G	N1-C6-O6	-5.75	116.45	119.90
21	AA	968	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	227	G	N1-C6-O6	-5.75	116.45	119.90
21	AA	720	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	1028	C	N3-C2-O2	-5.75	117.87	121.90
23	A2	79	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	483	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2055	C	C3'-C2'-C1'	5.75	106.10	101.50
54	BA	572	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	1446	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	2725	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	1036	A	C6-C5-N7	5.75	136.32	132.30
21	AA	1286	U	N3-C2-O2	-5.75	118.18	122.20
54	BA	58	G	N1-C6-O6	-5.75	116.45	119.90
54	BA	1745	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	1518	A	C6-C5-N7	5.75	136.32	132.30
54	BA	643	A	C1'-O4'-C4'	-5.75	105.30	109.90
54	BA	2023	C	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2417	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	2609	U	N3-C2-O2	-5.75	118.18	122.20
21	AA	403	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	2079	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	790	U	N3-C2-O2	-5.74	118.18	122.20
54	BA	810	U	C3'-C2'-C1'	5.74	106.09	101.50
54	BA	1057	A	O4'-C1'-N9	5.74	112.80	108.20
54	BA	1626	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1787	A	C5-C6-N1	5.74	120.57	117.70
21	AA	372	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1297	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1665	A	C5-C6-N1	5.74	120.57	117.70
55	BB	15	A	C4-C5-C6	-5.74	114.13	117.00
1	AB	73	ARG	NE-CZ-NH1	5.74	123.17	120.30
39	BQ	91	ARG	NE-CZ-NH1	5.74	123.17	120.30
54	BA	418	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1371	G	N3-C2-N2	-5.74	115.88	119.90
54	BA	2199	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2262	U	O4'-C1'-N1	5.74	112.79	108.20
54	BA	517	C	N1-C2-O2	5.74	122.34	118.90
54	BA	603	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1140	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1576	U	O4'-C1'-N1	5.74	112.79	108.20
12	AM	89	ARG	NE-CZ-NH1	5.74	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	AQ	5	ARG	NE-CZ-NH1	5.74	123.17	120.30
21	AA	690	G	N1-C6-O6	-5.74	116.46	119.90
21	AA	849	G	N1-C6-O6	-5.74	116.46	119.90
21	AA	179	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	907	A	N1-C6-N6	-5.74	115.16	118.60
21	AA	1151	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1089	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1638	C	N1-C2-O2	5.74	122.34	118.90
54	BA	2854	G	O4'-C1'-N9	5.74	112.79	108.20
55	BB	73	A	C4-C5-C6	-5.73	114.13	117.00
22	A1	31	C	N1-C2-O2	5.73	122.34	118.90
54	BA	497	A	C4-C5-C6	-5.73	114.13	117.00
54	BA	626	A	C6-C5-N7	5.73	136.31	132.30
21	AA	271	C	N3-C2-O2	-5.73	117.89	121.90
25	BC	68	ARG	NE-CZ-NH1	5.73	123.17	120.30
54	BA	1000	A	C4-C5-C6	-5.73	114.13	117.00
54	BA	1077	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	2732	G	O4'-C1'-N9	5.73	112.78	108.20
21	AA	412	A	C4-C5-C6	-5.73	114.14	117.00
21	AA	1056	U	O4'-C1'-N1	5.73	112.78	108.20
21	AA	1423	G	N3-C2-N2	-5.73	115.89	119.90
54	BA	2176	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	2507	C	O4'-C1'-N1	5.73	112.78	108.20
21	AA	1467	C	N1-C2-O2	5.73	122.33	118.90
21	AA	427	U	N3-C2-O2	-5.72	118.19	122.20
54	BA	101	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	403	U	N3-C2-O2	-5.72	118.19	122.20
54	BA	1005	C	N3-C2-O2	-5.72	117.89	121.90
21	AA	186	C	N1-C2-O2	5.72	122.33	118.90
21	AA	967	C	N3-C2-O2	-5.72	117.89	121.90
22	A1	48	C	N3-C2-O2	-5.72	117.89	121.90
31	BI	64	ARG	NE-CZ-NH1	5.72	123.16	120.30
54	BA	2462	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	2601	C	N3-C2-O2	-5.72	117.89	121.90
21	AA	937	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2030	A	C4-C5-C6	-5.72	114.14	117.00
55	BB	78	A	C4-C5-C6	-5.72	114.14	117.00
21	AA	971	G	C8-N9-C4	-5.72	104.11	106.40
54	BA	256	A	N1-C6-N6	-5.72	115.17	118.60
54	BA	620	G	O4'-C1'-N9	5.72	112.77	108.20
21	AA	341	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	733	G	N3-C4-C5	-5.72	125.74	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	599	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	737	C	N1-C2-O2	5.72	122.33	118.90
54	BA	1472	C	O4'-C1'-N1	5.72	112.77	108.20
54	BA	1764	C	N3-C2-O2	-5.72	117.90	121.90
21	AA	175	C	C1'-O4'-C4'	-5.71	105.33	109.90
21	AA	862	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	772	C	O4'-C1'-N1	5.71	112.77	108.20
54	BA	2090	A	C6-C5-N7	5.71	136.30	132.30
21	AA	559	A	C2-N3-C4	5.71	113.46	110.60
54	BA	1168	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	1495	A	C5-C6-N1	5.71	120.56	117.70
21	AA	295	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	847	U	N3-C2-O2	-5.71	118.20	122.20
54	BA	893	C	N1-C2-O2	5.71	122.33	118.90
54	BA	1129	A	C4-C5-C6	-5.71	114.14	117.00
55	BB	12	C	O4'-C1'-N1	5.71	112.77	108.20
21	AA	110	C	N1-C2-O2	5.71	122.32	118.90
54	BA	889	C	N1-C2-O2	5.71	122.32	118.90
54	BA	2388	A	C5'-C4'-O4'	5.71	115.95	109.10
21	AA	1399	C	P-O3'-C3'	5.71	126.55	119.70
54	BA	578	G	N3-C2-N2	-5.71	115.91	119.90
21	AA	184	G	N3-C2-N2	-5.70	115.91	119.90
21	AA	1149	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	832	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	948	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1048	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	84	A	C4-C5-C6	-5.70	114.15	117.00
11	AL	30	ARG	NE-CZ-NH2	-5.70	117.45	120.30
51	B2	12	ARG	NE-CZ-NH1	5.70	123.15	120.30
54	BA	225	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	876	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	972	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	1931	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	845	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2153	C	N1-C2-O2	5.70	122.32	118.90
21	AA	269	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	353	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	823	C	N3-C2-O2	-5.70	117.91	121.90
13	AN	61	ARG	NE-CZ-NH1	5.70	123.15	120.30
21	AA	1395	C	N3-C4-N4	-5.70	114.01	118.00
54	BA	675	A	C6-N1-C2	-5.70	115.18	118.60
54	BA	2263	C	N3-C2-O2	-5.70	117.91	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2416	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	1113	U	O4'-C1'-N1	5.69	112.75	108.20
24	A3	62	C	N3-C2-O2	-5.69	117.92	121.90
37	BO	9	ARG	NE-CZ-NH1	5.69	123.15	120.30
54	BA	1130	U	O4'-C1'-N1	5.69	112.75	108.20
54	BA	66	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	456	C	N1-C2-O2	5.69	122.31	118.90
54	BA	668	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	762	U	P-O3'-C3'	5.69	126.53	119.70
54	BA	1600	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	2354	C	O4'-C1'-N1	5.69	112.75	108.20
21	AA	962	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	1238	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	873	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	912	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1722	A	N1-C6-N6	-5.69	115.19	118.60
54	BA	1892	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	2730	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	452	A	C4-C5-C6	-5.69	114.16	117.00
21	AA	658	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1971	U	N3-C2-O2	-5.69	118.22	122.20
54	BA	246	C	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1697	G	N3-C4-C5	-5.68	125.76	128.60
54	BA	2154	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	1130	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	234	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	601	C	O4'-C1'-N1	5.68	112.75	108.20
54	BA	676	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1362	C	O4'-C1'-N1	5.68	112.75	108.20
21	AA	1382	C	N1-C2-O2	5.68	122.31	118.90
54	BA	505	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	262	A	C6-C5-N7	5.68	136.28	132.30
21	AA	702	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1032	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	1847	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	931	C	N3-C2-O2	-5.68	117.93	121.90
54	BA	1365	A	C4-C5-C6	-5.68	114.16	117.00
13	AN	90	ARG	NE-CZ-NH1	5.67	123.14	120.30
21	AA	539	A	C5-C6-N1	5.67	120.54	117.70
54	BA	115	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	817	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	1583	A	C4-C5-C6	-5.67	114.16	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1806	C	N1-C2-O2	5.67	122.31	118.90
7	AH	12	ARG	NE-CZ-NH1	5.67	123.14	120.30
54	BA	181	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1883	U	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2430	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	2755	C	O4'-C1'-N1	5.67	112.74	108.20
21	AA	155	A	C6-C5-N7	5.67	136.27	132.30
24	A3	26	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2648	G	N3-C2-N2	-5.67	115.93	119.90
21	AA	1263	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	479	A	C5-C6-N1	5.67	120.53	117.70
54	BA	2651	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2760	C	N3-C2-O2	-5.67	117.93	121.90
21	AA	149	A	C5-C6-N1	5.67	120.53	117.70
28	BF	147	ARG	NE-CZ-NH1	5.67	123.13	120.30
54	BA	211	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	436	C	O4'-C1'-N1	5.67	112.73	108.20
54	BA	1213	A	C4-C5-C6	-5.67	114.17	117.00
21	AA	211	G	N3-C4-C5	-5.67	125.77	128.60
39	BQ	47	ARG	NE-CZ-NH1	5.67	123.13	120.30
54	BA	2808	G	O4'-C1'-N9	5.67	112.73	108.20
21	AA	518	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	819	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	140	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	895	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	2843	G	N3-C2-N2	-5.66	115.94	119.90
54	BA	2655	G	N3-C4-C5	-5.66	125.77	128.60
54	BA	787	C	N1-C2-O2	5.66	122.30	118.90
54	BA	1490	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1564	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1865	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	2108	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2893	A	C4-C5-C6	-5.66	114.17	117.00
55	BB	68	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	422	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	482	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1415	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	2213	U	N3-C2-O2	-5.66	118.24	122.20
54	BA	581	C	N3-C2-O2	-5.66	117.94	121.90
21	AA	223	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	2297	A	O4'-C1'-N9	5.66	112.72	108.20
54	BA	2890	G	C3'-C2'-C1'	5.66	106.03	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1031	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	2271	G	O4'-C1'-N9	5.65	112.72	108.20
21	AA	525	C	N3-C2-O2	-5.65	117.94	121.90
21	AA	1501	C	N1-C2-O2	5.65	122.29	118.90
54	BA	385	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	1617	C	N3-C2-O2	-5.65	117.94	121.90
54	BA	1791	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	2825	G	N3-C2-N2	-5.65	115.94	119.90
54	BA	2232	C	N3-C2-O2	-5.65	117.95	121.90
21	AA	1397	C	C6-N1-C2	-5.65	118.04	120.30
54	BA	1025	G	O4'-C1'-N9	5.65	112.72	108.20
54	BA	2000	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	2721	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	252	U	N3-C2-O2	-5.65	118.25	122.20
21	AA	169	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	1132	C	N1-C2-O2	5.64	122.29	118.90
49	B0	15	ARG	NE-CZ-NH1	5.64	123.12	120.30
49	B0	49	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	1549	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2236	U	O4'-C1'-N1	5.64	112.72	108.20
55	BB	34	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	109	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1392	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	1993	U	O4'-C1'-N1	5.64	112.71	108.20
55	BB	100	G	N1-C6-O6	-5.64	116.52	119.90
21	AA	84	U	C3'-C2'-C1'	5.64	106.01	101.50
54	BA	532	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2439	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2496	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1221	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	2032	G	N3-C2-N2	-5.64	115.95	119.90
21	AA	199	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	221	C	N3-C2-O2	-5.64	117.95	121.90
43	BU	93	ARG	NE-CZ-NH1	5.64	123.12	120.30
54	BA	172	A	C5-C6-N1	5.64	120.52	117.70
21	AA	582	C	N3-C2-O2	-5.63	117.96	121.90
32	BJ	13	ARG	NE-CZ-NH1	5.63	123.12	120.30
54	BA	1928	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	601	C	N1-C2-O2	5.63	122.28	118.90
54	BA	676	A	C5-C6-N1	5.63	120.52	117.70
54	BA	1795	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	2126	A	C4-C5-C6	-5.63	114.18	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2493	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	2726	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	79	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	460	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	768	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	1558	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	2356	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	2461	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	288	A	C4-C5-C6	-5.63	114.19	117.00
36	BN	63	ARG	NE-CZ-NH1	5.63	123.11	120.30
54	BA	1440	U	O4'-C1'-N1	5.63	112.70	108.20
54	BA	2538	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	299	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2062	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2757	A	N1-C6-N6	-5.62	115.22	118.60
21	AA	443	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	789	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1122	G	C5-C6-N1	5.62	114.31	111.50
54	BA	1373	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1827	U	O4'-C1'-N1	5.62	112.70	108.20
54	BA	2471	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	2896	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	105	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	1593	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	1726	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	2607	G	O4'-C1'-N9	5.62	112.70	108.20
21	AA	1360	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	848	C	N1-C2-O2	5.62	122.27	118.90
21	AA	295	C	O4'-C1'-N1	5.62	112.69	108.20
54	BA	1161	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	367	G	O4'-C1'-N9	5.62	112.69	108.20
16	AQ	63	CYS	CA-C-N	5.62	129.56	117.20
21	AA	7	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	1161	C	N3-C2-O2	-5.62	117.97	121.90
54	BA	512	G	N1-C6-O6	-5.62	116.53	119.90
54	BA	848	C	N3-C4-N4	-5.61	114.07	118.00
54	BA	1104	C	N1-C2-O2	5.61	122.27	118.90
21	AA	1112	C	N3-C2-O2	-5.61	117.97	121.90
22	A1	16	C	N1-C2-O2	5.61	122.27	118.90
54	BA	882	G	N3-C2-N2	-5.61	115.97	119.90
54	BA	1936	A	P-O3'-C3'	5.61	126.43	119.70
54	BA	2542	A	C4-C5-C6	-5.61	114.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2566	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	1266	G	N3-C4-C5	-5.61	125.80	128.60
4	AE	68	ARG	NE-CZ-NH2	-5.61	117.50	120.30
21	AA	73	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	986	C	O4'-C1'-N1	5.61	112.69	108.20
55	BB	41	G	N3-C4-C5	-5.61	125.80	128.60
21	AA	148	G	N3-C2-N2	-5.61	115.98	119.90
54	BA	1200	C	N1-C2-O2	5.61	122.26	118.90
54	BA	2020	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	2863	C	N3-C2-O2	-5.61	117.98	121.90
21	AA	544	G	O4'-C1'-N9	5.60	112.68	108.20
54	BA	829	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	2448	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	1319	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1535	A	O4'-C1'-N9	5.60	112.68	108.20
21	AA	1446	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	1297	G	C3'-C2'-C1'	5.60	105.98	101.50
54	BA	2096	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	2338	C	N3-C2-O2	-5.60	117.98	121.90
21	AA	477	C	N3-C2-O2	-5.60	117.98	121.90
21	AA	1320	C	N1-C2-O2	5.60	122.26	118.90
22	A1	76	A	O4'-C1'-N9	5.60	112.68	108.20
54	BA	1286	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1655	A	N1-C6-N6	-5.60	115.24	118.60
54	BA	1913	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	263	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	520	A	C5-C6-N1	5.59	120.50	117.70
54	BA	342	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	1525	A	C6-C5-N7	5.59	136.22	132.30
54	BA	2687	U	O4'-C1'-N1	5.59	112.68	108.20
54	BA	560	C	N3-C2-O2	-5.59	117.98	121.90
54	BA	1780	A	C1'-O4'-C4'	-5.59	105.43	109.90
54	BA	2286	G	O4'-C4'-C3'	5.59	110.58	106.10
2	AC	126	ARG	NE-CZ-NH1	5.59	123.09	120.30
21	AA	361	G	C5-C6-N1	5.59	114.30	111.50
54	BA	459	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	1691	C	O4'-C1'-N1	5.59	112.67	108.20
55	BB	101	A	N1-C6-N6	-5.59	115.25	118.60
21	AA	806	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	1414	U	O4'-C1'-N1	5.59	112.67	108.20
33	BK	17	ARG	NE-CZ-NH1	5.59	123.09	120.30
54	BA	315	G	O4'-C1'-N9	5.59	112.67	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	736	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2163	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	2208	C	N3-C2-O2	-5.59	117.99	121.90
21	AA	210	C	C3'-C2'-C1'	5.59	105.97	101.50
21	AA	1069	C	O4'-C1'-N1	5.59	112.67	108.20
21	AA	1096	C	N1-C2-O2	5.59	122.25	118.90
54	BA	1356	G	N1-C6-O6	-5.59	116.55	119.90
54	BA	1872	A	C4-C5-C6	-5.59	114.21	117.00
54	BA	2494	G	O4'-C1'-N9	5.59	112.67	108.20
54	BA	2558	C	O4'-C1'-N1	5.58	112.67	108.20
54	BA	528	A	O4'-C1'-N9	5.58	112.67	108.20
54	BA	1838	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	2658	C	C5'-C4'-O4'	5.58	115.80	109.10
21	AA	85	U	O4'-C1'-N1	5.58	112.67	108.20
21	AA	663	A	C6-C5-N7	5.58	136.21	132.30
54	BA	691	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	1126	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2701	U	O4'-C1'-N1	5.58	112.67	108.20
54	BA	1185	G	O4'-C1'-N9	5.58	112.66	108.20
55	BB	54	G	N1-C6-O6	-5.58	116.55	119.90
21	AA	108	G	N3-C4-C5	-5.58	125.81	128.60
21	AA	830	G	C5-C6-N1	5.58	114.29	111.50
21	AA	1162	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	1388	C	O4'-C1'-N1	5.58	112.66	108.20
54	BA	32	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	52	A	C5'-C4'-C3'	-5.58	107.07	116.00
54	BA	831	G	N3-C2-N2	-5.58	115.99	119.90
54	BA	833	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2775	G	N1-C6-O6	-5.58	116.55	119.90
21	AA	586	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	69	C	O4'-C1'-N1	5.58	112.66	108.20
54	BA	889	C	C5'-C4'-C3'	-5.58	107.08	116.00
54	BA	1858	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	2499	C	O4'-C1'-N1	5.58	112.66	108.20
54	BA	2716	C	O4'-C1'-N1	5.58	112.66	108.20
21	AA	1069	C	C1'-O4'-C4'	-5.57	105.44	109.90
54	BA	862	G	N3-C4-C5	-5.57	125.81	128.60
55	BB	36	C	N1-C2-O2	5.57	122.24	118.90
46	BX	17	ARG	NE-CZ-NH1	5.57	123.09	120.30
54	BA	1940	U	N3-C2-O2	-5.57	118.30	122.20
54	BA	1990	C	O4'-C1'-N1	5.57	112.66	108.20
21	AA	556	C	N1-C2-O2	5.57	122.24	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1267	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	1447	A	C2-N3-C4	5.57	113.39	110.60
54	BA	433	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	976	G	N3-C4-N9	5.57	129.34	126.00
54	BA	692	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	2150	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	578	C	N1-C2-O2	5.57	122.24	118.90
21	AA	1331	G	N1-C6-O6	-5.57	116.56	119.90
22	A1	59	U	O4'-C1'-N1	5.57	112.65	108.20
54	BA	425	G	N1-C6-O6	-5.57	116.56	119.90
54	BA	740	C	N1-C2-O2	5.57	122.24	118.90
54	BA	887	U	O4'-C1'-N1	5.57	112.65	108.20
54	BA	1469	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	1876	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	504	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	670	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1837	C	N3-C2-O2	-5.56	118.01	121.90
21	AA	213	G	O4'-C1'-N9	5.56	112.65	108.20
21	AA	248	C	O4'-C1'-N1	5.56	112.65	108.20
21	AA	535	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	466	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	739	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1178	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	2501	C	N1-C2-O2	5.56	122.23	118.90
54	BA	1210	G	N1-C6-O6	-5.56	116.57	119.90
54	BA	2497	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	207	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	471	A	N1-C6-N6	-5.55	115.27	118.60
54	BA	843	G	O4'-C1'-N9	5.55	112.64	108.20
54	BA	1698	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	2319	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	2339	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	2612	C	N1-C2-O2	5.55	122.23	118.90
55	BB	9	G	N3-C2-N2	-5.55	116.01	119.90
54	BA	1393	A	C6-C5-N7	5.55	136.19	132.30
21	AA	1214	C	O4'-C1'-N1	5.55	112.64	108.20
21	AA	1427	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	1465	G	C3'-C2'-C1'	5.55	105.94	101.50
54	BA	1816	C	O4'-C1'-N1	5.55	112.64	108.20
55	BB	115	A	C4-C5-C6	-5.55	114.22	117.00
21	AA	631	C	N1-C2-O2	5.55	122.23	118.90
21	AA	1296	C	N1-C2-O2	5.55	122.23	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	851	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	2044	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	2359	C	O4'-C1'-N1	5.55	112.64	108.20
55	BB	105	G	N3-C2-N2	-5.55	116.02	119.90
54	BA	414	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	552	U	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1609	A	C4-C5-C6	-5.55	114.23	117.00
20	AU	30	GLU	C-N-CA	5.55	135.57	121.70
54	BA	210	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	602	A	C6-C5-N7	5.55	136.18	132.30
54	BA	964	C	N1-C2-O2	5.55	122.23	118.90
54	BA	2474	U	N3-C2-O2	-5.55	118.32	122.20
54	BA	2535	G	N3-C2-N2	-5.55	116.02	119.90
21	AA	461	A	O4'-C1'-N9	5.54	112.64	108.20
21	AA	492	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	992	U	O4'-C1'-N1	5.54	112.64	108.20
54	BA	765	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1754	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2626	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	1318	A	C4-C5-C6	-5.54	114.23	117.00
22	A1	30	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	1925	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	2660	A	O4'-C1'-N9	5.54	112.63	108.20
21	AA	487	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	856	C	N1-C2-O2	5.54	122.22	118.90
54	BA	858	G	O4'-C1'-N9	5.54	112.63	108.20
54	BA	1019	U	O4'-C1'-N1	5.54	112.63	108.20
21	AA	47	C	N1-C2-O2	5.54	122.22	118.90
21	AA	431	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	1101	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	574	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	1934	C	N3-C2-O2	-5.54	118.02	121.90
54	BA	2226	C	N1-C2-O2	5.54	122.22	118.90
54	BA	2534	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	2792	A	C4-C5-C6	-5.54	114.23	117.00
39	BQ	63	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
21	AA	20	U	O4'-C1'-N1	5.54	112.63	108.20
21	AA	610	U	O4'-C1'-N1	5.54	112.63	108.20
21	AA	898	G	N1-C6-O6	-5.54	116.58	119.90
21	AA	1447	A	C4-C5-C6	-5.54	114.23	117.00
22	A1	73	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	459	A	C4-C5-C6	-5.53	114.23	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	622	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	1070	U	O4'-C1'-N1	5.53	112.62	108.20
21	AA	1139	G	N3-C2-N2	-5.53	116.03	119.90
21	AA	1388	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	854	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	902	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	2478	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	805	C	O4'-C1'-N1	5.53	112.62	108.20
21	AA	900	A	O4'-C1'-N9	5.53	112.62	108.20
54	BA	1679	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	2794	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	597	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	256	A	O4'-C1'-N9	5.53	112.62	108.20
54	BA	274	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	820	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	979	A	C4-C5-C6	-5.53	114.24	117.00
21	AA	1339	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	1088	A	O4'-C1'-N9	5.53	112.62	108.20
54	BA	1306	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2512	C	O4'-C1'-N1	5.53	112.62	108.20
54	BA	6	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	253	C	O4'-C1'-N1	5.52	112.62	108.20
55	BB	38	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	493	A	O4'-C1'-N9	5.52	112.62	108.20
21	AA	569	C	N3-C2-O2	-5.52	118.03	121.90
21	AA	746	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	999	C	O4'-C1'-N1	5.52	112.62	108.20
34	BL	2	ARG	NE-CZ-NH1	5.52	123.06	120.30
54	BA	251	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	337	C	O4'-C1'-N1	5.52	112.62	108.20
54	BA	2772	C	N3-C2-O2	-5.52	118.03	121.90
55	BB	103	U	O4'-C1'-N1	5.52	112.62	108.20
54	BA	1614	A	C6-C5-N7	5.52	136.16	132.30
54	BA	1951	U	O4'-C1'-N1	5.52	112.62	108.20
21	AA	1229	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	706	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1540	G	N3-C2-N2	-5.52	116.04	119.90
54	BA	1884	G	N1-C6-O6	-5.52	116.59	119.90
54	BA	2145	C	N1-C2-O2	5.52	122.21	118.90
21	AA	40	C	N3-C2-O2	-5.52	118.04	121.90
21	AA	320	A	C3'-C2'-C1'	5.52	105.91	101.50
46	BX	44	ARG	NE-CZ-NH1	5.52	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1274	A	C4-C5-C6	-5.52	114.24	117.00
22	A1	62	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	509	C	N1-C2-O2	5.52	122.21	118.90
54	BA	896	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2019	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	1184	G	N3-C2-N2	-5.51	116.04	119.90
22	A1	53	G	N1-C6-O6	-5.51	116.59	119.90
54	BA	239	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	624	C	N1-C2-O2	5.51	122.21	118.90
54	BA	328	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	402	A	C5-C6-N1	5.51	120.46	117.70
54	BA	1029	A	C6-C5-N7	5.51	136.16	132.30
54	BA	2013	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	2191	A	C4-C5-C6	-5.51	114.25	117.00
8	AI	105	ARG	NE-CZ-NH2	-5.51	117.55	120.30
21	AA	85	U	N3-C2-O2	-5.51	118.34	122.20
54	BA	51	G	O4'-C1'-N9	5.51	112.61	108.20
54	BA	8	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	1742	U	O4'-C1'-N1	5.51	112.61	108.20
21	AA	1048	G	C3'-C2'-C1'	5.51	105.91	101.50
22	A1	66	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	1646	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	476	U	O4'-C1'-N1	5.50	112.60	108.20
24	A3	13	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	973	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	2655	G	C8-N9-C4	-5.50	104.20	106.40
54	BA	2030	A	O4'-C1'-N9	5.50	112.60	108.20
54	BA	162	U	N3-C2-O2	-5.50	118.35	122.20
4	AE	44	ARG	NE-CZ-NH1	5.50	123.05	120.30
21	AA	217	C	N1-C2-O2	5.50	122.20	118.90
21	AA	1252	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	528	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	857	G	C8-N9-C4	-5.50	104.20	106.40
54	BA	953	G	N1-C6-O6	-5.50	116.60	119.90
55	BB	109	A	O4'-C1'-N9	5.50	112.60	108.20
54	BA	807	U	O4'-C1'-N1	5.50	112.60	108.20
54	BA	1122	G	N3-C2-N2	-5.50	116.05	119.90
54	BA	2705	A	C6-C5-N7	5.50	136.15	132.30
21	AA	40	C	O4'-C1'-N1	5.50	112.60	108.20
21	AA	194	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	2380	C	O4'-C1'-N1	5.50	112.60	108.20
12	AM	59	VAL	C-N-CA	5.49	135.43	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	405	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	2657	A	C4-C5-C6	-5.49	114.25	117.00
52	B3	39	ARG	NE-CZ-NH1	5.49	123.05	120.30
54	BA	538	A	C4-C5-C6	-5.49	114.25	117.00
21	AA	1055	A	C4-C5-C6	-5.49	114.25	117.00
21	AA	1496	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	698	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	1354	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	1793	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1868	C	O4'-C1'-N1	5.49	112.59	108.20
21	AA	1012	A	C4-C5-C6	-5.49	114.25	117.00
22	A1	75	C	N1-C2-O2	5.49	122.19	118.90
24	A3	16	C	N1-C2-O2	5.49	122.19	118.90
54	BA	105	C	C5'-C4'-O4'	5.49	115.69	109.10
54	BA	1595	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1677	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	1782	U	O4'-C4'-C3'	5.49	110.49	106.10
54	BA	2109	U	O4'-C1'-N1	5.49	112.59	108.20
21	AA	366	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	1221	C	N1-C2-O2	5.49	122.19	118.90
54	BA	1254	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	2129	C	N1-C2-O2	5.49	122.19	118.90
21	AA	489	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	101	A	O4'-C1'-N9	5.48	112.59	108.20
54	BA	288	U	O4'-C1'-N1	5.48	112.59	108.20
21	AA	972	C	N1-C2-O2	5.48	122.19	118.90
54	BA	45	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	140	C	N3-C4-C5	5.48	124.09	121.90
54	BA	2076	U	N3-C2-O2	-5.48	118.36	122.20
54	BA	2587	A	C4-C5-C6	-5.48	114.26	117.00
55	BB	90	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	341	C	O4'-C1'-N1	5.48	112.58	108.20
54	BA	784	G	N3-C4-C5	-5.48	125.86	128.60
54	BA	2140	G	O4'-C1'-N9	5.48	112.58	108.20
54	BA	129	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	2521	C	N3-C2-O2	-5.48	118.06	121.90
54	BA	745	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	782	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	928	A	C6-C5-N7	5.48	136.13	132.30
54	BA	2662	A	N1-C6-N6	-5.48	115.31	118.60
55	BB	111	U	N3-C2-O2	-5.48	118.36	122.20
21	AA	708	C	N1-C2-O2	5.48	122.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1001	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	2286	G	N1-C6-O6	-5.48	116.61	119.90
54	BA	2644	G	N3-C2-N2	-5.48	116.07	119.90
21	AA	327	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	423	G	O4'-C1'-N9	5.47	112.58	108.20
54	BA	888	C	N1-C2-O2	5.47	122.18	118.90
54	BA	2084	C	N1-C2-O2	5.47	122.18	118.90
21	AA	225	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	1323	C	O4'-C1'-N1	5.47	112.58	108.20
55	BB	101	A	C4-C5-C6	-5.47	114.26	117.00
54	BA	158	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	201	C	N3-C2-O2	-5.47	118.07	121.90
54	BA	1729	U	N3-C2-O2	-5.47	118.37	122.20
21	AA	1190	G	N3-C4-C5	-5.47	125.86	128.60
54	BA	623	C	C5'-C4'-O4'	5.47	115.66	109.10
54	BA	1222	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	1542	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	523	C	N1-C2-O2	5.47	122.18	118.90
54	BA	1902	C	N1-C2-O2	5.47	122.18	118.90
21	AA	766	A	C6-C5-N7	5.47	136.13	132.30
54	BA	48	G	C5'-C4'-O4'	5.47	115.66	109.10
54	BA	1860	G	O4'-C1'-N9	5.47	112.57	108.20
54	BA	2715	C	N1-C2-O2	5.47	122.18	118.90
21	AA	688	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	455	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	675	A	C6-C5-N7	5.46	136.12	132.30
54	BA	1954	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	2068	U	O4'-C1'-N1	5.46	112.57	108.20
55	BB	99	A	C4-C5-C6	-5.46	114.27	117.00
9	AJ	62	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	2425	A	C6-C5-N7	5.46	136.12	132.30
54	BA	2449	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	2821	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1331	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	2040	G	O4'-C1'-N9	5.46	112.57	108.20
54	BA	2008	C	O4'-C1'-N1	5.46	112.57	108.20
54	BA	2195	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	2299	U	O4'-C1'-N1	5.46	112.57	108.20
21	AA	135	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	91	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	272	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1800	C	O4'-C1'-N1	5.46	112.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	483	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	2551	C	O4'-C1'-N1	5.46	112.57	108.20
21	AA	7	A	O4'-C1'-N9	5.46	112.56	108.20
21	AA	681	A	C6-C5-N7	5.46	136.12	132.30
54	BA	1431	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	2244	U	O4'-C1'-N1	5.46	112.56	108.20
12	AM	78	ARG	NE-CZ-NH1	5.45	123.03	120.30
21	AA	1167	A	C4-C5-C6	-5.45	114.27	117.00
21	AA	1236	A	C4-C5-C6	-5.45	114.27	117.00
45	BW	74	LYS	C-N-CA	5.45	135.33	121.70
54	BA	608	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	720	U	O4'-C1'-N1	5.45	112.56	108.20
54	BA	1189	A	C4-C5-C6	-5.45	114.27	117.00
22	A1	76	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	210	C	N1-C2-O2	5.45	122.17	118.90
21	AA	409	U	O4'-C1'-N1	5.45	112.56	108.20
21	AA	880	C	O4'-C1'-N1	5.45	112.56	108.20
21	AA	1450	U	N3-C2-O2	-5.45	118.39	122.20
54	BA	1621	U	O4'-C1'-N1	5.45	112.56	108.20
21	AA	1309	G	N7-C8-N9	5.45	115.82	113.10
54	BA	1378	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	1915	U	O4'-C1'-N1	5.45	112.56	108.20
21	AA	1203	C	N1-C2-O2	5.45	122.17	118.90
24	A3	38	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2001	C	N3-C4-C5	5.45	124.08	121.90
54	BA	2298	A	C4-C5-C6	-5.45	114.28	117.00
22	A1	17	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	2301	C	N3-C2-O2	-5.44	118.09	121.90
21	AA	335	C	C5'-C4'-C3'	-5.44	107.29	116.00
21	AA	461	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	16	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	723	C	O4'-C1'-N1	5.44	112.56	108.20
54	BA	743	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1818	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	1894	C	N1-C2-O2	5.44	122.16	118.90
54	BA	2531	A	C4-C5-C6	-5.44	114.28	117.00
55	BB	81	G	N1-C6-O6	-5.44	116.64	119.90
21	AA	371	A	C6-C5-N7	5.44	136.11	132.30
21	AA	785	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	300	A	C6-C5-N7	5.44	136.11	132.30
54	BA	2577	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	182	A	O4'-C1'-N9	5.44	112.55	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	195	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	621	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	987	C	N1-C2-O2	5.43	122.16	118.90
54	BA	1789	A	C6-C5-N7	5.43	136.10	132.30
14	AO	16	ARG	NE-CZ-NH2	-5.43	117.58	120.30
54	BA	247	G	N3-C2-N2	-5.43	116.10	119.90
54	BA	1010	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	2214	C	N1-C2-O2	5.43	122.16	118.90
21	AA	583	A	C6-C5-N7	5.43	136.10	132.30
21	AA	1108	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	989	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1339	G	N3-C2-N2	-5.43	116.10	119.90
54	BA	643	A	C4-C5-C6	-5.43	114.28	117.00
54	BA	2177	C	N3-C2-O2	-5.43	118.10	121.90
49	B0	16	ARG	NE-CZ-NH1	5.43	123.01	120.30
21	AA	120	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	125	U	C5'-C4'-C3'	-5.43	107.32	116.00
54	BA	1919	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	2014	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	2508	G	N1-C6-O6	-5.43	116.64	119.90
24	A3	10	G	N1-C6-O6	-5.42	116.64	119.90
54	BA	225	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	1790	C	N3-C2-O2	-5.42	118.10	121.90
54	BA	177	G	N3-C4-C5	-5.42	125.89	128.60
21	AA	661	G	N3-C2-N2	-5.42	116.11	119.90
23	A2	82	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	329	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	717	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	1089	A	O4'-C1'-C2'	-5.42	100.38	105.80
54	BA	1287	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1519	A	C6-C5-N7	5.42	136.09	132.30
54	BA	1669	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	1485	U	O4'-C1'-N1	5.42	112.53	108.20
54	BA	514	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2216	G	C8-N9-C4	-5.42	104.23	106.40
24	A3	45	A	C6-C5-N7	5.42	136.09	132.30
54	BA	1293	C	N1-C2-O2	5.42	122.15	118.90
22	A1	14	A	C5'-C4'-O4'	5.41	115.60	109.10
54	BA	221	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	1128	G	O4'-C1'-N9	5.41	112.53	108.20
54	BA	1597	A	C1'-O4'-C4'	-5.41	105.57	109.90
54	BA	2004	G	N1-C6-O6	-5.41	116.65	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BB	91	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1804	C	N1-C2-O2	5.41	122.15	118.90
14	AO	62	ARG	NE-CZ-NH1	5.41	123.00	120.30
21	AA	1490	U	O4'-C1'-N1	5.41	112.53	108.20
52	B3	41	ARG	NE-CZ-NH1	5.41	123.00	120.30
54	BA	1092	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	2078	C	N1-C2-O2	5.41	122.15	118.90
55	BB	109	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	1139	G	N1-C6-O6	-5.41	116.65	119.90
54	BA	1349	C	N1-C2-O2	5.41	122.14	118.90
54	BA	1855	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1774	C	O4'-C1'-N1	5.41	112.53	108.20
21	AA	96	U	O4'-C1'-N1	5.41	112.52	108.20
54	BA	308	G	C3'-C2'-C1'	5.41	105.83	101.50
21	AA	247	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	331	C	N1-C2-O2	5.40	122.14	118.90
21	AA	397	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	758	C	N1-C2-O2	5.40	122.14	118.90
21	AA	961	U	N3-C2-O2	-5.40	118.42	122.20
21	AA	1279	G	N3-C4-C5	-5.40	125.90	128.60
54	BA	764	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2173	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2205	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2345	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	558	U	N3-C2-O2	-5.40	118.42	122.20
54	BA	620	G	C5-C6-N1	5.40	114.20	111.50
54	BA	2043	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	2400	G	N1-C6-O6	-5.40	116.66	119.90
54	BA	2515	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2777	G	N1-C6-O6	-5.40	116.66	119.90
21	AA	1250	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	587	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	1311	G	O4'-C1'-N9	5.40	112.52	108.20
21	AA	77	A	C4-C5-C6	-5.40	114.30	117.00
21	AA	320	A	C6-C5-N7	5.40	136.08	132.30
21	AA	801	U	O4'-C1'-N1	5.40	112.52	108.20
24	A3	77	A	N7-C8-N9	5.40	116.50	113.80
54	BA	680	C	C5'-C4'-O4'	5.40	115.58	109.10
54	BA	1175	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	2183	A	N1-C6-N6	-5.40	115.36	118.60
54	BA	2889	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	1757	A	O4'-C1'-N9	5.40	112.52	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2222	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2683	C	O4'-C1'-N1	5.40	112.52	108.20
21	AA	833	G	N1-C6-O6	-5.39	116.66	119.90
54	BA	401	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	593	U	O4'-C1'-N1	5.39	112.52	108.20
54	BA	1008	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	1067	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	1957	C	N3-C2-O2	-5.39	118.12	121.90
21	AA	97	G	N1-C6-O6	-5.39	116.66	119.90
54	BA	372	G	N1-C6-O6	-5.39	116.66	119.90
54	BA	620	G	C2-N3-C4	5.39	114.60	111.90
54	BA	2204	G	C5-C6-N1	5.39	114.20	111.50
54	BA	2667	C	N1-C2-O2	5.39	122.14	118.90
54	BA	2857	G	N1-C6-O6	-5.39	116.67	119.90
55	BB	94	A	C6-C5-N7	5.39	136.07	132.30
21	AA	183	C	N1-C2-O2	5.39	122.14	118.90
21	AA	1345	U	O4'-C1'-N1	5.39	112.51	108.20
22	A1	61	C	N1-C2-O2	5.39	122.14	118.90
21	AA	261	U	N3-C2-O2	-5.39	118.43	122.20
21	AA	765	G	N3-C4-C5	-5.39	125.91	128.60
54	BA	1219	U	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1699	G	C1'-O4'-C4'	-5.39	105.59	109.90
54	BA	2171	A	P-O3'-C3'	5.39	126.17	119.70
54	BA	2531	A	C3'-C2'-C1'	5.39	105.81	101.50
54	BA	2886	A	C4-C5-C6	-5.39	114.31	117.00
22	A1	51	C	N3-C2-O2	-5.39	118.13	121.90
21	AA	29	U	O4'-C1'-N1	5.39	112.51	108.20
21	AA	164	G	N3-C2-N2	-5.39	116.13	119.90
21	AA	568	G	N3-C2-N2	-5.39	116.13	119.90
21	AA	651	C	N3-C2-O2	-5.39	118.13	121.90
21	AA	756	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	671	C	N1-C2-O2	5.39	122.13	118.90
54	BA	1022	G	O4'-C1'-N9	5.39	112.51	108.20
54	BA	1364	G	O4'-C1'-N9	5.39	112.51	108.20
54	BA	1404	C	O4'-C1'-N1	5.39	112.51	108.20
54	BA	1591	A	C6-C5-N7	5.39	136.07	132.30
1	AB	207	ARG	NE-CZ-NH2	-5.38	117.61	120.30
21	AA	447	G	N1-C6-O6	-5.38	116.67	119.90
24	A3	14	A	C5'-C4'-O4'	5.38	115.56	109.10
54	BA	835	C	C5'-C4'-O4'	5.38	115.56	109.10
54	BA	1731	G	O4'-C1'-N9	5.38	112.51	108.20
54	BA	235	U	O4'-C1'-N1	5.38	112.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2434	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	808	C	N3-C2-O2	-5.38	118.13	121.90
54	BA	561	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	1572	A	N1-C6-N6	-5.38	115.37	118.60
54	BA	2598	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	2814	A	C6-C5-N7	5.38	136.07	132.30
21	AA	852	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	2331	G	O4'-C1'-N9	5.38	112.50	108.20
21	AA	530	G	C5-C6-N1	5.38	114.19	111.50
21	AA	792	A	C1'-O4'-C4'	-5.38	105.60	109.90
54	BA	493	G	O4'-C1'-N9	5.38	112.50	108.20
54	BA	672	C	N1-C2-O2	5.38	122.13	118.90
54	BA	2146	C	N1-C2-O2	5.38	122.13	118.90
21	AA	43	C	N3-C2-O2	-5.38	118.14	121.90
21	AA	1191	A	C4-C5-C6	-5.38	114.31	117.00
21	AA	1358	U	O4'-C1'-N1	5.38	112.50	108.20
54	BA	2015	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	2406	A	C4-C5-C6	-5.38	114.31	117.00
54	BA	2608	G	N1-C6-O6	-5.38	116.67	119.90
54	BA	707	G	N3-C2-N2	-5.38	116.14	119.90
54	BA	1507	C	O4'-C1'-N1	5.38	112.50	108.20
21	AA	705	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	1069	A	O4'-C1'-N9	5.37	112.50	108.20
54	BA	2686	G	N3-C4-C5	-5.37	125.91	128.60
8	AI	40	ARG	NE-CZ-NH1	5.37	122.99	120.30
21	AA	825	A	C6-C5-N7	5.37	136.06	132.30
21	AA	911	U	O4'-C1'-N1	5.37	112.50	108.20
21	AA	1184	G	C5-C6-N1	5.37	114.19	111.50
35	BM	66	ARG	NE-CZ-NH2	-5.37	117.61	120.30
54	BA	853	C	N1-C2-O2	5.37	122.12	118.90
21	AA	1497	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	311	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	975	A	C4-C5-C6	-5.37	114.32	117.00
54	BA	1340	U	N3-C2-O2	-5.37	118.44	122.20
54	BA	1462	C	N1-C2-O2	5.37	122.12	118.90
1	AB	20	ARG	NE-CZ-NH1	5.37	122.98	120.30
3	AD	183	ARG	NE-CZ-NH1	5.37	122.98	120.30
54	BA	558	U	O4'-C1'-N1	5.37	112.49	108.20
54	BA	1241	A	C4-C5-C6	-5.37	114.32	117.00
54	BA	1675	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	1890	A	C4-C5-C6	-5.37	114.32	117.00
54	BA	2458	G	N3-C4-C5	-5.37	125.92	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2627	G	N1-C2-N2	5.37	121.03	116.20
54	BA	2650	U	O4'-C1'-N1	5.37	112.49	108.20
21	AA	1479	C	N1-C2-O2	5.36	122.12	118.90
54	BA	1053	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2009	A	C6-C5-N7	5.36	136.06	132.30
54	BA	732	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2885	G	O4'-C1'-N9	5.36	112.49	108.20
21	AA	1399	C	N1-C2-O2	5.36	122.12	118.90
54	BA	2358	A	C6-C5-N7	5.36	136.05	132.30
21	AA	971	G	O4'-C1'-N9	5.36	112.49	108.20
54	BA	835	C	N1-C2-O2	5.36	122.11	118.90
21	AA	1197	A	C4-C5-C6	-5.36	114.32	117.00
22	A1	70	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	179	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	192	C	O4'-C1'-N1	5.36	112.48	108.20
54	BA	426	C	O4'-C1'-N1	5.36	112.48	108.20
54	BA	435	C	N1-C2-O2	5.36	122.11	118.90
54	BA	1439	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	120	A	C3'-C2'-C1'	5.35	105.78	101.50
21	AA	1109	C	N1-C2-O2	5.35	122.11	118.90
22	A1	26	A	N1-C6-N6	-5.35	115.39	118.60
54	BA	1926	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2509	G	O4'-C1'-N9	5.35	112.48	108.20
54	BA	2647	U	N3-C2-O2	-5.35	118.45	122.20
21	AA	1333	A	C6-C5-N7	5.35	136.05	132.30
54	BA	804	A	C3'-C2'-C1'	5.35	105.78	101.50
21	AA	161	A	C4-C5-C6	-5.35	114.33	117.00
21	AA	336	A	C4-C5-C6	-5.35	114.33	117.00
54	BA	98	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	1841	U	N3-C2-O2	-5.35	118.45	122.20
21	AA	693	G	N3-C4-C5	-5.35	125.93	128.60
21	AA	814	A	C4-C5-C6	-5.35	114.33	117.00
21	AA	859	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	2164	C	N3-C4-C5	5.35	124.04	121.90
55	BB	19	C	O4'-C1'-N1	5.35	112.48	108.20
54	BA	2688	G	N1-C6-O6	-5.35	116.69	119.90
21	AA	193	C	N3-C2-O2	-5.34	118.16	121.90
21	AA	582	C	C5'-C4'-O4'	5.34	115.51	109.10
21	AA	1462	C	N1-C2-O2	5.34	122.11	118.90
54	BA	1507	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1644	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1978	A	C4-C5-C6	-5.34	114.33	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1994	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	2876	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	425	G	O4'-C1'-N9	5.34	112.47	108.20
54	BA	878	A	C6-C5-N7	5.34	136.04	132.30
54	BA	1111	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	1118	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1547	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	579	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	2741	A	O4'-C1'-N9	5.34	112.47	108.20
54	BA	2540	C	N1-C2-O2	5.34	122.10	118.90
21	AA	108	G	N1-C6-O6	-5.34	116.70	119.90
21	AA	890	G	C8-N9-C4	-5.34	104.27	106.40
54	BA	892	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	1271	G	N1-C6-O6	-5.34	116.70	119.90
54	BA	1499	C	N1-C2-O2	5.34	122.10	118.90
21	AA	697	U	N3-C2-O2	-5.33	118.47	122.20
21	AA	1403	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	1604	C	O4'-C1'-N1	5.33	112.47	108.20
21	AA	510	A	C6-C5-N7	5.33	136.03	132.30
21	AA	1533	C	N3-C4-C5	5.33	124.03	121.90
54	BA	1792	G	N1-C6-O6	-5.33	116.70	119.90
7	AH	14	ARG	NE-CZ-NH1	5.33	122.97	120.30
54	BA	1927	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	2852	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	200	U	O4'-C1'-N1	5.33	112.46	108.20
54	BA	2519	U	O3'-P-O5'	-5.33	93.87	104.00
21	AA	373	A	C4-C5-C6	-5.33	114.33	117.00
21	AA	498	A	O4'-C1'-N9	5.33	112.46	108.20
22	A1	36	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	737	C	N3-C4-C5	5.33	124.03	121.90
21	AA	746	A	N1-C6-N6	-5.33	115.41	118.60
54	BA	1115	G	C5-C6-N1	5.33	114.16	111.50
54	BA	1533	C	O4'-C1'-N1	5.33	112.46	108.20
54	BA	1805	A	C6-C5-N7	5.33	136.03	132.30
21	AA	275	G	C5-C6-N1	5.32	114.16	111.50
21	AA	1094	G	O4'-C1'-N9	5.32	112.46	108.20
24	A3	72	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	530	G	N3-C2-N2	-5.32	116.17	119.90
54	BA	622	G	N1-C6-O6	-5.32	116.70	119.90
54	BA	859	G	N3-C2-N2	-5.32	116.17	119.90
54	BA	1587	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	990	A	C4-C5-C6	-5.32	114.34	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2353	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	908	C	N3-C2-O2	-5.32	118.18	121.90
54	BA	1103	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	1809	A	O4'-C1'-N9	5.32	112.45	108.20
54	BA	2132	U	N3-C2-O2	-5.32	118.48	122.20
54	BA	2691	C	O4'-C1'-N1	5.32	112.45	108.20
21	AA	13	U	O4'-C1'-N1	5.32	112.45	108.20
21	AA	26	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	537	G	N3-C4-C5	-5.32	125.94	128.60
54	BA	1514	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	2083	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	2275	C	N1-C2-O2	5.32	122.09	118.90
54	BA	2418	A	O4'-C1'-N9	5.32	112.45	108.20
54	BA	2576	G	N3-C2-N2	-5.32	116.18	119.90
54	BA	2805	C	O4'-C1'-N1	5.32	112.45	108.20
54	BA	2826	A	C4-C5-C6	-5.32	114.34	117.00
21	AA	345	C	C1'-O4'-C4'	-5.32	105.65	109.90
21	AA	557	G	N1-C6-O6	-5.32	116.71	119.90
21	AA	1431	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	588	U	C3'-C2'-C1'	5.32	105.75	101.50
54	BA	1072	C	C1'-O4'-C4'	-5.32	105.65	109.90
54	BA	1217	U	O4'-C1'-N1	5.32	112.45	108.20
54	BA	2140	G	C5-C6-N1	5.32	114.16	111.50
54	BA	752	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	996	A	C6-C5-N7	5.31	136.02	132.30
54	BA	1513	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1656	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	2112	G	N1-C6-O6	-5.31	116.71	119.90
21	AA	19	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	443	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	974	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	2271	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	2883	A	C4-C5-C6	-5.31	114.34	117.00
21	AA	340	U	O4'-C1'-N1	5.31	112.45	108.20
21	AA	554	A	O4'-C1'-N9	5.31	112.45	108.20
54	BA	149	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	196	A	C1'-O4'-C4'	-5.31	105.65	109.90
54	BA	267	C	O4'-C1'-N1	5.31	112.45	108.20
54	BA	460	A	C4-C5-C6	-5.31	114.34	117.00
54	BA	2558	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	2676	C	N1-C2-O2	5.31	122.09	118.90
21	AA	562	U	N3-C2-O2	-5.31	118.48	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	378	C	N1-C2-O2	5.31	122.08	118.90
54	BA	824	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1674	G	O4'-C1'-N9	5.31	112.45	108.20
54	BA	2344	U	N3-C2-O2	-5.31	118.48	122.20
55	BB	69	G	N1-C6-O6	-5.31	116.72	119.90
21	AA	158	G	C2'-C3'-O3'	5.31	122.19	113.70
37	BO	102	ARG	NE-CZ-NH1	5.31	122.95	120.30
54	BA	330	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	441	U	O4'-C1'-N1	5.31	112.44	108.20
54	BA	1099	G	N1-C6-O6	-5.31	116.72	119.90
54	BA	1384	A	C6-C5-N7	5.31	136.01	132.30
54	BA	1445	G	C5-C6-N1	5.31	114.15	111.50
21	AA	466	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	650	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	893	C	N3-C2-O2	-5.30	118.19	121.90
21	AA	1206	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	1224	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	349	U	O4'-C1'-N1	5.30	112.44	108.20
21	AA	281	G	C3'-C2'-C1'	5.30	105.74	101.50
54	BA	1720	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2340	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	687	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	1179	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	1182	G	N3-C2-N2	-5.30	116.19	119.90
54	BA	366	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	540	C	O4'-C1'-N1	5.30	112.44	108.20
54	BA	1305	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	2441	U	N3-C2-O2	-5.30	118.49	122.20
21	AA	473	U	N3-C2-O2	-5.30	118.49	122.20
28	BF	101	ARG	NE-CZ-NH1	5.30	122.95	120.30
34	BL	60	ARG	NE-CZ-NH1	5.30	122.95	120.30
21	AA	1300	G	N1-C6-O6	-5.30	116.72	119.90
21	AA	624	C	O4'-C1'-N1	5.30	112.44	108.20
47	BY	29	ARG	NE-CZ-NH2	-5.30	117.65	120.30
54	BA	1315	C	N1-C2-O2	5.30	122.08	118.90
54	BA	1451	C	C2'-C3'-O3'	5.30	122.17	113.70
21	AA	1280	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	2200	C	O4'-C1'-N1	5.29	112.44	108.20
55	BB	70	C	C5'-C4'-O4'	5.29	115.45	109.10
6	AG	91	ARG	NE-CZ-NH1	5.29	122.95	120.30
21	AA	864	A	C4-C5-C6	-5.29	114.35	117.00
47	BY	7	ARG	NE-CZ-NH1	5.29	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1866	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	2330	G	O4'-C1'-N9	5.29	112.44	108.20
34	BL	18	ARG	NE-CZ-NH2	-5.29	117.65	120.30
54	BA	893	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	2748	A	C4-C5-C6	-5.29	114.35	117.00
21	AA	1126	U	O4'-C1'-N1	5.29	112.43	108.20
21	AA	1227	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	1674	G	C3'-C2'-C1'	5.29	105.73	101.50
54	BA	1820	U	N1-C2-N3	5.29	118.07	114.90
54	BA	2896	C	O4'-C1'-N1	5.29	112.43	108.20
21	AA	533	A	C4-C5-C6	-5.29	114.36	117.00
21	AA	770	C	O4'-C1'-N1	5.29	112.43	108.20
21	AA	1303	C	O4'-C1'-N1	5.29	112.43	108.20
54	BA	90	U	O4'-C1'-N1	5.29	112.43	108.20
54	BA	826	U	N3-C2-O2	-5.29	118.50	122.20
55	BB	106	G	C5-C6-N1	5.29	114.14	111.50
16	AQ	63	CYS	O-C-N	-5.28	114.25	122.70
21	AA	50	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	231	U	O4'-C1'-N1	5.28	112.43	108.20
21	AA	1410	A	C6-C5-N7	5.28	136.00	132.30
54	BA	2172	U	O4'-C1'-N1	5.28	112.43	108.20
21	AA	563	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1470	U	C1'-O4'-C4'	-5.28	105.67	109.90
54	BA	275	C	C3'-C2'-C1'	5.28	105.73	101.50
54	BA	316	C	N1-C2-O2	5.28	122.07	118.90
54	BA	1268	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	971	G	N9-C4-C5	5.28	107.51	105.40
21	AA	1021	A	C6-C5-N7	5.28	136.00	132.30
21	AA	1072	G	C8-N9-C4	-5.28	104.29	106.40
54	BA	732	C	N3-C2-O2	-5.28	118.20	121.90
54	BA	1176	U	O4'-C1'-N1	5.28	112.42	108.20
21	AA	1080	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1493	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1509	C	N1-C2-O2	5.28	122.07	118.90
54	BA	897	C	C5'-C4'-O4'	5.28	115.43	109.10
54	BA	1304	A	C6-C5-N7	5.28	135.99	132.30
54	BA	1655	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	2270	A	C6-C5-N7	5.28	135.99	132.30
54	BA	2524	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	2555	U	C4'-C3'-C2'	-5.28	97.32	102.60
54	BA	2750	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	1324	A	C4-C5-C6	-5.28	114.36	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	935	C	N3-C2-O2	-5.28	118.21	121.90
54	BA	1945	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	2395	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2698	U	N3-C2-O2	-5.28	118.51	122.20
21	AA	912	C	N1-C2-O2	5.27	122.06	118.90
21	AA	1366	C	N3-C2-O2	-5.27	118.21	121.90
24	A3	41	C	N1-C2-O2	5.27	122.06	118.90
54	BA	2295	C	O4'-C1'-N1	5.27	112.42	108.20
21	AA	415	A	C4-C5-C6	-5.27	114.36	117.00
21	AA	620	C	N1-C2-O2	5.27	122.06	118.90
54	BA	1597	A	O4'-C1'-N9	5.27	112.42	108.20
55	BB	107	G	C3'-C2'-C1'	5.27	105.72	101.50
21	AA	1477	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	421	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	744	U	C5'-C4'-O4'	5.27	115.42	109.10
54	BA	857	G	N3-C4-C5	-5.27	125.97	128.60
54	BA	1534	U	N3-C2-O2	-5.27	118.51	122.20
54	BA	1956	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2118	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2506	U	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2697	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	1539	U	C1'-O4'-C4'	-5.27	105.69	109.90
54	BA	1838	C	O4'-C1'-N1	5.27	112.41	108.20
4	AE	92	ARG	NE-CZ-NH1	5.26	122.93	120.30
21	AA	1183	U	O4'-C1'-N1	5.26	112.41	108.20
21	AA	1253	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	1168	G	N3-C2-N2	-5.26	116.22	119.90
54	BA	156	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	901	C	C5'-C4'-O4'	5.26	115.42	109.10
54	BA	921	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	1057	A	C1'-O4'-C4'	-5.26	105.69	109.90
54	BA	2462	C	O4'-C1'-N1	5.26	112.41	108.20
21	AA	57	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	549	C	N1-C2-O2	5.26	122.06	118.90
21	AA	607	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	890	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	1307	A	C4-C5-C6	-5.26	114.37	117.00
54	BA	2591	C	O4'-C1'-N1	5.26	112.41	108.20
54	BA	1169	A	C4-C5-C6	-5.26	114.37	117.00
23	A2	92	U	N3-C2-O2	-5.26	118.52	122.20
21	AA	1137	C	P-O3'-C3'	5.26	126.01	119.70
54	BA	1826	G	C3'-C2'-C1'	-5.26	97.29	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	600	A	C6-C5-N7	5.25	135.98	132.30
54	BA	1155	A	C4-C5-C6	-5.25	114.37	117.00
21	AA	411	A	C6-C5-N7	5.25	135.98	132.30
54	BA	351	C	N1-C2-O2	5.25	122.05	118.90
54	BA	587	C	N1-C2-O2	5.25	122.05	118.90
54	BA	838	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1420	A	C1'-O4'-C4'	-5.25	105.70	109.90
54	BA	1701	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	2282	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	2903	U	O4'-C1'-N1	5.25	112.40	108.20
21	AA	1076	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	503	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	695	G	N1-C6-O6	-5.25	116.75	119.90
18	AS	79	TYR	CB-CG-CD1	5.25	124.15	121.00
54	BA	1296	G	O4'-C1'-N9	5.25	112.40	108.20
6	AG	4	ARG	NE-CZ-NH1	5.25	122.92	120.30
21	AA	1106	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	632	A	N1-C6-N6	-5.25	115.45	118.60
54	BA	2675	A	C4-C5-C6	-5.25	114.38	117.00
21	AA	342	C	N1-C2-O2	5.25	122.05	118.90
21	AA	1183	U	N3-C2-O2	-5.25	118.53	122.20
21	AA	1500	A	C4-C5-C6	-5.25	114.38	117.00
24	A3	41	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1924	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2428	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	2602	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	1178	C	N1-C2-O2	5.25	122.05	118.90
54	BA	293	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	529	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	901	A	C4-C5-C6	-5.24	114.38	117.00
24	A3	59	A	C6-C5-N7	5.24	135.97	132.30
54	BA	2112	G	C5'-C4'-O4'	5.24	115.39	109.10
54	BA	141	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	486	C	N1-C2-O2	5.24	122.04	118.90
54	BA	2637	U	N3-C2-O2	-5.24	118.53	122.20
21	AA	503	C	N3-C2-O2	-5.24	118.23	121.90
21	AA	1280	A	O4'-C1'-N9	5.24	112.39	108.20
21	AA	1482	G	N1-C6-O6	-5.24	116.76	119.90
24	A3	18	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	33	C	N3-C2-O2	-5.24	118.23	121.90
54	BA	128	C	N3-C2-O2	-5.24	118.23	121.90
54	BA	164	C	N3-C2-O2	-5.24	118.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2728	U	O4'-C1'-N1	5.24	112.39	108.20
24	A3	66	C	N3-C2-O2	-5.24	118.23	121.90
54	BA	183	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	557	C	N3-C4-N4	-5.24	114.33	118.00
54	BA	806	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1571	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	1504	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	1327	A	C5'-C4'-C3'	-5.24	107.62	116.00
55	BB	47	C	N3-C2-O2	-5.24	118.23	121.90
54	BA	1087	G	N3-C2-N2	-5.23	116.24	119.90
54	BA	1559	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	1737	G	O4'-C1'-N9	5.23	112.39	108.20
55	BB	3	C	N1-C2-O2	5.23	122.04	118.90
21	AA	683	G	C5'-C4'-C3'	-5.23	107.63	116.00
21	AA	776	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	1411	C	N3-C2-O2	-5.23	118.24	121.90
25	BC	257	ARG	NE-CZ-NH2	-5.23	117.68	120.30
54	BA	130	C	N1-C2-O2	5.23	122.04	118.90
54	BA	635	C	N1-C2-O2	5.23	122.04	118.90
54	BA	1882	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2115	G	N3-C4-C5	-5.23	125.98	128.60
54	BA	2146	C	O4'-C1'-N1	5.23	112.39	108.20
54	BA	2207	C	N3-C2-O2	-5.23	118.24	121.90
54	BA	2752	C	O4'-C1'-N1	5.23	112.39	108.20
22	A1	56	C	N1-C2-O2	5.23	122.04	118.90
54	BA	249	C	C5'-C4'-O4'	5.23	115.38	109.10
54	BA	762	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	1257	C	N1-C2-O2	5.23	122.04	118.90
54	BA	1970	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	2073	C	O4'-C1'-N1	5.23	112.38	108.20
54	BA	829	A	N1-C6-N6	-5.23	115.46	118.60
54	BA	1553	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	1820	U	N3-C2-O2	-5.23	118.54	122.20
54	BA	2446	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	23	C	N1-C2-O2	5.23	122.04	118.90
21	AA	1506	U	C1'-O4'-C4'	-5.23	105.72	109.90
54	BA	1646	C	N3-C4-N4	-5.23	114.34	118.00
54	BA	2505	G	N3-C2-N2	-5.23	116.24	119.90
21	AA	332	G	N3-C2-N2	-5.22	116.24	119.90
21	AA	543	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	100	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	877	A	C6-C5-N7	5.22	135.96	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2530	A	C6-C5-N7	5.22	135.96	132.30
54	BA	2880	C	N1-C2-O2	5.22	122.03	118.90
21	AA	764	C	C6-N1-C2	-5.22	118.21	120.30
21	AA	911	U	C5-C6-N1	-5.22	120.09	122.70
21	AA	926	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	1531	C	N3-C2-O2	-5.22	118.25	121.90
55	BB	21	G	N1-C6-O6	-5.22	116.77	119.90
55	BB	111	U	O4'-C1'-N1	5.22	112.38	108.20
21	AA	382	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	595	A	C3'-C2'-C1'	5.22	105.67	101.50
23	A2	92	U	O4'-C1'-N1	5.22	112.38	108.20
54	BA	371	A	C6-C5-N7	5.22	135.95	132.30
54	BA	1229	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1690	A	C4-C5-C6	-5.22	114.39	117.00
21	AA	1453	G	O4'-C1'-N9	5.22	112.37	108.20
22	A1	74	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1290	C	N3-C2-O2	-5.22	118.25	121.90
21	AA	176	C	N1-C2-O2	5.22	122.03	118.90
21	AA	272	C	N1-C2-O2	5.22	122.03	118.90
54	BA	702	U	O4'-C1'-N1	5.22	112.37	108.20
21	AA	112	G	N3-C4-C5	-5.21	125.99	128.60
21	AA	226	G	N1-C6-O6	-5.21	116.77	119.90
31	BI	102	ARG	NH1-CZ-NH2	-5.21	113.66	119.40
54	BA	112	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	540	C	N1-C2-O2	5.21	122.03	118.90
54	BA	634	C	N1-C2-O2	5.21	122.03	118.90
54	BA	1557	C	N1-C2-O2	5.21	122.03	118.90
54	BA	1918	A	C6-C5-N7	5.21	135.95	132.30
54	BA	2308	G	N3-C2-N2	-5.21	116.25	119.90
21	AA	592	G	N1-C6-O6	-5.21	116.77	119.90
22	A1	16	C	N3-C4-C5	5.21	123.98	121.90
22	A1	11	C	N1-C2-O2	5.21	122.03	118.90
21	AA	1129	C	N1-C2-O2	5.21	122.03	118.90
33	BK	49	ARG	NE-CZ-NH1	5.21	122.91	120.30
21	AA	492	C	N1-C2-O2	5.21	122.03	118.90
37	BO	33	ARG	NE-CZ-NH2	5.21	122.90	120.30
54	BA	1256	G	N3-C2-N2	-5.21	116.25	119.90
54	BA	2196	C	O4'-C1'-N1	5.21	112.36	108.20
54	BA	2385	C	C1'-O4'-C4'	-5.21	105.73	109.90
43	BU	5	ARG	NE-CZ-NH1	5.21	122.90	120.30
54	BA	968	C	O4'-C1'-N1	5.21	112.36	108.20
55	BB	51	G	N1-C6-O6	-5.21	116.78	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	82	G	O4'-C1'-N9	5.20	112.36	108.20
54	BA	1150	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1570	A	C6-C5-N7	5.20	135.94	132.30
54	BA	1722	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	1749	A	C6-C5-N7	5.20	135.94	132.30
54	BA	2047	C	N1-C2-O2	5.20	122.02	118.90
2	AC	130	ARG	NE-CZ-NH2	5.20	122.90	120.30
54	BA	1592	C	N1-C2-O2	5.20	122.02	118.90
54	BA	2636	C	O4'-C1'-N1	5.20	112.36	108.20
54	BA	2841	C	N3-C2-O2	-5.20	118.26	121.90
54	BA	1068	G	N3-C2-N2	-5.20	116.26	119.90
54	BA	2266	A	C6-C5-N7	5.20	135.94	132.30
54	BA	2381	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	159	G	N1-C6-O6	-5.20	116.78	119.90
54	BA	2581	G	N3-C4-C5	-5.20	126.00	128.60
54	BA	554	U	C5-C6-N1	-5.20	120.10	122.70
21	AA	1061	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	1364	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	236	C	N3-C2-O2	-5.20	118.26	121.90
54	BA	744	U	C4'-C3'-C2'	-5.20	97.40	102.60
54	BA	1031	G	N1-C6-O6	-5.19	116.78	119.90
54	BA	108	G	N3-C2-N2	-5.19	116.27	119.90
54	BA	1288	G	C1'-O4'-C4'	-5.19	105.75	109.90
54	BA	1397	U	N3-C2-O2	-5.19	118.56	122.20
54	BA	1477	A	C4-C5-C6	-5.19	114.40	117.00
54	BA	1585	C	N1-C2-O2	5.19	122.02	118.90
54	BA	2395	C	N1-C2-O2	5.19	122.02	118.90
54	BA	2824	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	2374	C	N1-C2-O2	5.19	122.01	118.90
21	AA	17	U	C5'-C4'-O4'	5.19	115.32	109.10
21	AA	1460	C	O4'-C1'-N1	5.19	112.35	108.20
43	BU	21	ARG	NE-CZ-NH2	-5.19	117.71	120.30
54	BA	131	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	724	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	1255	U	C4'-C3'-C2'	-5.19	97.41	102.60
54	BA	1417	C	N1-C2-O2	5.19	122.01	118.90
54	BA	1515	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	1566	A	O4'-C1'-N9	5.19	112.35	108.20
54	BA	2169	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	2510	C	O4'-C1'-N1	5.19	112.35	108.20
55	BB	27	C	N1-C2-O2	5.19	122.01	118.90
21	AA	1075	U	O4'-C1'-N1	5.19	112.35	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	58	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	820	A	N1-C6-N6	-5.19	115.49	118.60
21	AA	532	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	1307	U	C5'-C4'-O4'	5.18	115.32	109.10
54	BA	275	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	1039	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	1105	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	1127	G	N3-C2-N2	-5.18	116.27	119.90
54	BA	815	C	O4'-C1'-N1	5.18	112.35	108.20
54	BA	1893	C	O4'-C1'-N1	5.18	112.34	108.20
21	AA	418	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1066	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	442	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	1612	C	N1-C2-O2	5.18	122.01	118.90
21	AA	426	U	O4'-C1'-N1	5.18	112.34	108.20
21	AA	1199	U	N3-C2-O2	-5.18	118.57	122.20
54	BA	1069	A	C2-N3-C4	5.18	113.19	110.60
54	BA	1983	G	C5-C6-N1	5.18	114.09	111.50
21	AA	520	A	C4-C5-C6	-5.18	114.41	117.00
33	BK	98	ARG	NE-CZ-NH1	5.18	122.89	120.30
54	BA	1174	U	N3-C2-O2	-5.18	118.58	122.20
54	BA	1578	U	C4'-C3'-C2'	-5.18	97.42	102.60
54	BA	1088	A	C2-N3-C4	5.17	113.19	110.60
54	BA	1248	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1489	C	N1-C2-O2	5.17	122.00	118.90
54	BA	1731	G	N3-C4-C5	-5.17	126.01	128.60
54	BA	1776	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1937	A	C3'-C2'-C1'	-5.17	97.36	101.50
21	AA	156	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	718	A	C4-C5-C6	-5.17	114.41	117.00
54	BA	2206	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	618	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	1131	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1941	C	N1-C2-O2	5.17	122.00	118.90
1	AB	73	ARG	NE-CZ-NH2	-5.17	117.72	120.30
22	A1	68	C	N1-C2-O2	5.17	122.00	118.90
54	BA	750	A	C4-C5-C6	-5.17	114.42	117.00
54	BA	1640	A	C4-C5-C6	-5.17	114.42	117.00
54	BA	2709	G	C5-C6-N1	5.17	114.08	111.50
21	AA	151	A	C6-C5-N7	5.17	135.92	132.30
21	AA	361	G	N1-C6-O6	-5.17	116.80	119.90
21	AA	897	C	N1-C2-O2	5.17	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1704	C	N1-C2-O2	5.17	122.00	118.90
54	BA	2067	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	2278	A	C6-C5-N7	5.17	135.91	132.30
21	AA	475	C	N1-C2-O2	5.16	122.00	118.90
21	AA	1181	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	1802	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	2010	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	2064	C	N3-C2-O2	-5.16	118.29	121.90
55	BB	32	U	O4'-C1'-N1	5.16	112.33	108.20
22	A1	2	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	2463	C	N1-C2-O2	5.16	122.00	118.90
21	AA	255	G	N1-C6-O6	-5.16	116.80	119.90
21	AA	326	G	N1-C6-O6	-5.16	116.80	119.90
21	AA	843	U	P-O3'-C3'	5.16	125.89	119.70
21	AA	1468	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	347	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1660	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	2469	A	C4-C5-C6	-5.16	114.42	117.00
5	AF	45	ARG	NE-CZ-NH1	5.16	122.88	120.30
54	BA	13	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1491	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	2297	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	148	G	C5-C6-N1	5.16	114.08	111.50
54	BA	1758	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	2439	A	O4'-C1'-N9	5.16	112.33	108.20
54	BA	2457	U	N3-C2-O2	-5.16	118.59	122.20
21	AA	846	G	N1-C6-O6	-5.16	116.81	119.90
21	AA	1107	C	N1-C2-O2	5.16	121.99	118.90
54	BA	125	A	C1'-O4'-C4'	-5.16	105.78	109.90
54	BA	1327	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	1829	A	C4-C5-C6	-5.16	114.42	117.00
55	BB	22	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	2366	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	2424	C	N1-C2-O2	5.15	121.99	118.90
54	BA	2805	C	N1-C2-O2	5.15	121.99	118.90
21	AA	277	C	N3-C2-O2	-5.15	118.29	121.90
54	BA	61	C	N1-C2-O2	5.15	121.99	118.90
54	BA	894	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	984	A	C4-C5-C6	-5.15	114.42	117.00
54	BA	1033	U	C3'-C2'-C1'	5.15	105.62	101.50
54	BA	2063	C	N3-C4-N4	-5.15	114.39	118.00
54	BA	2139	U	N3-C2-O2	-5.15	118.59	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2391	G	N3-C4-C5	-5.15	126.02	128.60
45	BW	54	ARG	NE-CZ-NH2	5.15	122.88	120.30
54	BA	765	C	N1-C2-O2	5.15	121.99	118.90
54	BA	1181	U	O4'-C1'-N1	5.15	112.32	108.20
21	AA	567	G	N1-C6-O6	-5.15	116.81	119.90
52	B3	41	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
54	BA	2633	G	C5'-C4'-O4'	5.15	115.28	109.10
21	AA	550	G	N1-C6-O6	-5.15	116.81	119.90
26	BD	33	ARG	NE-CZ-NH1	5.15	122.87	120.30
37	BO	102	ARG	NE-CZ-NH2	-5.15	117.73	120.30
54	BA	136	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	573	U	N3-C2-O2	-5.15	118.60	122.20
54	BA	1859	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2238	G	N1-C6-O6	-5.15	116.81	119.90
21	AA	305	G	C3'-C2'-C1'	5.15	105.62	101.50
54	BA	2160	C	N1-C2-O2	5.15	121.99	118.90
54	BA	2510	C	N1-C2-O2	5.15	121.99	118.90
21	AA	6	G	O4'-C4'-C3'	5.14	110.22	106.10
21	AA	614	C	O4'-C1'-N1	5.14	112.32	108.20
28	BF	109	ARG	NE-CZ-NH1	5.14	122.87	120.30
39	BQ	29	ARG	NE-CZ-NH1	5.14	122.87	120.30
54	BA	611	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	1064	C	O4'-C1'-N1	5.14	112.32	108.20
54	BA	1937	A	C6-C5-N7	5.14	135.90	132.30
54	BA	2134	A	C4-C5-C6	-5.14	114.43	117.00
21	AA	212	G	N3-C4-C5	-5.14	126.03	128.60
21	AA	564	C	N3-C4-C5	5.14	123.96	121.90
21	AA	1476	A	C6-C5-N7	5.14	135.90	132.30
54	BA	683	U	N3-C2-O2	-5.14	118.60	122.20
54	BA	726	G	N3-C4-C5	-5.14	126.03	128.60
54	BA	1090	A	C6-C5-N7	5.14	135.90	132.30
21	AA	469	C	N1-C2-O2	5.14	121.98	118.90
21	AA	1167	A	C3'-C2'-C1'	5.14	105.61	101.50
22	A1	14	A	O4'-C1'-N9	5.14	112.31	108.20
54	BA	596	U	C5'-C4'-O4'	5.14	115.27	109.10
54	BA	794	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	1291	C	N1-C2-O2	5.14	121.98	118.90
54	BA	1788	C	C4'-C3'-C2'	-5.14	97.46	102.60
54	BA	2157	G	C1'-O4'-C4'	-5.14	105.79	109.90
54	BA	2339	C	C1'-O4'-C4'	-5.14	105.79	109.90
21	AA	311	C	N1-C2-O2	5.14	121.98	118.90
54	BA	1040	A	C4-C5-C6	-5.14	114.43	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	65	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	621	A	C5'-C4'-C3'	-5.14	107.78	116.00
54	BA	1045	C	N3-C4-C5	5.14	123.95	121.90
54	BA	2399	G	O4'-C1'-N9	5.14	112.31	108.20
55	BB	10	G	N1-C6-O6	-5.14	116.82	119.90
21	AA	1316	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	1532	U	O4'-C1'-N1	5.13	112.31	108.20
38	BP	108	ARG	NE-CZ-NH1	5.13	122.87	120.30
54	BA	547	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	2306	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	2816	G	N3-C2-N2	-5.13	116.31	119.90
21	AA	964	A	C4-C5-C6	-5.13	114.43	117.00
54	BA	1567	G	N3-C2-N2	-5.13	116.31	119.90
54	BA	1804	C	C5'-C4'-O4'	5.13	115.26	109.10
54	BA	2194	U	O4'-C1'-N1	5.13	112.31	108.20
54	BA	2427	C	N1-C2-O2	5.13	121.98	118.90
8	AI	32	ARG	NE-CZ-NH2	-5.13	117.73	120.30
8	AI	98	ARG	NH1-CZ-NH2	-5.13	113.75	119.40
54	BA	384	A	C6-C5-N7	5.13	135.89	132.30
54	BA	993	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	1234	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	2182	U	O4'-C1'-N1	5.13	112.31	108.20
54	BA	2307	G	O4'-C1'-N9	5.13	112.31	108.20
54	BA	2359	C	N1-C2-O2	5.13	121.98	118.90
11	AL	13	ARG	NE-CZ-NH1	5.13	122.86	120.30
54	BA	444	C	N1-C2-O2	5.13	121.98	118.90
54	BA	1385	A	C1'-O4'-C4'	-5.13	105.80	109.90
21	AA	14	U	N3-C2-O2	-5.13	118.61	122.20
21	AA	467	U	N3-C2-O2	-5.13	118.61	122.20
21	AA	1273	C	N1-C2-O2	5.13	121.98	118.90
54	BA	1102	C	N1-C2-O2	5.13	121.98	118.90
54	BA	1485	U	O4'-C1'-N1	5.12	112.30	108.20
55	BB	12	C	N1-C2-O2	5.12	121.97	118.90
21	AA	1436	U	O4'-C1'-N1	5.12	112.30	108.20
54	BA	837	C	N3-C2-O2	-5.12	118.31	121.90
54	BA	1030	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1132	U	N3-C2-O2	-5.12	118.61	122.20
54	BA	1584	U	N3-C2-O2	-5.12	118.61	122.20
54	BA	2562	U	N3-C2-O2	-5.12	118.61	122.20
54	BA	2562	U	O4'-C1'-N1	5.12	112.30	108.20
9	AJ	16	ARG	NE-CZ-NH2	-5.12	117.74	120.30
21	AA	726	C	N1-C2-O2	5.12	121.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A3	26	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	417	C	N3-C2-O2	-5.12	118.31	121.90
54	BA	1706	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	2355	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2539	C	N1-C2-O2	5.12	121.97	118.90
54	BA	2665	A	C4-C5-C6	-5.12	114.44	117.00
22	A1	18	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2492	U	N3-C2-O2	-5.12	118.62	122.20
30	BH	68	ARG	NE-CZ-NH2	-5.12	117.74	120.30
54	BA	2328	A	C6-C5-N7	5.12	135.88	132.30
21	AA	485	U	O4'-C1'-N1	5.12	112.29	108.20
21	AA	1489	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	440	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	2706	A	O4'-C1'-N9	5.12	112.29	108.20
21	AA	478	A	C4-C5-C6	-5.11	114.44	117.00
21	AA	957	U	C5-C6-N1	-5.11	120.14	122.70
21	AA	1172	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	993	G	N3-C2-N2	-5.11	116.32	119.90
54	BA	2783	U	O4'-C1'-N1	5.11	112.29	108.20
55	BB	29	A	O4'-C1'-N9	5.11	112.29	108.20
21	AA	632	U	N3-C2-O2	-5.11	118.62	122.20
21	AA	680	C	N1-C2-O2	5.11	121.97	118.90
50	B1	5	ARG	NE-CZ-NH1	5.11	122.86	120.30
54	BA	240	C	N1-C2-O2	5.11	121.97	118.90
54	BA	465	G	N3-C2-N2	-5.11	116.32	119.90
21	AA	356	A	C6-C5-N7	5.11	135.88	132.30
21	AA	552	U	C1'-O4'-C4'	-5.11	105.81	109.90
21	AA	590	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	360	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	1770	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	1895	C	N1-C2-O2	5.11	121.97	118.90
54	BA	1011	G	O4'-C1'-N9	5.11	112.29	108.20
21	AA	267	C	N1-C2-O2	5.11	121.97	118.90
21	AA	629	A	C6-C5-N7	5.11	135.88	132.30
21	AA	659	U	N3-C2-O2	-5.11	118.62	122.20
21	AA	1459	G	N3-C4-C5	-5.11	126.05	128.60
21	AA	1525	G	N1-C6-O6	-5.11	116.84	119.90
54	BA	458	G	C3'-C2'-C1'	-5.11	97.41	101.50
54	BA	957	C	N1-C2-O2	5.11	121.96	118.90
54	BA	2402	U	N3-C2-O2	-5.11	118.62	122.20
54	BA	2628	C	C5'-C4'-O4'	5.11	115.23	109.10
55	BB	17	C	N1-C2-O2	5.11	121.97	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	587	G	N1-C6-O6	-5.11	116.84	119.90
51	B2	14	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
54	BA	343	C	N1-C2-O2	5.11	121.96	118.90
54	BA	1146	C	N3-C2-O2	-5.11	118.33	121.90
21	AA	242	G	N3-C2-N2	-5.10	116.33	119.90
22	A1	15	G	C3'-C2'-C1'	5.10	105.58	101.50
54	BA	92	U	N3-C2-O2	-5.10	118.63	122.20
54	BA	164	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	673	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	839	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	1542	U	N1-C2-N3	5.10	117.96	114.90
17	AR	42	ARG	NE-CZ-NH1	5.10	122.85	120.30
54	BA	2585	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	166	U	C5-C6-N1	-5.10	120.15	122.70
21	AA	293	G	N3-C2-N2	-5.10	116.33	119.90
21	AA	1042	A	C4-C5-C6	-5.10	114.45	117.00
21	AA	1242	G	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1474	U	O4'-C1'-N1	5.10	112.28	108.20
54	BA	211	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2797	U	N3-C2-O2	-5.10	118.63	122.20
21	AA	225	C	O4'-C1'-N1	5.10	112.28	108.20
21	AA	254	G	N1-C6-O6	-5.10	116.84	119.90
21	AA	1071	C	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1300	G	C5-C6-N1	5.10	114.05	111.50
21	AA	1307	U	O4'-C1'-N1	5.10	112.28	108.20
23	A2	93	U	N3-C2-O2	-5.10	118.63	122.20
45	BW	76	ARG	NE-CZ-NH1	5.10	122.85	120.30
54	BA	962	G	N1-C6-O6	-5.10	116.84	119.90
54	BA	1025	G	N3-C4-C5	-5.10	126.05	128.60
54	BA	1545	A	C6-C5-N7	5.10	135.87	132.30
54	BA	2204	G	N3-C2-N2	-5.10	116.33	119.90
54	BA	2508	G	O4'-C1'-N9	5.10	112.28	108.20
55	BB	57	A	C4-C5-C6	-5.10	114.45	117.00
15	AP	56	ARG	NE-CZ-NH1	5.10	122.85	120.30
29	BG	148	ARG	NE-CZ-NH1	5.10	122.85	120.30
21	AA	435	A	C4-C5-C6	-5.09	114.45	117.00
54	BA	444	C	N3-C4-C5	5.09	123.94	121.90
54	BA	595	C	O4'-C1'-N1	5.09	112.28	108.20
54	BA	873	C	C4'-C3'-C2'	-5.09	97.51	102.60
54	BA	2888	C	O4'-C1'-N1	5.09	112.28	108.20
21	AA	1444	U	C1'-O4'-C4'	-5.09	105.83	109.90
21	AA	1521	C	N1-C2-O2	5.09	121.95	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1152	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2557	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	2704	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	2718	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	2749	A	C4-C5-C6	-5.09	114.45	117.00
21	AA	218	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	867	C	O4'-C1'-N1	5.09	112.27	108.20
21	AA	576	C	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1310	G	O4'-C1'-N9	5.09	112.27	108.20
54	BA	2311	A	C4-C5-C6	-5.09	114.46	117.00
21	AA	163	C	O4'-C1'-N1	5.09	112.27	108.20
21	AA	1078	U	C5-C6-N1	-5.09	120.16	122.70
21	AA	1259	C	N1-C2-O2	5.09	121.95	118.90
54	BA	573	U	C5'-C4'-C3'	-5.09	107.86	116.00
54	BA	72	U	N3-C2-O2	-5.08	118.64	122.20
54	BA	1437	C	O4'-C1'-N1	5.08	112.27	108.20
54	BA	1634	A	P-O3'-C3'	5.08	125.80	119.70
21	AA	1172	C	N1-C2-O2	5.08	121.95	118.90
54	BA	1023	U	O4'-C1'-N1	5.08	112.27	108.20
54	BA	2563	U	C5'-C4'-O4'	5.08	115.20	109.10
21	AA	163	C	P-O3'-C3'	5.08	125.80	119.70
21	AA	889	A	C6-C5-N7	5.08	135.86	132.30
54	BA	199	A	O4'-C1'-N9	5.08	112.27	108.20
54	BA	1293	C	O4'-C1'-N1	5.08	112.27	108.20
54	BA	1451	C	P-O3'-C3'	5.08	125.80	119.70
21	AA	1140	C	N3-C2-O2	-5.08	118.34	121.90
54	BA	1285	A	C6-C5-N7	5.08	135.86	132.30
54	BA	1428	C	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1888	G	O4'-C1'-N9	5.08	112.26	108.20
54	BA	2066	C	N3-C2-O2	-5.08	118.34	121.90
21	AA	159	G	N1-C6-O6	-5.08	116.85	119.90
51	B2	41	ARG	NE-CZ-NH1	5.08	122.84	120.30
54	BA	1258	U	C3'-C2'-C1'	5.08	105.56	101.50
54	BA	1822	C	C4'-C3'-C2'	-5.08	97.52	102.60
54	BA	1945	G	C5-C6-N1	5.08	114.04	111.50
54	BA	2165	C	N1-C2-O2	5.08	121.95	118.90
54	BA	2452	C	N1-C2-O2	5.08	121.95	118.90
55	BB	13	G	N3-C2-N2	-5.08	116.34	119.90
35	BM	51	ARG	NE-CZ-NH2	-5.08	117.76	120.30
54	BA	797	G	C4'-C3'-C2'	-5.08	97.52	102.60
41	BS	11	ARG	NH1-CZ-NH2	-5.08	113.82	119.40
54	BA	1587	G	C8-N9-C4	-5.08	104.37	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	2825	G	N3-C4-C5	-5.08	126.06	128.60
12	AM	112	ARG	NE-CZ-NH1	5.07	122.84	120.30
21	AA	554	A	C6-C5-N7	5.07	135.85	132.30
54	BA	2	G	O4'-C1'-N9	5.07	112.26	108.20
54	BA	1568	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1968	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	2347	C	N1-C2-O2	5.07	121.94	118.90
21	AA	686	U	O4'-C1'-N1	5.07	112.26	108.20
21	AA	1051	C	N3-C2-O2	-5.07	118.35	121.90
54	BA	678	C	O4'-C1'-N1	5.07	112.26	108.20
54	BA	2686	G	C5-C6-N1	5.07	114.04	111.50
21	AA	538	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	756	C	N1-C2-O2	5.07	121.94	118.90
36	BN	90	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
54	BA	24	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	780	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	919	U	N3-C2-O2	-5.07	118.65	122.20
54	BA	1120	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1861	G	O4'-C1'-N9	5.07	112.26	108.20
54	BA	1958	C	N1-C2-O2	5.07	121.94	118.90
54	BA	2214	C	O4'-C1'-N1	5.07	112.26	108.20
54	BA	2453	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	467	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1822	C	O4'-C1'-N1	5.07	112.25	108.20
55	BB	23	G	C5-C6-N1	5.07	114.03	111.50
21	AA	735	C	O4'-C1'-N1	5.07	112.25	108.20
21	AA	1223	C	N1-C2-O2	5.07	121.94	118.90
54	BA	435	C	C5'-C4'-O4'	5.07	115.18	109.10
54	BA	500	G	O4'-C1'-N9	5.07	112.25	108.20
54	BA	759	G	C5-C6-N1	5.07	114.03	111.50
54	BA	883	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1798	U	C5-C6-N1	-5.07	120.17	122.70
21	AA	158	G	C8-N9-C4	-5.07	104.37	106.40
22	A1	14	A	C1'-O4'-C4'	-5.07	105.85	109.90
54	BA	197	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	1270	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1573	G	O4'-C1'-N9	5.07	112.25	108.20
54	BA	2476	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	2502	G	C5'-C4'-C3'	-5.07	107.90	116.00
54	BA	2717	C	N1-C2-O2	5.07	121.94	118.90
21	AA	572	A	O4'-C1'-N9	5.06	112.25	108.20
21	AA	888	G	N7-C8-N9	5.06	115.63	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	1227	A	O4'-C1'-N9	5.06	112.25	108.20
51	B2	19	ARG	CD-NE-CZ	5.06	130.69	123.60
55	BB	23	G	C3'-C2'-C1'	5.06	105.55	101.50
21	AA	675	A	C6-C5-N7	5.06	135.84	132.30
21	AA	109	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	112	G	C5-C6-N1	5.06	114.03	111.50
21	AA	1166	G	N1-C6-O6	-5.06	116.86	119.90
24	A3	11	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	142	A	C6-C5-N7	5.06	135.84	132.30
54	BA	1965	C	N3-C2-O2	-5.06	118.36	121.90
6	AG	108	ARG	NE-CZ-NH1	5.06	122.83	120.30
21	AA	97	G	C5-C6-N1	5.06	114.03	111.50
54	BA	181	A	C5'-C4'-O4'	5.06	115.17	109.10
54	BA	642	U	C5'-C4'-O4'	5.06	115.17	109.10
54	BA	1075	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	1602	U	P-O3'-C3'	5.06	125.77	119.70
54	BA	2188	U	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2531	A	C2-N3-C4	5.06	113.13	110.60
54	BA	2556	C	N1-C2-O2	5.06	121.94	118.90
21	AA	1398	A	C6-C5-N7	5.06	135.84	132.30
25	BC	47	ARG	NE-CZ-NH1	5.06	122.83	120.30
21	AA	1447	A	C1'-O4'-C4'	-5.05	105.86	109.90
52	B3	29	ARG	NE-CZ-NH1	5.05	122.83	120.30
54	BA	546	U	N3-C2-O2	-5.05	118.66	122.20
54	BA	993	G	N9-C4-C5	5.05	107.42	105.40
54	BA	1773	A	C6-C5-N7	5.05	135.84	132.30
21	AA	211	G	C5-C6-N1	5.05	114.03	111.50
54	BA	1934	C	C4'-C3'-C2'	-5.05	97.55	102.60
54	BA	2307	G	N3-C4-C5	-5.05	126.07	128.60
54	BA	2483	C	N1-C2-O2	5.05	121.93	118.90
21	AA	595	A	C4-C5-C6	-5.05	114.47	117.00
21	AA	899	C	N3-C2-O2	-5.05	118.36	121.90
21	AA	1192	C	N1-C2-O2	5.05	121.93	118.90
21	AA	1379	G	C5'-C4'-C3'	-5.05	107.92	116.00
21	AA	1505	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	153	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	656	G	N3-C4-C5	-5.05	126.07	128.60
54	BA	1348	C	O4'-C1'-N1	5.05	112.24	108.20
54	BA	1536	C	N1-C2-O2	5.05	121.93	118.90
21	AA	513	C	N1-C2-O2	5.05	121.93	118.90
21	AA	951	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	985	C	N1-C2-O2	5.05	121.93	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	25	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	586	A	C6-N1-C2	-5.05	115.57	118.60
54	BA	1588	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1636	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	1691	C	N1-C2-O2	5.05	121.93	118.90
54	BA	2334	U	N3-C2-O2	-5.05	118.67	122.20
54	BA	2554	U	C3'-C2'-C1'	-5.05	97.46	101.50
21	AA	483	C	C3'-C2'-C1'	5.05	105.54	101.50
54	BA	165	A	C6-C5-N7	5.05	135.83	132.30
54	BA	412	A	C4-C5-C6	-5.05	114.48	117.00
54	BA	869	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	2035	G	C5-C6-N1	5.05	114.02	111.50
3	AD	164	ARG	NH1-CZ-NH2	-5.05	113.85	119.40
11	AL	8	ARG	NE-CZ-NH2	-5.05	117.78	120.30
21	AA	314	C	N3-C2-O2	-5.05	118.37	121.90
21	AA	496	A	C4-C5-C6	-5.05	114.48	117.00
22	A1	6	A	C6-C5-N7	5.05	135.83	132.30
54	BA	458	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	1327	A	C5'-C4'-O4'	5.05	115.16	109.10
21	AA	54	C	N3-C2-O2	-5.04	118.37	121.90
21	AA	1026	G	N1-C6-O6	-5.04	116.87	119.90
54	BA	2215	C	N1-C2-O2	5.04	121.93	118.90
54	BA	2403	C	N1-C2-O2	5.04	121.93	118.90
21	AA	559	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	665	A	C6-C5-N7	5.04	135.83	132.30
22	A1	18	G	C1'-O4'-C4'	-5.04	105.87	109.90
54	BA	539	G	N1-C6-O6	-5.04	116.87	119.90
54	BA	2034	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2324	U	O4'-C1'-N1	5.04	112.24	108.20
21	AA	490	C	N1-C2-O2	5.04	121.92	118.90
21	AA	606	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	118	A	C5'-C4'-O4'	5.04	115.15	109.10
54	BA	897	C	N1-C2-O2	5.04	121.92	118.90
54	BA	1480	C	C4'-C3'-C2'	-5.04	97.56	102.60
54	BA	1560	G	C5-C6-N1	5.04	114.02	111.50
54	BA	1643	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	2093	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	2094	A	C6-C5-N7	5.04	135.83	132.30
21	AA	82	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	398	C	N1-C2-O2	5.04	121.92	118.90
54	BA	1148	U	C3'-C2'-C1'	5.04	105.53	101.50
54	BA	1544	A	C4-C5-C6	-5.04	114.48	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AA	43	C	C5'-C4'-O4'	5.04	115.15	109.10
21	AA	316	C	N1-C2-O2	5.04	121.92	118.90
54	BA	678	C	N1-C2-O2	5.04	121.92	118.90
54	BA	1503	A	C6-C5-N7	5.04	135.83	132.30
45	BW	40	ARG	NE-CZ-NH1	5.04	122.82	120.30
54	BA	1251	C	N3-C2-O2	-5.04	118.37	121.90
54	BA	1259	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	2476	A	C4'-C3'-C2'	-5.04	97.56	102.60
54	BA	533	G	N1-C6-O6	-5.04	116.88	119.90
54	BA	661	A	C6-C5-N7	5.04	135.82	132.30
54	BA	955	U	N3-C2-O2	-5.04	118.68	122.20
54	BA	1928	A	C4'-C3'-C2'	-5.04	97.56	102.60
54	BA	2055	C	C6-N1-C2	-5.04	118.29	120.30
54	BA	2248	C	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2377	A	C4-C5-C6	-5.04	114.48	117.00
21	AA	282	A	C6-C5-N7	5.03	135.82	132.30
21	AA	923	A	C6-C5-N7	5.03	135.82	132.30
23	A2	88	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	580	U	O4'-C1'-N1	5.03	112.23	108.20
54	BA	686	U	O4'-C1'-N1	5.03	112.23	108.20
54	BA	722	A	O4'-C1'-N9	5.03	112.23	108.20
54	BA	1908	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2692	G	N7-C8-N9	5.03	115.62	113.10
54	BA	1232	G	C5-C6-N1	5.03	114.02	111.50
54	BA	1300	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	2616	C	O4'-C1'-N1	5.03	112.23	108.20
8	AI	10	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
54	BA	357	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	1582	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2485	G	N3-C2-N2	-5.03	116.38	119.90
55	BB	20	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	115	G	N1-C6-O6	-5.03	116.88	119.90
22	A1	41	A	C6-C5-N7	5.03	135.82	132.30
54	BA	980	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	2021	C	P-O3'-C3'	5.03	125.73	119.70
54	BA	2420	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2438	U	O4'-C1'-N1	5.03	112.22	108.20
54	BA	2603	G	N1-C6-O6	-5.03	116.88	119.90
9	AJ	5	ARG	NE-CZ-NH1	5.03	122.81	120.30
14	AO	76	ARG	NE-CZ-NH1	5.03	122.81	120.30
21	AA	1423	G	C1'-O4'-C4'	-5.03	105.88	109.90
22	A1	10	G	N3-C4-C5	-5.03	126.09	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	20	G	N1-C6-O6	-5.03	116.89	119.90
54	BA	817	C	C4'-C3'-C2'	-5.03	97.58	102.60
54	BA	2182	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	921	C	N1-C2-O2	5.02	121.92	118.90
54	BA	1736	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1997	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	624	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	747	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1371	G	O4'-C1'-N9	5.02	112.22	108.20
54	BA	2512	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2544	G	N1-C6-O6	-5.02	116.89	119.90
5	AF	86	ARG	NE-CZ-NH2	-5.02	117.79	120.30
54	BA	1269	A	C6-C5-N7	5.02	135.81	132.30
54	BA	2183	A	C4-C5-C6	-5.02	114.49	117.00
21	AA	25	C	N1-C2-O2	5.02	121.91	118.90
21	AA	531	U	C3'-C2'-C1'	5.02	105.52	101.50
21	AA	545	C	N1-C2-O2	5.02	121.91	118.90
21	AA	971	G	N3-C4-C5	-5.02	126.09	128.60
21	AA	1160	G	C4'-C3'-C2'	-5.02	97.58	102.60
54	BA	1296	G	N3-C2-N2	-5.02	116.39	119.90
54	BA	1488	C	N3-C2-O2	-5.02	118.39	121.90
54	BA	1685	C	N1-C2-O2	5.02	121.91	118.90
54	BA	160	A	C6-C5-N7	5.02	135.81	132.30
54	BA	249	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	320	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	1097	U	O4'-C1'-N1	5.02	112.21	108.20
54	BA	1209	U	O4'-C1'-N1	5.02	112.21	108.20
54	BA	1973	G	N1-C6-O6	-5.02	116.89	119.90
21	AA	164	G	C1'-O4'-C4'	-5.02	105.89	109.90
21	AA	913	A	C4-C5-C6	-5.02	114.49	117.00
25	BC	155	ARG	NE-CZ-NH1	5.02	122.81	120.30
54	BA	298	G	N3-C4-C5	-5.02	126.09	128.60
54	BA	2872	A	C4-C5-C6	-5.02	114.49	117.00
21	AA	339	C	N1-C2-O2	5.01	121.91	118.90
21	AA	909	A	C4-C5-C6	-5.01	114.49	117.00
21	AA	1117	A	C6-C5-N7	5.01	135.81	132.30
54	BA	168	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	735	A	N1-C6-N6	-5.01	115.59	118.60
54	BA	1465	G	O4'-C4'-C3'	5.01	110.11	106.10
54	BA	828	U	N3-C2-O2	-5.01	118.69	122.20
55	BB	24	G	O4'-C4'-C3'	5.01	110.11	106.10
21	AA	1347	G	N3-C2-N2	-5.01	116.39	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BA	1129	A	C5'-C4'-C3'	-5.01	107.98	116.00
21	AA	1335	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	1202	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	1832	C	N1-C2-O2	5.01	121.91	118.90
21	AA	894	G	N1-C6-O6	-5.01	116.89	119.90
54	BA	368	A	C6-C5-N7	5.01	135.81	132.30
54	BA	2585	U	N3-C2-O2	-5.01	118.69	122.20
21	AA	1059	C	N1-C2-O2	5.01	121.90	118.90
21	AA	1358	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	256	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	402	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	1702	G	N1-C6-O6	-5.01	116.90	119.90
54	BA	2586	U	O4'-C1'-N1	5.01	112.20	108.20
54	BA	2667	C	O4'-C1'-N1	5.01	112.20	108.20
54	BA	2831	G	N1-C6-O6	-5.01	116.90	119.90
55	BB	70	C	N1-C2-O2	5.01	121.90	118.90
21	AA	537	G	O4'-C1'-N9	5.00	112.20	108.20
24	A3	31	G	N3-C4-C5	-5.00	126.10	128.60
54	BA	174	U	O4'-C1'-N1	5.00	112.20	108.20
54	BA	2300	C	O4'-C1'-N1	5.00	112.20	108.20
21	AA	463	U	C5'-C4'-C3'	-5.00	107.99	116.00
21	AA	617	G	N1-C6-O6	-5.00	116.90	119.90
21	AA	1531	A	O4'-C1'-N9	5.00	112.20	108.20
54	BA	756	A	C6-C5-N7	5.00	135.80	132.30
54	BA	857	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	1211	C	N1-C2-O2	5.00	121.90	118.90
54	BA	1639	C	N1-C2-O2	5.00	121.90	118.90
54	BA	1912	A	O4'-C1'-N9	5.00	112.20	108.20
54	BA	2250	G	C5-C6-N1	5.00	114.00	111.50
54	BA	2621	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	2158	A	C6-C5-N7	5.00	135.80	132.30

There are no chirality outliers.

All (1062) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	18	G	Sidechain
22	A1	25	C	Sidechain
22	A1	27	C	Sidechain
22	A1	31	C	Sidechain
22	A1	35	A	Sidechain
22	A1	36	C	Sidechain

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Mol	Chain	Res	Type	Group
22	A1	39	G	Sidechain
22	A1	45	G	Sidechain
22	A1	57	G	Sidechain
22	A1	61	C	Sidechain
22	A1	62	C	Sidechain
22	A1	74	C	Sidechain
22	A1	76	A	Sidechain
23	A2	81	U	Sidechain
23	A2	82	A	Sidechain
23	A2	87	U	Sidechain
23	A2	88	U	Sidechain
23	A2	89	U	Sidechain
24	A3	1	C	Sidechain
24	A3	18	U	Sidechain
24	A3	20	G	Sidechain
24	A3	25	U	Sidechain
24	A3	28	U	Sidechain
24	A3	34	U	Sidechain
24	A3	4	G	Sidechain
24	A3	42	C	Sidechain
24	A3	44	A	Sidechain
24	A3	47	G	Sidechain
24	A3	5	G	Sidechain
24	A3	6	G	Sidechain
24	A3	62	C	Sidechain
24	A3	66	C	Sidechain
24	A3	69	C	Sidechain
24	A3	77	A	Sidechain
24	A3	9	G	Sidechain
21	AA	100	G	Sidechain
21	AA	1002	G	Sidechain
21	AA	1006	G	Sidechain
21	AA	1030	U	Sidechain
21	AA	1038	C	Sidechain
21	AA	105	G	Sidechain
21	AA	1059	C	Sidechain
21	AA	1065	U	Sidechain
21	AA	1068	G	Sidechain
21	AA	1072	G	Sidechain
21	AA	1077	G	Sidechain
21	AA	108	G	Sidechain
21	AA	1083	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1087	G	Sidechain
21	AA	1089	G	Sidechain
21	AA	1092	A	Sidechain
21	AA	1096	C	Sidechain
21	AA	1099	G	Sidechain
21	AA	1108	G	Sidechain
21	AA	1109	C	Sidechain
21	AA	111	G	Sidechain
21	AA	1114	C	Sidechain
21	AA	1116	U	Sidechain
21	AA	1120	C	Sidechain
21	AA	1125	U	Sidechain
21	AA	1133	G	Sidechain
21	AA	1137	C	Sidechain
21	AA	1139	G	Sidechain
21	AA	1140	C	Sidechain
21	AA	1142	G	Sidechain
21	AA	1146	A	Sidechain
21	AA	1147	C	Sidechain
21	AA	1149	C	Sidechain
21	AA	1158	C	Sidechain
21	AA	1161	C	Sidechain
21	AA	1166	G	Sidechain
21	AA	1167	A	Sidechain
21	AA	1169	A	Sidechain
21	AA	1175	G	Sidechain
21	AA	1178	G	Sidechain
21	AA	1179	A	Sidechain
21	AA	1181	G	Sidechain
21	AA	1182	G	Sidechain
21	AA	1187	G	Sidechain
21	AA	1194	U	Sidechain
21	AA	1198	G	Sidechain
21	AA	1201	A	Sidechain
21	AA	1202	U	Sidechain
21	AA	1211	U	Sidechain
21	AA	1213	A	Sidechain
21	AA	1216	A	Sidechain
21	AA	1220	G	Sidechain
21	AA	1221	G	Sidechain
21	AA	1222	G	Sidechain
21	AA	1228	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1234	C	Sidechain
21	AA	1239	A	Sidechain
21	AA	1256	A	Sidechain
21	AA	1266	G	Sidechain
21	AA	1276	G	Sidechain
21	AA	1278	G	Sidechain
21	AA	1282	C	Sidechain
21	AA	1283	U	Sidechain
21	AA	1286	U	Sidechain
21	AA	1290	G	Sidechain
21	AA	1292	G	Sidechain
21	AA	13	U	Sidechain
21	AA	130	A	Sidechain
21	AA	1303	C	Sidechain
21	AA	1305	G	Sidechain
21	AA	1306	A	Sidechain
21	AA	1316	G	Sidechain
21	AA	1321	U	Sidechain
21	AA	1326	U	Sidechain
21	AA	1329	A	Sidechain
21	AA	1332	A	Sidechain
21	AA	1337	G	Sidechain
21	AA	1339	A	Sidechain
21	AA	1340	A	Sidechain
21	AA	1358	U	Sidechain
21	AA	1360	A	Sidechain
21	AA	1362	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	1377	A	Sidechain
21	AA	1380	U	Sidechain
21	AA	1385	G	Sidechain
21	AA	1391	U	Sidechain
21	AA	1393	U	Sidechain
21	AA	1397	C	Sidechain
21	AA	1405	G	Sidechain
21	AA	1409	C	Sidechain
21	AA	1411	C	Sidechain
21	AA	1414	U	Sidechain
21	AA	1416	G	Sidechain
21	AA	142	G	Sidechain
21	AA	1421	G	Sidechain
21	AA	1439	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	144	G	Sidechain
21	AA	1443	C	Sidechain
21	AA	1446	A	Sidechain
21	AA	1447	A	Sidechain
21	AA	1451	U	Sidechain
21	AA	1453	G	Sidechain
21	AA	1455	G	Sidechain
21	AA	1456	A	Sidechain
21	AA	1464	U	Sidechain
21	AA	1470	U	Sidechain
21	AA	1473	G	Sidechain
21	AA	1478	U	Sidechain
21	AA	148	G	Sidechain
21	AA	1483	A	Sidechain
21	AA	1485	U	Sidechain
21	AA	1487	G	Sidechain
21	AA	1489	G	Sidechain
21	AA	1494	G	Sidechain
21	AA	1495	U	Sidechain
21	AA	1496	C	Sidechain
21	AA	1502	A	Sidechain
21	AA	1505	G	Sidechain
21	AA	1507	A	Sidechain
21	AA	1509	C	Sidechain
21	AA	1510	C	Sidechain
21	AA	1514	G	Sidechain
21	AA	1517	G	Sidechain
21	AA	1518	A	Sidechain
21	AA	1521	C	Sidechain
21	AA	1526	G	Sidechain
21	AA	153	C	Sidechain
21	AA	1530	G	Sidechain
21	AA	1532	U	Sidechain
21	AA	1533	C	Sidechain
21	AA	155	A	Sidechain
21	AA	16	A	Sidechain
21	AA	162	A	Sidechain
21	AA	163	C	Sidechain
21	AA	164	G	Sidechain
21	AA	166	U	Sidechain
21	AA	17	U	Sidechain
21	AA	173	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	174	A	Sidechain
21	AA	179	A	Sidechain
21	AA	185	U	Sidechain
21	AA	187	G	Sidechain
21	AA	190	A	Sidechain
21	AA	191	G	Sidechain
21	AA	196	A	Sidechain
21	AA	197	A	Sidechain
21	AA	20	U	Sidechain
21	AA	201	G	Sidechain
21	AA	205	A	Sidechain
21	AA	206	C	Sidechain
21	AA	211	G	Sidechain
21	AA	217	C	Sidechain
21	AA	218	U	Sidechain
21	AA	220	G	Sidechain
21	AA	228	A	Sidechain
21	AA	229	U	Sidechain
21	AA	237	G	Sidechain
21	AA	241	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	262	A	Sidechain
21	AA	269	C	Sidechain
21	AA	274	A	Sidechain
21	AA	278	G	Sidechain
21	AA	279	A	Sidechain
21	AA	283	U	Sidechain
21	AA	284	C	Sidechain
21	AA	286	C	Sidechain
21	AA	29	U	Sidechain
21	AA	292	G	Sidechain
21	AA	295	C	Sidechain
21	AA	297	G	Sidechain
21	AA	314	C	Sidechain
21	AA	315	A	Sidechain
21	AA	316	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	324	G	Sidechain
21	AA	325	A	Sidechain
21	AA	328	C	Sidechain
21	AA	331	G	Sidechain
21	AA	332	G	Sidechain
21	AA	333	U	Sidechain
21	AA	338	A	Sidechain
21	AA	340	U	Sidechain
21	AA	341	C	Sidechain
21	AA	343	U	Sidechain
21	AA	35	G	Sidechain
21	AA	350	G	Sidechain
21	AA	351	G	Sidechain
21	AA	355	C	Sidechain
21	AA	362	G	Sidechain
21	AA	366	A	Sidechain
21	AA	373	A	Sidechain
21	AA	375	U	Sidechain
21	AA	376	G	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	384	G	Sidechain
21	AA	39	G	Sidechain
21	AA	391	G	Sidechain
21	AA	394	G	Sidechain
21	AA	397	A	Sidechain
21	AA	399	G	Sidechain
21	AA	406	G	Sidechain
21	AA	407	U	Sidechain
21	AA	409	U	Sidechain
21	AA	41	G	Sidechain
21	AA	411	A	Sidechain
21	AA	414	A	Sidechain
21	AA	420	U	Sidechain
21	AA	421	U	Sidechain
21	AA	428	G	Sidechain
21	AA	43	C	Sidechain
21	AA	430	A	Sidechain
21	AA	433	G	Sidechain
21	AA	442	G	Sidechain
21	AA	444	G	Sidechain
21	AA	447	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	450	G	Sidechain
21	AA	453	G	Sidechain
21	AA	458	U	Sidechain
21	AA	462	G	Sidechain
21	AA	463	U	Sidechain
21	AA	467	U	Sidechain
21	AA	471	U	Sidechain
21	AA	481	G	Sidechain
21	AA	491	G	Sidechain
21	AA	496	A	Sidechain
21	AA	5	U	Sidechain
21	AA	505	G	Sidechain
21	AA	506	G	Sidechain
21	AA	509	A	Sidechain
21	AA	51	A	Sidechain
21	AA	512	U	Sidechain
21	AA	514	C	Sidechain
21	AA	515	G	Sidechain
21	AA	519	C	Sidechain
21	AA	522	C	Sidechain
21	AA	526	C	Sidechain
21	AA	527	G	Sidechain
21	AA	530	G	Sidechain
21	AA	54	C	Sidechain
21	AA	540	G	Sidechain
21	AA	542	G	Sidechain
21	AA	547	A	Sidechain
21	AA	553	A	Sidechain
21	AA	558	G	Sidechain
21	AA	566	G	Sidechain
21	AA	57	G	Sidechain
21	AA	575	G	Sidechain
21	AA	580	C	Sidechain
21	AA	581	G	Sidechain
21	AA	594	U	Sidechain
21	AA	595	A	Sidechain
21	AA	598	U	Sidechain
21	AA	602	A	Sidechain
21	AA	606	G	Sidechain
21	AA	607	A	Sidechain
21	AA	611	C	Sidechain
21	AA	618	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	623	C	Sidechain
21	AA	626	G	Sidechain
21	AA	629	A	Sidechain
21	AA	632	U	Sidechain
21	AA	633	G	Sidechain
21	AA	634	C	Sidechain
21	AA	642	A	Sidechain
21	AA	648	A	Sidechain
21	AA	657	U	Sidechain
21	AA	658	C	Sidechain
21	AA	66	A	Sidechain
21	AA	664	G	Sidechain
21	AA	669	G	Sidechain
21	AA	670	G	Sidechain
21	AA	674	G	Sidechain
21	AA	676	A	Sidechain
21	AA	678	U	Sidechain
21	AA	682	G	Sidechain
21	AA	686	U	Sidechain
21	AA	699	C	Sidechain
21	AA	705	G	Sidechain
21	AA	706	A	Sidechain
21	AA	710	G	Sidechain
21	AA	717	U	Sidechain
21	AA	718	A	Sidechain
21	AA	729	A	Sidechain
21	AA	73	C	Sidechain
21	AA	737	C	Sidechain
21	AA	740	U	Sidechain
21	AA	741	G	Sidechain
21	AA	752	G	Sidechain
21	AA	756	C	Sidechain
21	AA	760	G	Sidechain
21	AA	771	G	Sidechain
21	AA	789	U	Sidechain
21	AA	790	A	Sidechain
21	AA	792	A	Sidechain
21	AA	794	A	Sidechain
21	AA	807	A	Sidechain
21	AA	809	G	Sidechain
21	AA	81	A	Sidechain
21	AA	811	C	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	813	U	Sidechain
21	AA	817	C	Sidechain
21	AA	82	G	Sidechain
21	AA	822	U	Sidechain
21	AA	827	U	Sidechain
21	AA	829	G	Sidechain
21	AA	834	U	Sidechain
21	AA	836	G	Sidechain
21	AA	838	G	Sidechain
21	AA	84	U	Sidechain
21	AA	848	C	Sidechain
21	AA	85	U	Sidechain
21	AA	852	G	Sidechain
21	AA	856	C	Sidechain
21	AA	857	C	Sidechain
21	AA	859	G	Sidechain
21	AA	862	C	Sidechain
21	AA	863	U	Sidechain
21	AA	867	G	Sidechain
21	AA	868	C	Sidechain
21	AA	87	C	Sidechain
21	AA	871	U	Sidechain
21	AA	873	A	Sidechain
21	AA	882	C	Sidechain
21	AA	883	C	Sidechain
21	AA	885	G	Sidechain
21	AA	890	G	Sidechain
21	AA	891	U	Sidechain
21	AA	895	G	Sidechain
21	AA	898	G	Sidechain
21	AA	9	G	Sidechain
21	AA	900	A	Sidechain
21	AA	906	A	Sidechain
21	AA	910	C	Sidechain
21	AA	926	G	Sidechain
21	AA	93	U	Sidechain
21	AA	931	C	Sidechain
21	AA	938	A	Sidechain
21	AA	942	G	Sidechain
21	AA	946	A	Sidechain
21	AA	949	A	Sidechain
21	AA	954	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	955	U	Sidechain
21	AA	957	U	Sidechain
21	AA	958	A	Sidechain
21	AA	959	A	Sidechain
21	AA	96	U	Sidechain
21	AA	960	U	Sidechain
21	AA	961	U	Sidechain
21	AA	964	A	Sidechain
21	AA	970	C	Sidechain
21	AA	971	G	Sidechain
21	AA	973	G	Sidechain
21	AA	975	A	Sidechain
21	AA	986	U	Sidechain
21	AA	99	C	Sidechain
21	AA	994	A	Sidechain
21	AA	998	C	Sidechain
2	AC	172	VAL	Peptide
8	AI	123	ARG	Peptide
9	AJ	37	ARG	Sidechain
10	AK	115	ILE	Peptide
54	BA	1002	G	Sidechain
54	BA	1005	C	Sidechain
54	BA	1006	C	Sidechain
54	BA	1012	U	Sidechain
54	BA	1014	A	Sidechain
54	BA	1018	U	Sidechain
54	BA	1022	G	Sidechain
54	BA	1023	U	Sidechain
54	BA	1025	G	Sidechain
54	BA	1028	A	Sidechain
54	BA	1029	A	Sidechain
54	BA	103	A	Sidechain
54	BA	1032	A	Sidechain
54	BA	1033	U	Sidechain
54	BA	1041	G	Sidechain
54	BA	1044	C	Sidechain
54	BA	1049	C	Sidechain
54	BA	1055	G	Sidechain
54	BA	1061	U	Sidechain
54	BA	1062	G	Sidechain
54	BA	1068	G	Sidechain
54	BA	1069	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1073	A	Sidechain
54	BA	1079	C	Sidechain
54	BA	108	G	Sidechain
54	BA	1080	A	Sidechain
54	BA	1082	U	Sidechain
54	BA	1083	U	Sidechain
54	BA	1086	A	Sidechain
54	BA	1089	A	Sidechain
54	BA	1091	G	Sidechain
54	BA	1093	G	Sidechain
54	BA	1096	A	Sidechain
54	BA	1098	A	Sidechain
54	BA	11	C	Sidechain
54	BA	1107	G	Sidechain
54	BA	112	U	Sidechain
54	BA	1130	U	Sidechain
54	BA	1133	A	Sidechain
54	BA	1139	G	Sidechain
54	BA	114	U	Sidechain
54	BA	1142	A	Sidechain
54	BA	115	C	Sidechain
54	BA	1151	A	Sidechain
54	BA	1152	C	Sidechain
54	BA	1153	C	Sidechain
54	BA	1155	A	Sidechain
54	BA	1156	A	Sidechain
54	BA	116	C	Sidechain
54	BA	1162	G	Sidechain
54	BA	117	G	Sidechain
54	BA	1185	G	Sidechain
54	BA	1186	G	Sidechain
54	BA	119	A	Sidechain
54	BA	1194	A	Sidechain
54	BA	12	U	Sidechain
54	BA	1200	C	Sidechain
54	BA	1205	A	Sidechain
54	BA	1208	C	Sidechain
54	BA	1209	U	Sidechain
54	BA	1211	C	Sidechain
54	BA	1214	A	Sidechain
54	BA	1224	U	Sidechain
54	BA	1236	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1237	A	Sidechain
54	BA	1238	G	Sidechain
54	BA	1239	G	Sidechain
54	BA	1240	U	Sidechain
54	BA	1242	U	Sidechain
54	BA	125	A	Sidechain
54	BA	1252	G	Sidechain
54	BA	1253	A	Sidechain
54	BA	1256	G	Sidechain
54	BA	1259	G	Sidechain
54	BA	1275	A	Sidechain
54	BA	1276	A	Sidechain
54	BA	1283	G	Sidechain
54	BA	1290	C	Sidechain
54	BA	1292	G	Sidechain
54	BA	1301	A	Sidechain
54	BA	1311	G	Sidechain
54	BA	1313	U	Sidechain
54	BA	1314	C	Sidechain
54	BA	1315	C	Sidechain
54	BA	1317	G	Sidechain
54	BA	1321	A	Sidechain
54	BA	1339	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1346	G	Sidechain
54	BA	1349	C	Sidechain
54	BA	135	U	Sidechain
54	BA	1352	U	Sidechain
54	BA	1360	G	Sidechain
54	BA	1362	C	Sidechain
54	BA	1365	A	Sidechain
54	BA	1373	A	Sidechain
54	BA	1377	G	Sidechain
54	BA	1380	G	Sidechain
54	BA	1385	A	Sidechain
54	BA	1387	A	Sidechain
54	BA	139	U	Sidechain
54	BA	1390	U	Sidechain
54	BA	1395	A	Sidechain
54	BA	1396	U	Sidechain
54	BA	1399	C	Sidechain
54	BA	14	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1400	U	Sidechain
54	BA	1401	G	Sidechain
54	BA	1404	C	Sidechain
54	BA	1405	U	Sidechain
54	BA	141	G	Sidechain
54	BA	1412	U	Sidechain
54	BA	1419	A	Sidechain
54	BA	1424	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1429	G	Sidechain
54	BA	1431	A	Sidechain
54	BA	1442	U	Sidechain
54	BA	1445	G	Sidechain
54	BA	1450	G	Sidechain
54	BA	1453	A	Sidechain
54	BA	1455	G	Sidechain
54	BA	146	A	Sidechain
54	BA	1464	G	Sidechain
54	BA	1475	G	Sidechain
54	BA	1487	U	Sidechain
54	BA	1490	A	Sidechain
54	BA	1492	G	Sidechain
54	BA	1495	A	Sidechain
54	BA	1497	U	Sidechain
54	BA	15	G	Sidechain
54	BA	150	U	Sidechain
54	BA	1509	A	Sidechain
54	BA	152	A	Sidechain
54	BA	1521	G	Sidechain
54	BA	1534	U	Sidechain
54	BA	1537	G	Sidechain
54	BA	1545	A	Sidechain
54	BA	1546	G	Sidechain
54	BA	1569	A	Sidechain
54	BA	1581	G	Sidechain
54	BA	1590	A	Sidechain
54	BA	1595	C	Sidechain
54	BA	1599	U	Sidechain
54	BA	1600	C	Sidechain
54	BA	1601	G	Sidechain
54	BA	1602	U	Sidechain
54	BA	1604	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	162	U	Sidechain
54	BA	1621	U	Sidechain
54	BA	1623	G	Sidechain
54	BA	1625	C	Sidechain
54	BA	1628	G	Sidechain
54	BA	1631	G	Sidechain
54	BA	1632	A	Sidechain
54	BA	1641	A	Sidechain
54	BA	1642	G	Sidechain
54	BA	1651	G	Sidechain
54	BA	1656	C	Sidechain
54	BA	1659	G	Sidechain
54	BA	1664	A	Sidechain
54	BA	1666	G	Sidechain
54	BA	1667	G	Sidechain
54	BA	1671	U	Sidechain
54	BA	1672	A	Sidechain
54	BA	1673	G	Sidechain
54	BA	1680	U	Sidechain
54	BA	1681	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1683	U	Sidechain
54	BA	1688	U	Sidechain
54	BA	1698	A	Sidechain
54	BA	17	G	Sidechain
54	BA	170	U	Sidechain
54	BA	1700	A	Sidechain
54	BA	1701	A	Sidechain
54	BA	1703	G	Sidechain
54	BA	1705	A	Sidechain
54	BA	1706	C	Sidechain
54	BA	1709	U	Sidechain
54	BA	1710	G	Sidechain
54	BA	1711	A	Sidechain
54	BA	1716	U	Sidechain
54	BA	172	A	Sidechain
54	BA	1720	U	Sidechain
54	BA	1725	U	Sidechain
54	BA	1734	G	Sidechain
54	BA	1735	A	Sidechain
54	BA	1737	G	Sidechain
54	BA	1738	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1744	A	Sidechain
54	BA	1749	A	Sidechain
54	BA	175	G	Sidechain
54	BA	1750	G	Sidechain
54	BA	1753	G	Sidechain
54	BA	1759	A	Sidechain
54	BA	1763	G	Sidechain
54	BA	177	G	Sidechain
54	BA	1771	C	Sidechain
54	BA	1772	A	Sidechain
54	BA	1773	A	Sidechain
54	BA	1775	U	Sidechain
54	BA	1779	U	Sidechain
54	BA	1781	U	Sidechain
54	BA	1788	C	Sidechain
54	BA	1790	C	Sidechain
54	BA	1796	U	Sidechain
54	BA	1797	G	Sidechain
54	BA	1802	A	Sidechain
54	BA	1813	G	Sidechain
54	BA	1821	A	Sidechain
54	BA	1828	G	Sidechain
54	BA	1830	C	Sidechain
54	BA	1831	G	Sidechain
54	BA	1832	C	Sidechain
54	BA	1834	U	Sidechain
54	BA	1837	C	Sidechain
54	BA	1840	G	Sidechain
54	BA	1843	C	Sidechain
54	BA	1845	G	Sidechain
54	BA	1847	A	Sidechain
54	BA	1848	A	Sidechain
54	BA	1852	U	Sidechain
54	BA	1859	U	Sidechain
54	BA	186	G	Sidechain
54	BA	1860	G	Sidechain
54	BA	1872	A	Sidechain
54	BA	1882	U	Sidechain
54	BA	1885	A	Sidechain
54	BA	1886	U	Sidechain
54	BA	189	G	Sidechain
54	BA	1897	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1909	C	Sidechain
54	BA	1910	G	Sidechain
54	BA	1913	A	Sidechain
54	BA	1918	A	Sidechain
54	BA	1923	U	Sidechain
54	BA	1924	C	Sidechain
54	BA	1929	G	Sidechain
54	BA	1936	A	Sidechain
54	BA	1940	U	Sidechain
54	BA	1941	C	Sidechain
54	BA	1948	G	Sidechain
54	BA	1956	U	Sidechain
54	BA	1963	U	Sidechain
54	BA	1966	A	Sidechain
54	BA	197	A	Sidechain
54	BA	1976	U	Sidechain
54	BA	198	C	Sidechain
54	BA	1989	G	Sidechain
54	BA	199	A	Sidechain
54	BA	1993	U	Sidechain
54	BA	1996	C	Sidechain
54	BA	200	U	Sidechain
54	BA	2012	G	Sidechain
54	BA	2014	A	Sidechain
54	BA	2016	U	Sidechain
54	BA	202	U	Sidechain
54	BA	2024	G	Sidechain
54	BA	2031	A	Sidechain
54	BA	2035	G	Sidechain
54	BA	2039	U	Sidechain
54	BA	2040	G	Sidechain
54	BA	2044	C	Sidechain
54	BA	2046	G	Sidechain
54	BA	2056	G	Sidechain
54	BA	2059	A	Sidechain
54	BA	206	U	Sidechain
54	BA	2065	C	Sidechain
54	BA	2066	C	Sidechain
54	BA	2068	U	Sidechain
54	BA	2069	G	Sidechain
54	BA	207	A	Sidechain
54	BA	2070	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2071	A	Sidechain
54	BA	2075	U	Sidechain
54	BA	2076	U	Sidechain
54	BA	2082	A	Sidechain
54	BA	209	C	Sidechain
54	BA	2097	A	Sidechain
54	BA	2104	C	Sidechain
54	BA	2112	G	Sidechain
54	BA	2113	U	Sidechain
54	BA	2115	G	Sidechain
54	BA	2116	G	Sidechain
54	BA	2119	A	Sidechain
54	BA	2120	G	Sidechain
54	BA	2127	G	Sidechain
54	BA	2130	U	Sidechain
54	BA	2131	U	Sidechain
54	BA	2134	A	Sidechain
54	BA	2138	G	Sidechain
54	BA	214	G	Sidechain
54	BA	2159	G	Sidechain
54	BA	2160	C	Sidechain
54	BA	2161	C	Sidechain
54	BA	2162	G	Sidechain
54	BA	2163	A	Sidechain
54	BA	2168	G	Sidechain
54	BA	2169	A	Sidechain
54	BA	2172	U	Sidechain
54	BA	2177	C	Sidechain
54	BA	2188	U	Sidechain
54	BA	2194	U	Sidechain
54	BA	220	G	Sidechain
54	BA	2207	C	Sidechain
54	BA	2208	C	Sidechain
54	BA	221	A	Sidechain
54	BA	2216	G	Sidechain
54	BA	2217	G	Sidechain
54	BA	2228	G	Sidechain
54	BA	2236	U	Sidechain
54	BA	2238	G	Sidechain
54	BA	2240	U	Sidechain
54	BA	2254	C	Sidechain
54	BA	2258	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2260	C	Sidechain
54	BA	2267	A	Sidechain
54	BA	2269	G	Sidechain
54	BA	227	A	Sidechain
54	BA	2277	G	Sidechain
54	BA	228	C	Sidechain
54	BA	2281	A	Sidechain
54	BA	2282	G	Sidechain
54	BA	2283	C	Sidechain
54	BA	2287	A	Sidechain
54	BA	2290	G	Sidechain
54	BA	2294	G	Sidechain
54	BA	2295	C	Sidechain
54	BA	2301	C	Sidechain
54	BA	2302	U	Sidechain
54	BA	2305	U	Sidechain
54	BA	2307	G	Sidechain
54	BA	2309	A	Sidechain
54	BA	2312	U	Sidechain
54	BA	2313	C	Sidechain
54	BA	2324	U	Sidechain
54	BA	2325	G	Sidechain
54	BA	2327	A	Sidechain
54	BA	2328	A	Sidechain
54	BA	233	A	Sidechain
54	BA	2336	A	Sidechain
54	BA	2338	C	Sidechain
54	BA	2341	G	Sidechain
54	BA	2344	U	Sidechain
54	BA	2345	G	Sidechain
54	BA	2354	C	Sidechain
54	BA	2357	G	Sidechain
54	BA	2367	G	Sidechain
54	BA	2368	C	Sidechain
54	BA	2375	G	Sidechain
54	BA	2378	A	Sidechain
54	BA	2382	G	Sidechain
54	BA	2383	G	Sidechain
54	BA	2390	U	Sidechain
54	BA	2391	G	Sidechain
54	BA	240	C	Sidechain
54	BA	2406	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2407	A	Sidechain
54	BA	2416	C	Sidechain
54	BA	2428	G	Sidechain
54	BA	2430	A	Sidechain
54	BA	2431	U	Sidechain
54	BA	2433	A	Sidechain
54	BA	2434	A	Sidechain
54	BA	244	A	Sidechain
54	BA	2442	C	Sidechain
54	BA	2444	G	Sidechain
54	BA	2448	A	Sidechain
54	BA	2453	A	Sidechain
54	BA	2454	G	Sidechain
54	BA	2459	A	Sidechain
54	BA	2460	U	Sidechain
54	BA	2462	C	Sidechain
54	BA	2463	C	Sidechain
54	BA	247	G	Sidechain
54	BA	2470	G	Sidechain
54	BA	2475	C	Sidechain
54	BA	2478	A	Sidechain
54	BA	2482	A	Sidechain
54	BA	2483	C	Sidechain
54	BA	2485	G	Sidechain
54	BA	2486	C	Sidechain
54	BA	2489	U	Sidechain
54	BA	249	C	Sidechain
54	BA	2493	U	Sidechain
54	BA	2495	G	Sidechain
54	BA	2498	C	Sidechain
54	BA	25	U	Sidechain
54	BA	250	G	Sidechain
54	BA	2502	G	Sidechain
54	BA	2509	G	Sidechain
54	BA	2516	A	Sidechain
54	BA	2530	A	Sidechain
54	BA	2542	A	Sidechain
54	BA	2546	U	Sidechain
54	BA	2549	G	Sidechain
54	BA	2551	C	Sidechain
54	BA	2555	U	Sidechain
54	BA	2559	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2571	U	Sidechain
54	BA	2581	G	Sidechain
54	BA	2586	U	Sidechain
54	BA	2591	C	Sidechain
54	BA	2595	G	Sidechain
54	BA	2603	G	Sidechain
54	BA	2607	G	Sidechain
54	BA	2609	U	Sidechain
54	BA	261	G	Sidechain
54	BA	2615	U	Sidechain
54	BA	2618	G	Sidechain
54	BA	262	A	Sidechain
54	BA	2620	C	Sidechain
54	BA	2623	G	Sidechain
54	BA	2627	G	Sidechain
54	BA	2630	G	Sidechain
54	BA	2637	U	Sidechain
54	BA	2638	G	Sidechain
54	BA	2643	G	Sidechain
54	BA	2645	G	Sidechain
54	BA	2646	C	Sidechain
54	BA	2649	C	Sidechain
54	BA	2653	U	Sidechain
54	BA	2658	C	Sidechain
54	BA	2660	A	Sidechain
54	BA	2668	G	Sidechain
54	BA	2679	A	Sidechain
54	BA	2694	G	Sidechain
54	BA	2699	C	Sidechain
54	BA	2701	U	Sidechain
54	BA	272	A	Sidechain
54	BA	273	G	Sidechain
54	BA	2732	G	Sidechain
54	BA	274	C	Sidechain
54	BA	2743	U	Sidechain
54	BA	2757	A	Sidechain
54	BA	2767	C	Sidechain
54	BA	2772	C	Sidechain
54	BA	2774	C	Sidechain
54	BA	2775	G	Sidechain
54	BA	278	A	Sidechain
54	BA	2781	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2784	U	Sidechain
54	BA	2787	C	Sidechain
54	BA	279	A	Sidechain
54	BA	2798	U	Sidechain
54	BA	2804	U	Sidechain
54	BA	2809	A	Sidechain
54	BA	2811	G	Sidechain
54	BA	2812	G	Sidechain
54	BA	2814	A	Sidechain
54	BA	2820	A	Sidechain
54	BA	2822	G	Sidechain
54	BA	2833	U	Sidechain
54	BA	2843	G	Sidechain
54	BA	2847	U	Sidechain
54	BA	2849	U	Sidechain
54	BA	285	G	Sidechain
54	BA	2851	A	Sidechain
54	BA	2852	G	Sidechain
54	BA	2854	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2863	C	Sidechain
54	BA	2867	G	Sidechain
54	BA	2868	A	Sidechain
54	BA	287	G	Sidechain
54	BA	2874	C	Sidechain
54	BA	2879	A	Sidechain
54	BA	2883	A	Sidechain
54	BA	2885	G	Sidechain
54	BA	2889	C	Sidechain
54	BA	2893	A	Sidechain
54	BA	291	G	Sidechain
54	BA	295	G	Sidechain
54	BA	30	G	Sidechain
54	BA	31	C	Sidechain
54	BA	317	G	Sidechain
54	BA	318	C	Sidechain
54	BA	319	G	Sidechain
54	BA	32	C	Sidechain
54	BA	321	U	Sidechain
54	BA	323	C	Sidechain
54	BA	33	C	Sidechain
54	BA	330	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	333	G	Sidechain
54	BA	336	C	Sidechain
54	BA	339	U	Sidechain
54	BA	342	A	Sidechain
54	BA	343	C	Sidechain
54	BA	354	A	Sidechain
54	BA	370	G	Sidechain
54	BA	373	U	Sidechain
54	BA	39	G	Sidechain
54	BA	390	U	Sidechain
54	BA	392	U	Sidechain
54	BA	395	U	Sidechain
54	BA	399	U	Sidechain
54	BA	40	U	Sidechain
54	BA	401	A	Sidechain
54	BA	403	U	Sidechain
54	BA	405	U	Sidechain
54	BA	41	C	Sidechain
54	BA	418	C	Sidechain
54	BA	420	C	Sidechain
54	BA	422	A	Sidechain
54	BA	426	C	Sidechain
54	BA	429	A	Sidechain
54	BA	43	G	Sidechain
54	BA	435	C	Sidechain
54	BA	437	U	Sidechain
54	BA	446	G	Sidechain
54	BA	452	G	Sidechain
54	BA	460	A	Sidechain
54	BA	461	C	Sidechain
54	BA	463	G	Sidechain
54	BA	479	A	Sidechain
54	BA	481	G	Sidechain
54	BA	49	A	Sidechain
54	BA	490	C	Sidechain
54	BA	492	A	Sidechain
54	BA	498	G	Sidechain
54	BA	500	G	Sidechain
54	BA	502	A	Sidechain
54	BA	507	A	Sidechain
54	BA	51	G	Sidechain
54	BA	511	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	517	C	Sidechain
54	BA	528	A	Sidechain
54	BA	529	A	Sidechain
54	BA	530	G	Sidechain
54	BA	533	G	Sidechain
54	BA	541	A	Sidechain
54	BA	545	U	Sidechain
54	BA	548	G	Sidechain
54	BA	551	G	Sidechain
54	BA	553	G	Sidechain
54	BA	568	U	Sidechain
54	BA	570	G	Sidechain
54	BA	576	U	Sidechain
54	BA	578	G	Sidechain
54	BA	581	C	Sidechain
54	BA	584	C	Sidechain
54	BA	586	A	Sidechain
54	BA	588	U	Sidechain
54	BA	608	A	Sidechain
54	BA	612	G	Sidechain
54	BA	615	U	Sidechain
54	BA	617	G	Sidechain
54	BA	62	U	Sidechain
54	BA	620	G	Sidechain
54	BA	621	A	Sidechain
54	BA	622	G	Sidechain
54	BA	628	G	Sidechain
54	BA	629	G	Sidechain
54	BA	630	G	Sidechain
54	BA	636	G	Sidechain
54	BA	640	C	Sidechain
54	BA	645	C	Sidechain
54	BA	652	U	Sidechain
54	BA	674	G	Sidechain
54	BA	676	A	Sidechain
54	BA	679	C	Sidechain
54	BA	680	C	Sidechain
54	BA	69	C	Sidechain
54	BA	690	G	Sidechain
54	BA	692	C	Sidechain
54	BA	697	G	Sidechain
54	BA	699	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	7	G	Sidechain
54	BA	700	G	Sidechain
54	BA	711	G	Sidechain
54	BA	713	G	Sidechain
54	BA	726	G	Sidechain
54	BA	729	G	Sidechain
54	BA	732	C	Sidechain
54	BA	741	U	Sidechain
54	BA	746	U	Sidechain
54	BA	750	A	Sidechain
54	BA	752	A	Sidechain
54	BA	77	G	Sidechain
54	BA	772	C	Sidechain
54	BA	773	U	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain
54	BA	780	G	Sidechain
54	BA	783	A	Sidechain
54	BA	790	U	Sidechain
54	BA	797	G	Sidechain
54	BA	80	G	Sidechain
54	BA	804	A	Sidechain
54	BA	817	C	Sidechain
54	BA	818	G	Sidechain
54	BA	827	U	Sidechain
54	BA	828	U	Sidechain
54	BA	829	A	Sidechain
54	BA	831	G	Sidechain
54	BA	837	C	Sidechain
54	BA	840	C	Sidechain
54	BA	841	G	Sidechain
54	BA	843	G	Sidechain
54	BA	85	G	Sidechain
54	BA	858	G	Sidechain
54	BA	875	G	Sidechain
54	BA	888	C	Sidechain
54	BA	890	C	Sidechain
54	BA	891	G	Sidechain
54	BA	893	C	Sidechain
54	BA	898	C	Sidechain
54	BA	907	G	Sidechain
54	BA	912	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	920	A	Sidechain
54	BA	921	C	Sidechain
54	BA	922	C	Sidechain
54	BA	923	G	Sidechain
54	BA	929	U	Sidechain
54	BA	934	U	Sidechain
54	BA	943	A	Sidechain
54	BA	945	A	Sidechain
54	BA	949	G	Sidechain
54	BA	950	G	Sidechain
54	BA	955	U	Sidechain
54	BA	956	G	Sidechain
54	BA	960	A	Sidechain
54	BA	961	C	Sidechain
54	BA	964	C	Sidechain
54	BA	966	G	Sidechain
54	BA	968	C	Sidechain
54	BA	97	C	Sidechain
54	BA	972	A	Sidechain
54	BA	974	G	Sidechain
54	BA	983	A	Sidechain
54	BA	984	A	Sidechain
54	BA	985	C	Sidechain
54	BA	989	G	Sidechain
54	BA	991	C	Sidechain
54	BA	994	C	Sidechain
55	BB	108	A	Sidechain
55	BB	112	G	Sidechain
55	BB	113	C	Sidechain
55	BB	13	G	Sidechain
55	BB	15	A	Sidechain
55	BB	24	G	Sidechain
55	BB	29	A	Sidechain
55	BB	31	C	Sidechain
55	BB	40	U	Sidechain
55	BB	41	G	Sidechain
55	BB	49	C	Sidechain
55	BB	50	A	Sidechain
55	BB	57	A	Sidechain
55	BB	6	G	Sidechain
55	BB	64	G	Sidechain
55	BB	69	G	Sidechain

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Mol	Chain	Res	Type	Group
55	BB	73	A	Sidechain
55	BB	75	G	Sidechain
55	BB	89	U	Sidechain
55	BB	96	G	Sidechain
25	BC	155	ARG	Sidechain
43	BU	21	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	0	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	0	0
9	AJ	790	0	832	1	0
10	AK	880	0	891	0	0
11	AL	955	0	1019	0	0
12	AM	877	0	937	0	0
13	AN	805	0	844	0	0
14	AO	714	0	737	0	0
15	AP	639	0	656	0	0
16	AQ	652	0	695	0	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16522	0	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	1	0
25	BC	2083	0	2157	0	0
26	BD	1565	0	1616	1	0
27	BE	1552	0	1619	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
36	BN	961	0	1000	0	0
37	BO	892	0	923	0	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	1	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	0	0
43	BU	780	0	834	0	0
44	BV	753	0	780	0	0
45	BW	599	0	614	0	0
46	BX	625	0	655	0	0
47	BY	509	0	543	0	0
48	BZ	449	0	491	0	0
49	B0	444	0	461	0	0
50	B1	413	0	444	0	0
51	B2	377	0	418	0	0
52	B3	504	0	574	0	0
53	B4	302	0	343	1	0
54	BA	62317	0	31345	6	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	1	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99665	12	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 (12) 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)
35:BM:126:ILE:H	35:BM:126:ILE:HD13	1.74	0.53
54:BA:2105:U:HO2'	56:B5:2:ALA:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A3:24:C:H2'	24:A3:25:U:C6	2.53	0.43
54:BA:480:A:H3'	54:BA:481:G:C5'	2.48	0.43
54:BA:2352:A:C5	54:BA:2353:G:H1'	2.53	0.43
53:B4:1:MET:SD	53:B4:34:LYS:HE3	2.59	0.42
54:BA:1247:A:H3'	54:BA:1248:G:H5"	2.02	0.42
39:BQ:23:TYR:CD1	54:BA:533:G:H5'	2.56	0.41
5:AF:94:HIS:CG	5:AF:95:ALA:H	2.40	0.40
26:BD:33:ARG:HD2	26:BD:33:ARG:H	1.86	0.40
2:AC:22:PHE:CE2	9:AJ:11:LYS:HE3	2.57	0.40
54:BA:83:A:H2'	54:BA:84:A:C8	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%)	198 (91%)	17 (8%)	3 (1%)	11 46
2	AC	205/208 (99%)	185 (90%)	15 (7%)	5 (2%)	6 33
3	AD	203/206 (98%)	189 (93%)	11 (5%)	3 (2%)	10 46
4	AE	150/152 (99%)	137 (91%)	12 (8%)	1 (1%)	22 63
5	AF	99/101 (98%)	83 (84%)	10 (10%)	6 (6%)	1 17
6	AG	150/152 (99%)	134 (89%)	11 (7%)	5 (3%)	4 26
7	AH	127/130 (98%)	121 (95%)	5 (4%)	1 (1%)	19 60
8	AI	126/128 (98%)	109 (86%)	12 (10%)	5 (4%)	3 23
9	AJ	98/100 (98%)	91 (93%)	4 (4%)	3 (3%)	4 27
10	AK	116/118 (98%)	108 (93%)	8 (7%)	0	100 100
11	AL	121/124 (98%)	107 (88%)	10 (8%)	4 (3%)	4 26
12	AM	112/115 (97%)	98 (88%)	11 (10%)	3 (3%)	5 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	AN	98/101 (97%)	84 (86%)	13 (13%)	1 (1%)	15 55
14	AO	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13 50
15	AP	79/81 (98%)	69 (87%)	6 (8%)	4 (5%)	2 19
16	AQ	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	12 48
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	8 40
18	AS	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	12 48
19	AT	84/86 (98%)	78 (93%)	3 (4%)	3 (4%)	3 25
20	AU	51/53 (96%)	40 (78%)	7 (14%)	4 (8%)	1 13
25	BC	270/273 (99%)	242 (90%)	25 (9%)	3 (1%)	14 52
26	BD	207/209 (99%)	176 (85%)	16 (8%)	15 (7%)	1 14
27	BE	199/201 (99%)	174 (87%)	17 (8%)	8 (4%)	3 23
28	BF	176/179 (98%)	158 (90%)	11 (6%)	7 (4%)	3 23
29	BG	174/177 (98%)	148 (85%)	24 (14%)	2 (1%)	14 52
30	BH	147/149 (99%)	133 (90%)	14 (10%)	0	100 100
31	BI	139/142 (98%)	121 (87%)	14 (10%)	4 (3%)	4 29
32	BJ	140/142 (99%)	127 (91%)	8 (6%)	5 (4%)	3 25
33	BK	121/123 (98%)	106 (88%)	12 (10%)	3 (2%)	5 32
34	BL	141/144 (98%)	125 (89%)	10 (7%)	6 (4%)	2 22
35	BM	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	6 35
36	BN	119/121 (98%)	105 (88%)	10 (8%)	4 (3%)	3 26
37	BO	114/117 (97%)	105 (92%)	8 (7%)	1 (1%)	17 57
38	BP	112/115 (97%)	97 (87%)	11 (10%)	4 (4%)	3 25
39	BQ	115/118 (98%)	103 (90%)	8 (7%)	4 (4%)	3 25
40	BR	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	4 28
41	BS	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	8 38
42	BT	92/94 (98%)	81 (88%)	7 (8%)	4 (4%)	2 22
43	BU	101/104 (97%)	87 (86%)	5 (5%)	9 (9%)	1 11
44	BV	92/94 (98%)	88 (96%)	3 (3%)	1 (1%)	14 52
45	BW	78/80 (98%)	58 (74%)	17 (22%)	3 (4%)	3 24
46	BX	75/79 (95%)	62 (83%)	8 (11%)	5 (7%)	1 15
47	BY	61/63 (97%)	55 (90%)	3 (5%)	3 (5%)	2 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
48	BZ	56/59 (95%)	50 (89%)	6 (11%)	0	100 100
49	B0	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	8 38
50	B1	50/52 (96%)	46 (92%)	1 (2%)	3 (6%)	1 17
51	B2	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
52	B3	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	4 26
53	B4	36/38 (95%)	31 (86%)	5 (14%)	0	100 100
56	B5	221/234 (94%)	206 (93%)	12 (5%)	3 (1%)	11 46
All	All	5876/6008 (98%)	5263 (90%)	450 (8%)	163 (3%)	8 30

All (163) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	206	ILE
6	AG	11	ILE
9	AJ	75	ASP
11	AL	43	LYS
17	AR	20	ILE
20	AU	9	GLU
26	BD	134	HIS
26	BD	150	GLN
26	BD	201	LEU
27	BE	96	VAL
28	BF	32	LYS
28	BF	176	PHE
31	BI	119	ALA
33	BK	103	VAL
37	BO	100	HIS
38	BP	63	ILE
39	BQ	87	VAL
43	BU	70	ALA
44	BV	71	LYS
50	B1	36	LYS
50	B1	50	GLU
52	B3	31	ILE
56	B5	50	ILE
2	AC	176	THR
3	AD	33	ILE
4	AE	105	ILE
5	AF	6	ILE

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Mol	Chain	Res	Type
6	AG	4	ARG
6	AG	74	VAL
7	AH	69	ALA
8	AI	120	ALA
12	AM	42	VAL
14	AO	10	ILE
15	AP	79	ASN
19	AT	43	LYS
25	BC	191	LEU
26	BD	51	THR
26	BD	80	TRP
26	BD	119	ALA
26	BD	145	SER
27	BE	61	ARG
27	BE	147	LEU
34	BL	4	ASN
34	BL	36	LYS
36	BN	47	VAL
38	BP	31	VAL
38	BP	109	ILE
40	BR	91	GLN
43	BU	83	GLY
45	BW	20	LEU
46	BX	26	ARG
47	BY	9	LYS
47	BY	48	ARG
49	B0	27	LEU
1	AB	18	GLN
5	AF	10	VAL
5	AF	59	TYR
5	AF	63	ASN
5	AF	87	SER
8	AI	122	ARG
8	AI	126	PHE
9	AJ	57	VAL
15	AP	25	ARG
18	AS	5	LYS
20	AU	25	ALA
25	BC	36	ASN
26	BD	31	ALA
26	BD	34	VAL
26	BD	40	LEU

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Mol	Chain	Res	Type
26	BD	77	ARG
26	BD	167	ASN
27	BE	165	HIS
29	BG	22	VAL
31	BI	18	ASN
32	BJ	15	TRP
32	BJ	46	PRO
32	BJ	53	TYR
33	BK	92	GLU
35	BM	23	GLY
36	BN	91	ALA
36	BN	102	PHE
40	BR	37	GLU
41	BS	33	LEU
41	BS	92	ARG
42	BT	66	LYS
42	BT	68	LYS
42	BT	78	SER
43	BU	43	LYS
43	BU	45	GLN
46	BX	27	ARG
46	BX	52	ALA
47	BY	7	ARG
52	B3	3	ILE
56	B5	3	LYS
1	AB	224	ARG
2	AC	167	TYR
3	AD	28	ASP
3	AD	34	GLU
6	AG	56	SER
8	AI	55	ASP
13	AN	63	ARG
15	AP	43	ALA
15	AP	80	LYS
16	AQ	64	ARG
19	AT	65	LEU
26	BD	112	THR
27	BE	45	ALA
28	BF	136	ILE
33	BK	14	SER
34	BL	3	LEU
34	BL	27	LEU

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Mol	Chain	Res	Type
35	BM	117	PHE
39	BQ	21	LYS
39	BQ	86	SER
43	BU	12	VAL
43	BU	19	GLY
43	BU	95	PHE
46	BX	17	ARG
46	BX	21	LEU
56	B5	91	GLY
5	AF	93	LYS
6	AG	5	VAL
11	AL	33	CYS
11	AL	78	VAL
12	AM	82	LEU
20	AU	23	GLU
26	BD	22	ILE
27	BE	46	GLN
28	BF	46	LYS
28	BF	103	ILE
29	BG	108	PHE
32	BJ	72	LYS
32	BJ	81	ILE
34	BL	94	THR
38	BP	50	ARG
39	BQ	20	ALA
40	BR	44	GLY
43	BU	59	GLU
1	AB	128	LEU
11	AL	46	SER
26	BD	87	GLY
28	BF	110	ILE
31	BI	56	VAL
35	BM	36	VAL
43	BU	5	ARG
45	BW	11	ASN
8	AI	57	VAL
25	BC	98	GLY
42	BT	2	ILE
2	AC	195	ILE
9	AJ	42	LEU
50	B1	4	ILE
12	AM	8	ILE

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Mol	Chain	Res	Type
19	AT	3	ILE
20	AU	31	VAL
27	BE	120	VAL
27	BE	186	VAL
31	BI	24	GLY
34	BL	55	MET
36	BN	84	GLY
45	BW	6	GLY
28	BF	12	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%)	176 (98%)	4 (2%)	52 71
2	AC	170/171 (99%)	167 (98%)	3 (2%)	59 77
3	AD	172/173 (99%)	169 (98%)	3 (2%)	60 78
4	AE	113/113 (100%)	112 (99%)	1 (1%)	78 87
5	AF	87/87 (100%)	87 (100%)	0	100 100
6	AG	123/123 (100%)	122 (99%)	1 (1%)	81 89
7	AH	104/105 (99%)	102 (98%)	2 (2%)	57 75
8	AI	105/105 (100%)	104 (99%)	1 (1%)	76 86
9	AJ	86/86 (100%)	86 (100%)	0	100 100
10	AK	90/90 (100%)	90 (100%)	0	100 100
11	AL	103/104 (99%)	102 (99%)	1 (1%)	76 86
12	AM	91/92 (99%)	90 (99%)	1 (1%)	73 84
13	AN	83/84 (99%)	80 (96%)	3 (4%)	35 59
14	AO	76/77 (99%)	76 (100%)	0	100 100
15	AP	65/65 (100%)	64 (98%)	1 (2%)	65 80
16	AQ	74/74 (100%)	71 (96%)	3 (4%)	30 55
17	AR	48/48 (100%)	48 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	AS	70/70 (100%)	67 (96%)	3 (4%)	29 53
19	AT	65/65 (100%)	63 (97%)	2 (3%)	40 62
20	AU	44/44 (100%)	44 (100%)	0	100 100
25	BC	216/217 (100%)	208 (96%)	8 (4%)	34 58
26	BD	164/164 (100%)	159 (97%)	5 (3%)	41 63
27	BE	165/165 (100%)	165 (100%)	0	100 100
28	BF	149/150 (99%)	149 (100%)	0	100 100
29	BG	137/138 (99%)	135 (98%)	2 (2%)	65 80
30	BH	114/114 (100%)	108 (95%)	6 (5%)	22 47
31	BI	109/110 (99%)	108 (99%)	1 (1%)	78 87
32	BJ	116/116 (100%)	110 (95%)	6 (5%)	23 48
33	BK	103/103 (100%)	103 (100%)	0	100 100
34	BL	102/103 (99%)	102 (100%)	0	100 100
35	BM	109/109 (100%)	107 (98%)	2 (2%)	59 77
36	BN	100/100 (100%)	99 (99%)	1 (1%)	76 86
37	BO	86/87 (99%)	86 (100%)	0	100 100
38	BP	99/100 (99%)	96 (97%)	3 (3%)	41 63
39	BQ	89/90 (99%)	88 (99%)	1 (1%)	73 84
40	BR	84/84 (100%)	84 (100%)	0	100 100
41	BS	93/93 (100%)	92 (99%)	1 (1%)	73 84
42	BT	80/80 (100%)	79 (99%)	1 (1%)	69 81
43	BU	83/84 (99%)	80 (96%)	3 (4%)	35 59
44	BV	78/78 (100%)	77 (99%)	1 (1%)	69 81
45	BW	59/59 (100%)	56 (95%)	3 (5%)	24 48
46	BX	67/68 (98%)	60 (90%)	7 (10%)	7 24
47	BY	55/55 (100%)	55 (100%)	0	100 100
48	BZ	48/49 (98%)	48 (100%)	0	100 100
49	B0	47/48 (98%)	46 (98%)	1 (2%)	53 72
50	B1	45/45 (100%)	43 (96%)	2 (4%)	28 53
51	B2	38/38 (100%)	37 (97%)	1 (3%)	46 66
52	B3	51/52 (98%)	50 (98%)	1 (2%)	55 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	4755 (98%)	87 (2%)	61 77

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	17	HIS
1	AB	22	TRP
1	AB	71	THR
1	AB	124	THR
2	AC	128	MET
2	AC	133	MET
2	AC	191	THR
3	AD	2	ARG
3	AD	49	ASP
3	AD	50	TYR
4	AE	155	LYS
6	AG	129	ASN
7	AH	20	ASN
7	AH	65	PHE
8	AI	80	HIS
11	AL	120	ARG
12	AM	104	ASN
13	AN	61	ARG
13	AN	82	ILE
13	AN	101	TRP
15	AP	8	ARG
16	AQ	41	THR
16	AQ	62	GLU
16	AQ	69	THR
18	AS	4	LEU
18	AS	13	HIS
18	AS	73	PHE
19	AT	19	HIS
19	AT	30	PHE
25	BC	34	GLU
25	BC	62	ARG
25	BC	80	LEU
25	BC	153	LEU
25	BC	156	SER

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Mol	Chain	Res	Type
25	BC	179	GLU
25	BC	200	MET
25	BC	212	TRP
26	BD	33	ARG
26	BD	42	ASN
26	BD	134	HIS
26	BD	136	ASN
26	BD	181	ASP
29	BG	34	ARG
29	BG	154	GLU
30	BH	1	MET
30	BH	18	GLN
30	BH	40	THR
30	BH	58	LEU
30	BH	113	SER
30	BH	132	PHE
31	BI	125	THR
32	BJ	43	GLU
32	BJ	53	TYR
32	BJ	65	THR
32	BJ	77	HIS
32	BJ	119	PHE
32	BJ	128	ASN
35	BM	97	GLN
35	BM	126	ILE
36	BN	4	ARG
38	BP	12	MET
38	BP	31	VAL
38	BP	98	TYR
39	BQ	50	ARG
41	BS	57	ASN
42	BT	61	LEU
43	BU	5	ARG
43	BU	57	ILE
43	BU	80	ASP
44	BV	12	GLN
45	BW	23	LYS
45	BW	39	GLN
45	BW	54	ARG
46	BX	31	ASN
46	BX	33	HIS
46	BX	35	HIS

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Mol	Chain	Res	Type
46	BX	36	ARG
46	BX	40	GLU
46	BX	56	ARG
46	BX	73	ARG
49	B0	3	GLN
50	B1	16	THR
50	B1	34	GLU
51	B2	43	THR
52	B3	7	ARG
56	B5	13	GLU
56	B5	165	ASN

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

Mol	Chain	Res	Type
5	AF	58	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1529/1533 (99%)	271 (17%)	84 (5%)
22	A1	73/76 (96%)	11 (15%)	3 (4%)
23	A2	14/15 (93%)	6 (42%)	2 (14%)
24	A3	77/77 (100%)	13 (16%)	1 (1%)
54	BA	2902/2903 (99%)	460 (15%)	131 (4%)
55	BB	116/118 (98%)	21 (18%)	4 (3%)
All	All	4711/4722 (99%)	782 (16%)	225 (4%)

All (782) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	7	A
21	AA	9	G
21	AA	13	U
21	AA	14	U
21	AA	17	U
21	AA	26	A
21	AA	27	G
21	AA	32	A
21	AA	36	C

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Mol	Chain	Res	Type
21	AA	39	G
21	AA	40	C
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	52	C
21	AA	54	C
21	AA	55	A
21	AA	66	A
21	AA	69	G
21	AA	83	C
21	AA	86	G
21	AA	87	C
21	AA	94	G
21	AA	95	C
21	AA	109	A
21	AA	110	C
21	AA	112	G
21	AA	120	A
21	AA	121	U
21	AA	124	C
21	AA	125	U
21	AA	131	A
21	AA	136	C
21	AA	144	G
21	AA	159	G
21	AA	161	A
21	AA	163	C
21	AA	164	G
21	AA	165	G
21	AA	171	A
21	AA	188	C
21	AA	189	A
21	AA	190	A
21	AA	191	G
21	AA	195	A
21	AA	198	G
21	AA	207	C
21	AA	211	G
21	AA	212	G
21	AA	230	G
21	AA	240	G

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Mol	Chain	Res	Type
21	AA	244	U
21	AA	245	U
21	AA	246	A
21	AA	247	G
21	AA	249	U
21	AA	250	A
21	AA	251	G
21	AA	252	U
21	AA	266	G
21	AA	267	C
21	AA	273	U
21	AA	279	A
21	AA	282	A
21	AA	289	G
21	AA	306	A
21	AA	307	C
21	AA	308	C
21	AA	309	A
21	AA	321	A
21	AA	324	G
21	AA	328	C
21	AA	329	A
21	AA	344	A
21	AA	345	C
21	AA	347	G
21	AA	348	G
21	AA	352	C
21	AA	354	G
21	AA	358	U
21	AA	363	A
21	AA	367	U
21	AA	372	C
21	AA	373	A
21	AA	374	A
21	AA	381	C
21	AA	384	G
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	412	A
21	AA	421	U
21	AA	422	C

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Mol	Chain	Res	Type
21	AA	424	G
21	AA	429	U
21	AA	451	A
21	AA	463	U
21	AA	465	A
21	AA	467	U
21	AA	468	A
21	AA	473	U
21	AA	481	G
21	AA	494	G
21	AA	499	A
21	AA	505	G
21	AA	511	C
21	AA	512	U
21	AA	513	C
21	AA	518	C
21	AA	522	C
21	AA	527	G
21	AA	532	A
21	AA	533	A
21	AA	547	A
21	AA	559	A
21	AA	562	U
21	AA	566	G
21	AA	572	A
21	AA	576	C
21	AA	582	C
21	AA	611	C
21	AA	612	C
21	AA	618	C
21	AA	633	G
21	AA	653	U
21	AA	665	A
21	AA	687	A
21	AA	694	A
21	AA	695	A
21	AA	714	G
21	AA	718	A
21	AA	719	C
21	AA	731	G
21	AA	755	G
21	AA	777	A

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Mol	Chain	Res	Type
21	AA	793	U
21	AA	794	A
21	AA	812	G
21	AA	817	C
21	AA	821	G
21	AA	827	U
21	AA	828	U
21	AA	841	C
21	AA	843	U
21	AA	844	G
21	AA	845	A
21	AA	846	G
21	AA	849	G
21	AA	872	A
21	AA	873	A
21	AA	889	A
21	AA	914	A
21	AA	926	G
21	AA	927	G
21	AA	931	C
21	AA	932	C
21	AA	934	C
21	AA	935	A
21	AA	939	G
21	AA	945	G
21	AA	946	A
21	AA	958	A
21	AA	960	U
21	AA	961	U
21	AA	966	G
21	AA	969	A
21	AA	971	G
21	AA	975	A
21	AA	978	A
21	AA	979	C
21	AA	980	C
21	AA	983	A
21	AA	992	U
21	AA	993	G
21	AA	994	A
21	AA	995	C
21	AA	996	A

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Mol	Chain	Res	Type
21	AA	1004	A
21	AA	1030	U
21	AA	1031	C
21	AA	1032	G
21	AA	1033	G
21	AA	1045	C
21	AA	1054	C
21	AA	1056	U
21	AA	1065	U
21	AA	1068	G
21	AA	1081	A
21	AA	1094	G
21	AA	1101	A
21	AA	1102	A
21	AA	1125	U
21	AA	1126	U
21	AA	1130	A
21	AA	1136	C
21	AA	1148	U
21	AA	1151	A
21	AA	1160	G
21	AA	1161	C
21	AA	1167	A
21	AA	1168	U
21	AA	1181	G
21	AA	1182	G
21	AA	1183	U
21	AA	1184	G
21	AA	1185	G
21	AA	1191	A
21	AA	1196	A
21	AA	1197	A
21	AA	1202	U
21	AA	1203	C
21	AA	1212	U
21	AA	1214	C
21	AA	1215	G
21	AA	1221	G
21	AA	1222	G
21	AA	1223	C
21	AA	1225	A
21	AA	1226	C

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Mol	Chain	Res	Type
21	AA	1227	A
21	AA	1228	C
21	AA	1238	A
21	AA	1240	U
21	AA	1241	G
21	AA	1256	A
21	AA	1257	A
21	AA	1266	G
21	AA	1270	G
21	AA	1279	G
21	AA	1281	C
21	AA	1282	C
21	AA	1286	U
21	AA	1297	G
21	AA	1300	G
21	AA	1301	U
21	AA	1302	C
21	AA	1303	C
21	AA	1317	C
21	AA	1321	U
21	AA	1331	G
21	AA	1337	G
21	AA	1338	G
21	AA	1348	U
21	AA	1360	A
21	AA	1363	A
21	AA	1378	C
21	AA	1379	G
21	AA	1380	U
21	AA	1381	U
21	AA	1382	C
21	AA	1396	A
21	AA	1397	C
21	AA	1399	C
21	AA	1400	C
21	AA	1401	G
21	AA	1432	G
21	AA	1446	A
21	AA	1451	U
21	AA	1452	C
21	AA	1470	U
21	AA	1471	U

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Mol	Chain	Res	Type
21	AA	1487	G
21	AA	1493	A
21	AA	1502	A
21	AA	1503	A
21	AA	1505	G
21	AA	1506	U
21	AA	1507	A
21	AA	1517	G
21	AA	1529	G
21	AA	1530	G
22	A1	10	G
22	A1	17	U
22	A1	20	G
22	A1	21	A
22	A1	46	7MG
22	A1	47	U
22	A1	59	U
22	A1	61	C
22	A1	62	C
22	A1	63	G
22	A1	76	A
23	A2	80	C
23	A2	81	U
23	A2	82	A
23	A2	83	U
23	A2	92	U
23	A2	93	U
24	A3	9	G
24	A3	14	A
24	A3	16	C
24	A3	18	U
24	A3	20	G
24	A3	22	A
24	A3	35	C
24	A3	36	A
24	A3	48	U
24	A3	60	A
24	A3	74	A
24	A3	75	C
24	A3	77	A
54	BA	9	G
54	BA	12	U

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Mol	Chain	Res	Type
54	BA	13	A
54	BA	14	A
54	BA	15	G
54	BA	31	C
54	BA	34	U
54	BA	52	A
54	BA	53	A
54	BA	61	C
54	BA	71	A
54	BA	72	U
54	BA	74	A
54	BA	75	G
54	BA	91	A
54	BA	100	U
54	BA	101	A
54	BA	102	U
54	BA	119	A
54	BA	120	U
54	BA	121	G
54	BA	122	G
54	BA	142	A
54	BA	143	C
54	BA	144	A
54	BA	145	C
54	BA	149	A
54	BA	172	A
54	BA	180	G
54	BA	181	A
54	BA	196	A
54	BA	199	A
54	BA	200	U
54	BA	204	A
54	BA	216	A
54	BA	222	A
54	BA	228	C
54	BA	245	G
54	BA	248	G
54	BA	250	G
54	BA	266	G
54	BA	272	A
54	BA	278	A
54	BA	279	A

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Mol	Chain	Res	Type
54	BA	299	A
54	BA	302	C
54	BA	316	C
54	BA	330	A
54	BA	332	A
54	BA	346	A
54	BA	347	A
54	BA	370	G
54	BA	373	U
54	BA	374	A
54	BA	385	C
54	BA	386	G
54	BA	387	U
54	BA	405	U
54	BA	412	A
54	BA	444	C
54	BA	448	U
54	BA	454	A
54	BA	455	C
54	BA	457	A
54	BA	480	A
54	BA	481	G
54	BA	482	A
54	BA	491	G
54	BA	503	A
54	BA	504	A
54	BA	505	A
54	BA	507	A
54	BA	508	A
54	BA	509	C
54	BA	510	C
54	BA	511	U
54	BA	518	G
54	BA	526	A
54	BA	527	C
54	BA	529	A
54	BA	530	G
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	547	A
54	BA	549	G

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Mol	Chain	Res	Type
54	BA	550	C
54	BA	557	C
54	BA	573	U
54	BA	574	A
54	BA	586	A
54	BA	603	A
54	BA	613	A
54	BA	614	A
54	BA	616	A
54	BA	620	G
54	BA	627	A
54	BA	631	A
54	BA	637	A
54	BA	642	U
54	BA	655	A
54	BA	672	C
54	BA	685	A
54	BA	686	U
54	BA	717	C
54	BA	736	C
54	BA	747	U
54	BA	750	A
54	BA	751	A
54	BA	754	U
54	BA	763	G
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	783	A
54	BA	784	G
54	BA	791	C
54	BA	805	G
54	BA	810	U
54	BA	812	C
54	BA	822	G
54	BA	823	C
54	BA	827	U
54	BA	844	A
54	BA	846	U
54	BA	847	U
54	BA	856	G

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Mol	Chain	Res	Type
54	BA	858	G
54	BA	859	G
54	BA	860	U
54	BA	874	G
54	BA	889	C
54	BA	890	C
54	BA	897	C
54	BA	910	A
54	BA	914	G
54	BA	915	C
54	BA	941	A
54	BA	946	C
54	BA	958	U
54	BA	959	A
54	BA	961	C
54	BA	962	G
54	BA	974	G
54	BA	976	G
54	BA	977	G
54	BA	981	A
54	BA	983	A
54	BA	996	A
54	BA	1005	C
54	BA	1009	A
54	BA	1012	U
54	BA	1022	G
54	BA	1026	G
54	BA	1033	U
54	BA	1034	G
54	BA	1057	A
54	BA	1063	G
54	BA	1069	A
54	BA	1070	A
54	BA	1071	G
54	BA	1072	C
54	BA	1073	A
54	BA	1075	C
54	BA	1084	A
54	BA	1085	A
54	BA	1088	A
54	BA	1089	A
54	BA	1090	A

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Mol	Chain	Res	Type
54	BA	1094	U
54	BA	1112	G
54	BA	1126	A
54	BA	1127	A
54	BA	1129	A
54	BA	1130	U
54	BA	1132	U
54	BA	1133	A
54	BA	1135	C
54	BA	1144	A
54	BA	1148	U
54	BA	1175	A
54	BA	1176	U
54	BA	1188	U
54	BA	1189	A
54	BA	1204	A
54	BA	1248	G
54	BA	1252	G
54	BA	1253	A
54	BA	1254	A
54	BA	1266	G
54	BA	1272	A
54	BA	1276	A
54	BA	1292	G
54	BA	1300	G
54	BA	1301	A
54	BA	1308	A
54	BA	1313	U
54	BA	1314	C
54	BA	1315	C
54	BA	1317	G
54	BA	1325	U
54	BA	1326	U
54	BA	1327	A
54	BA	1328	A
54	BA	1341	G
54	BA	1350	C
54	BA	1365	A
54	BA	1378	A
54	BA	1379	U
54	BA	1383	A
54	BA	1385	A

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Mol	Chain	Res	Type
54	BA	1388	G
54	BA	1391	U
54	BA	1396	U
54	BA	1416	G
54	BA	1427	A
54	BA	1428	C
54	BA	1440	U
54	BA	1452	G
54	BA	1453	A
54	BA	1459	G
54	BA	1460	U
54	BA	1476	U
54	BA	1482	G
54	BA	1490	A
54	BA	1493	C
54	BA	1503	A
54	BA	1534	U
54	BA	1535	A
54	BA	1537	G
54	BA	1539	U
54	BA	1540	G
54	BA	1566	A
54	BA	1569	A
54	BA	1584	U
54	BA	1585	C
54	BA	1597	A
54	BA	1603	A
54	BA	1606	C
54	BA	1607	C
54	BA	1608	A
54	BA	1615	C
54	BA	1616	A
54	BA	1618	A
54	BA	1622	G
54	BA	1625	C
54	BA	1626	A
54	BA	1627	G
54	BA	1635	A
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1651	G

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Mol	Chain	Res	Type
54	BA	1656	C
54	BA	1669	A
54	BA	1674	G
54	BA	1684	G
54	BA	1696	G
54	BA	1715	G
54	BA	1730	C
54	BA	1758	U
54	BA	1761	C
54	BA	1764	C
54	BA	1773	A
54	BA	1783	A
54	BA	1784	A
54	BA	1799	G
54	BA	1800	C
54	BA	1808	A
54	BA	1810	A
54	BA	1827	U
54	BA	1829	A
54	BA	1847	A
54	BA	1848	A
54	BA	1861	G
54	BA	1871	A
54	BA	1877	A
54	BA	1884	G
54	BA	1886	U
54	BA	1900	A
54	BA	1906	G
54	BA	1912	A
54	BA	1913	A
54	BA	1914	C
54	BA	1915	U
54	BA	1937	A
54	BA	1938	A
54	BA	1940	U
54	BA	1943	U
54	BA	1952	A
54	BA	1953	A
54	BA	1955	U
54	BA	1963	U
54	BA	1964	G
54	BA	1965	C

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Mol	Chain	Res	Type
54	BA	1966	A
54	BA	1967	C
54	BA	1970	A
54	BA	1971	U
54	BA	1972	G
54	BA	1992	G
54	BA	1993	U
54	BA	1997	C
54	BA	2001	C
54	BA	2018	G
54	BA	2019	A
54	BA	2020	A
54	BA	2021	C
54	BA	2022	U
54	BA	2023	C
54	BA	2030	A
54	BA	2032	G
54	BA	2034	U
54	BA	2043	C
54	BA	2061	G
54	BA	2062	A
54	BA	2077	A
54	BA	2092	U
54	BA	2112	G
54	BA	2113	U
54	BA	2117	A
54	BA	2119	A
54	BA	2126	A
54	BA	2127	G
54	BA	2132	U
54	BA	2135	A
54	BA	2138	G
54	BA	2157	G
54	BA	2159	G
54	BA	2160	C
54	BA	2163	A
54	BA	2169	A
54	BA	2172	U
54	BA	2173	A
54	BA	2174	C
54	BA	2181	U
54	BA	2210	U

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Mol	Chain	Res	Type
54	BA	2211	A
54	BA	2212	A
54	BA	2213	U
54	BA	2214	C
54	BA	2225	A
54	BA	2226	C
54	BA	2238	G
54	BA	2239	G
54	BA	2251	G
54	BA	2266	A
54	BA	2267	A
54	BA	2269	G
54	BA	2270	A
54	BA	2283	C
54	BA	2296	U
54	BA	2297	A
54	BA	2306	C
54	BA	2307	G
54	BA	2308	G
54	BA	2310	C
54	BA	2311	A
54	BA	2312	U
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2333	A
54	BA	2335	A
54	BA	2339	C
54	BA	2345	G
54	BA	2346	A
54	BA	2347	C
54	BA	2353	G
54	BA	2383	G
54	BA	2385	C
54	BA	2391	G
54	BA	2406	A
54	BA	2407	A
54	BA	2409	G
54	BA	2423	U
54	BA	2424	C
54	BA	2425	A
54	BA	2429	G

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Mol	Chain	Res	Type
54	BA	2433	A
54	BA	2441	U
54	BA	2442	C
54	BA	2447	G
54	BA	2448	A
54	BA	2459	A
54	BA	2460	U
54	BA	2473	U
54	BA	2474	U
54	BA	2475	C
54	BA	2486	C
54	BA	2491	U
54	BA	2495	G
54	BA	2496	C
54	BA	2499	C
54	BA	2502	G
54	BA	2503	A
54	BA	2505	G
54	BA	2506	U
54	BA	2531	A
54	BA	2532	G
54	BA	2534	A
54	BA	2540	C
54	BA	2547	A
54	BA	2554	U
54	BA	2555	U
54	BA	2565	A
54	BA	2566	A
54	BA	2567	G
54	BA	2573	C
54	BA	2575	C
54	BA	2576	G
54	BA	2599	G
54	BA	2602	A
54	BA	2603	G
54	BA	2609	U
54	BA	2610	C
54	BA	2614	A
54	BA	2628	C
54	BA	2630	G
54	BA	2638	G
54	BA	2640	G

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Mol	Chain	Res	Type
54	BA	2646	C
54	BA	2655	G
54	BA	2660	A
54	BA	2661	G
54	BA	2666	C
54	BA	2667	C
54	BA	2689	U
54	BA	2690	U
54	BA	2702	G
54	BA	2707	U
54	BA	2718	G
54	BA	2744	G
54	BA	2765	A
54	BA	2766	A
54	BA	2778	A
54	BA	2779	U
54	BA	2780	G
54	BA	2781	A
54	BA	2784	U
54	BA	2791	G
54	BA	2798	U
54	BA	2799	A
54	BA	2808	G
54	BA	2816	G
54	BA	2817	U
54	BA	2820	A
54	BA	2833	U
54	BA	2835	A
54	BA	2850	A
54	BA	2852	G
54	BA	2872	A
54	BA	2873	A
54	BA	2876	G
54	BA	2879	A
54	BA	2890	G
54	BA	2891	U
54	BA	2894	G
54	BA	2895	G
55	BB	9	G
55	BB	13	G
55	BB	14	U
55	BB	15	A

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Mol	Chain	Res	Type
55	BB	16	G
55	BB	25	U
55	BB	30	C
55	BB	36	C
55	BB	38	C
55	BB	42	C
55	BB	44	G
55	BB	45	A
55	BB	50	A
55	BB	66	A
55	BB	67	G
55	BB	74	U
55	BB	87	U
55	BB	88	C
55	BB	107	G
55	BB	108	A
55	BB	109	A

All (225) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	13	U
21	AA	26	A
21	AA	51	A
21	AA	54	C
21	AA	66	A
21	AA	70	U
21	AA	109	A
21	AA	120	A
21	AA	124	C
21	AA	151	A
21	AA	158	G
21	AA	163	C
21	AA	188	C
21	AA	190	A
21	AA	210	C
21	AA	249	U
21	AA	250	A
21	AA	251	G
21	AA	305	G
21	AA	307	C

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Mol	Chain	Res	Type
21	AA	328	C
21	AA	344	A
21	AA	345	C
21	AA	347	G
21	AA	373	A
21	AA	412	A
21	AA	420	U
21	AA	446	G
21	AA	451	A
21	AA	472	U
21	AA	481	G
21	AA	522	C
21	AA	559	A
21	AA	575	G
21	AA	611	C
21	AA	653	U
21	AA	718	A
21	AA	755	G
21	AA	793	U
21	AA	811	C
21	AA	872	A
21	AA	913	A
21	AA	931	C
21	AA	945	G
21	AA	968	A
21	AA	974	A
21	AA	978	A
21	AA	983	A
21	AA	994	A
21	AA	1029	U
21	AA	1032	G
21	AA	1049	U
21	AA	1092	A
21	AA	1101	A
21	AA	1125	U
21	AA	1129	C
21	AA	1181	G
21	AA	1184	G
21	AA	1190	G
21	AA	1191	A
21	AA	1201	A
21	AA	1212	U

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Mol	Chain	Res	Type
21	AA	1214	C
21	AA	1222	G
21	AA	1227	A
21	AA	1238	A
21	AA	1265	C
21	AA	1297	G
21	AA	1300	G
21	AA	1319	A
21	AA	1337	G
21	AA	1345	U
21	AA	1377	A
21	AA	1379	G
21	AA	1396	A
21	AA	1399	C
21	AA	1400	C
21	AA	1447	A
21	AA	1470	U
21	AA	1471	U
21	AA	1504	G
21	AA	1505	G
21	AA	1506	U
22	A1	10	G
22	A1	20	G
22	A1	61	C
23	A2	82	A
23	A2	92	U
24	A3	1	C
54	BA	12	U
54	BA	14	A
54	BA	33	C
54	BA	34	U
54	BA	52	A
54	BA	72	U
54	BA	118	A
54	BA	121	G
54	BA	142	A
54	BA	196	A
54	BA	199	A
54	BA	244	A
54	BA	249	C
54	BA	308	G
54	BA	330	A

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Mol	Chain	Res	Type
54	BA	332	A
54	BA	345	A
54	BA	346	A
54	BA	386	G
54	BA	401	A
54	BA	454	A
54	BA	455	C
54	BA	479	A
54	BA	503	A
54	BA	506	G
54	BA	508	A
54	BA	510	C
54	BA	530	G
54	BA	531	C
54	BA	532	A
54	BA	571	U
54	BA	574	A
54	BA	674	G
54	BA	685	A
54	BA	716	A
54	BA	750	A
54	BA	762	U
54	BA	764	A
54	BA	775	G
54	BA	790	U
54	BA	827	U
54	BA	957	C
54	BA	976	G
54	BA	983	A
54	BA	990	A
54	BA	1021	A
54	BA	1038	G
54	BA	1045	C
54	BA	1069	A
54	BA	1070	A
54	BA	1089	A
54	BA	1126	A
54	BA	1128	G
54	BA	1132	U
54	BA	1204	A
54	BA	1236	G
54	BA	1253	A

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Mol	Chain	Res	Type
54	BA	1300	G
54	BA	1312	U
54	BA	1314	C
54	BA	1344	U
54	BA	1420	A
54	BA	1427	A
54	BA	1428	C
54	BA	1451	C
54	BA	1539	U
54	BA	1584	U
54	BA	1606	C
54	BA	1607	C
54	BA	1615	C
54	BA	1625	C
54	BA	1626	A
54	BA	1634	A
54	BA	1647	U
54	BA	1655	A
54	BA	1668	A
54	BA	1699	G
54	BA	1782	U
54	BA	1783	A
54	BA	1786	A
54	BA	1787	A
54	BA	1799	G
54	BA	1819	A
54	BA	1826	G
54	BA	1847	A
54	BA	1899	A
54	BA	1912	A
54	BA	1936	A
54	BA	1952	A
54	BA	2000	C
54	BA	2018	G
54	BA	2021	C
54	BA	2022	U
54	BA	2033	A
54	BA	2035	G
54	BA	2062	A
54	BA	2111	U
54	BA	2117	A
54	BA	2118	U

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Mol	Chain	Res	Type
54	BA	2126	A
54	BA	2135	A
54	BA	2157	G
54	BA	2163	A
54	BA	2172	U
54	BA	2176	A
54	BA	2212	A
54	BA	2213	U
54	BA	2225	A
54	BA	2296	U
54	BA	2307	G
54	BA	2310	C
54	BA	2345	G
54	BA	2422	C
54	BA	2423	U
54	BA	2432	A
54	BA	2434	A
54	BA	2441	U
54	BA	2459	A
54	BA	2485	G
54	BA	2495	G
54	BA	2501	C
54	BA	2539	C
54	BA	2555	U
54	BA	2565	A
54	BA	2575	C
54	BA	2598	A
54	BA	2609	U
54	BA	2681	C
54	BA	2780	G
54	BA	2872	A
54	BA	2890	G
55	BB	13	G
55	BB	24	G
55	BB	57	A
55	BB	107	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	4SU	A3	8	24	18,21,22	1.34	1 (5%)	26,30,33	0.65	1 (3%)
24	H2U	A3	21	24	18,21,22	1.33	2 (11%)	21,30,33	1.16	3 (14%)
24	PSU	A3	56	24	18,21,22	0.88	0	22,30,33	1.18	2 (9%)
22	6MZ	A1	37	22	18,25,26	0.96	1 (5%)	16,36,39	1.54	2 (12%)
24	5MU	A3	55	24	19,22,23	0.72	0	28,32,35	1.35	4 (14%)
22	7MG	A1	46	22	22,26,27	4.70	2 (9%)	29,39,42	1.37	1 (3%)
22	CM0	A1	34	22,23	22,26,27	1.28	2 (9%)	28,37,40	1.21	2 (7%)
22	5MU	A1	54	22	19,22,23	0.73	0	28,32,35	1.22	3 (10%)
22	4SU	A1	7	22	18,21,22	1.36	1 (5%)	26,30,33	0.97	1 (3%)
22	PSU	A1	55	22	18,21,22	0.90	0	22,30,33	1.08	1 (4%)
24	OMC	A3	33	24	19,22,23	0.78	0	26,31,34	1.11	1 (3%)

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

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-21.78	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	7	4SU	C5-C4	-4.83	1.36	1.42
24	A3	8	4SU	C5-C4	-4.69	1.36	1.42
22	A1	34	CM0	O5-C5	-4.33	1.26	1.36
24	A3	21	H2U	C2-N3	-3.45	1.31	1.38
24	A3	21	H2U	C4-N3	-3.20	1.32	1.37
22	A1	34	CM0	C6-C5	2.35	1.37	1.34
22	A1	46	7MG	C5-N7	2.16	1.38	1.35
22	A1	37	6MZ	C8-N7	-2.15	1.30	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A1	46	7MG	N9-C8-N7	5.81	111.68	103.38
22	A1	37	6MZ	C9-N6-C6	4.46	126.71	122.87
24	A3	55	5MU	C5M-C5-C6	-3.50	118.18	122.85
24	A3	33	OMC	O2-C2-N3	-3.30	116.97	122.33
24	A3	56	PSU	C6-C5-C4	3.26	120.48	118.20
24	A3	21	H2U	N3-C2-N1	3.17	120.01	116.65
22	A1	37	6MZ	C2-N1-C6	3.11	119.25	116.59
22	A1	54	5MU	C5M-C5-C6	-2.98	118.87	122.85
22	A1	54	5MU	C6-C5-C4	2.97	120.51	118.03
24	A3	55	5MU	C6-C5-C4	2.94	120.49	118.03
24	A3	56	PSU	O4'-C1'-C2'	2.80	109.09	105.14
22	A1	34	CM0	C7-O5-C5	2.61	120.99	117.58
22	A1	55	PSU	C6-C5-C4	2.57	120.00	118.20
24	A3	21	H2U	O2-C2-N3	-2.45	116.93	121.50
24	A3	55	5MU	C5M-C5-C4	2.33	121.33	118.77
22	A1	7	4SU	C6-C5-C4	2.28	121.92	119.95
24	A3	55	5MU	C5-C6-N1	-2.27	121.00	123.34
24	A3	21	H2U	C5-C4-N3	2.20	119.12	116.65
24	A3	8	4SU	C6-C5-C4	2.18	121.84	119.95
22	A1	34	CM0	O4'-C4'-C3'	2.17	109.40	105.11
22	A1	54	5MU	C5-C6-N1	-2.11	121.17	123.34

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
22	A1	55	PSU	O4'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	FME	BA	3001	57	8,9,10	0.73	0	7,9,11	1.41	1 (14%)
57	VAL	A1	101	22,58	4,6,7	0.76	0	6,7,9	1.22	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	22,58	-	2/5/6/8	-

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	-2.92	117.12	124.78
58	BA	3001	FME	C-CA-N	2.60	114.43	109.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A1	101	VAL	C-CA-CB-CG1
57	A1	101	VAL	C-CA-CB-CG2
58	BA	3001	FME	O1-CN-N-CA
58	BA	3001	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

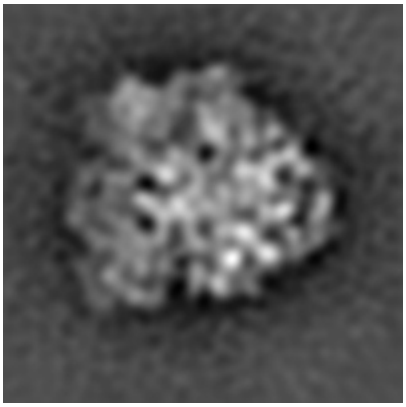
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1718. These allow visual inspection of the internal detail of the map and identification of artifacts.

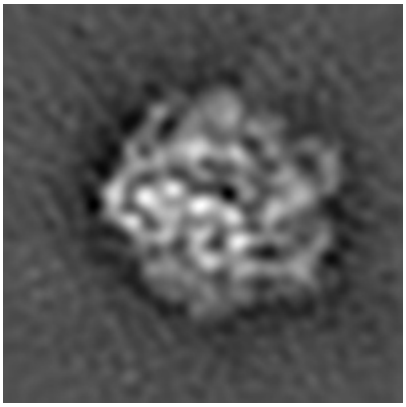
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

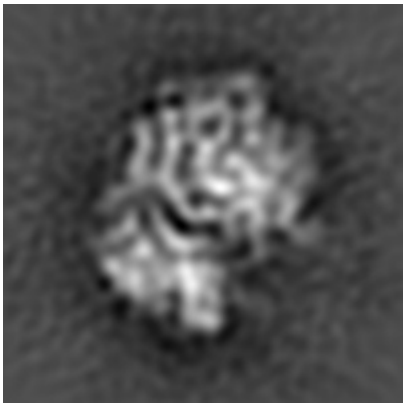
6.1.1 Primary map



X



Y



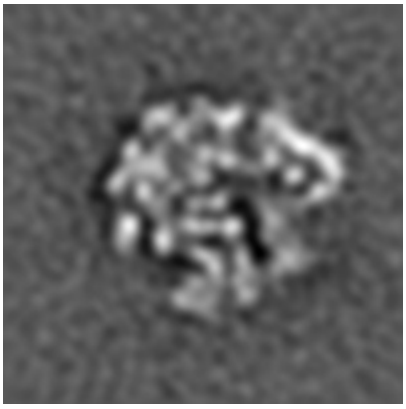
Z

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

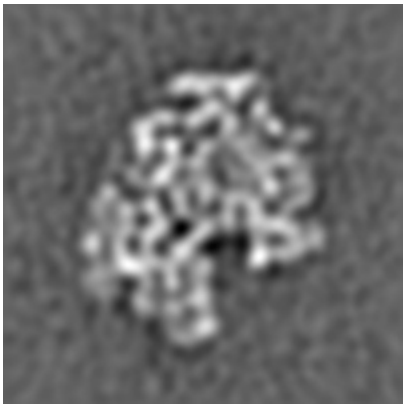
6.2 Central slices

6.2.1 Primary map

X Index: 64



Y Index: 64



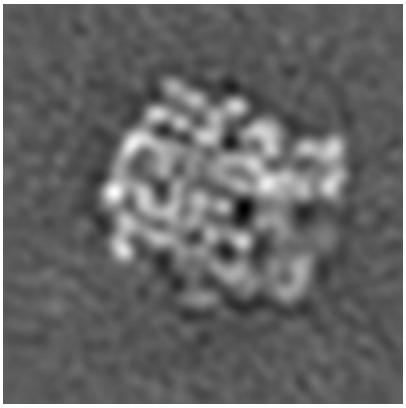
Z Index: 64

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

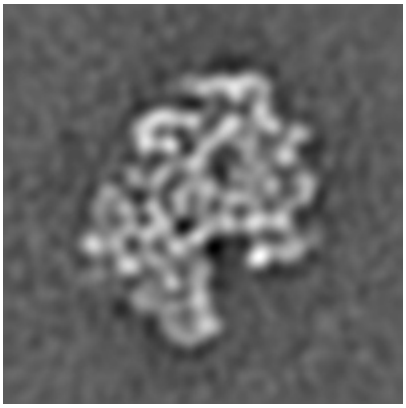
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 66



Y Index: 69

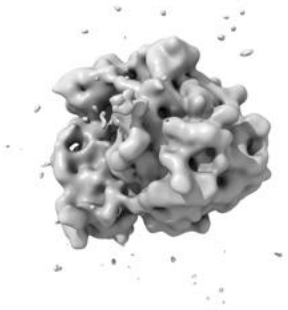


Z Index: 62

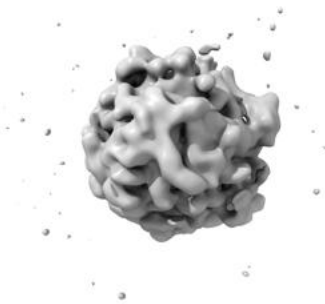
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

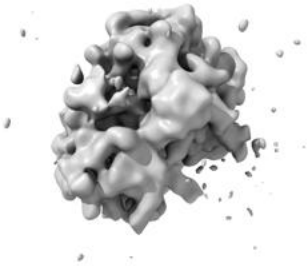
6.4.1 Primary map



X



Y



Z

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

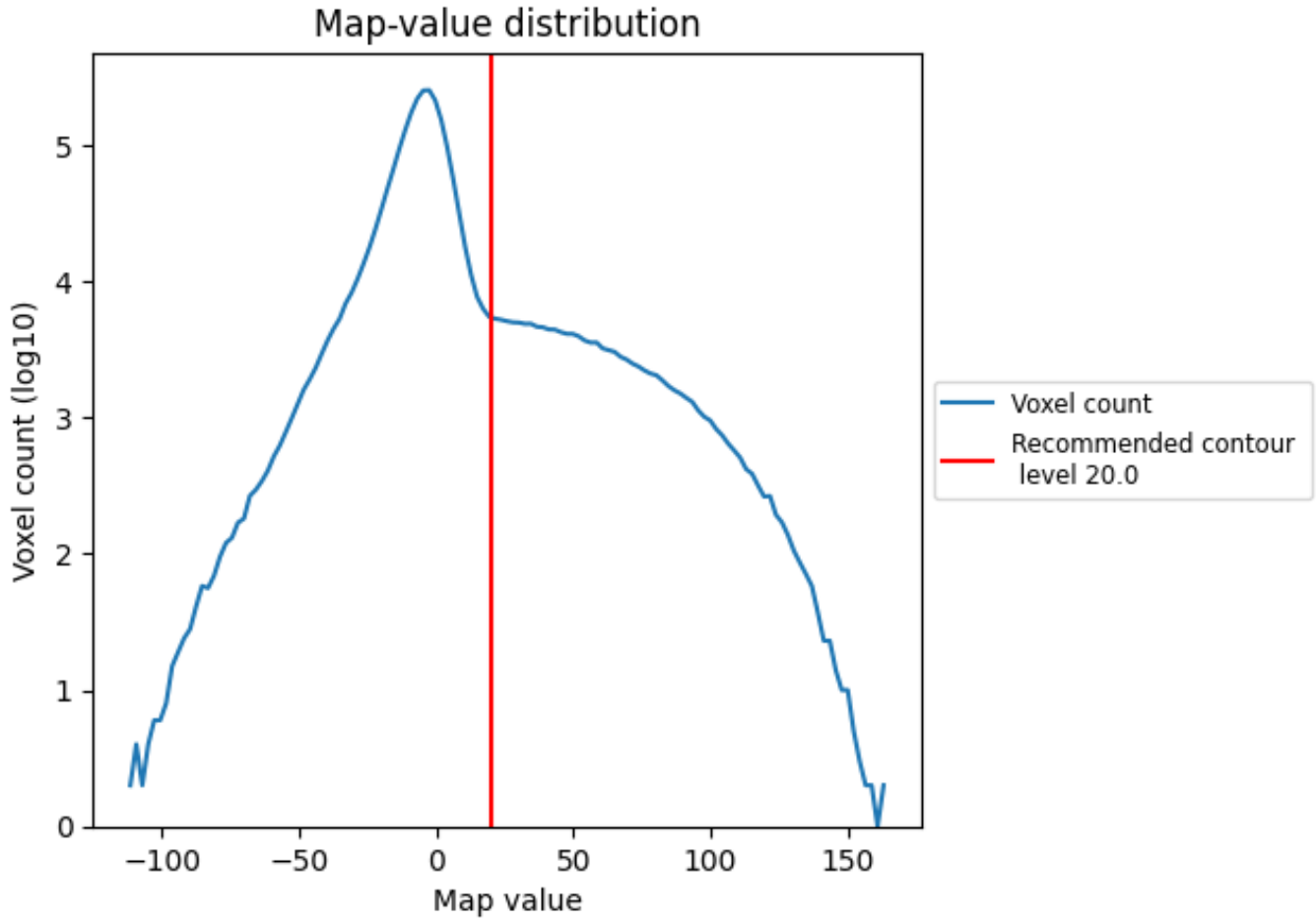
6.5 Mask visualisation (i)

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

7 Map analysis

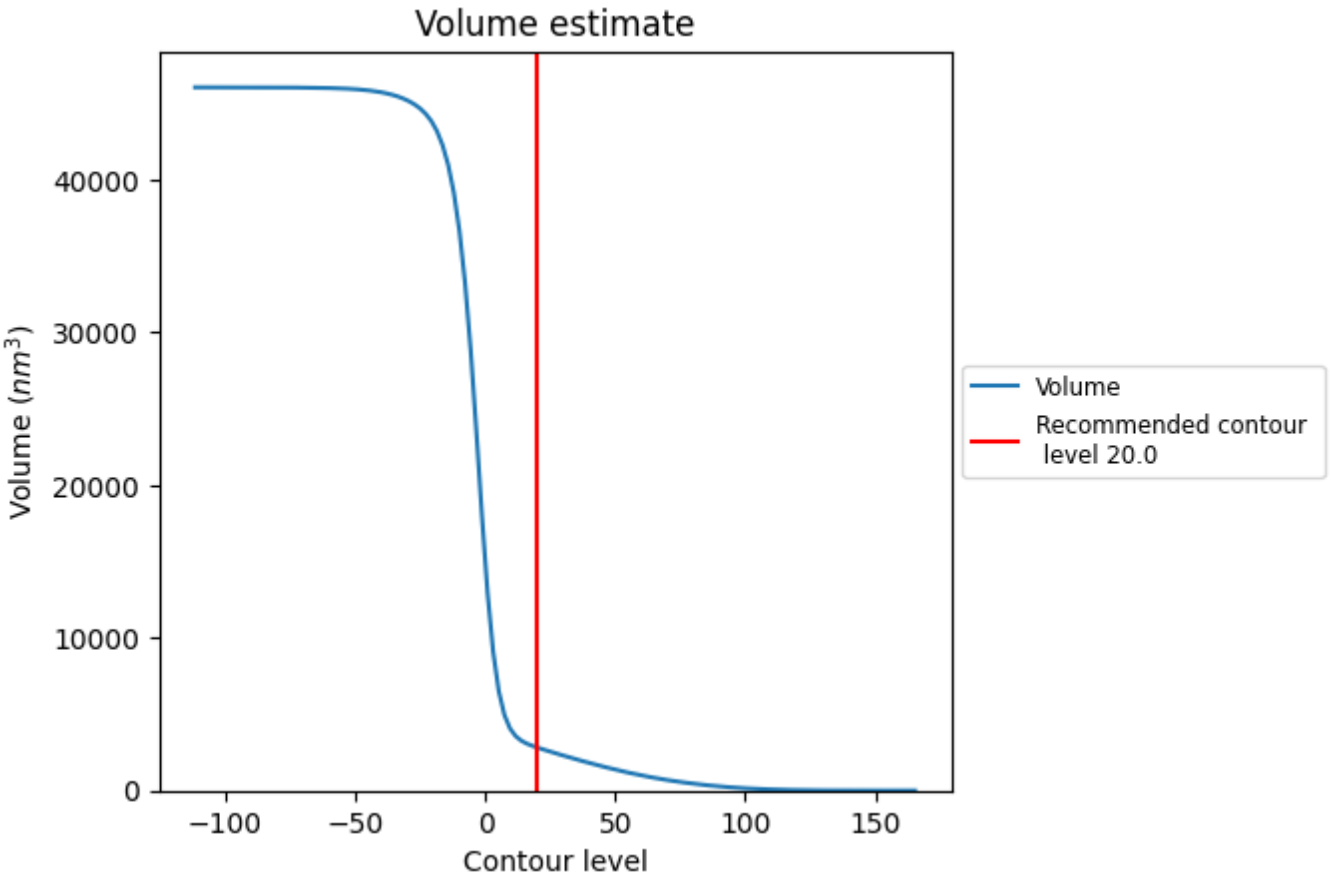
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

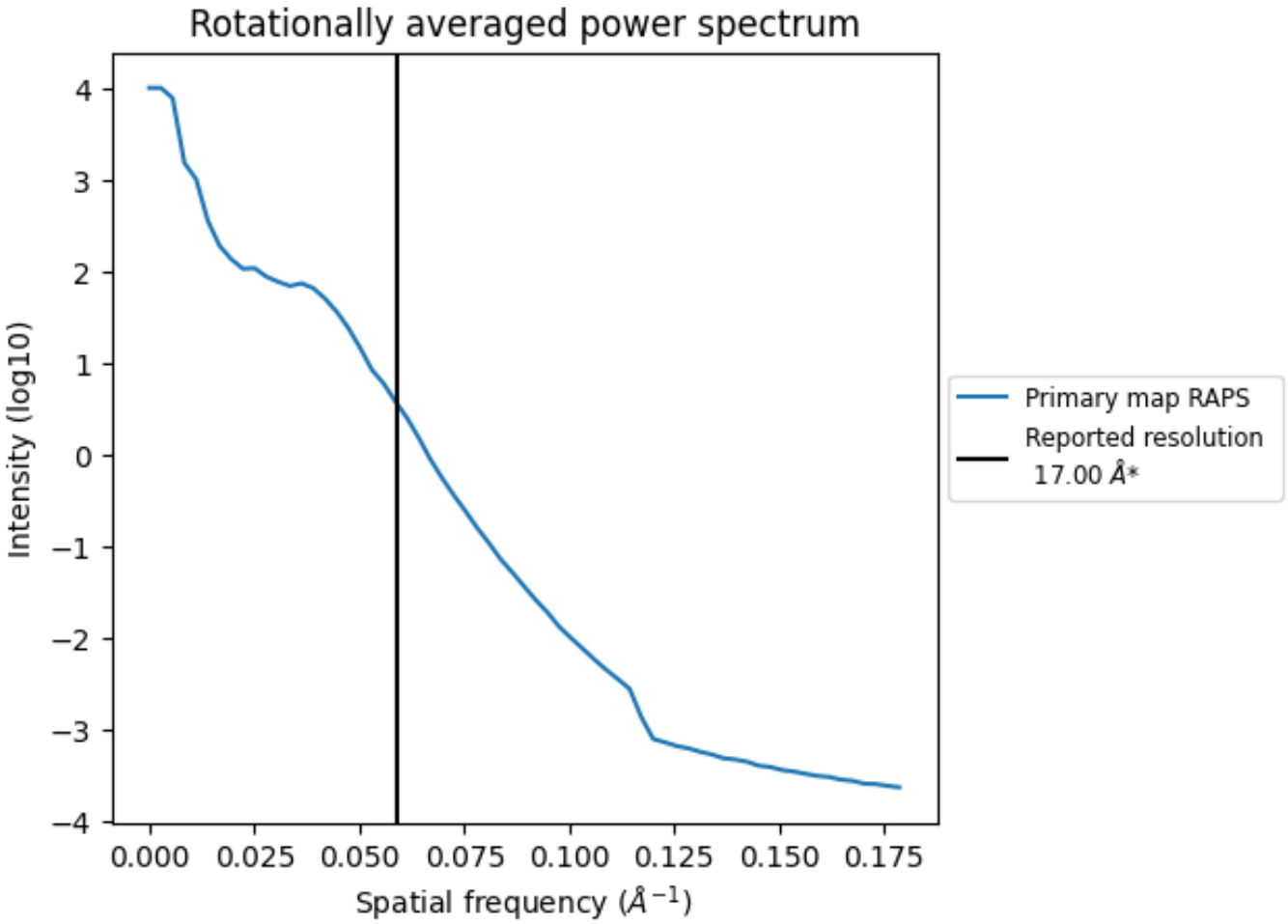
7.2 Volume estimate



The volume at the recommended contour level is 2816 nm^3; this corresponds to an approximate mass of 2544 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.059 Å^{-1}

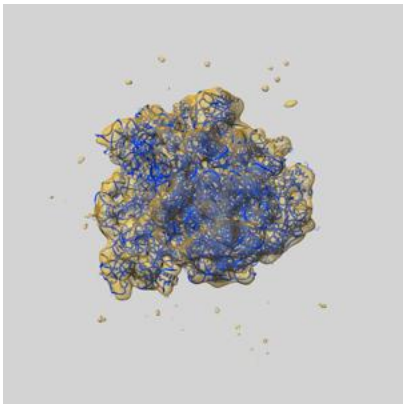
8 Fourier-Shell correlation (i)

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

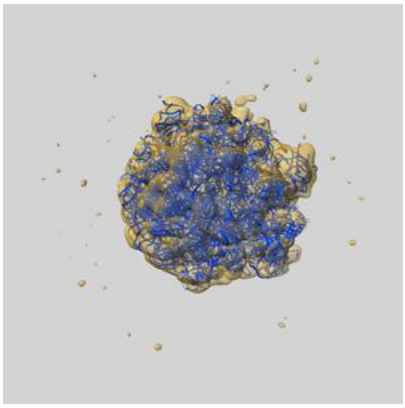
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1718 and PDB model 4V70. Per-residue inclusion information can be found in section 3 on page 17.

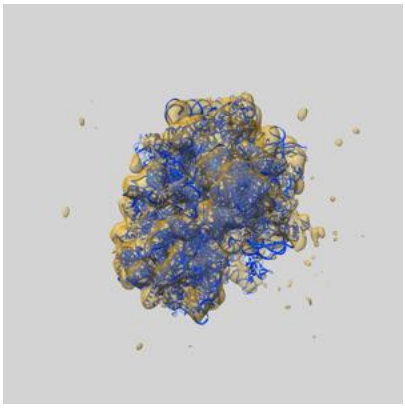
9.1 Map-model overlay



X



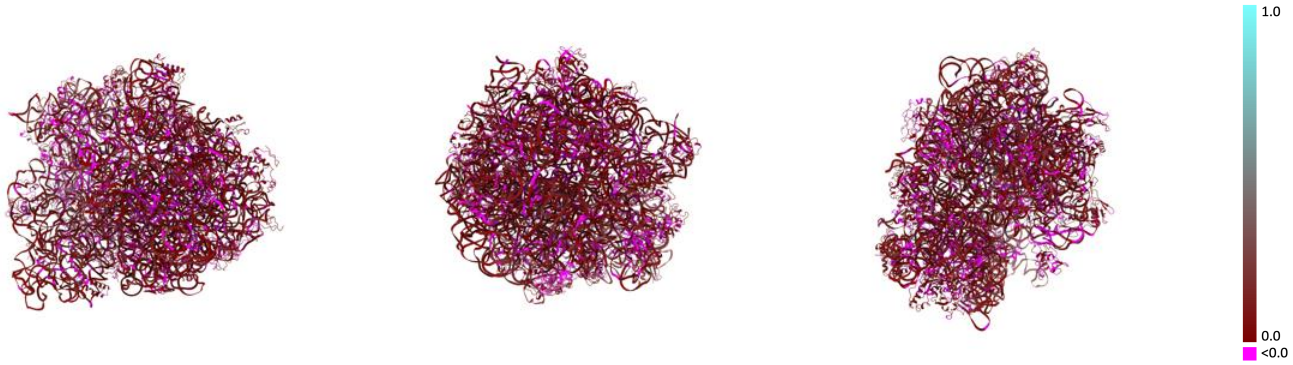
Y



Z

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

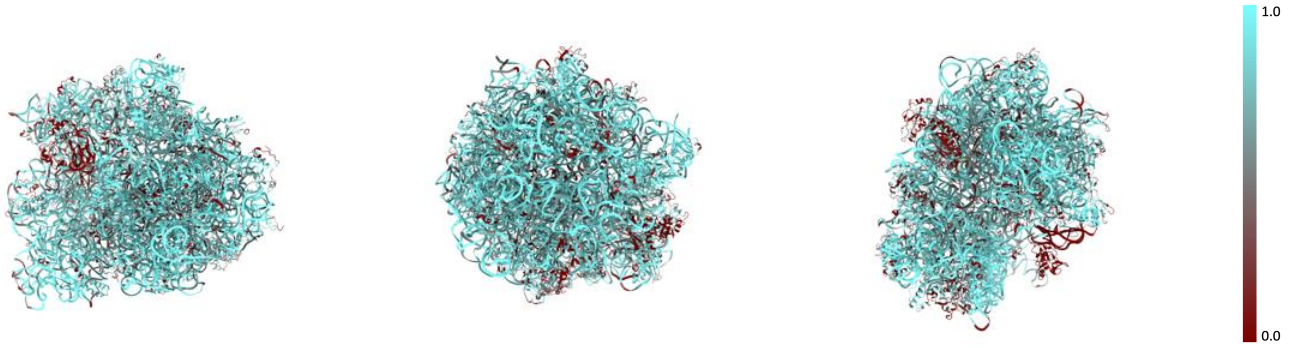
9.2 Q-score mapped to coordinate model



X Y Z

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

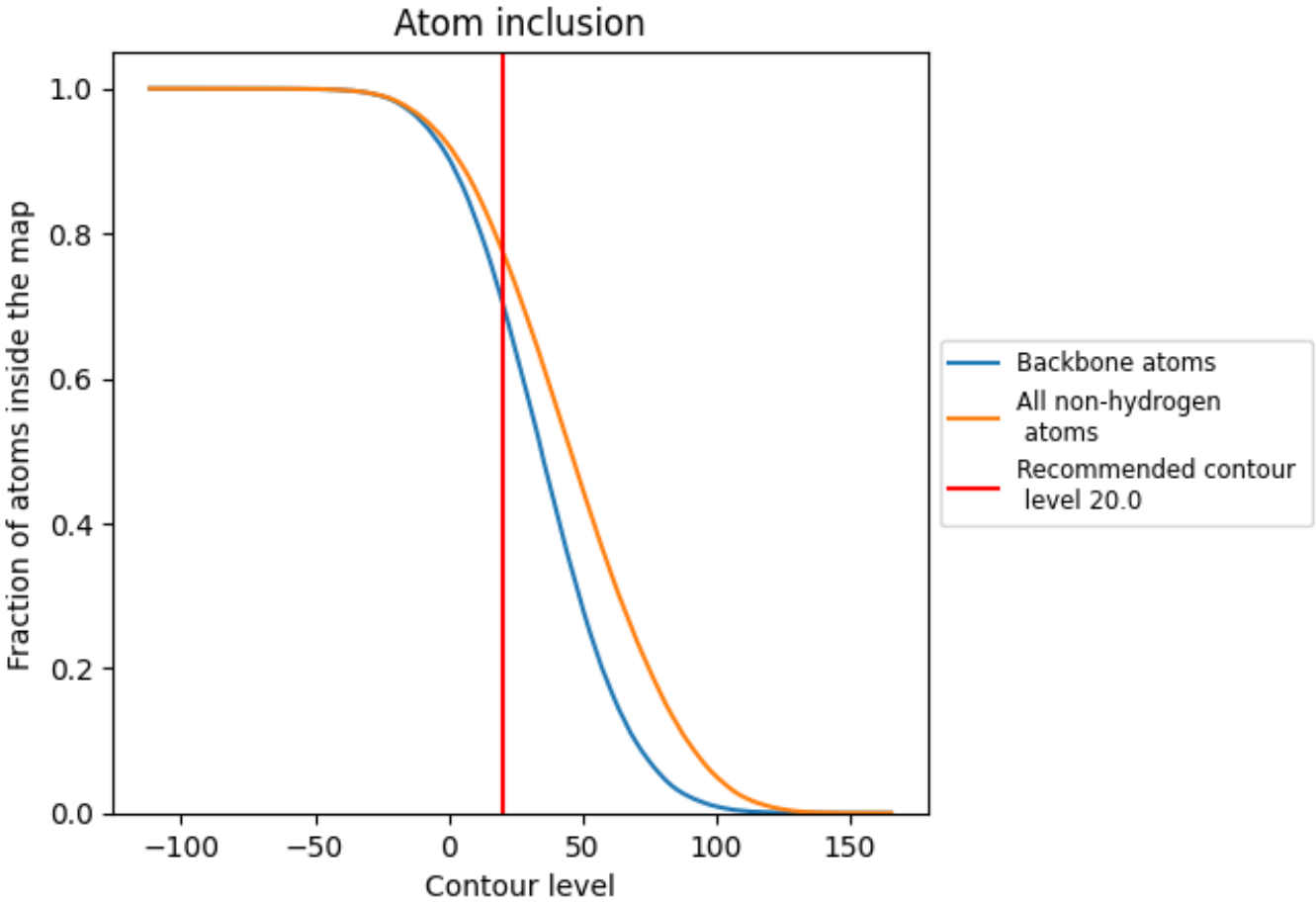
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (20.0).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.7765	0.0610
A1	0.5900	0.0500
A2	0.6375	0.0550
A3	0.6206	0.0660
AA	0.8748	0.0770
AB	0.5495	0.0440
AC	0.5301	0.0470
AD	0.4679	0.0190
AE	0.7284	0.0520
AF	0.7491	0.0640
AG	0.5825	0.0270
AH	0.7667	0.0360
AI	0.6932	0.0280
AJ	0.6073	0.0130
AK	0.7520	0.0450
AL	0.7231	0.0230
AM	0.7325	0.0550
AN	0.6990	0.0230
AO	0.6855	0.0380
AP	0.6823	0.0310
AQ	0.6992	0.0350
AR	0.6879	-0.0070
AS	0.8061	0.0390
AT	0.7699	0.0150
AU	0.6015	0.0230
B0	0.6636	0.0160
B1	0.7550	0.0590
B2	0.4507	-0.0110
B3	0.5336	-0.0500
B4	0.7877	0.0430
B5	0.1562	0.0100
BA	0.8514	0.0770
BB	0.9193	0.0890
BC	0.5062	0.0120
BD	0.6606	0.0140

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Chain	Atom inclusion	Q-score
BE	0.6237	0.0290
BF	0.7397	0.0490
BG	0.6916	0.0510
BH	0.2838	0.0060
BI	0.0127	0.0220
BJ	0.6327	0.0250
BK	0.4967	0.0240
BL	0.6368	0.0060
BM	0.5173	0.0040
BN	0.7465	0.0120
BO	0.8806	0.0320
BP	0.5923	0.0360
BQ	0.6960	0.0060
BR	0.7026	0.0350
BS	0.6830	0.0250
BT	0.6902	0.0260
BU	0.5677	0.0370
BV	0.7507	0.0510
BW	0.7577	0.0320
BX	0.5141	-0.0080
BY	0.5131	0.0150
BZ	0.7071	0.0420