



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:55 PM BST

PDB ID : 4V77
EMDB ID: : EMD-2474
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate post-translocation state (post2b)
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 PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

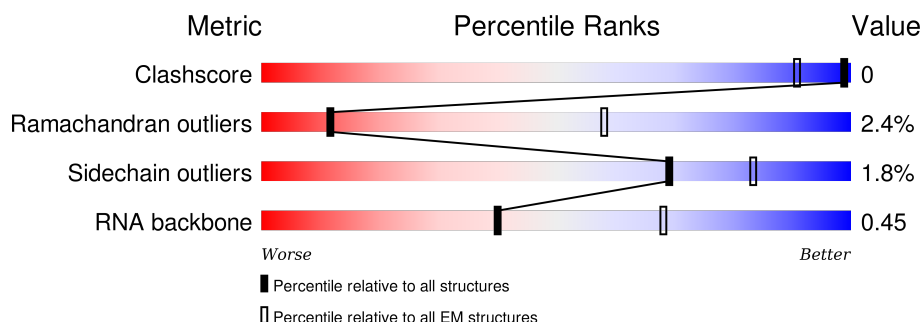
1 Overall quality at a glance

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.













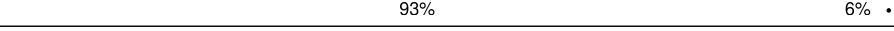
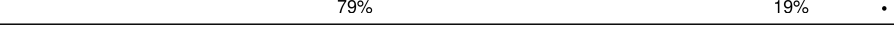
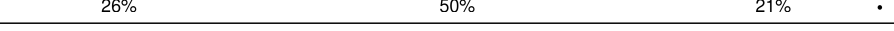
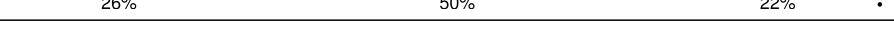





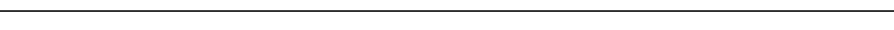

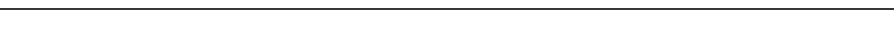
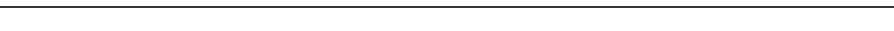


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	AB	220	94% 6%
2	AC	208	90% 9% .
3	AD	206	87% 12%
4	AE	152	91% 9%
5	AF	101	87% 13%
6	AG	152	88% 12% .
7	AH	130	92% 7% ..
8	AI	128	84% 16% .





















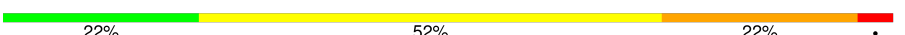
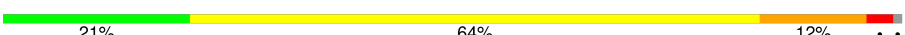

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Mol	Chain	Length	Quality of chain
9	AJ	100	
10	AK	118	
11	AL	124	
12	AM	115	
13	AN	101	
14	AO	89	
15	AP	81	
16	AQ	82	
17	AR	57	
18	AS	81	
19	AT	86	
20	AU	53	
21	AA	1533	
22	A1	76	
23	A2	15	
24	A3	77	
25	BC	273	
26	BD	209	
27	BE	201	
28	BF	179	
29	BG	177	
30	BH	149	
31	BI	142	
32	BJ	142	
33	BK	123	

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Mol	Chain	Length	Quality of chain
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

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
1	AB	220	Total	C	N	O	S	0	1
			1708	1083	306	312	7		

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

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

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

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

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

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

- Molecule 24 is a 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		

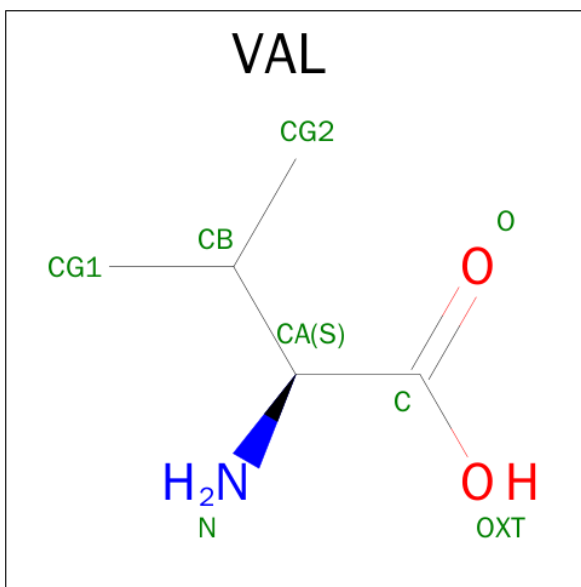
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

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.

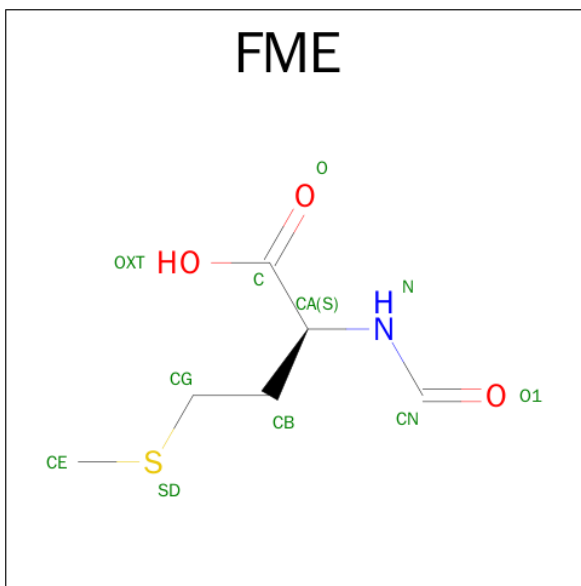
Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	223	Total	C	N	O	S	0	0
			1658	1038	302	312	6		

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C₅H₁₁NO₂).



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: C₆H₁₁NO₃S).

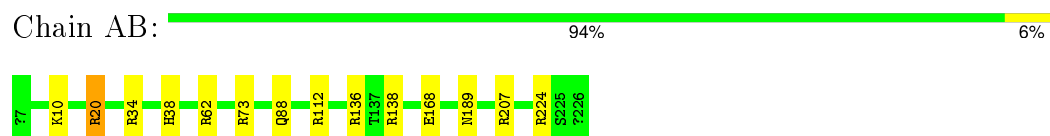


Mol	Chain	Residues	Atoms					AltConf
58	BA	1	Total	C	N	O	S	0
			10	6	1	2	1	

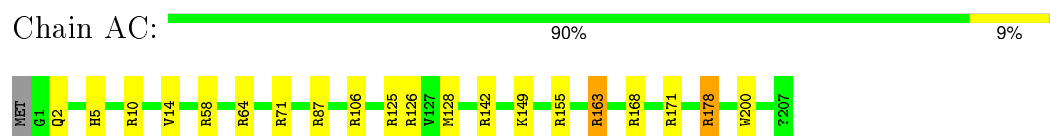
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

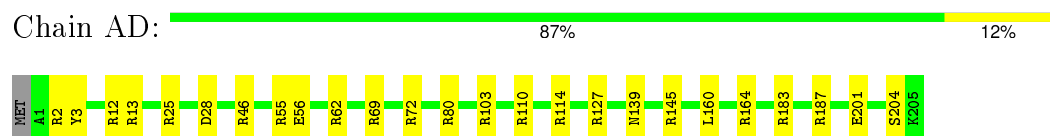
- Molecule 1: 30S ribosomal protein S2



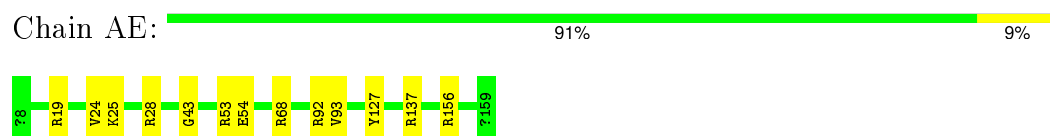
- Molecule 2: 30S ribosomal protein S3



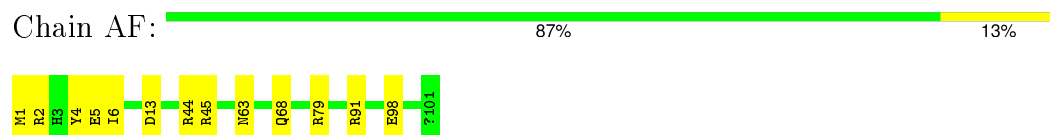
- Molecule 3: 30S ribosomal protein S4



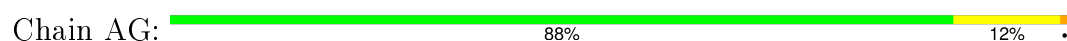
- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6




- Molecule 6: 30S ribosomal protein S7





- Molecule 14: 30S ribosomal protein S15

Chain AO:  83% 15% ..



- Molecule 15: 30S ribosomal protein S16

Chain AP:  88% 12%



- Molecule 16: 30S ribosomal protein S17

Chain AQ:  89% 11%



- Molecule 17: 30S ribosomal protein S18

Chain AR:  89% 11%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  90% 9% .




- Molecule 19: 30S ribosomal protein S20

Chain AT:  93% 6% .



- Molecule 20: 30S ribosomal protein S21

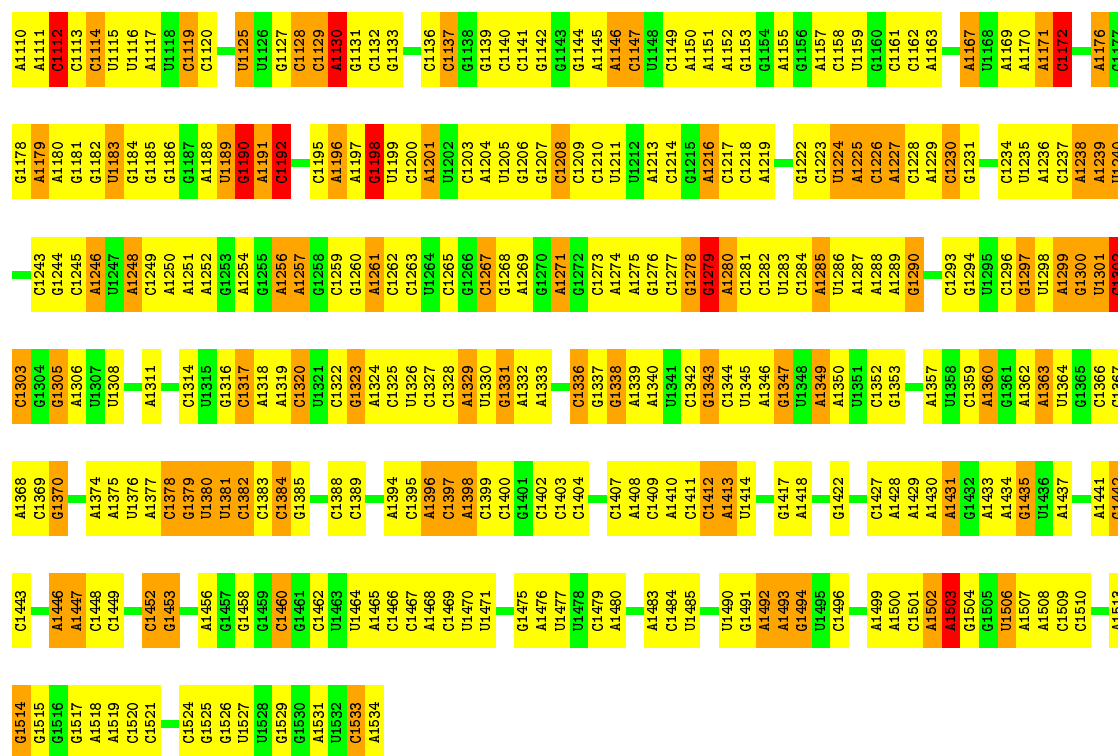
Chain AU:  79% 19% .



- Molecule 21: 16S ribosomal RNA

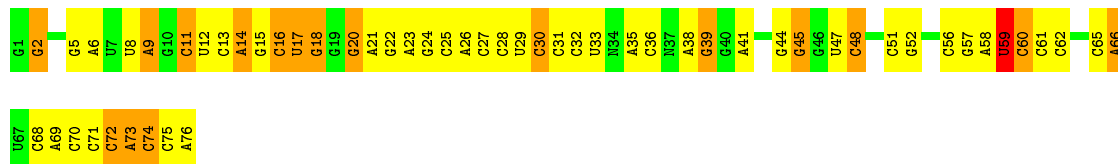
Chain AA:  26% 50% 21% .

A1044	C1045	A1046	G1047	G1048	G1049	G1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	G1058	C1059	U1060	G1061	U1062	C1063	G1064	U1065	C1066	A1067	G1068	C1069	U1070	C1071	U1072	U1073	G1077	A1080	A1081	A1082	U1086	G1089	U1090	U1091	A1092	A1093	G1094	U1095	C1096	C1097	C1098	G1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1109					
C980	U981	U982	A983	C984	C985	U986	C987	C990	U991	U992	G993	A994	C995	U996	U997	C998	C999	A1000	C1001	G1002	G1003	A1004	A1005	G1006	U1007	U1008	U1009	U1010	C1011	A1012	G1013	A1014	G1015	A1016	A1019	G1020	A1021	A1022	U1025	G1026	C1027	U1028	U1029	U1030	C1031	G1032	G1033	G1034	A1035	A1036	C1037	A1038	G1039	A1042	G1043					
A784	C720	G721	G722	U723	C724	C725	G726	G727	A728	A729	G730	G731	C732	G733	G734	C735	A736	C737	C738	C739	U740	G741	G742	A743	C744	G745	A746	U747	G748	A749	C750	U751	G752	C753	C754	G755	C756	U757	C758	A759	G760	G761	C764	G765	A766	G767	C768	A769	C770	G775	G776	A777	G778	C779	A780	A781	A782	C783		
A649	G650	C651	U652	U653	G654	A655	G656	U657	C658	U659	C660	G661	U662	A663	A664	A665	A666	U667	A668	A669	A670	A671	A672	A673	A674	A675	A676	C679	C680	A681	G682	U686	A687	G688	C689	G690	G691	U692	G693	A694	A695	A696	U697	G698	C699	A702	G703	A704	C705	A706	U707	C708	A712	G713	G714	A715	A716	U717	A718	C719
C580	U581	C582	A583	C586	U590	U591	U592	U593	U594	A595	A596	C599	A600	G601	A602	G606	A607	A608	A609	U610	C611	C612	A613	C614	C615	C616	A617	A618	U619	C620	A621	A622	C623	C624	U625	G626	G627	G628	A629	A630	C631	C632	G633	C634	A635	A636	A637	U638	A639	C640	U641	A642	C643	C647	A648					
U515	U516	C517	C518	C519	A520	G521	C522	A523	G524	C525	C526	C527	C528	G529	C530	U531	A532	A533	U534	A535	C536	C537	A538	A539	C545	A546	A547	A548	U549	U550	U551	U552	A553	A554	U555	C556	G557	C558	A559	A560	U561	U562	A563	C564	U565	U566	U567	A568	C569	A572	C573	A574	A575	A576	C577	C578	A579			
G453	U490	C491	C492	A493	C494	C495	C496	U497	A498	C499	A500	A501	A502	C503	C504	C507	U508	A509	A510	C511	U512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545						
A199	G200	G203	C204	A205	C206	C207	U208	U209	C210	A211	G212	G213	C214	C215	U216	C217	U218	U219	G220	C221	C222	C223	A224	C225	A228	U229	C233	C234	C235	A236	G237	U173	C106	G107	G108	C109	C110	G111	G112	G113	U114	C115	A116	G117	U118	C119	A120	U121	G122	U123	C124	A60	G128	A129	A130	A131	A132	A133	A134	
C264	G265	C266	C267	U268	C269	A270	C271	C272	U273	A274	G275	C276	C277	C278	A279	C280	U281	U282	U283	C284	C285	C286	U287	A288	C289	C290	U291	C292	G293	U294	C295	U296	G297	A298	G299	A300	A303	U304	G305	A306	C307	C308	A309	G310	C311	C312	A313	C314	A315	C316	U317	G318	C319	A320	A321	C322	U323	A263	G198	
A325	G326	A327	C328	A329	C330	C334	C335	A336	G337	A338	C400	A401	G402	C403	A404	C405	U406	A407	A408	A409	G410	A411	A412	G413	C414	A415	C418	C419	U420	U421	G422	G423	A424	G425	A426	A427	G428	U429	A430	A431	A432	C433	A434	C437	C438	A439	C440	A441	C442	U443	A444	A445	G446	C447	A448	G449	A450	C451	A452	
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G515	U516	C517	C518	C519	A520	G521	C522	A523	G524	C525	C526	C527	C528	G529	C530	U531	A532	A533	U534	A535	C536	C537	A538	A539	C545	A546	A547	A548	U549	U550	U551	U552	A553	A554	U555	C556	G557	C558	A559	A560	U561	U562	A563	C564	U565	U566	U567	A568	C569	A572	C573	A574	A575	A576	C577	C578	A579			
A549	G550	C551	U552	U553	G554	A555	G556	U557	C558	U559	C560	G561	U562	A563	A564	A565	A566	U567	A568	A569	A570	A571	A572	A573	A574	A575	A576	C579	C580	A581	G582	U586	A587	G588	C589	G590	G591	U592	G593	A594	A595	A596	U597	G598	C599	A702	G703	A704	C705	A706	U707	C708	A712	G713	G714	A715	A716	U717	A718	C719
G720	G721	G722	U723	C724	C725	G726	G727	A728	A729	G730	G731	C732	G733	G734	C735	A736	C737	C738	C739	U740	G741	G742	A743	C744	G745	A746	U747	G748	A749	C750	U751	G752	C753	C754	G755	C756	U757	C758	A759	G760	G761	C764	G765	A766	G767	C768	A769	C770	G775	G776	A777	G778	C779	A780	A781	A782	C783			
A784	C785	C786	C787	C788	C789	C790	C791	A792	U793	A794	C795	C796	C797	G800	U801	C802	G803	U804	C805	C806	A807	C808	G809	C810	C811	G812	U813	A814	C815	A816	C817	G818	U819	A820	C821	G822	C823	G824	A825	C826	U827	U828	A831	G838	C839	C840	C841	U842	U843	G844	A845	G846	U847	C848	C853	U854	C856			
C857	C858	C859	A860	C861	C862	U863	A864	C865	C866	C867	C868	C869	U870	U871	A872	A873	C874	U875	C876	C877	A878	C879	C880	C881	C882	C883	U884	C885	C886	C887	C888	C889	C890	U891	A892	U893	U894	C895	C896	C897	C898	C899	A900	A901	U902	G903	G904	U905	U906	U907	A908	A909	C910	U911	C912	A913	A914	A915	U916	
G917	A918	A919	U920	U921	G922	A923	C924	G925	G926	G927	C930	C931	C932	G933	A934	C935	A936	C937	A938	C939	G940	C941	G945	A946	C947	C948	U949	A950	C951	U952	G953	A954	U955	U956	U957	A958	A959	U960	U961	C962	G963	A964	U965	G966	C967	A968	A969	C970	C971	G972	C973	A974	A975	G976	A977	A978	C979			
C980	U981	U982	C983	C984	C985	U986	C987	C990	U991	U992	G993	A994	C995	U996	U997	C998	C999	A1000	C1001	G1002	G1003	A1004	A1005	G1006	U1007	U1008	U1009	U1010	C1011	A1012	G1013	A1014	G1015	A1016	A1019	G1020	A1021	A1022	U1025	G1026	C1027	U1028	U1029	U1030	C1031	G1032	G1033	G1034	A1035	A1036	C1037	A1038	G1039	A1042	G1043					



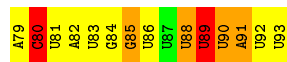
• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 26% 50% 22%



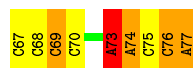
• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

Chain A2: 7% 53% 27% 13%

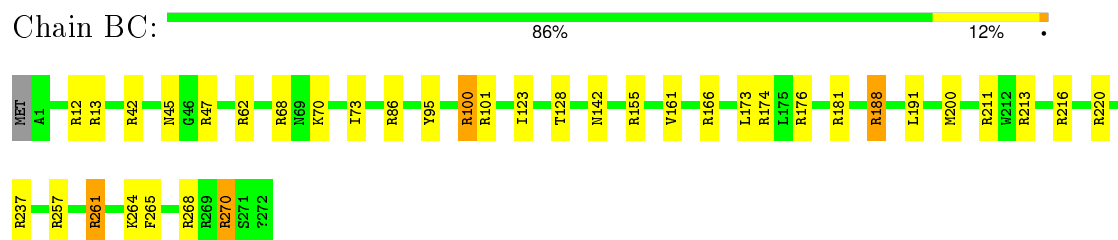


• Molecule 24: tRNA-fMet

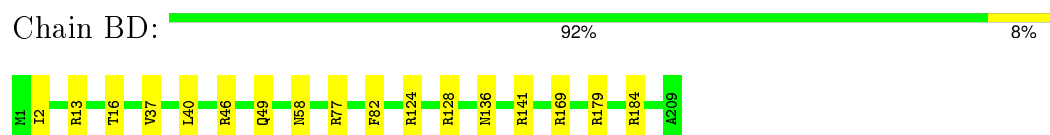
Chain A3: 29% 53% 16%



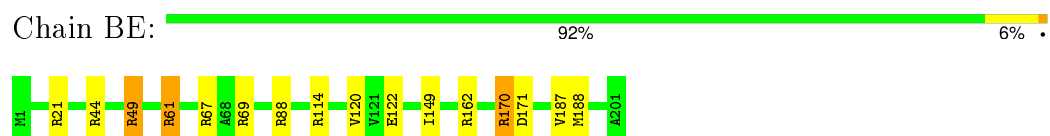
• Molecule 25: 50S ribosomal protein L2



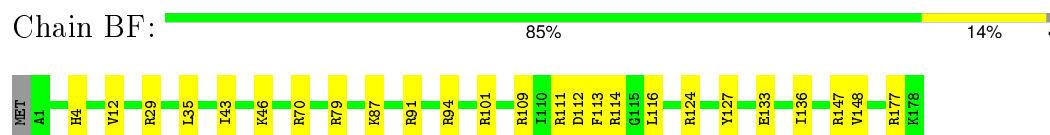
- Molecule 26: 50S ribosomal protein L3



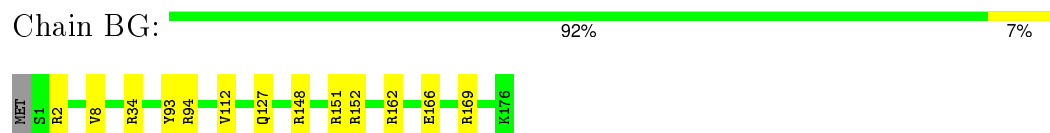
- Molecule 27: 50S ribosomal protein L4



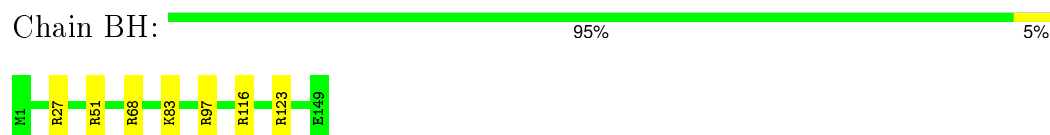
- Molecule 28: 50S ribosomal protein L5



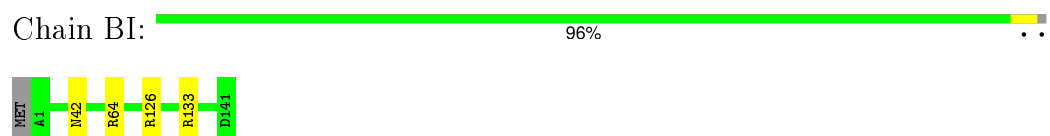
- Molecule 29: 50S ribosomal protein L6




- Molecule 30: 50S ribosomal protein L9

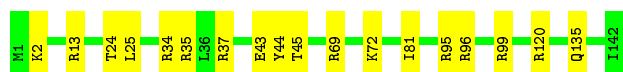


- Molecule 31: 50S ribosomal protein L11



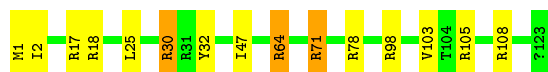
- Molecule 32: 50S ribosomal protein L13

Chain BJ:  87% 13%




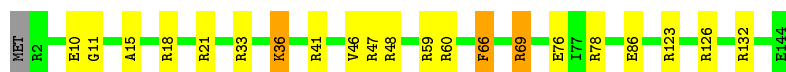
- Molecule 33: 50S ribosomal protein L14

Chain BK:  88% 10%



- Molecule 34: 50S ribosomal protein L15

Chain BL:  85% 13%



- Molecule 35: 50S ribosomal protein L16

Chain BM:  85% 15%



- Molecule 36: 50S ribosomal protein L17

Chain BN:  88% 12%




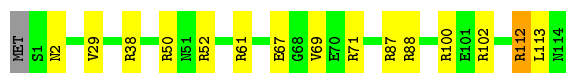
- Molecule 37: 50S ribosomal protein L18

Chain BO:  87% 11%




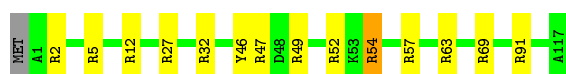
- Molecule 38: 50S ribosomal protein L19

Chain BP:  86% 12%



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  87% 11%



- Molecule 40: 50S ribosomal protein L21

Chain BR: 91% 9%



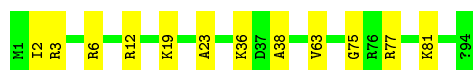
- Molecule 41: 50S ribosomal protein L22

Chain BS: 92% 8%



- Molecule 42: 50S ribosomal protein L23

Chain BT: 87% 13%



- Molecule 43: 50S ribosomal protein L24

Chain BU: 87% 12% ..



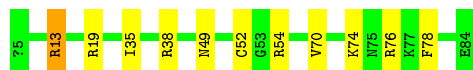
- Molecule 44: 50S ribosomal protein L25

Chain BV: 91% 9%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 86% 13% .



- Molecule 46: 50S ribosomal protein L28

Chain BX: 86% 10% ..



- Molecule 47: 50S ribosomal protein L29

Chain BY:  92% 8%




- Molecule 48: 50S ribosomal protein L30

Chain BZ:  86% 12%



- Molecule 49: 50S ribosomal protein L32

Chain B0:  84% 14%



- Molecule 50: 50S ribosomal protein L33

Chain B1:  92% 8%




- Molecule 51: 50S ribosomal protein L34

Chain B2:  74% 26%



- Molecule 52: 50S ribosomal protein L35

Chain B3:  86% 12%

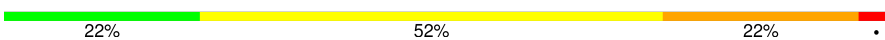


- Molecule 53: 50S ribosomal protein L36

Chain B4:  92% 8%



- Molecule 54: 23S ribosomal RNA

Chain BA:  22% 52% 22%

G1024	C957	A896	G831	G768	G704	A643	C581	A515	U451	U387	G254	A195	A127	A63	G1
G1025	U958	C997	U832	G768	A705	A644	A552	C516	G452	G388	A255	A196	C128	A64	U4
G1026	A959	C998	A833	G772	A706	U646	G583	C517	A453	G389	A256	A197	C129	U65	A5
A1027	A960	A989	G834	U773		U646	C584		A454	U390	C257	A198	C130	C66	A6
A1028	G961	A900	C835	G774	U709	G647	G585	G520	C455	A391		C198	A131	U67	G7
A1029	G962	C901	G836	G775	U710		A586	U521	C456	U392	A262	A199	G132	G68	C8
C1030	U963	C902	G837	G776			G587	A522	A457	C393	G263	U200	U133	C69	G9
C1031	C964	G903	C838	G777	U714	C850	U588	G523	G458	C394	A264	U202	G134	G70	A10
A1032	C965	A905	U839	G778	A715	G851	U589		U459	U395	A265			A71	A11
U1033			C840	U779	A716	U653	A590	A526	A460	G396	G266	A203	U138	U72	C11
G1034			G841	U780	C717	A654	U591	C527	C461	U397	C267	A204	U139	A73	U12
U1035			U842	A781	C718	A655	A592	A528	C462	C398	C268	G205	C140	A74	A13
A1039	G969	C908	G843	A782	C719	G856	U593	A529	G463	U399	C269	U206	G141	G75	A14
A1040	G971	A910	A844	A783	U720	U857	U594	G530	U464	G400	A270	A207	A142	C76	G15
A1041	A972	A911	A845	G784	A721	U858	C595	C531	G465	A401	G271	C208	C143	G77	C16
G1042	A973	C912	U846	G785	A722	U859	U596	A532	A466	A402	G272	C209	A144	U78	G17
C1043	G974	U913	U847	C786	C723	C660	G597	G533	C467	U403	G273	C210	C145	U79	U18
G1044		G914	C848	C787	U724	A661	U598	U534		A404	C274	C211	A146	A19	A19
C1045		C915	A849	A788	G725	G662	A599	G535	A470	U405	C275	G212	C147	C20	C20
C1046	A979	G916	U850	A789	G726	G663	G600	G536	A471		U276	A213	U148	A83	A21
A1046	A980	A917	C851	U790	A727	G664	C601	G537	A472	G408	G277	G214	A149	G85	C22
G1047	A981	A918	U852	A791	G728	U665	A602	A538	C473		A278	G215	U150	G86	G23
A1048	C982	U919	C853	A792	G729	A666	A603	G539	C474	G411	A279	A216	C151	U87	G24
C1049	A983	A920	C854	A793	A730	U667		C540	C475	A412	U280	A217	A152	G88	U25
A1050	A984	C921	G855	A794	C731	A668	U606	A541	C476	C413	C281	A218		G26	G26
G1051	C985	C922	G856	C795	C732	G669	U607	C542	A477	C414	A282	A219		A89	G27
C1052	C986	G923	G857	G796	G733	A670	A608	G543	A478	A415	G283	G220	A155	U90	C37
C1053	C987	G924	C858		G734	C671	A609	G544	A479	U416	U284	A221	C157	A91	A28
A1054	A988	A925	G859	G799	A735	C672	C610	U545	A480	C417	G285	A222	U158	U92	U29
G1055	G989	G926	U860	A800	C736	C673	C611	U546	A481	C418	U286	A223	G93	G86	G30
A1056	A990	A927	A861	G801	C737	G674	G612	A547	A482	U419	G287	U224	A160	A94	C31
A1057	C991	A928	G862	A802	G738	A675	A613	G548	A483	C420	U288	C225	A161	C96	C32
C1058	C992	U929	A863	U803	A739	A676	A614	G549	C484	C421	G289	A226	U162	C97	C33
G1059	G993	G930	C864	A804	C740	A677	U615	G550	C485	A422	U290	A227	U163	G98	G34
U1060	C994	U931	C865	G805	U741	C678	A616	G551	C486	A423	G291	C228	C164	U99	A44
C995	C995	U932	A866	C806	A742	C679	G617		C487	G359	C229	A165	U171	C106	G45
G1062	A996	A933	C867	A743	A743	C680		U554	C488	U427	A294	G230	U166	A101	G46
G1063	G997	U934		U744	U744	G681	G620	G555	G489	A428		A231	A167	U102	C37
	C998	C935	U870	G809	G745	U682	A621	A556	C490	A429	A299	G232	G168	A103	A38
	U999	A936	U871	U810	U746	G683	G622	C557	G491	A430	A300	A233	G169	A104	U40
A1001	A1000	C937	U872	U811	U747	G684	C623	U558	A492	U431	C302	U235	U170	C105	A42
		G938	C873	C812	G748	A685	C624	G559	G493	U432	G303	C236	U172	G107	A44
		G939		U813	A749	U686	G625	G560		A433	U304	C237	A173	G45	G45
A1070		G940	A877	C814	A750	C687	A626		A497	C433	C305	C238	U174	C109	G46
G1071	C1006	A941	A878	C815	A751	U688	A627	A563		U434	U306	C239	G175	C37	G47
	U1007	G942	G879	C816	A752	A689	G628	C564	G500	C435	U307	C240	G176	G48	G48
A1008	A1008	A943		C817	A753	G690	G629	C565	A501	C436	G307	A241	A177	A11	A49
A1009	C944	C944	G883	G818		C691	A631	U566	A502	U437	G308	A242	G177	U112	U50
A1010	A945	A945	C884	A819	A756	C692	A632	U567	A503	G438	A309	G243	G178	U113	G51
C1075		C946	C885	A820	G757	A693	A633	U568	A504	A439	U310	A244	C179	U114	A52
C1076	U1012	A947	U887	A821	C758	U694	A634	U569	A505	C440	A311	G245	G180	C115	A53
A1077	C1013	C948	C888	G822	G759	G695	C634	G370		A443	G312	G246	A182	C116	G54
U1078	A1014	G950	C889	U824	G760	G696	C635	U571	A507	A444	G313	C247	A183	G117	G55
		G951	C890	U825	A761	G697	C636	A572	A508	C445	C314	G248	C183	A118	A56
		C951	C891	A826	U762	C698	A637	U573	C509	G446	G315	G249	C184	A119	C57
U1083	U1019	G952	G891	U826	G763	A699	G638	A574	C510	G447	C316	C250	G189	U120	G58
A1084	A1020	G953	A892	U827	A764	G700	U639	A575	U511	A447	G317	G251	G190	G121	U59
A1085	G1022	U954	C893	U828	C765	G701	C640	U512	A448	U449	C318	A251	A191	C60	G60
A1086	A1021	U955	U894	U702	U766	U702	U641	G513	U449	U449	G319	G252	A191	C61	G61
G1087	U1023	G956	U895	G830	U767	U703	U642	G578	A514	G450	A320	C253	C192	A126	U62

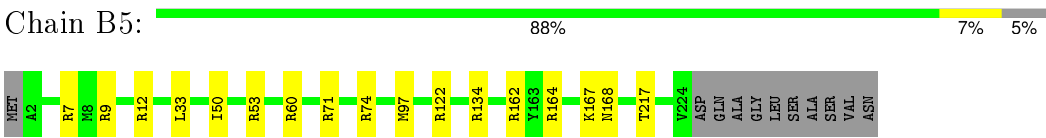
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G2035	G1973	G1910	A1780	G1649	G1538	G1459	A1395	G1333	U1273	G1210	G1149	A1089
C2036	C1974	U1911	U1781	G1650	U1589	U1460	U1589	G1334	U1274	G1211	G1150	A1090
A2037	G1975	G1912	U1782	G1651	A1590	C1461	U1397	G1335	A1275	G1212	A1151	G1091
G2038	U1976	C1913	A1783	G1652	A1591	C1462	C1398	G1336	A1276	A1213	C1152	C1092
U2039	A1977	G1914	A1784	G1653	A1592	C1463	C1399	G1337	A1277	A1214	C1153	G1093
G2040	A1978	C1915	A1785	G1654	A1593	G1464	U1400	G1338	G1278	G1215	G1154	U1094
U2041	A1979	U1916	A1786	A1655	U1594		G1401	G1339	G1279	G1216	A1155	A1095
A2042	U1980	U1917	A1787	C1656	A1595		U1402	U1340	G1280	U1217	A1156	A1096
C2043	A1981	A1918	C1788	A1657	C1536	A1470	A1403	G1341	G1281	G1218	G1157	U1097
C2044	U1982	A1919	A1789	C1658	A1596	G1471	A1404	G1342	U1282	U1219	C1158	A1098
C2045		G1920	A1790		A1597	C1472	U1405	G1343	G1283	G1220	U1159	G1099
G2046	C1985	U1921	A1791	U1662	U1598		U1406	U1344	A1284	C1221	U1160	G1100
C2047	C1986		G1792	G1663	C1600	G1475	G1407	C1345	A1285	U1222	C1161	U1101
	A1987	C1924	C1793	A1664	G1601	U1476	G1408	G1346	A1286	G1223	G1162	C1102
C2050		C1925	U1794	A1665	U1602	U1477	U1409	A1347	A1287		G1163	A1103
A2051	U1990	U1926	C1795		A1603	G1478		C1348	G1288		C1164	C1104
A2052	G1992	A1928	U1796	A1668	C1604	G1479	A1413	C1349	C1289		A1165	U1105
G2053	G1993	G1929	G1797	A1669	C1605	U1480	C1414	C1350	C1290	G1228	G1166	G1106
A2054	C1994	G1930	U1798	A1670	C1606	U1481	U1415	C1351	G1291	A1230	C1167	G1107
G2055	U1995	U1931	G1799	A1671	C1547	G1482	G1416	C1352	G1292	U1231	G1168	U1108
G2056	U1996	G1932	A1800	G1672	A1608		C1417	A1353	C1293	G1232	A1169	C1109
G2057	C1997	A1933	A1801	G1673	A1548		G1418	A1354	U1294	C1233	C1170	G1110
A2058	A1998	G1934	A1739	G1674	A1610	U1485	A1419	G1355	C1295	U1234	G1171	A1111
C2059	C1999	C1935	A1802	G1675	A1551		A1420	G1356	G1296	G1235	G1172	G1112
A2060	C2000	U1936	C1804	A1676	C1612	C1488		C1357	C1297	G1236	U1173	U1113
G2061	C2001	A1937	A1805	A1677	G1613	A1490	G1423	G1358	C1298	A1237	U1174	C1114
A2062	G2002	U1938	G1743	A1678	U1554		G1424	A1359	G1299	G1238	A1175	G1115
C2063	G2003	U1939	A1744	A1679	G1615	C1493	G1425	A1360	G1300	U1239	U1176	G1116
C2064	A2003	A1940	A1745	A1680	C1556	U1494	G1426	A1367	G1239	U1240	G1177	C1117
G2065	G2004	U1946	G1746	G1681	C1557	A1495	A1427	G1368	A1307	A1246	U1184	C1123
C2066	A2005	C1941	U1747	G1682	U1563	U1502	A1433	G1369	A1308	A1247	G1185	G1124
G2067	C2006	U1942	C1748	G1683	C1564	A1503	A1434	C1370	G1309	G1248	G1186	G1125
U2068	U2007	U1943	A1749	A1684	C1565	A1504	G1435	G1371	G1310		G1187	A1126
G2069	C2008	U1944	A1750	C1685	A1566	A1505	U1436	U1372	G1311	C1251	U1188	A1127
A2070	A2009	G1945	G1751	G1686	G1567	U1506	C1437	A1373	U1312	G1252	A1189	G1128
G2071	G2010	U1946	U1752	G1687	G1568	C1507	U1438	G1374	U1313	A1253	G1190	A1129
C2072	U2011	C1947	G1753	U1688	U1569	A1508	A1439	U1375	G1314	U1254	G1191	U1130
C2073	G2012	U1951	A1754	A1689	A1570	A1509	U1440	C1376	C1315	U1255	G1192	G1131
U2074	A2013	A1952	A1755	A1690	C1568	A1510	G1441	G1377	U1316	G1256	G1193	U1132
U2075	A2014	A1953	G1756	C1691	G1567	U1512	U1442	U1378	G1317	C1257	A1194	A1133
A2076	A2015	G1954	A1757	G1692	G1568	C1512	U1443	U1379	U1318	U1258	G1195	A1134
G2077	U2016	U1955	U1758	U1693	A1569	U1513	G1444	G1380	C1319	G1259	C1196	C1135
C2078	U2017	C1956	A1759	G1694	A1630	A1515	G1445	G1381	C1320	A1260	G1197	G1136
U2079	G2018	U1956	C1760	C1695	U1570	G1516	G1446	G1382	A1321	C1261	U1198	G1137
A2080	A2019	C1957	C1761	A1696	A1571	G1517	C1447	A1383	A1322	A1262	U1199	G1138
U2081	A2020	C1958	A1762	A1697	A1572	U1518	G1448	A1384	C1323	U1263	C1200	G1139
A2082	C2021	G1959	G1763	G1699	G1573	U1519	U1449	A1385	G1324	A1264	U1201	C1140
G2083	C2022	A1960	C1764	A1700	A1574	U1520	G1450	C1386	U1325	A1265	G1202	U1141
C2084	C2023	C1961	U1765	A1701	A1635	G1521	G1452	A1387	U1326	G1266	U1203	A1142
U2085	G2024	U1962	U1766	A1702	U1575	G1522	C1453	G1388	A1327	U1267	A1204	A1143
G2086	C2025	U1963	C1768	G1703	C1577	U1523			A1328	A1268	A1205	A1144
G2087	U2026	G1964		G1704	U1578	G1524			U1329	A1269	G1206	C1145
A2088	G2027	U1965	A1772	A1705	A1579	U1525	C1451	C1389	U1329	C1270	C1146	C1147
C2089	U2028	A1966	A1773	G1706	A1580	A1526	G1453	A1387				
A2090	G2029	C1967	C1774	G1707	C1581	U1527	C1454	G1388				
C2091	A2030	G1968	U1775	C1708	A1583	U1528						
U2092	A2031	A1969	G1776	G1709	U1584	G1529						
G2093	C2032	U1970	U1777	G1710	C1585	A1526						
A2094	A2033	U1971	U1778	A1711	A1586	C1526						



Response	Percentage
Yes	21%
No	64%
Don't know	12%



● Molecule 56: 50S ribosomal protein L1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, FME, ACE, H2U, CM0, 6MZ, NH2, 4SU, 7MG, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	AB	0.72	0/1736	1.05	12/2340 (0.5%)
10	AK	0.74	0/894	1.20	12/1207 (1.0%)
11	AL	0.76	0/969	1.32	18/1300 (1.4%)
12	AM	0.76	0/884	1.23	16/1181 (1.4%)
13	AN	0.79	0/817	1.32	12/1088 (1.1%)
14	AO	0.73	0/722	1.12	9/964 (0.9%)
15	AP	0.76	0/648	1.22	9/870 (1.0%)
16	AQ	0.71	0/658	1.14	6/883 (0.7%)
17	AR	0.81	0/463	1.28	6/623 (1.0%)
18	AS	0.78	0/653	1.29	8/879 (0.9%)
19	AT	0.71	0/672	1.08	6/890 (0.7%)
2	AC	0.72	0/1651	1.12	14/2225 (0.6%)
20	AU	0.83	0/431	1.48	10/572 (1.7%)
21	AA	1.52	2/36759 (0.0%)	2.21	1934/57346 (3.4%)
22	A1	1.53	0/1668	2.22	92/2595 (3.5%)
23	A2	1.51	0/343	2.43	24/531 (4.5%)
24	A3	1.53	0/1722	2.18	82/2685 (3.1%)
25	BC	0.75	0/2121	1.27	26/2852 (0.9%)
26	BD	0.68	0/1586	1.11	8/2134 (0.4%)
27	BE	0.68	0/1571	1.12	9/2113 (0.4%)
28	BF	0.76	0/1444	1.21	13/1937 (0.7%)
29	BG	0.69	0/1343	1.13	10/1816 (0.6%)
3	AD	0.77	0/1665	1.23	21/2227 (0.9%)
30	BH	0.67	0/1122	1.08	6/1515 (0.4%)
31	BI	0.66	0/1046	1.02	3/1410 (0.2%)
32	BJ	0.72	0/1152	1.19	11/1551 (0.7%)
33	BK	0.73	0/947	1.28	10/1268 (0.8%)
34	BL	0.74	0/1054	1.32	14/1403 (1.0%)
35	BM	0.75	0/1093	1.22	14/1460 (1.0%)
36	BN	0.77	0/973	1.31	14/1301 (1.1%)
37	BO	0.75	0/902	1.25	11/1209 (0.9%)
38	BP	0.73	0/929	1.20	10/1242 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	BQ	0.79	0/960	1.30	14/1278 (1.1%)
4	AE	0.70	0/1119	1.09	9/1506 (0.6%)
40	BR	0.72	0/829	1.19	7/1107 (0.6%)
41	BS	0.65	0/864	1.13	7/1156 (0.6%)
42	BT	0.68	0/744	1.21	5/994 (0.5%)
43	BU	0.70	0/787	1.14	6/1051 (0.6%)
44	BV	0.72	0/766	1.18	6/1025 (0.6%)
45	BW	0.75	0/604	1.27	5/799 (0.6%)
46	BX	0.76	0/635	1.32	10/848 (1.2%)
47	BY	0.67	0/510	1.24	6/677 (0.9%)
48	BZ	0.68	0/453	1.21	4/605 (0.7%)
49	B0	0.72	0/450	1.18	5/599 (0.8%)
5	AF	0.74	0/835	1.09	5/1128 (0.4%)
50	B1	0.72	0/417	1.04	2/556 (0.4%)
51	B2	0.80	0/380	1.47	10/498 (2.0%)
52	B3	0.71	0/513	1.20	5/676 (0.7%)
53	B4	0.70	0/303	1.17	2/397 (0.5%)
54	BA	1.40	0/69796	2.22	4069/108888 (3.7%)
55	BB	1.40	0/2800	2.18	144/4367 (3.3%)
56	B5	0.66	0/1673	1.12	11/2255 (0.5%)
6	AG	0.75	0/1188	1.21	17/1593 (1.1%)
7	AH	0.70	0/989	1.10	9/1326 (0.7%)
8	AI	0.81	0/1035	1.28	20/1377 (1.5%)
9	AJ	0.72	0/797	1.21	14/1079 (1.3%)
All	All	1.28	2/160085 (0.0%)	2.00	6842/239402 (2.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AB	0	1
10	AK	0	1
14	AO	0	1
2	AC	0	1
21	AA	0	350
22	A1	0	16
23	A2	0	5
24	A3	0	17
26	BD	0	1
27	BE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	BO	0	1
5	AF	0	1
54	BA	0	705
55	BB	0	21
All	All	0	1122

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	AA	1382	C	C4-N4	-5.09	1.29	1.33
21	AA	476	U	C5'-C4'	5.08	1.57	1.51

All (6842) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1932	A	N1-C6-N6	-13.19	110.69	118.60
54	BA	371	A	N1-C6-N6	-12.55	111.07	118.60
21	AA	1239	A	N1-C6-N6	-12.45	111.13	118.60
54	BA	2432	A	N1-C6-N6	-12.35	111.19	118.60
54	BA	1635	A	N1-C6-N6	-12.24	111.26	118.60
54	BA	2813	A	N1-C6-N6	-12.08	111.35	118.60
54	BA	2589	A	N1-C6-N6	-12.07	111.36	118.60
10	AK	52	ARG	NE-CZ-NH2	12.03	126.32	120.30
54	BA	1098	A	N1-C6-N6	-11.76	111.54	118.60
54	BA	2820	A	N1-C6-N6	-11.76	111.55	118.60
54	BA	309	A	N1-C6-N6	-11.66	111.61	118.60
54	BA	878	A	N1-C6-N6	-11.61	111.63	118.60
54	BA	1609	A	N1-C6-N6	-11.58	111.65	118.60
54	BA	311	A	N1-C6-N6	-11.56	111.66	118.60
6	AG	77	ARG	NE-CZ-NH1	11.52	126.06	120.30
21	AA	329	A	N1-C6-N6	-11.34	111.80	118.60
54	BA	794	A	N1-C6-N6	-11.33	111.80	118.60
54	BA	1352	U	O4'-C1'-N1	11.33	117.27	108.20
54	BA	324	A	N1-C6-N6	-11.27	111.84	118.60
54	BA	125	A	N1-C6-N6	-11.27	111.84	118.60
21	AA	1476	A	N1-C6-N6	-11.23	111.86	118.60
21	AA	573	A	N1-C6-N6	-11.21	111.87	118.60
3	AD	110	ARG	NE-CZ-NH1	11.19	125.89	120.30
21	AA	320	A	N1-C6-N6	-11.19	111.89	118.60
54	BA	632	A	N1-C6-N6	-11.18	111.89	118.60
54	BA	613	A	N1-C6-N6	-11.16	111.90	118.60
21	AA	1219	A	N1-C6-N6	-11.16	111.91	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2781	A	N1-C6-N6	-11.14	111.92	118.60
54	BA	1347	A	N1-C6-N6	-11.13	111.92	118.60
21	AA	728	A	N1-C6-N6	-11.08	111.95	118.60
54	BA	1308	A	N1-C6-N6	-11.07	111.96	118.60
21	AA	889	A	N1-C6-N6	-11.05	111.97	118.60
54	BA	1780	A	N1-C6-N6	-11.05	111.97	118.60
21	AA	1188	A	N1-C6-N6	-11.03	111.98	118.60
18	AS	2	ARG	NE-CZ-NH1	11.02	125.81	120.30
21	AA	704	A	N1-C6-N6	-10.99	112.01	118.60
54	BA	1046	A	N1-C6-N6	-10.99	112.01	118.60
54	BA	497	A	N1-C6-N6	-10.98	112.01	118.60
54	BA	2076	U	O4'-C1'-N1	10.96	116.97	108.20
54	BA	1496	A	N1-C6-N6	-10.96	112.02	118.60
54	BA	752	A	O4'-C1'-N9	10.94	116.95	108.20
54	BA	2274	A	N1-C6-N6	-10.93	112.04	118.60
21	AA	780	A	N1-C6-N6	-10.92	112.05	118.60
21	AA	199	A	N1-C6-N6	-10.90	112.06	118.60
54	BA	2749	A	N1-C6-N6	-10.89	112.06	118.60
54	BA	1583	A	N1-C6-N6	-10.87	112.08	118.60
21	AA	608	A	N1-C6-N6	-10.85	112.09	118.60
21	AA	781	A	N1-C6-N6	-10.85	112.09	118.60
54	BA	1385	A	N1-C6-N6	-10.84	112.09	118.60
21	AA	139	A	N1-C6-N6	-10.82	112.11	118.60
54	BA	633	A	N1-C6-N6	-10.82	112.11	118.60
54	BA	900	A	N1-C6-N6	-10.81	112.11	118.60
54	BA	928	A	N1-C6-N6	-10.80	112.12	118.60
54	BA	223	A	N1-C6-N6	-10.80	112.12	118.60
11	AL	82	ARG	NE-CZ-NH1	10.76	125.68	120.30
54	BA	2600	A	N1-C6-N6	-10.74	112.15	118.60
54	BA	222	A	N1-C6-N6	-10.72	112.17	118.60
47	BY	52	ARG	NE-CZ-NH1	10.72	125.66	120.30
54	BA	507	A	N1-C6-N6	-10.71	112.17	118.60
54	BA	1919	A	N1-C6-N6	-10.71	112.18	118.60
3	AD	2	ARG	NE-CZ-NH1	10.70	125.65	120.30
21	AA	746	A	N1-C6-N6	-10.68	112.19	118.60
54	BA	354	A	N1-C6-N6	-10.67	112.20	118.60
54	BA	74	A	N1-C6-N6	-10.67	112.20	118.60
54	BA	526	A	O4'-C1'-N9	10.65	116.72	108.20
7	AH	12	ARG	NE-CZ-NH1	10.65	125.62	120.30
54	BA	262	A	N1-C6-N6	-10.64	112.22	118.60
21	AA	129	A	N1-C6-N6	-10.64	112.22	118.60
54	BA	1260	A	N1-C6-N6	-10.60	112.24	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2547	A	N1-C6-N6	-10.60	112.24	118.60
21	AA	448	A	N1-C6-N6	-10.59	112.24	118.60
21	AA	1248	A	N1-C6-N6	-10.59	112.25	118.60
54	BA	1901	A	N1-C6-N6	-10.59	112.25	118.60
54	BA	910	A	N1-C6-N6	-10.58	112.25	118.60
54	BA	2126	A	N1-C6-N6	-10.57	112.26	118.60
21	AA	192	A	N1-C6-N6	-10.56	112.26	118.60
21	AA	279	A	N1-C6-N6	-10.55	112.27	118.60
21	AA	1163	A	N1-C6-N6	-10.54	112.27	118.60
21	AA	681	A	N1-C6-N6	-10.52	112.29	118.60
21	AA	977	A	N1-C6-N6	-10.51	112.30	118.60
23	A2	91	A	N1-C6-N6	-10.51	112.30	118.60
54	BA	1129	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	1089	A	N1-C6-N6	-10.50	112.30	118.60
54	BA	204	A	N1-C6-N6	-10.49	112.31	118.60
54	BA	1553	A	N1-C6-N6	-10.49	112.31	118.60
20	AU	46	ARG	NE-CZ-NH1	10.48	125.54	120.30
54	BA	2241	A	N1-C6-N6	-10.48	112.31	118.60
54	BA	2734	A	N1-C6-N6	-10.48	112.31	118.60
21	AA	59	A	N1-C6-N6	-10.47	112.31	118.60
54	BA	478	A	N1-C6-N6	-10.47	112.31	118.60
54	BA	294	A	N1-C6-N6	-10.46	112.32	118.60
54	BA	2887	A	N1-C6-N6	-10.45	112.33	118.60
21	AA	1502	A	N1-C6-N6	-10.45	112.33	118.60
54	BA	1872	A	N1-C6-N6	-10.43	112.34	118.60
54	BA	2406	A	N1-C6-N6	-10.43	112.34	118.60
54	BA	670	A	N1-C6-N6	-10.43	112.34	118.60
54	BA	1713	A	N1-C6-N6	-10.42	112.35	118.60
21	AA	563	A	N1-C6-N6	-10.42	112.35	118.60
55	BB	101	A	N1-C6-N6	-10.42	112.35	118.60
10	AK	36	ARG	NE-CZ-NH1	10.41	125.50	120.30
21	AA	648	A	N1-C6-N6	-10.41	112.36	118.60
21	AA	172	A	N1-C6-N6	-10.40	112.36	118.60
55	BB	15	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	616	A	N1-C6-N6	-10.40	112.36	118.60
54	BA	2646	C	N3-C2-O2	-10.39	114.63	121.90
17	AR	56	ARG	NE-CZ-NH1	10.38	125.49	120.30
55	BB	50	A	N1-C6-N6	-10.37	112.38	118.60
54	BA	793	A	N1-C6-N6	-10.36	112.39	118.60
54	BA	1607	C	O4'-C1'-N1	10.36	116.48	108.20
21	AA	160	A	N1-C6-N6	-10.35	112.39	118.60
54	BA	1434	A	N1-C6-N6	-10.33	112.40	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1057	A	N1-C6-N6	-10.33	112.40	118.60
54	BA	2333	A	N1-C6-N6	-10.33	112.40	118.60
54	BA	1014	A	N1-C6-N6	-10.32	112.41	118.60
21	AA	676	A	N1-C6-N6	-10.31	112.41	118.60
21	AA	327	A	N1-C6-N6	-10.31	112.42	118.60
21	AA	197	A	N1-C6-N6	-10.30	112.42	118.60
21	AA	179	A	N1-C6-N6	-10.29	112.42	118.60
54	BA	866	A	N1-C6-N6	-10.29	112.43	118.60
21	AA	909	A	N1-C6-N6	-10.28	112.43	118.60
54	BA	1505	A	N1-C6-N6	-10.27	112.44	118.60
7	AH	14	ARG	NE-CZ-NH1	10.27	125.43	120.30
21	AA	872	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	91	A	N1-C6-N6	-10.27	112.44	118.60
54	BA	1237	A	N1-C6-N6	-10.26	112.44	118.60
54	BA	1781	U	O4'-C1'-N1	10.26	116.41	108.20
54	BA	2439	A	O4'-C1'-N9	10.26	116.41	108.20
54	BA	547	A	N1-C6-N6	-10.25	112.45	118.60
21	AA	298	A	N1-C6-N6	-10.23	112.46	118.60
21	AA	860	A	N1-C6-N6	-10.22	112.47	118.60
21	AA	1410	A	N1-C6-N6	-10.22	112.47	118.60
54	BA	458	G	O4'-C1'-N9	10.22	116.37	108.20
54	BA	2020	A	N1-C6-N6	-10.20	112.48	118.60
54	BA	1960	A	N1-C6-N6	-10.20	112.48	118.60
3	AD	12	ARG	NE-CZ-NH1	10.19	125.40	120.30
21	AA	81	A	N1-C6-N6	-10.19	112.48	118.60
54	BA	384	A	N1-C6-N6	-10.19	112.49	118.60
21	AA	996	A	N1-C6-N6	-10.18	112.49	118.60
54	BA	931	U	O4'-C1'-N1	10.17	116.34	108.20
21	AA	149	A	N1-C6-N6	-10.16	112.50	118.60
21	AA	1213	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	2097	A	N1-C6-N6	-10.16	112.50	118.60
54	BA	2792	A	N1-C6-N6	-10.15	112.51	118.60
54	BA	960	A	N1-C6-N6	-10.15	112.51	118.60
54	BA	1067	A	N1-C6-N6	-10.15	112.51	118.60
54	BA	2352	A	N1-C6-N6	-10.15	112.51	118.60
54	BA	788	A	N1-C6-N6	-10.14	112.51	118.60
54	BA	821	A	N1-C6-N6	-10.13	112.52	118.60
54	BA	1853	A	N1-C6-N6	-10.12	112.53	118.60
21	AA	53	A	N1-C6-N6	-10.12	112.53	118.60
21	AA	609	A	N1-C6-N6	-10.11	112.54	118.60
54	BA	2655	G	O4'-C1'-N9	10.11	116.28	108.20
21	AA	466	A	N1-C6-N6	-10.10	112.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2654	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	130	A	N1-C6-N6	-10.10	112.54	118.60
54	BA	2809	A	N1-C6-N6	-10.10	112.54	118.60
21	AA	1396	A	N1-C6-N6	-10.09	112.55	118.60
54	BA	1614	A	N1-C6-N6	-10.07	112.56	118.60
54	BA	2886	A	N1-C6-N6	-10.06	112.56	118.60
25	BC	216	ARG	NE-CZ-NH1	10.05	125.32	120.30
21	AA	468	A	N1-C6-N6	-10.04	112.58	118.60
21	AA	1441	A	N1-C6-N6	-10.04	112.58	118.60
21	AA	162	A	N1-C6-N6	-10.04	112.58	118.60
54	BA	362	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	913	A	N1-C6-N6	-10.02	112.59	118.60
21	AA	1368	A	N1-C6-N6	-10.01	112.60	118.60
54	BA	119	A	N1-C6-N6	-10.01	112.60	118.60
36	BN	8	ARG	NE-CZ-NH1	10.00	125.30	120.30
54	BA	423	A	N1-C6-N6	-10.00	112.60	118.60
54	BA	432	A	N1-C6-N6	-9.99	112.60	118.60
21	AA	300	A	N1-C6-N6	-9.99	112.61	118.60
21	AA	1274	A	N1-C6-N6	-9.99	112.61	118.60
21	AA	1036	A	N1-C6-N6	-9.98	112.61	118.60
25	BC	188	ARG	NE-CZ-NH1	9.98	125.29	120.30
54	BA	2632	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	1156	A	N1-C6-N6	-9.98	112.61	118.60
54	BA	2369	A	N1-C6-N6	-9.98	112.61	118.60
21	AA	325	A	N1-C6-N6	-9.97	112.62	118.60
22	A1	35	A	N1-C6-N6	-9.97	112.62	118.60
54	BA	943	A	N1-C6-N6	-9.96	112.62	118.60
21	AA	1287	A	N1-C6-N6	-9.96	112.62	118.60
54	BA	792	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	1551	A	N1-C6-N6	-9.95	112.63	118.60
54	BA	449	A	N1-C6-N6	-9.95	112.63	118.60
21	AA	968	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	1145	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	1981	A	N1-C6-N6	-9.94	112.64	118.60
54	BA	2726	A	N1-C6-N6	-9.94	112.64	118.60
21	AA	26	A	N1-C6-N6	-9.93	112.64	118.60
54	BA	945	A	N1-C6-N6	-9.93	112.64	118.60
55	BB	109	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	1938	A	N1-C6-N6	-9.92	112.65	118.60
25	BC	213	ARG	NE-CZ-NH1	9.92	125.26	120.30
54	BA	2518	A	N1-C6-N6	-9.92	112.65	118.60
54	BA	1773	A	N1-C6-N6	-9.91	112.65	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1340	U	O4'-C1'-N1	9.91	116.13	108.20
21	AA	892	A	N1-C6-N6	-9.91	112.66	118.60
54	BA	323	C	O4'-C1'-N1	9.90	116.12	108.20
21	AA	1447	A	N1-C6-N6	-9.88	112.67	118.60
11	AL	30	ARG	NE-CZ-NH1	9.88	125.24	120.30
54	BA	800	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	905	A	N1-C6-N6	-9.88	112.67	118.60
54	BA	1253	A	N1-C6-N6	-9.88	112.67	118.60
22	A1	21	A	N1-C6-N6	-9.87	112.68	118.60
22	A1	41	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	2042	A	N1-C6-N6	-9.87	112.68	118.60
54	BA	2443	C	N3-C2-O2	-9.87	114.99	121.90
21	AA	743	A	N1-C6-N6	-9.86	112.68	118.60
54	BA	1590	A	N1-C6-N6	-9.86	112.69	118.60
54	BA	1077	A	N1-C6-N6	-9.86	112.69	118.60
21	AA	131	A	N1-C6-N6	-9.84	112.69	118.60
21	AA	747	A	N1-C6-N6	-9.84	112.69	118.60
54	BA	404	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	1927	A	N1-C6-N6	-9.84	112.70	118.60
54	BA	1515	A	N1-C6-N6	-9.83	112.70	118.60
54	BA	1580	A	N1-C6-N6	-9.83	112.70	118.60
21	AA	546	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	1759	A	N1-C6-N6	-9.81	112.71	118.60
21	AA	1492	A	N1-C6-N6	-9.81	112.71	118.60
54	BA	2882	A	N1-C6-N6	-9.81	112.72	118.60
21	AA	498	A	N1-C6-N6	-9.81	112.72	118.60
54	BA	2590	A	N1-C6-N6	-9.80	112.72	118.60
21	AA	1136	C	N3-C2-O2	-9.80	115.04	121.90
21	AA	1480	A	N1-C6-N6	-9.80	112.72	118.60
21	AA	389	A	N1-C6-N6	-9.79	112.72	118.60
21	AA	706	A	N1-C6-N6	-9.79	112.72	118.60
54	BA	1378	A	N1-C6-N6	-9.79	112.72	118.60
55	BB	104	A	N1-C6-N6	-9.79	112.73	118.60
21	AA	51	A	N1-C6-N6	-9.78	112.73	118.60
21	AA	1256	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	1785	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	1095	A	N1-C6-N6	-9.78	112.73	118.60
54	BA	429	A	N1-C6-N6	-9.78	112.73	118.60
21	AA	412	A	N1-C6-N6	-9.77	112.74	118.60
54	BA	1943	U	O4'-C1'-N1	9.76	116.01	108.20
54	BA	1085	A	N1-C6-N6	-9.76	112.75	118.60
54	BA	368	A	N1-C6-N6	-9.75	112.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1815	A	N1-C6-N6	-9.75	112.75	118.60
54	BA	443	A	N1-C6-N6	-9.74	112.75	118.60
54	BA	278	A	N1-C6-N6	-9.74	112.75	118.60
54	BA	1080	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	2814	A	N1-C6-N6	-9.74	112.76	118.60
54	BA	2873	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1937	A	N1-C6-N6	-9.73	112.76	118.60
45	BW	19	ARG	NE-CZ-NH1	9.73	125.17	120.30
54	BA	2835	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	2899	A	N1-C6-N6	-9.73	112.76	118.60
54	BA	1630	A	N1-C6-N6	-9.73	112.76	118.60
21	AA	520	A	N1-C6-N6	-9.73	112.76	118.60
21	AA	1280	A	N1-C6-N6	-9.72	112.77	118.60
21	AA	1428	A	N1-C6-N6	-9.72	112.77	118.60
54	BA	1439	A	O4'-C1'-N9	9.72	115.98	108.20
54	BA	1204	A	O4'-C1'-N9	9.72	115.98	108.20
21	AA	819	A	N1-C6-N6	-9.72	112.77	118.60
21	AA	152	A	N1-C6-N6	-9.71	112.77	118.60
21	AA	414	A	N1-C6-N6	-9.71	112.77	118.60
54	BA	1791	A	N1-C6-N6	-9.71	112.78	118.60
54	BA	2741	A	N1-C6-N6	-9.71	112.78	118.60
21	AA	1169	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	49	A	N1-C6-N6	-9.70	112.78	118.60
22	A1	58	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	2682	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	2530	A	N1-C6-N6	-9.70	112.78	118.60
54	BA	1916	A	N1-C6-N6	-9.69	112.78	118.60
54	BA	1469	A	N1-C6-N6	-9.68	112.79	118.60
54	BA	867	C	N3-C2-O2	-9.67	115.13	121.90
21	AA	344	A	N1-C6-N6	-9.67	112.80	118.60
21	AA	975	A	N1-C6-N6	-9.67	112.80	118.60
54	BA	972	A	N1-C6-N6	-9.66	112.81	118.60
21	AA	532	A	N1-C6-N6	-9.65	112.81	118.60
21	AA	397	A	N1-C6-N6	-9.65	112.81	118.60
54	BA	572	A	N1-C6-N6	-9.64	112.81	118.60
55	BB	34	A	N1-C6-N6	-9.64	112.82	118.60
55	BB	94	A	N1-C6-N6	-9.64	112.82	118.60
21	AA	978	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	155	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	941	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	2142	A	N1-C6-N6	-9.63	112.82	118.60
54	BA	526	A	N1-C6-N6	-9.62	112.83	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	499	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	804	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	1808	A	N1-C6-N6	-9.62	112.83	118.60
54	BA	527	C	N3-C2-O2	-9.61	115.17	121.90
54	BA	1009	A	N1-C6-N6	-9.61	112.84	118.60
54	BA	1534	U	O4'-C1'-N1	9.60	115.88	108.20
54	BA	1900	A	N1-C6-N6	-9.60	112.84	118.60
54	BA	1029	A	N1-C6-N6	-9.59	112.84	118.60
54	BA	1420	A	N1-C6-N6	-9.59	112.85	118.60
21	AA	787	A	N1-C6-N6	-9.58	112.85	118.60
55	BB	45	A	N1-C6-N6	-9.58	112.85	118.60
21	AA	572	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1427	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1632	A	N1-C6-N6	-9.57	112.86	118.60
54	BA	1677	A	N1-C6-N6	-9.56	112.86	118.60
21	AA	1250	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	715	A	N1-C6-N6	-9.56	112.87	118.60
54	BA	621	A	N1-C6-N6	-9.55	112.87	118.60
54	BA	382	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	408	A	N1-C6-N6	-9.55	112.87	118.60
21	AA	366	A	N1-C6-N6	-9.54	112.87	118.60
21	AA	873	A	N1-C6-N6	-9.54	112.87	118.60
54	BA	1420	A	O4'-C1'-N9	9.53	115.82	108.20
24	A3	36	A	N1-C6-N6	-9.53	112.88	118.60
54	BA	541	A	N1-C6-N6	-9.53	112.89	118.60
54	BA	213	A	N1-C6-N6	-9.52	112.89	118.60
21	AA	1254	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	751	A	N1-C6-N6	-9.52	112.89	118.60
54	BA	1387	A	N1-C6-N6	-9.51	112.89	118.60
21	AA	60	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	2062	A	N1-C6-N6	-9.51	112.90	118.60
54	BA	1522	A	N1-C6-N6	-9.50	112.90	118.60
55	BB	108	A	N1-C6-N6	-9.50	112.90	118.60
54	BA	845	A	N1-C6-N6	-9.49	112.91	118.60
21	AA	935	A	N1-C6-N6	-9.48	112.91	118.60
21	AA	1216	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	2311	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	1534	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	2101	A	N1-C6-N6	-9.47	112.92	118.60
54	BA	1054	A	N1-C6-N6	-9.47	112.92	118.60
21	AA	872	A	C1'-O4'-C4'	-9.46	102.33	109.90
21	AA	845	A	N1-C6-N6	-9.46	112.93	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	447	A	N1-C6-N6	-9.46	112.93	118.60
21	AA	282	A	N1-C6-N6	-9.46	112.93	118.60
21	AA	1111	A	N1-C6-N6	-9.45	112.93	118.60
21	AA	716	A	N1-C6-N6	-9.45	112.93	118.60
54	BA	2761	A	N1-C6-N6	-9.44	112.93	118.60
21	AA	914	A	N1-C6-N6	-9.44	112.93	118.60
54	BA	1021	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	766	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	1127	A	N1-C6-N6	-9.44	112.94	118.60
54	BA	2298	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	635	A	N1-C6-N6	-9.44	112.94	118.60
21	AA	441	A	N1-C6-N6	-9.43	112.94	118.60
21	AA	687	A	N1-C6-N6	-9.43	112.94	118.60
54	BA	103	A	N1-C6-N6	-9.42	112.95	118.60
21	AA	1150	A	N1-C6-N6	-9.41	112.95	118.60
21	AA	831	A	N1-C6-N6	-9.41	112.95	118.60
54	BA	2169	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	1525	A	N1-C6-N6	-9.40	112.96	118.60
21	AA	629	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	2108	A	N1-C6-N6	-9.40	112.96	118.60
54	BA	2037	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	1314	C	N3-C2-O2	-9.39	115.33	121.90
54	BA	13	A	N1-C6-N6	-9.39	112.97	118.60
54	BA	654	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	706	A	N1-C6-N6	-9.38	112.97	118.60
54	BA	867	C	O4'-C1'-N1	9.37	115.70	108.20
54	BA	833	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	1912	A	N1-C6-N6	-9.37	112.98	118.60
33	BK	71	ARG	NE-CZ-NH1	9.37	124.98	120.30
21	AA	949	A	N1-C6-N6	-9.37	112.98	118.60
54	BA	556	A	N1-C6-N6	-9.37	112.98	118.60
21	AA	1346	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	265	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	231	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	1603	A	N1-C6-N6	-9.35	112.99	118.60
54	BA	1672	A	N1-C6-N6	-9.35	112.99	118.60
13	AN	9	ARG	NE-CZ-NH1	9.34	124.97	120.30
21	AA	155	A	N1-C6-N6	-9.34	112.99	118.60
54	BA	2191	A	N1-C6-N6	-9.34	112.99	118.60
54	BA	1175	A	N1-C6-N6	-9.33	113.00	118.60
21	AA	393	A	N1-C6-N6	-9.32	113.00	118.60
21	AA	816	A	N1-C6-N6	-9.32	113.01	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	560	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	825	A	N1-C6-N6	-9.32	113.01	118.60
21	AA	1105	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	959	A	N1-C6-N6	-9.32	113.01	118.60
54	BA	1618	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	947	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	1503	A	N1-C6-N6	-9.31	113.01	118.60
54	BA	727	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1569	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	160	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	783	A	N1-C6-N6	-9.30	113.02	118.60
54	BA	1847	A	N1-C6-N6	-9.30	113.02	118.60
21	AA	906	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	279	A	N1-C6-N6	-9.29	113.03	118.60
54	BA	1801	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	504	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	2063	C	N3-C2-O2	-9.28	115.40	121.90
47	BY	47	ARG	NE-CZ-NH1	9.28	124.94	120.30
54	BA	1086	A	C5-C6-N1	9.28	122.34	117.70
54	BA	2376	A	N1-C6-N6	-9.28	113.03	118.60
54	BA	825	A	N1-C6-N6	-9.27	113.04	118.60
24	A3	58	A	N1-C6-N6	-9.27	113.04	118.60
54	BA	1255	U	O4'-C1'-N1	9.26	115.61	108.20
54	BA	2799	A	N1-C6-N6	-9.26	113.04	118.60
54	BA	716	A	N1-C6-N6	-9.26	113.04	118.60
21	AA	1275	A	N1-C6-N6	-9.26	113.05	118.60
54	BA	71	A	N1-C6-N6	-9.26	113.05	118.60
54	BA	1275	A	N1-C6-N6	-9.26	113.05	118.60
54	BA	348	A	N1-C6-N6	-9.25	113.05	118.60
22	A1	73	A	N1-C6-N6	-9.25	113.05	118.60
21	AA	1500	A	N1-C6-N6	-9.25	113.05	118.60
40	BR	90	ARG	NE-CZ-NH1	9.24	124.92	120.30
54	BA	1701	A	N1-C6-N6	-9.24	113.05	118.60
54	BA	761	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	1952	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	2439	A	N1-C6-N6	-9.24	113.06	118.60
54	BA	867	C	N1-C2-O2	9.24	124.44	118.90
54	BA	2009	A	N1-C6-N6	-9.24	113.06	118.60
21	AA	274	A	N1-C6-N6	-9.23	113.06	118.60
21	AA	459	A	N1-C6-N6	-9.23	113.06	118.60
54	BA	1545	A	N1-C6-N6	-9.23	113.06	118.60
54	BA	2321	U	O4'-C1'-N1	9.23	115.58	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	496	A	N1-C6-N6	-9.22	113.06	118.60
45	BW	76	ARG	NE-CZ-NH1	9.22	124.91	120.30
21	AA	1431	A	N1-C6-N6	-9.22	113.07	118.60
54	BA	1552	A	N1-C6-N6	-9.22	113.07	118.60
21	AA	1340	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	689	A	N1-C6-N6	-9.21	113.07	118.60
54	BA	889	C	N3-C2-O2	-9.20	115.46	121.90
54	BA	1008	A	N1-C6-N6	-9.20	113.08	118.60
54	BA	1650	A	N1-C6-N6	-9.20	113.08	118.60
9	AJ	9	ARG	NE-CZ-NH1	9.20	124.90	120.30
54	BA	527	C	N1-C2-O2	9.20	124.42	118.90
21	AA	1434	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	503	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	753	A	N1-C6-N6	-9.19	113.08	118.60
54	BA	1977	A	N1-C6-N6	-9.19	113.08	118.60
21	AA	547	A	N1-C6-N6	-9.19	113.09	118.60
54	BA	1654	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1655	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	2059	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1088	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	1268	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	743	A	N1-C6-N6	-9.18	113.09	118.60
54	BA	146	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	207	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1755	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	2565	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1214	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1284	A	N1-C6-N6	-9.17	113.10	118.60
54	BA	1783	A	N1-C6-N6	-9.16	113.11	118.60
54	BA	2433	A	N1-C6-N6	-9.16	113.11	118.60
21	AA	794	A	N1-C6-N6	-9.15	113.11	118.60
55	BB	115	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2173	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2450	A	N1-C6-N6	-9.15	113.11	118.60
21	AA	1170	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	661	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	981	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1143	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	1353	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	2482	A	N1-C6-N6	-9.15	113.11	118.60
54	BA	515	A	N1-C6-N6	-9.14	113.11	118.60
21	AA	994	A	N1-C6-N6	-9.14	113.12	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1333	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	990	A	N1-C6-N6	-9.14	113.12	118.60
40	BR	68	ARG	NE-CZ-NH1	9.14	124.87	120.30
54	BA	1953	A	N1-C6-N6	-9.14	113.12	118.60
54	BA	1502	A	N1-C6-N6	-9.13	113.12	118.60
21	AA	431	A	N1-C6-N6	-9.13	113.12	118.60
37	BO	111	ARG	NE-CZ-NH1	9.13	124.86	120.30
54	BA	280	U	O4'-C1'-N1	9.13	115.50	108.20
54	BA	345	A	N1-C6-N6	-9.12	113.12	118.60
22	A1	74	C	N3-C2-O2	-9.12	115.51	121.90
55	BB	41	G	O4'-C1'-N9	9.12	115.50	108.20
21	AA	1269	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1304	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1490	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	973	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	574	A	N1-C6-N6	-9.12	113.13	118.60
54	BA	1395	A	N1-C6-N6	-9.11	113.13	118.60
54	BA	2015	A	N1-C6-N6	-9.11	113.13	118.60
8	AI	105	ARG	NE-CZ-NH1	9.11	124.85	120.30
54	BA	1803	A	N1-C6-N6	-9.11	113.14	118.60
54	BA	101	A	N1-C6-N6	-9.10	113.14	118.60
21	AA	518	C	N3-C2-O2	-9.10	115.53	121.90
54	BA	2358	A	N1-C6-N6	-9.10	113.14	118.60
17	AR	52	ARG	NE-CZ-NH1	9.09	124.85	120.30
54	BA	936	A	N1-C6-N6	-9.09	113.14	118.60
54	BA	2212	A	N1-C6-N6	-9.09	113.14	118.60
21	AA	415	A	C5-C6-N1	9.09	122.25	117.70
21	AA	1191	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	2335	A	N1-C6-N6	-9.09	113.15	118.60
21	AA	72	A	N1-C6-N6	-9.09	113.15	118.60
54	BA	789	A	N1-C6-N6	-9.08	113.15	118.60
4	AE	68	ARG	NE-CZ-NH1	9.08	124.84	120.30
21	AA	1238	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	422	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	1809	A	N1-C6-N6	-9.08	113.15	118.60
54	BA	1746	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	996	A	N1-C6-N6	-9.07	113.16	118.60
21	AA	8	A	N1-C6-N6	-9.07	113.16	118.60
54	BA	1758	U	O4'-C1'-N1	9.07	115.45	108.20
24	A3	60	A	N1-C6-N6	-9.06	113.16	118.60
32	BJ	13	ARG	NE-CZ-NH1	9.06	124.83	120.30
21	AA	478	A	N1-C6-N6	-9.06	113.17	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2422	C	N3-C2-O2	-9.05	115.56	121.90
54	BA	2266	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	199	A	N1-C6-N6	-9.05	113.17	118.60
54	BA	1700	A	N1-C6-N6	-9.04	113.17	118.60
54	BA	1548	A	N1-C6-N6	-9.04	113.18	118.60
21	AA	195	A	N1-C6-N6	-9.03	113.18	118.60
54	BA	1606	C	O4'-C1'-N1	9.04	115.43	108.20
54	BA	2095	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	607	A	N1-C6-N6	-9.03	113.18	118.60
21	AA	1465	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	78	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	918	A	N1-C6-N6	-9.02	113.19	118.60
54	BA	1169	A	N1-C6-N6	-9.02	113.19	118.60
34	BL	78	ARG	NE-CZ-NH1	9.02	124.81	120.30
54	BA	877	A	N1-C6-N6	-9.02	113.19	118.60
21	AA	119	A	N1-C6-N6	-9.01	113.19	118.60
24	A3	77	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	21	A	N1-C6-N6	-9.01	113.19	118.60
54	BA	2388	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	219	A	N1-C6-N6	-9.00	113.20	118.60
54	BA	1354	A	N1-C6-N6	-9.00	113.20	118.60
56	B5	7	ARG	NE-CZ-NH1	9.00	124.80	120.30
13	AN	13	ARG	NE-CZ-NH1	8.99	124.80	120.30
54	BA	196	A	N1-C6-N6	-8.99	113.20	118.60
54	BA	575	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	171	A	N1-C6-N6	-8.99	113.21	118.60
21	AA	782	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	2071	A	N1-C6-N6	-8.99	113.21	118.60
54	BA	2740	A	C5-C6-N1	8.99	122.19	117.70
21	AA	364	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	1136	C	N1-C2-O2	8.98	124.29	118.90
54	BA	1288	G	O4'-C1'-N9	8.98	115.39	108.20
54	BA	1762	A	N1-C6-N6	-8.98	113.21	118.60
21	AA	371	A	N1-C6-N6	-8.98	113.21	118.60
54	BA	1610	A	N1-C6-N6	-8.98	113.21	118.60
27	BE	162	ARG	NE-CZ-NH1	8.97	124.79	120.30
21	AA	432	A	N1-C6-N6	-8.97	113.22	118.60
21	AA	1493	A	N1-C6-N6	-8.97	113.22	118.60
54	BA	482	A	N1-C6-N6	-8.96	113.22	118.60
54	BA	676	A	N1-C6-N6	-8.96	113.22	118.60
18	AS	35	ARG	NE-CZ-NH1	8.96	124.78	120.30
54	BA	415	A	N1-C6-N6	-8.96	113.23	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	739	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	2407	A	N1-C6-N6	-8.96	113.23	118.60
54	BA	2033	A	N1-C6-N6	-8.95	113.23	118.60
54	BA	2560	A	N1-C6-N6	-8.95	113.23	118.60
21	AA	315	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	227	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	2211	A	C5-C6-N1	8.94	122.17	117.70
54	BA	2868	A	N1-C6-N6	-8.94	113.23	118.60
54	BA	1327	A	N1-C6-N6	-8.94	113.24	118.60
21	AA	1167	A	N1-C6-N6	-8.94	113.24	118.60
54	BA	2346	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	454	A	N1-C6-N6	-8.93	113.24	118.60
54	BA	2727	A	N1-C6-N6	-8.93	113.24	118.60
21	AA	80	A	N1-C6-N6	-8.93	113.25	118.60
54	BA	1821	A	N1-C6-N6	-8.93	113.25	118.60
54	BA	1133	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	1301	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	1664	A	N1-C6-N6	-8.92	113.25	118.60
21	AA	1042	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	2497	A	N1-C6-N6	-8.92	113.25	118.60
54	BA	2825	G	O4'-C1'-N9	8.92	115.33	108.20
21	AA	1225	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	2425	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	1307	A	N1-C6-N6	-8.91	113.25	118.60
54	BA	2516	A	N1-C6-N6	-8.91	113.25	118.60
21	AA	19	A	N1-C6-N6	-8.91	113.26	118.60
21	AA	1377	A	N1-C6-N6	-8.91	113.26	118.60
23	A2	82	A	N1-C6-N6	-8.91	113.26	118.60
54	BA	627	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	721	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	28	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	1322	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2154	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2147	A	N1-C6-N6	-8.90	113.26	118.60
11	AL	55	ARG	NE-CZ-NH1	8.90	124.75	120.30
21	AA	1101	A	N1-C6-N6	-8.90	113.26	118.60
21	AA	1317	C	C1'-O4'-C4'	-8.90	102.78	109.90
54	BA	2587	A	N1-C6-N6	-8.90	113.26	118.60
54	BA	2476	A	N1-C6-N6	-8.89	113.26	118.60
21	AA	1117	A	N1-C6-N6	-8.89	113.27	118.60
54	BA	861	A	N1-C6-N6	-8.89	113.27	118.60
21	AA	1225	A	C5-C6-N1	8.87	122.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1705	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	2227	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1899	A	N1-C6-N6	-8.87	113.28	118.60
21	AA	600	A	N1-C6-N6	-8.86	113.28	118.60
21	AA	1092	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	63	A	N1-C6-N6	-8.87	113.28	118.60
54	BA	1204	A	N1-C6-N6	-8.86	113.28	118.60
54	BA	372	G	O4'-C1'-N9	8.86	115.29	108.20
54	BA	149	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	165	A	N1-C6-N6	-8.85	113.29	118.60
54	BA	1594	U	O4'-C1'-N1	8.85	115.28	108.20
54	BA	2211	A	N1-C6-N6	-8.84	113.29	118.60
55	BB	15	A	O4'-C1'-N9	8.84	115.27	108.20
25	BC	220	ARG	NE-CZ-NH1	8.84	124.72	120.30
54	BA	1508	A	O4'-C1'-N9	8.84	115.27	108.20
54	BA	2270	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	104	A	N1-C6-N6	-8.84	113.30	118.60
54	BA	1272	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	2646	C	N1-C2-O2	8.83	124.20	118.90
54	BA	2660	A	N1-C6-N6	-8.83	113.30	118.60
21	AA	1319	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	1413	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	2198	A	N1-C6-N6	-8.83	113.30	118.60
54	BA	1383	A	N1-C6-N6	-8.82	113.31	118.60
54	BA	2386	A	N1-C6-N6	-8.82	113.31	118.60
21	AA	171	A	C5-C6-N1	8.81	122.11	117.70
54	BA	322	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	479	A	N1-C6-N6	-8.81	113.31	118.60
24	A3	22	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	167	A	N1-C6-N6	-8.81	113.31	118.60
21	AA	919	A	N1-C6-N6	-8.81	113.31	118.60
54	BA	99	U	O4'-C1'-N1	8.81	115.25	108.20
54	BA	5	A	N1-C6-N6	-8.80	113.32	118.60
54	BA	241	A	N1-C6-N6	-8.80	113.32	118.60
21	AA	374	A	N1-C6-N6	-8.80	113.32	118.60
46	BX	2	ARG	NE-CZ-NH1	8.80	124.70	120.30
23	A2	88	U	O4'-C1'-N1	8.80	115.24	108.20
54	BA	191	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	2090	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	2736	A	N1-C6-N6	-8.79	113.32	118.60
54	BA	2171	A	N1-C6-N6	-8.79	113.33	118.60
21	AA	55	A	N1-C6-N6	-8.79	113.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2503	A	N1-C6-N6	-8.79	113.33	118.60
54	BA	2670	A	N1-C6-N6	-8.79	113.33	118.60
1	AB	207	ARG	NE-CZ-NH1	8.78	124.69	120.30
54	BA	2030	A	N1-C6-N6	-8.78	113.33	118.60
21	AA	190	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	878	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2170	A	N1-C6-N6	-8.77	113.34	118.60
21	AA	120	A	N1-C6-N6	-8.77	113.34	118.60
40	BR	13	ARG	NE-CZ-NH1	8.77	124.68	120.30
54	BA	1772	A	N1-C6-N6	-8.77	113.34	118.60
54	BA	2314	A	N1-C6-N6	-8.76	113.34	118.60
28	BF	101	ARG	NE-CZ-NH1	8.76	124.68	120.30
22	A1	69	A	N1-C6-N6	-8.75	113.35	118.60
27	BE	114	ARG	NE-CZ-NH1	8.75	124.68	120.30
54	BA	620	G	O4'-C1'-N9	8.75	115.20	108.20
21	AA	1433	A	N1-C6-N6	-8.74	113.35	118.60
22	A1	6	A	N1-C6-N6	-8.74	113.35	118.60
54	BA	2564	A	N1-C6-N6	-8.74	113.35	118.60
54	BA	2675	A	N1-C6-N6	-8.74	113.36	118.60
54	BA	2453	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	338	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	131	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	1668	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	196	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	723	U	C1'-O4'-C4'	-8.73	102.92	109.90
54	BA	1328	A	N1-C6-N6	-8.73	113.36	118.60
21	AA	74	A	N1-C6-N6	-8.73	113.36	118.60
54	BA	589	U	O4'-C1'-N1	8.73	115.18	108.20
21	AA	1261	A	N1-C6-N6	-8.72	113.36	118.60
54	BA	1262	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	1403	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	1393	A	N1-C6-N6	-8.72	113.37	118.60
54	BA	2821	A	N1-C6-N6	-8.71	113.37	118.60
44	BV	93	ARG	NE-CZ-NH1	8.71	124.66	120.30
54	BA	490	C	N3-C2-O2	-8.71	115.80	121.90
54	BA	1593	A	N1-C6-N6	-8.71	113.37	118.60
21	AA	675	A	N1-C6-N6	-8.71	113.38	118.60
54	BA	371	A	C5-C6-N1	8.71	122.05	117.70
5	AF	91	ARG	NE-CZ-NH1	8.70	124.65	120.30
21	AA	1246	A	N1-C6-N6	-8.70	113.38	118.60
21	AA	1360	A	N1-C6-N6	-8.70	113.38	118.60
54	BA	472	A	N1-C6-N6	-8.70	113.38	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2711	A	N1-C6-N6	-8.69	113.38	118.60
23	A2	79	A	N1-C6-N6	-8.69	113.38	118.60
54	BA	2800	A	N1-C6-N6	-8.69	113.39	118.60
21	AA	1359	C	N3-C2-O2	-8.69	115.82	121.90
21	AA	872	A	O4'-C1'-N9	8.69	115.15	108.20
21	AA	1398	A	N1-C6-N6	-8.69	113.39	118.60
54	BA	1634	A	C5-C6-N1	8.68	122.04	117.70
21	AA	559	A	O4'-C1'-N9	8.68	115.14	108.20
54	BA	637	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	2850	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1936	A	N1-C6-N6	-8.68	113.39	118.60
54	BA	1155	A	N1-C6-N6	-8.68	113.39	118.60
21	AA	802	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1365	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	111	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	1885	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	2003	A	N1-C6-N6	-8.67	113.40	118.60
54	BA	2225	A	N1-C6-N6	-8.67	113.40	118.60
21	AA	1080	A	N1-C6-N6	-8.66	113.40	118.60
54	BA	2893	A	N1-C6-N6	-8.66	113.41	118.60
54	BA	332	A	N1-C6-N6	-8.66	113.41	118.60
21	AA	807	A	N1-C6-N6	-8.65	113.41	118.60
54	BA	888	C	O4'-C1'-N1	8.65	115.12	108.20
24	A3	74	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	44	A	N1-C6-N6	-8.64	113.41	118.60
54	BA	603	A	N1-C6-N6	-8.64	113.42	118.60
21	AA	161	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	1591	A	N1-C6-N6	-8.64	113.42	118.60
54	BA	346	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	1532	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	2092	U	O4'-C1'-N1	8.63	115.11	108.20
21	AA	1227	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	927	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	1285	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	509	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	554	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	52	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	460	A	N1-C6-N6	-8.63	113.42	118.60
21	AA	908	A	N1-C6-N6	-8.62	113.42	118.60
24	A3	45	A	N1-C6-N6	-8.62	113.42	118.60
54	BA	181	A	N1-C6-N6	-8.63	113.42	118.60
54	BA	1854	A	N1-C6-N6	-8.62	113.43	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2778	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	2860	A	N1-C6-N6	-8.62	113.42	118.60
54	BA	2158	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	1566	A	N1-C6-N6	-8.62	113.43	118.60
54	BA	574	A	C5-C6-N1	8.61	122.01	117.70
54	BA	1147	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	2468	A	N1-C6-N6	-8.61	113.43	118.60
54	BA	2435	A	N1-C6-N6	-8.61	113.43	118.60
21	AA	321	A	N1-C6-N6	-8.61	113.44	118.60
24	A3	11	A	N1-C6-N6	-8.61	113.44	118.60
54	BA	83	A	N1-C6-N6	-8.61	113.44	118.60
21	AA	958	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	23	G	O4'-C1'-N9	8.60	115.08	108.20
54	BA	982	C	N1-C2-O2	8.60	124.06	118.90
21	AA	790	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	89	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	167	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1679	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1858	A	N1-C6-N6	-8.60	113.44	118.60
54	BA	1932	A	C4-C5-C6	-8.60	112.70	117.00
21	AA	579	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	844	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	1134	A	N1-C6-N6	-8.59	113.44	118.60
54	BA	1749	A	N1-C6-N6	-8.59	113.44	118.60
36	BN	69	ARG	NE-CZ-NH1	8.59	124.59	120.30
54	BA	2602	A	N1-C6-N6	-8.59	113.45	118.60
28	BF	109	ARG	NE-CZ-NH1	8.59	124.59	120.30
21	AA	461	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	1535	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	1020	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	508	A	N1-C6-N6	-8.58	113.45	118.60
54	BA	614	A	N1-C6-N6	-8.57	113.45	118.60
21	AA	1155	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	616	A	C5-C6-N1	8.57	121.98	117.70
34	BL	48	ARG	NE-CZ-NH1	8.57	124.58	120.30
54	BA	1637	A	N1-C6-N6	-8.57	113.46	118.60
54	BA	982	C	N3-C2-O2	-8.56	115.91	121.90
21	AA	938	A	N1-C6-N6	-8.56	113.46	118.60
24	A3	35	C	N3-C2-O2	-8.56	115.91	121.90
54	BA	2287	A	N1-C6-N6	-8.56	113.46	118.60
34	BL	126	ARG	NE-CZ-NH1	8.56	124.58	120.30
21	AA	77	A	N1-C6-N6	-8.56	113.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	988	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	1067	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	1531	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	1205	A	N1-C6-N6	-8.55	113.47	118.60
54	BA	2750	A	N1-C6-N6	-8.55	113.47	118.60
24	A3	73	A	N1-C6-N6	-8.55	113.47	118.60
21	AA	71	A	N1-C6-N6	-8.54	113.47	118.60
22	A1	66	A	N1-C6-N6	-8.54	113.47	118.60
54	BA	666	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	729	A	N1-C6-N6	-8.54	113.48	118.60
21	AA	1044	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	975	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	1254	A	N1-C6-N6	-8.53	113.48	118.60
21	AA	109	A	N1-C6-N6	-8.53	113.48	118.60
54	BA	197	A	N1-C6-N6	-8.53	113.48	118.60
16	AQ	76	ARG	NE-CZ-NH1	8.52	124.56	120.30
21	AA	665	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	704	A	C5-C6-N1	8.52	121.96	117.70
21	AA	1329	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	768	A	N1-C6-N6	-8.52	113.49	118.60
54	BA	272	A	N1-C6-N6	-8.52	113.49	118.60
21	AA	465	A	N1-C6-N6	-8.51	113.50	118.60
21	AA	1507	A	N1-C6-N6	-8.51	113.50	118.60
54	BA	975	A	C5-C6-N1	8.51	121.95	117.70
54	BA	1754	A	N1-C6-N6	-8.51	113.50	118.60
21	AA	1204	A	N1-C6-N6	-8.50	113.50	118.60
54	BA	330	A	N1-C6-N6	-8.50	113.50	118.60
15	AP	25	ARG	NE-CZ-NH1	8.50	124.55	120.30
18	AS	80	ARG	NE-CZ-NH1	8.49	124.55	120.30
21	AA	1031	C	N3-C2-O2	-8.49	115.95	121.90
54	BA	2054	A	N1-C6-N6	-8.49	113.50	118.60
21	AA	749	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	730	A	N1-C6-N6	-8.49	113.51	118.60
21	AA	487	A	N1-C6-N6	-8.49	113.51	118.60
54	BA	2741	A	C5-C6-N1	8.48	121.94	117.70
21	AA	1197	A	N1-C6-N6	-8.48	113.51	118.60
54	BA	2135	A	N1-C6-N6	-8.48	113.51	118.60
21	AA	814	A	N1-C6-N6	-8.47	113.52	118.60
21	AA	969	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	2679	A	N1-C6-N6	-8.47	113.52	118.60
54	BA	2439	A	C5-C6-N1	8.47	121.93	117.70
54	BA	299	A	N1-C6-N6	-8.46	113.52	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	493	A	C5-C6-N1	8.46	121.93	117.70
21	AA	1014	A	C5-C6-N1	8.46	121.93	117.70
21	AA	1152	A	N1-C6-N6	-8.46	113.53	118.60
21	AA	1456	A	N1-C6-N6	-8.46	113.53	118.60
54	BA	71	A	C5-C6-N1	8.45	121.93	117.70
54	BA	2412	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2322	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	2411	A	C5-C6-N1	8.45	121.92	117.70
21	AA	214	C	N3-C2-O2	-8.45	115.99	121.90
21	AA	815	A	N1-C6-N6	-8.45	113.53	118.60
54	BA	1784	A	N1-C6-N6	-8.44	113.53	118.60
21	AA	1236	A	C5-C6-N1	8.44	121.92	117.70
21	AA	530	G	C1'-O4'-C4'	-8.43	103.15	109.90
54	BA	2443	C	N1-C2-O2	8.43	123.96	118.90
54	BA	311	A	C4-C5-C6	-8.43	112.79	117.00
54	BA	590	A	N1-C6-N6	-8.43	113.54	118.60
54	BA	1451	C	N3-C2-O2	-8.43	116.00	121.90
54	BA	2700	A	N1-C6-N6	-8.43	113.54	118.60
42	BT	3	ARG	NE-CZ-NH1	8.43	124.51	120.30
54	BA	1010	A	N1-C6-N6	-8.43	113.54	118.60
2	AC	10	ARG	NE-CZ-NH1	8.42	124.51	120.30
54	BA	599	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	1501	C	N3-C2-O2	-8.42	116.00	121.90
21	AA	1046	A	N1-C6-N6	-8.42	113.55	118.60
34	BL	59	ARG	NE-CZ-NH1	8.42	124.51	120.30
54	BA	94	A	N1-C6-N6	-8.42	113.55	118.60
54	BA	693	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	120	A	C5-C6-N1	8.42	121.91	117.70
21	AA	1151	A	N1-C6-N6	-8.42	113.55	118.60
21	AA	306	A	C5-C6-N1	8.41	121.91	117.70
21	AA	1229	A	N1-C6-N6	-8.41	113.55	118.60
54	BA	505	A	N1-C6-N6	-8.41	113.55	118.60
21	AA	382	A	N1-C6-N6	-8.41	113.56	118.60
21	AA	1101	A	C5-C6-N1	8.41	121.90	117.70
44	BV	19	ARG	NE-CZ-NH1	8.41	124.50	120.30
54	BA	582	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	1745	A	N1-C6-N6	-8.41	113.56	118.60
54	BA	2541	A	N1-C6-N6	-8.41	113.56	118.60
55	BB	15	A	C5-C6-N1	8.41	121.90	117.70
54	BA	917	A	N1-C6-N6	-8.40	113.56	118.60
54	BA	2030	A	O4'-C1'-N9	8.40	114.92	108.20
54	BA	750	A	N1-C6-N6	-8.40	113.56	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2020	A	C5-C6-N1	8.40	121.90	117.70
54	BA	2654	A	C5-C6-N1	8.40	121.90	117.70
21	AA	356	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	1981	A	C5-C6-N1	8.39	121.90	117.70
54	BA	2503	A	C5-C6-N1	8.39	121.90	117.70
54	BA	152	A	N1-C6-N6	-8.39	113.56	118.60
54	BA	2070	A	N1-C6-N6	-8.39	113.57	118.60
21	AA	1285	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	2411	A	N1-C6-N6	-8.39	113.57	118.60
54	BA	2628	C	N3-C2-O2	-8.38	116.03	121.90
55	BB	66	A	C5-C6-N1	8.39	121.89	117.70
18	AS	31	ARG	NE-CZ-NH1	8.38	124.49	120.30
54	BA	1606	C	N3-C2-O2	-8.38	116.03	121.90
54	BA	1096	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	1194	A	N1-C6-N6	-8.38	113.57	118.60
54	BA	347	A	N1-C6-N6	-8.38	113.58	118.60
18	AS	54	ARG	NE-CZ-NH1	8.37	124.49	120.30
21	AA	946	A	N1-C6-N6	-8.38	113.58	118.60
54	BA	2055	C	N3-C2-O2	-8.38	116.04	121.90
54	BA	2469	A	N1-C6-N6	-8.37	113.58	118.60
24	A3	76	C	N3-C2-O2	-8.37	116.04	121.90
54	BA	528	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	2666	C	N3-C2-O2	-8.37	116.04	121.90
54	BA	2740	A	N1-C6-N6	-8.37	113.58	118.60
54	BA	1929	G	O4'-C1'-N9	8.36	114.89	108.20
21	AA	253	A	N1-C6-N6	-8.36	113.58	118.60
48	BZ	15	ARG	NE-CZ-NH1	8.36	124.48	120.30
35	BM	59	ARG	NE-CZ-NH1	8.36	124.48	120.30
54	BA	118	A	N1-C6-N6	-8.36	113.58	118.60
54	BA	2392	A	N1-C6-N6	-8.36	113.58	118.60
24	A3	14	A	N1-C6-N6	-8.36	113.58	118.60
21	AA	1311	A	N1-C6-N6	-8.35	113.59	118.60
24	A3	59	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	1453	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	303	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1201	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1362	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1196	A	N1-C6-N6	-8.35	113.59	118.60
21	AA	1446	A	N1-C6-N6	-8.35	113.59	118.60
54	BA	1085	A	C5-C6-N1	8.35	121.87	117.70
54	BA	2778	A	C5-C6-N1	8.34	121.87	117.70
54	BA	1928	A	N1-C6-N6	-8.34	113.60	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	50	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1241	A	N1-C6-N6	-8.33	113.60	118.60
54	BA	1130	U	O4'-C1'-N1	8.33	114.87	108.20
54	BA	2468	A	C5-C6-N1	8.33	121.86	117.70
54	BA	2518	A	C5-C6-N1	8.33	121.86	117.70
54	BA	2014	A	N1-C6-N6	-8.32	113.61	118.60
54	BA	344	A	N1-C6-N6	-8.32	113.61	118.60
21	AA	702	A	N1-C6-N6	-8.32	113.61	118.60
32	BJ	35	ARG	NE-CZ-NH1	8.32	124.46	120.30
54	BA	1586	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	2721	A	N1-C6-N6	-8.31	113.61	118.60
54	BA	453	A	N1-C6-N6	-8.31	113.62	118.60
54	BA	1005	C	N3-C2-O2	-8.31	116.08	121.90
21	AA	228	A	N1-C6-N6	-8.30	113.62	118.60
1	AB	62	ARG	NE-CZ-NH1	8.29	124.45	120.30
54	BA	613	A	C5-C6-N1	8.29	121.85	117.70
55	BB	66	A	N1-C6-N6	-8.29	113.62	118.60
54	BA	1336	A	C5-C6-N1	8.28	121.84	117.70
54	BA	1423	G	O4'-C1'-N9	8.29	114.83	108.20
21	AA	523	A	N1-C6-N6	-8.28	113.64	118.60
54	BA	196	A	C5-C6-N1	8.28	121.84	117.70
54	BA	6	A	N1-C6-N6	-8.27	113.64	118.60
54	BA	204	A	C5-C6-N1	8.27	121.83	117.70
3	AD	72	ARG	NE-CZ-NH1	8.27	124.43	120.30
54	BA	1019	U	O4'-C1'-N1	8.27	114.81	108.20
55	BB	73	A	N1-C6-N6	-8.27	113.64	118.60
46	BX	17	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	222	A	C5-C6-N1	8.26	121.83	117.70
54	BA	2432	A	C5-C6-N1	8.26	121.83	117.70
19	AT	9	ARG	NE-CZ-NH1	8.26	124.43	120.30
54	BA	2327	A	N1-C6-N6	-8.26	113.65	118.60
54	BA	2051	A	N1-C6-N6	-8.25	113.65	118.60
13	AN	59	ARG	NE-CZ-NH1	8.25	124.42	120.30
21	AA	1288	A	N1-C6-N6	-8.25	113.65	118.60
54	BA	2542	A	C5-C6-N1	8.25	121.82	117.70
21	AA	199	A	C5-C6-N1	8.24	121.82	117.70
21	AA	499	A	C5-C6-N1	8.24	121.82	117.70
54	BA	1317	G	O4'-C1'-N9	8.24	114.80	108.20
54	BA	1876	A	N1-C6-N6	-8.24	113.66	118.60
54	BA	1970	A	N1-C6-N6	-8.24	113.65	118.60
54	BA	2879	A	N1-C6-N6	-8.24	113.66	118.60
21	AA	1251	A	N1-C6-N6	-8.24	113.66	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2171	A	C5-C6-N1	8.24	121.82	117.70
54	BA	984	A	O4'-C1'-N9	8.23	114.79	108.20
54	BA	2114	A	N1-C6-N6	-8.23	113.66	118.60
19	AT	17	ARG	NE-CZ-NH1	8.23	124.42	120.30
24	A3	3	C	N3-C2-O2	-8.23	116.14	121.90
54	BA	2765	A	C5-C6-N1	8.23	121.82	117.70
54	BA	2430	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	712	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2317	A	N1-C6-N6	-8.23	113.66	118.60
54	BA	2471	A	N1-C6-N6	-8.23	113.66	118.60
21	AA	223	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	466	A	C5-C6-N1	8.22	121.81	117.70
54	BA	1073	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	356	A	C5-C6-N1	8.22	121.81	117.70
21	AA	1022	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	1110	A	N1-C6-N6	-8.22	113.67	118.60
21	AA	631	C	N3-C2-O2	-8.22	116.15	121.90
54	BA	2082	A	N1-C6-N6	-8.21	113.67	118.60
21	AA	728	A	C5-C6-N1	8.21	121.80	117.70
34	BL	33	ARG	NE-CZ-NH1	8.21	124.40	120.30
6	AG	108	ARG	NE-CZ-NH1	8.20	124.40	120.30
54	BA	1040	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	182	A	N1-C6-N6	-8.20	113.68	118.60
21	AA	621	A	N1-C6-N6	-8.20	113.68	118.60
54	BA	1730	C	N3-C2-O2	-8.20	116.16	121.90
21	AA	1429	A	N1-C6-N6	-8.19	113.69	118.60
54	BA	866	A	C5-C6-N1	8.19	121.79	117.70
30	BH	123	ARG	NE-CZ-NH1	8.18	124.39	120.30
54	BA	2129	C	N3-C2-O2	-8.18	116.18	121.90
21	AA	1413	A	N1-C6-N6	-8.18	113.69	118.60
54	BA	1253	A	C5-C6-N1	8.18	121.79	117.70
54	BA	2614	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	592	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	1664	A	C5-C6-N1	8.17	121.78	117.70
54	BA	2025	C	N3-C2-O2	-8.17	116.18	121.90
22	A1	26	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	19	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	675	A	N1-C6-N6	-8.17	113.70	118.60
54	BA	2433	A	C5-C6-N1	8.17	121.78	117.70
21	AA	327	A	C4-C5-C6	-8.16	112.92	117.00
44	BV	9	ARG	NE-CZ-NH1	8.16	124.38	120.30
21	AA	728	A	C4-C5-C6	-8.16	112.92	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	532	A	N1-C6-N6	-8.16	113.71	118.60
54	BA	1967	C	O4'-C1'-N1	8.16	114.72	108.20
21	AA	1519	A	N1-C6-N6	-8.15	113.71	118.60
24	A3	11	A	C5-C6-N1	8.15	121.78	117.70
54	BA	474	G	O4'-C1'-N9	8.15	114.72	108.20
54	BA	1571	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	327	A	C5-C6-N1	8.15	121.77	117.70
54	BA	1379	U	O3'-P-O5'	-8.15	88.52	104.00
54	BA	1829	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	2031	A	N1-C6-N6	-8.15	113.71	118.60
54	BA	2451	A	N1-C6-N6	-8.15	113.71	118.60
55	BB	39	A	N1-C6-N6	-8.15	113.71	118.60
21	AA	1016	A	N1-C6-N6	-8.14	113.72	118.60
54	BA	453	A	C5-C6-N1	8.13	121.77	117.70
54	BA	2639	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	649	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	915	A	N1-C6-N6	-8.13	113.72	118.60
23	A2	91	A	C5-C6-N1	8.13	121.77	117.70
24	A3	38	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	60	A	C5-C6-N1	8.13	121.76	117.70
21	AA	1324	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	718	A	N1-C6-N6	-8.13	113.72	118.60
54	BA	1597	A	N1-C6-N6	-8.13	113.72	118.60
21	AA	1289	A	C5-C6-N1	8.12	121.76	117.70
54	BA	1678	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1819	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1888	G	O4'-C1'-N9	8.12	114.70	108.20
54	BA	609	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	752	A	N1-C6-N6	-8.12	113.73	118.60
54	BA	1847	A	C5-C6-N1	8.12	121.76	117.70
37	BO	7	ARG	NE-CZ-NH1	8.12	124.36	120.30
21	AA	1499	A	N1-C6-N6	-8.11	113.73	118.60
54	BA	2765	A	N1-C6-N6	-8.12	113.73	118.60
21	AA	602	A	N1-C6-N6	-8.11	113.73	118.60
21	AA	32	A	N1-C6-N6	-8.11	113.74	118.60
21	AA	1493	A	C5-C6-N1	8.10	121.75	117.70
54	BA	466	A	N1-C6-N6	-8.10	113.74	118.60
21	AA	98	A	N1-C6-N6	-8.10	113.74	118.60
13	AN	63	ARG	NE-CZ-NH1	8.10	124.35	120.30
21	AA	608	A	C5-C6-N1	8.10	121.75	117.70
54	BA	896	A	N1-C6-N6	-8.10	113.74	118.60
55	BB	52	A	N1-C6-N6	-8.09	113.74	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1238	A	C5-C6-N1	8.09	121.75	117.70
3	AD	127	ARG	NE-CZ-NH1	8.09	124.34	120.30
21	AA	320	A	C4-C5-C6	-8.09	112.96	117.00
22	A1	14	A	N1-C6-N6	-8.09	113.75	118.60
46	BX	2	ARG	NE-CZ-NH2	-8.09	116.26	120.30
54	BA	710	U	O4'-C1'-N1	8.08	114.67	108.20
21	AA	974	A	N1-C6-N6	-8.08	113.75	118.60
8	AI	17	ARG	NE-CZ-NH1	8.08	124.34	120.30
21	AA	1229	A	C1'-O4'-C4'	-8.08	103.44	109.90
54	BA	195	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	1021	A	N1-C6-N6	-8.08	113.75	118.60
21	AA	1518	A	N1-C6-N6	-8.07	113.76	118.60
23	A2	79	A	C5-C6-N1	8.07	121.74	117.70
54	BA	311	A	C5-C6-N1	8.07	121.73	117.70
54	BA	1494	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	1230	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	1889	A	N1-C6-N6	-8.07	113.76	118.60
54	BA	131	A	C5-C6-N1	8.06	121.73	117.70
54	BA	2266	A	C5-C6-N1	8.06	121.73	117.70
54	BA	2667	C	N3-C2-O2	-8.06	116.26	121.90
28	BF	91	ARG	NE-CZ-NH1	8.06	124.33	120.30
21	AA	250	A	N1-C6-N6	-8.06	113.76	118.60
54	BA	1962	C	N3-C2-O2	-8.05	116.26	121.90
54	BA	216	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	2377	A	N1-C6-N6	-8.05	113.77	118.60
55	BB	29	A	N1-C6-N6	-8.05	113.77	118.60
21	AA	937	A	N1-C6-N6	-8.05	113.77	118.60
54	BA	984	A	N1-C6-N6	-8.05	113.77	118.60
15	AP	31	ARG	NE-CZ-NH1	8.05	124.32	120.30
21	AA	279	A	C5-C6-N1	8.05	121.72	117.70
5	AF	79	ARG	NE-CZ-NH1	8.04	124.32	120.30
54	BA	362	A	C5-C6-N1	8.04	121.72	117.70
54	BA	2459	A	C5-C6-N1	8.05	121.72	117.70
54	BA	2734	A	C5-C6-N1	8.04	121.72	117.70
54	BA	1932	A	C5-C6-N1	8.04	121.72	117.70
54	BA	477	A	N1-C6-N6	-8.04	113.78	118.60
54	BA	2376	A	C5-C6-N1	8.04	121.72	117.70
2	AC	142	ARG	NE-CZ-NH1	8.03	124.31	120.30
52	B3	44	ARG	NE-CZ-NH1	8.03	124.31	120.30
54	BA	1393	A	C5-C6-N1	8.03	121.71	117.70
54	BA	1451	C	N1-C2-O2	8.03	123.72	118.90
54	BA	2758	A	N1-C6-N6	-8.03	113.78	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	547	A	C5-C6-N1	8.03	121.71	117.70
54	BA	655	A	N1-C6-N6	-8.03	113.78	118.60
54	BA	961	C	N3-C2-O2	-8.03	116.28	121.90
21	AA	470	C	N3-C2-O2	-8.02	116.28	121.90
21	AA	493	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	1644	C	O4'-C1'-N1	8.02	114.62	108.20
54	BA	2007	U	O4'-C1'-N1	8.02	114.62	108.20
3	AD	187	ARG	NE-CZ-NH1	8.02	124.31	120.30
21	AA	983	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	2872	A	N1-C6-N6	-8.02	113.79	118.60
54	BA	443	A	C5-C6-N1	8.01	121.71	117.70
54	BA	1677	A	C5-C6-N1	8.01	121.71	117.70
21	AA	574	A	N1-C6-N6	-8.01	113.80	118.60
55	BB	59	A	N1-C6-N6	-8.01	113.79	118.60
8	AI	98	ARG	NE-CZ-NH1	8.01	124.30	120.30
21	AA	250	A	C5-C6-N1	8.01	121.70	117.70
21	AA	1035	A	N1-C6-N6	-8.01	113.80	118.60
22	A1	58	A	C5-C6-N1	8.01	121.70	117.70
54	BA	718	A	C5-C6-N1	8.01	121.70	117.70
26	BD	13	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	282	A	N1-C6-N6	-8.00	113.80	118.60
21	AA	189	A	C5-C6-N1	8.00	121.70	117.70
25	BC	86	ARG	NE-CZ-NH1	8.00	124.30	120.30
54	BA	1978	A	N1-C6-N6	-8.00	113.80	118.60
54	BA	2776	A	C5-C6-N1	8.00	121.70	117.70
54	BA	14	A	C5-C6-N1	7.99	121.70	117.70
54	BA	1523	U	O4'-C1'-N1	7.99	114.59	108.20
17	AR	42	ARG	NE-CZ-NH1	7.99	124.30	120.30
54	BA	2270	A	C5-C6-N1	7.99	121.69	117.70
21	AA	1446	A	C5-C6-N1	7.99	121.69	117.70
54	BA	633	A	C5-C6-N1	7.98	121.69	117.70
54	BA	1384	A	N1-C6-N6	-7.98	113.81	118.60
55	BB	57	A	C5-C6-N1	7.97	121.69	117.70
54	BA	176	A	N1-C6-N6	-7.97	113.82	118.60
54	BA	1952	A	C5-C6-N1	7.97	121.69	117.70
54	BA	1672	A	C5-C6-N1	7.97	121.68	117.70
54	BA	457	A	N1-C6-N6	-7.96	113.82	118.60
21	AA	414	A	C5-C6-N1	7.96	121.68	117.70
54	BA	1045	C	N3-C2-O2	-7.96	116.33	121.90
54	BA	1383	A	C5-C6-N1	7.96	121.68	117.70
3	AD	183	ARG	NE-CZ-NH1	7.96	124.28	120.30
21	AA	152	A	C5-C6-N1	7.96	121.68	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	863	A	C5-C6-N1	7.96	121.68	117.70
41	BS	25	ARG	NE-CZ-NH1	7.95	124.28	120.30
54	BA	218	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	263	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	270	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	238	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	977	A	C5-C6-N1	7.95	121.67	117.70
54	BA	1451	C	O4'-C1'-N1	7.95	114.56	108.20
54	BA	1786	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	2381	A	N1-C6-N6	-7.95	113.83	118.60
54	BA	91	A	C5-C6-N1	7.95	121.67	117.70
54	BA	643	A	N1-C6-N6	-7.95	113.83	118.60
21	AA	630	A	C5-C6-N1	7.94	121.67	117.70
21	AA	901	A	N1-C6-N6	-7.94	113.83	118.60
54	BA	223	A	C5-C6-N1	7.94	121.67	117.70
54	BA	2835	A	C5-C6-N1	7.94	121.67	117.70
54	BA	1570	A	N1-C6-N6	-7.94	113.84	118.60
33	BK	30	ARG	NE-CZ-NH1	7.94	124.27	120.30
21	AA	621	A	C5-C6-N1	7.94	121.67	117.70
21	AA	1350	A	N1-C6-N6	-7.94	113.84	118.60
54	BA	1899	A	C5-C6-N1	7.94	121.67	117.70
21	AA	780	A	C5-C6-N1	7.93	121.67	117.70
54	BA	2725	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1029	A	C5-C6-N1	7.93	121.67	117.70
54	BA	941	A	C5-C6-N1	7.93	121.67	117.70
54	BA	2675	A	C5-C6-N1	7.93	121.67	117.70
21	AA	101	A	C5-C6-N1	7.93	121.67	117.70
24	A3	60	A	C5-C6-N1	7.93	121.66	117.70
21	AA	959	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1204	A	C5-C6-N1	7.93	121.66	117.70
54	BA	1607	C	N3-C2-O2	-7.93	116.35	121.90
21	AA	236	A	N1-C6-N6	-7.93	113.84	118.60
54	BA	1652	A	N1-C6-N6	-7.92	113.84	118.60
54	BA	2572	A	C5-C6-N1	7.92	121.66	117.70
21	AA	611	C	N3-C2-O2	-7.92	116.36	121.90
54	BA	161	A	N1-C6-N6	-7.92	113.85	118.60
54	BA	679	C	O4'-C1'-N1	7.92	114.53	108.20
21	AA	811	C	N3-C2-O2	-7.91	116.36	121.90
21	AA	909	A	C5-C6-N1	7.91	121.66	117.70
54	BA	2513	A	C5-C6-N1	7.91	121.66	117.70
54	BA	320	A	N1-C6-N6	-7.91	113.85	118.60
21	AA	172	A	C5-C6-N1	7.91	121.66	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1382	C	N3-C2-O2	-7.91	116.36	121.90
54	BA	337	C	N3-C2-O2	-7.91	116.36	121.90
54	BA	1669	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	2513	A	N1-C6-N6	-7.91	113.86	118.60
54	BA	497	A	C5-C6-N1	7.91	121.65	117.70
21	AA	1318	A	N1-C6-N6	-7.91	113.86	118.60
21	AA	865	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	2340	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	1998	A	N1-C6-N6	-7.90	113.86	118.60
21	AA	1531	A	C5-C6-N1	7.90	121.65	117.70
54	BA	28	A	N1-C6-N6	-7.90	113.86	118.60
54	BA	310	A	N1-C6-N6	-7.90	113.86	118.60
13	AN	90	ARG	NE-CZ-NH1	7.90	124.25	120.30
54	BA	2311	A	C5-C6-N1	7.90	121.65	117.70
54	BA	309	A	C5-C6-N1	7.89	121.65	117.70
21	AA	1332	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	173	A	N1-C6-N6	-7.89	113.86	118.60
54	BA	1646	C	N3-C2-O2	-7.89	116.38	121.90
54	BA	1431	A	N1-C6-N6	-7.89	113.86	118.60
21	AA	1217	C	N3-C2-O2	-7.89	116.38	121.90
54	BA	2284	A	N1-C6-N6	-7.89	113.87	118.60
21	AA	1261	A	C5-C6-N1	7.89	121.64	117.70
54	BA	900	A	C5-C6-N1	7.89	121.64	117.70
21	AA	559	A	C5-C6-N1	7.89	121.64	117.70
54	BA	2887	A	C5-C6-N1	7.89	121.64	117.70
54	BA	1054	A	C4-C5-C6	-7.88	113.06	117.00
54	BA	127	A	N1-C6-N6	-7.88	113.87	118.60
54	BA	1275	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1509	A	C5-C6-N1	7.88	121.64	117.70
54	BA	789	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1028	A	C5-C6-N1	7.88	121.64	117.70
54	BA	1247	A	N1-C6-N6	-7.88	113.88	118.60
21	AA	151	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	754	C	N3-C2-O2	-7.87	116.39	121.90
54	BA	323	C	N3-C2-O2	-7.87	116.39	121.90
54	BA	2418	A	C5-C6-N1	7.87	121.64	117.70
21	AA	478	A	C5-C6-N1	7.87	121.64	117.70
54	BA	233	A	C5-C6-N1	7.87	121.64	117.70
54	BA	2572	A	O4'-C1'-N9	7.87	114.50	108.20
54	BA	1953	A	C5-C6-N1	7.87	121.64	117.70
21	AA	33	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	746	A	C5-C6-N1	7.87	121.63	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	936	C	N3-C2-O2	-7.87	116.39	121.90
21	AA	1014	A	N1-C6-N6	-7.87	113.88	118.60
55	BB	109	A	C5-C6-N1	7.87	121.64	117.70
54	BA	1264	A	N1-C6-N6	-7.87	113.88	118.60
21	AA	913	A	P-O3'-C3'	7.87	129.14	119.70
54	BA	156	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	764	A	N1-C6-N6	-7.87	113.88	118.60
54	BA	2189	U	O4'-C1'-N1	7.87	114.49	108.20
54	BA	2358	A	C5-C6-N1	7.87	121.63	117.70
8	AI	10	ARG	NE-CZ-NH1	7.86	124.23	120.30
21	AA	495	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	217	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	300	A	N1-C6-N6	-7.86	113.88	118.60
21	AA	1349	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	397	U	O4'-C1'-N1	7.86	114.49	108.20
54	BA	1634	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	1735	A	N1-C6-N6	-7.86	113.88	118.60
54	BA	2425	A	C5-C6-N1	7.86	121.63	117.70
21	AA	28	A	C5-C6-N1	7.86	121.63	117.70
54	BA	1535	A	C5-C6-N1	7.86	121.63	117.70
54	BA	2665	A	N1-C6-N6	-7.86	113.89	118.60
21	AA	1004	A	C5-C6-N1	7.86	121.63	117.70
21	AA	1374	A	C5-C6-N1	7.85	121.63	117.70
54	BA	342	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	670	A	C5-C6-N1	7.85	121.63	117.70
55	BB	46	A	N1-C6-N6	-7.85	113.89	118.60
21	AA	1500	A	C5-C6-N1	7.85	121.63	117.70
54	BA	1089	A	C5-C6-N1	7.85	121.62	117.70
21	AA	498	A	C5-C6-N1	7.85	121.62	117.70
54	BA	626	A	N1-C6-N6	-7.85	113.89	118.60
54	BA	2030	A	C5-C6-N1	7.85	121.62	117.70
21	AA	935	A	C5-C6-N1	7.84	121.62	117.70
54	BA	668	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	734	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	892	A	N1-C6-N6	-7.84	113.89	118.60
54	BA	1265	A	N1-C6-N6	-7.84	113.89	118.60
21	AA	630	A	N1-C6-N6	-7.84	113.90	118.60
54	BA	705	A	C5-C6-N1	7.84	121.62	117.70
21	AA	448	A	C5-C6-N1	7.84	121.62	117.70
21	AA	573	A	C5-C6-N1	7.84	121.62	117.70
56	B5	9	ARG	NE-CZ-NH1	7.84	124.22	120.30
37	BO	94	ARG	NE-CZ-NH1	7.83	124.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	373	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	759	A	N1-C6-N6	-7.83	113.90	118.60
21	AA	1158	C	N3-C2-O2	-7.83	116.42	121.90
1	AB	73	ARG	NE-CZ-NH1	7.83	124.22	120.30
54	BA	241	A	C5-C6-N1	7.83	121.61	117.70
21	AA	913	A	C5-C6-N1	7.83	121.61	117.70
54	BA	144	A	N1-C6-N6	-7.83	113.90	118.60
54	BA	990	A	C5-C6-N1	7.83	121.61	117.70
54	BA	793	A	C5-C6-N1	7.83	121.61	117.70
54	BA	1735	A	C5-C6-N1	7.83	121.61	117.70
21	AA	583	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	1794	A	N1-C6-N6	-7.82	113.91	118.60
54	BA	2497	A	C5-C6-N1	7.82	121.61	117.70
54	BA	2886	A	O4'-C1'-N9	7.82	114.46	108.20
54	BA	2267	A	C5-C6-N1	7.82	121.61	117.70
54	BA	404	A	C5-C6-N1	7.81	121.61	117.70
54	BA	2749	A	C5-C6-N1	7.81	121.60	117.70
54	BA	1608	A	C5-C6-N1	7.81	121.60	117.70
21	AA	50	A	C5-C6-N1	7.81	121.60	117.70
21	AA	313	A	N1-C6-N6	-7.80	113.92	118.60
21	AA	456	A	N1-C6-N6	-7.80	113.92	118.60
54	BA	2114	A	C5-C6-N1	7.80	121.60	117.70
25	BC	268	ARG	NE-CZ-NH1	7.80	124.20	120.30
54	BA	2748	A	C5-C6-N1	7.80	121.60	117.70
33	BK	64	ARG	NE-CZ-NH1	7.80	124.20	120.30
54	BA	477	A	C5-C6-N1	7.80	121.60	117.70
11	AL	120	ARG	NE-CZ-NH1	7.79	124.20	120.30
21	AA	119	A	C5-C6-N1	7.79	121.60	117.70
21	AA	320	A	C5-C6-N1	7.79	121.60	117.70
54	BA	849	A	N1-C6-N6	-7.79	113.92	118.60
54	BA	1616	A	N1-C6-N6	-7.79	113.92	118.60
54	BA	2821	A	C5-C6-N1	7.79	121.60	117.70
21	AA	364	A	C5-C6-N1	7.79	121.60	117.70
21	AA	1213	A	C5-C6-N1	7.79	121.60	117.70
27	BE	67	ARG	NE-CZ-NH1	7.79	124.20	120.30
54	BA	222	A	C4-C5-C6	-7.79	113.10	117.00
54	BA	2268	A	C5-C6-N1	7.79	121.59	117.70
54	BA	1757	A	C5-C6-N1	7.79	121.59	117.70
54	BA	373	U	O4'-C1'-N1	7.79	114.43	108.20
54	BA	614	A	C5-C6-N1	7.79	121.59	117.70
54	BA	756	A	N1-C6-N6	-7.79	113.93	118.60
54	BA	1635	A	C5-C6-N1	7.79	121.59	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	160	A	C5-C6-N1	7.78	121.59	117.70
54	BA	340	A	N1-C6-N6	-7.78	113.93	118.60
54	BA	981	A	C5-C6-N1	7.78	121.59	117.70
54	BA	1151	A	C5-C6-N1	7.78	121.59	117.70
54	BA	2451	A	C5-C6-N1	7.78	121.59	117.70
54	BA	592	A	C5-C6-N1	7.78	121.59	117.70
2	AC	155	ARG	NE-CZ-NH1	7.78	124.19	120.30
21	AA	1201	A	C5-C6-N1	7.78	121.59	117.70
54	BA	1913	A	N1-C6-N6	-7.78	113.93	118.60
21	AA	792	A	C5-C6-N1	7.78	121.59	117.70
54	BA	675	A	C5-C6-N1	7.78	121.59	117.70
14	AO	88	ARG	NE-CZ-NH1	7.77	124.19	120.30
21	AA	640	A	C5-C6-N1	7.77	121.59	117.70
21	AA	1360	A	C5-C6-N1	7.77	121.59	117.70
54	BA	322	A	C5-C6-N1	7.77	121.59	117.70
54	BA	2163	A	C5-C6-N1	7.77	121.59	117.70
54	BA	190	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	363	A	N1-C6-N6	-7.77	113.94	118.60
54	BA	1169	A	C4-C5-C6	-7.77	113.12	117.00
54	BA	1890	A	C5-C6-N1	7.77	121.58	117.70
54	BA	2183	A	N1-C6-N6	-7.77	113.94	118.60
29	BG	2	ARG	NE-CZ-NH1	7.77	124.18	120.30
54	BA	2005	A	C5-C6-N1	7.77	121.58	117.70
21	AA	430	A	N1-C6-N6	-7.77	113.94	118.60
21	AA	1430	A	C5-C6-N1	7.77	121.58	117.70
54	BA	1098	A	C4-C5-C6	-7.76	113.12	117.00
54	BA	2176	A	N1-C6-N6	-7.76	113.94	118.60
21	AA	720	C	N3-C2-O2	-7.76	116.47	121.90
39	BQ	2	ARG	NE-CZ-NH1	7.76	124.18	120.30
54	BA	2542	A	N1-C6-N6	-7.76	113.94	118.60
54	BA	2713	U	O4'-C1'-N1	7.76	114.41	108.20
24	A3	59	A	C5-C6-N1	7.76	121.58	117.70
54	BA	73	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	544	C	N3-C2-O2	-7.75	116.47	121.90
54	BA	632	A	C5-C6-N1	7.75	121.58	117.70
54	BA	2577	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	2886	A	C5-C6-N1	7.75	121.58	117.70
21	AA	767	A	C5-C6-N1	7.75	121.57	117.70
21	AA	1375	A	N1-C6-N6	-7.75	113.95	118.60
22	A1	48	C	N3-C2-O2	-7.75	116.48	121.90
22	A1	73	A	C5-C6-N1	7.75	121.57	117.70
54	BA	735	A	N1-C6-N6	-7.75	113.95	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1591	A	C5-C6-N1	7.75	121.57	117.70
54	BA	1936	A	C5-C6-N1	7.75	121.57	117.70
55	BB	25	U	O4'-C1'-N1	7.75	114.40	108.20
21	AA	792	A	N1-C6-N6	-7.75	113.95	118.60
54	BA	676	A	C5-C6-N1	7.74	121.57	117.70
54	BA	716	A	C5-C6-N1	7.74	121.57	117.70
54	BA	2071	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1641	A	N1-C6-N6	-7.74	113.96	118.60
54	BA	504	A	C5-C6-N1	7.74	121.57	117.70
54	BA	1213	A	N1-C6-N6	-7.73	113.96	118.60
22	A1	20	G	N3-C2-N2	-7.73	114.49	119.90
54	BA	2346	A	C5-C6-N1	7.73	121.56	117.70
54	BA	278	A	C5-C6-N1	7.73	121.56	117.70
54	BA	1237	A	C5-C6-N1	7.73	121.56	117.70
54	BA	2799	A	C5-C6-N1	7.73	121.56	117.70
54	BA	1745	A	C5-C6-N1	7.73	121.56	117.70
55	BB	101	A	C5-C6-N1	7.73	121.56	117.70
54	BA	2726	A	C5-C6-N1	7.73	121.56	117.70
54	BA	103	A	C5-C6-N1	7.72	121.56	117.70
54	BA	602	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	833	A	C5-C6-N1	7.72	121.56	117.70
54	BA	1008	A	C5-C6-N1	7.72	121.56	117.70
54	BA	2052	A	C5-C6-N1	7.72	121.56	117.70
21	AA	959	A	C5-C6-N1	7.72	121.56	117.70
21	AA	1157	A	C5-C6-N1	7.72	121.56	117.70
54	BA	742	A	C5-C6-N1	7.72	121.56	117.70
54	BA	547	A	C5-C6-N1	7.72	121.56	117.70
12	AM	28	ARG	NE-CZ-NH1	7.72	124.16	120.30
54	BA	10	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	1598	A	N1-C6-N6	-7.72	113.97	118.60
54	BA	14	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	654	A	C5-C6-N1	7.71	121.56	117.70
54	BA	1848	A	N1-C6-N6	-7.71	113.97	118.60
54	BA	2829	A	C5-C6-N1	7.71	121.56	117.70
21	AA	1352	C	N3-C2-O2	-7.71	116.50	121.90
21	AA	1229	A	C4-C5-C6	-7.71	113.15	117.00
54	BA	1439	A	C5-C6-N1	7.71	121.55	117.70
54	BA	2080	A	N1-C6-N6	-7.71	113.98	118.60
21	AA	48	C	N3-C2-O2	-7.70	116.51	121.90
24	A3	73	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1301	A	O4'-C1'-N9	7.70	114.36	108.20
21	AA	306	A	N1-C6-N6	-7.70	113.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	608	A	C4-C5-C6	-7.70	113.15	117.00
21	AA	1130	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	391	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	802	A	C5-C6-N1	7.70	121.55	117.70
21	AA	1230	C	O4'-C1'-N1	7.70	114.36	108.20
54	BA	422	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1544	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	960	A	C5-C6-N1	7.70	121.55	117.70
54	BA	1504	A	N1-C6-N6	-7.70	113.98	118.60
54	BA	2267	A	N1-C6-N6	-7.70	113.98	118.60
21	AA	7	A	N1-C6-N6	-7.69	113.98	118.60
21	AA	1179	A	N1-C6-N6	-7.69	113.98	118.60
21	AA	596	A	N1-C6-N6	-7.69	113.99	118.60
54	BA	1133	A	C5-C6-N1	7.69	121.55	117.70
54	BA	1454	C	N3-C2-O2	-7.69	116.52	121.90
54	BA	2792	A	C4-C5-C6	-7.69	113.15	117.00
54	BA	2476	A	C5-C6-N1	7.69	121.54	117.70
54	BA	1783	A	C5-C6-N1	7.69	121.54	117.70
21	AA	900	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	1872	A	C5-C6-N1	7.68	121.54	117.70
21	AA	972	C	N3-C2-O2	-7.68	116.52	121.90
54	BA	2328	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	74	A	C5-C6-N1	7.68	121.54	117.70
9	AJ	31	ARG	NE-CZ-NH1	7.68	124.14	120.30
54	BA	2163	A	N1-C6-N6	-7.68	113.99	118.60
54	BA	2628	C	N1-C2-O2	7.68	123.51	118.90
41	BS	11	ARG	NE-CZ-NH1	7.67	124.14	120.30
21	AA	181	A	N1-C6-N6	-7.67	114.00	118.60
4	AE	53	ARG	NE-CZ-NH1	7.67	124.14	120.30
21	AA	704	A	C4-C5-C6	-7.67	113.17	117.00
54	BA	531	C	N3-C2-O2	-7.67	116.53	121.90
54	BA	1565	C	O4'-C1'-N1	7.67	114.34	108.20
17	AR	72	ARG	NE-CZ-NH1	7.67	124.14	120.30
54	BA	1084	A	N1-C6-N6	-7.67	114.00	118.60
39	BQ	69	ARG	NE-CZ-NH1	7.67	124.13	120.30
54	BA	1000	A	C5-C6-N1	7.67	121.53	117.70
54	BA	2856	A	C5-C6-N1	7.67	121.53	117.70
54	BA	928	A	C5-C6-N1	7.67	121.53	117.70
54	BA	2169	A	O4'-C1'-N9	7.67	114.33	108.20
21	AA	371	A	C5-C6-N1	7.66	121.53	117.70
54	BA	221	A	C5-C6-N1	7.66	121.53	117.70
54	BA	1001	A	N1-C6-N6	-7.66	114.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BN	17	ARG	NE-CZ-NH1	7.66	124.13	120.30
54	BA	983	A	C5-C6-N1	7.66	121.53	117.70
3	AD	80	ARG	NE-CZ-NH1	7.66	124.13	120.30
21	AA	1502	A	C5-C6-N1	7.66	121.53	117.70
21	AA	1510	C	N3-C2-O2	-7.66	116.54	121.90
54	BA	2727	A	C5-C6-N1	7.66	121.53	117.70
54	BA	2781	A	C5-C6-N1	7.66	121.53	117.70
15	AP	35	ARG	NE-CZ-NH1	7.66	124.13	120.30
21	AA	742	G	N3-C2-N2	-7.66	114.54	119.90
54	BA	56	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	149	A	C5-C6-N1	7.66	121.53	117.70
54	BA	1966	A	N1-C6-N6	-7.66	114.01	118.60
54	BA	2021	C	N3-C2-O2	-7.65	116.54	121.90
54	BA	2567	G	O4'-C1'-N9	7.65	114.32	108.20
21	AA	183	C	N3-C2-O2	-7.65	116.54	121.90
54	BA	2378	A	N1-C6-N6	-7.65	114.01	118.60
21	AA	190	A	C5-C6-N1	7.65	121.52	117.70
21	AA	673	A	C5-C6-N1	7.65	121.52	117.70
44	BV	18	ARG	NE-CZ-NH1	7.65	124.12	120.30
54	BA	1014	A	C4-C5-C6	-7.65	113.18	117.00
21	AA	1357	A	N1-C6-N6	-7.64	114.01	118.60
54	BA	1866	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2043	C	N3-C2-O2	-7.64	116.55	121.90
21	AA	640	A	N1-C6-N6	-7.64	114.01	118.60
54	BA	979	A	N1-C6-N6	-7.64	114.01	118.60
54	BA	2776	A	N1-C6-N6	-7.64	114.01	118.60
54	BA	1169	A	C5-C6-N1	7.64	121.52	117.70
33	BK	108	ARG	NE-CZ-NH1	7.64	124.12	120.30
21	AA	101	A	N1-C6-N6	-7.64	114.02	118.60
2	AC	106	ARG	NE-CZ-NH1	7.64	124.12	120.30
54	BA	2327	A	C5-C6-N1	7.64	121.52	117.70
54	BA	2461	A	N1-C6-N6	-7.64	114.02	118.60
21	AA	1004	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	233	A	N1-C6-N6	-7.63	114.02	118.60
54	BA	877	A	C5-C6-N1	7.63	121.52	117.70
54	BA	2815	C	N3-C2-O2	-7.63	116.56	121.90
54	BA	608	A	N1-C6-N6	-7.63	114.02	118.60
21	AA	129	A	C5-C6-N1	7.63	121.52	117.70
21	AA	560	A	C5-C6-N1	7.63	121.52	117.70
54	BA	1127	A	C5-C6-N1	7.63	121.52	117.70
42	BT	77	ARG	NE-CZ-NH1	7.63	124.11	120.30
54	BA	821	A	C5-C6-N1	7.63	121.51	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1327	A	C5-C6-N1	7.63	121.52	117.70
21	AA	1169	A	C5-C6-N1	7.62	121.51	117.70
21	AA	1357	A	C5-C6-N1	7.62	121.51	117.70
54	BA	2614	A	C5-C6-N1	7.62	121.51	117.70
21	AA	95	C	N3-C2-O2	-7.62	116.56	121.90
21	AA	182	A	C5-C6-N1	7.62	121.51	117.70
21	AA	300	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1287	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	873	A	C5-C6-N1	7.62	121.51	117.70
43	BU	6	ARG	NE-CZ-NH1	7.62	124.11	120.30
54	BA	1268	A	C5-C6-N1	7.62	121.51	117.70
21	AA	328	C	N3-C2-O2	-7.62	116.57	121.90
54	BA	352	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	1808	A	C5-C6-N1	7.62	121.51	117.70
21	AA	665	A	C5-C6-N1	7.62	121.51	117.70
21	AA	923	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	1180	A	N1-C6-N6	-7.62	114.03	118.60
54	BA	2503	A	O4'-C1'-N9	7.62	114.30	108.20
54	BA	1668	A	C5-C6-N1	7.62	121.51	117.70
21	AA	151	A	C5-C6-N1	7.62	121.51	117.70
21	AA	349	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1046	A	C5-C6-N1	7.62	121.51	117.70
54	BA	1626	A	N1-C6-N6	-7.62	114.03	118.60
21	AA	26	A	C5-C6-N1	7.61	121.51	117.70
21	AA	373	A	C5-C6-N1	7.61	121.51	117.70
21	AA	655	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	1522	A	C5-C6-N1	7.61	121.51	117.70
54	BA	2478	A	C5-C6-N1	7.61	121.51	117.70
55	BB	39	A	C5-C6-N1	7.61	121.51	117.70
21	AA	1493	A	O4'-C1'-N9	7.61	114.29	108.20
55	BB	73	A	C5-C6-N1	7.61	121.51	117.70
21	AA	1339	A	C5-C6-N1	7.61	121.51	117.70
21	AA	1394	A	C5-C6-N1	7.61	121.50	117.70
21	AA	502	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	1102	C	N3-C2-O2	-7.61	116.57	121.90
54	BA	1366	A	N1-C6-N6	-7.61	114.03	118.60
54	BA	1700	A	C5-C6-N1	7.61	121.50	117.70
54	BA	2145	C	N3-C2-O2	-7.61	116.57	121.90
28	BF	111	ARG	NE-CZ-NH1	7.61	124.10	120.30
54	BA	1942	C	N3-C2-O2	-7.61	116.58	121.90
21	AA	19	A	C4-C5-C6	-7.61	113.20	117.00
54	BA	1892	C	N3-C2-O2	-7.61	116.58	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1332	A	C5-C6-N1	7.60	121.50	117.70
54	BA	2748	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	1050	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	1340	U	N3-C2-O2	-7.60	116.88	122.20
55	BB	99	A	N1-C6-N6	-7.60	114.04	118.60
21	AA	696	A	N1-C6-N6	-7.60	114.04	118.60
54	BA	310	A	C5-C6-N1	7.60	121.50	117.70
54	BA	2452	C	N3-C2-O2	-7.60	116.58	121.90
21	AA	264	C	N3-C2-O2	-7.59	116.58	121.90
21	AA	452	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	1439	A	N1-C6-N6	-7.59	114.04	118.60
21	AA	262	A	N1-C6-N6	-7.59	114.04	118.60
54	BA	1737	G	O4'-C1'-N9	7.59	114.27	108.20
54	BA	1470	A	N1-C6-N6	-7.59	114.05	118.60
54	BA	471	A	C5-C6-N1	7.59	121.49	117.70
54	BA	2340	A	C5-C6-N1	7.59	121.50	117.70
21	AA	307	C	N3-C2-O2	-7.59	116.59	121.90
21	AA	1306	A	C5-C6-N1	7.59	121.49	117.70
21	AA	345	C	N3-C2-O2	-7.59	116.59	121.90
21	AA	790	A	C5-C6-N1	7.59	121.49	117.70
11	AL	30	ARG	NE-CZ-NH2	-7.58	116.51	120.30
13	AN	75	ARG	NE-CZ-NH1	7.58	124.09	120.30
54	BA	1156	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1913	A	C5-C6-N1	7.58	121.49	117.70
21	AA	631	C	N1-C2-O2	7.58	123.45	118.90
21	AA	814	A	C5-C6-N1	7.58	121.49	117.70
54	BA	699	A	N1-C6-N6	-7.58	114.05	118.60
21	AA	1093	A	C5-C6-N1	7.58	121.49	117.70
54	BA	2406	A	C5-C6-N1	7.58	121.49	117.70
54	BA	550	C	N3-C2-O2	-7.58	116.60	121.90
54	BA	788	A	C5-C6-N1	7.58	121.49	117.70
54	BA	1111	A	N1-C6-N6	-7.58	114.05	118.60
21	AA	6	G	P-O3'-C3'	7.58	128.79	119.70
21	AA	974	A	C5-C6-N1	7.58	121.49	117.70
54	BA	621	A	C5-C6-N1	7.58	121.49	117.70
54	BA	909	A	N1-C6-N6	-7.58	114.05	118.60
7	AH	113	ARG	NE-CZ-NH1	7.57	124.09	120.30
21	AA	1400	C	N3-C2-O2	-7.57	116.60	121.90
21	AA	1418	A	N1-C6-N6	-7.57	114.06	118.60
25	BC	155	ARG	NE-CZ-NH1	7.57	124.09	120.30
54	BA	627	A	C5-C6-N1	7.57	121.49	117.70
54	BA	739	A	C5-C6-N1	7.57	121.49	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AL	113	ARG	NE-CZ-NH1	7.57	124.09	120.30
54	BA	42	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	2369	A	C4-C5-C6	-7.57	113.21	117.00
54	BA	1574	C	N3-C2-O2	-7.57	116.60	121.90
21	AA	274	A	C5-C6-N1	7.57	121.48	117.70
54	BA	2031	A	C5-C6-N1	7.57	121.48	117.70
54	BA	492	A	N1-C6-N6	-7.57	114.06	118.60
54	BA	2281	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2766	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1916	A	C5-C6-N1	7.56	121.48	117.70
54	BA	323	C	N1-C2-O2	7.56	123.44	118.90
21	AA	412	A	C5-C6-N1	7.56	121.48	117.70
22	A1	23	A	C5-C6-N1	7.56	121.48	117.70
54	BA	1205	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2809	A	C5-C6-N1	7.56	121.48	117.70
54	BA	2858	C	N3-C2-O2	-7.56	116.61	121.90
54	BA	1433	A	N1-C6-N6	-7.55	114.07	118.60
54	BA	1129	A	C5-C6-N1	7.55	121.48	117.70
21	AA	532	A	C5-C6-N1	7.55	121.48	117.70
54	BA	447	A	C5-C6-N1	7.55	121.48	117.70
54	BA	1032	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2564	A	C5-C6-N1	7.55	121.48	117.70
21	AA	65	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	172	A	C4-C5-C6	-7.55	113.22	117.00
54	BA	819	A	N1-C6-N6	-7.55	114.07	118.60
21	AA	795	C	N3-C2-O2	-7.55	116.62	121.90
54	BA	271	G	O4'-C1'-N9	7.55	114.24	108.20
54	BA	282	A	C5-C6-N1	7.55	121.47	117.70
54	BA	2383	G	O4'-C1'-N9	7.55	114.24	108.20
21	AA	1375	A	C5-C6-N1	7.54	121.47	117.70
40	BR	84	ARG	NE-CZ-NH1	7.54	124.07	120.30
54	BA	2657	A	N1-C6-N6	-7.54	114.07	118.60
21	AA	451	A	N1-C6-N6	-7.54	114.08	118.60
23	A2	88	U	N3-C2-O2	-7.54	116.92	122.20
54	BA	507	A	C5-C6-N1	7.54	121.47	117.70
21	AA	1145	A	C5-C6-N1	7.54	121.47	117.70
54	BA	2448	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	2278	A	N1-C6-N6	-7.54	114.08	118.60
54	BA	345	A	C5-C6-N1	7.54	121.47	117.70
21	AA	72	A	C5-C6-N1	7.53	121.47	117.70
21	AA	81	A	C5-C6-N1	7.53	121.47	117.70
21	AA	1146	A	C5-C6-N1	7.53	121.47	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	B2	39	ARG	NE-CZ-NH1	7.53	124.07	120.30
54	BA	653	U	O4'-C1'-N1	7.53	114.23	108.20
22	A1	23	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	756	A	C5-C6-N1	7.53	121.47	117.70
54	BA	1553	A	C5-C6-N1	7.53	121.46	117.70
54	BA	1365	A	C5-C6-N1	7.53	121.46	117.70
54	BA	1544	A	C5-C6-N1	7.53	121.46	117.70
54	BA	2058	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	2706	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	1866	A	N1-C6-N6	-7.53	114.08	118.60
54	BA	2274	A	C5-C6-N1	7.53	121.46	117.70
54	BA	279	A	C5-C6-N1	7.52	121.46	117.70
54	BA	946	C	O4'-C1'-N1	7.52	114.22	108.20
54	BA	1943	U	N3-C2-O2	-7.52	116.93	122.20
21	AA	476	U	O4'-C1'-N1	7.52	114.22	108.20
39	BQ	91	ARG	NE-CZ-NH1	7.52	124.06	120.30
54	BA	95	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	761	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1392	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	2534	A	N1-C6-N6	-7.52	114.09	118.60
21	AA	518	C	N1-C2-O2	7.52	123.41	118.90
21	AA	1280	A	C5-C6-N1	7.52	121.46	117.70
54	BA	244	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	430	A	N1-C6-N6	-7.52	114.09	118.60
54	BA	1459	G	O4'-C1'-N9	7.52	114.22	108.20
21	AA	1362	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1518	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1678	A	C5-C6-N1	7.52	121.46	117.70
54	BA	2247	A	C5-C6-N1	7.52	121.46	117.70
54	BA	1786	A	C5-C6-N1	7.52	121.46	117.70
21	AA	1503	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	461	A	C5-C6-N1	7.51	121.46	117.70
21	AA	44	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	468	A	C5-C6-N1	7.51	121.45	117.70
21	AA	1176	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	1757	A	N1-C6-N6	-7.51	114.09	118.60
54	BA	182	A	N1-C6-N6	-7.51	114.09	118.60
21	AA	1418	A	C5-C6-N1	7.51	121.45	117.70
36	BN	90	ARG	NE-CZ-NH1	7.51	124.05	120.30
41	BS	88	ARG	NE-CZ-NH1	7.51	124.05	120.30
54	BA	1598	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2799	A	O4'-C1'-N9	7.50	114.20	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	564	C	N3-C2-O2	-7.50	116.65	121.90
21	AA	994	A	C5-C6-N1	7.50	121.45	117.70
22	A1	26	A	C4-C5-C6	-7.50	113.25	117.00
37	BO	33	ARG	NE-CZ-NH1	7.50	124.05	120.30
39	BQ	57	ARG	NE-CZ-NH1	7.50	124.05	120.30
54	BA	213	A	C5-C6-N1	7.50	121.45	117.70
54	BA	988	A	C5-C6-N1	7.50	121.45	117.70
54	BA	582	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1272	A	C5-C6-N1	7.50	121.45	117.70
21	AA	702	A	C5-C6-N1	7.50	121.45	117.70
54	BA	933	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1342	A	N1-C6-N6	-7.50	114.10	118.60
21	AA	559	A	N1-C6-N6	-7.50	114.10	118.60
22	A1	60	C	N3-C2-O2	-7.50	116.65	121.90
54	BA	1073	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1829	A	C5-C6-N1	7.50	121.45	117.70
54	BA	2541	A	C5-C6-N1	7.50	121.45	117.70
54	BA	1246	A	N1-C6-N6	-7.50	114.10	118.60
39	BQ	32	ARG	NE-CZ-NH1	7.49	124.05	120.30
54	BA	510	C	N3-C2-O2	-7.49	116.65	121.90
54	BA	1302	A	N1-C6-N6	-7.49	114.10	118.60
54	BA	1969	A	N1-C6-N6	-7.49	114.10	118.60
21	AA	8	A	C5-C6-N1	7.49	121.45	117.70
54	BA	959	A	C5-C6-N1	7.49	121.45	117.70
21	AA	246	A	N1-C6-N6	-7.49	114.11	118.60
21	AA	915	A	C5-C6-N1	7.49	121.44	117.70
21	AA	1238	A	C4-C5-C6	-7.49	113.25	117.00
54	BA	1780	A	C5-C6-N1	7.49	121.45	117.70
21	AA	353	A	N1-C6-N6	-7.49	114.11	118.60
54	BA	2573	C	N3-C2-O2	-7.49	116.66	121.90
55	BB	53	A	C5-C6-N1	7.49	121.44	117.70
21	AA	889	A	C5-C6-N1	7.49	121.44	117.70
54	BA	2867	G	O4'-C1'-N9	7.49	114.19	108.20
54	BA	2899	A	C5-C6-N1	7.49	121.44	117.70
21	AA	130	A	C4-C5-C6	-7.48	113.26	117.00
54	BA	218	A	C5-C6-N1	7.48	121.44	117.70
21	AA	1431	A	C5-C6-N1	7.48	121.44	117.70
54	BA	1328	A	C5-C6-N1	7.48	121.44	117.70
54	BA	1609	A	C4-C5-C6	-7.48	113.26	117.00
54	BA	1787	A	C5-C6-N1	7.48	121.44	117.70
54	BA	2268	A	N1-C6-N6	-7.48	114.11	118.60
21	AA	344	A	C4-C5-C6	-7.47	113.26	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BJ	96	ARG	NE-CZ-NH1	7.47	124.04	120.30
54	BA	118	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1403	A	C5-C6-N1	7.47	121.44	117.70
21	AA	1036	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1260	A	C4-C5-C6	-7.47	113.26	117.00
54	BA	2381	A	C5-C6-N1	7.47	121.44	117.70
21	AA	969	A	C5-C6-N1	7.47	121.44	117.70
54	BA	1395	A	C5-C6-N1	7.47	121.44	117.70
54	BA	249	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	2456	C	N3-C2-O2	-7.47	116.67	121.90
21	AA	764	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	587	C	N3-C2-O2	-7.47	116.67	121.90
54	BA	1054	A	C5-C6-N1	7.47	121.43	117.70
54	BA	1815	A	C5-C6-N1	7.47	121.43	117.70
54	BA	2091	C	N3-C2-O2	-7.47	116.67	121.90
21	AA	382	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2483	C	N3-C2-O2	-7.46	116.67	121.90
21	AA	622	A	N1-C6-N6	-7.46	114.12	118.60
35	BM	10	ARG	NE-CZ-NH1	7.46	124.03	120.30
54	BA	96	C	N3-C2-O2	-7.46	116.68	121.90
54	BA	126	A	N1-C6-N6	-7.46	114.12	118.60
54	BA	231	A	C4-C5-C6	-7.46	113.27	117.00
21	AA	1434	A	C5-C6-N1	7.46	121.43	117.70
24	A3	22	A	C5-C6-N1	7.46	121.43	117.70
54	BA	538	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1609	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2243	U	O4'-C1'-N1	7.46	114.17	108.20
21	AA	282	A	C5-C6-N1	7.46	121.43	117.70
54	BA	160	A	C5-C6-N1	7.46	121.43	117.70
54	BA	2810	A	N1-C6-N6	-7.46	114.12	118.60
21	AA	349	A	N1-C6-N6	-7.46	114.13	118.60
21	AA	841	C	N3-C2-O2	-7.46	116.68	121.90
21	AA	1188	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1717	A	C5-C6-N1	7.46	121.43	117.70
54	BA	1495	A	N1-C6-N6	-7.46	114.13	118.60
54	BA	743	A	C5-C6-N1	7.45	121.43	117.70
54	BA	1086	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	2314	A	C5-C6-N1	7.45	121.42	117.70
21	AA	1229	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1057	A	C4-C5-C6	-7.45	113.28	117.00
54	BA	1143	A	C5-C6-N1	7.45	121.42	117.70
54	BA	1927	A	C5-C6-N1	7.45	121.42	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	129	A	C4-C5-C6	-7.45	113.28	117.00
54	BA	1640	A	N1-C6-N6	-7.45	114.13	118.60
54	BA	1069	A	N1-C6-N6	-7.44	114.13	118.60
54	BA	1332	G	O4'-C1'-N9	7.44	114.16	108.20
21	AA	819	A	C5-C6-N1	7.44	121.42	117.70
33	BK	105	ARG	NE-CZ-NH1	7.44	124.02	120.30
54	BA	2660	A	C5-C6-N1	7.44	121.42	117.70
21	AA	1483	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	563	A	N1-C6-N6	-7.44	114.14	118.60
54	BA	1632	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1614	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1079	C	N3-C2-O2	-7.44	116.69	121.90
54	BA	1713	A	C5-C6-N1	7.44	121.42	117.70
54	BA	1810	A	C5-C6-N1	7.44	121.42	117.70
54	BA	900	A	C4-C5-C6	-7.44	113.28	117.00
54	BA	1103	A	N1-C6-N6	-7.43	114.14	118.60
54	BA	1552	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2637	U	O4'-C1'-N1	7.43	114.15	108.20
21	AA	366	A	C5-C6-N1	7.43	121.42	117.70
34	BL	47	ARG	NE-CZ-NH1	7.43	124.02	120.30
21	AA	1229	A	O4'-C1'-N9	7.43	114.14	108.20
54	BA	2042	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2600	A	C4-C5-C6	-7.43	113.28	117.00
21	AA	1520	C	N3-C2-O2	-7.43	116.70	121.90
54	BA	1805	A	C5-C6-N1	7.43	121.42	117.70
54	BA	2602	A	C5-C6-N1	7.43	121.41	117.70
21	AA	1377	A	C5-C6-N1	7.43	121.41	117.70
54	BA	2813	A	C4-C5-C6	-7.43	113.29	117.00
15	AP	56	ARG	NE-CZ-NH1	7.43	124.01	120.30
21	AA	131	A	C5-C6-N1	7.43	121.41	117.70
21	AA	1227	A	C5-C6-N1	7.43	121.41	117.70
54	BA	2837	A	N1-C6-N6	-7.43	114.14	118.60
21	AA	918	A	C5-C6-N1	7.42	121.41	117.70
54	BA	172	A	N1-C6-N6	-7.42	114.14	118.60
54	BA	933	A	N1-C6-N6	-7.42	114.14	118.60
21	AA	74	A	C5-C6-N1	7.42	121.41	117.70
21	AA	195	A	C5-C6-N1	7.42	121.41	117.70
21	AA	432	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1403	C	N3-C2-O2	-7.42	116.70	121.90
54	BA	56	A	C5-C6-N1	7.42	121.41	117.70
54	BA	905	A	C5-C6-N1	7.42	121.41	117.70
21	AA	1534	A	C5-C6-N1	7.42	121.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	722	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	794	A	C5-C6-N1	7.42	121.41	117.70
54	BA	1572	A	N1-C6-N6	-7.42	114.15	118.60
54	BA	2288	A	C5-C6-N1	7.42	121.41	117.70
10	AK	92	ARG	NE-CZ-NH1	7.42	124.01	120.30
54	BA	2298	A	C5-C6-N1	7.41	121.41	117.70
21	AA	509	A	C5-C6-N1	7.41	121.41	117.70
54	BA	2682	A	C5-C6-N1	7.41	121.40	117.70
21	AA	1214	C	N3-C2-O2	-7.41	116.72	121.90
54	BA	1978	A	C5-C6-N1	7.41	121.40	117.70
54	BA	2893	A	C5-C6-N1	7.41	121.40	117.70
54	BA	265	A	C5-C6-N1	7.41	121.40	117.70
54	BA	661	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1170	A	C5-C6-N1	7.40	121.40	117.70
54	BA	49	A	C5-C6-N1	7.40	121.40	117.70
54	BA	1579	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	2764	A	C5-C6-N1	7.40	121.40	117.70
55	BB	108	A	C5-C6-N1	7.40	121.40	117.70
21	AA	1171	A	N1-C6-N6	-7.40	114.16	118.60
54	BA	608	A	C5-C6-N1	7.40	121.40	117.70
55	BB	97	C	O4'-C1'-N1	7.40	114.12	108.20
21	AA	315	A	C5-C6-N1	7.40	121.40	117.70
23	A2	91	A	C4-C5-C6	-7.40	113.30	117.00
54	BA	1885	A	C5-C6-N1	7.40	121.40	117.70
54	BA	2022	U	O4'-C1'-N1	7.40	114.12	108.20
54	BA	2856	A	N1-C6-N6	-7.40	114.16	118.60
21	AA	499	A	C4-C5-C6	-7.39	113.30	117.00
21	AA	695	A	N1-C6-N6	-7.39	114.16	118.60
22	A1	36	C	N3-C2-O2	-7.39	116.72	121.90
54	BA	2823	A	N1-C6-N6	-7.39	114.16	118.60
3	AD	69	ARG	NE-CZ-NH1	7.39	124.00	120.30
21	AA	234	C	N3-C2-O2	-7.39	116.73	121.90
21	AA	1468	A	C5-C6-N1	7.39	121.40	117.70
21	AA	1533	C	N3-C2-O2	-7.39	116.72	121.90
21	AA	498	A	C4-C5-C6	-7.39	113.30	117.00
54	BA	1254	A	C5-C6-N1	7.39	121.39	117.70
54	BA	354	A	C4-C5-C6	-7.39	113.31	117.00
54	BA	2547	A	C4-C5-C6	-7.39	113.31	117.00
21	AA	694	A	C5-C6-N1	7.38	121.39	117.70
21	AA	1394	A	N1-C6-N6	-7.38	114.17	118.60
54	BA	73	A	C5-C6-N1	7.38	121.39	117.70
54	BA	532	A	C5-C6-N1	7.38	121.39	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	889	C	N1-C2-O2	7.38	123.33	118.90
54	BA	1937	A	C5-C6-N1	7.38	121.39	117.70
54	BA	721	A	C5-C6-N1	7.38	121.39	117.70
21	AA	1441	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2070	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2191	A	C5-C6-N1	7.38	121.39	117.70
54	BA	2407	A	C5-C6-N1	7.38	121.39	117.70
21	AA	673	A	N1-C6-N6	-7.38	114.17	118.60
22	A1	21	A	C5-C6-N1	7.38	121.39	117.70
21	AA	143	A	C5-C6-N1	7.38	121.39	117.70
21	AA	968	A	C5-C6-N1	7.38	121.39	117.70
54	BA	368	A	C5-C6-N1	7.38	121.39	117.70
54	BA	1367	A	C5-C6-N1	7.37	121.39	117.70
55	BB	53	A	N1-C6-N6	-7.37	114.18	118.60
1	AB	224	ARG	NE-CZ-NH1	7.37	123.99	120.30
21	AA	1239	A	C4-C5-C6	-7.37	113.31	117.00
22	A1	59	U	O4'-C1'-N1	7.37	114.10	108.20
54	BA	146	A	C4-C5-C6	-7.37	113.31	117.00
54	BA	734	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1096	A	C5-C6-N1	7.37	121.39	117.70
54	BA	1151	A	N1-C6-N6	-7.37	114.18	118.60
21	AA	279	A	C4-C5-C6	-7.37	113.31	117.00
23	A2	80	C	N3-C2-O2	-7.37	116.74	121.90
54	BA	2054	A	C5-C6-N1	7.37	121.38	117.70
54	BA	2184	A	N1-C6-N6	-7.37	114.18	118.60
54	BA	689	A	C5-C6-N1	7.37	121.38	117.70
21	AA	59	A	C5-C6-N1	7.37	121.38	117.70
21	AA	523	A	C5-C6-N1	7.36	121.38	117.70
21	AA	768	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2560	A	C5-C6-N1	7.36	121.38	117.70
21	AA	1519	A	C5-C6-N1	7.36	121.38	117.70
54	BA	631	A	C5-C6-N1	7.36	121.38	117.70
21	AA	81	A	C4-C5-C6	-7.36	113.32	117.00
21	AA	914	A	C5-C6-N1	7.36	121.38	117.70
21	AA	535	A	N1-C6-N6	-7.36	114.19	118.60
21	AA	583	A	C5-C6-N1	7.36	121.38	117.70
21	AA	607	A	C5-C6-N1	7.36	121.38	117.70
54	BA	2212	A	C5-C6-N1	7.36	121.38	117.70
54	BA	384	A	C5-C6-N1	7.36	121.38	117.70
54	BA	1028	A	N1-C6-N6	-7.36	114.19	118.60
54	BA	1126	A	C5-C6-N1	7.36	121.38	117.70
55	BB	104	A	C5-C6-N1	7.36	121.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2874	C	N3-C2-O2	-7.35	116.75	121.90
21	AA	1467	C	N3-C2-O2	-7.35	116.75	121.90
54	BA	899	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	1140	C	N3-C2-O2	-7.35	116.75	121.90
54	BA	2060	A	C5-C6-N1	7.35	121.38	117.70
54	BA	2088	A	N1-C6-N6	-7.35	114.19	118.60
21	AA	663	A	C5-C6-N1	7.35	121.38	117.70
54	BA	432	A	C5-C6-N1	7.35	121.38	117.70
54	BA	509	C	N3-C2-O2	-7.35	116.75	121.90
54	BA	1505	A	C5-C6-N1	7.35	121.38	117.70
21	AA	1082	A	C5-C6-N1	7.35	121.38	117.70
25	BC	270	ARG	NE-CZ-NH1	7.35	123.97	120.30
54	BA	1515	A	C5-C6-N1	7.35	121.37	117.70
54	BA	1255	U	N3-C2-O2	-7.35	117.06	122.20
21	AA	1055	A	N1-C6-N6	-7.35	114.19	118.60
54	BA	309	A	C4-C5-C6	-7.35	113.33	117.00
55	BB	45	A	C5-C6-N1	7.35	121.37	117.70
21	AA	1369	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	912	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	1090	A	C5-C6-N1	7.34	121.37	117.70
54	BA	1013	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	2721	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2733	A	N1-C6-N6	-7.34	114.19	118.60
21	AA	1042	A	C5-C6-N1	7.34	121.37	117.70
54	BA	698	C	N3-C2-O2	-7.34	116.76	121.90
54	BA	1095	A	C5-C6-N1	7.34	121.37	117.70
54	BA	2781	A	C4-C5-C6	-7.34	113.33	117.00
21	AA	205	A	N1-C6-N6	-7.34	114.20	118.60
21	AA	1271	A	N1-C6-N6	-7.34	114.20	118.60
54	BA	2154	A	C5-C6-N1	7.34	121.37	117.70
54	BA	449	A	C5-C6-N1	7.33	121.37	117.70
54	BA	119	A	C5-C6-N1	7.33	121.37	117.70
54	BA	1801	A	C5-C6-N1	7.33	121.37	117.70
21	AA	1368	A	C4-C5-C6	-7.33	113.33	117.00
54	BA	911	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	1504	A	C5-C6-N1	7.33	121.37	117.70
54	BA	2750	A	C5-C6-N1	7.33	121.37	117.70
21	AA	765	G	O4'-C1'-N9	7.33	114.06	108.20
21	AA	784	A	C5-C6-N1	7.33	121.36	117.70
54	BA	1590	A	C4-C5-C6	-7.33	113.33	117.00
21	AA	808	C	N3-C2-O2	-7.33	116.77	121.90
54	BA	1848	A	C5-C6-N1	7.33	121.36	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2059	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2062	A	C5-C6-N1	7.33	121.36	117.70
21	AA	1363	A	N1-C6-N6	-7.33	114.20	118.60
54	BA	825	A	C5-C6-N1	7.33	121.36	117.70
54	BA	2572	A	N1-C6-N6	-7.33	114.20	118.60
21	AA	1151	A	C5-C6-N1	7.32	121.36	117.70
21	AA	1180	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1871	A	C5-C6-N1	7.32	121.36	117.70
21	AA	872	A	C5-C6-N1	7.32	121.36	117.70
21	AA	1483	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2309	A	N1-C6-N6	-7.32	114.21	118.60
21	AA	371	A	C4-C5-C6	-7.32	113.34	117.00
21	AA	1302	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	197	A	C5-C6-N1	7.32	121.36	117.70
54	BA	979	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2426	A	C5-C6-N1	7.32	121.36	117.70
54	BA	2434	A	N1-C6-N6	-7.32	114.21	118.60
54	BA	2129	C	N1-C2-O2	7.32	123.29	118.90
21	AA	1346	A	C5-C6-N1	7.32	121.36	117.70
22	A1	69	A	C5-C6-N1	7.32	121.36	117.70
54	BA	412	A	C5-C6-N1	7.32	121.36	117.70
54	BA	1836	C	O4'-C1'-N1	7.32	114.05	108.20
54	BA	2084	C	N3-C2-O2	-7.32	116.78	121.90
54	BA	2711	A	C5-C6-N1	7.32	121.36	117.70
54	BA	767	U	O4'-C1'-N1	7.32	114.05	108.20
54	BA	2430	A	C5-C6-N1	7.32	121.36	117.70
54	BA	643	A	O4'-C1'-N9	7.31	114.05	108.20
54	BA	16	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	2829	A	N1-C6-N6	-7.31	114.21	118.60
54	BA	472	A	C5-C6-N1	7.31	121.36	117.70
54	BA	1175	A	C5-C6-N1	7.31	121.36	117.70
21	AA	572	A	C5-C6-N1	7.31	121.36	117.70
21	AA	747	A	C4-C5-C6	-7.31	113.34	117.00
21	AA	1081	A	N1-C6-N6	-7.31	114.21	118.60
21	AA	1287	A	C5-C6-N1	7.31	121.35	117.70
21	AA	1363	A	C5-C6-N1	7.31	121.35	117.70
21	AA	1428	A	C5-C6-N1	7.31	121.35	117.70
54	BA	507	A	C4-C5-C6	-7.31	113.35	117.00
54	BA	2478	A	N1-C6-N6	-7.31	114.22	118.60
55	BB	36	C	N3-C2-O2	-7.31	116.78	121.90
54	BA	685	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2835	A	C4-C5-C6	-7.30	113.35	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	643	A	C5-C6-N1	7.30	121.35	117.70
54	BA	947	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2598	A	C5-C6-N1	7.30	121.35	117.70
21	AA	1167	A	C5-C6-N1	7.30	121.35	117.70
22	A1	74	C	N1-C2-O2	7.30	123.28	118.90
54	BA	28	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1275	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	1321	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1610	A	C5-C6-N1	7.30	121.35	117.70
54	BA	2887	A	C4-C5-C6	-7.30	113.35	117.00
54	BA	1098	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1165	A	N1-C6-N6	-7.30	114.22	118.60
54	BA	1987	A	C5-C6-N1	7.30	121.35	117.70
54	BA	1284	A	C5-C6-N1	7.29	121.35	117.70
18	AS	2	ARG	NE-CZ-NH2	-7.29	116.65	120.30
21	AA	130	A	C5-C6-N1	7.29	121.35	117.70
21	AA	156	C	N3-C2-O2	-7.29	116.80	121.90
21	AA	676	A	C5-C6-N1	7.29	121.35	117.70
22	A1	26	A	C5-C6-N1	7.29	121.35	117.70
55	BB	35	C	N3-C2-O2	-7.29	116.80	121.90
54	BA	1419	A	N1-C6-N6	-7.29	114.22	118.60
54	BA	925	A	C5-C6-N1	7.29	121.34	117.70
55	BB	99	A	C5-C6-N1	7.29	121.34	117.70
7	AH	76	ARG	NE-CZ-NH1	7.29	123.94	120.30
21	AA	38	G	N1-C6-O6	-7.29	115.53	119.90
54	BA	861	A	C5-C6-N1	7.29	121.34	117.70
54	BA	1675	C	N3-C2-O2	-7.29	116.80	121.90
12	AM	112	ARG	NE-CZ-NH1	7.28	123.94	120.30
21	AA	1019	A	N1-C6-N6	-7.28	114.23	118.60
54	BA	668	A	C5-C6-N1	7.28	121.34	117.70
21	AA	1287	A	C4-C5-C6	-7.28	113.36	117.00
54	BA	346	A	C5-C6-N1	7.28	121.34	117.70
21	AA	177	G	O4'-C1'-N9	7.28	114.03	108.20
21	AA	1256	A	C5-C6-N1	7.28	121.34	117.70
34	BL	123	ARG	NE-CZ-NH1	7.28	123.94	120.30
54	BA	515	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1772	A	C5-C6-N1	7.28	121.34	117.70
21	AA	712	A	C5-C6-N1	7.28	121.34	117.70
54	BA	706	A	C5-C6-N1	7.28	121.34	117.70
54	BA	980	A	C5-C6-N1	7.28	121.34	117.70
54	BA	1321	A	N1-C6-N6	-7.28	114.23	118.60
21	AA	65	A	C5-C6-N1	7.28	121.34	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	246	A	C5-C6-N1	7.28	121.34	117.70
54	BA	320	A	C5-C6-N1	7.27	121.34	117.70
21	AA	980	C	N3-C2-O2	-7.27	116.81	121.90
21	AA	1408	A	C5-C6-N1	7.27	121.34	117.70
54	BA	2717	C	N3-C2-O2	-7.27	116.81	121.90
21	AA	653	U	N3-C2-O2	-7.27	117.11	122.20
54	BA	262	A	C4-C5-C6	-7.27	113.36	117.00
54	BA	2014	A	C5-C6-N1	7.27	121.33	117.70
54	BA	2278	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1572	A	C5-C6-N1	7.27	121.33	117.70
54	BA	1785	A	C4-C5-C6	-7.27	113.37	117.00
54	BA	1308	A	C4-C5-C6	-7.27	113.37	117.00
54	BA	2711	A	C4-C5-C6	-7.27	113.37	117.00
2	AC	125	ARG	NE-CZ-NH1	7.26	123.93	120.30
21	AA	169	C	N3-C2-O2	-7.26	116.81	121.90
21	AA	397	A	C5-C6-N1	7.26	121.33	117.70
50	B1	27	ARG	NE-CZ-NH1	7.26	123.93	120.30
7	AH	83	ARG	NE-CZ-NH1	7.26	123.93	120.30
15	AP	14	ARG	NE-CZ-NH1	7.26	123.93	120.30
21	AA	233	C	N3-C2-O2	-7.26	116.82	121.90
21	AA	781	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2766	A	N1-C6-N6	-7.26	114.24	118.60
21	AA	1111	A	C5-C6-N1	7.26	121.33	117.70
54	BA	2654	A	C4-C5-C6	-7.26	113.37	117.00
23	A2	82	A	C5-C6-N1	7.26	121.33	117.70
54	BA	1217	U	O4'-C1'-N1	7.26	114.00	108.20
54	BA	1644	C	N3-C2-O2	-7.26	116.82	121.90
54	BA	1579	A	C5-C6-N1	7.25	121.33	117.70
21	AA	217	C	N3-C2-O2	-7.25	116.82	121.90
21	AA	1096	C	N3-C2-O2	-7.25	116.82	121.90
54	BA	1900	A	C5-C6-N1	7.25	121.33	117.70
21	AA	595	A	N1-C6-N6	-7.25	114.25	118.60
21	AA	1101	A	P-O3'-C3'	7.25	128.40	119.70
54	BA	2342	C	N3-C2-O2	-7.25	116.83	121.90
54	BA	567	U	O4'-C1'-N1	7.25	114.00	108.20
54	BA	1635	A	C4-C5-C6	-7.25	113.38	117.00
21	AA	907	A	C5-C6-N1	7.25	121.32	117.70
54	BA	299	A	C5-C6-N1	7.25	121.32	117.70
21	AA	51	A	C5-C6-N1	7.24	121.32	117.70
21	AA	270	A	N1-C6-N6	-7.24	114.25	118.60
54	BA	1276	A	N1-C6-N6	-7.24	114.25	118.60
54	BA	1359	A	N1-C6-N6	-7.24	114.25	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1384	A	C5-C6-N1	7.24	121.32	117.70
54	BA	274	C	N3-C2-O2	-7.24	116.83	121.90
21	AA	546	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2225	A	C5-C6-N1	7.24	121.32	117.70
54	BA	2556	C	N3-C2-O2	-7.24	116.83	121.90
54	BA	2676	C	N3-C2-O2	-7.24	116.83	121.90
55	BB	50	A	C4-C5-C6	-7.24	113.38	117.00
21	AA	309	A	N1-C6-N6	-7.24	114.26	118.60
54	BA	155	A	C5-C6-N1	7.24	121.32	117.70
54	BA	1877	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	433	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	1286	A	N1-C6-N6	-7.23	114.26	118.60
54	BA	1938	A	C5-C6-N1	7.23	121.32	117.70
54	BA	1419	A	C5-C6-N1	7.23	121.31	117.70
56	B5	164	ARG	NE-CZ-NH2	7.23	123.92	120.30
54	BA	2589	A	C4-C5-C6	-7.23	113.39	117.00
21	AA	280	C	N3-C2-O2	-7.23	116.84	121.90
54	BA	127	A	C5-C6-N1	7.23	121.31	117.70
54	BA	1977	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2531	A	C5-C6-N1	7.23	121.31	117.70
21	AA	815	A	C5-C6-N1	7.23	121.31	117.70
21	AA	1447	A	C5-C6-N1	7.23	121.31	117.70
54	BA	644	A	C5-C6-N1	7.23	121.31	117.70
54	BA	2900	A	C5-C6-N1	7.23	121.31	117.70
21	AA	496	A	C5-C6-N1	7.22	121.31	117.70
21	AA	629	A	C5-C6-N1	7.22	121.31	117.70
54	BA	294	A	C4-C5-C6	-7.22	113.39	117.00
54	BA	130	C	O4'-C1'-N1	7.22	113.98	108.20
54	BA	911	A	C5-C6-N1	7.22	121.31	117.70
54	BA	2758	A	C5-C6-N1	7.22	121.31	117.70
54	BA	886	A	N1-C6-N6	-7.22	114.27	118.60
54	BA	2448	A	C5-C6-N1	7.22	121.31	117.70
21	AA	1296	C	N3-C2-O2	-7.22	116.85	121.90
54	BA	1711	A	C5-C6-N1	7.22	121.31	117.70
21	AA	476	U	P-O3'-C3'	7.21	128.36	119.70
21	AA	975	A	C5-C6-N1	7.21	121.31	117.70
54	BA	482	A	C5-C6-N1	7.21	121.31	117.70
54	BA	1785	A	C5-C6-N1	7.21	121.31	117.70
9	AJ	45	ARG	NE-CZ-NH1	7.21	123.91	120.30
54	BA	866	A	C4-C5-C6	-7.21	113.39	117.00
54	BA	1905	C	N3-C2-O2	-7.21	116.85	121.90
54	BA	2764	A	N1-C6-N6	-7.21	114.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	98	A	C5-C6-N1	7.21	121.30	117.70
21	AA	553	A	C5-C6-N1	7.21	121.30	117.70
54	BA	198	C	N3-C2-O2	-7.21	116.86	121.90
54	BA	2330	G	O4'-C1'-N9	7.21	113.97	108.20
21	AA	139	A	C4-C5-C6	-7.21	113.40	117.00
21	AA	336	A	N1-C6-N6	-7.21	114.28	118.60
21	AA	502	A	C5-C6-N1	7.21	121.30	117.70
21	AA	718	A	C5-C6-N1	7.21	121.30	117.70
21	AA	1250	A	C5-C6-N1	7.21	121.30	117.70
35	BM	38	ARG	NE-CZ-NH1	7.21	123.90	120.30
55	BB	58	A	N1-C6-N6	-7.21	114.28	118.60
54	BA	478	A	C4-C5-C6	-7.21	113.40	117.00
54	BA	1090	A	N1-C6-N6	-7.21	114.28	118.60
54	BA	2566	A	N1-C6-N6	-7.21	114.28	118.60
16	AQ	10	ARG	NE-CZ-NH1	7.20	123.90	120.30
21	AA	181	A	C5-C6-N1	7.20	121.30	117.70
21	AA	238	A	C5-C6-N1	7.20	121.30	117.70
54	BA	563	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1132	C	N3-C2-O2	-7.20	116.86	121.90
22	A1	38	A	N1-C6-N6	-7.20	114.28	118.60
35	BM	114	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	330	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1354	A	C5-C6-N1	7.20	121.30	117.70
21	AA	1410	A	C4-C5-C6	-7.20	113.40	117.00
54	BA	165	A	C5-C6-N1	7.20	121.30	117.70
54	BA	722	A	C5-C6-N1	7.20	121.30	117.70
54	BA	996	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1711	A	N1-C6-N6	-7.20	114.28	118.60
54	BA	2639	A	C5-C6-N1	7.20	121.30	117.70
10	AK	68	ARG	NE-CZ-NH1	7.20	123.90	120.30
54	BA	878	A	C5-C6-N1	7.20	121.30	117.70
54	BA	1067	A	C5-C6-N1	7.20	121.30	117.70
21	AA	549	C	N3-C2-O2	-7.19	116.86	121.90
21	AA	344	A	C5-C6-N1	7.19	121.30	117.70
21	AA	716	A	C4-C5-C6	-7.19	113.40	117.00
21	AA	1054	C	N3-C2-O2	-7.19	116.86	121.90
21	AA	1136	C	O4'-C1'-N1	7.19	113.95	108.20
54	BA	141	G	O4'-C1'-N9	7.19	113.95	108.20
54	BA	227	A	C5-C6-N1	7.19	121.30	117.70
54	BA	1815	A	C4-C5-C6	-7.19	113.40	117.00
54	BA	2095	A	C4-C5-C6	-7.19	113.40	117.00
54	BA	2899	A	C4-C5-C6	-7.19	113.40	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2297	A	C5-C6-N1	7.19	121.30	117.70
54	BA	391	A	C5-C6-N1	7.19	121.30	117.70
21	AA	563	A	C5-C6-N1	7.19	121.29	117.70
54	BA	480	A	C5-C6-N1	7.19	121.29	117.70
3	AD	55	ARG	NE-CZ-NH1	7.18	123.89	120.30
21	AA	805	C	N3-C2-O2	-7.18	116.87	121.90
21	AA	899	C	N3-C2-O2	-7.18	116.87	121.90
21	AA	1197	A	C5-C6-N1	7.18	121.29	117.70
54	BA	53	A	C5-C6-N1	7.18	121.29	117.70
54	BA	348	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1269	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	631	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	2119	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	528	A	C5-C6-N1	7.18	121.29	117.70
54	BA	792	A	C5-C6-N1	7.18	121.29	117.70
54	BA	1477	A	N1-C6-N6	-7.18	114.29	118.60
54	BA	2792	A	C5-C6-N1	7.18	121.29	117.70
21	AA	441	A	C5-C6-N1	7.18	121.29	117.70
22	A1	66	A	C5-C6-N1	7.18	121.29	117.70
21	AA	1012	A	C5-C6-N1	7.17	121.29	117.70
24	A3	36	A	C5-C6-N1	7.17	121.29	117.70
26	BD	128	ARG	NE-CZ-NH2	7.17	123.89	120.30
54	BA	1373	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	1583	A	C5-C6-N1	7.17	121.29	117.70
54	BA	2422	C	N1-C2-O2	7.17	123.20	118.90
22	A1	27	C	N3-C2-O2	-7.17	116.88	121.90
21	AA	794	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1112	G	O4'-C1'-N9	7.17	113.94	108.20
54	BA	1701	A	C5-C6-N1	7.17	121.29	117.70
54	BA	1803	A	C5-C6-N1	7.17	121.28	117.70
21	AA	753	A	N1-C6-N6	-7.17	114.30	118.60
21	AA	1433	A	C5-C6-N1	7.17	121.28	117.70
25	BC	68	ARG	NE-CZ-NH1	7.17	123.88	120.30
21	AA	1306	A	N1-C6-N6	-7.17	114.30	118.60
24	A3	17	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	53	A	N1-C6-N6	-7.17	114.30	118.60
54	BA	787	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	1493	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	2090	A	C5-C6-N1	7.17	121.28	117.70
54	BA	2214	C	N3-C2-O2	-7.17	116.88	121.90
54	BA	2531	A	N1-C6-N6	-7.17	114.30	118.60
21	AA	160	A	C4-C5-C6	-7.17	113.42	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1244	A	C5-C6-N1	7.17	121.28	117.70
21	AA	747	A	C5-C6-N1	7.16	121.28	117.70
21	AA	1037	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	480	A	N1-C6-N6	-7.16	114.30	118.60
54	BA	829	A	C5-C6-N1	7.16	121.28	117.70
21	AA	10	A	N1-C6-N6	-7.16	114.30	118.60
43	BU	5	ARG	NE-CZ-NH1	7.16	123.88	120.30
54	BA	2066	C	N3-C2-O2	-7.16	116.89	121.90
54	BA	2170	A	C5-C6-N1	7.16	121.28	117.70
21	AA	574	A	C5-C6-N1	7.16	121.28	117.70
21	AA	716	A	C5-C6-N1	7.16	121.28	117.70
54	BA	529	A	C5-C6-N1	7.16	121.28	117.70
54	BA	1713	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	777	A	C5-C6-N1	7.16	121.28	117.70
21	AA	1362	A	C4-C5-C6	-7.16	113.42	117.00
54	BA	300	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2058	A	C5-C6-N1	7.16	121.28	117.70
54	BA	2326	C	N3-C2-O2	-7.16	116.89	121.90
55	BB	104	A	C4-C5-C6	-7.16	113.42	117.00
21	AA	151	A	C4-C5-C6	-7.15	113.42	117.00
25	BC	42	ARG	NE-CZ-NH1	7.15	123.88	120.30
54	BA	1070	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1142	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	595	A	C5-C6-N1	7.15	121.28	117.70
21	AA	1093	A	N1-C6-N6	-7.15	114.31	118.60
21	AA	1111	A	C4-C5-C6	-7.15	113.42	117.00
54	BA	602	A	C5-C6-N1	7.15	121.28	117.70
54	BA	1809	A	C5-C6-N1	7.15	121.28	117.70
21	AA	1395	C	N3-C2-O2	-7.15	116.90	121.90
33	BK	18	ARG	NE-CZ-NH1	7.15	123.88	120.30
54	BA	899	A	C5-C6-N1	7.15	121.28	117.70
54	BA	403	U	O4'-C1'-N1	7.15	113.92	108.20
54	BA	676	A	C4-C5-C6	-7.15	113.43	117.00
54	BA	1027	A	C5-C6-N1	7.15	121.27	117.70
54	BA	2199	A	C5-C6-N1	7.15	121.27	117.70
54	BA	2211	A	O4'-C1'-N9	7.15	113.92	108.20
21	AA	58	C	N3-C2-O2	-7.15	116.90	121.90
51	B2	21	ARG	NE-CZ-NH1	7.15	123.87	120.30
54	BA	637	A	C5-C6-N1	7.15	121.27	117.70
54	BA	1353	A	C5-C6-N1	7.15	121.27	117.70
9	AJ	7	ARG	NE-CZ-NH2	7.14	123.87	120.30
54	BA	1508	A	C5-C6-N1	7.14	121.27	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1625	C	O4'-C1'-N1	7.14	113.92	108.20
21	AA	28	A	C4-C5-C6	-7.14	113.43	117.00
21	AA	1462	C	N3-C2-O2	-7.14	116.90	121.90
54	BA	344	A	C5-C6-N1	7.14	121.27	117.70
54	BA	1367	A	N1-C6-N6	-7.14	114.31	118.60
2	AC	178	ARG	NE-CZ-NH1	7.14	123.87	120.30
21	AA	85	U	O4'-C1'-N1	7.14	113.91	108.20
21	AA	80	A	C5-C6-N1	7.14	121.27	117.70
54	BA	145	C	N3-C2-O2	-7.14	116.91	121.90
21	AA	1130	A	C5-C6-N1	7.13	121.27	117.70
25	BC	237	ARG	NE-CZ-NH1	7.13	123.87	120.30
21	AA	1080	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1043	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	2336	A	N1-C6-N6	-7.13	114.32	118.60
54	BA	342	A	C5-C6-N1	7.13	121.27	117.70
54	BA	1746	A	C5-C6-N1	7.13	121.27	117.70
55	BB	115	A	C4-C5-C6	-7.13	113.43	117.00
36	BN	64	ARG	NE-CZ-NH1	7.13	123.86	120.30
44	BV	21	ARG	NE-CZ-NH1	7.13	123.86	120.30
54	BA	1816	C	N3-C2-O2	-7.13	116.91	121.90
54	BA	1876	A	C5-C6-N1	7.13	121.27	117.70
23	A2	89	U	P-O3'-C3'	7.13	128.25	119.70
21	AA	642	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2134	A	C5-C6-N1	7.12	121.26	117.70
21	AA	864	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	627	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	1105	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1188	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	94	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2530	A	C5-C6-N1	7.12	121.26	117.70
22	A1	9	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2037	A	C4-C5-C6	-7.12	113.44	117.00
21	AA	1480	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	1916	A	C4-C5-C6	-7.12	113.44	117.00
54	BA	2198	A	C5-C6-N1	7.12	121.26	117.70
54	BA	2469	A	C5-C6-N1	7.12	121.26	117.70
21	AA	1299	A	N1-C6-N6	-7.12	114.33	118.60
54	BA	2715	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	1149	C	N3-C2-O2	-7.12	116.92	121.90
21	AA	1503	A	C5-C6-N1	7.12	121.26	117.70
54	BA	661	A	O4'-C1'-N9	7.12	113.89	108.20
21	AA	784	A	N1-C6-N6	-7.11	114.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1342	C	N3-C2-O2	-7.11	116.92	121.90
54	BA	217	A	C5-C6-N1	7.11	121.26	117.70
54	BA	1503	A	C4-C5-C6	-7.11	113.44	117.00
54	BA	2169	A	C5-C6-N1	7.11	121.25	117.70
54	BA	2426	A	N1-C6-N6	-7.11	114.33	118.60
21	AA	681	A	C4-C5-C6	-7.11	113.45	117.00
54	BA	2666	C	N1-C2-O2	7.11	123.17	118.90
21	AA	1101	A	C4-C5-C6	-7.11	113.45	117.00
35	BM	50	ARG	NE-CZ-NH1	7.11	123.85	120.30
54	BA	361	G	O4'-C1'-N9	7.11	113.89	108.20
54	BA	478	A	C5-C6-N1	7.11	121.25	117.70
54	BA	709	U	O4'-C1'-N1	7.11	113.89	108.20
54	BA	2587	A	C5-C6-N1	7.11	121.25	117.70
21	AA	1340	A	C5-C6-N1	7.11	121.25	117.70
39	BQ	63	ARG	NE-CZ-NH1	7.11	123.85	120.30
49	B0	15	ARG	NE-CZ-NH1	7.11	123.85	120.30
54	BA	2171	A	C4-C5-C6	-7.11	113.45	117.00
21	AA	1456	A	C5-C6-N1	7.10	121.25	117.70
54	BA	471	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	742	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	783	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1827	U	O4'-C1'-N1	7.10	113.88	108.20
54	BA	2097	A	C5-C6-N1	7.10	121.25	117.70
21	AA	207	C	N3-C2-O2	-7.10	116.93	121.90
54	BA	735	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1322	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1791	A	C5-C6-N1	7.10	121.25	117.70
54	BA	781	A	N1-C6-N6	-7.10	114.34	118.60
54	BA	782	A	C5-C6-N1	7.10	121.25	117.70
54	BA	1304	A	C4-C5-C6	-7.10	113.45	117.00
54	BA	1665	A	N1-C6-N6	-7.10	114.34	118.60
11	AL	49	ARG	NE-CZ-NH1	7.09	123.85	120.30
19	AT	73	ARG	NE-CZ-NH1	7.09	123.85	120.30
21	AA	726	C	N3-C2-O2	-7.09	116.93	121.90
21	AA	1251	A	C5-C6-N1	7.09	121.25	117.70
21	AA	990	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	294	A	C5-C6-N1	7.09	121.25	117.70
21	AA	215	C	N3-C2-O2	-7.09	116.94	121.90
39	BQ	27	ARG	NE-CZ-NH1	7.09	123.85	120.30
54	BA	1434	A	C5-C6-N1	7.09	121.25	117.70
54	BA	2227	A	C5-C6-N1	7.09	121.25	117.70
24	A3	76	C	N1-C2-O2	7.09	123.15	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	63	A	C5-C6-N1	7.09	121.25	117.70
54	BA	1918	A	C5-C6-N1	7.09	121.25	117.70
2	AC	58	ARG	NE-CZ-NH1	7.09	123.84	120.30
21	AA	1092	A	C5-C6-N1	7.09	121.24	117.70
21	AA	1230	C	N3-C2-O2	-7.09	116.94	121.90
21	AA	1262	C	N3-C2-O2	-7.09	116.94	121.90
54	BA	749	A	C5-C6-N1	7.09	121.24	117.70
54	BA	1027	A	N1-C6-N6	-7.09	114.35	118.60
54	BA	1084	A	C5-C6-N1	7.09	121.24	117.70
54	BA	2037	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1889	A	C5-C6-N1	7.08	121.24	117.70
54	BA	2275	C	N3-C2-O2	-7.08	116.94	121.90
54	BA	2347	C	N3-C2-O2	-7.08	116.94	121.90
21	AA	66	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	1699	G	O4'-C1'-N9	7.08	113.86	108.20
54	BA	2097	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	2753	A	N1-C6-N6	-7.08	114.35	118.60
20	AU	16	ARG	NE-CZ-NH1	7.08	123.84	120.30
21	AA	161	A	C5-C6-N1	7.08	121.24	117.70
24	A3	14	A	C5-C6-N1	7.08	121.24	117.70
54	BA	529	A	N1-C6-N6	-7.08	114.35	118.60
54	BA	1348	C	O4'-C1'-N1	7.08	113.86	108.20
54	BA	1392	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1528	A	C5-C6-N1	7.08	121.24	117.70
54	BA	142	A	C5-C6-N1	7.08	121.24	117.70
54	BA	523	C	N3-C2-O2	-7.08	116.95	121.90
21	AA	1109	C	N3-C2-O2	-7.08	116.95	121.90
21	AA	1329	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	190	A	C5-C6-N1	7.08	121.24	117.70
54	BA	661	A	C4-C5-C6	-7.08	113.46	117.00
54	BA	1545	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1597	A	C5-C6-N1	7.08	121.24	117.70
54	BA	1901	A	C4-C5-C6	-7.08	113.46	117.00
28	BF	177	ARG	NE-CZ-NH1	7.07	123.84	120.30
54	BA	173	A	C5-C6-N1	7.07	121.24	117.70
54	BA	1226	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	1260	A	C5-C6-N1	7.07	121.24	117.70
54	BA	717	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1286	A	C5-C6-N1	7.07	121.24	117.70
54	BA	2902	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	191	A	C5-C6-N1	7.07	121.24	117.70
54	BA	677	A	C5-C6-N1	7.07	121.23	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1630	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	1744	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	1872	A	C4-C5-C6	-7.07	113.47	117.00
54	BA	2173	A	C5-C6-N1	7.07	121.23	117.70
54	BA	2440	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	1958	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	2657	A	C5-C6-N1	7.07	121.23	117.70
21	AA	188	C	N3-C2-O2	-7.07	116.95	121.90
21	AA	979	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	914	G	O4'-C1'-N9	7.07	113.86	108.20
21	AA	553	A	N1-C6-N6	-7.07	114.36	118.60
54	BA	556	A	C5-C6-N1	7.07	121.23	117.70
54	BA	575	A	C5-C6-N1	7.07	121.23	117.70
54	BA	645	C	N3-C2-O2	-7.07	116.95	121.90
54	BA	2070	A	C4-C5-C6	-7.07	113.47	117.00
24	A3	1	C	N3-C2-O2	-7.06	116.95	121.90
24	A3	44	A	C5-C6-N1	7.06	121.23	117.70
21	AA	501	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	1100	C	N3-C2-O2	-7.06	116.96	121.90
54	BA	19	A	C5-C6-N1	7.06	121.23	117.70
54	BA	1509	A	N1-C6-N6	-7.06	114.36	118.60
54	BA	324	A	C5-C6-N1	7.06	121.23	117.70
2	AC	126	ARG	NE-CZ-NH1	7.06	123.83	120.30
54	BA	497	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	526	A	C5-C6-N1	7.06	121.23	117.70
21	AA	199	A	C4-C5-C6	-7.06	113.47	117.00
21	AA	624	C	N3-C2-O2	-7.06	116.96	121.90
21	AA	1246	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	423	A	C5-C6-N1	7.06	121.23	117.70
54	BA	945	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2412	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2725	A	C5-C6-N1	7.06	121.23	117.70
54	BA	2734	A	C4-C5-C6	-7.06	113.47	117.00
22	A1	21	A	C4-C5-C6	-7.06	113.47	117.00
54	BA	2743	U	O4'-C1'-N1	7.06	113.84	108.20
31	BI	64	ARG	NE-CZ-NH1	7.05	123.83	120.30
54	BA	1966	A	C5-C6-N1	7.05	121.23	117.70
54	BA	2015	A	C5-C6-N1	7.05	121.23	117.70
51	B2	14	ARG	NE-CZ-NH1	7.05	123.83	120.30
54	BA	142	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	1029	A	C4-C5-C6	-7.05	113.47	117.00
21	AA	51	A	C4-C5-C6	-7.05	113.47	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	983	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	1427	A	C5-C6-N1	7.05	121.23	117.70
54	BA	1676	A	C5-C6-N1	7.05	121.23	117.70
54	BA	2612	C	N3-C2-O2	-7.05	116.96	121.90
54	BA	205	G	O4'-C1'-N9	7.05	113.84	108.20
54	BA	2322	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2566	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2820	A	C4-C5-C6	-7.05	113.48	117.00
54	BA	34	U	O4'-C1'-N1	7.05	113.84	108.20
54	BA	371	A	O4'-C1'-N9	7.05	113.84	108.20
21	AA	1000	A	N1-C6-N6	-7.05	114.37	118.60
54	BA	1387	A	C5-C6-N1	7.05	121.22	117.70
54	BA	1616	A	C5-C6-N1	7.05	121.22	117.70
54	BA	2309	A	C5-C6-N1	7.05	121.22	117.70
54	BA	457	A	C5-C6-N1	7.04	121.22	117.70
54	BA	788	A	C4-C5-C6	-7.04	113.48	117.00
21	AA	533	A	C5-C6-N1	7.04	121.22	117.70
21	AA	1170	A	C4-C5-C6	-7.04	113.48	117.00
54	BA	1953	A	C4-C5-C6	-7.04	113.48	117.00
22	A1	38	A	C5-C6-N1	7.04	121.22	117.70
52	B3	29	ARG	NE-CZ-NH1	7.04	123.82	120.30
54	BA	1378	A	C5-C6-N1	7.04	121.22	117.70
54	BA	1615	C	N3-C2-O2	-7.04	116.97	121.90
54	BA	2288	A	N1-C6-N6	-7.04	114.38	118.60
54	BA	2391	G	O4'-C1'-N9	7.04	113.83	108.20
54	BA	2619	C	O4'-C1'-N1	7.04	113.83	108.20
21	AA	298	A	C5-C6-N1	7.04	121.22	117.70
9	AJ	9	ARG	NE-CZ-NH2	-7.03	116.78	120.30
54	BA	2700	A	C5-C6-N1	7.03	121.22	117.70
21	AA	1480	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1039	A	C5-C6-N1	7.03	121.22	117.70
54	BA	1420	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2706	A	C5-C6-N1	7.03	121.22	117.70
21	AA	729	A	C5-C6-N1	7.03	121.22	117.70
21	AA	1012	A	N1-C6-N6	-7.03	114.38	118.60
21	AA	1437	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	443	A	C4-C5-C6	-7.03	113.48	117.00
54	BA	2060	A	N1-C6-N6	-7.03	114.38	118.60
54	BA	2126	A	C5-C6-N1	7.03	121.22	117.70
54	BA	2364	C	O4'-C1'-N1	7.03	113.83	108.20
54	BA	1618	A	C5-C6-N1	7.03	121.21	117.70
45	BW	13	ARG	NE-CZ-NH1	7.03	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	144	A	C5-C6-N1	7.03	121.21	117.70
54	BA	511	U	O4'-C1'-N1	7.03	113.82	108.20
54	BA	1287	A	C5-C6-N1	7.03	121.21	117.70
54	BA	1760	C	N3-C2-O2	-7.03	116.98	121.90
54	BA	1040	A	C5-C6-N1	7.03	121.21	117.70
54	BA	820	A	N1-C6-N6	-7.02	114.39	118.60
54	BA	1152	C	N3-C2-O2	-7.02	116.98	121.90
54	BA	1314	C	N1-C2-O2	7.02	123.11	118.90
54	BA	111	A	C5-C6-N1	7.02	121.21	117.70
21	AA	171	A	C4-C5-C6	-7.02	113.49	117.00
21	AA	1027	C	N3-C2-O2	-7.02	116.99	121.90
25	BC	174	ARG	NE-CZ-NH1	7.02	123.81	120.30
54	BA	479	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	972	A	C5-C6-N1	7.02	121.21	117.70
21	AA	329	A	C4-C5-C6	-7.02	113.49	117.00
54	BA	918	A	C5-C6-N1	7.02	121.21	117.70
54	BA	2879	A	C5-C6-N1	7.02	121.21	117.70
21	AA	1289	A	N1-C6-N6	-7.01	114.39	118.60
24	A3	22	A	C1'-O4'-C4'	-7.01	104.29	109.90
24	A3	74	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1211	C	O4'-C1'-N1	7.01	113.81	108.20
54	BA	1490	A	C5-C6-N1	7.01	121.21	117.70
54	BA	1549	A	N1-C6-N6	-7.01	114.39	118.60
54	BA	1566	A	C5-C6-N1	7.01	121.21	117.70
21	AA	964	A	C5-C6-N1	7.01	121.21	117.70
3	AD	46	ARG	NE-CZ-NH1	7.01	123.81	120.30
21	AA	411	A	N1-C6-N6	-7.01	114.39	118.60
22	A1	41	A	C5-C6-N1	7.01	121.20	117.70
24	A3	58	A	C5-C6-N1	7.01	121.21	117.70
54	BA	163	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	2333	A	C5-C6-N1	7.01	121.21	117.70
54	BA	385	C	N3-C2-O2	-7.01	117.00	121.90
54	BA	1833	C	N3-C2-O2	-7.01	116.99	121.90
54	BA	2459	A	N1-C6-N6	-7.01	114.39	118.60
21	AA	1246	A	C5-C6-N1	7.01	121.20	117.70
21	AA	1248	A	C4-C5-C6	-7.01	113.50	117.00
25	BC	13	ARG	NE-CZ-NH1	7.01	123.80	120.30
54	BA	1919	A	C5-C6-N1	7.00	121.20	117.70
2	AC	163	ARG	NE-CZ-NH1	7.00	123.80	120.30
21	AA	6	G	O4'-C1'-N9	7.00	113.80	108.20
21	AA	298	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	2868	A	C5-C6-N1	7.00	121.20	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AM	70	ARG	NE-CZ-NH1	7.00	123.80	120.30
21	AA	143	A	N1-C6-N6	-7.00	114.40	118.60
54	BA	264	C	N3-C2-O2	-7.00	117.00	121.90
54	BA	2001	C	N3-C2-O2	-7.00	117.00	121.90
42	BT	12	ARG	NE-CZ-NH1	7.00	123.80	120.30
54	BA	910	A	C5-C6-N1	7.00	121.20	117.70
54	BA	2126	A	C4-C5-C6	-7.00	113.50	117.00
54	BA	262	A	C5-C6-N1	7.00	121.20	117.70
26	BD	179	ARG	NE-CZ-NH1	6.99	123.80	120.30
51	B2	35	ARG	NE-CZ-NH1	6.99	123.80	120.30
54	BA	727	A	C5-C6-N1	6.99	121.20	117.70
54	BA	1784	A	C5-C6-N1	6.99	121.20	117.70
37	BO	16	ARG	NE-CZ-NH1	6.99	123.80	120.30
54	BA	1773	A	C5-C6-N1	6.99	121.20	117.70
6	AG	78	ARG	NE-CZ-NH1	6.99	123.80	120.30
21	AA	958	A	C5-C6-N1	6.99	121.20	117.70
21	AA	967	C	N3-C2-O2	-6.99	117.01	121.90
54	BA	586	A	N1-C6-N6	-6.99	114.41	118.60
7	AH	87	ARG	NE-CZ-NH2	6.99	123.79	120.30
21	AA	596	A	C5-C6-N1	6.99	121.19	117.70
21	AA	1059	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	1112	C	N3-C2-O2	-6.99	117.01	121.90
21	AA	1288	A	C5-C6-N1	6.99	121.19	117.70
35	BM	40	ARG	NE-CZ-NH1	6.99	123.79	120.30
54	BA	1128	G	O4'-C1'-N9	6.99	113.79	108.20
21	AA	780	A	C4-C5-C6	-6.99	113.51	117.00
21	AA	906	A	C4-C5-C6	-6.99	113.51	117.00
54	BA	1586	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2565	A	C5-C6-N1	6.99	121.19	117.70
54	BA	2851	A	N1-C6-N6	-6.99	114.41	118.60
21	AA	197	A	C5-C6-N1	6.99	121.19	117.70
21	AA	460	A	N1-C6-N6	-6.99	114.41	118.60
54	BA	892	A	C5-C6-N1	6.99	121.19	117.70
54	BA	943	A	C5-C6-N1	6.98	121.19	117.70
21	AA	174	A	N1-C6-N6	-6.98	114.41	118.60
21	AA	465	A	C5-C6-N1	6.98	121.19	117.70
30	BH	27	ARG	NE-CZ-NH1	6.98	123.79	120.30
54	BA	362	A	C4-C5-C6	-6.98	113.51	117.00
54	BA	456	C	N3-C2-O2	-6.98	117.01	121.90
54	BA	1189	A	N1-C6-N6	-6.98	114.41	118.60
54	BA	2336	A	C5-C6-N1	6.98	121.19	117.70
54	BA	2704	C	N3-C2-O2	-6.98	117.01	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1285	A	C5-C6-N1	6.98	121.19	117.70
54	BA	10	A	C5-C6-N1	6.98	121.19	117.70
54	BA	896	A	C5-C6-N1	6.98	121.19	117.70
54	BA	1226	A	C5-C6-N1	6.98	121.19	117.70
24	A3	39	A	N1-C6-N6	-6.98	114.42	118.60
54	BA	508	A	C5-C6-N1	6.98	121.19	117.70
21	AA	286	C	N3-C2-O2	-6.97	117.02	121.90
21	AA	1317	C	N3-C2-O2	-6.97	117.02	121.90
39	BQ	54	ARG	NE-CZ-NH1	6.97	123.79	120.30
54	BA	1009	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2266	A	C4-C5-C6	-6.97	113.51	117.00
21	AA	1466	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	225	C	N3-C2-O2	-6.97	117.02	121.90
54	BA	2461	A	C5-C6-N1	6.97	121.19	117.70
54	BA	2577	A	C5-C6-N1	6.97	121.19	117.70
11	AL	35	ARG	NE-CZ-NH1	6.97	123.78	120.30
21	AA	389	A	C5-C6-N1	6.97	121.19	117.70
21	AA	435	A	C5-C6-N1	6.97	121.19	117.70
21	AA	865	A	C5-C6-N1	6.97	121.19	117.70
54	BA	371	A	C4-C5-C6	-6.97	113.52	117.00
54	BA	1469	A	C5-C6-N1	6.97	121.18	117.70
54	BA	2753	A	C5-C6-N1	6.97	121.18	117.70
21	AA	1046	A	C5-C6-N1	6.97	121.18	117.70
54	BA	324	A	C4-C5-C6	-6.97	113.52	117.00
55	BB	12	C	N3-C2-O2	-6.97	117.02	121.90
55	BB	46	A	C4-C5-C6	-6.97	113.52	117.00
21	AA	909	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	1239	A	C5-C6-N1	6.96	121.18	117.70
22	A1	58	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	503	A	C5-C6-N1	6.96	121.18	117.70
54	BA	1505	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1969	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2119	A	C5-C6-N1	6.96	121.18	117.70
13	AN	81	ARG	NE-CZ-NH1	6.96	123.78	120.30
54	BA	1268	A	C4-C5-C6	-6.96	113.52	117.00
21	AA	807	A	C5-C6-N1	6.96	121.18	117.70
22	A1	72	C	N3-C2-O2	-6.96	117.03	121.90
24	A3	38	A	C5-C6-N1	6.96	121.18	117.70
54	BA	514	A	N1-C6-N6	-6.96	114.42	118.60
54	BA	2386	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2682	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	38	A	N1-C6-N6	-6.96	114.42	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1998	A	C5-C6-N1	6.96	121.18	117.70
54	BA	2430	A	O4'-C1'-N9	6.96	113.77	108.20
21	AA	392	C	N3-C2-O2	-6.96	117.03	121.90
54	BA	1073	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	1278	C	N3-C2-O2	-6.96	117.03	121.90
24	A3	77	A	C5-C6-N1	6.96	121.18	117.70
54	BA	677	A	N1-C6-N6	-6.96	114.43	118.60
54	BA	449	A	C4-C5-C6	-6.96	113.52	117.00
54	BA	2281	A	N1-C6-N6	-6.96	114.43	118.60
21	AA	539	A	C5-C6-N1	6.95	121.18	117.70
21	AA	1063	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	6	A	C5-C6-N1	6.95	121.18	117.70
14	AO	71	ARG	NE-CZ-NH1	6.95	123.78	120.30
54	BA	897	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	1014	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1246	A	C5-C6-N1	6.95	121.17	117.70
54	BA	1902	C	N3-C2-O2	-6.95	117.03	121.90
54	BA	2393	U	O4'-C1'-N1	6.95	113.76	108.20
9	AJ	68	ARG	NE-CZ-NH1	6.95	123.77	120.30
54	BA	2820	A	C5-C6-N1	6.94	121.17	117.70
21	AA	32	A	C5-C6-N1	6.94	121.17	117.70
21	AA	1333	A	C5-C6-N1	6.94	121.17	117.70
21	AA	1340	A	C4-C5-C6	-6.94	113.53	117.00
21	AA	313	A	C5-C6-N1	6.94	121.17	117.70
54	BA	1385	A	C5-C6-N1	6.94	121.17	117.70
54	BA	2314	A	O4'-C1'-N9	6.94	113.75	108.20
54	BA	2063	C	N1-C2-O2	6.94	123.06	118.90
13	AN	63	ARG	NE-CZ-NH2	-6.94	116.83	120.30
54	BA	1415	U	O4'-C1'-N1	6.94	113.75	108.20
54	BA	2020	A	C4-C5-C6	-6.94	113.53	117.00
54	BA	2362	C	N3-C2-O2	-6.94	117.04	121.90
54	BA	1097	U	O4'-C1'-N1	6.94	113.75	108.20
54	BA	572	A	C5-C6-N1	6.93	121.17	117.70
54	BA	1503	A	C5-C6-N1	6.93	121.17	117.70
54	BA	2856	A	C4-C5-C6	-6.93	113.53	117.00
21	AA	1274	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	404	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	2205	A	N1-C6-N6	-6.93	114.44	118.60
54	BA	2560	A	C4-C5-C6	-6.93	113.53	117.00
54	BA	2712	C	N3-C2-O2	-6.93	117.05	121.90
54	BA	2726	A	C4-C5-C6	-6.93	113.54	117.00
21	AA	1069	C	N3-C2-O2	-6.93	117.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1380	U	P-O3'-C3'	6.93	128.01	119.70
21	AA	1476	A	C5-C6-N1	6.93	121.16	117.70
54	BA	2823	A	C5-C6-N1	6.93	121.16	117.70
54	BA	2826	A	C5-C6-N1	6.93	121.16	117.70
43	BU	21	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	541	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	1261	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	344	A	C4-C5-C6	-6.92	113.54	117.00
54	BA	925	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	2628	C	O4'-C1'-N1	6.92	113.74	108.20
54	BA	2727	A	C4-C5-C6	-6.92	113.54	117.00
21	AA	648	A	C5-C6-N1	6.92	121.16	117.70
21	AA	797	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	1739	A	N1-C6-N6	-6.92	114.45	118.60
54	BA	1853	A	C5-C6-N1	6.92	121.16	117.70
15	AP	70	ARG	NE-CZ-NH1	6.92	123.76	120.30
54	BA	302	C	N3-C2-O2	-6.92	117.06	121.90
54	BA	1877	A	C5-C6-N1	6.92	121.16	117.70
48	BZ	37	ARG	NE-CZ-NH1	6.91	123.76	120.30
54	BA	1691	C	N3-C2-O2	-6.91	117.06	121.90
21	AA	1502	A	O4'-C1'-N9	6.91	113.73	108.20
54	BA	1046	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	1836	C	N3-C2-O2	-6.91	117.06	121.90
54	BA	2082	A	C5-C6-N1	6.91	121.16	117.70
54	BA	2388	A	C5-C6-N1	6.91	121.16	117.70
21	AA	983	A	C5-C6-N1	6.91	121.15	117.70
54	BA	1987	A	N1-C6-N6	-6.91	114.45	118.60
54	BA	632	A	C4-C5-C6	-6.91	113.55	117.00
54	BA	730	A	C5-C6-N1	6.91	121.15	117.70
54	BA	1057	A	C5-C6-N1	6.91	121.15	117.70
54	BA	1537	G	O4'-C1'-N9	6.91	113.72	108.20
21	AA	826	C	N3-C2-O2	-6.90	117.07	121.90
21	AA	353	A	C5-C6-N1	6.90	121.15	117.70
23	A2	85	G	C5'-C4'-C3'	-6.90	104.96	116.00
42	BT	6	ARG	NE-CZ-NH2	6.90	123.75	120.30
54	BA	1045	C	O4'-C1'-N1	6.90	113.72	108.20
54	BA	1912	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2077	A	N1-C6-N6	-6.90	114.46	118.60
54	BA	2900	A	N1-C6-N6	-6.90	114.46	118.60
15	AP	28	ARG	NE-CZ-NH1	6.90	123.75	120.30
21	AA	116	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1596	A	N1-C6-N6	-6.90	114.46	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	655	A	C5-C6-N1	6.90	121.15	117.70
21	AA	1163	A	C4-C5-C6	-6.90	113.55	117.00
22	A1	76	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1652	A	C5-C6-N1	6.90	121.15	117.70
54	BA	2463	C	O4'-C1'-N1	6.90	113.72	108.20
21	AA	714	G	N3-C2-N2	-6.90	115.07	119.90
21	AA	892	A	C5-C6-N1	6.90	121.15	117.70
54	BA	1591	A	C4-C5-C6	-6.90	113.55	117.00
54	BA	2227	A	C4-C5-C6	-6.90	113.55	117.00
21	AA	44	A	C5-C6-N1	6.89	121.15	117.70
12	AM	78	ARG	NE-CZ-NH1	6.89	123.75	120.30
21	AA	1200	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	973	A	C5-C6-N1	6.89	121.15	117.70
21	AA	136	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	1269	A	C5-C6-N1	6.89	121.15	117.70
54	BA	878	A	C4-C5-C6	-6.89	113.55	117.00
54	BA	2432	A	C4-C5-C6	-6.89	113.56	117.00
21	AA	1216	A	C5-C6-N1	6.89	121.14	117.70
21	AA	1428	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	795	C	N3-C2-O2	-6.89	117.08	121.90
54	BA	1241	A	C5-C6-N1	6.89	121.14	117.70
21	AA	131	A	C4-C5-C6	-6.89	113.56	117.00
54	BA	226	A	C5-C6-N1	6.89	121.14	117.70
54	BA	2165	C	N3-C2-O2	-6.89	117.08	121.90
21	AA	602	A	C5-C6-N1	6.88	121.14	117.70
21	AA	642	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	978	A	C5-C6-N1	6.88	121.14	117.70
4	AE	19	ARG	NE-CZ-NH1	6.88	123.74	120.30
31	BI	133	ARG	NE-CZ-NH1	6.88	123.74	120.30
54	BA	147	C	N3-C2-O2	-6.88	117.08	121.90
54	BA	2598	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	383	A	N1-C6-N6	-6.88	114.47	118.60
21	AA	1105	A	C4-C5-C6	-6.88	113.56	117.00
21	AA	1430	A	N1-C6-N6	-6.88	114.47	118.60
22	A1	66	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	83	A	C5-C6-N1	6.88	121.14	117.70
54	BA	819	A	C5-C6-N1	6.88	121.14	117.70
21	AA	1226	C	N3-C2-O2	-6.88	117.08	121.90
21	AA	1396	A	C4-C5-C6	-6.88	113.56	117.00
54	BA	2872	A	C5-C6-N1	6.88	121.14	117.70
54	BA	1895	C	N3-C2-O2	-6.88	117.09	121.90
21	AA	196	A	C5-C6-N1	6.88	121.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	660	C	N3-C2-O2	-6.88	117.09	121.90
21	AA	974	A	C4-C5-C6	-6.87	113.56	117.00
21	AA	1274	A	C5-C6-N1	6.87	121.14	117.70
54	BA	854	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	928	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	1156	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	1247	A	C5-C6-N1	6.87	121.14	117.70
54	BA	1536	C	N3-C2-O2	-6.87	117.09	121.90
21	AA	782	A	C5-C6-N1	6.87	121.14	117.70
54	BA	226	A	N1-C6-N6	-6.87	114.48	118.60
54	BA	941	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	2736	A	C5-C6-N1	6.87	121.14	117.70
54	BA	472	A	C4-C5-C6	-6.87	113.56	117.00
54	BA	513	A	N1-C6-N6	-6.87	114.48	118.60
21	AA	55	A	C5-C6-N1	6.87	121.14	117.70
21	AA	576	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	2527	C	N3-C2-O2	-6.87	117.09	121.90
23	A2	82	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	125	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1270	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	1532	A	C5-C6-N1	6.87	121.13	117.70
54	BA	1745	A	C4-C5-C6	-6.87	113.57	117.00
54	BA	2534	A	C5-C6-N1	6.87	121.13	117.70
54	BA	2880	C	N3-C2-O2	-6.87	117.09	121.90
54	BA	239	C	N3-C2-O2	-6.86	117.09	121.90
54	BA	1902	C	O4'-C1'-N1	6.86	113.69	108.20
37	BO	10	ARG	NE-CZ-NH1	6.86	123.73	120.30
46	BX	10	ARG	NE-CZ-NH1	6.86	123.73	120.30
54	BA	503	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	802	A	C5-C6-N1	6.86	121.13	117.70
54	BA	95	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1414	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	1717	A	N1-C6-N6	-6.86	114.48	118.60
54	BA	2422	C	O4'-C1'-N1	6.86	113.69	108.20
21	AA	897	C	N3-C2-O2	-6.86	117.10	121.90
21	AA	1169	A	C4-C5-C6	-6.86	113.57	117.00
21	AA	535	A	C5-C6-N1	6.86	121.13	117.70
24	A3	39	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1213	A	C5-C6-N1	6.86	121.13	117.70
54	BA	1928	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2517	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2806	C	N3-C2-O2	-6.86	117.10	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	401	A	N1-C6-N6	-6.86	114.49	118.60
54	BA	522	A	C5-C6-N1	6.86	121.13	117.70
54	BA	984	A	C5-C6-N1	6.86	121.13	117.70
54	BA	2226	C	N3-C2-O2	-6.86	117.10	121.90
54	BA	2590	A	C4-C5-C6	-6.86	113.57	117.00
54	BA	270	A	C5-C6-N1	6.85	121.13	117.70
21	AA	890	G	O4'-C1'-N9	6.85	113.68	108.20
54	BA	1626	A	C5-C6-N1	6.85	121.13	117.70
54	BA	1689	A	N1-C6-N6	-6.85	114.49	118.60
21	AA	309	A	C5-C6-N1	6.85	121.12	117.70
54	BA	1580	A	C5-C6-N1	6.85	121.12	117.70
54	BA	2176	A	C5-C6-N1	6.85	121.12	117.70
21	AA	270	A	C4-C5-C6	-6.85	113.58	117.00
54	BA	804	A	C5-C6-N1	6.85	121.12	117.70
54	BA	1681	G	O4'-C1'-N9	6.84	113.68	108.20
54	BA	1808	A	O4'-C1'-N9	6.84	113.67	108.20
21	AA	270	A	C5-C6-N1	6.84	121.12	117.70
21	AA	71	A	C5-C6-N1	6.84	121.12	117.70
21	AA	1102	A	N1-C6-N6	-6.84	114.50	118.60
54	BA	2427	C	N3-C2-O2	-6.84	117.11	121.90
54	BA	354	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1134	A	C5-C6-N1	6.84	121.12	117.70
54	BA	1385	A	C4-C5-C6	-6.84	113.58	117.00
54	BA	2094	A	N1-C6-N6	-6.84	114.50	118.60
36	BN	86	ARG	NE-CZ-NH1	6.84	123.72	120.30
29	BG	169	ARG	NE-CZ-NH1	6.84	123.72	120.30
54	BA	586	A	C5-C6-N1	6.84	121.12	117.70
54	BA	839	U	O4'-C1'-N1	6.84	113.67	108.20
54	BA	1007	C	O4'-C1'-N1	6.84	113.67	108.20
25	BC	101	ARG	NE-CZ-NH1	6.83	123.72	120.30
54	BA	2705	A	C5-C6-N1	6.83	121.12	117.70
54	BA	1181	U	O4'-C1'-N1	6.83	113.67	108.20
54	BA	2757	A	C5-C6-N1	6.83	121.12	117.70
21	AA	746	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	118	A	C4-C5-C6	-6.83	113.58	117.00
54	BA	782	A	N1-C6-N6	-6.83	114.50	118.60
21	AA	715	A	C5-C6-N1	6.83	121.11	117.70
54	BA	203	A	N1-C6-N6	-6.83	114.50	118.60
54	BA	927	A	C5-C6-N1	6.83	121.11	117.70
54	BA	1954	G	O4'-C1'-N9	6.83	113.66	108.20
51	B2	3	ARG	NE-CZ-NH1	6.83	123.71	120.30
54	BA	560	C	N3-C2-O2	-6.83	117.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1548	A	C5-C6-N1	6.83	121.11	117.70
6	AG	2	ARG	NE-CZ-NH2	6.83	123.71	120.30
21	AA	155	A	C4-C5-C6	-6.83	113.59	117.00
21	AA	262	A	C5-C6-N1	6.83	121.11	117.70
54	BA	718	A	O4'-C1'-N9	6.83	113.66	108.20
54	BA	1802	A	C5-C6-N1	6.83	121.11	117.70
54	BA	2740	A	C4-C5-C6	-6.83	113.59	117.00
11	AL	109	ARG	NE-CZ-NH1	6.82	123.71	120.30
21	AA	1163	A	C5-C6-N1	6.82	121.11	117.70
55	BB	46	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1092	C	O4'-C1'-N1	6.82	113.66	108.20
54	BA	2051	A	C5-C6-N1	6.82	121.11	117.70
21	AA	1066	C	N3-C2-O2	-6.82	117.13	121.90
22	A1	35	A	C5-C6-N1	6.82	121.11	117.70
54	BA	603	A	C5-C6-N1	6.82	121.11	117.70
54	BA	917	A	C5-C6-N1	6.82	121.11	117.70
54	BA	1960	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	2284	A	C5-C6-N1	6.82	121.11	117.70
2	AC	171	ARG	NE-CZ-NH1	6.82	123.71	120.30
54	BA	79	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	1044	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	1142	A	C5-C6-N1	6.82	121.11	117.70
54	BA	2810	A	C5-C6-N1	6.82	121.11	117.70
21	AA	510	A	C5-C6-N1	6.82	121.11	117.70
21	AA	1210	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	430	A	C5-C6-N1	6.82	121.11	117.70
54	BA	737	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	1990	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	2358	A	C4-C5-C6	-6.82	113.59	117.00
54	BA	2516	A	C4-C5-C6	-6.82	113.59	117.00
21	AA	1267	C	N3-C2-O2	-6.82	117.13	121.90
21	AA	1322	C	N3-C2-O2	-6.82	117.13	121.90
54	BA	1739	A	C5-C6-N1	6.82	121.11	117.70
21	AA	546	A	C4-C5-C6	-6.81	113.59	117.00
54	BA	1676	A	N1-C6-N6	-6.81	114.51	118.60
4	AE	92	ARG	NE-CZ-NH1	6.81	123.70	120.30
21	AA	19	A	C5-C6-N1	6.81	121.10	117.70
21	AA	949	A	C4-C5-C6	-6.81	113.60	117.00
21	AA	1368	A	C5-C6-N1	6.81	121.10	117.70
54	BA	1634	A	C4-C5-C6	-6.81	113.60	117.00
54	BA	2840	C	N3-C2-O2	-6.81	117.13	121.90
21	AA	179	A	C4-C5-C6	-6.81	113.60	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2783	U	O4'-C1'-N1	6.81	113.64	108.20
24	A3	44	A	N1-C6-N6	-6.80	114.52	118.60
54	BA	184	C	O4'-C1'-N1	6.80	113.64	108.20
54	BA	347	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1010	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1640	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2559	C	N3-C2-O2	-6.80	117.14	121.90
21	AA	715	A	N1-C6-N6	-6.80	114.52	118.60
21	AA	1513	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1035	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1376	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	1495	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2179	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	2333	A	C4-C5-C6	-6.80	113.60	117.00
54	BA	2352	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2733	A	C5-C6-N1	6.80	121.10	117.70
7	AH	12	ARG	NE-CZ-NH2	-6.80	116.90	120.30
21	AA	1110	A	C5-C6-N1	6.80	121.10	117.70
21	AA	1396	A	C5-C6-N1	6.80	121.10	117.70
54	BA	352	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1502	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2287	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2006	C	N3-C2-O2	-6.80	117.14	121.90
54	BA	2094	A	C5-C6-N1	6.80	121.10	117.70
14	AO	53	ARG	NE-CZ-NH1	6.80	123.70	120.30
54	BA	1744	A	C5-C6-N1	6.80	121.10	117.70
54	BA	2019	A	N1-C6-N6	-6.80	114.52	118.60
55	BB	58	A	C5-C6-N1	6.80	121.10	117.70
54	BA	1551	A	C4-C5-C6	-6.79	113.60	117.00
22	A1	51	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	2238	G	O4'-C1'-N9	6.79	113.64	108.20
21	AA	906	A	C5-C6-N1	6.79	121.10	117.70
54	BA	557	C	N3-C2-O2	-6.79	117.14	121.90
54	BA	922	C	N3-C2-O2	-6.79	117.15	121.90
54	BA	2738	A	N1-C6-N6	-6.79	114.53	118.60
21	AA	487	A	C5-C6-N1	6.79	121.09	117.70
21	AA	975	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	502	A	N1-C6-N6	-6.79	114.53	118.60
21	AA	530	G	O4'-C1'-N9	6.79	113.63	108.20
21	AA	1257	A	C5-C6-N1	6.79	121.09	117.70
54	BA	1352	U	N3-C2-O2	-6.79	117.45	122.20
55	BB	94	A	C4-C5-C6	-6.79	113.61	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	325	A	C4-C5-C6	-6.79	113.61	117.00
54	BA	825	A	C4-C5-C6	-6.79	113.61	117.00
21	AA	1383	C	N3-C2-O2	-6.79	117.15	121.90
36	BN	63	ARG	NE-CZ-NH1	6.79	123.69	120.30
21	AA	1343	G	N3-C2-N2	-6.78	115.15	119.90
54	BA	1443	U	O4'-C1'-N1	6.78	113.63	108.20
54	BA	1882	U	O4'-C1'-N1	6.78	113.63	108.20
54	BA	1480	C	N3-C2-O2	-6.78	117.15	121.90
21	AA	1036	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2420	C	N3-C2-O2	-6.78	117.15	121.90
6	AG	3	ARG	NE-CZ-NH1	6.78	123.69	120.30
54	BA	1759	A	C5-C6-N1	6.78	121.09	117.70
54	BA	1819	A	C5-C6-N1	6.78	121.09	117.70
54	BA	2778	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	949	A	C5-C6-N1	6.78	121.09	117.70
21	AA	1402	C	N3-C2-O2	-6.78	117.16	121.90
54	BA	382	A	C5-C6-N1	6.78	121.09	117.70
54	BA	781	A	C5-C6-N1	6.78	121.09	117.70
54	BA	990	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	1669	A	C5-C6-N1	6.78	121.09	117.70
21	AA	648	A	C4-C5-C6	-6.78	113.61	117.00
54	BA	2749	A	C4-C5-C6	-6.78	113.61	117.00
21	AA	23	C	N3-C2-O2	-6.77	117.16	121.90
30	BH	68	ARG	NE-CZ-NH1	6.77	123.69	120.30
54	BA	203	A	C5-C6-N1	6.77	121.09	117.70
54	BA	1147	A	C4-C5-C6	-6.77	113.61	117.00
8	AI	129	ARG	NE-CZ-NH1	6.77	123.69	120.30
21	AA	665	A	C4-C5-C6	-6.77	113.61	117.00
21	AA	1254	A	C5-C6-N1	6.77	121.08	117.70
33	BK	78	ARG	NE-CZ-NH1	6.77	123.69	120.30
54	BA	84	A	C5-C6-N1	6.77	121.08	117.70
54	BA	140	C	N3-C2-O2	-6.77	117.16	121.90
21	AA	1196	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2142	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2183	A	C5-C6-N1	6.77	121.08	117.70
54	BA	2411	A	C4-C5-C6	-6.77	113.62	117.00
54	BA	2558	C	O4'-C1'-N1	6.77	113.61	108.20
21	AA	176	C	N3-C2-O2	-6.76	117.17	121.90
21	AA	325	A	C5-C6-N1	6.76	121.08	117.70
21	AA	918	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	2883	A	C5-C6-N1	6.76	121.08	117.70
55	BB	115	A	C5-C6-N1	6.76	121.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	192	A	C4-C5-C6	-6.76	113.62	117.00
38	BP	38	ARG	NE-CZ-NH1	6.76	123.68	120.30
54	BA	1001	A	C5-C6-N1	6.76	121.08	117.70
21	AA	33	A	C5-C6-N1	6.76	121.08	117.70
54	BA	2879	A	O4'-C1'-N9	6.76	113.61	108.20
54	BA	106	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	1147	A	C5-C6-N1	6.76	121.08	117.70
21	AA	78	A	C5-C6-N1	6.76	121.08	117.70
21	AA	901	A	C5-C6-N1	6.76	121.08	117.70
54	BA	368	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1794	A	C5-C6-N1	6.76	121.08	117.70
21	AA	706	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	207	A	C5-C6-N1	6.76	121.08	117.70
54	BA	342	A	C4-C5-C6	-6.76	113.62	117.00
54	BA	1894	C	N3-C2-O2	-6.76	117.17	121.90
54	BA	2482	A	C5-C6-N1	6.76	121.08	117.70
21	AA	1252	A	C5-C6-N1	6.75	121.08	117.70
54	BA	1048	A	C5-C6-N1	6.75	121.08	117.70
21	AA	962	C	N3-C2-O2	-6.75	117.17	121.90
25	BC	12	ARG	NE-CZ-NH1	6.75	123.68	120.30
54	BA	1070	A	N1-C6-N6	-6.75	114.55	118.60
54	BA	1789	A	C5-C6-N1	6.75	121.08	117.70
54	BA	2381	A	C4-C5-C6	-6.75	113.62	117.00
54	BA	2317	A	C5-C6-N1	6.75	121.08	117.70
54	BA	2706	A	C4-C5-C6	-6.75	113.62	117.00
21	AA	228	A	C5-C6-N1	6.75	121.08	117.70
21	AA	640	A	C4-C5-C6	-6.75	113.63	117.00
51	B2	33	ARG	NE-CZ-NH1	6.75	123.67	120.30
54	BA	945	A	C5-C6-N1	6.75	121.07	117.70
54	BA	2283	C	O4'-C1'-N1	6.75	113.60	108.20
4	AE	68	ARG	NE-CZ-NH2	-6.75	116.93	120.30
54	BA	219	A	C5-C6-N1	6.75	121.07	117.70
54	BA	257	C	O4'-C1'-N1	6.75	113.60	108.20
54	BA	514	A	C5-C6-N1	6.75	121.07	117.70
55	BB	34	A	C5-C6-N1	6.75	121.07	117.70
21	AA	1016	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	1311	A	C5-C6-N1	6.75	121.07	117.70
54	BA	1237	A	C4-C5-C6	-6.75	113.63	117.00
21	AA	1327	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	695	G	O4'-C1'-N9	6.74	113.59	108.20
54	BA	1088	A	C5-C6-N1	6.74	121.07	117.70
21	AA	459	A	C5-C6-N1	6.74	121.07	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	490	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1379	U	O4'-C1'-N1	6.74	113.59	108.20
54	BA	2530	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	2873	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	810	C	N3-C2-O2	-6.74	117.18	121.90
21	AA	878	A	C4-C5-C6	-6.74	113.63	117.00
51	B2	34	ARG	NE-CZ-NH1	6.74	123.67	120.30
54	BA	640	C	N3-C2-O2	-6.74	117.18	121.90
54	BA	1603	A	C4-C5-C6	-6.74	113.63	117.00
54	BA	1978	A	C4-C5-C6	-6.74	113.63	117.00
21	AA	1408	A	N1-C6-N6	-6.73	114.56	118.60
24	A3	45	A	C5-C6-N1	6.73	121.07	117.70
54	BA	1301	A	C5-C6-N1	6.73	121.07	117.70
54	BA	2297	A	N1-C6-N6	-6.73	114.56	118.60
32	BJ	34	ARG	NE-CZ-NH1	6.73	123.67	120.30
54	BA	592	A	C4-C5-C6	-6.73	113.63	117.00
21	AA	553	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	1386	C	N3-C2-O2	-6.73	117.19	121.90
54	BA	2675	A	C4-C5-C6	-6.73	113.64	117.00
54	BA	823	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	206	C	N3-C2-O2	-6.73	117.19	121.90
21	AA	1219	A	C5-C6-N1	6.73	121.06	117.70
54	BA	2902	C	O4'-C1'-N1	6.73	113.58	108.20
21	AA	132	C	N3-C2-O2	-6.73	117.19	121.90
34	BL	69	ARG	NE-CZ-NH1	6.73	123.66	120.30
21	AA	124	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	839	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	1053	C	N3-C2-O2	-6.72	117.19	121.90
21	AA	66	A	C5-C6-N1	6.72	121.06	117.70
21	AA	575	G	P-O3'-C3'	6.72	127.77	119.70
54	BA	1095	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1347	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	2134	A	N1-C6-N6	-6.72	114.57	118.60
54	BA	2463	C	N3-C2-O2	-6.72	117.19	121.90
54	BA	1365	A	C4-C5-C6	-6.72	113.64	117.00
9	AJ	62	ARG	NE-CZ-NH1	6.72	123.66	120.30
21	AA	40	C	O4'-C1'-N1	6.72	113.58	108.20
21	AA	606	G	N3-C2-N2	-6.72	115.20	119.90
54	BA	845	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1843	C	O4'-C1'-N1	6.72	113.58	108.20
55	BB	95	U	O4'-C1'-N1	6.72	113.58	108.20
54	BA	1535	A	O4'-C1'-N9	6.72	113.57	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2723	C	N3-C2-O2	-6.72	117.20	121.90
21	AA	308	C	N3-C2-O2	-6.72	117.20	121.90
54	BA	13	A	C5-C6-N1	6.72	121.06	117.70
54	BA	19	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	1829	A	C4-C5-C6	-6.72	113.64	117.00
54	BA	890	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	985	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	1264	A	C5-C6-N1	6.71	121.06	117.70
54	BA	2088	A	C5-C6-N1	6.71	121.06	117.70
21	AA	675	A	C5-C6-N1	6.71	121.06	117.70
54	BA	693	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	1571	A	C5-C6-N1	6.71	121.06	117.70
54	BA	1991	U	O4'-C1'-N1	6.71	113.57	108.20
21	AA	872	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	31	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	2278	A	C4-C5-C6	-6.71	113.64	117.00
54	BA	2164	C	N3-C2-O2	-6.71	117.20	121.90
21	AA	609	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	1311	A	C4-C5-C6	-6.71	113.65	117.00
54	BA	378	C	N3-C2-O2	-6.71	117.20	121.90
54	BA	513	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1406	U	O4'-C1'-N1	6.71	113.56	108.20
54	BA	2268	A	C4-C5-C6	-6.71	113.65	117.00
21	AA	189	A	N1-C6-N6	-6.71	114.58	118.60
39	BQ	49	ARG	NE-CZ-NH1	6.71	123.65	120.30
54	BA	242	G	O4'-C1'-N9	6.71	113.56	108.20
54	BA	272	A	C5-C6-N1	6.71	121.05	117.70
54	BA	1128	G	C1'-O4'-C4'	-6.71	104.54	109.90
54	BA	2378	A	C5-C6-N1	6.71	121.05	117.70
21	AA	73	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2539	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	2639	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	764	A	C5-C6-N1	6.70	121.05	117.70
21	AA	26	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	120	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	514	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	1408	A	C4-C5-C6	-6.70	113.65	117.00
22	A1	41	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	190	A	C4-C5-C6	-6.70	113.65	117.00
21	AA	374	A	C5-C6-N1	6.70	121.05	117.70
21	AA	448	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	2814	A	C4-C5-C6	-6.70	113.65	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2814	A	C5-C6-N1	6.70	121.05	117.70
55	BB	35	C	N1-C2-O2	6.70	122.92	118.90
54	BA	961	C	N1-C2-O2	6.70	122.92	118.90
54	BA	1999	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	845	A	C5-C6-N1	6.70	121.05	117.70
21	AA	923	A	C5-C6-N1	6.70	121.05	117.70
21	AA	1150	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	33	C	N3-C2-O2	-6.70	117.21	121.90
54	BA	231	A	C5-C6-N1	6.70	121.05	117.70
54	BA	1175	A	C4-C5-C6	-6.70	113.65	117.00
54	BA	1291	C	N3-C2-O2	-6.70	117.21	121.90
21	AA	50	A	C4-C5-C6	-6.69	113.65	117.00
21	AA	338	A	C5-C6-N1	6.69	121.05	117.70
54	BA	181	A	C5-C6-N1	6.69	121.05	117.70
54	BA	182	A	C5-C6-N1	6.69	121.05	117.70
55	BB	45	A	C4-C5-C6	-6.69	113.65	117.00
21	AA	787	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	2000	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2104	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	2108	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	2352	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	2533	U	O4'-C1'-N1	6.69	113.55	108.20
54	BA	2662	A	N1-C6-N6	-6.69	114.59	118.60
21	AA	1299	A	C5-C6-N1	6.69	121.04	117.70
54	BA	2154	A	C4-C5-C6	-6.69	113.66	117.00
54	BA	2364	C	N3-C2-O2	-6.69	117.22	121.90
21	AA	1129	C	N3-C2-O2	-6.69	117.22	121.90
54	BA	655	A	C5-C6-N1	6.69	121.04	117.70
54	BA	1262	A	C5-C6-N1	6.69	121.04	117.70
56	B5	162	ARG	NE-CZ-NH1	6.69	123.64	120.30
54	BA	1569	A	C5-C6-N1	6.69	121.04	117.70
21	AA	52	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	332	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1330	C	N3-C2-O2	-6.68	117.22	121.90
20	AU	6	ARG	NE-CZ-NH2	6.68	123.64	120.30
22	A1	9	A	C5-C6-N1	6.68	121.04	117.70
21	AA	948	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1772	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	2135	A	O4'-C1'-N9	6.68	113.55	108.20
54	BA	2283	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	1853	A	C4-C5-C6	-6.68	113.66	117.00
54	BA	1924	C	N3-C2-O2	-6.68	117.22	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2060	A	O4'-C1'-N9	6.68	113.54	108.20
54	BA	2501	C	N3-C2-O2	-6.68	117.22	121.90
54	BA	2860	A	C5-C6-N1	6.68	121.04	117.70
21	AA	1349	A	C5-C6-N1	6.68	121.04	117.70
30	BH	51	ARG	NE-CZ-NH1	6.68	123.64	120.30
42	BT	77	ARG	NE-CZ-NH2	-6.68	116.96	120.30
54	BA	620	G	N3-C2-N2	-6.68	115.23	119.90
54	BA	1749	A	C5-C6-N1	6.68	121.04	117.70
54	BA	1854	A	C5-C6-N1	6.68	121.04	117.70
21	AA	74	A	C4-C5-C6	-6.67	113.66	117.00
21	AA	866	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	1367	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	996	A	C4-C5-C6	-6.67	113.66	117.00
54	BA	2434	A	C5-C6-N1	6.67	121.04	117.70
55	BB	114	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	708	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	146	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1433	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1927	A	C4-C5-C6	-6.67	113.66	117.00
22	A1	32	C	N3-C2-O2	-6.67	117.23	121.90
22	A1	61	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	750	A	C5-C6-N1	6.67	121.04	117.70
54	BA	1288	G	N1-C6-O6	-6.67	115.90	119.90
54	BA	1428	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	1031	C	N1-C2-O2	6.67	122.90	118.90
54	BA	2647	U	O4'-C1'-N1	6.67	113.54	108.20
21	AA	338	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	820	A	C5-C6-N1	6.67	121.03	117.70
54	BA	1319	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2575	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	2875	C	N3-C2-O2	-6.67	117.23	121.90
55	BB	70	C	N3-C2-O2	-6.67	117.23	121.90
17	AR	52	ARG	NE-CZ-NH2	-6.67	116.97	120.30
21	AA	251	G	P-O3'-C3'	6.67	127.70	119.70
29	BG	34	ARG	NE-CZ-NH1	6.67	123.63	120.30
54	BA	1472	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1664	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	2314	A	C4-C5-C6	-6.67	113.67	117.00
21	AA	139	A	C5-C6-N1	6.67	121.03	117.70
21	AA	806	C	N3-C2-O2	-6.67	117.23	121.90
21	AA	1011	C	N3-C2-O2	-6.67	117.23	121.90
54	BA	1533	C	N3-C2-O2	-6.67	117.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1654	A	C4-C5-C6	-6.67	113.67	117.00
54	BA	2366	A	N1-C6-N6	-6.67	114.60	118.60
6	AG	118	ARG	NE-CZ-NH1	6.66	123.63	120.30
54	BA	501	A	C5-C6-N1	6.66	121.03	117.70
54	BA	784	G	O4'-C1'-N9	6.66	113.53	108.20
54	BA	800	A	C5-C6-N1	6.66	121.03	117.70
54	BA	888	C	C1'-O4'-C4'	-6.66	104.57	109.90
21	AA	495	A	C5-C6-N1	6.66	121.03	117.70
54	BA	2594	C	N3-C2-O2	-6.66	117.24	121.90
11	AL	98	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	649	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1265	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1603	A	C5-C6-N1	6.66	121.03	117.70
21	AA	1499	A	C5-C6-N1	6.66	121.03	117.70
54	BA	1261	C	N3-C2-O2	-6.66	117.24	121.90
21	AA	1051	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	601	C	N3-C2-O2	-6.66	117.24	121.90
54	BA	1553	A	C4-C5-C6	-6.66	113.67	117.00
54	BA	2013	A	N1-C6-N6	-6.66	114.61	118.60
56	B5	74	ARG	NE-CZ-NH1	6.66	123.63	120.30
21	AA	1275	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	143	C	N3-C2-O2	-6.65	117.24	121.90
21	AA	825	A	C5-C6-N1	6.65	121.03	117.70
21	AA	946	A	C5-C6-N1	6.65	121.03	117.70
32	BJ	69	ARG	NE-CZ-NH1	6.65	123.63	120.30
54	BA	89	A	C4-C5-C6	-6.65	113.67	117.00
54	BA	1665	A	C5-C6-N1	6.65	121.03	117.70
54	BA	2147	A	C5-C6-N1	6.65	121.03	117.70
54	BA	2565	A	C4-C5-C6	-6.65	113.67	117.00
21	AA	937	A	C5-C6-N1	6.65	121.03	117.70
24	A3	69	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	84	A	N1-C6-N6	-6.65	114.61	118.60
54	BA	2089	C	O4'-C1'-N1	6.65	113.52	108.20
21	AA	919	A	O4'-C1'-N9	6.65	113.52	108.20
54	BA	1784	A	C4-C5-C6	-6.65	113.68	117.00
21	AA	1218	C	N3-C2-O2	-6.65	117.25	121.90
54	BA	1274	A	N1-C6-N6	-6.65	114.61	118.60
54	BA	2072	C	N3-C2-O2	-6.65	117.25	121.90
21	AA	1117	A	C5-C6-N1	6.64	121.02	117.70
23	A2	80	C	N3-C4-C5	6.64	124.56	121.90
54	BA	165	A	C4-C5-C6	-6.64	113.68	117.00
55	BB	78	A	C5-C6-N1	6.64	121.02	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	45	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	460	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1077	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1732	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	1618	A	C4-C5-C6	-6.64	113.68	117.00
55	BB	26	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	1213	A	C4-C5-C6	-6.64	113.68	117.00
38	BP	71	ARG	NE-CZ-NH1	6.64	123.62	120.30
47	BY	7	ARG	NE-CZ-NH1	6.64	123.62	120.30
54	BA	693	A	C5-C6-N1	6.64	121.02	117.70
54	BA	1431	A	C5-C6-N1	6.64	121.02	117.70
54	BA	2610	C	N3-C2-O2	-6.64	117.25	121.90
21	AA	182	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1089	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	1566	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2153	C	N3-C2-O2	-6.64	117.25	121.90
54	BA	2376	A	C4-C5-C6	-6.64	113.68	117.00
54	BA	2589	A	C5-C6-N1	6.64	121.02	117.70
11	AL	85	ARG	NE-CZ-NH1	6.63	123.62	120.30
21	AA	1433	A	C4-C5-C6	-6.63	113.68	117.00
54	BA	1342	A	C5-C6-N1	6.63	121.02	117.70
54	BA	1871	A	N1-C6-N6	-6.63	114.62	118.60
21	AA	879	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1918	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	401	A	C5-C6-N1	6.63	121.02	117.70
21	AA	1429	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	1290	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	53	A	C5-C6-N1	6.63	121.01	117.70
21	AA	896	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	5	A	C5-C6-N1	6.63	121.02	117.70
54	BA	1403	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	2439	A	C1'-O4'-C4'	-6.63	104.60	109.90
54	BA	2730	C	O4'-C1'-N1	6.63	113.50	108.20
55	BB	11	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	934	C	N3-C2-O2	-6.63	117.26	121.90
21	AA	1257	A	N1-C6-N6	-6.63	114.62	118.60
54	BA	655	A	C4-C5-C6	-6.63	113.69	117.00
54	BA	946	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	1570	A	C5-C6-N1	6.63	121.01	117.70
54	BA	1607	C	N1-C2-O2	6.63	122.88	118.90
54	BA	1832	C	N3-C2-O2	-6.63	117.26	121.90
54	BA	2632	A	C5-C6-N1	6.63	121.01	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1113	C	N3-C2-O2	-6.62	117.26	121.90
54	BA	1005	C	N1-C2-O2	6.62	122.88	118.90
54	BA	2687	U	O4'-C1'-N1	6.62	113.50	108.20
21	AA	10	A	C5-C6-N1	6.62	121.01	117.70
21	AA	831	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	1135	C	N3-C2-O2	-6.62	117.26	121.90
54	BA	1144	A	C5-C6-N1	6.62	121.01	117.70
54	BA	1284	A	C4-C5-C6	-6.62	113.69	117.00
54	BA	2117	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2205	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2670	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2883	A	N1-C6-N6	-6.62	114.63	118.60
54	BA	1628	G	N1-C6-O6	-6.62	115.93	119.90
54	BA	1698	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2850	A	C5-C6-N1	6.62	121.01	117.70
16	AQ	61	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	267	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	1499	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	2660	A	O4'-C1'-N9	6.62	113.50	108.20
12	AM	56	ARG	NE-CZ-NH1	6.62	123.61	120.30
14	AO	62	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	400	C	N3-C2-O2	-6.62	117.27	121.90
21	AA	403	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	870	U	O4'-C1'-N1	6.62	113.49	108.20
54	BA	2851	A	C5-C6-N1	6.62	121.01	117.70
29	BG	151	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	AA	364	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	768	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	1053	G	N3-C2-N2	-6.62	115.27	119.90
54	BA	334	C	N3-C2-O2	-6.62	117.27	121.90
54	BA	886	A	C5-C6-N1	6.62	121.01	117.70
54	BA	2882	A	C4-C5-C6	-6.62	113.69	117.00
21	AA	174	A	C5-C6-N1	6.61	121.01	117.70
21	AA	900	A	C5-C6-N1	6.61	121.01	117.70
33	BK	17	ARG	NE-CZ-NH1	6.61	123.61	120.30
54	BA	47	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	986	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1542	U	O4'-C1'-N1	6.61	113.49	108.20
54	BA	1754	A	C5-C6-N1	6.61	121.01	117.70
54	BA	2721	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	104	A	C5-C6-N1	6.61	121.01	117.70
54	BA	340	A	C5-C6-N1	6.61	121.01	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1253	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	1575	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	2273	A	C5-C6-N1	6.61	121.01	117.70
55	BB	99	A	C4-C5-C6	-6.61	113.69	117.00
35	BM	44	ARG	NE-CZ-NH1	6.61	123.61	120.30
54	BA	487	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	1706	C	N3-C2-O2	-6.61	117.27	121.90
21	AA	110	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	21	A	C5-C6-N1	6.61	121.00	117.70
54	BA	453	A	C4-C5-C6	-6.61	113.69	117.00
54	BA	1512	C	N3-C2-O2	-6.61	117.27	121.90
54	BA	2736	A	C4-C5-C6	-6.61	113.69	117.00
1	AB	112	ARG	NE-CZ-NH1	6.61	123.60	120.30
54	BA	753	A	C5-C6-N1	6.61	121.00	117.70
54	BA	2665	A	C5-C6-N1	6.61	121.00	117.70
54	BA	671	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	1961	C	N3-C2-O2	-6.61	117.28	121.90
54	BA	2108	A	C5-C6-N1	6.61	121.00	117.70
21	AA	913	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	1369	C	N1-C2-O2	6.60	122.86	118.90
54	BA	1404	C	O4'-C1'-N1	6.60	113.48	108.20
21	AA	67	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	607	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	157	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	893	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1269	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1970	A	C5-C6-N1	6.60	121.00	117.70
54	BA	439	A	C5-C6-N1	6.60	121.00	117.70
54	BA	1626	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	1722	A	C5-C6-N1	6.60	121.00	117.70
54	BA	2497	A	C4-C5-C6	-6.60	113.70	117.00
21	AA	251	G	N3-C2-N2	-6.60	115.28	119.90
21	AA	1250	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	564	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	1249	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	1592	C	N3-C2-O2	-6.60	117.28	121.90
54	BA	2720	U	O4'-C1'-N1	6.60	113.48	108.20
1	AB	136	ARG	NE-CZ-NH1	6.60	123.60	120.30
21	AA	72	A	C4-C5-C6	-6.60	113.70	117.00
54	BA	42	A	C5-C6-N1	6.60	121.00	117.70
54	BA	699	A	C5-C6-N1	6.60	121.00	117.70
54	BA	2065	C	N3-C2-O2	-6.60	117.28	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	97	C	N3-C2-O2	-6.60	117.28	121.90
21	AA	1352	C	N1-C2-O2	6.59	122.86	118.90
54	BA	845	A	C5-C6-N1	6.59	121.00	117.70
47	BY	23	ARG	NE-CZ-NH1	6.59	123.60	120.30
21	AA	466	A	C4-C5-C6	-6.59	113.70	117.00
21	AA	352	C	N3-C2-O2	-6.59	117.29	121.90
24	A3	73	A	P-O3'-C3'	6.59	127.61	119.70
54	BA	751	A	C5-C6-N1	6.59	121.00	117.70
54	BA	2241	A	C5-C6-N1	6.59	121.00	117.70
21	AA	777	A	N1-C6-N6	-6.59	114.65	118.60
54	BA	2813	A	C5-C6-N1	6.59	120.99	117.70
55	BB	22	U	O4'-C1'-N1	6.59	113.47	108.20
55	BB	101	A	C4-C5-C6	-6.59	113.71	117.00
21	AA	919	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	860	U	O4'-C1'-N1	6.58	113.47	108.20
54	BA	1494	A	C5-C6-N1	6.58	120.99	117.70
21	AA	1150	A	C5-C6-N1	6.58	120.99	117.70
54	BA	556	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	838	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	1481	U	O4'-C1'-N1	6.58	113.47	108.20
54	BA	1890	A	N1-C6-N6	-6.58	114.65	118.60
21	AA	152	A	C4-C5-C6	-6.58	113.71	117.00
21	AA	1500	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	515	A	C4-C5-C6	-6.58	113.71	117.00
54	BA	1596	A	C5-C6-N1	6.58	120.99	117.70
21	AA	612	C	N3-C2-O2	-6.58	117.29	121.90
54	BA	1366	A	C5-C6-N1	6.58	120.99	117.70
54	BA	2273	A	N1-C6-N6	-6.58	114.65	118.60
21	AA	1190	G	P-O3'-C3'	6.58	127.59	119.70
54	BA	1940	U	O4'-C1'-N1	6.58	113.46	108.20
55	BB	4	C	N3-C2-O2	-6.58	117.30	121.90
21	AA	756	C	N3-C2-O2	-6.58	117.30	121.90
54	BA	1349	C	N3-C2-O2	-6.58	117.30	121.90
17	AR	60	ARG	NE-CZ-NH1	6.58	123.59	120.30
54	BA	1306	C	N3-C2-O2	-6.58	117.30	121.90
21	AA	910	C	N3-C2-O2	-6.57	117.30	121.90
21	AA	982	U	P-O3'-C3'	6.57	127.59	119.70
54	BA	89	A	C5-C6-N1	6.57	120.99	117.70
54	BA	422	A	C4-C5-C6	-6.57	113.71	117.00
54	BA	610	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	715	A	C5-C6-N1	6.57	120.99	117.70
54	BA	1879	C	N3-C2-O2	-6.57	117.30	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2009	A	C5-C6-N1	6.57	120.99	117.70
54	BA	2512	C	O4'-C1'-N1	6.57	113.46	108.20
54	BA	2515	C	N3-C2-O2	-6.57	117.30	121.90
3	AD	62	ARG	NE-CZ-NH1	6.57	123.58	120.30
21	AA	609	A	C5-C6-N1	6.57	120.98	117.70
21	AA	892	A	C4-C5-C6	-6.57	113.72	117.00
24	A3	16	C	N3-C2-O2	-6.57	117.30	121.90
54	BA	1952	A	O4'-C1'-N9	6.57	113.45	108.20
54	BA	590	A	C5-C6-N1	6.57	120.98	117.70
54	BA	1562	U	O4'-C1'-N1	6.57	113.45	108.20
21	AA	167	A	C5-C6-N1	6.56	120.98	117.70
21	AA	1145	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	73	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	905	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	16	A	C5-C6-N1	6.56	120.98	117.70
21	AA	59	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	32	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2901	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	119	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	1549	A	C5-C6-N1	6.56	120.98	117.70
54	BA	2191	A	C4-C5-C6	-6.56	113.72	117.00
21	AA	483	C	N3-C2-O2	-6.56	117.31	121.90
21	AA	883	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	1453	A	C5-C6-N1	6.56	120.98	117.70
54	BA	1496	A	C4-C5-C6	-6.56	113.72	117.00
54	BA	126	A	C5-C6-N1	6.56	120.98	117.70
21	AA	179	A	C5-C6-N1	6.56	120.98	117.70
54	BA	992	C	N3-C2-O2	-6.56	117.31	121.90
54	BA	2006	C	O4'-C1'-N1	6.56	113.44	108.20
54	BA	255	A	C5-C6-N1	6.55	120.98	117.70
54	BA	793	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	2308	G	O4'-C1'-N9	6.55	113.44	108.20
22	A1	76	A	N1-C6-N6	-6.55	114.67	118.60
21	AA	1203	C	N3-C2-O2	-6.55	117.31	121.90
54	BA	1189	A	C5-C6-N1	6.55	120.98	117.70
54	BA	1194	A	C5-C6-N1	6.55	120.98	117.70
54	BA	1454	C	N1-C2-O2	6.55	122.83	118.90
54	BA	2590	A	C5-C6-N1	6.55	120.98	117.70
21	AA	149	A	C5-C6-N1	6.55	120.97	117.70
21	AA	1531	A	C4-C5-C6	-6.55	113.72	117.00
54	BA	221	A	N1-C6-N6	-6.55	114.67	118.60
21	AA	274	A	C4-C5-C6	-6.55	113.73	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BG	94	ARG	NE-CZ-NH1	6.55	123.57	120.30
54	BA	516	C	N3-C2-O2	-6.55	117.32	121.90
54	BA	2089	C	N3-C2-O2	-6.55	117.32	121.90
21	AA	155	A	C5-C6-N1	6.54	120.97	117.70
54	BA	269	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	753	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	2538	C	N3-C2-O2	-6.54	117.32	121.90
21	AA	321	A	C5-C6-N1	6.54	120.97	117.70
21	AA	629	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1127	A	C4-C5-C6	-6.54	113.73	117.00
16	AQ	64	ARG	NE-CZ-NH1	6.54	123.57	120.30
24	A3	40	C	N3-C2-O2	-6.54	117.32	121.90
54	BA	1525	A	C4-C5-C6	-6.54	113.73	117.00
45	BW	38	ARG	NE-CZ-NH1	6.54	123.57	120.30
21	AA	55	A	C4-C5-C6	-6.54	113.73	117.00
21	AA	263	A	C5-C6-N1	6.54	120.97	117.70
21	AA	735	C	N3-C2-O2	-6.54	117.33	121.90
54	BA	541	A	C5-C6-N1	6.54	120.97	117.70
54	BA	972	A	C4-C5-C6	-6.54	113.73	117.00
54	BA	1266	G	O4'-C1'-N9	6.54	113.43	108.20
54	BA	2486	C	N3-C2-O2	-6.54	117.33	121.90
21	AA	451	A	C5-C6-N1	6.53	120.97	117.70
24	A3	49	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1722	A	N1-C6-N6	-6.53	114.68	118.60
55	BB	80	U	O4'-C1'-N1	6.53	113.43	108.20
54	BA	944	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1433	A	C4-C5-C6	-6.53	113.73	117.00
4	AE	28	ARG	NE-CZ-NH1	6.53	123.57	120.30
21	AA	389	A	C4-C5-C6	-6.53	113.73	117.00
21	AA	753	A	C5-C6-N1	6.53	120.97	117.70
21	AA	970	C	N3-C2-O2	-6.53	117.33	121.90
24	A3	22	A	C4-C5-C6	-6.53	113.73	117.00
54	BA	2482	A	C4-C5-C6	-6.53	113.73	117.00
22	A1	39	G	C1'-O4'-C4'	-6.53	104.68	109.90
54	BA	1774	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	2633	G	O4'-C1'-N9	6.53	113.42	108.20
21	AA	363	A	C5-C6-N1	6.53	120.96	117.70
54	BA	477	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	794	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1780	A	O4'-C1'-N9	6.53	113.42	108.20
25	BC	257	ARG	NE-CZ-NH1	6.53	123.56	120.30
54	BA	719	C	N3-C2-O2	-6.53	117.33	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1308	A	C5-C6-N1	6.53	120.96	117.70
54	BA	1489	C	N3-C2-O2	-6.53	117.33	121.90
54	BA	1495	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1677	A	C4-C5-C6	-6.53	113.74	117.00
54	BA	1805	A	N1-C6-N6	-6.53	114.69	118.60
54	BA	282	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1638	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	2346	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	312	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	1967	C	N3-C2-O2	-6.52	117.33	121.90
54	BA	2480	C	O4'-C1'-N1	6.52	113.42	108.20
21	AA	563	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	761	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2211	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	2264	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	622	A	C5-C6-N1	6.52	120.96	117.70
21	AA	1022	A	C5-C6-N1	6.52	120.96	117.70
21	AA	1158	C	N1-C2-O2	6.52	122.81	118.90
21	AA	1399	C	N3-C2-O2	-6.52	117.34	121.90
54	BA	1327	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1821	A	C5-C6-N1	6.52	120.96	117.70
54	BA	2270	A	O4'-C1'-N9	6.52	113.42	108.20
54	BA	2518	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	292	G	N1-C6-O6	-6.52	115.99	119.90
21	AA	908	A	C5-C6-N1	6.52	120.96	117.70
54	BA	947	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1143	A	C4-C5-C6	-6.52	113.74	117.00
54	BA	1754	A	C4-C5-C6	-6.52	113.74	117.00
21	AA	739	C	N3-C2-O2	-6.52	117.34	121.90
21	AA	1465	A	C5-C6-N1	6.52	120.96	117.70
21	AA	767	A	C4-C5-C6	-6.51	113.74	117.00
22	A1	73	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	241	A	C4-C5-C6	-6.51	113.74	117.00
54	BA	951	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	2635	A	C5-C6-N1	6.51	120.96	117.70
54	BA	330	A	P-O3'-C3'	6.51	127.51	119.70
54	BA	359	G	N1-C6-O6	-6.51	115.99	119.90
54	BA	1307	A	C5-C6-N1	6.51	120.96	117.70
54	BA	1700	A	C4-C5-C6	-6.51	113.74	117.00
21	AA	578	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	965	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	1757	A	C4-C5-C6	-6.51	113.75	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2752	C	N3-C2-O2	-6.51	117.34	121.90
21	AA	288	A	C5-C6-N1	6.51	120.95	117.70
54	BA	1208	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	2013	A	C5-C6-N1	6.51	120.95	117.70
21	AA	342	C	N3-C2-O2	-6.51	117.34	121.90
54	BA	402	A	C5-C6-N1	6.51	120.95	117.70
54	BA	1577	C	N3-C2-O2	-6.51	117.35	121.90
54	BA	1655	A	C5-C6-N1	6.51	120.95	117.70
21	AA	681	A	C5-C6-N1	6.50	120.95	117.70
54	BA	348	A	C4-C5-C6	-6.50	113.75	117.00
55	BB	59	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	285	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	1065	U	C3'-C2'-C1'	6.50	106.70	101.50
54	BA	434	U	O4'-C1'-N1	6.50	113.40	108.20
21	AA	313	A	C4-C5-C6	-6.50	113.75	117.00
21	AA	452	A	C5-C6-N1	6.50	120.95	117.70
54	BA	398	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	414	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	429	A	C5-C6-N1	6.50	120.95	117.70
54	BA	665	U	O4'-C1'-N1	6.50	113.40	108.20
54	BA	1708	C	N3-C2-O2	-6.50	117.35	121.90
56	B5	12	ARG	NE-CZ-NH1	6.50	123.55	120.30
54	BA	8	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	256	A	C5-C6-N1	6.50	120.95	117.70
54	BA	2547	A	C5-C6-N1	6.50	120.95	117.70
54	BA	338	G	N3-C2-N2	-6.50	115.35	119.90
54	BA	1287	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1821	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2079	U	O4'-C1'-N1	6.50	113.40	108.20
54	BA	2626	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	487	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	351	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	1762	A	C5-C6-N1	6.50	120.95	117.70
54	BA	1937	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2710	C	N3-C2-O2	-6.50	117.35	121.90
21	AA	341	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	721	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	1129	A	C4-C5-C6	-6.50	113.75	117.00
54	BA	2248	C	N3-C2-O2	-6.50	117.35	121.90
54	BA	2634	A	C5-C6-N1	6.50	120.95	117.70
12	AM	108	ARG	NE-CZ-NH1	6.49	123.55	120.30
21	AA	1411	C	N3-C2-O2	-6.49	117.35	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	57	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	2392	A	C5-C6-N1	6.49	120.95	117.70
54	BA	1868	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	183	C	N3-C2-O2	-6.49	117.36	121.90
54	BA	1020	A	C5-C6-N1	6.49	120.94	117.70
54	BA	1413	A	C4-C5-C6	-6.49	113.75	117.00
56	B5	60	ARG	NE-CZ-NH1	6.49	123.55	120.30
39	BQ	52	ARG	NE-CZ-NH1	6.49	123.54	120.30
54	BA	1373	A	C5-C6-N1	6.49	120.94	117.70
54	BA	1477	A	C5-C6-N1	6.49	120.94	117.70
55	BB	50	A	C5-C6-N1	6.49	120.94	117.70
21	AA	969	A	C4-C5-C6	-6.49	113.76	117.00
41	BS	110	ARG	NE-CZ-NH2	6.49	123.54	120.30
54	BA	470	A	N1-C6-N6	-6.49	114.71	118.60
54	BA	1679	A	C5-C6-N1	6.49	120.94	117.70
22	A1	38	A	C4-C5-C6	-6.49	113.76	117.00
54	BA	479	A	C5-C6-N1	6.49	120.94	117.70
54	BA	1304	A	C5-C6-N1	6.49	120.94	117.70
18	AS	36	ARG	NE-CZ-NH1	6.48	123.54	120.30
21	AA	1410	A	C5-C6-N1	6.48	120.94	117.70
54	BA	2335	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1508	A	N1-C6-N6	-6.48	114.71	118.60
27	BE	44	ARG	NE-CZ-NH1	6.48	123.54	120.30
28	BF	147	ARG	NE-CZ-NH1	6.48	123.54	120.30
54	BA	1453	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1641	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1783	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	109	A	C5-C6-N1	6.48	120.94	117.70
54	BA	1336	A	N1-C6-N6	-6.48	114.71	118.60
21	AA	860	A	C4-C5-C6	-6.48	113.76	117.00
21	AA	1021	A	C5-C6-N1	6.48	120.94	117.70
22	A1	31	C	N3-C2-O2	-6.48	117.37	121.90
54	BA	833	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	1289	C	N3-C2-O2	-6.48	117.37	121.90
54	BA	2142	A	C4-C5-C6	-6.48	113.76	117.00
54	BA	2369	A	C5-C6-N1	6.48	120.94	117.70
21	AA	435	A	N1-C6-N6	-6.48	114.71	118.60
21	AA	1248	A	C5-C6-N1	6.48	120.94	117.70
21	AA	1518	A	C4-C5-C6	-6.48	113.76	117.00
22	A1	35	A	C4-C5-C6	-6.48	113.76	117.00
38	BP	87	ARG	NE-CZ-NH1	6.48	123.54	120.30
55	BB	62	C	N3-C2-O2	-6.48	117.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1082	A	N1-C6-N6	-6.47	114.72	118.60
28	BF	79	ARG	NE-CZ-NH1	6.47	123.54	120.30
54	BA	208	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	752	A	C5-C6-N1	6.47	120.94	117.70
54	BA	2741	A	C4-C5-C6	-6.47	113.76	117.00
4	AE	156	ARG	NE-CZ-NH2	6.47	123.54	120.30
21	AA	489	C	N3-C2-O2	-6.47	117.37	121.90
21	AA	533	A	N1-C6-N6	-6.47	114.72	118.60
24	A3	73	A	C4-C5-C6	-6.47	113.76	117.00
54	BA	1737	G	N1-C6-O6	-6.47	116.02	119.90
54	BA	2025	C	N1-C2-O2	6.47	122.78	118.90
54	BA	2174	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	2465	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1755	A	C5-C6-N1	6.47	120.94	117.70
54	BA	155	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1103	A	C5-C6-N1	6.47	120.94	117.70
54	BA	1705	A	C5-C6-N1	6.47	120.93	117.70
21	AA	1398	A	C5-C6-N1	6.47	120.93	117.70
54	BA	965	C	O4'-C1'-N1	6.47	113.37	108.20
54	BA	1957	C	N3-C2-O2	-6.47	117.37	121.90
3	AD	2	ARG	NE-CZ-NH2	-6.47	117.07	120.30
21	AA	1000	A	C5-C6-N1	6.47	120.93	117.70
23	A2	85	G	P-O3'-C3'	6.47	127.46	119.70
54	BA	742	A	C4-C5-C6	-6.47	113.77	117.00
54	BA	1727	C	N3-C2-O2	-6.47	117.37	121.90
54	BA	1880	U	O4'-C1'-N1	6.47	113.37	108.20
54	BA	2868	A	C4-C5-C6	-6.47	113.77	117.00
21	AA	53	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	621	A	C5'-C4'-C3'	-6.46	105.66	116.00
54	BA	1069	A	C5-C6-N1	6.46	120.93	117.70
21	AA	1055	A	C5-C6-N1	6.46	120.93	117.70
24	A3	67	C	N3-C2-O2	-6.46	117.38	121.90
27	BE	49	ARG	NE-CZ-NH1	6.46	123.53	120.30
54	BA	634	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	925	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1585	C	N3-C2-O2	-6.46	117.38	121.90
54	BA	1781	U	N3-C2-O2	-6.46	117.68	122.20
21	AA	196	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	325	G	O4'-C1'-N9	6.46	113.37	108.20
54	BA	416	U	O4'-C1'-N1	6.46	113.37	108.20
54	BA	726	G	O4'-C1'-N9	6.46	113.37	108.20
54	BA	1551	A	C5-C6-N1	6.46	120.93	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1728	C	N3-C2-O2	-6.46	117.38	121.90
21	AA	411	A	C5-C6-N1	6.46	120.93	117.70
21	AA	706	A	C5-C6-N1	6.46	120.93	117.70
54	BA	104	A	C4-C5-C6	-6.46	113.77	117.00
21	AA	1219	A	C4-C5-C6	-6.46	113.77	117.00
54	BA	1965	C	N3-C2-O2	-6.46	117.38	121.90
55	BB	52	A	C5-C6-N1	6.46	120.93	117.70
54	BA	156	A	C5-C6-N1	6.46	120.93	117.70
21	AA	236	A	C5-C6-N1	6.45	120.93	117.70
21	AA	1180	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	929	U	O4'-C1'-N1	6.45	113.36	108.20
54	BA	1064	C	N3-C2-O2	-6.45	117.38	121.90
21	AA	635	A	C5-C6-N1	6.45	120.93	117.70
21	AA	807	A	C4-C5-C6	-6.45	113.77	117.00
54	BA	829	A	N1-C6-N6	-6.45	114.73	118.60
54	BA	1580	A	C4-C5-C6	-6.45	113.77	117.00
55	BB	3	C	O4'-C1'-N1	6.45	113.36	108.20
21	AA	7	A	C5-C6-N1	6.45	120.92	117.70
21	AA	938	A	C4-C5-C6	-6.45	113.78	117.00
28	BF	29	ARG	NE-CZ-NH1	6.45	123.53	120.30
54	BA	149	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	599	A	C5-C6-N1	6.45	120.93	117.70
54	BA	1548	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1939	U	O4'-C1'-N1	6.45	113.36	108.20
21	AA	907	A	N1-C6-N6	-6.45	114.73	118.60
24	A3	11	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1701	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1793	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	2521	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	42	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	213	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	1233	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	2873	A	C5-C6-N1	6.45	120.92	117.70
21	AA	78	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	223	A	C5-C6-N1	6.45	120.92	117.70
21	AA	470	C	N1-C2-O2	6.45	122.77	118.90
21	AA	573	A	C4-C5-C6	-6.45	113.78	117.00
21	AA	985	C	N3-C2-O2	-6.45	117.39	121.90
24	A3	58	A	C4-C5-C6	-6.45	113.78	117.00
54	BA	623	C	N3-C2-O2	-6.45	117.39	121.90
54	BA	2745	C	N3-C2-O2	-6.45	117.39	121.90
55	BB	94	A	C5-C6-N1	6.45	120.92	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	429	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1071	G	C3'-C2'-C1'	6.44	106.66	101.50
21	AA	938	A	C5-C6-N1	6.44	120.92	117.70
54	BA	470	A	C5-C6-N1	6.44	120.92	117.70
54	BA	1305	C	O4'-C1'-N1	6.44	113.35	108.20
54	BA	1616	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2059	A	C4-C5-C6	-6.44	113.78	117.00
21	AA	1429	A	C5-C6-N1	6.44	120.92	117.70
54	BA	37	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	227	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1599	U	O4'-C1'-N1	6.44	113.35	108.20
54	BA	1761	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	1934	C	O4'-C1'-N1	6.44	113.35	108.20
54	BA	2184	A	C5-C6-N1	6.44	120.92	117.70
54	BA	2306	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2425	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	2830	C	N3-C2-O2	-6.44	117.39	121.90
21	AA	787	A	C5-C6-N1	6.44	120.92	117.70
21	AA	1374	A	N1-C6-N6	-6.44	114.74	118.60
54	BA	765	C	N3-C2-O2	-6.44	117.39	121.90
54	BA	2600	A	C5-C6-N1	6.44	120.92	117.70
21	AA	532	A	C4-C5-C6	-6.44	113.78	117.00
54	BA	1469	A	C4-C5-C6	-6.44	113.78	117.00
24	A3	60	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	1362	C	O4'-C1'-N1	6.43	113.35	108.20
54	BA	1787	A	N1-C6-N6	-6.43	114.74	118.60
21	AA	978	A	C4-C5-C6	-6.43	113.78	117.00
54	BA	732	C	N3-C2-O2	-6.43	117.40	121.90
54	BA	1799	G	P-O3'-C3'	6.43	127.42	119.70
21	AA	848	C	N3-C2-O2	-6.43	117.40	121.90
21	AA	60	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	1144	A	N1-C6-N6	-6.43	114.74	118.60
54	BA	1230	A	C5-C6-N1	6.43	120.92	117.70
54	BA	2019	A	C5-C6-N1	6.43	120.91	117.70
21	AA	177	G	N3-C4-C5	-6.43	125.39	128.60
54	BA	2769	U	O4'-C1'-N1	6.43	113.34	108.20
54	BA	2809	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	1306	A	C4-C5-C6	-6.43	113.79	117.00
54	BA	960	A	C4-C5-C6	-6.43	113.79	117.00
21	AA	34	C	N3-C2-O2	-6.42	117.40	121.90
22	A1	69	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	101	A	C5-C6-N1	6.42	120.91	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	255	A	N1-C6-N6	-6.42	114.75	118.60
54	BA	1448	G	O4'-C1'-N9	6.42	113.34	108.20
54	BA	1755	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	339	C	N3-C2-O2	-6.42	117.40	121.90
21	AA	1204	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	86	G	O4'-C1'-N9	6.42	113.34	108.20
54	BA	251	A	C5-C6-N1	6.42	120.91	117.70
21	AA	760	G	N1-C6-O6	-6.42	116.05	119.90
54	BA	804	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1705	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	459	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1191	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1413	A	C5-C6-N1	6.42	120.91	117.70
54	BA	2619	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	789	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	911	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	1080	A	C5-C6-N1	6.42	120.91	117.70
54	BA	1650	A	C4-C5-C6	-6.42	113.79	117.00
54	BA	2073	C	N3-C2-O2	-6.42	117.41	121.90
54	BA	2616	C	N3-C2-O2	-6.42	117.41	121.90
3	AD	114	ARG	NE-CZ-NH1	6.42	123.51	120.30
54	BA	2860	A	C4-C5-C6	-6.42	113.79	117.00
21	AA	1275	A	C5-C6-N1	6.41	120.91	117.70
21	AA	1502	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	432	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	739	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	204	A	C4-C5-C6	-6.41	113.79	117.00
54	BA	210	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	832	U	O4'-C1'-N1	6.41	113.33	108.20
54	BA	1290	C	P-O3'-C3'	6.41	127.39	119.70
21	AA	149	A	C4-C5-C6	-6.41	113.80	117.00
21	AA	329	A	C5-C6-N1	6.41	120.90	117.70
21	AA	932	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	2135	A	C5-C6-N1	6.41	120.90	117.70
54	BA	2498	C	N3-C2-O2	-6.41	117.41	121.90
54	BA	988	A	C4-C5-C6	-6.41	113.80	117.00
54	BA	2150	C	O4'-C1'-N1	6.41	113.33	108.20
21	AA	702	A	O4'-C1'-N9	6.41	113.32	108.20
21	AA	766	A	C5-C6-N1	6.41	120.90	117.70
54	BA	1196	C	N3-C2-O2	-6.41	117.42	121.90
54	BA	1641	A	C5-C6-N1	6.41	120.90	117.70
54	BA	2377	A	C5-C6-N1	6.41	120.90	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	70	ARG	NE-CZ-NH1	6.40	123.50	120.30
54	BA	5	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1383	A	O4'-C1'-N9	6.40	113.32	108.20
21	AA	630	A	C4-C5-C6	-6.40	113.80	117.00
36	BN	46	ARG	NE-CZ-NH1	6.40	123.50	120.30
55	BB	34	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	919	A	C5-C6-N1	6.40	120.90	117.70
54	BA	1936	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	2800	A	C5-C6-N1	6.40	120.90	117.70
8	AI	44	ARG	NE-CZ-NH1	6.40	123.50	120.30
21	AA	482	A	C5-C6-N1	6.40	120.90	117.70
26	BD	184	ARG	NE-CZ-NH1	6.40	123.50	120.30
54	BA	1359	A	C5-C6-N1	6.40	120.90	117.70
54	BA	2178	C	N3-C2-O2	-6.40	117.42	121.90
21	AA	696	A	C5-C6-N1	6.40	120.90	117.70
21	AA	1014	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	1097	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	223	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	1028	A	C4-C5-C6	-6.40	113.80	117.00
54	BA	2888	C	N3-C2-O2	-6.40	117.42	121.90
54	BA	800	A	C4-C5-C6	-6.40	113.80	117.00
21	AA	816	A	C4-C5-C6	-6.39	113.80	117.00
21	AA	1167	A	C4-C5-C6	-6.39	113.80	117.00
25	BC	62	ARG	NE-CZ-NH1	6.39	123.50	120.30
54	BA	1735	A	C4-C5-C6	-6.39	113.80	117.00
54	BA	1908	C	N3-C2-O2	-6.39	117.42	121.90
21	AA	493	A	O4'-C1'-N9	6.39	113.31	108.20
54	BA	723	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	837	C	N3-C2-O2	-6.39	117.43	121.90
5	AF	45	ARG	NE-CZ-NH1	6.39	123.50	120.30
21	AA	935	A	C4-C5-C6	-6.39	113.81	117.00
21	AA	816	A	C5-C6-N1	6.39	120.89	117.70
21	AA	1318	A	C5-C6-N1	6.39	120.89	117.70
54	BA	61	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	877	A	C4-C5-C6	-6.39	113.81	117.00
54	BA	1153	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2160	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2340	A	C4-C5-C6	-6.39	113.81	117.00
55	BB	118	C	N3-C2-O2	-6.39	117.43	121.90
54	BA	2458	G	O4'-C1'-N9	6.39	113.31	108.20
54	BA	1011	G	O4'-C1'-N9	6.39	113.31	108.20
54	BA	1819	A	C4-C5-C6	-6.39	113.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1155	A	C4-C5-C6	-6.38	113.81	117.00
34	BL	41	ARG	NE-CZ-NH1	6.38	123.49	120.30
54	BA	44	A	C5-C6-N1	6.38	120.89	117.70
21	AA	675	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1654	A	C5-C6-N1	6.38	120.89	117.70
21	AA	205	A	C5-C6-N1	6.38	120.89	117.70
21	AA	1086	U	O4'-C1'-N1	6.38	113.31	108.20
21	AA	1092	A	C4-C5-C6	-6.38	113.81	117.00
22	A1	48	C	N1-C2-O2	6.38	122.73	118.90
54	BA	1478	G	O4'-C1'-N9	6.38	113.31	108.20
54	BA	2426	A	C4-C5-C6	-6.38	113.81	117.00
21	AA	383	A	C5-C6-N1	6.38	120.89	117.70
54	BA	422	A	O4'-C1'-N9	6.38	113.30	108.20
55	BB	59	A	C5-C6-N1	6.38	120.89	117.70
21	AA	90	C	N3-C2-O2	-6.38	117.44	121.90
21	AA	1067	A	C5-C6-N1	6.38	120.89	117.70
21	AA	1281	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	166	U	O4'-C1'-N1	6.38	113.30	108.20
54	BA	927	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	1336	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	2261	C	O4'-C1'-N1	6.38	113.30	108.20
54	BA	2542	A	C4-C5-C6	-6.38	113.81	117.00
54	BA	66	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	1947	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	2760	C	N3-C2-O2	-6.38	117.44	121.90
54	BA	1730	C	N1-C2-O2	6.38	122.72	118.90
21	AA	280	C	N1-C2-O2	6.37	122.72	118.90
21	AA	759	A	C5-C6-N1	6.37	120.89	117.70
21	AA	1350	A	C5-C6-N1	6.37	120.89	117.70
54	BA	182	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	1672	A	C4-C5-C6	-6.37	113.81	117.00
54	BA	18	U	O4'-C1'-N1	6.37	113.30	108.20
54	BA	2476	A	C4-C5-C6	-6.37	113.81	117.00
14	AO	52	ARG	NE-CZ-NH1	6.37	123.48	120.30
21	AA	167	A	C4-C5-C6	-6.37	113.81	117.00
21	AA	222	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	736	C	N3-C2-O2	-6.37	117.44	121.90
21	AA	878	A	C5-C6-N1	6.37	120.89	117.70
5	AF	44	ARG	NE-CZ-NH1	6.37	123.48	120.30
21	AA	248	C	N3-C2-O2	-6.37	117.44	121.90
51	B2	12	ARG	NE-CZ-NH1	6.37	123.48	120.30
54	BA	1870	C	N3-C2-O2	-6.37	117.44	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	71	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	1052	C	N3-C2-O2	-6.37	117.44	121.90
15	AP	8	ARG	NE-CZ-NH1	6.37	123.48	120.30
54	BA	637	A	C4-C5-C6	-6.37	113.82	117.00
54	BA	1847	A	C4-C5-C6	-6.37	113.82	117.00
21	AA	192	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1244	A	N1-C6-N6	-6.36	114.78	118.60
54	BA	1252	G	O4'-C1'-N9	6.36	113.29	108.20
54	BA	2247	A	N1-C6-N6	-6.36	114.78	118.60
21	AA	460	A	C5-C6-N1	6.36	120.88	117.70
21	AA	1102	A	C5-C6-N1	6.36	120.88	117.70
21	AA	1534	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	21	A	C4-C5-C6	-6.36	113.82	117.00
54	BA	791	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	1749	A	C4-C5-C6	-6.36	113.82	117.00
21	AA	1508	A	C5-C6-N1	6.36	120.88	117.70
21	AA	108	G	O4'-C1'-N9	6.36	113.29	108.20
21	AA	1179	A	C5-C6-N1	6.36	120.88	117.70
21	AA	1397	C	N3-C2-O2	-6.36	117.45	121.90
54	BA	454	A	C5-C6-N1	6.36	120.88	117.70
54	BA	2579	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	1060	U	O4'-C1'-N1	6.36	113.28	108.20
21	AA	1155	A	C5-C6-N1	6.36	120.88	117.70
54	BA	195	A	C5-C6-N1	6.36	120.88	117.70
54	BA	1118	C	N3-C2-O2	-6.36	117.45	121.90
21	AA	99	C	N3-C2-O2	-6.35	117.45	121.90
21	AA	687	A	C5-C6-N1	6.35	120.88	117.70
4	AE	24	VAL	C-N-CA	6.35	137.58	121.70
21	AA	1271	A	C5-C6-N1	6.35	120.88	117.70
54	BA	233	A	C4-C5-C6	-6.35	113.82	117.00
54	BA	1050	A	C5-C6-N1	6.35	120.88	117.70
54	BA	2903	U	O4'-C1'-N1	6.35	113.28	108.20
54	BA	2578	G	N1-C6-O6	-6.35	116.09	119.90
54	BA	2829	A	C4-C5-C6	-6.35	113.82	117.00
21	AA	796	C	N3-C2-O2	-6.35	117.45	121.90
54	BA	737	C	O4'-C1'-N1	6.35	113.28	108.20
38	BP	102	ARG	NE-CZ-NH1	6.35	123.47	120.30
54	BA	1359	A	O4'-C1'-N9	6.35	113.28	108.20
54	BA	2507	C	N3-C2-O2	-6.35	117.46	121.90
55	BB	113	C	N3-C2-O2	-6.35	117.46	121.90
21	AA	379	C	N3-C2-O2	-6.35	117.46	121.90
54	BA	815	C	O4'-C1'-N1	6.35	113.28	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AM	97	ARG	NE-CZ-NH1	6.34	123.47	120.30
21	AA	843	U	O4'-C1'-N1	6.34	113.28	108.20
21	AA	1181	G	C1'-O4'-C4'	-6.34	104.83	109.90
54	BA	63	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	821	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	2288	A	C4-C5-C6	-6.34	113.83	117.00
54	BA	2794	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	143	C	O4'-C1'-N1	6.34	113.27	108.20
54	BA	2015	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	600	A	C5-C6-N1	6.34	120.87	117.70
54	BA	1593	A	C5-C6-N1	6.34	120.87	117.70
21	AA	235	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	936	A	C5-C6-N1	6.34	120.87	117.70
54	BA	958	U	O4'-C1'-N1	6.34	113.27	108.20
54	BA	1133	A	C4-C5-C6	-6.34	113.83	117.00
38	BP	88	ARG	NE-CZ-NH1	6.34	123.47	120.30
21	AA	1151	A	C4-C5-C6	-6.34	113.83	117.00
21	AA	1359	C	N1-C2-O2	6.34	122.70	118.90
54	BA	1806	C	N3-C2-O2	-6.34	117.46	121.90
54	BA	2540	C	N3-C2-O2	-6.34	117.46	121.90
56	B5	53	ARG	NE-CZ-NH1	6.34	123.47	120.30
6	AG	137	ARG	NE-CZ-NH1	6.33	123.47	120.30
21	AA	243	A	N1-C6-N6	-6.33	114.80	118.60
54	BA	1515	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	2372	U	O4'-C1'-N1	6.33	113.27	108.20
22	A1	59	U	N3-C2-O2	-6.33	117.77	122.20
46	BX	36	ARG	NE-CZ-NH1	6.33	123.47	120.30
54	BA	2183	A	C4-C5-C6	-6.33	113.83	117.00
21	AA	880	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	440	C	N3-C2-O2	-6.33	117.47	121.90
54	BA	621	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	817	C	N3-C2-O2	-6.33	117.47	121.90
21	AA	1329	A	C5-C6-N1	6.33	120.86	117.70
32	BJ	34	ARG	NE-CZ-NH2	-6.33	117.14	120.30
54	BA	167	A	C5-C6-N1	6.33	120.86	117.70
21	AA	687	A	C4-C5-C6	-6.33	113.84	117.00
21	AA	994	A	O4'-C1'-N9	6.33	113.26	108.20
54	BA	975	A	C4-C5-C6	-6.33	113.84	117.00
54	BA	2322	A	C4-C5-C6	-6.33	113.83	117.00
54	BA	724	U	O4'-C1'-N1	6.33	113.26	108.20
54	BA	1165	A	C5-C6-N1	6.33	120.86	117.70
54	BA	504	A	C4-C5-C6	-6.32	113.84	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	685	A	N1-C6-N6	-6.32	114.81	118.60
54	BA	981	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	802	A	N1-C6-N6	-6.32	114.81	118.60
21	AA	349	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	575	A	C4-C5-C6	-6.32	113.84	117.00
54	BA	2207	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2332	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2653	U	O4'-C1'-N1	6.32	113.26	108.20
21	AA	40	C	N3-C2-O2	-6.32	117.48	121.90
21	AA	396	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	1313	U	N3-C2-O2	-6.32	117.78	122.20
54	BA	2161	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2291	U	O4'-C1'-N1	6.32	113.25	108.20
54	BA	2583	G	N3-C2-N2	-6.32	115.48	119.90
54	BA	2761	A	C5-C6-N1	6.32	120.86	117.70
21	AA	754	C	N1-C2-O2	6.32	122.69	118.90
21	AA	857	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	277	G	O4'-C1'-N9	6.32	113.25	108.20
54	BA	2003	A	C5-C6-N1	6.32	120.86	117.70
54	BA	2036	C	N3-C2-O2	-6.32	117.48	121.90
54	BA	2837	A	C5-C6-N1	6.32	120.86	117.70
54	BA	164	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	2088	A	C4-C5-C6	-6.31	113.84	117.00
54	BA	1341	G	O4'-C1'-N9	6.31	113.25	108.20
54	BA	1685	C	N3-C2-O2	-6.31	117.48	121.90
54	BA	1802	A	N1-C6-N6	-6.31	114.81	118.60
54	BA	2841	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	254	G	N1-C6-O6	-6.31	116.11	119.90
21	AA	411	A	C4-C5-C6	-6.31	113.84	117.00
21	AA	1413	A	C5-C6-N1	6.31	120.86	117.70
54	BA	1650	A	C5-C6-N1	6.31	120.86	117.70
54	BA	2730	C	N3-C2-O2	-6.31	117.48	121.90
21	AA	996	A	C5-C6-N1	6.31	120.86	117.70
21	AA	523	A	C4-C5-C6	-6.31	113.85	117.00
54	BA	1746	A	C4-C5-C6	-6.31	113.85	117.00
54	BA	2679	A	C5-C6-N1	6.31	120.85	117.70
54	BA	445	C	N3-C2-O2	-6.31	117.49	121.90
54	BA	1596	A	C4-C5-C6	-6.31	113.85	117.00
21	AA	33	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	569	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	1254	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	201	C	N3-C2-O2	-6.30	117.49	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1395	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	1686	C	O4'-C1'-N1	6.30	113.24	108.20
54	BA	2328	A	C5-C6-N1	6.30	120.85	117.70
54	BA	2866	U	O4'-C1'-N1	6.30	113.24	108.20
14	AO	63	ARG	NE-CZ-NH1	6.30	123.45	120.30
21	AA	315	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	1284	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	1868	C	O4'-C1'-N1	6.30	113.24	108.20
54	BA	505	A	C5-C6-N1	6.30	120.85	117.70
54	BA	2406	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2512	C	N3-C2-O2	-6.30	117.49	121.90
54	BA	2636	C	N3-C2-O2	-6.30	117.49	121.90
21	AA	602	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	1179	A	C4-C5-C6	-6.30	113.85	117.00
21	AA	1252	A	N1-C6-N6	-6.30	114.82	118.60
54	BA	265	A	O4'-C1'-N9	6.30	113.24	108.20
54	BA	715	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2602	A	O4'-C1'-N9	6.30	113.24	108.20
54	BA	1272	A	C4-C5-C6	-6.30	113.85	117.00
54	BA	2299	U	O4'-C1'-N1	6.30	113.24	108.20
21	AA	732	C	N3-C2-O2	-6.30	117.49	121.90
55	BB	76	G	O4'-C1'-N9	6.30	113.24	108.20
21	AA	815	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	1324	A	C5-C6-N1	6.29	120.85	117.70
54	BA	1941	C	N3-C2-O2	-6.29	117.49	121.90
54	BA	2003	A	C4-C5-C6	-6.29	113.85	117.00
54	BA	2270	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	1228	C	N3-C2-O2	-6.29	117.49	121.90
54	BA	1274	A	C5-C6-N1	6.29	120.85	117.70
54	BA	1630	A	C5-C6-N1	6.29	120.85	117.70
54	BA	1637	A	C5-C6-N1	6.29	120.85	117.70
54	BA	1780	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	572	A	C4-C5-C6	-6.29	113.85	117.00
21	AA	694	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	522	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	980	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	2870	C	N3-C2-O2	-6.29	117.50	121.90
9	AJ	72	ARG	NE-CZ-NH1	6.29	123.44	120.30
21	AA	282	A	C4-C5-C6	-6.29	113.86	117.00
21	AA	528	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	152	A	C5-C6-N1	6.29	120.84	117.70
54	BA	796	C	N3-C2-O2	-6.29	117.50	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2395	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	1302	A	C5-C6-N1	6.29	120.84	117.70
54	BA	2116	G	N1-C6-O6	-6.29	116.13	119.90
21	AA	623	C	N3-C2-O2	-6.29	117.50	121.90
54	BA	483	A	N1-C6-N6	-6.29	114.83	118.60
54	BA	1496	A	C5-C6-N1	6.29	120.84	117.70
54	BA	2751	G	O4'-C1'-N9	6.29	113.23	108.20
25	BC	166	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	601	C	O4'-C1'-N1	6.28	113.23	108.20
54	BA	1590	A	C5-C6-N1	6.28	120.84	117.70
36	BN	103	ARG	NE-CZ-NH1	6.28	123.44	120.30
54	BA	582	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1020	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	440	C	N3-C2-O2	-6.28	117.50	121.90
54	BA	1605	C	N3-C2-O2	-6.28	117.50	121.90
21	AA	253	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	1977	A	C4-C5-C6	-6.28	113.86	117.00
54	BA	2258	C	N3-C2-O2	-6.28	117.51	121.90
55	BB	93	C	N3-C2-O2	-6.28	117.51	121.90
8	AI	112	ARG	NE-CZ-NH2	-6.28	117.16	120.30
8	AI	118	ARG	NE-CZ-NH1	6.28	123.44	120.30
21	AA	766	A	C4-C5-C6	-6.28	113.86	117.00
21	AA	1140	C	N3-C2-O2	-6.28	117.51	121.90
54	BA	1252	G	N3-C2-N2	-6.28	115.51	119.90
21	AA	579	A	C5-C6-N1	6.27	120.84	117.70
40	BR	78	ARG	NE-CZ-NH1	6.27	123.44	120.30
54	BA	38	A	C5-C6-N1	6.27	120.84	117.70
54	BA	1828	G	C5-C6-N1	6.27	114.64	111.50
54	BA	2755	C	N3-C2-O2	-6.27	117.51	121.90
22	A1	28	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	1698	A	N1-C6-N6	-6.27	114.84	118.60
11	AL	53	ARG	NE-CZ-NH1	6.27	123.44	120.30
21	AA	695	A	C5-C6-N1	6.27	120.83	117.70
54	BA	125	A	C4-C5-C6	-6.27	113.87	117.00
54	BA	336	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	210	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	1223	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2611	C	N3-C2-O2	-6.27	117.51	121.90
54	BA	2635	A	N1-C6-N6	-6.27	114.84	118.60
55	BB	29	A	C5-C6-N1	6.27	120.83	117.70
55	BB	30	C	N3-C2-O2	-6.27	117.51	121.90
21	AA	634	C	N3-C2-O2	-6.26	117.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	421	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	611	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2009	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2759	G	N1-C6-O6	-6.26	116.14	119.90
21	AA	999	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	1045	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1367	A	C4-C5-C6	-6.26	113.87	117.00
55	BB	49	C	N3-C2-O2	-6.26	117.52	121.90
11	AL	11	ARG	NE-CZ-NH1	6.26	123.43	120.30
21	AA	77	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	172	A	C5-C6-N1	6.26	120.83	117.70
54	BA	1263	U	C3'-C2'-C1'	6.26	106.51	101.50
54	BA	1928	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2480	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	2703	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	303	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	1157	A	C4-C5-C6	-6.26	113.87	117.00
21	AA	1441	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	898	C	N3-C2-O2	-6.26	117.52	121.90
54	BA	1324	G	C3'-C2'-C1'	6.26	106.51	101.50
21	AA	83	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	1363	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	998	C	N3-C2-O2	-6.26	117.52	121.90
21	AA	456	A	C5-C6-N1	6.26	120.83	117.70
21	AA	996	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2386	A	C4-C5-C6	-6.26	113.87	117.00
54	BA	2814	A	O4'-C1'-N9	6.26	113.21	108.20
54	BA	1077	A	C4-C5-C6	-6.25	113.87	117.00
21	AA	825	A	C4-C5-C6	-6.25	113.87	117.00
21	AA	1277	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	610	U	N3-C2-O2	-6.25	117.82	122.20
54	BA	482	A	C4-C5-C6	-6.25	113.87	117.00
54	BA	2699	C	N3-C2-O2	-6.25	117.53	121.90
55	BB	42	C	N3-C2-O2	-6.25	117.52	121.90
21	AA	10	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	718	A	N1-C6-N6	-6.25	114.85	118.60
53	B4	36	ARG	NE-CZ-NH1	6.25	123.42	120.30
54	BA	41	C	N3-C2-O2	-6.25	117.53	121.90
54	BA	547	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	748	G	N1-C6-O6	-6.25	116.15	119.90
54	BA	1676	A	C4-C5-C6	-6.25	113.88	117.00
21	AA	873	A	C4-C5-C6	-6.25	113.88	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BX	27	ARG	NE-CZ-NH1	6.25	123.42	120.30
54	BA	931	U	N3-C2-O2	-6.25	117.83	122.20
54	BA	1652	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	2226	C	O4'-C1'-N1	6.25	113.20	108.20
21	AA	431	A	C5-C6-N1	6.25	120.82	117.70
54	BA	727	A	C4-C5-C6	-6.25	113.88	117.00
54	BA	762	U	P-O3'-C3'	6.24	127.19	119.70
54	BA	1276	A	C5-C6-N1	6.24	120.82	117.70
54	BA	1323	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	2620	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	1209	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	52	A	C5-C6-N1	6.24	120.82	117.70
54	BA	722	A	C4-C5-C6	-6.24	113.88	117.00
54	BA	731	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	840	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	77	A	C5-C6-N1	6.24	120.82	117.70
21	AA	1044	A	C5-C6-N1	6.24	120.82	117.70
54	BA	211	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	130	C	N3-C2-O2	-6.24	117.54	121.90
54	BA	237	C	N3-C2-O2	-6.24	117.53	121.90
54	BA	1282	U	O4'-C1'-N1	6.24	113.19	108.20
54	BA	1804	C	N3-C2-O2	-6.24	117.53	121.90
21	AA	915	A	C4-C5-C6	-6.23	113.88	117.00
21	AA	1333	A	C4-C5-C6	-6.23	113.88	117.00
54	BA	466	A	C5-C6-N1	6.23	120.82	117.70
54	BA	686	U	O4'-C1'-N1	6.23	113.19	108.20
54	BA	903	C	N3-C2-O2	-6.23	117.54	121.90
54	BA	909	A	C5-C6-N1	6.23	120.82	117.70
21	AA	193	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	386	C	N3-C2-O2	-6.23	117.54	121.90
21	AA	767	A	N1-C6-N6	-6.23	114.86	118.60
21	AA	1456	A	C4-C5-C6	-6.23	113.89	117.00
54	BA	1237	A	O4'-C1'-N9	6.23	113.18	108.20
12	AM	100	ARG	NE-CZ-NH1	6.23	123.41	120.30
54	BA	1295	C	N3-C2-O2	-6.23	117.54	121.90
1	AB	10	LYS	C-N-CA	6.23	137.27	121.70
20	AU	20	ARG	NE-CZ-NH1	6.23	123.41	120.30
21	AA	1509	C	N3-C2-O2	-6.23	117.54	121.90
34	BL	18	ARG	NE-CZ-NH1	6.23	123.41	120.30
54	BA	828	U	N3-C2-O2	-6.23	117.84	122.20
21	AA	385	C	N3-C2-O2	-6.23	117.54	121.90
19	AT	59	ARG	NE-CZ-NH1	6.22	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	80	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	782	A	C4-C5-C6	-6.22	113.89	117.00
21	AA	1086	U	C1'-O4'-C4'	-6.22	104.92	109.90
21	AA	1201	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	1485	U	O4'-C1'-N1	6.22	113.18	108.20
54	BA	2417	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	2863	C	N3-C2-O2	-6.22	117.54	121.90
21	AA	853	C	N3-C2-O2	-6.22	117.54	121.90
31	BI	126	ARG	NE-CZ-NH1	6.22	123.41	120.30
37	BO	15	ARG	NE-CZ-NH1	6.22	123.41	120.30
54	BA	2050	C	N3-C2-O2	-6.22	117.54	121.90
54	BA	2076	U	C1'-O4'-C4'	-6.22	104.92	109.90
21	AA	1234	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	161	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1328	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	2591	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	335	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	370	C	N3-C2-O2	-6.22	117.55	121.90
21	AA	1192	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	318	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	586	A	C4-C5-C6	-6.22	113.89	117.00
54	BA	873	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	920	A	C5-C6-N1	6.22	120.81	117.70
54	BA	1032	A	N1-C6-N6	-6.22	114.87	118.60
55	BB	28	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1170	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1178	C	O4'-C1'-N1	6.22	113.17	108.20
54	BA	2106	U	O4'-C1'-N1	6.22	113.17	108.20
54	BA	1039	A	N1-C6-N6	-6.22	114.87	118.60
54	BA	1795	C	N3-C2-O2	-6.22	117.55	121.90
54	BA	1960	A	C5-C6-N1	6.22	120.81	117.70
54	BA	2453	A	C5-C6-N1	6.22	120.81	117.70
39	BQ	12	ARG	NE-CZ-NH2	6.21	123.41	120.30
54	BA	915	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1463	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1525	A	C5-C6-N1	6.21	120.81	117.70
54	BA	2551	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	228	A	C4-C5-C6	-6.21	113.89	117.00
54	BA	1809	A	C4-C5-C6	-6.21	113.89	117.00
1	AB	20	ARG	NE-CZ-NH1	6.21	123.41	120.30
21	AA	1146	A	N1-C6-N6	-6.21	114.87	118.60
23	A2	88	U	C3'-C2'-C1'	6.21	106.47	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	103	A	C4-C5-C6	-6.21	113.89	117.00
8	AI	128	LYS	C-N-CA	6.21	137.22	121.70
21	AA	243	A	C5-C6-N1	6.21	120.81	117.70
21	AA	1098	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	64	A	C5-C6-N1	6.21	120.81	117.70
21	AA	1314	C	N3-C2-O2	-6.21	117.55	121.90
24	A3	24	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	378	C	O4'-C1'-N1	6.21	113.17	108.20
54	BA	756	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1117	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	1189	A	C4'-C3'-C2'	-6.21	96.39	102.60
54	BA	2338	C	N3-C2-O2	-6.21	117.55	121.90
54	BA	2785	C	N3-C2-O2	-6.21	117.55	121.90
21	AA	163	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	221	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	477	C	N3-C2-O2	-6.21	117.56	121.90
34	BL	21	ARG	NE-CZ-NH2	6.21	123.40	120.30
54	BA	1522	A	C4-C5-C6	-6.21	113.90	117.00
54	BA	1686	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	2652	C	N3-C2-O2	-6.21	117.56	121.90
54	BA	2882	A	C5-C6-N1	6.21	120.80	117.70
54	BA	415	A	C5-C6-N1	6.21	120.80	117.70
54	BA	775	G	O4'-C1'-N9	6.21	113.16	108.20
55	BB	71	C	N3-C2-O2	-6.21	117.56	121.90
21	AA	25	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	111	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	1507	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2147	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	668	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	816	C	O4'-C1'-N1	6.20	113.16	108.20
21	AA	998	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	1259	C	N3-C2-O2	-6.20	117.56	121.90
22	A1	20	G	N1-C6-O6	-6.20	116.18	119.90
54	BA	613	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	635	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	1583	A	C4-C5-C6	-6.20	113.90	117.00
54	BA	2023	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	408	A	C5-C6-N1	6.20	120.80	117.70
54	BA	16	C	N1-C2-O2	6.20	122.62	118.90
54	BA	1350	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2514	U	O4'-C1'-N1	6.20	113.16	108.20
21	AA	1377	A	C4-C5-C6	-6.20	113.90	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1796	U	O4'-C1'-N1	6.20	113.16	108.20
54	BA	1981	A	C4-C5-C6	-6.20	113.90	117.00
21	AA	1060	U	N3-C2-O2	-6.20	117.86	122.20
54	BA	1357	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2200	C	N3-C2-O2	-6.20	117.56	121.90
54	BA	2649	C	N3-C2-O2	-6.20	117.56	121.90
21	AA	430	A	C5-C6-N1	6.19	120.80	117.70
21	AA	556	C	N3-C2-O2	-6.19	117.56	121.90
54	BA	1974	C	N3-C2-O2	-6.19	117.56	121.90
21	AA	393	A	C4-C5-C6	-6.19	113.90	117.00
21	AA	647	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1001	C	N3-C2-O2	-6.19	117.56	121.90
54	BA	2175	C	N3-C2-O2	-6.19	117.57	121.90
21	AA	1236	A	N1-C6-N6	-6.19	114.89	118.60
37	BO	25	ARG	NE-CZ-NH1	6.19	123.39	120.30
43	BU	85	ARG	NE-CZ-NH1	6.19	123.39	120.30
54	BA	1398	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	2055	C	N1-C2-O2	6.19	122.61	118.90
54	BA	256	A	N1-C6-N6	-6.19	114.89	118.60
54	BA	806	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1858	A	C5-C6-N1	6.19	120.79	117.70
54	BA	2439	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	831	A	C5-C6-N1	6.19	120.79	117.70
54	BA	184	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	849	A	C5-C6-N1	6.19	120.79	117.70
54	BA	1293	C	N3-C2-O2	-6.19	117.57	121.90
54	BA	1750	G	N1-C6-O6	-6.19	116.19	119.90
54	BA	2063	C	C3'-C2'-C1'	6.19	106.45	101.50
54	BA	644	A	N1-C6-N6	-6.19	114.89	118.60
54	BA	943	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	2212	A	C4-C5-C6	-6.19	113.91	117.00
54	BA	2821	A	C4-C5-C6	-6.19	113.91	117.00
21	AA	316	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	1005	A	C5-C6-N1	6.18	120.79	117.70
21	AA	1172	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	1216	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	311	A	C6-C5-N7	6.18	136.63	132.30
54	BA	657	U	O4'-C1'-N1	6.18	113.15	108.20
54	BA	1731	G	O4'-C1'-N9	6.18	113.15	108.20
55	BB	108	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1606	C	N1-C2-O2	6.18	122.61	118.90
54	BA	1844	C	N3-C2-O2	-6.18	117.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2774	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	1639	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	2313	C	N3-C2-O2	-6.18	117.57	121.90
54	BA	2510	C	N3-C2-O2	-6.18	117.57	121.90
21	AA	1382	C	N3-C4-N4	-6.18	113.67	118.00
54	BA	2757	A	N1-C6-N6	-6.18	114.89	118.60
54	BA	131	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	286	U	O4'-C1'-N1	6.18	113.14	108.20
54	BA	1544	A	C4-C5-C6	-6.18	113.91	117.00
54	BA	1932	A	C6-C5-N7	6.18	136.62	132.30
21	AA	1520	C	N1-C2-O2	6.17	122.60	118.90
46	BX	49	ARG	NE-CZ-NH1	6.17	123.39	120.30
54	BA	199	A	C5-C6-N1	6.17	120.79	117.70
54	BA	1399	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2700	A	C4-C5-C6	-6.17	113.91	117.00
14	AO	16	ARG	NE-CZ-NH1	6.17	123.39	120.30
21	AA	431	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	758	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1561	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	2407	A	C4-C5-C6	-6.17	113.91	117.00
54	BA	2799	A	C4-C5-C6	-6.17	113.91	117.00
55	BB	8	C	N3-C2-O2	-6.17	117.58	121.90
24	A3	75	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	374	A	C4-C5-C6	-6.17	113.92	117.00
54	BA	435	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	1214	A	C5-C6-N1	6.17	120.78	117.70
21	AA	436	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	465	A	C4-C5-C6	-6.17	113.92	117.00
21	AA	1404	C	N3-C2-O2	-6.17	117.58	121.90
54	BA	134	G	O4'-C1'-N9	6.17	113.13	108.20
54	BA	2368	C	N3-C2-O2	-6.17	117.58	121.90
21	AA	794	A	C4-C5-C6	-6.16	113.92	117.00
34	BL	132	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	1021	A	C5-C6-N1	6.16	120.78	117.70
54	BA	1572	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1656	C	N3-C2-O2	-6.16	117.58	121.90
54	BA	1912	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	2380	C	N3-C2-O2	-6.16	117.58	121.90
21	AA	1317	C	N1-C2-O2	6.16	122.60	118.90
54	BA	1085	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	2095	A	C5-C6-N1	6.16	120.78	117.70
54	BA	603	A	C4-C5-C6	-6.16	113.92	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	861	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	197	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1354	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	1938	A	C4-C5-C6	-6.16	113.92	117.00
54	BA	2031	A	C4-C5-C6	-6.16	113.92	117.00
6	AG	95	ARG	NE-CZ-NH1	6.16	123.38	120.30
21	AA	328	C	N1-C2-O2	6.16	122.59	118.90
21	AA	1093	A	C4-C5-C6	-6.16	113.92	117.00
33	BK	98	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	566	U	O4'-C1'-N1	6.16	113.13	108.20
54	BA	2208	C	N3-C2-O2	-6.16	117.59	121.90
54	BA	2513	A	C4-C5-C6	-6.16	113.92	117.00
21	AA	1407	C	N3-C2-O2	-6.16	117.59	121.90
25	BC	261	ARG	NE-CZ-NH1	6.16	123.38	120.30
54	BA	744	U	O4'-C1'-N1	6.16	113.12	108.20
54	BA	1126	A	N1-C6-N6	-6.16	114.91	118.60
54	BA	1559	U	O4'-C1'-N1	6.16	113.12	108.20
8	AI	11	ARG	NE-CZ-NH1	6.15	123.38	120.30
21	AA	1519	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	141	G	N3-C4-C5	-6.15	125.52	128.60
54	BA	584	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	865	A	C4-C5-C6	-6.15	113.92	117.00
21	AA	912	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	1465	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	10	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	109	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	218	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	2558	C	N3-C2-O2	-6.15	117.59	121.90
21	AA	435	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	76	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	1625	C	C1'-O4'-C4'	-6.15	104.98	109.90
54	BA	2117	A	N1-C6-N6	-6.15	114.91	118.60
21	AA	1476	A	C4-C5-C6	-6.15	113.92	117.00
54	BA	192	C	N3-C2-O2	-6.15	117.59	121.90
54	BA	2170	A	C4-C5-C6	-6.15	113.92	117.00
21	AA	940	C	N3-C2-O2	-6.15	117.60	121.90
22	A1	6	A	C5-C6-N1	6.15	120.77	117.70
54	BA	1889	A	C4-C5-C6	-6.15	113.93	117.00
21	AA	106	C	N3-C2-O2	-6.15	117.60	121.90
21	AA	946	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	599	A	C4-C5-C6	-6.15	113.93	117.00
54	BA	1261	C	O4'-C1'-N1	6.15	113.12	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2103	C	N3-C2-O2	-6.15	117.60	121.90
21	AA	1016	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1257	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	2469	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	408	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	995	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	1280	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	244	A	C5-C6-N1	6.14	120.77	117.70
54	BA	565	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	734	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	1161	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1637	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2080	A	C5-C6-N1	6.14	120.77	117.70
21	AA	356	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	599	C	N3-C2-O2	-6.14	117.60	121.90
21	AA	635	A	C4-C5-C6	-6.14	113.93	117.00
21	AA	945	G	N3-C4-C5	-6.14	125.53	128.60
21	AA	1120	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	1040	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	2359	C	N3-C2-O2	-6.14	117.60	121.90
54	BA	705	A	N1-C6-N6	-6.14	114.92	118.60
21	AA	194	C	N3-C2-O2	-6.14	117.61	121.90
21	AA	1319	A	C5-C6-N1	6.14	120.77	117.70
54	BA	1269	A	C4-C5-C6	-6.14	113.93	117.00
54	BA	374	A	C5-C6-N1	6.13	120.77	117.70
54	BA	1881	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2247	A	C4-C5-C6	-6.13	113.93	117.00
54	BA	2264	C	O4'-C1'-N1	6.13	113.11	108.20
25	BC	181	ARG	NE-CZ-NH1	6.13	123.37	120.30
54	BA	2564	A	C4-C5-C6	-6.13	113.93	117.00
21	AA	1529	G	O4'-C1'-N9	6.13	113.11	108.20
54	BA	314	C	N3-C2-O2	-6.13	117.61	121.90
54	BA	2374	C	N3-C2-O2	-6.13	117.61	121.90
21	AA	885	G	N1-C6-O6	-6.13	116.22	119.90
54	BA	1679	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	1689	A	C5-C6-N1	6.13	120.77	117.70
54	BA	1230	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	1314	C	N1-C1'-C2'	6.13	121.97	114.00
54	BA	1427	A	C4-C5-C6	-6.13	113.94	117.00
54	BA	2644	G	O4'-C1'-N9	6.13	113.10	108.20
54	BA	2281	A	C4-C5-C6	-6.13	113.94	117.00
24	A3	44	A	C4-C5-C6	-6.12	113.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2158	A	C5-C6-N1	6.12	120.76	117.70
16	AQ	76	ARG	NE-CZ-NH2	-6.12	117.24	120.30
24	A3	38	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	609	A	C5-C6-N1	6.12	120.76	117.70
54	BA	1526	C	N3-C2-O2	-6.12	117.61	121.90
54	BA	1803	A	C4-C5-C6	-6.12	113.94	117.00
1	AB	138	ARG	NE-CZ-NH1	6.12	123.36	120.30
21	AA	478	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	490	C	N1-C2-O2	6.12	122.57	118.90
54	BA	589	U	C1'-O4'-C4'	-6.12	105.00	109.90
54	BA	933	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	2516	A	C5-C6-N1	6.12	120.76	117.70
22	A1	11	C	N3-C2-O2	-6.12	117.62	121.90
51	B2	28	ARG	NE-CZ-NH1	6.12	123.36	120.30
54	BA	602	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	633	A	C4-C5-C6	-6.12	113.94	117.00
54	BA	824	U	O4'-C1'-N1	6.12	113.09	108.20
54	BA	1030	C	O4'-C1'-N1	6.12	113.09	108.20
54	BA	1272	A	O4'-C1'-N9	6.12	113.09	108.20
21	AA	1389	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	491	G	O4'-C1'-N9	6.11	113.09	108.20
54	BA	1049	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2202	U	O4'-C1'-N1	6.11	113.09	108.20
54	BA	1115	G	N1-C6-O6	-6.11	116.23	119.90
54	BA	2466	C	N3-C2-O2	-6.11	117.62	121.90
55	BB	35	C	O4'-C1'-N1	6.11	113.09	108.20
21	AA	750	C	N3-C2-O2	-6.11	117.62	121.90
21	AA	1109	C	N1-C2-O2	6.11	122.57	118.90
21	AA	1400	C	N1-C2-O2	6.11	122.57	118.90
54	BA	466	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	492	A	C5-C6-N1	6.11	120.75	117.70
54	BA	2058	A	C4-C5-C6	-6.11	113.94	117.00
54	BA	680	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	1866	A	C4-C5-C6	-6.11	113.94	117.00
21	AA	814	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	64	A	N1-C6-N6	-6.11	114.94	118.60
54	BA	300	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	626	A	C5-C6-N1	6.11	120.75	117.70
54	BA	1200	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2241	A	C4-C5-C6	-6.11	113.95	117.00
55	BB	90	C	N3-C2-O2	-6.11	117.62	121.90
54	BA	2176	A	C4-C5-C6	-6.11	113.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2274	A	C4-C5-C6	-6.11	113.95	117.00
54	BA	2831	G	N1-C6-O6	-6.11	116.24	119.90
21	AA	680	C	N3-C2-O2	-6.10	117.63	121.90
11	AL	49	ARG	NE-CZ-NH2	6.10	123.35	120.30
54	BA	784	G	N1-C6-O6	-6.10	116.24	119.90
54	BA	1370	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	1471	G	N1-C6-O6	-6.10	116.24	119.90
54	BA	2101	A	C5-C6-N1	6.10	120.75	117.70
54	BA	530	G	O4'-C1'-N9	6.10	113.08	108.20
54	BA	2604	U	O4'-C1'-N1	6.10	113.08	108.20
54	BA	2762	C	O4'-C1'-N1	6.10	113.08	108.20
54	BA	2827	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	6	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	864	G	O4'-C1'-N9	6.10	113.08	108.20
54	BA	1347	A	C5-C6-N1	6.10	120.75	117.70
21	AA	419	C	N3-C2-O2	-6.10	117.63	121.90
46	BX	73	ARG	NE-CZ-NH1	6.10	123.35	120.30
54	BA	97	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	439	A	N1-C6-N6	-6.10	114.94	118.60
54	BA	687	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	750	A	C4-C5-C6	-6.10	113.95	117.00
54	BA	1741	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	2451	A	C4-C5-C6	-6.10	113.95	117.00
26	BD	46	ARG	NE-CZ-NH1	6.10	123.35	120.30
54	BA	1417	C	N3-C2-O2	-6.10	117.63	121.90
54	BA	2163	A	O4'-C1'-N9	6.10	113.08	108.20
54	BA	2435	A	C5-C6-N1	6.10	120.75	117.70
54	BA	2748	A	C4-C5-C6	-6.10	113.95	117.00
21	AA	624	C	O4'-C1'-N1	6.09	113.08	108.20
38	BP	61	ARG	NE-CZ-NH1	6.09	123.35	120.30
54	BA	179	C	N3-C2-O2	-6.09	117.63	121.90
54	BA	83	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	490	C	O4'-C1'-N1	6.09	113.08	108.20
54	BA	1297	C	N3-C2-O2	-6.09	117.64	121.90
21	AA	320	A	C6-C5-N7	6.09	136.56	132.30
21	AA	452	A	C4-C5-C6	-6.09	113.95	117.00
21	AA	718	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	743	A	C4-C5-C6	-6.09	113.95	117.00
54	BA	1608	A	N1-C6-N6	-6.09	114.94	118.60
8	AI	108	ARG	NE-CZ-NH1	6.09	123.34	120.30
21	AA	85	U	N3-C2-O2	-6.09	117.94	122.20
54	BA	2366	A	C5-C6-N1	6.09	120.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	600	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	1553	A	C1'-O4'-C4'	-6.09	105.03	109.90
54	BA	1570	A	C4-C5-C6	-6.09	113.96	117.00
54	BA	2377	A	C4-C5-C6	-6.09	113.96	117.00
21	AA	860	A	C5-C6-N1	6.09	120.74	117.70
32	BJ	120	ARG	NE-CZ-NH1	6.09	123.34	120.30
37	BO	102	ARG	NE-CZ-NH1	6.09	123.34	120.30
32	BJ	37	ARG	NE-CZ-NH1	6.08	123.34	120.30
54	BA	2771	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	36	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	1496	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	69	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	251	A	N1-C6-N6	-6.08	114.95	118.60
54	BA	1893	C	N3-C2-O2	-6.08	117.64	121.90
54	BA	2312	U	N3-C2-O2	-6.08	117.94	122.20
21	AA	175	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	579	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	1492	A	C5-C6-N1	6.08	120.74	117.70
54	BA	1569	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2143	C	N3-C2-O2	-6.08	117.64	121.90
21	AA	336	A	C5-C6-N1	6.08	120.74	117.70
54	BA	2033	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	2311	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	125	A	O4'-C1'-N9	6.08	113.06	108.20
54	BA	1925	C	N3-C2-O2	-6.08	117.65	121.90
55	BB	109	A	C4-C5-C6	-6.08	113.96	117.00
54	BA	1830	C	N3-C2-O2	-6.08	117.65	121.90
54	BA	2094	A	C4-C5-C6	-6.08	113.96	117.00
21	AA	1328	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	352	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	1488	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	1899	A	C4-C5-C6	-6.07	113.96	117.00
21	AA	1332	A	C4-C5-C6	-6.07	113.96	117.00
54	BA	1013	C	N1-C2-O2	6.07	122.54	118.90
21	AA	1437	A	C5-C6-N1	6.07	120.73	117.70
54	BA	1810	A	N1-C6-N6	-6.07	114.96	118.60
54	BA	2173	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	2614	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	650	G	N1-C6-O6	-6.07	116.26	119.90
21	AA	1176	A	C4-C5-C6	-6.07	113.97	117.00
21	AA	1452	C	N3-C2-O2	-6.07	117.65	121.90
23	A2	82	A	O4'-C1'-N9	6.07	113.05	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BF	124	ARG	NE-CZ-NH1	6.07	123.33	120.30
29	BG	152	ARG	NE-CZ-NH1	6.07	123.33	120.30
54	BA	217	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	666	A	C5-C6-N1	6.07	120.73	117.70
54	BA	1100	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	94	A	C4-C5-C6	-6.07	113.97	117.00
54	BA	1547	C	N3-C2-O2	-6.07	117.65	121.90
54	BA	2101	A	C4-C5-C6	-6.07	113.97	117.00
12	AM	89	ARG	NE-CZ-NH1	6.06	123.33	120.30
24	A3	9	G	C1'-O4'-C4'	-6.06	105.05	109.90
29	BG	148	ARG	NE-CZ-NH1	6.06	123.33	120.30
54	BA	310	A	C4-C5-C6	-6.06	113.97	117.00
54	BA	736	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	1335	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	1303	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	921	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2254	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2634	A	N1-C6-N6	-6.06	114.96	118.60
54	BA	2662	A	O4'-C1'-N9	6.06	113.05	108.20
24	A3	42	C	N3-C2-O2	-6.06	117.66	121.90
55	BB	88	C	N3-C2-O2	-6.06	117.66	121.90
21	AA	1114	C	N3-C2-O2	-6.06	117.66	121.90
47	BY	7	ARG	NE-CZ-NH2	-6.06	117.27	120.30
54	BA	987	C	N3-C2-O2	-6.06	117.66	121.90
54	BA	2261	C	N3-C2-O2	-6.05	117.66	121.90
55	BB	17	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	539	G	N3-C2-N2	-6.05	115.66	119.90
22	A1	16	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	1461	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	1788	C	N3-C2-O2	-6.05	117.66	121.90
54	BA	1578	U	O4'-C1'-N1	6.05	113.04	108.20
54	BA	1624	U	O4'-C1'-N1	6.05	113.04	108.20
54	BA	2315	G	O4'-C1'-N9	6.05	113.04	108.20
54	BA	2670	A	C4-C5-C6	-6.05	113.97	117.00
21	AA	924	C	N3-C2-O2	-6.05	117.67	121.90
54	BA	1194	A	C4-C5-C6	-6.05	113.98	117.00
21	AA	277	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	643	C	N3-C2-O2	-6.05	117.67	121.90
21	AA	1256	A	C4-C5-C6	-6.05	113.98	117.00
54	BA	1901	A	C5-C6-N1	6.05	120.72	117.70
54	BA	1918	A	C4-C5-C6	-6.05	113.98	117.00
21	AA	792	A	C4-C5-C6	-6.04	113.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1507	A	C5-C6-N1	6.04	120.72	117.70
32	BJ	99	ARG	NE-CZ-NH1	6.04	123.32	120.30
54	BA	2461	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	2479	U	O4'-C1'-N1	6.04	113.03	108.20
54	BA	95	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	865	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1251	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1326	U	O4'-C1'-N1	6.04	113.03	108.20
54	BA	2579	C	O4'-C1'-N1	6.04	113.03	108.20
21	AA	511	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	977	A	C4-C5-C6	-6.04	113.98	117.00
21	AA	1366	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	639	U	O4'-C1'-N1	6.04	113.03	108.20
54	BA	2206	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	251	G	O4'-C1'-N9	6.04	113.03	108.20
54	BA	382	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	595	C	N3-C2-O2	-6.04	117.67	121.90
54	BA	1545	A	C4-C5-C6	-6.04	113.98	117.00
54	BA	1614	A	C4-C5-C6	-6.04	113.98	117.00
55	BB	91	C	N3-C2-O2	-6.04	117.67	121.90
21	AA	1269	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	1658	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	1996	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	1244	G	N1-C6-O6	-6.03	116.28	119.90
54	BA	1332	G	N3-C4-C5	-6.03	125.58	128.60
21	AA	658	C	N3-C2-O2	-6.03	117.68	121.90
24	A3	74	A	C4-C5-C6	-6.03	113.98	117.00
54	BA	428	A	C5-C6-N1	6.03	120.71	117.70
54	BA	1348	C	N3-C2-O2	-6.03	117.68	121.90
54	BA	2077	A	C5-C6-N1	6.03	120.71	117.70
54	BA	2541	A	C4-C5-C6	-6.03	113.99	117.00
54	BA	2667	C	N1-C2-O2	6.03	122.52	118.90
55	BB	60	C	N3-C2-O2	-6.03	117.68	121.90
21	AA	176	C	N1-C2-O2	6.02	122.51	118.90
21	AA	726	C	N1-C2-O2	6.02	122.51	118.90
25	BC	100	ARG	NE-CZ-NH1	6.02	123.31	120.30
53	B4	4	ARG	NE-CZ-NH1	6.02	123.31	120.30
54	BA	1253	A	O4'-C1'-N9	6.02	113.02	108.20
21	AA	510	A	N1-C6-N6	-6.02	114.99	118.60
21	AA	536	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	842	U	C3'-C2'-C1'	6.02	106.32	101.50
54	BA	270	A	C4-C5-C6	-6.02	113.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2008	C	N3-C2-O2	-6.02	117.69	121.90
54	BA	2298	A	C4-C5-C6	-6.02	113.99	117.00
54	BA	452	G	N1-C6-O6	-6.02	116.29	119.90
54	BA	660	C	N3-C2-O2	-6.02	117.69	121.90
21	AA	1290	G	N3-C2-N2	-6.01	115.69	119.90
54	BA	546	U	O4'-C1'-N1	6.01	113.01	108.20
54	BA	1167	C	N3-C2-O2	-6.01	117.69	121.90
21	AA	311	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1571	A	C4-C5-C6	-6.01	113.99	117.00
54	BA	2134	A	C4-C5-C6	-6.01	113.99	117.00
9	AJ	89	ARG	NE-CZ-NH1	6.01	123.31	120.30
21	AA	547	A	C4-C5-C6	-6.01	113.99	117.00
24	A3	52	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1254	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2199	A	N1-C6-N6	-6.01	114.99	118.60
54	BA	2234	G	N7-C8-N9	6.01	116.11	113.10
54	BA	2813	A	C6-C5-N7	6.01	136.51	132.30
11	AL	49	ARG	NH1-CZ-NH2	-6.01	112.79	119.40
21	AA	272	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	423	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	787	C	N1-C2-O2	6.01	122.51	118.90
54	BA	1007	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1936	A	P-O3'-C3'	6.01	126.91	119.70
54	BA	2078	C	N3-C2-O2	-6.01	117.69	121.90
54	BA	1096	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	54	C	N3-C2-O2	-6.01	117.70	121.90
21	AA	611	C	N1-C2-O2	6.01	122.50	118.90
48	BZ	44	ARG	NE-CZ-NH1	6.01	123.30	120.30
54	BA	1952	A	C4-C5-C6	-6.01	114.00	117.00
54	BA	2339	C	N3-C2-O2	-6.01	117.70	121.90
55	BB	29	A	C4-C5-C6	-6.01	114.00	117.00
21	AA	580	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	1046	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	1427	C	N3-C2-O2	-6.00	117.70	121.90
10	AK	121	ARG	NE-CZ-NH1	6.00	123.30	120.30
21	AA	246	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	1114	C	O4'-C1'-N1	6.00	113.00	108.20
21	AA	1225	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	959	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	2263	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	2757	A	C5'-C4'-O4'	6.00	116.30	109.10
21	AA	744	C	N3-C2-O2	-6.00	117.70	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	749	A	C5-C6-N1	6.00	120.70	117.70
21	AA	983	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	152	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	888	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1900	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	554	A	C5-C6-N1	6.00	120.70	117.70
21	AA	1152	A	C5-C6-N1	6.00	120.70	117.70
54	BA	172	A	C4-C5-C6	-6.00	114.00	117.00
54	BA	1090	A	C4-C5-C6	-6.00	114.00	117.00
21	AA	329	A	C6-C5-N7	6.00	136.50	132.30
21	AA	422	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1078	U	N3-C2-O2	-6.00	118.00	122.20
21	AA	1289	A	C4-C5-C6	-6.00	114.00	117.00
24	A3	35	C	N1-C2-O2	6.00	122.50	118.90
54	BA	1363	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1762	A	C4-C5-C6	-6.00	114.00	117.00
16	AQ	5	ARG	NE-CZ-NH1	6.00	123.30	120.30
21	AA	1293	C	N3-C2-O2	-6.00	117.70	121.90
54	BA	1357	C	O4'-C1'-N1	6.00	113.00	108.20
54	BA	670	A	P-O3'-C3'	5.99	126.89	119.70
54	BA	1655	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	1874	C	N3-C2-O2	-5.99	117.70	121.90
55	BB	66	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	844	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	2327	A	C4-C5-C6	-5.99	114.00	117.00
21	AA	76	G	N3-C2-N2	-5.99	115.71	119.90
21	AA	1449	C	N3-C2-O2	-5.99	117.71	121.90
22	A1	6	A	C4-C5-C6	-5.99	114.00	117.00
54	BA	4	U	O4'-C1'-N1	5.99	112.99	108.20
54	BA	246	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	844	A	C5-C6-N1	5.99	120.69	117.70
54	BA	1556	C	N3-C2-O2	-5.99	117.71	121.90
6	AG	142	ARG	NE-CZ-NH1	5.99	123.29	120.30
20	AU	17	ARG	NE-CZ-NH1	5.99	123.29	120.30
21	AA	183	C	C1'-O4'-C4'	-5.99	105.11	109.90
21	AA	1019	A	C5-C6-N1	5.99	120.69	117.70
21	AA	1117	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	2297	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	2786	U	O4'-C1'-N1	5.99	112.99	108.20
21	AA	162	A	C5-C6-N1	5.99	120.69	117.70
21	AA	363	A	C4-C5-C6	-5.99	114.01	117.00
21	AA	1492	A	C4-C5-C6	-5.99	114.01	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1086	A	C4-C5-C6	-5.99	114.01	117.00
54	BA	1437	C	N3-C2-O2	-5.99	117.71	121.90
54	BA	1493	C	N1-C2-O2	5.99	122.49	118.90
54	BA	1362	C	N3-C2-O2	-5.98	117.71	121.90
22	A1	14	A	C5-C6-N1	5.98	120.69	117.70
54	BA	197	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	704	G	N3-C4-C5	-5.98	125.61	128.60
21	AA	300	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1236	A	C4-C5-C6	-5.98	114.01	117.00
38	BP	100	ARG	NE-CZ-NH1	5.98	123.29	120.30
54	BA	1246	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	2498	C	O4'-C1'-N1	5.98	112.98	108.20
41	BS	99	ARG	NE-CZ-NH1	5.98	123.29	120.30
54	BA	1843	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	2453	A	C4-C5-C6	-5.98	114.01	117.00
19	AT	9	ARG	NH1-CZ-NH2	-5.98	112.82	119.40
21	AA	586	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	958	A	C4-C5-C6	-5.98	114.01	117.00
21	AA	1176	A	C5-C6-N1	5.98	120.69	117.70
54	BA	216	A	C5-C6-N1	5.98	120.69	117.70
54	BA	408	G	N1-C6-O6	-5.98	116.31	119.90
54	BA	892	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1301	A	C4-C5-C6	-5.98	114.01	117.00
54	BA	1694	C	N3-C2-O2	-5.98	117.72	121.90
21	AA	520	A	C5-C6-N1	5.98	120.69	117.70
54	BA	2232	C	N3-C2-O2	-5.98	117.72	121.90
54	BA	2388	A	C4-C5-C6	-5.98	114.01	117.00
6	AG	52	ARG	NE-CZ-NH1	5.97	123.29	120.30
21	AA	1281	C	N1-C2-O2	5.97	122.48	118.90
54	BA	85	G	O4'-C1'-N9	5.97	112.98	108.20
54	BA	203	A	C4-C5-C6	-5.97	114.01	117.00
54	BA	540	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	812	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	2772	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	1217	C	N1-C2-O2	5.97	122.48	118.90
24	A3	62	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	581	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1534	U	N3-C2-O2	-5.97	118.02	122.20
21	AA	6	G	N3-C4-C5	-5.97	125.61	128.60
21	AA	784	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	792	A	C1'-O4'-C4'	-5.97	105.12	109.90
22	A1	2	G	N3-C2-N2	-5.97	115.72	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2047	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	502	A	C4-C5-C6	-5.97	114.02	117.00
21	AA	712	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	792	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	2300	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	651	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	209	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	730	A	C4-C5-C6	-5.97	114.02	117.00
54	BA	1114	C	N3-C2-O2	-5.97	117.72	121.90
54	BA	1822	C	N3-C2-O2	-5.97	117.72	121.90
21	AA	238	A	C4-C5-C6	-5.96	114.02	117.00
21	AA	1049	U	C1'-O4'-C4'	-5.96	105.13	109.90
54	BA	2655	G	C8-N9-C4	-5.96	104.01	106.40
21	AA	1227	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	1067	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2716	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	760	G	O4'-C1'-N9	5.96	112.97	108.20
54	BA	964	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1131	G	O4'-C1'-N9	5.96	112.97	108.20
54	BA	1727	C	O4'-C1'-N1	5.96	112.97	108.20
54	BA	2776	A	C4-C5-C6	-5.96	114.02	117.00
54	BA	2896	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	816	A	C1'-O4'-C4'	-5.96	105.13	109.90
54	BA	1470	A	C5-C6-N1	5.96	120.68	117.70
54	BA	1704	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2382	G	O4'-C1'-N9	5.96	112.97	108.20
21	AA	1484	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	1800	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2301	C	N3-C2-O2	-5.96	117.73	121.90
54	BA	2474	U	N3-C2-O2	-5.96	118.03	122.20
54	BA	455	C	N3-C2-O2	-5.96	117.73	121.90
21	AA	414	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	469	C	N3-C2-O2	-5.95	117.73	121.90
27	BE	88	ARG	NE-CZ-NH1	5.95	123.28	120.30
54	BA	700	G	O4'-C1'-N9	5.95	112.96	108.20
54	BA	1625	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	1668	A	C4-C5-C6	-5.95	114.02	117.00
54	BA	2761	A	C4-C5-C6	-5.95	114.02	117.00
21	AA	637	C	N3-C2-O2	-5.95	117.73	121.90
35	BM	66	ARG	NE-CZ-NH1	5.95	123.28	120.30
54	BA	1123	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	2350	C	N3-C2-O2	-5.95	117.73	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2853	C	N3-C2-O2	-5.95	117.73	121.90
54	BA	347	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	20	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	1535	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	2257	U	O4'-C1'-N1	5.95	112.96	108.20
54	BA	2317	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	18	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	1665	A	C4-C5-C6	-5.95	114.03	117.00
54	BA	2606	C	N3-C2-O2	-5.95	117.74	121.90
54	BA	2753	A	C4-C5-C6	-5.95	114.03	117.00
21	AA	309	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	420	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	900	A	C6-C5-N7	5.94	136.46	132.30
12	AM	2	ARG	NE-CZ-NH2	5.94	123.27	120.30
21	AA	432	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	740	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	749	A	N1-C6-N6	-5.94	115.03	118.60
54	BA	2177	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2546	U	O4'-C1'-N1	5.94	112.95	108.20
54	BA	2666	C	O4'-C1'-N1	5.94	112.95	108.20
21	AA	303	A	C5-C6-N1	5.94	120.67	117.70
21	AA	382	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	1237	C	N3-C2-O2	-5.94	117.74	121.90
21	AA	1359	C	C1'-O4'-C4'	-5.94	105.15	109.90
21	AA	1370	G	N3-C4-C5	-5.94	125.63	128.60
21	AA	1443	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	38	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	483	A	C5-C6-N1	5.94	120.67	117.70
54	BA	1752	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	2042	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	1000	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	1248	A	O4'-C1'-N9	5.94	112.95	108.20
54	BA	1069	A	C4-C5-C6	-5.94	114.03	117.00
54	BA	1315	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	1557	C	N3-C2-O2	-5.94	117.74	121.90
54	BA	211	C	O4'-C1'-N1	5.94	112.95	108.20
54	BA	1980	G	O4'-C1'-N9	5.94	112.95	108.20
54	BA	2090	A	C4-C5-C6	-5.94	114.03	117.00
21	AA	1357	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1317	G	C3'-C2'-C1'	5.93	106.25	101.50
54	BA	1475	G	O4'-C1'-N9	5.93	112.95	108.20
54	BA	1807	G	O4'-C1'-N9	5.93	112.95	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	B5	71	ARG	NE-CZ-NH1	5.93	123.27	120.30
54	BA	116	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	1151	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	1402	U	O4'-C1'-N1	5.93	112.95	108.20
54	BA	1509	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2284	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2632	A	C4-C5-C6	-5.93	114.03	117.00
21	AA	334	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	699	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	1513	A	N1-C6-N6	-5.93	115.04	118.60
22	A1	68	C	N3-C2-O2	-5.93	117.75	121.90
54	BA	896	A	C4-C5-C6	-5.93	114.03	117.00
54	BA	2871	U	O4'-C1'-N1	5.93	112.94	108.20
21	AA	876	C	N3-C2-O2	-5.93	117.75	121.90
21	AA	412	A	C4-C5-C6	-5.93	114.04	117.00
54	BA	1103	A	C4-C5-C6	-5.93	114.04	117.00
54	BA	1298	C	N3-C2-O2	-5.93	117.75	121.90
55	BB	88	C	O4'-C1'-N1	5.92	112.94	108.20
21	AA	574	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	1273	C	N3-C2-O2	-5.92	117.75	121.90
54	BA	142	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	732	C	O4'-C1'-N1	5.92	112.94	108.20
54	BA	2580	U	N3-C2-O2	-5.92	118.05	122.20
54	BA	2602	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2655	G	N3-C4-C5	-5.92	125.64	128.60
54	BA	2762	C	N3-C2-O2	-5.92	117.75	121.90
38	BP	50	ARG	NE-CZ-NH1	5.92	123.26	120.30
9	AJ	5	ARG	NE-CZ-NH1	5.92	123.26	120.30
21	AA	560	A	C4-C5-C6	-5.92	114.04	117.00
54	BA	2096	C	N3-C2-O2	-5.92	117.76	121.90
12	AM	91	ARG	NE-CZ-NH1	5.92	123.26	120.30
21	AA	1035	A	C4-C5-C6	-5.92	114.04	117.00
21	AA	1317	C	O4'-C1'-N1	5.92	112.93	108.20
24	A3	29	C	O4'-C1'-N1	5.92	112.93	108.20
21	AA	1103	C	N3-C2-O2	-5.92	117.76	121.90
54	BA	2093	G	O4'-C1'-N9	5.92	112.93	108.20
54	BA	2705	A	N1-C6-N6	-5.92	115.05	118.60
21	AA	143	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	1553	A	O4'-C1'-N9	5.91	112.93	108.20
54	BA	1021	A	C4-C5-C6	-5.91	114.04	117.00
54	BA	2496	C	N3-C2-O2	-5.91	117.76	121.90
6	AG	9	ARG	NE-CZ-NH1	5.91	123.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	525	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	624	C	N3-C2-O2	-5.91	117.76	121.90
54	BA	1795	C	O4'-C1'-N1	5.91	112.93	108.20
54	BA	2456	C	N1-C2-O2	5.91	122.45	118.90
55	BB	79	G	O4'-C1'-N9	5.91	112.93	108.20
54	BA	666	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	1998	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	2448	A	C4-C5-C6	-5.91	114.05	117.00
21	AA	729	A	C4-C5-C6	-5.91	114.05	117.00
29	BG	151	ARG	NE-CZ-NH2	-5.91	117.35	120.30
54	BA	2169	A	C4-C5-C6	-5.91	114.05	117.00
10	AK	127	ARG	NE-CZ-NH2	5.91	123.25	120.30
21	AA	87	C	N3-C2-O2	-5.91	117.77	121.90
21	AA	1003	G	O4'-C1'-N9	5.91	112.92	108.20
54	BA	11	C	N3-C2-O2	-5.91	117.77	121.90
54	BA	471	A	C4-C5-C6	-5.91	114.05	117.00
54	BA	663	G	N3-C2-N2	-5.91	115.77	119.90
54	BA	1871	A	O4'-C1'-N9	5.91	112.92	108.20
21	AA	1028	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	395	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1157	A	N1-C6-N6	-5.90	115.06	118.60
54	BA	1039	A	C4-C5-C6	-5.90	114.05	117.00
54	BA	1962	C	N1-C2-O2	5.90	122.44	118.90
54	BA	2260	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	2697	G	N1-C6-O6	-5.90	116.36	119.90
2	AC	168	ARG	NE-CZ-NH1	5.90	123.25	120.30
21	AA	95	C	N1-C2-O2	5.90	122.44	118.90
21	AA	366	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	631	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	462	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	2845	U	O4'-C1'-N1	5.90	112.92	108.20
54	BA	2886	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	880	C	O4'-C1'-N1	5.90	112.92	108.20
54	BA	2691	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	116	A	N1-C6-N6	-5.90	115.06	118.60
21	AA	271	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	314	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	493	A	C4-C5-C6	-5.90	114.05	117.00
21	AA	1065	U	O4'-C1'-N1	5.90	112.92	108.20
21	AA	1141	C	N3-C2-O2	-5.90	117.77	121.90
21	AA	1453	G	O4'-C1'-N9	5.90	112.92	108.20
54	BA	1985	C	N3-C2-O2	-5.90	117.77	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2767	C	N3-C2-O2	-5.90	117.77	121.90
54	BA	833	A	O4'-C1'-N9	5.89	112.92	108.20
21	AA	418	C	N3-C2-O2	-5.89	117.78	121.90
21	AA	679	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	2738	A	C5-C6-N1	5.89	120.65	117.70
21	AA	647	C	O4'-C1'-N1	5.89	112.91	108.20
54	BA	673	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	1738	G	O4'-C1'-N9	5.89	112.91	108.20
54	BA	2104	C	O4'-C1'-N1	5.89	112.91	108.20
21	AA	676	A	C4-C5-C6	-5.89	114.06	117.00
21	AA	1128	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	28	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	2617	U	O4'-C1'-N1	5.89	112.91	108.20
21	AA	703	G	O4'-C1'-N9	5.89	112.91	108.20
54	BA	456	C	N1-C2-O2	5.89	122.43	118.90
54	BA	1262	A	C4-C5-C6	-5.89	114.06	117.00
54	BA	2403	C	N3-C2-O2	-5.89	117.78	121.90
54	BA	242	G	N3-C4-C5	-5.88	125.66	128.60
54	BA	346	A	O4'-C1'-N9	5.88	112.91	108.20
54	BA	1502	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1565	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	1632	A	O4'-C1'-N9	5.88	112.91	108.20
56	B5	134	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	1598	A	C4-C5-C6	-5.88	114.06	117.00
22	A1	62	C	N3-C2-O2	-5.88	117.78	121.90
36	BN	45	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	716	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	848	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	973	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	1048	A	N1-C6-N6	-5.88	115.07	118.60
54	BA	1790	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	2528	U	O4'-C1'-N1	5.88	112.91	108.20
54	BA	1345	C	N3-C2-O2	-5.88	117.78	121.90
54	BA	2486	C	O4'-C1'-N1	5.88	112.90	108.20
54	BA	2766	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	101	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	485	C	N3-C2-O2	-5.88	117.79	121.90
54	BA	1532	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	1004	A	C4-C5-C6	-5.88	114.06	117.00
21	AA	1282	C	N3-C2-O2	-5.88	117.79	121.90
43	BU	93	ARG	NE-CZ-NH1	5.88	123.24	120.30
54	BA	816	C	N3-C2-O2	-5.88	117.79	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1302	A	C4-C5-C6	-5.88	114.06	117.00
54	BA	2030	A	C4-C5-C6	-5.88	114.06	117.00
38	BP	112	ARG	NE-CZ-NH1	5.87	123.24	120.30
54	BA	486	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	1231	U	O4'-C1'-N1	5.87	112.90	108.20
54	BA	1885	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	1994	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2884	U	O4'-C1'-N1	5.87	112.90	108.20
21	AA	295	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	968	C	N3-C2-O2	-5.87	117.79	121.90
54	BA	2054	A	C4-C5-C6	-5.87	114.06	117.00
54	BA	2433	A	C4-C5-C6	-5.87	114.06	117.00
21	AA	937	A	C4-C5-C6	-5.87	114.07	117.00
21	AA	673	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	917	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	2184	A	C4-C5-C6	-5.87	114.07	117.00
18	AS	3	SER	C-N-CA	5.87	136.36	121.70
21	AA	1288	A	C4-C5-C6	-5.87	114.07	117.00
54	BA	107	G	O4'-C1'-N9	5.87	112.89	108.20
54	BA	1157	G	N1-C6-O6	-5.87	116.38	119.90
54	BA	1921	G	O4'-C1'-N9	5.87	112.89	108.20
54	BA	2249	U	O4'-C1'-N1	5.87	112.89	108.20
54	BA	2649	C	O4'-C1'-N1	5.87	112.89	108.20
21	AA	1171	A	C5-C6-N1	5.86	120.63	117.70
21	AA	1271	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	514	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	1839	G	C5-C6-N1	5.86	114.43	111.50
54	BA	2171	A	C3'-C2'-C1'	-5.86	96.81	101.50
21	AA	758	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	770	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	779	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	1469	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	1320	C	N3-C2-O2	-5.86	117.80	121.90
55	BB	5	U	O4'-C1'-N1	5.86	112.89	108.20
54	BA	835	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	508	U	N3-C2-O2	-5.86	118.10	122.20
21	AA	764	C	N1-C2-O2	5.86	122.41	118.90
54	BA	1221	C	N3-C2-O2	-5.86	117.80	121.90
54	BA	2396	G	O4'-C1'-N9	5.86	112.89	108.20
23	A2	82	A	C1'-O4'-C4'	-5.86	105.22	109.90
54	BA	219	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	994	C	N3-C2-O2	-5.86	117.80	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1789	A	C4-C5-C6	-5.86	114.07	117.00
54	BA	2805	C	N3-C2-O2	-5.86	117.80	121.90
21	AA	110	C	N1-C2-O2	5.85	122.41	118.90
21	AA	703	G	C3'-C2'-C1'	5.85	106.18	101.50
21	AA	743	A	C5-C6-N1	5.85	120.63	117.70
21	AA	900	A	C4-C5-C6	-5.85	114.07	117.00
54	BA	1768	C	N3-C2-O2	-5.85	117.80	121.90
21	AA	441	A	C4-C5-C6	-5.85	114.07	117.00
21	AA	783	C	N3-C2-O2	-5.85	117.80	121.90
21	AA	1071	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	393	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	1600	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	1611	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	2285	C	N3-C2-O2	-5.85	117.80	121.90
54	BA	2662	A	C5-C6-N1	5.85	120.63	117.70
55	BB	77	U	O4'-C1'-N1	5.85	112.88	108.20
21	AA	108	G	N3-C4-C5	-5.85	125.67	128.60
24	A3	36	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	158	U	O4'-C1'-N1	5.85	112.88	108.20
54	BA	236	C	N3-C2-O2	-5.85	117.81	121.90
54	BA	322	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	602	A	O4'-C1'-N9	5.85	112.88	108.20
54	BA	849	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	1586	A	C4-C5-C6	-5.85	114.08	117.00
24	A3	39	A	C4-C5-C6	-5.85	114.08	117.00
54	BA	2084	C	N1-C2-O2	5.85	122.41	118.90
54	BA	2321	U	N3-C2-O2	-5.85	118.11	122.20
54	BA	650	C	N3-C2-O2	-5.85	117.81	121.90
10	AK	126	ARG	NE-CZ-NH1	5.84	123.22	120.30
36	BN	96	ARG	NE-CZ-NH1	5.84	123.22	120.30
54	BA	1111	A	C5-C6-N1	5.84	120.62	117.70
21	AA	889	A	C4-C5-C6	-5.84	114.08	117.00
24	A3	3	C	N1-C2-O2	5.84	122.41	118.90
54	BA	1494	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	135	C	N3-C2-O2	-5.84	117.81	121.90
21	AA	307	C	N1-C2-O2	5.84	122.40	118.90
21	AA	519	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	785	G	N1-C6-O6	-5.84	116.40	119.90
54	BA	2222	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	2326	C	O4'-C1'-N1	5.84	112.87	108.20
54	BA	2418	A	N1-C6-N6	-5.84	115.10	118.60
54	BA	2442	C	N3-C2-O2	-5.84	117.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AT	28	ARG	NE-CZ-NH1	5.84	123.22	120.30
21	AA	65	A	C4-C5-C6	-5.84	114.08	117.00
21	AA	977	A	O4'-C1'-N9	5.84	112.87	108.20
54	BA	156	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	814	C	N3-C2-O2	-5.84	117.81	121.90
54	BA	1431	A	C4-C5-C6	-5.84	114.08	117.00
54	BA	2746	U	O4'-C1'-N1	5.84	112.87	108.20
21	AA	186	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	443	C	N3-C2-O2	-5.83	117.82	121.90
41	BS	8	ARG	NE-CZ-NH1	5.83	123.22	120.30
12	AM	91	ARG	NE-CZ-NH2	-5.83	117.38	120.30
21	AA	381	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	2732	G	N3-C4-C5	-5.83	125.68	128.60
21	AA	1279	G	N3-C4-C5	-5.83	125.69	128.60
21	AA	1524	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	1158	C	N3-C2-O2	-5.83	117.82	121.90
47	BY	48	ARG	NE-CZ-NH1	5.83	123.21	120.30
21	AA	153	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	337	C	N1-C2-O2	5.83	122.40	118.90
21	AA	868	C	N3-C2-O2	-5.83	117.82	121.90
21	AA	964	A	N1-C6-N6	-5.83	115.10	118.60
21	AA	1265	C	N3-C2-O2	-5.83	117.82	121.90
54	BA	108	G	N3-C2-N2	-5.83	115.82	119.90
54	BA	334	C	O4'-C1'-N1	5.83	112.86	108.20
54	BA	1764	C	N3-C2-O2	-5.83	117.82	121.90
12	AM	69	ARG	NE-CZ-NH1	5.82	123.21	120.30
21	AA	482	A	N1-C6-N6	-5.82	115.11	118.60
54	BA	786	C	N3-C2-O2	-5.82	117.82	121.90
21	AA	353	A	C1'-O4'-C4'	-5.82	105.24	109.90
21	AA	236	A	C4-C5-C6	-5.82	114.09	117.00
22	A1	23	A	C4-C5-C6	-5.82	114.09	117.00
55	BB	58	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	74	A	C4-C5-C6	-5.82	114.09	117.00
54	BA	1172	C	N3-C2-O2	-5.82	117.83	121.90
21	AA	728	A	C6-C5-N7	5.82	136.37	132.30
54	BA	222	A	C1'-O4'-C4'	-5.82	105.25	109.90
54	BA	1221	C	O4'-C1'-N1	5.82	112.86	108.20
54	BA	1670	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	2764	A	C4-C5-C6	-5.82	114.09	117.00
21	AA	897	C	N1-C2-O2	5.82	122.39	118.90
54	BA	229	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	901	C	N3-C2-O2	-5.82	117.83	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2045	C	N3-C2-O2	-5.82	117.83	121.90
54	BA	912	C	N1-C2-O2	5.81	122.39	118.90
54	BA	2646	C	C2-N1-C1'	5.81	125.19	118.80
54	BA	56	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	705	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	746	U	O4'-C1'-N1	5.81	112.85	108.20
54	BA	1321	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1378	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1726	C	N3-C2-O2	-5.81	117.83	121.90
21	AA	930	C	N3-C2-O2	-5.81	117.83	121.90
20	AU	33	ARG	NE-CZ-NH1	5.81	123.20	120.30
21	AA	1324	A	C4-C5-C6	-5.81	114.09	117.00
54	BA	1285	A	C5-C6-N1	5.81	120.60	117.70
54	BA	1528	A	N1-C6-N6	-5.81	115.11	118.60
54	BA	1790	C	O4'-C1'-N1	5.81	112.85	108.20
21	AA	214	C	N1-C2-O2	5.81	122.39	118.90
21	AA	1251	A	C4-C5-C6	-5.81	114.10	117.00
22	A1	25	C	N3-C2-O2	-5.81	117.83	121.90
54	BA	1805	A	C4-C5-C6	-5.81	114.10	117.00
21	AA	355	C	N3-C2-O2	-5.81	117.84	121.90
21	AA	1054	C	N1-C2-O2	5.81	122.38	118.90
54	BA	609	A	C4-C5-C6	-5.81	114.10	117.00
54	BA	92	U	N3-C2-O2	-5.80	118.14	122.20
54	BA	283	G	N1-C6-O6	-5.80	116.42	119.90
54	BA	353	C	N3-C2-O2	-5.80	117.84	121.90
21	AA	157	U	O4'-C1'-N1	5.80	112.84	108.20
8	AI	121	ARG	NE-CZ-NH1	5.80	123.20	120.30
21	AA	621	A	C4-C5-C6	-5.80	114.10	117.00
30	BH	116	ARG	NE-CZ-NH1	5.80	123.20	120.30
54	BA	1264	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2765	A	C4-C5-C6	-5.80	114.10	117.00
55	BB	15	A	C4-C5-C6	-5.80	114.10	117.00
21	AA	1081	A	C5-C6-N1	5.80	120.60	117.70
21	AA	1479	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1247	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	22	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	238	C	N3-C2-O2	-5.80	117.84	121.90
54	BA	1854	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2800	A	C4-C5-C6	-5.80	114.10	117.00
54	BA	2478	A	C4-C5-C6	-5.79	114.10	117.00
21	AA	984	C	N3-C2-O2	-5.79	117.84	121.90
24	A3	77	A	C4-C5-C6	-5.79	114.10	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	345	A	C4-C5-C6	-5.79	114.10	117.00
54	BA	366	C	N3-C2-O2	-5.79	117.84	121.90
15	AP	51	ARG	NE-CZ-NH1	5.79	123.20	120.30
54	BA	2554	U	O4'-C1'-N1	5.79	112.83	108.20
54	BA	678	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	2651	C	N3-C2-O2	-5.79	117.85	121.90
21	AA	328	C	P-O3'-C3'	5.79	126.65	119.70
54	BA	422	A	C3'-C2'-C1'	5.79	106.13	101.50
54	BA	902	C	N3-C2-O2	-5.79	117.85	121.90
54	BA	2577	A	C4-C5-C6	-5.79	114.11	117.00
14	AO	87	ARG	NE-CZ-NH1	5.79	123.19	120.30
54	BA	1196	C	O4'-C1'-N1	5.79	112.83	108.20
54	BA	1312	U	P-O3'-C3'	5.78	126.64	119.70
21	AA	393	A	C5-C6-N1	5.78	120.59	117.70
21	AA	856	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	1593	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	1877	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2791	G	O4'-C1'-N9	5.78	112.83	108.20
21	AA	1054	C	C1'-O4'-C4'	-5.78	105.28	109.90
54	BA	846	U	N3-C2-O2	-5.78	118.15	122.20
54	BA	1121	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2132	U	N3-C2-O2	-5.78	118.15	122.20
54	BA	2658	C	N3-C2-O2	-5.78	117.85	121.90
55	BB	27	C	N3-C2-O2	-5.78	117.85	121.90
54	BA	2146	C	N3-C2-O2	-5.78	117.86	121.90
21	AA	642	A	C4-C5-C6	-5.78	114.11	117.00
21	AA	1030	U	N3-C2-O2	-5.78	118.16	122.20
21	AA	1430	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	333	G	O4'-C1'-N9	5.78	112.82	108.20
54	BA	554	U	O4'-C1'-N1	5.78	112.82	108.20
54	BA	1126	A	O4'-C1'-N9	5.78	112.82	108.20
54	BA	1742	U	O4'-C1'-N1	5.78	112.82	108.20
21	AA	608	A	C6-C5-N7	5.78	136.34	132.30
21	AA	1038	C	N3-C2-O2	-5.78	117.86	121.90
21	AA	1204	A	C5-C6-N1	5.78	120.59	117.70
54	BA	53	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2534	A	C4-C5-C6	-5.78	114.11	117.00
54	BA	2648	G	N1-C6-O6	-5.78	116.43	119.90
23	A2	79	A	C4-C5-C6	-5.77	114.11	117.00
22	A1	18	G	N1-C6-O6	-5.77	116.44	119.90
25	BC	176	ARG	NE-CZ-NH1	5.77	123.19	120.30
54	BA	2220	U	O4'-C1'-N1	5.77	112.82	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	980	C	N1-C2-O2	5.77	122.36	118.90
54	BA	1748	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1876	A	C4-C5-C6	-5.77	114.11	117.00
54	BA	2068	U	O4'-C1'-N1	5.77	112.82	108.20
54	BA	2587	A	C4-C5-C6	-5.77	114.11	117.00
21	AA	456	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	914	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	994	A	C4-C5-C6	-5.77	114.12	117.00
21	AA	1339	A	N1-C6-N6	-5.77	115.14	118.60
25	BC	47	ARG	NE-CZ-NH1	5.77	123.18	120.30
39	BQ	5	ARG	NE-CZ-NH1	5.77	123.18	120.30
54	BA	277	G	N1-C6-O6	-5.77	116.44	119.90
54	BA	281	C	N3-C2-O2	-5.77	117.86	121.90
54	BA	1462	C	N3-C2-O2	-5.77	117.86	121.90
21	AA	71	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	454	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	475	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	650	C	O4'-C1'-N1	5.76	112.81	108.20
54	BA	1582	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	1604	C	N3-C2-O2	-5.76	117.86	121.90
54	BA	1851	U	O4'-C1'-N1	5.76	112.81	108.20
21	AA	819	A	C4-C5-C6	-5.76	114.12	117.00
4	AE	137	ARG	NE-CZ-NH1	5.76	123.18	120.30
33	BK	71	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
21	AA	614	C	N3-C2-O2	-5.76	117.87	121.90
54	BA	91	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	374	A	N1-C6-N6	-5.76	115.14	118.60
54	BA	531	C	N1-C2-O2	5.76	122.36	118.90
54	BA	587	C	N1-C2-O2	5.76	122.36	118.90
54	BA	608	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	1692	U	O4'-C1'-N1	5.76	112.81	108.20
54	BA	2471	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2679	A	C4-C5-C6	-5.76	114.12	117.00
43	BU	6	ARG	NE-CZ-NH2	-5.76	117.42	120.30
49	B0	12	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	BA	1204	A	C4-C5-C6	-5.76	114.12	117.00
21	AA	1183	U	O4'-C1'-N1	5.76	112.81	108.20
54	BA	936	A	C4-C5-C6	-5.76	114.12	117.00
54	BA	2262	U	O4'-C1'-N1	5.76	112.81	108.20
21	AA	1107	C	N3-C2-O2	-5.75	117.87	121.90
21	AA	1320	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	859	G	O4'-C1'-N9	5.75	112.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	415	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	655	A	C4-C5-C6	-5.75	114.12	117.00
21	AA	696	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	331	C	N3-C2-O2	-5.75	117.87	121.90
54	BA	819	A	C4-C5-C6	-5.75	114.12	117.00
54	BA	2213	U	N3-C2-O2	-5.75	118.17	122.20
21	AA	47	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	618	C	N3-C2-O2	-5.75	117.88	121.90
21	AA	960	U	N3-C2-O2	-5.75	118.17	122.20
54	BA	427	U	O4'-C1'-N1	5.75	112.80	108.20
21	AA	44	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	723	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	127	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	1344	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	2567	G	C1'-O4'-C4'	-5.75	105.30	109.90
54	BA	96	C	N1-C2-O2	5.75	122.35	118.90
54	BA	278	A	C4-C5-C6	-5.75	114.13	117.00
54	BA	2510	C	O4'-C1'-N1	5.75	112.80	108.20
54	BA	813	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	1078	U	O4'-C1'-N1	5.75	112.80	108.20
54	BA	1104	C	N3-C2-O2	-5.75	117.88	121.90
54	BA	1890	A	C4-C5-C6	-5.75	114.13	117.00
21	AA	596	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	1434	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	412	A	N1-C6-N6	-5.74	115.15	118.60
21	AA	223	A	C4-C5-C6	-5.74	114.13	117.00
21	AA	373	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2571	U	O4'-C1'-N1	5.74	112.79	108.20
55	BB	31	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	246	A	C1'-O4'-C4'	-5.74	105.31	109.90
21	AA	253	A	C5-C6-N1	5.74	120.57	117.70
21	AA	269	C	N3-C2-O2	-5.74	117.88	121.90
21	AA	539	A	N1-C6-N6	-5.74	115.16	118.60
54	BA	250	G	N3-C2-N2	-5.74	115.88	119.90
54	BA	616	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2033	A	C5-C6-N1	5.74	120.57	117.70
54	BA	2071	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	2452	C	O4'-C1'-N1	5.74	112.79	108.20
54	BA	2572	A	C4-C5-C6	-5.74	114.13	117.00
55	BB	19	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	129	C	N3-C2-O2	-5.74	117.88	121.90
54	BA	1898	U	O4'-C1'-N1	5.74	112.79	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	984	A	C4-C5-C6	-5.74	114.13	117.00
54	BA	1498	C	N3-C2-O2	-5.74	117.89	121.90
54	BA	1690	A	C5-C6-N1	5.74	120.57	117.70
54	BA	2091	C	N1-C2-O2	5.74	122.34	118.90
54	BA	2535	G	O4'-C1'-N9	5.74	112.79	108.20
21	AA	1431	A	C4-C5-C6	-5.73	114.13	117.00
54	BA	1205	A	C4-C5-C6	-5.73	114.13	117.00
54	BA	1271	G	O4'-C1'-N9	5.73	112.79	108.20
21	AA	1448	C	N3-C2-O2	-5.73	117.89	121.90
54	BA	2850	A	C4-C5-C6	-5.73	114.13	117.00
54	BA	808	G	O4'-C1'-N9	5.73	112.78	108.20
54	BA	2429	G	N3-C2-N2	-5.73	115.89	119.90
21	AA	526	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	1413	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	528	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	842	U	O4'-C1'-N1	5.73	112.78	108.20
54	BA	1794	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	2828	G	N1-C6-O6	-5.73	116.46	119.90
21	AA	174	A	C4-C5-C6	-5.73	114.14	117.00
34	BL	60	ARG	NE-CZ-NH2	5.73	123.16	120.30
54	BA	508	A	C4-C5-C6	-5.73	114.14	117.00
21	AA	194	C	N1-C2-O2	5.73	122.34	118.90
21	AA	1147	C	N3-C2-O2	-5.73	117.89	121.90
21	AA	1350	A	C4-C5-C6	-5.73	114.14	117.00
54	BA	210	C	O4'-C1'-N1	5.73	112.78	108.20
54	BA	1167	C	O4'-C1'-N1	5.72	112.78	108.20
54	BA	2462	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	357	C	N3-C2-O2	-5.72	117.89	121.90
54	BA	2471	A	C5-C6-N1	5.72	120.56	117.70
54	BA	2826	A	N1-C6-N6	-5.72	115.17	118.60
54	BA	615	U	N3-C2-O2	-5.72	118.19	122.20
54	BA	718	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2639	A	O4'-C1'-N9	5.72	112.78	108.20
54	BA	691	C	O4'-C1'-N1	5.72	112.78	108.20
54	BA	2328	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	1653	G	O4'-C1'-N9	5.72	112.78	108.20
54	BA	1848	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	2435	A	C4-C5-C6	-5.72	114.14	117.00
54	BA	417	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	1188	U	N3-C2-O2	-5.72	118.20	122.20
54	BA	1447	C	N3-C2-O2	-5.72	117.90	121.90
54	BA	1285	A	C4-C5-C6	-5.71	114.14	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2589	A	C6-C5-N7	5.71	136.30	132.30
21	AA	1501	C	N1-C2-O2	5.71	122.33	118.90
54	BA	1864	U	O4'-C1'-N1	5.71	112.77	108.20
54	BA	2014	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2592	G	N1-C6-O6	-5.71	116.47	119.90
54	BA	176	A	C4-C5-C6	-5.71	114.14	117.00
21	AA	795	C	N1-C2-O2	5.71	122.33	118.90
21	AA	1378	C	N3-C2-O2	-5.71	117.90	121.90
22	A1	52	G	N3-C2-N2	-5.71	115.90	119.90
54	BA	1773	A	C4-C5-C6	-5.71	114.14	117.00
54	BA	2076	U	N3-C2-O2	-5.71	118.20	122.20
54	BA	2392	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	2725	A	C4-C5-C6	-5.71	114.15	117.00
55	BB	92	C	N3-C2-O2	-5.71	117.90	121.90
54	BA	72	U	O4'-C1'-N1	5.71	112.77	108.20
54	BA	99	U	N3-C2-O2	-5.71	118.21	122.20
54	BA	863	A	N1-C6-N6	-5.71	115.18	118.60
55	BB	57	A	N1-C6-N6	-5.71	115.18	118.60
21	AA	707	U	O4'-C1'-N1	5.71	112.76	108.20
54	BA	384	A	C4-C5-C6	-5.71	114.15	117.00
54	BA	1010	A	C4-C5-C6	-5.71	114.15	117.00
21	AA	1044	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	1226	C	N1-C2-O2	5.70	122.32	118.90
21	AA	1409	C	N3-C2-O2	-5.70	117.91	121.90
21	AA	1447	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	528	A	O4'-C1'-N9	5.70	112.76	108.20
54	BA	2601	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	2703	C	O4'-C1'-N1	5.70	112.76	108.20
21	AA	101	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	1136	C	C6-N1-C2	-5.70	118.02	120.30
54	BA	1617	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	1806	C	C5'-C4'-O4'	5.70	115.94	109.10
21	AA	1230	C	C5'-C4'-O4'	5.70	115.94	109.10
21	AA	1442	G	N3-C2-N2	-5.70	115.91	119.90
54	BA	578	G	N1-C6-O6	-5.70	116.48	119.90
21	AA	195	A	C4-C5-C6	-5.70	114.15	117.00
21	AA	881	G	N1-C6-O6	-5.70	116.48	119.90
54	BA	477	A	C3'-C2'-C1'	5.70	106.06	101.50
54	BA	1434	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2198	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2236	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	2485	G	C2'-C3'-O3'	5.70	122.82	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	176	A	C5-C6-N1	5.70	120.55	117.70
54	BA	1229	C	N3-C2-O2	-5.70	117.91	121.90
9	AJ	48	ARG	NE-CZ-NH1	5.70	123.15	120.30
21	AA	494	G	O4'-C1'-N9	5.70	112.76	108.20
21	AA	738	C	N3-C2-O2	-5.70	117.91	121.90
54	BA	444	C	O4'-C1'-N1	5.70	112.76	108.20
54	BA	460	A	C4-C5-C6	-5.70	114.15	117.00
54	BA	2195	U	O4'-C1'-N1	5.70	112.76	108.20
54	BA	2391	G	C1'-O4'-C4'	-5.70	105.34	109.90
21	AA	1005	A	N1-C6-N6	-5.69	115.18	118.60
54	BA	781	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2795	C	N3-C2-O2	-5.69	117.91	121.90
54	BA	253	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1053	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	1146	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1711	A	C4-C5-C6	-5.69	114.15	117.00
54	BA	2450	A	C5-C6-N1	5.69	120.55	117.70
10	AK	55	ARG	NE-CZ-NH1	5.69	123.15	120.30
21	AA	284	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	700	G	N1-C6-O6	-5.69	116.48	119.90
54	BA	1226	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1241	A	C4-C5-C6	-5.69	114.16	117.00
54	BA	1475	G	N1-C6-O6	-5.69	116.49	119.90
54	BA	772	C	N3-C2-O2	-5.69	117.92	121.90
8	AI	79	ARG	NE-CZ-NH1	5.69	123.14	120.30
21	AA	1137	C	N3-C2-O2	-5.69	117.92	121.90
21	AA	1347	G	O4'-C1'-N9	5.69	112.75	108.20
54	BA	305	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	812	C	O4'-C1'-N1	5.69	112.75	108.20
54	BA	2320	U	N3-C2-O2	-5.69	118.22	122.20
54	BA	2520	C	N3-C2-O2	-5.69	117.92	121.90
54	BA	1504	A	C4-C5-C6	-5.69	114.16	117.00
13	AN	53	ARG	NE-CZ-NH1	5.68	123.14	120.30
54	BA	330	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	405	U	O4'-C1'-N1	5.68	112.75	108.20
54	BA	1207	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	1986	C	N3-C2-O2	-5.68	117.92	121.90
21	AA	749	A	C4-C5-C6	-5.68	114.16	117.00
21	AA	1325	C	N3-C2-O2	-5.68	117.92	121.90
24	A3	66	C	N3-C2-O2	-5.68	117.92	121.90
54	BA	249	C	N1-C2-O2	5.68	122.31	118.90
54	BA	505	A	C4-C5-C6	-5.68	114.16	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1533	C	N1-C2-O2	5.68	122.31	118.90
54	BA	294	A	C1'-O4'-C4'	-5.68	105.36	109.90
54	BA	1590	A	C6-C5-N7	5.68	136.28	132.30
54	BA	275	C	N3-C2-O2	-5.68	117.93	121.90
54	BA	1155	A	C4-C5-C6	-5.68	114.16	117.00
54	BA	885	C	N3-C2-O2	-5.68	117.93	121.90
54	BA	1575	C	O4'-C1'-N1	5.68	112.74	108.20
54	BA	2755	C	O4'-C1'-N1	5.68	112.74	108.20
21	AA	1003	G	N1-C6-O6	-5.67	116.50	119.90
54	BA	1006	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2215	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2722	G	O4'-C1'-N9	5.67	112.74	108.20
55	BB	63	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	173	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1239	G	N3-C2-N2	-5.67	115.93	119.90
54	BA	2499	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2863	C	O4'-C1'-N1	5.67	112.74	108.20
54	BA	2900	A	C4-C5-C6	-5.67	114.16	117.00
54	BA	1644	C	N1-C2-O2	5.67	122.30	118.90
21	AA	451	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	272	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	402	A	N1-C6-N6	-5.67	115.20	118.60
54	BA	2553	G	N1-C6-O6	-5.67	116.50	119.90
21	AA	507	C	N3-C2-O2	-5.67	117.93	121.90
22	A1	71	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	67	U	O4'-C1'-N1	5.67	112.73	108.20
21	AA	1349	A	C4-C5-C6	-5.67	114.17	117.00
54	BA	780	G	N1-C6-O6	-5.67	116.50	119.90
54	BA	1092	C	N3-C2-O2	-5.67	117.93	121.90
54	BA	2867	G	N3-C4-C5	-5.67	125.77	128.60
21	AA	415	A	O4'-C1'-N9	5.66	112.73	108.20
21	AA	864	A	C5-C6-N1	5.66	120.53	117.70
21	AA	1344	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	413	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1552	A	O4'-C1'-N9	5.66	112.73	108.20
54	BA	1613	G	N1-C6-O6	-5.66	116.50	119.90
54	BA	2433	A	O4'-C1'-N9	5.66	112.73	108.20
21	AA	601	G	N1-C6-O6	-5.66	116.50	119.90
54	BA	115	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	1632	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	358	U	O4'-C1'-N1	5.66	112.73	108.20
54	BA	475	C	O4'-C1'-N1	5.66	112.73	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	640	C	O4'-C1'-N1	5.66	112.73	108.20
54	BA	1050	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1919	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	743	A	C4-C5-C6	-5.66	114.17	117.00
21	AA	1152	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	1351	C	N3-C2-O2	-5.66	117.94	121.90
54	BA	2179	C	N1-C2-O2	5.66	122.30	118.90
54	BA	2458	G	N1-C6-O6	-5.66	116.50	119.90
54	BA	2517	C	O4'-C1'-N1	5.66	112.73	108.20
21	AA	1045	C	N1-C2-O2	5.66	122.29	118.90
41	BS	92	ARG	NE-CZ-NH1	5.66	123.13	120.30
54	BA	920	A	N1-C6-N6	-5.66	115.21	118.60
21	AA	258	G	N3-C2-N2	-5.66	115.94	119.90
54	BA	14	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	52	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	161	A	C4-C5-C6	-5.66	114.17	117.00
54	BA	986	C	N1-C2-O2	5.66	122.29	118.90
54	BA	2678	C	N3-C2-O2	-5.66	117.94	121.90
55	BB	26	C	N3-C4-N4	-5.66	114.04	118.00
21	AA	1503	A	C4-C5-C6	-5.65	114.17	117.00
21	AA	1100	C	N1-C2-O2	5.65	122.29	118.90
46	BX	44	ARG	NE-CZ-NH1	5.65	123.13	120.30
54	BA	1480	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1760	C	O4'-C1'-N1	5.65	112.72	108.20
21	AA	1238	A	C6-C5-N7	5.65	136.25	132.30
28	BF	94	ARG	NE-CZ-NH1	5.65	123.12	120.30
54	BA	1214	A	C4-C5-C6	-5.65	114.17	117.00
54	BA	1741	C	O4'-C1'-N1	5.65	112.72	108.20
54	BA	1134	A	C4-C5-C6	-5.65	114.18	117.00
54	BA	2395	C	O4'-C1'-N1	5.65	112.72	108.20
8	AI	112	ARG	NE-CZ-NH1	5.65	123.12	120.30
21	AA	322	C	N3-C2-O2	-5.65	117.95	121.90
54	BA	20	C	N3-C2-O2	-5.65	117.95	121.90
54	BA	1942	C	N1-C2-O2	5.65	122.29	118.90
54	BA	2644	G	O4'-C4'-C3'	5.65	110.62	106.10
54	BA	1717	A	C4-C5-C6	-5.65	114.18	117.00
21	AA	290	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	299	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2177	C	N1-C2-O2	5.64	122.29	118.90
11	AL	13	ARG	NE-CZ-NH1	5.64	123.12	120.30
21	AA	656	G	N1-C6-O6	-5.64	116.51	119.90
21	AA	1201	A	O4'-C1'-N9	5.64	112.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	584	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	239	C	O4'-C1'-N1	5.64	112.71	108.20
21	AA	169	C	N1-C2-O2	5.64	122.28	118.90
21	AA	884	U	C1'-O4'-C4'	-5.64	105.39	109.90
21	AA	899	C	O4'-C1'-N1	5.64	112.71	108.20
54	BA	1054	A	C6-C5-N7	5.64	136.25	132.30
21	AA	1012	A	C4-C5-C6	-5.64	114.18	117.00
21	AA	1346	A	C4-C5-C6	-5.64	114.18	117.00
54	BA	2039	U	O4'-C1'-N1	5.64	112.71	108.20
54	BA	2787	C	N3-C2-O2	-5.64	117.95	121.90
21	AA	1037	C	N1-C2-O2	5.64	122.28	118.90
21	AA	1243	C	N3-C2-O2	-5.64	117.95	121.90
54	BA	1199	U	O4'-C1'-N1	5.64	112.71	108.20
21	AA	263	A	C4-C5-C6	-5.63	114.18	117.00
21	AA	1032	G	O4'-C1'-N9	5.63	112.71	108.20
54	BA	2099	U	C3'-C2'-C1'	5.63	106.01	101.50
54	BA	749	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	2416	C	N3-C2-O2	-5.63	117.96	121.90
5	AF	2	ARG	NE-CZ-NH1	5.63	123.12	120.30
22	A1	52	G	O4'-C1'-N9	5.63	112.70	108.20
54	BA	33	C	N1-C2-O2	5.63	122.28	118.90
54	BA	415	A	C4-C5-C6	-5.63	114.18	117.00
54	BA	1914	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	191	A	C4-C5-C6	-5.63	114.19	117.00
54	BA	418	C	N3-C2-O2	-5.63	117.96	121.90
21	AA	321	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1081	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	1452	C	P-O3'-C3'	5.63	126.45	119.70
21	AA	397	A	C4-C5-C6	-5.63	114.19	117.00
21	AA	583	A	C4-C5-C6	-5.63	114.19	117.00
22	A1	70	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	343	C	N3-C2-O2	-5.63	117.96	121.90
54	BA	2524	G	N1-C6-O6	-5.63	116.53	119.90
24	A3	70	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	2430	A	C4-C5-C6	-5.62	114.19	117.00
21	AA	689	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	679	C	N3-C2-O2	-5.62	117.96	121.90
54	BA	203	A	O4'-C1'-N9	5.62	112.70	108.20
54	BA	1612	C	N3-C2-O2	-5.62	117.97	121.90
11	AL	113	ARG	NE-CZ-NH2	-5.62	117.49	120.30
54	BA	957	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	98	A	C4-C5-C6	-5.62	114.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	B0	16	ARG	NE-CZ-NH1	5.62	123.11	120.30
54	BA	2065	C	N1-C2-O2	5.62	122.27	118.90
54	BA	1966	A	C4-C5-C6	-5.62	114.19	117.00
54	BA	148	U	C1'-O4'-C4'	-5.62	105.41	109.90
54	BA	1920	C	N3-C2-O2	-5.62	117.97	121.90
21	AA	162	A	C4-C5-C6	-5.61	114.19	117.00
21	AA	1263	C	N3-C2-O2	-5.61	117.97	121.90
38	BP	52	ARG	NE-CZ-NH1	5.61	123.11	120.30
54	BA	643	A	C4-C5-C6	-5.61	114.19	117.00
54	BA	898	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	1731	G	N1-C6-O6	-5.61	116.53	119.90
54	BA	69	C	O4'-C1'-N1	5.61	112.69	108.20
54	BA	2371	G	O4'-C1'-N9	5.61	112.69	108.20
54	BA	2468	A	C4-C5-C6	-5.61	114.19	117.00
21	AA	1021	A	C4-C5-C6	-5.61	114.19	117.00
21	AA	1279	G	N1-C6-O6	-5.61	116.53	119.90
21	AA	1398	A	C4-C5-C6	-5.61	114.20	117.00
26	BD	169	ARG	NE-CZ-NH1	5.61	123.10	120.30
54	BA	672	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	692	C	N3-C2-O2	-5.61	117.97	121.90
54	BA	799	G	N1-C6-O6	-5.61	116.54	119.90
54	BA	1142	A	C4-C5-C6	-5.61	114.20	117.00
21	AA	250	A	C4-C5-C6	-5.61	114.20	117.00
54	BA	75	G	O4'-C1'-N9	5.61	112.68	108.20
54	BA	558	U	O4'-C1'-N1	5.61	112.68	108.20
54	BA	1098	A	C6-C5-N7	5.61	136.22	132.30
54	BA	590	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1211	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1346	G	C5'-C4'-O4'	5.60	115.82	109.10
21	AA	262	A	C4-C5-C6	-5.60	114.20	117.00
21	AA	1067	A	C4-C5-C6	-5.60	114.20	117.00
24	A3	57	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	689	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	2385	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	614	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	1838	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1997	C	N3-C2-O2	-5.60	117.98	121.90
55	BB	38	C	N3-C2-O2	-5.60	117.98	121.90
21	AA	845	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	574	A	C4-C5-C6	-5.60	114.20	117.00
54	BA	851	C	N3-C2-O2	-5.60	117.98	121.90
54	BA	1305	C	N3-C2-O2	-5.60	117.98	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2873	A	O4'-C1'-N9	5.60	112.68	108.20
21	AA	327	A	C6-C5-N7	5.60	136.22	132.30
24	A3	9	G	N3-C2-N2	-5.59	115.98	119.90
30	BH	97	ARG	NE-CZ-NH1	5.59	123.10	120.30
11	AL	93	ARG	NE-CZ-NH1	5.59	123.10	120.30
54	BA	368	A	O4'-C1'-N9	5.59	112.67	108.20
54	BA	847	U	N3-C2-O2	-5.59	118.29	122.20
54	BA	910	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	1075	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2459	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	306	A	C4-C5-C6	-5.59	114.21	117.00
21	AA	1082	A	C4-C5-C6	-5.59	114.20	117.00
21	AA	1130	A	C4-C5-C6	-5.59	114.20	117.00
22	A1	65	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	87	U	O4'-C1'-N1	5.59	112.67	108.20
54	BA	1387	A	C4-C5-C6	-5.59	114.20	117.00
54	BA	2150	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	2384	U	O4'-C1'-N1	5.59	112.67	108.20
22	A1	56	C	N3-C2-O2	-5.59	117.99	121.90
54	BA	1560	G	N1-C6-O6	-5.59	116.55	119.90
24	A3	49	C	N1-C2-O2	5.59	122.25	118.90
54	BA	2858	C	O4'-C1'-N1	5.59	112.67	108.20
54	BA	1490	A	C4-C5-C6	-5.58	114.21	117.00
22	A1	13	C	O4'-C1'-N1	5.58	112.67	108.20
54	BA	251	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	1595	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	503	C	N3-C2-O2	-5.58	117.99	121.90
21	AA	1529	G	N3-C4-C5	-5.58	125.81	128.60
24	A3	41	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	1243	C	N3-C2-O2	-5.58	117.99	121.90
54	BA	2019	A	C4-C5-C6	-5.58	114.21	117.00
21	AA	148	G	N1-C6-O6	-5.58	116.55	119.90
21	AA	538	G	O4'-C1'-N9	5.58	112.66	108.20
21	AA	1228	C	O4'-C1'-N1	5.58	112.66	108.20
54	BA	1178	C	N3-C2-O2	-5.58	118.00	121.90
54	BA	1508	A	N1-C6-N6	-5.58	115.25	118.60
54	BA	1509	A	C1'-O4'-C4'	-5.58	105.44	109.90
54	BA	2276	G	N3-C2-N2	-5.58	116.00	119.90
54	BA	2421	G	O4'-C1'-N9	5.58	112.66	108.20
21	AA	805	C	O4'-C1'-N1	5.58	112.66	108.20
21	AA	923	A	C4-C5-C6	-5.58	114.21	117.00
54	BA	341	C	N3-C2-O2	-5.58	118.00	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	521	U	O4'-C1'-N1	5.58	112.66	108.20
21	AA	460	A	C4-C5-C6	-5.57	114.21	117.00
54	BA	1000	A	C4-C5-C6	-5.57	114.21	117.00
54	BA	57	C	O4'-C1'-N1	5.57	112.66	108.20
21	AA	1279	G	N3-C2-N2	-5.57	116.00	119.90
54	BA	1076	C	N3-C2-O2	-5.57	118.00	121.90
54	BA	1393	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	2005	A	N1-C6-N6	-5.57	115.26	118.60
54	BA	2205	A	C4-C5-C6	-5.57	114.21	117.00
21	AA	264	C	N1-C2-O2	5.57	122.24	118.90
54	BA	593	U	O4'-C1'-N1	5.57	112.66	108.20
54	BA	2225	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	2412	A	C4-C5-C6	-5.57	114.22	117.00
21	AA	1418	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	222	A	C6-C5-N7	5.57	136.20	132.30
54	BA	234	U	O4'-C1'-N1	5.57	112.65	108.20
54	BA	366	C	O4'-C1'-N1	5.57	112.66	108.20
54	BA	1101	U	O4'-C1'-N1	5.57	112.65	108.20
54	BA	1244	A	C4-C5-C6	-5.57	114.22	117.00
54	BA	2309	A	C4-C5-C6	-5.57	114.22	117.00
55	BB	57	A	C4-C5-C6	-5.57	114.22	117.00
55	BB	78	A	N1-C6-N6	-5.57	115.26	118.60
21	AA	649	A	C4-C5-C6	-5.57	114.22	117.00
22	A1	9	A	C4-C5-C6	-5.57	114.22	117.00
22	A1	72	C	N1-C2-O2	5.57	122.24	118.90
54	BA	544	C	N1-C2-O2	5.57	122.24	118.90
54	BA	1934	C	N3-C2-O2	-5.57	118.00	121.90
21	AA	1339	A	C1'-O4'-C4'	-5.56	105.45	109.90
54	BA	935	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	2135	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	2467	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	563	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	39	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	782	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1112	G	N1-C6-O6	-5.56	116.56	119.90
54	BA	2044	C	N3-C2-O2	-5.56	118.01	121.90
21	AA	336	A	C4-C5-C6	-5.56	114.22	117.00
21	AA	353	A	O4'-C1'-N9	5.56	112.64	108.20
54	BA	572	A	C4-C5-C6	-5.56	114.22	117.00
54	BA	1394	U	N3-C2-O2	-5.56	118.31	122.20
54	BA	2699	C	O4'-C1'-N1	5.56	112.65	108.20
54	BA	332	A	O4'-C1'-N9	5.56	112.64	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	436	C	N3-C2-O2	-5.56	118.01	121.90
54	BA	667	U	O4'-C1'-N1	5.56	112.64	108.20
54	BA	2661	G	N1-C6-O6	-5.56	116.57	119.90
21	AA	82	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	225	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1884	G	N1-C6-O6	-5.55	116.57	119.90
54	BA	2774	C	O4'-C1'-N1	5.55	112.64	108.20
21	AA	172	A	C6-C5-N7	5.55	136.19	132.30
21	AA	1510	C	N1-C2-O2	5.55	122.23	118.90
54	BA	2883	A	C4-C5-C6	-5.55	114.22	117.00
21	AA	383	A	C4-C5-C6	-5.55	114.22	117.00
22	A1	75	C	N3-C2-O2	-5.55	118.01	121.90
54	BA	1288	G	N3-C4-C5	-5.55	125.82	128.60
54	BA	1518	C	N3-C2-O2	-5.55	118.01	121.90
21	AA	461	A	C4-C5-C6	-5.55	114.22	117.00
21	AA	882	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	522	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	687	C	O4'-C1'-N1	5.55	112.64	108.20
54	BA	1032	A	C4-C5-C6	-5.55	114.22	117.00
54	BA	1111	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	1414	C	N1-C2-O2	5.55	122.23	118.90
21	AA	839	C	N1-C2-O2	5.55	122.23	118.90
21	AA	1196	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	2082	A	C4-C5-C6	-5.55	114.23	117.00
21	AA	1287	A	C6-C5-N7	5.55	136.18	132.30
21	AA	1346	A	C1'-O4'-C4'	-5.55	105.46	109.90
54	BA	1353	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	1791	A	C4-C5-C6	-5.55	114.23	117.00
54	BA	1887	C	N3-C2-O2	-5.55	118.02	121.90
54	BA	1313	U	C3'-C2'-C1'	5.54	105.94	101.50
54	BA	2531	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	178	C	N3-C2-O2	-5.54	118.02	121.90
55	BB	37	C	N3-C2-O2	-5.54	118.02	121.90
21	AA	215	C	N1-C2-O2	5.54	122.22	118.90
54	BA	294	A	C6-C5-N7	5.54	136.18	132.30
54	BA	527	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1335	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	1888	G	N3-C4-C5	-5.54	125.83	128.60
54	BA	2581	G	N1-C6-O6	-5.54	116.58	119.90
54	BA	644	A	C4-C5-C6	-5.54	114.23	117.00
7	AH	79	ARG	NE-CZ-NH1	5.54	123.07	120.30
8	AI	84	ARG	NE-CZ-NH1	5.54	123.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1375	A	C4-C5-C6	-5.54	114.23	117.00
21	AA	1493	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	398	C	O4'-C1'-N1	5.54	112.63	108.20
54	BA	2367	G	N3-C2-N2	-5.54	116.02	119.90
55	BB	73	A	C4-C5-C6	-5.54	114.23	117.00
54	BA	549	G	N1-C6-O6	-5.54	116.58	119.90
54	BA	695	G	C4'-C3'-C2'	-5.54	97.06	102.60
54	BA	1738	G	N3-C4-C5	-5.54	125.83	128.60
21	AA	968	A	C4-C5-C6	-5.54	114.23	117.00
40	BR	21	ARG	NE-CZ-NH1	5.54	123.07	120.30
54	BA	1990	C	N1-C2-O2	5.54	122.22	118.90
21	AA	1374	A	C4-C5-C6	-5.53	114.23	117.00
54	BA	304	U	O4'-C1'-N1	5.53	112.63	108.20
54	BA	1071	G	N1-C6-O6	-5.53	116.58	119.90
54	BA	2507	C	O4'-C1'-N1	5.53	112.63	108.20
54	BA	2739	U	O4'-C1'-N1	5.53	112.63	108.20
54	BA	2305	U	O4'-C1'-N1	5.53	112.63	108.20
21	AA	161	A	C4-C5-C6	-5.53	114.23	117.00
21	AA	953	G	N3-C2-N2	-5.53	116.03	119.90
21	AA	1468	A	N1-C6-N6	-5.53	115.28	118.60
54	BA	476	G	N7-C8-N9	5.53	115.86	113.10
21	AA	225	C	N3-C2-O2	-5.53	118.03	121.90
21	AA	535	A	C4-C5-C6	-5.53	114.24	117.00
54	BA	198	C	C5'-C4'-O4'	5.53	115.73	109.10
54	BA	807	U	N3-C2-O2	-5.53	118.33	122.20
21	AA	111	G	O4'-C1'-N9	5.53	112.62	108.20
21	AA	566	G	N1-C6-O6	-5.53	116.58	119.90
21	AA	752	G	O4'-C1'-N9	5.53	112.62	108.20
21	AA	1300	G	O4'-C1'-N9	5.53	112.62	108.20
54	BA	908	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2773	C	N3-C2-O2	-5.53	118.03	121.90
54	BA	2021	C	O4'-C1'-N1	5.52	112.62	108.20
54	BA	49	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	1447	C	O4'-C1'-N1	5.52	112.62	108.20
21	AA	1469	C	N1-C2-O2	5.52	122.21	118.90
54	BA	1799	G	O4'-C1'-N9	5.52	112.62	108.20
54	BA	1980	G	N3-C2-N2	-5.52	116.03	119.90
21	AA	766	A	C1'-O4'-C4'	-5.52	105.48	109.90
21	AA	1507	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	417	C	O4'-C1'-N1	5.52	112.61	108.20
54	BA	1419	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	2212	A	O4'-C1'-N9	5.52	112.61	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2788	C	N3-C2-O2	-5.52	118.04	121.90
3	AD	13	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	AA	189	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	1412	C	N3-C2-O2	-5.52	118.04	121.90
51	B2	41	ARG	NE-CZ-NH1	5.52	123.06	120.30
54	BA	240	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	863	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	899	A	C4-C5-C6	-5.52	114.24	117.00
54	BA	937	C	N3-C2-O2	-5.52	118.04	121.90
54	BA	1957	C	N1-C2-O2	5.52	122.21	118.90
54	BA	2872	A	C4-C5-C6	-5.52	114.24	117.00
55	BB	81	G	C5-C6-N1	5.52	114.26	111.50
54	BA	1080	A	C4-C5-C6	-5.52	114.24	117.00
21	AA	266	G	N3-C4-C5	-5.51	125.84	128.60
54	BA	1325	U	N3-C2-O2	-5.51	118.34	122.20
54	BA	1837	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	2342	C	N1-C2-O2	5.51	122.21	118.90
54	BA	2855	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	901	C	O4'-C1'-N1	5.51	112.61	108.20
21	AA	522	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	102	U	O4'-C1'-N1	5.51	112.61	108.20
54	BA	256	A	C4-C5-C6	-5.51	114.24	117.00
54	BA	640	C	N1-C2-O2	5.51	122.21	118.90
54	BA	691	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	2005	A	C4-C5-C6	-5.51	114.25	117.00
54	BA	2378	A	C4-C5-C6	-5.51	114.24	117.00
21	AA	1195	C	N3-C2-O2	-5.51	118.04	121.90
54	BA	2559	C	N1-C2-O2	5.51	122.21	118.90
21	AA	788	U	N3-C2-O2	-5.51	118.34	122.20
21	AA	1026	G	N3-C2-N2	-5.51	116.04	119.90
21	AA	720	C	N1-C2-O2	5.51	122.20	118.90
54	BA	1340	U	P-O3'-C3'	5.51	126.31	119.70
54	BA	2784	U	O4'-C1'-N1	5.51	112.61	108.20
21	AA	129	A	O4'-C1'-N9	5.50	112.60	108.20
54	BA	1549	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1601	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	2781	A	C6-C5-N7	5.50	136.15	132.30
21	AA	1422	G	C5-C6-N1	5.50	114.25	111.50
54	BA	1341	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	2126	A	O4'-C1'-N9	5.50	112.60	108.20
21	AA	504	C	N3-C2-O2	-5.50	118.05	121.90
21	AA	840	C	N3-C2-O2	-5.50	118.05	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	31	C	O4'-C1'-N1	5.50	112.60	108.20
54	BA	426	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	853	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	1786	A	C4-C5-C6	-5.50	114.25	117.00
54	BA	1828	G	O4'-C1'-N9	5.50	112.60	108.20
54	BA	1347	A	C6-C5-N7	5.50	136.15	132.30
54	BA	2027	G	N1-C6-O6	-5.50	116.60	119.90
54	BA	2811	G	N3-C2-N2	-5.50	116.05	119.90
24	A3	26	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	361	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	1248	A	C1'-O4'-C4'	-5.50	105.50	109.90
24	A3	63	C	N3-C2-O2	-5.50	118.05	121.90
54	BA	523	C	N1-C2-O2	5.50	122.20	118.90
54	BA	1301	A	C1'-O4'-C4'	-5.50	105.50	109.90
21	AA	351	G	P-O3'-C3'	5.50	126.29	119.70
54	BA	2201	G	N1-C6-O6	-5.50	116.60	119.90
21	AA	8	A	C4-C5-C6	-5.49	114.25	117.00
21	AA	842	U	N3-C2-O2	-5.49	118.36	122.20
54	BA	334	C	N1-C2-O2	5.49	122.20	118.90
54	BA	784	G	C5-C6-N1	5.49	114.25	111.50
54	BA	1366	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	1463	C	O4'-C1'-N1	5.49	112.59	108.20
21	AA	280	C	O4'-C1'-N1	5.49	112.59	108.20
21	AA	622	A	C4-C5-C6	-5.49	114.25	117.00
21	AA	690	G	N1-C6-O6	-5.49	116.61	119.90
54	BA	37	C	N1-C2-O2	5.49	122.19	118.90
54	BA	569	U	O4'-C1'-N1	5.49	112.59	108.20
3	AD	204	SER	C-N-CA	5.49	135.42	121.70
21	AA	1462	C	N1-C2-O2	5.49	122.19	118.90
54	BA	167	A	C4-C5-C6	-5.49	114.25	117.00
54	BA	606	U	O4'-C1'-N1	5.49	112.59	108.20
54	BA	806	C	O4'-C1'-N1	5.49	112.59	108.20
54	BA	1905	C	C5'-C4'-O4'	5.49	115.69	109.10
54	BA	2815	C	N1-C2-O2	5.49	122.19	118.90
8	AI	48	ARG	NE-CZ-NH1	5.49	123.05	120.30
54	BA	181	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	1125	G	O4'-C1'-N9	5.49	112.59	108.20
21	AA	702	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	2810	A	C4-C5-C6	-5.49	114.26	117.00
54	BA	316	C	N3-C2-O2	-5.49	118.06	121.90
54	BA	728	G	N3-C2-N2	-5.49	116.06	119.90
54	BA	1140	C	N1-C2-O2	5.49	122.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1295	C	C4'-C3'-C2'	-5.49	97.11	102.60
54	BA	2710	C	N1-C2-O2	5.49	122.19	118.90
54	BA	2823	A	C4-C5-C6	-5.49	114.26	117.00
21	AA	265	G	N1-C6-O6	-5.48	116.61	119.90
21	AA	488	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	975	A	C6-C5-N7	5.48	136.14	132.30
54	BA	54	G	O4'-C1'-N9	5.48	112.58	108.20
54	BA	321	U	N3-C2-O2	-5.48	118.36	122.20
54	BA	2369	A	C6-C5-N7	5.48	136.14	132.30
21	AA	869	G	P-O3'-C3'	5.48	126.28	119.70
28	BF	114	ARG	NE-CZ-NH1	5.48	123.04	120.30
54	BA	59	U	O4'-C1'-N1	5.48	112.58	108.20
54	BA	1356	G	O4'-C1'-N9	5.48	112.58	108.20
54	BA	2011	U	O4'-C1'-N1	5.48	112.58	108.20
21	AA	496	A	C4-C5-C6	-5.48	114.26	117.00
21	AA	1197	A	C4-C5-C6	-5.48	114.26	117.00
54	BA	1564	C	N3-C2-O2	-5.48	118.06	121.90
21	AA	1395	C	N1-C2-O2	5.48	122.19	118.90
54	BA	1541	C	N3-C2-O2	-5.48	118.07	121.90
21	AA	19	A	C6-C5-N7	5.47	136.13	132.30
21	AA	501	C	N1-C2-O2	5.47	122.18	118.90
21	AA	1057	G	C5'-C4'-C3'	-5.47	107.24	116.00
54	BA	2492	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	2750	A	C4-C5-C6	-5.47	114.26	117.00
21	AA	1216	A	O4'-C1'-N9	5.47	112.58	108.20
21	AA	1410	A	C6-C5-N7	5.47	136.13	132.30
54	BA	430	A	C4-C5-C6	-5.47	114.26	117.00
54	BA	1520	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	1678	A	C4-C5-C6	-5.47	114.26	117.00
54	BA	1710	G	O4'-C1'-N9	5.47	112.58	108.20
54	BA	1881	C	O4'-C1'-N1	5.47	112.58	108.20
21	AA	251	G	N3-C4-C5	-5.47	125.86	128.60
22	A1	5	G	N1-C6-O6	-5.47	116.62	119.90
54	BA	503	A	O4'-C1'-N9	5.47	112.58	108.20
54	BA	1018	U	O4'-C1'-N1	5.47	112.58	108.20
54	BA	2047	C	O4'-C1'-N1	5.47	112.58	108.20
2	AC	64	ARG	NE-CZ-NH1	5.47	123.03	120.30
21	AA	139	A	C6-C5-N7	5.47	136.13	132.30
54	BA	670	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	1428	C	O4'-C1'-N1	5.47	112.58	108.20
54	BA	1806	C	O4'-C1'-N1	5.47	112.58	108.20
1	AB	10	LYS	CA-C-N	5.47	129.23	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2752	C	O4'-C1'-N1	5.47	112.57	108.20
21	AA	43	C	N3-C2-O2	-5.47	118.07	121.90
21	AA	1302	C	N1-C2-O2	5.47	122.18	118.90
54	BA	144	A	C4-C5-C6	-5.47	114.27	117.00
54	BA	2375	G	C5-C6-N1	5.47	114.23	111.50
21	AA	1336	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	1446	A	C4-C5-C6	-5.46	114.27	117.00
55	BB	9	G	O4'-C1'-N9	5.46	112.57	108.20
54	BA	957	C	C3'-C2'-C1'	5.46	105.87	101.50
54	BA	1139	G	N1-C6-O6	-5.46	116.62	119.90
54	BA	1662	U	O4'-C1'-N1	5.46	112.57	108.20
54	BA	1760	C	N1-C2-O2	5.46	122.18	118.90
54	BA	2581	G	O4'-C1'-N9	5.46	112.57	108.20
54	BA	2676	C	N1-C2-O2	5.46	122.18	118.90
54	BA	2196	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	1229	A	C6-C5-N7	5.46	136.12	132.30
39	BQ	47	ARG	NE-CZ-NH1	5.46	123.03	120.30
54	BA	119	A	O4'-C1'-N9	5.46	112.57	108.20
54	BA	696	G	N3-C4-C5	-5.46	125.87	128.60
54	BA	948	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	1030	C	N3-C2-O2	-5.46	118.08	121.90
54	BA	2705	A	O4'-C1'-N9	5.46	112.57	108.20
21	AA	564	C	N1-C2-O2	5.46	122.17	118.90
54	BA	979	A	C4-C5-C6	-5.46	114.27	117.00
54	BA	1975	G	N1-C6-O6	-5.46	116.63	119.90
54	BA	2600	A	C6-C5-N7	5.46	136.12	132.30
54	BA	268	C	N3-C2-O2	-5.46	118.08	121.90
21	AA	964	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	1615	C	O4'-C1'-N1	5.45	112.56	108.20
54	BA	2119	A	C4-C5-C6	-5.45	114.27	117.00
21	AA	595	A	C4-C5-C6	-5.45	114.27	117.00
21	AA	908	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	13	A	C4-C5-C6	-5.45	114.27	117.00
54	BA	1917	U	O4'-C1'-N1	5.45	112.56	108.20
21	AA	1342	C	N1-C2-O2	5.45	122.17	118.90
54	BA	1229	C	O4'-C1'-N1	5.45	112.56	108.20
54	BA	1260	A	C6-C5-N7	5.45	136.12	132.30
54	BA	1432	G	N1-C6-O6	-5.45	116.63	119.90
54	BA	2137	U	N3-C2-O2	-5.45	118.38	122.20
54	BA	2826	A	C4-C5-C6	-5.45	114.28	117.00
24	A3	29	C	N3-C2-O2	-5.45	118.09	121.90
54	BA	502	A	C5-C6-N1	5.45	120.42	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2851	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	811	C	N1-C2-O2	5.45	122.17	118.90
21	AA	1064	G	N3-C2-N2	-5.45	116.09	119.90
21	AA	1225	A	C2-N3-C4	5.45	113.32	110.60
21	AA	554	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	1322	C	N3-C4-C5	5.45	124.08	121.90
54	BA	795	C	N1-C2-O2	5.45	122.17	118.90
54	BA	1286	A	C4-C5-C6	-5.45	114.28	117.00
54	BA	2335	A	C4-C5-C6	-5.45	114.28	117.00
21	AA	692	U	N3-C2-O2	-5.44	118.39	122.20
21	AA	1053	G	N1-C6-O6	-5.44	116.63	119.90
21	AA	1245	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	1333	G	C5'-C4'-O4'	5.44	115.63	109.10
54	BA	2117	A	O4'-C1'-N9	5.44	112.56	108.20
21	AA	328	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	1466	C	N1-C2-O2	5.44	122.17	118.90
54	BA	1276	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	2806	C	O4'-C1'-N1	5.44	112.55	108.20
21	AA	624	C	P-O3'-C3'	5.44	126.23	119.70
21	AA	765	G	N3-C4-C5	-5.44	125.88	128.60
54	BA	1531	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	2889	C	N3-C2-O2	-5.44	118.09	121.90
21	AA	1043	G	N1-C6-O6	-5.44	116.64	119.90
54	BA	394	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	714	U	N3-C2-O2	-5.44	118.39	122.20
54	BA	2097	A	C6-C5-N7	5.44	136.11	132.30
21	AA	240	G	N1-C6-O6	-5.44	116.64	119.90
21	AA	330	C	N3-C2-O2	-5.44	118.09	121.90
54	BA	240	C	O4'-C1'-N1	5.44	112.55	108.20
54	BA	283	G	O4'-C1'-N9	5.44	112.55	108.20
54	BA	311	A	O4'-C1'-N9	5.44	112.55	108.20
54	BA	1669	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	2671	G	N1-C6-O6	-5.44	116.64	119.90
55	BB	39	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	685	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	1608	A	C4-C5-C6	-5.44	114.28	117.00
54	BA	2425	A	P-O3'-C3'	5.44	126.22	119.70
21	AA	1163	A	C6-C5-N7	5.43	136.10	132.30
54	BA	1278	C	C3'-C2'-C1'	5.43	105.85	101.50
54	BA	1314	C	C6-N1-C2	-5.43	118.13	120.30
54	BA	1798	U	O4'-C1'-N1	5.43	112.55	108.20
54	BA	2554	U	N3-C2-O2	-5.43	118.40	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	63	C	N3-C2-O2	-5.43	118.10	121.90
54	BA	318	C	O4'-C1'-N1	5.43	112.55	108.20
54	BA	289	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	473	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1796	U	C5-C6-N1	-5.43	119.98	122.70
21	AA	298	A	C6-C5-N7	5.43	136.10	132.30
21	AA	660	C	N1-C2-O2	5.43	122.16	118.90
21	AA	492	C	N3-C2-O2	-5.43	118.10	121.90
21	AA	1042	A	C4-C5-C6	-5.43	114.29	117.00
21	AA	1383	C	N1-C2-O2	5.43	122.16	118.90
54	BA	224	U	C5'-C4'-O4'	5.43	115.61	109.10
54	BA	1084	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	1248	G	N1-C6-O6	-5.43	116.64	119.90
54	BA	1420	A	C4-C5-C6	-5.43	114.29	117.00
54	BA	2172	U	O4'-C1'-N1	5.43	112.54	108.20
12	AM	106	ARG	NE-CZ-NH1	5.42	123.01	120.30
54	BA	502	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	560	C	N1-C2-O2	5.42	122.16	118.90
54	BA	1001	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	1698	A	C4-C5-C6	-5.42	114.29	117.00
6	AG	4	ARG	NE-CZ-NH1	5.42	123.01	120.30
54	BA	1027	A	C4-C5-C6	-5.42	114.29	117.00
21	AA	802	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	854	C	O4'-C1'-N1	5.42	112.54	108.20
54	BA	1992	G	N3-C2-N2	-5.42	116.10	119.90
54	BA	2418	A	C4-C5-C6	-5.42	114.29	117.00
55	BB	53	A	C4-C5-C6	-5.42	114.29	117.00
7	AH	127	TYR	CB-CG-CD2	-5.42	117.75	121.00
54	BA	1184	U	O4'-C1'-N1	5.42	112.54	108.20
54	BA	2802	G	N1-C6-O6	-5.42	116.65	119.90
54	BA	1270	C	C3'-C2'-C1'	5.42	105.83	101.50
21	AA	114	U	O4'-C1'-N1	5.42	112.53	108.20
54	BA	1805	A	C4'-C3'-C2'	-5.42	97.18	102.60
54	BA	1893	C	O4'-C1'-N1	5.42	112.53	108.20
54	BA	2506	U	N3-C2-O2	-5.42	118.41	122.20
54	BA	2511	U	O4'-C1'-N1	5.42	112.53	108.20
21	AA	940	C	O4'-C1'-N1	5.42	112.53	108.20
54	BA	479	A	C3'-C2'-C1'	-5.42	97.17	101.50
54	BA	698	C	N1-C2-O2	5.42	122.15	118.90
54	BA	1927	A	C3'-C2'-C1'	5.42	105.83	101.50
54	BA	2114	A	C4-C5-C6	-5.42	114.29	117.00
54	BA	2825	G	N3-C4-C5	-5.42	125.89	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	970	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1198	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1342	A	C4-C5-C6	-5.41	114.29	117.00
54	BA	1630	A	C6-C5-N7	5.41	136.09	132.30
54	BA	2001	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	2160	C	N1-C2-O2	5.41	122.15	118.90
54	BA	2255	G	N1-C6-O6	-5.41	116.65	119.90
3	AD	164	ARG	NE-CZ-NH1	5.41	123.01	120.30
21	AA	1170	A	C6-C5-N7	5.41	136.09	132.30
54	BA	177	G	O4'-C1'-N9	5.41	112.53	108.20
54	BA	340	A	C4-C5-C6	-5.41	114.29	117.00
21	AA	58	C	N1-C2-O2	5.41	122.15	118.90
21	AA	234	C	O4'-C1'-N1	5.41	112.53	108.20
21	AA	343	U	N3-C2-O2	-5.41	118.41	122.20
21	AA	627	G	N1-C6-O6	-5.41	116.65	119.90
21	AA	1128	C	O4'-C1'-N1	5.41	112.53	108.20
22	A1	22	G	O4'-C1'-N9	5.41	112.53	108.20
54	BA	1174	U	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1202	G	N1-C6-O6	-5.41	116.65	119.90
54	BA	1981	A	O4'-C1'-N9	5.41	112.53	108.20
54	BA	444	C	N3-C2-O2	-5.41	118.11	121.90
54	BA	1759	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	2080	A	C4-C5-C6	-5.41	114.30	117.00
54	BA	2174	C	C5'-C4'-O4'	5.41	115.59	109.10
54	BA	704	G	C8-N9-C4	-5.41	104.24	106.40
54	BA	2338	C	N1-C2-O2	5.41	122.14	118.90
54	BA	1499	C	O4'-C1'-N1	5.41	112.53	108.20
54	BA	1758	U	N3-C2-O2	-5.41	118.42	122.20
54	BA	2273	A	C4-C5-C6	-5.41	114.30	117.00
21	AA	808	C	N1-C2-O2	5.40	122.14	118.90
54	BA	538	A	N1-C6-N6	-5.40	115.36	118.60
54	BA	2210	U	C3'-C2'-C1'	-5.40	97.18	101.50
54	BA	2605	U	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2820	A	C6-C5-N7	5.40	136.08	132.30
21	AA	545	C	N3-C2-O2	-5.40	118.12	121.90
54	BA	544	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	994	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	1804	C	O4'-C1'-N1	5.40	112.52	108.20
54	BA	2361	G	O4'-C1'-N9	5.40	112.52	108.20
21	AA	1019	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	457	A	C4-C5-C6	-5.40	114.30	117.00
54	BA	634	C	N3-C4-C5	5.40	124.06	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1323	G	N3-C4-C5	-5.40	125.90	128.60
29	BG	93	TYR	CB-CG-CD2	-5.40	117.76	121.00
21	AA	68	G	C5-C6-N1	5.40	114.20	111.50
22	A1	51	C	N1-C2-O2	5.40	122.14	118.90
54	BA	228	C	N3-C2-O2	-5.40	118.12	121.90
21	AA	249	U	O4'-C1'-N1	5.39	112.52	108.20
54	BA	433	C	N1-C2-O2	5.39	122.14	118.90
54	BA	654	A	C4-C5-C6	-5.39	114.30	117.00
54	BA	2207	C	N1-C2-O2	5.39	122.14	118.90
54	BA	2543	G	C3'-C2'-C1'	5.39	105.82	101.50
54	BA	2573	C	O4'-C1'-N1	5.39	112.52	108.20
54	BA	2892	G	C3'-C2'-C1'	5.39	105.82	101.50
54	BA	2715	C	N1-C2-O2	5.39	122.14	118.90
21	AA	945	G	C5-C6-N1	5.39	114.19	111.50
21	AA	1278	G	N3-C2-N2	-5.39	116.13	119.90
21	AA	1388	C	N3-C2-O2	-5.39	118.13	121.90
21	AA	185	U	O4'-C1'-N1	5.39	112.51	108.20
21	AA	790	A	C4-C5-C6	-5.39	114.31	117.00
21	AA	931	C	N3-C2-O2	-5.39	118.13	121.90
54	BA	1012	U	O4'-C1'-N1	5.39	112.51	108.20
21	AA	481	G	N3-C4-C5	-5.39	125.91	128.60
54	BA	428	A	N1-C6-N6	-5.39	115.37	118.60
54	BA	1251	C	C1'-O4'-C4'	-5.39	105.59	109.90
54	BA	2519	U	N3-C2-O2	-5.39	118.43	122.20
54	BA	955	U	O4'-C1'-N1	5.38	112.51	108.20
22	A1	32	C	N1-C2-O2	5.38	122.13	118.90
21	AA	719	C	N3-C2-O2	-5.38	118.13	121.90
21	AA	1149	C	N1-C2-O2	5.38	122.13	118.90
49	B0	51	ARG	NE-CZ-NH1	5.38	122.99	120.30
54	BA	1690	A	N1-C6-N6	-5.38	115.37	118.60
54	BA	2041	U	O4'-C1'-N1	5.38	112.50	108.20
55	BB	68	C	N3-C2-O2	-5.38	118.13	121.90
21	AA	100	G	C5-C6-N1	5.38	114.19	111.50
21	AA	653	U	C3'-C2'-C1'	5.38	105.80	101.50
21	AA	1283	U	O4'-C1'-N1	5.38	112.50	108.20
23	A2	93	U	C5-C6-N1	-5.38	120.01	122.70
21	AA	890	G	N3-C4-C5	-5.38	125.91	128.60
54	BA	1045	C	N1-C2-O2	5.38	122.13	118.90
54	BA	1331	G	P-O3'-C3'	5.38	126.15	119.70
54	BA	1533	C	N1-C2-O2	5.38	122.13	118.90
21	AA	737	C	N3-C2-O2	-5.38	118.14	121.90
24	A3	20	G	N1-C6-O6	-5.38	116.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2824	C	O4'-C1'-N1	5.38	112.50	108.20
21	AA	620	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	676	A	C6-C5-N7	5.37	136.06	132.30
54	BA	677	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	1155	A	C5-C6-N1	5.37	120.39	117.70
54	BA	1550	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1712	U	O4'-C1'-N1	5.37	112.50	108.20
54	BA	1952	A	C1'-O4'-C4'	-5.37	105.60	109.90
54	BA	2350	C	O4'-C1'-N1	5.37	112.50	108.20
54	BA	221	A	C4-C5-C6	-5.37	114.31	117.00
54	BA	991	C	N3-C2-O2	-5.37	118.14	121.90
54	BA	1610	A	O4'-C1'-N9	5.37	112.50	108.20
54	BA	2248	C	N1-C2-O2	5.37	122.12	118.90
21	AA	327	A	P-O3'-C3'	5.37	126.14	119.70
21	AA	1231	G	N3-C2-N2	-5.37	116.14	119.90
54	BA	757	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	2158	A	C4-C5-C6	-5.37	114.31	117.00
21	AA	992	U	P-O3'-C3'	5.37	126.14	119.70
21	AA	1477	U	O4'-C1'-N1	5.37	112.50	108.20
54	BA	2556	C	N1-C2-O2	5.37	122.12	118.90
6	AG	6	ILE	C-N-CA	5.37	133.57	122.30
55	BB	50	A	C6-C5-N7	5.37	136.06	132.30
52	B3	29	ARG	NE-CZ-NH2	-5.37	117.62	120.30
54	BA	196	A	C4-C5-C6	-5.37	114.32	117.00
54	BA	232	G	N1-C6-O6	-5.37	116.68	119.90
54	BA	565	C	O4'-C1'-N1	5.37	112.49	108.20
54	BA	741	U	N3-C2-O2	-5.37	118.44	122.20
54	BA	1083	U	N3-C2-O2	-5.37	118.44	122.20
54	BA	2758	A	C4-C5-C6	-5.37	114.32	117.00
21	AA	217	C	N1-C2-O2	5.36	122.12	118.90
54	BA	1920	C	O4'-C1'-N1	5.36	112.49	108.20
54	BA	2295	C	N3-C2-O2	-5.36	118.15	121.90
55	BB	63	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	1499	A	C4-C5-C6	-5.36	114.32	117.00
25	BC	12	ARG	NE-CZ-NH2	-5.36	117.62	120.30
54	BA	1446	C	N3-C2-O2	-5.36	118.15	121.90
21	AA	179	A	C6-C5-N7	5.36	136.05	132.30
21	AA	638	U	O4'-C1'-N1	5.36	112.49	108.20
21	AA	690	G	C5-C6-N1	5.36	114.18	111.50
21	AA	1239	A	C6-C5-N7	5.36	136.05	132.30
24	A3	1	C	C1'-O4'-C4'	-5.36	105.61	109.90
54	BA	335	C	N3-C2-O2	-5.36	118.15	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2896	C	O4'-C1'-N1	5.36	112.49	108.20
3	AD	145	ARG	NE-CZ-NH1	5.36	122.98	120.30
21	AA	903	G	N1-C6-O6	-5.36	116.69	119.90
21	AA	1110	A	C4-C5-C6	-5.36	114.32	117.00
21	AA	1119	C	N3-C2-O2	-5.36	118.15	121.90
52	B3	12	ARG	NE-CZ-NH1	5.36	122.98	120.30
54	BA	128	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	440	C	O4'-C1'-N1	5.36	112.48	108.20
54	BA	1145	C	N3-C2-O2	-5.36	118.15	121.90
54	BA	1311	G	O4'-C1'-N9	5.35	112.48	108.20
22	A1	12	U	C3'-C2'-C1'	5.35	105.78	101.50
54	BA	815	C	N3-C2-O2	-5.35	118.15	121.90
54	BA	2590	A	C6-C5-N7	5.35	136.05	132.30
54	BA	2837	A	C4-C5-C6	-5.35	114.32	117.00
21	AA	1189	U	N3-C2-O2	-5.35	118.45	122.20
54	BA	287	G	N1-C6-O6	-5.35	116.69	119.90
54	BA	2064	C	N3-C2-O2	-5.35	118.15	121.90
21	AA	632	U	N3-C2-O2	-5.35	118.45	122.20
21	AA	843	U	N3-C2-O2	-5.35	118.46	122.20
54	BA	542	C	N3-C2-O2	-5.35	118.16	121.90
54	BA	827	U	O4'-C1'-N1	5.35	112.48	108.20
21	AA	346	G	N3-C4-C5	-5.35	125.93	128.60
21	AA	1106	G	N1-C6-O6	-5.35	116.69	119.90
23	A2	92	U	O4'-C1'-N1	5.35	112.48	108.20
35	BM	55	ARG	NE-CZ-NH1	5.35	122.97	120.30
54	BA	974	G	O4'-C1'-N9	5.35	112.48	108.20
54	BA	2423	U	O4'-C1'-N1	5.35	112.48	108.20
54	BA	109	C	O4'-C1'-N1	5.34	112.47	108.20
54	BA	145	C	N1-C2-O2	5.34	122.11	118.90
54	BA	820	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	1072	C	N3-C2-O2	-5.34	118.16	121.90
54	BA	1341	G	C5-C6-N1	5.34	114.17	111.50
24	A3	54	G	N1-C6-O6	-5.34	116.69	119.90
39	BQ	54	ARG	NE-CZ-NH2	-5.34	117.63	120.30
54	BA	64	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2254	C	O4'-C1'-N1	5.34	112.47	108.20
21	AA	415	A	N1-C6-N6	-5.34	115.40	118.60
21	AA	1115	U	C5-C6-N1	-5.34	120.03	122.70
54	BA	90	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1149	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	1346	G	N1-C6-O6	-5.34	116.69	119.90
54	BA	2062	A	C4-C5-C6	-5.34	114.33	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	777	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	199	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	1373	A	C4-C5-C6	-5.34	114.33	117.00
54	BA	2095	A	C6-C5-N7	5.34	136.04	132.30
54	BA	2457	U	N3-C2-O2	-5.34	118.46	122.20
54	BA	2792	A	C6-C5-N7	5.34	136.04	132.30
21	AA	305	G	N3-C4-C5	-5.34	125.93	128.60
21	AA	1296	C	N1-C2-O2	5.34	122.10	118.90
54	BA	301	G	O4'-C1'-N9	5.34	112.47	108.20
54	BA	1777	U	O4'-C1'-N1	5.34	112.47	108.20
54	BA	1930	G	C5-C6-N1	5.34	114.17	111.50
21	AA	1460	C	N3-C2-O2	-5.34	118.17	121.90
54	BA	1976	U	N3-C2-O2	-5.33	118.47	122.20
10	AK	52	ARG	NE-CZ-NH1	-5.33	117.63	120.30
22	A1	30	C	N3-C4-C5	5.33	124.03	121.90
54	BA	274	C	O4'-C1'-N1	5.33	112.47	108.20
54	BA	285	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	320	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	1954	G	C3'-C2'-C1'	5.33	105.77	101.50
21	AA	1364	U	N3-C2-O2	-5.33	118.47	122.20
26	BD	124	ARG	NE-CZ-NH1	5.33	122.97	120.30
54	BA	1801	A	C4-C5-C6	-5.33	114.33	117.00
54	BA	2371	G	N3-C2-N2	-5.33	116.17	119.90
21	AA	430	A	C4-C5-C6	-5.33	114.34	117.00
21	AA	1384	C	N3-C2-O2	-5.33	118.17	121.90
54	BA	1182	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	1439	A	C4-C5-C6	-5.33	114.34	117.00
55	BB	90	C	O4'-C1'-N1	5.33	112.46	108.20
12	AM	92	ARG	NE-CZ-NH1	5.33	122.96	120.30
54	BA	2202	U	C3'-C2'-C1'	5.33	105.76	101.50
21	AA	352	C	N3-C4-N4	-5.33	114.27	118.00
54	BA	77	G	N1-C6-O6	-5.33	116.70	119.90
54	BA	2555	U	O4'-C1'-N1	5.33	112.46	108.20
21	AA	756	C	N1-C2-O2	5.32	122.09	118.90
54	BA	946	C	C1'-O4'-C4'	-5.32	105.64	109.90
54	BA	1897	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	2424	C	N3-C2-O2	-5.32	118.17	121.90
54	BA	1006	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	2527	C	N1-C2-O2	5.32	122.09	118.90
54	BA	915	C	O4'-C1'-N1	5.32	112.46	108.20
54	BA	1	G	N1-C6-O6	-5.32	116.71	119.90
54	BA	391	A	C4-C5-C6	-5.32	114.34	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1347	A	O4'-C1'-N9	5.32	112.45	108.20
54	BA	1355	G	O4'-C1'-N9	5.32	112.45	108.20
54	BA	1909	C	N3-C2-O2	-5.32	118.18	121.90
21	AA	666	G	N3-C2-N2	-5.32	116.18	119.90
54	BA	79	C	O4'-C1'-N1	5.32	112.45	108.20
54	BA	706	A	C4-C5-C6	-5.32	114.34	117.00
54	BA	1035	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1087	G	C3'-C2'-C1'	5.31	105.75	101.50
21	AA	81	A	C6-C5-N7	5.31	136.02	132.30
21	AA	298	A	C3'-C2'-C1'	5.31	105.75	101.50
21	AA	590	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	952	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	1374	G	N1-C6-O6	-5.31	116.71	119.90
54	BA	2702	G	N3-C2-N2	-5.31	116.18	119.90
14	AO	83	ARG	NE-CZ-NH1	5.31	122.96	120.30
54	BA	257	C	N3-C2-O2	-5.31	118.18	121.90
54	BA	2338	C	N3-C4-C5	5.31	124.03	121.90
54	BA	2793	C	N3-C2-O2	-5.31	118.18	121.90
55	BB	3	C	N3-C2-O2	-5.31	118.18	121.90
24	A3	76	C	O4'-C1'-N1	5.31	112.45	108.20
54	BA	2450	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	2859	G	O4'-C1'-N9	5.31	112.45	108.20
54	BA	1372	U	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1528	A	C4-C5-C6	-5.31	114.35	117.00
54	BA	1800	C	O4'-C1'-N1	5.31	112.45	108.20
54	BA	1980	G	C1'-O4'-C4'	-5.31	105.65	109.90
21	AA	612	C	N1-C2-O2	5.31	122.08	118.90
54	BA	2313	C	N3-C4-C5	5.31	124.02	121.90
21	AA	509	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	1509	C	O4'-C1'-N1	5.30	112.44	108.20
24	A3	67	C	N1-C2-O2	5.30	122.08	118.90
10	AK	105	ARG	NE-CZ-NH1	5.30	122.95	120.30
21	AA	663	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	823	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	190	A	C4-C5-C6	-5.30	114.35	117.00
54	BA	788	A	O4'-C1'-N9	5.30	112.44	108.20
54	BA	802	A	C4-C5-C6	-5.30	114.35	117.00
21	AA	1022	A	C4-C5-C6	-5.30	114.35	117.00
1	AB	73	ARG	NE-CZ-NH2	-5.30	117.65	120.30
21	AA	48	C	N1-C2-O2	5.30	122.08	118.90
54	BA	517	C	N3-C2-O2	-5.30	118.19	121.90
54	BA	1189	A	C4-C5-C6	-5.30	114.35	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	398	U	O4'-C1'-N1	5.30	112.44	108.20
35	BM	51	ARG	NE-CZ-NH1	5.30	122.95	120.30
54	BA	421	C	N1-C2-O2	5.30	122.08	118.90
54	BA	1009	A	C4-C5-C6	-5.30	114.35	117.00
55	BB	9	G	N1-C6-O6	-5.30	116.72	119.90
54	BA	897	C	N1-C2-O2	5.30	122.08	118.90
54	BA	1576	U	O4'-C1'-N1	5.30	112.44	108.20
54	BA	2344	U	N3-C2-O2	-5.30	118.49	122.20
54	BA	1974	C	O4'-C1'-N1	5.29	112.44	108.20
54	BA	2092	U	N3-C2-O2	-5.29	118.49	122.20
54	BA	2336	A	C4-C5-C6	-5.29	114.35	117.00
21	AA	183	C	N1-C2-O2	5.29	122.08	118.90
35	BM	114	ARG	NE-CZ-NH2	-5.29	117.65	120.30
54	BA	1299	G	N3-C2-N2	-5.29	116.19	119.90
54	BA	1398	C	N1-C2-O2	5.29	122.08	118.90
21	AA	137	U	N3-C2-O2	-5.29	118.50	122.20
21	AA	303	A	O4'-C1'-N9	5.29	112.43	108.20
21	AA	1394	A	C4-C5-C6	-5.29	114.35	117.00
54	BA	510	C	N1-C2-O2	5.29	122.08	118.90
54	BA	1537	G	N3-C4-C5	-5.29	125.95	128.60
54	BA	2028	U	O4'-C1'-N1	5.29	112.43	108.20
20	AU	8	ASN	C-N-CA	5.29	134.92	121.70
21	AA	1080	A	C4-C5-C6	-5.29	114.36	117.00
21	AA	1360	A	C4-C5-C6	-5.29	114.36	117.00
54	BA	1278	C	N1-C2-O2	5.29	122.07	118.90
54	BA	2452	C	N1-C2-O2	5.29	122.07	118.90
54	BA	2638	G	N3-C4-C5	-5.29	125.96	128.60
54	BA	2811	G	O4'-C1'-N9	5.29	112.43	108.20
21	AA	108	G	C5-C6-N1	5.29	114.14	111.50
21	AA	962	C	N1-C2-O2	5.29	122.07	118.90
54	BA	151	C	N3-C2-O2	-5.29	118.20	121.90
21	AA	75	G	N1-C6-O6	-5.28	116.73	119.90
24	A3	64	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	313	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	904	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	1164	C	N3-C2-O2	-5.28	118.20	121.90
54	BA	2824	C	N3-C2-O2	-5.28	118.20	121.90
21	AA	1198	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	2024	G	C5-C6-N1	5.28	114.14	111.50
21	AA	517	G	N1-C6-O6	-5.28	116.73	119.90
54	BA	145	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	1213	A	C4-C5-C6	-5.28	114.36	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1382	G	N3-C4-C5	-5.28	125.96	128.60
54	BA	1855	U	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2566	A	C4-C5-C6	-5.28	114.36	117.00
21	AA	392	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	479	A	C6-C5-N7	5.28	136.00	132.30
54	BA	735	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1026	G	O4'-C1'-N9	5.28	112.42	108.20
54	BA	2776	A	O4'-C1'-N9	5.28	112.42	108.20
21	AA	267	C	N1-C2-O2	5.28	122.07	118.90
54	BA	246	C	O4'-C1'-N1	5.28	112.42	108.20
54	BA	2657	A	C4-C5-C6	-5.28	114.36	117.00
54	BA	1322	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	2308	G	N3-C4-C5	-5.27	125.96	128.60
54	BA	2807	U	O4'-C1'-N1	5.27	112.42	108.20
21	AA	1112	C	N1-C2-O2	5.27	122.06	118.90
54	BA	231	A	C6-C5-N7	5.27	135.99	132.30
50	B1	5	ARG	NE-CZ-NH2	5.27	122.94	120.30
54	BA	1165	A	C4-C5-C6	-5.27	114.36	117.00
54	BA	1895	C	N1-C2-O2	5.27	122.06	118.90
54	BA	1945	G	C3'-C2'-C1'	5.27	105.72	101.50
21	AA	203	G	N3-C2-N2	-5.27	116.21	119.90
21	AA	396	C	N1-C2-O2	5.27	122.06	118.90
21	AA	1322	C	N1-C2-O2	5.27	122.06	118.90
22	A1	70	C	O4'-C1'-N1	5.27	112.42	108.20
54	BA	2024	G	N1-C6-O6	-5.27	116.74	119.90
54	BA	2464	G	O4'-C1'-N9	5.27	112.41	108.20
9	AJ	68	ARG	NE-CZ-NH2	-5.27	117.67	120.30
21	AA	1162	C	N3-C2-O2	-5.27	118.21	121.90
54	BA	1814	G	N3-C4-C5	-5.27	125.97	128.60
54	BA	2581	G	C5-C6-N1	5.27	114.13	111.50
21	AA	51	A	C6-C5-N7	5.26	135.99	132.30
21	AA	131	A	C6-C5-N7	5.26	135.98	132.30
21	AA	715	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	951	G	N3-C4-C5	-5.26	125.97	128.60
54	BA	205	G	N3-C4-C5	-5.26	125.97	128.60
21	AA	498	A	C6-C5-N7	5.26	135.98	132.30
21	AA	973	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	1297	G	N1-C6-O6	-5.26	116.74	119.90
54	BA	140	C	N1-C2-O2	5.26	122.06	118.90
21	AA	733	G	O4'-C1'-N9	5.26	112.41	108.20
54	BA	918	A	N1-C6-N6	-5.26	115.44	118.60
54	BA	946	C	N3-C4-N4	-5.26	114.32	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1270	C	N1-C2-O2	5.26	122.06	118.90
54	BA	2864	G	N1-C6-O6	-5.26	116.74	119.90
21	AA	286	C	N1-C2-O2	5.26	122.06	118.90
54	BA	245	G	O4'-C1'-N9	5.26	112.41	108.20
21	AA	181	A	C4-C5-C6	-5.26	114.37	117.00
21	AA	1331	G	N1-C6-O6	-5.26	116.75	119.90
21	AA	1336	C	C3'-C2'-C1'	5.26	105.70	101.50
54	BA	23	G	C1'-O4'-C4'	-5.26	105.69	109.90
54	BA	1256	G	N1-C6-O6	-5.26	116.75	119.90
54	BA	526	A	C4-C5-C6	-5.25	114.37	117.00
54	BA	2099	U	O4'-C1'-N1	5.25	112.40	108.20
21	AA	285	C	N1-C2-O2	5.25	122.05	118.90
21	AA	463	U	N3-C2-O2	-5.25	118.52	122.20
21	AA	920	U	N3-C2-O2	-5.25	118.52	122.20
21	AA	1230	C	C1'-O4'-C4'	-5.25	105.70	109.90
54	BA	497	A	C6-C5-N7	5.25	135.98	132.30
54	BA	1927	A	O4'-C4'-C3'	5.25	110.30	106.10
54	BA	2218	G	N3-C2-N2	-5.25	116.22	119.90
21	AA	66	A	C4-C5-C6	-5.25	114.37	117.00
21	AA	631	C	C1'-O4'-C4'	-5.25	105.70	109.90
21	AA	1188	A	C6-C5-N7	5.25	135.97	132.30
54	BA	436	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1319	C	O4'-C1'-N1	5.25	112.40	108.20
54	BA	1955	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	808	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	2021	C	N1-C2-O2	5.25	122.05	118.90
21	AA	1458	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	1470	U	C5-C6-N1	-5.25	120.08	122.70
54	BA	1392	A	C4-C5-C6	-5.25	114.38	117.00
54	BA	1629	U	O4'-C1'-N1	5.25	112.40	108.20
37	BO	9	ARG	NE-CZ-NH1	5.25	122.92	120.30
54	BA	664	G	N1-C6-O6	-5.25	116.75	119.90
54	BA	1291	C	N1-C2-O2	5.25	122.05	118.90
54	BA	1409	U	O4'-C1'-N1	5.25	112.40	108.20
54	BA	2226	C	N1-C2-O2	5.25	122.05	118.90
54	BA	2742	G	N1-C6-O6	-5.25	116.75	119.90
21	AA	615	G	C5-C6-N1	5.25	114.12	111.50
21	AA	817	C	N3-C2-O2	-5.25	118.23	121.90
54	BA	344	A	O4'-C1'-N9	5.25	112.40	108.20
10	AK	126	ARG	NE-CZ-NH2	-5.24	117.68	120.30
21	AA	1214	C	N1-C2-O2	5.24	122.05	118.90
54	BA	91	A	O4'-C1'-N9	5.24	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	992	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1144	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1597	A	C4-C5-C6	-5.24	114.38	117.00
54	BA	1996	C	N1-C2-O2	5.24	122.05	118.90
54	BA	2646	C	N1-C1'-C2'	5.24	120.82	114.00
54	BA	2717	C	O4'-C1'-N1	5.24	112.40	108.20
56	B5	122	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BA	433	C	O4'-C1'-N1	5.24	112.39	108.20
21	AA	121	U	O4'-C1'-N1	5.24	112.39	108.20
21	AA	132	C	N1-C2-O2	5.24	122.04	118.90
21	AA	951	G	N1-C6-O6	-5.24	116.75	119.90
21	AA	1072	G	N7-C8-N9	5.24	115.72	113.10
21	AA	1526	G	N3-C4-C5	-5.24	125.98	128.60
54	BA	641	U	C5'-C4'-O4'	5.24	115.39	109.10
54	BA	758	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1402	U	C4'-C3'-C2'	-5.24	97.36	102.60
54	BA	1708	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2103	C	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2568	U	O4'-C1'-N1	5.24	112.39	108.20
55	BB	60	C	O4'-C1'-N1	5.24	112.39	108.20
55	BB	110	C	N3-C2-O2	-5.24	118.23	121.90
22	A1	36	C	N1-C2-O2	5.24	122.04	118.90
54	BA	723	C	N1-C2-O2	5.24	122.04	118.90
54	BA	1234	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	1747	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2341	G	N1-C6-O6	-5.24	116.76	119.90
21	AA	108	G	N3-C2-N2	-5.24	116.23	119.90
21	AA	1127	G	N1-C6-O6	-5.24	116.76	119.90
54	BA	2356	U	O4'-C1'-N1	5.24	112.39	108.20
54	BA	2365	G	C5'-C4'-O4'	5.24	115.39	109.10
21	AA	1171	A	C4-C5-C6	-5.24	114.38	117.00
21	AA	1446	A	O4'-C1'-N9	5.24	112.39	108.20
52	B3	39	ARG	NE-CZ-NH1	5.24	122.92	120.30
54	BA	491	G	N3-C2-N2	-5.24	116.23	119.90
54	BA	671	C	N1-C2-O2	5.24	122.04	118.90
54	BA	1702	G	N1-C6-O6	-5.24	116.76	119.90
55	BB	12	C	N1-C2-O2	5.24	122.04	118.90
55	BB	27	C	N1-C2-O2	5.24	122.04	118.90
21	AA	1089	G	N1-C6-O6	-5.23	116.76	119.90
46	BX	71	ARG	NE-CZ-NH1	5.23	122.92	120.30
54	BA	25	U	O4'-C1'-N1	5.23	112.39	108.20
54	BA	174	U	O4'-C1'-N1	5.23	112.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1117	C	O4'-C1'-N1	5.23	112.39	108.20
54	BA	1924	C	N1-C2-O2	5.23	122.04	118.90
54	BA	2730	C	C4'-C3'-C2'	-5.23	97.37	102.60
54	BA	2840	C	O4'-C1'-N1	5.23	112.39	108.20
3	AD	103	ARG	NE-CZ-NH1	5.23	122.92	120.30
12	AM	111	PRO	C-N-CA	5.23	134.78	121.70
54	BA	1008	A	C4-C5-C6	-5.23	114.38	117.00
54	BA	2669	G	N1-C6-O6	-5.23	116.76	119.90
21	AA	367	U	O4'-C1'-N1	5.23	112.38	108.20
21	AA	1347	G	N3-C4-C5	-5.23	125.98	128.60
22	A1	29	U	O4'-C1'-N1	5.23	112.39	108.20
45	BW	54	ARG	NE-CZ-NH1	5.23	122.92	120.30
54	BA	450	G	N7-C8-N9	5.23	115.72	113.10
54	BA	2593	U	O4'-C1'-N1	5.23	112.38	108.20
21	AA	410	G	C5-C6-N1	5.23	114.11	111.50
54	BA	1987	A	C4-C5-C6	-5.23	114.39	117.00
54	BA	269	C	O4'-C1'-N1	5.23	112.38	108.20
54	BA	2157	G	C3'-C2'-C1'	5.23	105.68	101.50
54	BA	2313	C	N1-C2-O2	5.23	122.04	118.90
54	BA	2517	C	N1-C2-O2	5.23	122.04	118.90
20	AU	37	TYR	CB-CG-CD2	-5.23	117.86	121.00
54	BA	2244	U	O4'-C1'-N1	5.23	112.38	108.20
21	AA	1318	A	C4-C5-C6	-5.22	114.39	117.00
27	BE	170	ARG	NE-CZ-NH1	5.22	122.91	120.30
54	BA	1452	G	N3-C2-N2	-5.22	116.24	119.90
6	AG	6	ILE	CA-C-N	5.22	126.65	116.20
21	AA	207	C	N1-C2-O2	5.22	122.03	118.90
21	AA	234	C	N1-C2-O2	5.22	122.03	118.90
21	AA	415	A	C2-N3-C4	5.22	113.21	110.60
21	AA	476	U	N3-C2-O2	-5.22	118.54	122.20
21	AA	661	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	1823	G	N3-C2-N2	-5.22	116.24	119.90
21	AA	1327	C	N1-C2-O2	5.22	122.03	118.90
22	A1	13	C	N3-C2-O2	-5.22	118.25	121.90
54	BA	653	U	N3-C2-O2	-5.22	118.55	122.20
54	BA	1043	C	N1-C2-O2	5.22	122.03	118.90
54	BA	2562	U	O4'-C1'-N1	5.22	112.38	108.20
13	AN	69	ARG	NE-CZ-NH1	5.22	122.91	120.30
54	BA	565	C	C4'-C3'-C2'	-5.22	97.38	102.60
13	AN	41	ARG	NE-CZ-NH1	5.22	122.91	120.30
21	AA	23	C	N1-C2-O2	5.22	122.03	118.90
21	AA	392	C	N1-C2-O2	5.22	122.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	922	C	N1-C2-O2	5.22	122.03	118.90
54	BA	1168	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	325	A	C6-C5-N7	5.22	135.95	132.30
21	AA	894	G	C5-C6-N1	5.22	114.11	111.50
21	AA	1339	A	C5'-C4'-O4'	5.22	115.36	109.10
54	BA	954	G	N1-C6-O6	-5.22	116.77	119.90
54	BA	1732	C	N1-C2-O2	5.22	122.03	118.90
55	BB	69	G	N1-C6-O6	-5.22	116.77	119.90
21	AA	199	A	C6-C5-N7	5.21	135.95	132.30
21	AA	1027	C	N1-C2-O2	5.21	122.03	118.90
24	A3	24	C	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1813	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	1940	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	2873	A	C6-C5-N7	5.21	135.95	132.30
55	BB	113	C	C4'-C3'-C2'	-5.21	97.39	102.60
54	BA	280	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	2233	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	2543	G	C5-C6-N1	5.21	114.11	111.50
21	AA	288	A	N1-C6-N6	-5.21	115.47	118.60
54	BA	113	U	N3-C2-O2	-5.21	118.55	122.20
54	BA	1380	G	C5'-C4'-C3'	-5.21	107.66	116.00
54	BA	1859	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	1892	C	N1-C2-O2	5.21	122.03	118.90
54	BA	2065	C	N3-C4-C5	5.21	123.98	121.90
55	BB	21	G	N1-C6-O6	-5.21	116.77	119.90
54	BA	568	U	O4'-C1'-N1	5.21	112.37	108.20
21	AA	613	C	N3-C2-O2	-5.21	118.25	121.90
21	AA	694	A	C4-C5-C6	-5.21	114.40	117.00
54	BA	1993	U	O4'-C1'-N1	5.21	112.37	108.20
54	BA	939	G	C3'-C2'-C1'	-5.21	97.33	101.50
54	BA	1140	C	C5'-C4'-O4'	5.21	115.35	109.10
54	BA	2567	G	N3-C2-N2	-5.21	116.26	119.90
55	BB	16	G	N3-C4-C5	-5.21	126.00	128.60
55	BB	18	G	N3-C2-N2	-5.21	116.25	119.90
21	AA	1146	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	492	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	1870	C	N1-C2-O2	5.20	122.02	118.90
21	AA	428	G	N3-C4-C5	-5.20	126.00	128.60
54	BA	546	U	N3-C2-O2	-5.20	118.56	122.20
21	AA	39	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	865	A	O4'-C1'-N9	5.20	112.36	108.20
27	BE	21	ARG	NE-CZ-NH1	5.20	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	BJ	95	ARG	NE-CZ-NH1	5.20	122.90	120.30
54	BA	132	G	O4'-C1'-N9	5.20	112.36	108.20
54	BA	1383	A	C4-C5-C6	-5.20	114.40	117.00
21	AA	569	C	N3-C4-C5	5.20	123.98	121.90
21	AA	747	A	C6-C5-N7	5.20	135.94	132.30
21	AA	979	C	N1-C2-O2	5.20	122.02	118.90
40	BR	90	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
54	BA	44	A	C4-C5-C6	-5.20	114.40	117.00
54	BA	51	G	N3-C2-N2	-5.20	116.26	119.90
54	BA	267	C	N3-C2-O2	-5.20	118.26	121.90
54	BA	2655	G	N1-C6-O6	-5.20	116.78	119.90
21	AA	401	C	N3-C2-O2	-5.20	118.26	121.90
21	AA	1228	C	C3'-C2'-C1'	5.20	105.66	101.50
54	BA	573	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	894	U	O4'-C1'-N1	5.20	112.36	108.20
54	BA	1404	C	N3-C2-O2	-5.20	118.26	121.90
54	BA	1503	A	O4'-C1'-N9	5.20	112.36	108.20
54	BA	1656	C	O4'-C1'-N1	5.20	112.36	108.20
55	BB	36	C	N1-C2-O2	5.20	122.02	118.90
21	AA	34	C	N1-C2-O2	5.19	122.02	118.90
54	BA	2806	C	N1-C2-O2	5.19	122.02	118.90
21	AA	1161	C	N3-C2-O2	-5.19	118.27	121.90
36	BN	4	ARG	NE-CZ-NH1	5.19	122.90	120.30
54	BA	1376	C	N1-C2-O2	5.19	122.02	118.90
54	BA	1150	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	1289	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	1617	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	2031	A	C5'-C4'-C3'	-5.19	107.69	116.00
54	BA	2681	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	383	C	N3-C2-O2	-5.19	118.27	121.90
54	BA	652	U	O4'-C1'-N1	5.19	112.35	108.20
54	BA	893	C	O4'-C1'-N1	5.19	112.35	108.20
21	AA	857	C	O4'-C1'-N1	5.19	112.35	108.20
54	BA	1198	U	C5-C6-N1	-5.19	120.11	122.70
54	BA	1536	C	N1-C2-O2	5.19	122.01	118.90
54	BA	2768	U	O4'-C1'-N1	5.19	112.35	108.20
21	AA	48	C	C5'-C4'-C3'	-5.19	107.70	116.00
21	AA	494	G	N1-C6-O6	-5.19	116.79	119.90
54	BA	513	A	C4-C5-C6	-5.19	114.41	117.00
54	BA	2547	A	C6-C5-N7	5.19	135.93	132.30
21	AA	216	U	N3-C2-O2	-5.18	118.57	122.20
21	AA	573	A	C6-C5-N7	5.18	135.93	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	968	A	O4'-C1'-N9	5.18	112.35	108.20
54	BA	594	U	O4'-C1'-N1	5.18	112.35	108.20
54	BA	760	G	N1-C6-O6	-5.18	116.79	119.90
54	BA	1646	C	N1-C2-O2	5.18	122.01	118.90
54	BA	2367	G	O4'-C1'-N9	5.18	112.35	108.20
54	BA	2402	U	N3-C2-O2	-5.18	118.57	122.20
21	AA	879	C	N1-C2-O2	5.18	122.01	118.90
21	AA	1353	G	N3-C4-C5	-5.18	126.01	128.60
54	BA	439	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	626	A	C4-C5-C6	-5.18	114.41	117.00
54	BA	2405	G	O4'-C1'-N9	5.18	112.35	108.20
54	BA	2060	A	C4-C5-C6	-5.18	114.41	117.00
21	AA	110	C	C3'-C2'-C1'	5.18	105.64	101.50
21	AA	438	U	O4'-C1'-N1	5.18	112.34	108.20
21	AA	724	G	N3-C2-N2	-5.18	116.27	119.90
21	AA	961	U	O4'-C1'-N1	5.18	112.34	108.20
21	AA	1237	C	N1-C2-O2	5.18	122.01	118.90
54	BA	1150	C	N3-C2-O2	-5.18	118.27	121.90
54	BA	2263	C	O4'-C1'-N1	5.18	112.34	108.20
21	AA	1514	G	O4'-C1'-N9	5.18	112.34	108.20
54	BA	1879	C	O4'-C1'-N1	5.18	112.34	108.20
54	BA	706	A	O4'-C1'-N9	5.18	112.34	108.20
21	AA	131	A	C1'-O4'-C4'	-5.17	105.76	109.90
54	BA	75	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	794	A	C6-C5-N7	5.17	135.92	132.30
55	BB	96	G	O4'-C1'-N9	5.17	112.34	108.20
2	AC	71	ARG	NE-CZ-NH1	5.17	122.89	120.30
8	AI	32	ARG	NE-CZ-NH1	5.17	122.89	120.30
21	AA	490	C	N1-C2-O2	5.17	122.00	118.90
23	A2	82	A	C6-C5-N7	5.17	135.92	132.30
54	BA	2330	G	N9-C4-C5	5.17	107.47	105.40
21	AA	1231	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	793	A	O4'-C1'-N9	5.17	112.34	108.20
54	BA	841	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	1505	A	C6-C5-N7	5.17	135.92	132.30
21	AA	1475	G	N1-C6-O6	-5.17	116.80	119.90
54	BA	927	A	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	2329	U	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	2333	A	C6-C5-N7	5.17	135.92	132.30
54	BA	2828	G	O4'-C1'-N9	5.17	112.34	108.20
21	AA	475	C	N3-C2-O2	-5.17	118.28	121.90
54	BA	354	A	C6-C5-N7	5.17	135.92	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	37	C	O4'-C1'-N1	5.17	112.33	108.20
6	AG	43	TYR	CB-CG-CD1	-5.17	117.90	121.00
54	BA	555	G	C5-C6-N1	5.17	114.08	111.50
54	BA	803	U	O4'-C1'-N1	5.17	112.33	108.20
54	BA	1035	U	C4'-C3'-C2'	-5.17	97.43	102.60
54	BA	1489	C	O4'-C1'-N1	5.17	112.33	108.20
1	AB	34	ARG	NE-CZ-NH1	5.17	122.88	120.30
21	AA	681	A	C6-C5-N7	5.17	135.91	132.30
54	BA	2163	A	C4-C5-C6	-5.17	114.42	117.00
21	AA	934	C	N1-C2-O2	5.16	122.00	118.90
21	AA	1098	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1367	C	N1-C2-O2	5.16	122.00	118.90
21	AA	1484	C	O4'-C1'-N1	5.16	112.33	108.20
34	BL	59	ARG	NH1-CZ-NH2	-5.16	113.72	119.40
54	BA	1789	A	N1-C6-N6	-5.16	115.50	118.60
54	BA	2540	C	N1-C2-O2	5.16	122.00	118.90
54	BA	2893	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	707	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	143	C	N1-C2-O2	5.16	122.00	118.90
54	BA	401	A	C4-C5-C6	-5.16	114.42	117.00
54	BA	2195	U	C4'-C3'-C2'	-5.16	97.44	102.60
54	BA	1139	G	O4'-C1'-N9	5.16	112.33	108.20
54	BA	1209	U	N3-C2-O2	-5.16	118.59	122.20
54	BA	1937	A	O4'-C1'-N9	5.16	112.33	108.20
54	BA	2043	C	N1-C2-O2	5.16	122.00	118.90
54	BA	2773	C	O4'-C1'-N1	5.16	112.33	108.20
21	AA	294	U	O4'-C1'-N1	5.16	112.33	108.20
21	AA	1274	A	C6-C5-N7	5.16	135.91	132.30
54	BA	597	G	N1-C6-O6	-5.16	116.80	119.90
54	BA	778	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	1264	A	O4'-C1'-N9	5.16	112.33	108.20
54	BA	1459	G	N1-C6-O6	-5.16	116.81	119.90
54	BA	1868	C	N1-C2-O2	5.16	122.00	118.90
54	BA	2164	C	N1-C2-O2	5.16	122.00	118.90
55	BB	52	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	1467	C	N1-C2-O2	5.16	121.99	118.90
54	BA	1722	A	C4-C5-C6	-5.16	114.42	117.00
21	AA	64	G	O4'-C1'-N9	5.16	112.32	108.20
22	A1	44	G	N3-C2-N2	-5.16	116.29	119.90
54	BA	862	G	N3-C2-N2	-5.16	116.29	119.90
54	BA	1713	A	C6-C5-N7	5.16	135.91	132.30
54	BA	2539	C	O4'-C1'-N1	5.16	112.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	94	G	O4'-C1'-N9	5.15	112.32	108.20
54	BA	669	G	O4'-C1'-N9	5.15	112.32	108.20
54	BA	2045	C	O4'-C1'-N1	5.15	112.32	108.20
21	AA	1284	C	O4'-C1'-N1	5.15	112.32	108.20
54	BA	951	C	O4'-C1'-N1	5.15	112.32	108.20
21	AA	458	U	O4'-C1'-N1	5.15	112.32	108.20
21	AA	998	C	N1-C2-O2	5.15	121.99	118.90
21	AA	1449	C	N1-C2-O2	5.15	121.99	118.90
22	A1	45	G	N1-C6-O6	-5.15	116.81	119.90
54	BA	704	G	O4'-C1'-N9	5.15	112.32	108.20
54	BA	2576	G	N3-C4-C5	-5.15	126.03	128.60
54	BA	2646	C	C6-N1-C2	-5.15	118.24	120.30
54	BA	2493	U	O4'-C1'-N1	5.15	112.32	108.20
54	BA	2749	A	C6-C5-N7	5.15	135.90	132.30
21	AA	513	C	N3-C2-O2	-5.15	118.30	121.90
54	BA	1609	A	C6-C5-N7	5.15	135.90	132.30
54	BA	2214	C	N1-C2-O2	5.15	121.99	118.90
54	BA	265	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	385	C	N1-C2-O2	5.14	121.99	118.90
54	BA	1493	C	O4'-C1'-N1	5.14	112.32	108.20
54	BA	2052	A	C4-C5-C6	-5.14	114.43	117.00
37	BO	81	ARG	NE-CZ-NH2	5.14	122.87	120.30
54	BA	480	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	686	U	N3-C2-O2	-5.14	118.60	122.20
54	BA	2178	C	N1-C2-O2	5.14	121.99	118.90
54	BA	2312	U	O4'-C1'-N1	5.14	112.31	108.20
10	AK	52	ARG	CD-NE-CZ	5.14	130.80	123.60
21	AA	546	A	C6-C5-N7	5.14	135.90	132.30
21	AA	632	U	O4'-C1'-N1	5.14	112.31	108.20
21	AA	1060	U	N1-C1'-C2'	-5.14	106.35	112.00
21	AA	1063	C	N1-C2-O2	5.14	121.98	118.90
54	BA	526	A	C1'-O4'-C4'	-5.14	105.79	109.90
54	BA	542	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	1014	A	C6-C5-N7	5.14	135.90	132.30
54	BA	1575	C	N1-C2-O2	5.14	121.98	118.90
54	BA	2209	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	2707	U	C4'-C3'-C2'	-5.14	97.46	102.60
21	AA	119	A	C4-C5-C6	-5.14	114.43	117.00
54	BA	364	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	386	G	N1-C6-O6	-5.14	116.82	119.90
54	BA	1924	C	O4'-C1'-N1	5.14	112.31	108.20
54	BA	2043	C	C6-N1-C2	-5.14	118.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	323	U	C5'-C4'-C3'	-5.13	107.78	116.00
21	AA	559	A	C1'-O4'-C4'	-5.13	105.79	109.90
21	AA	735	C	N1-C2-O2	5.13	121.98	118.90
27	BE	61	ARG	NE-CZ-NH1	5.13	122.87	120.30
54	BA	1128	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2375	G	N1-C6-O6	-5.13	116.82	119.90
54	BA	2449	U	N3-C2-O2	-5.13	118.61	122.20
54	BA	2541	A	C3'-C2'-C1'	5.13	105.61	101.50
54	BA	177	G	N3-C4-C5	-5.13	126.03	128.60
54	BA	458	G	C3'-C2'-C1'	-5.13	97.39	101.50
54	BA	564	C	N1-C2-O2	5.13	121.98	118.90
21	AA	403	C	N1-C2-O2	5.13	121.98	118.90
21	AA	723	U	N3-C2-O2	-5.13	118.61	122.20
21	AA	1137	C	O4'-C1'-N1	5.13	112.31	108.20
54	BA	105	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	290	U	O4'-C1'-N1	5.13	112.31	108.20
54	BA	1059	G	O4'-C1'-N9	5.13	112.31	108.20
54	BA	1273	U	O4'-C1'-N1	5.13	112.31	108.20
21	AA	9	G	N3-C2-N2	-5.13	116.31	119.90
21	AA	860	A	C6-C5-N7	5.13	135.89	132.30
54	BA	364	C	N3-C2-O2	-5.13	118.31	121.90
21	AA	450	G	N1-C6-O6	-5.13	116.82	119.90
21	AA	582	C	N3-C2-O2	-5.13	118.31	121.90
54	BA	192	C	O4'-C1'-N1	5.13	112.30	108.20
54	BA	1640	A	C4-C5-C6	-5.13	114.44	117.00
21	AA	1051	C	O4'-C1'-N1	5.13	112.30	108.20
21	AA	1111	A	O4'-C1'-N9	5.13	112.30	108.20
21	AA	1379	G	C1'-O4'-C4'	-5.13	105.80	109.90
54	BA	631	A	C4-C5-C6	-5.13	114.44	117.00
54	BA	2032	G	N3-C4-C5	-5.13	126.04	128.60
54	BA	2509	G	O4'-C1'-N9	5.13	112.30	108.20
54	BA	1881	C	N1-C2-O2	5.12	121.97	118.90
54	BA	395	U	C5-C6-N1	-5.12	120.14	122.70
54	BA	557	C	N1-C2-O2	5.12	121.97	118.90
54	BA	792	A	C5'-C4'-O4'	5.12	115.25	109.10
54	BA	1913	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2038	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2423	U	N1-C2-N3	5.12	117.97	114.90
54	BA	2595	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	2858	C	N1-C2-O2	5.12	121.97	118.90
54	BA	2902	C	N1-C2-O2	5.12	121.97	118.90
55	BB	67	G	N1-C6-O6	-5.12	116.83	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A1	14	A	C4-C5-C6	-5.12	114.44	117.00
35	BM	81	ARG	NE-CZ-NH1	5.12	122.86	120.30
54	BA	889	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1109	C	O4'-C1'-N1	5.12	112.30	108.20
54	BA	1307	A	C4-C5-C6	-5.12	114.44	117.00
54	BA	2583	G	C5-C6-N1	5.12	114.06	111.50
21	AA	933	G	N1-C6-O6	-5.12	116.83	119.90
21	AA	1521	C	N3-C2-O2	-5.12	118.32	121.90
54	BA	1129	A	C6-C5-N7	5.12	135.88	132.30
21	AA	1260	G	N1-C6-O6	-5.12	116.83	119.90
54	BA	554	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	1921	G	N1-C6-O6	-5.12	116.83	119.90
55	BB	47	C	N3-C2-O2	-5.12	118.32	121.90
21	AA	372	C	N3-C4-C5	5.12	123.95	121.90
21	AA	518	C	O4'-C1'-N1	5.12	112.29	108.20
54	BA	1871	A	C4-C5-C6	-5.12	114.44	117.00
21	AA	611	C	N3-C4-C5	5.12	123.95	121.90
54	BA	163	C	N1-C2-O2	5.12	121.97	118.90
54	BA	2155	U	N3-C2-O2	-5.12	118.62	122.20
54	BA	2723	C	N1-C2-O2	5.12	121.97	118.90
22	A1	20	G	C6-C5-N7	5.11	133.47	130.40
54	BA	548	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	1349	C	O4'-C4'-C3'	5.11	110.19	106.10
54	BA	699	A	C4-C5-C6	-5.11	114.44	117.00
54	BA	1316	U	O4'-C1'-N1	5.11	112.29	108.20
54	BA	1954	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	2374	C	N1-C2-O2	5.11	121.97	118.90
35	BM	40	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
54	BA	367	G	C4'-C3'-C2'	-5.11	97.49	102.60
54	BA	1153	C	N1-C2-O2	5.11	121.97	118.90
54	BA	1185	G	N1-C6-O6	-5.11	116.83	119.90
54	BA	2462	C	O4'-C1'-N1	5.11	112.29	108.20
54	BA	1809	A	C6-C5-N7	5.11	135.88	132.30
21	AA	591	U	O4'-C1'-N1	5.11	112.29	108.20
24	A3	13	C	N3-C2-O2	-5.11	118.33	121.90
54	BA	1793	C	N1-C2-O2	5.11	121.96	118.90
54	BA	2420	C	N1-C2-O2	5.11	121.97	118.90
55	BB	71	C	O4'-C1'-N1	5.11	112.29	108.20
21	AA	1213	A	C6-C5-N7	5.11	135.87	132.30
54	BA	461	C	N3-C2-O2	-5.11	118.33	121.90
54	BA	634	C	C5'-C4'-O4'	5.11	115.23	109.10
54	BA	748	G	C1'-O4'-C4'	-5.11	105.81	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1338	G	C5-C6-N1	5.11	114.05	111.50
54	BA	2200	C	O4'-C1'-N1	5.11	112.28	108.20
54	BA	2704	C	N1-C2-O2	5.11	121.96	118.90
21	AA	532	A	O4'-C1'-N9	5.10	112.28	108.20
54	BA	1646	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2347	C	N1-C2-O2	5.10	121.96	118.90
54	BA	274	C	N1-C2-O2	5.10	121.96	118.90
54	BA	964	C	C4'-C3'-C2'	-5.10	97.50	102.60
54	BA	2440	C	N1-C2-O2	5.10	121.96	118.90
54	BA	2763	G	O4'-C1'-N9	5.10	112.28	108.20
55	BB	27	C	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1483	A	C4-C5-C6	-5.10	114.45	117.00
54	BA	262	A	C6-C5-N7	5.10	135.87	132.30
54	BA	601	C	C4'-C3'-C2'	-5.10	97.50	102.60
54	BA	865	C	O4'-C1'-N1	5.10	112.28	108.20
54	BA	2052	A	N1-C6-N6	-5.10	115.54	118.60
21	AA	206	C	N1-C2-O2	5.10	121.96	118.90
21	AA	243	A	P-O3'-C3'	5.10	125.82	119.70
54	BA	1296	G	C5'-C4'-O4'	5.10	115.22	109.10
54	BA	1901	A	C6-C5-N7	5.10	135.87	132.30
54	BA	2300	C	N1-C2-O2	5.10	121.96	118.90
54	BA	2573	C	N1-C2-O2	5.10	121.96	118.90
21	AA	204	G	O4'-C1'-N9	5.10	112.28	108.20
21	AA	1218	C	N1-C2-O2	5.10	121.96	118.90
21	AA	1471	U	O4'-C1'-N1	5.10	112.28	108.20
29	BG	162	ARG	NE-CZ-NH2	-5.10	117.75	120.30
54	BA	2194	U	O4'-C1'-N1	5.10	112.28	108.20
55	BB	54	G	N1-C6-O6	-5.10	116.84	119.90
22	A1	26	A	C6-C5-N7	5.09	135.87	132.30
54	BA	491	G	N1-C6-O6	-5.09	116.84	119.90
54	BA	595	C	O4'-C1'-N1	5.09	112.28	108.20
54	BA	1437	C	O4'-C1'-N1	5.09	112.28	108.20
9	AJ	9	ARG	CD-NE-CZ	5.09	130.73	123.60
54	BA	571	U	N3-C2-O2	-5.09	118.64	122.20
54	BA	2707	U	O4'-C1'-N1	5.09	112.28	108.20
54	BA	2871	U	N3-C2-O2	-5.09	118.64	122.20
21	AA	211	G	N3-C4-C5	-5.09	126.05	128.60
21	AA	552	U	O4'-C1'-N1	5.09	112.27	108.20
3	AD	187	ARG	NE-CZ-NH2	-5.09	117.75	120.30
21	AA	841	C	N1-C2-O2	5.09	121.95	118.90
54	BA	703	U	O4'-C1'-N1	5.09	112.27	108.20
54	BA	1195	G	C4'-C3'-C2'	-5.09	97.51	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2122	U	O4'-C1'-N1	5.09	112.27	108.20
21	AA	17	U	C1'-O4'-C4'	-5.09	105.83	109.90
21	AA	521	G	N1-C6-O6	-5.09	116.85	119.90
24	A3	76	C	C6-N1-C2	-5.09	118.27	120.30
54	BA	1982	U	C5'-C4'-O4'	5.09	115.21	109.10
8	AI	118	ARG	NE-CZ-NH2	-5.09	117.76	120.30
21	AA	52	C	N1-C2-O2	5.09	121.95	118.90
21	AA	959	A	C4-C5-C6	-5.09	114.46	117.00
21	AA	1007	U	O4'-C1'-N1	5.09	112.27	108.20
21	AA	1115	U	O4'-C1'-N1	5.09	112.27	108.20
28	BF	29	ARG	NE-CZ-NH2	-5.09	117.76	120.30
54	BA	829	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	984	A	C3'-C2'-C1'	5.09	105.57	101.50
54	BA	1000	A	N1-C6-N6	-5.09	115.55	118.60
54	BA	1088	A	C4-C5-C6	-5.09	114.46	117.00
54	BA	2892	G	N1-C6-O6	-5.09	116.85	119.90
54	BA	371	A	C6-C5-N7	5.08	135.86	132.30
54	BA	879	G	N1-C6-O6	-5.08	116.85	119.90
22	A1	52	G	N9-C4-C5	5.08	107.43	105.40
54	BA	507	A	C6-C5-N7	5.08	135.86	132.30
54	BA	2728	U	O4'-C1'-N1	5.08	112.27	108.20
54	BA	478	A	C6-C5-N7	5.08	135.86	132.30
54	BA	636	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	1143	A	C6-C5-N7	5.08	135.86	132.30
54	BA	1187	G	N3-C4-C5	-5.08	126.06	128.60
54	BA	1271	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2419	U	C5-C6-N1	-5.08	120.16	122.70
54	BA	2789	C	N3-C2-O2	-5.08	118.34	121.90
25	BC	220	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
21	AA	210	C	N1-C2-O2	5.08	121.95	118.90
21	AA	559	A	C4-C5-C6	-5.08	114.46	117.00
54	BA	1143	A	O4'-C1'-N9	5.08	112.26	108.20
54	BA	2853	C	O4'-C1'-N1	5.08	112.26	108.20
6	AG	94	ARG	NE-CZ-NH1	5.08	122.84	120.30
21	AA	952	U	C5'-C4'-C3'	-5.08	107.88	116.00
54	BA	596	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1061	U	O4'-C1'-N1	5.08	112.26	108.20
54	BA	1863	G	N1-C6-O6	-5.08	116.85	119.90
54	BA	2825	G	N7-C8-N9	5.08	115.64	113.10
54	BA	2855	C	O4'-C1'-N1	5.08	112.26	108.20
21	AA	109	A	C5'-C4'-C3'	-5.08	107.88	116.00
21	AA	192	A	C6-C5-N7	5.08	135.85	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	1802	A	C4-C5-C6	-5.08	114.46	117.00
2	AC	87	ARG	NE-CZ-NH1	5.07	122.84	120.30
21	AA	1053	G	C5-C6-N1	5.07	114.04	111.50
54	BA	365	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	2112	G	O4'-C1'-N9	5.07	112.26	108.20
54	BA	2614	A	O4'-C1'-N9	5.07	112.26	108.20
54	BA	2751	G	N3-C4-C5	-5.07	126.06	128.60
54	BA	539	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	2539	C	N1-C2-O2	5.07	121.94	118.90
21	AA	392	C	N3-C4-C5	5.07	123.93	121.90
21	AA	495	A	C4-C5-C6	-5.07	114.46	117.00
54	BA	235	U	O4'-C1'-N1	5.07	112.26	108.20
54	BA	493	G	N1-C6-O6	-5.07	116.86	119.90
54	BA	1384	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	1810	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	2395	C	N1-C2-O2	5.07	121.94	118.90
21	AA	235	C	N1-C2-O2	5.07	121.94	118.90
49	B0	39	ARG	NE-CZ-NH1	5.07	122.83	120.30
54	BA	1577	C	O4'-C1'-N1	5.07	112.25	108.20
9	AJ	37	ARG	NE-CZ-NH1	5.07	122.83	120.30
21	AA	805	C	N1-C2-O2	5.07	121.94	118.90
36	BN	71	ARG	NE-CZ-NH1	5.07	122.83	120.30
54	BA	133	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	683	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	1808	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	2051	A	C4-C5-C6	-5.07	114.47	117.00
21	AA	38	G	C5-C6-N1	5.07	114.03	111.50
21	AA	328	C	N3-C4-N4	-5.07	114.45	118.00
21	AA	1480	A	C6-C5-N7	5.07	135.85	132.30
54	BA	279	A	C4-C5-C6	-5.07	114.47	117.00
54	BA	737	C	N1-C2-O2	5.07	121.94	118.90
54	BA	878	A	C6-C5-N7	5.07	135.85	132.30
54	BA	1135	C	N1-C2-O2	5.07	121.94	118.90
54	BA	1951	U	O4'-C1'-N1	5.07	112.25	108.20
54	BA	2405	G	N1-C6-O6	-5.07	116.86	119.90
21	AA	151	A	C6-C5-N7	5.06	135.84	132.30
21	AA	695	A	C4-C5-C6	-5.06	114.47	117.00
21	AA	978	A	C3'-C2'-C1'	5.06	105.55	101.50
54	BA	481	G	O4'-C1'-N9	5.06	112.25	108.20
3	AD	25	ARG	NE-CZ-NH1	5.06	122.83	120.30
8	AI	94	ARG	NE-CZ-NH1	5.06	122.83	120.30
21	AA	307	C	N3-C4-C5	5.06	123.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	716	A	C6-C5-N7	5.06	135.84	132.30
54	BA	1437	C	N1-C2-O2	5.06	121.94	118.90
54	BA	1827	U	N1-C2-N3	5.06	117.94	114.90
21	AA	257	G	N1-C6-O6	-5.06	116.86	119.90
21	AA	1490	U	C5'-C4'-C3'	-5.06	107.90	116.00
44	BV	19	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
54	BA	2714	G	N3-C2-N2	-5.06	116.36	119.90
21	AA	1066	C	N1-C2-O2	5.06	121.94	118.90
24	A3	31	G	C3'-C2'-C1'	5.06	105.55	101.50
54	BA	1610	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	1739	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	2143	C	O4'-C1'-N1	5.06	112.25	108.20
54	BA	2488	G	N1-C6-O6	-5.06	116.86	119.90
54	BA	2652	C	O4'-C1'-N1	5.06	112.25	108.20
6	AG	77	ARG	NE-CZ-NH2	-5.06	117.77	120.30
21	AA	219	U	N3-C2-O2	-5.06	118.66	122.20
21	AA	697	U	N1-C2-N3	5.06	117.93	114.90
54	BA	1126	A	C4-C5-C6	-5.06	114.47	117.00
54	BA	1742	U	N3-C2-O2	-5.06	118.66	122.20
54	BA	2733	A	C5'-C4'-O4'	5.06	115.17	109.10
54	BA	2636	C	N1-C2-O2	5.06	121.93	118.90
21	AA	406	G	C5'-C4'-C3'	-5.05	107.91	116.00
21	AA	706	A	C6-C5-N7	5.05	135.84	132.30
21	AA	866	C	N1-C2-O2	5.05	121.93	118.90
54	BA	2234	G	C8-N9-C4	-5.05	104.38	106.40
21	AA	425	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	1186	G	N1-C6-O6	-5.05	116.87	119.90
21	AA	549	C	N1-C2-O2	5.05	121.93	118.90
54	BA	509	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1460	U	O4'-C1'-N1	5.05	112.24	108.20
54	BA	2544	G	N3-C4-C5	-5.05	126.07	128.60
55	BB	80	U	C5-C6-N1	-5.05	120.17	122.70
20	AU	46	ARG	CD-NE-CZ	5.05	130.67	123.60
21	AA	972	C	C1'-O4'-C4'	-5.05	105.86	109.90
54	BA	738	G	C5-C6-N1	5.05	114.02	111.50
54	BA	1816	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1908	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1982	U	O4'-C1'-N1	5.05	112.24	108.20
55	BB	86	G	O4'-C1'-N9	5.05	112.24	108.20
21	AA	1252	A	C4-C5-C6	-5.05	114.48	117.00
54	BA	98	G	N1-C6-O6	-5.05	116.87	119.90
54	BA	2238	G	N3-C4-C5	-5.05	126.08	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	1	C	N1-C2-O2	5.05	121.93	118.90
48	BZ	29	ARG	NE-CZ-NH2	5.05	122.82	120.30
54	BA	398	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1503	A	C6-C5-N7	5.05	135.83	132.30
54	BA	1526	C	N1-C2-O2	5.05	121.93	118.90
54	BA	1654	A	O4'-C1'-N9	5.05	112.24	108.20
54	BA	2161	C	N1-C2-O2	5.05	121.93	118.90
54	BA	2515	C	O4'-C1'-N1	5.05	112.24	108.20
21	AA	106	C	N1-C2-O2	5.04	121.93	118.90
54	BA	1765	U	O4'-C1'-N1	5.04	112.24	108.20
21	AA	732	C	N1-C2-O2	5.04	121.93	118.90
54	BA	1386	C	N3-C4-N4	-5.04	114.47	118.00
54	BA	1979	U	O4'-C1'-N1	5.04	112.23	108.20
54	BA	2083	G	O4'-C1'-N9	5.04	112.23	108.20
54	BA	2612	C	N1-C2-O2	5.04	121.93	118.90
8	AI	105	ARG	CD-NE-CZ	5.04	130.66	123.60
21	AA	152	A	C6-C5-N7	5.04	135.83	132.30
54	BA	1290	C	N1-C2-O2	5.04	121.92	118.90
55	BB	23	G	N3-C4-C5	-5.04	126.08	128.60
35	BM	16	ARG	NE-CZ-NH1	5.04	122.82	120.30
54	BA	783	A	C4-C5-C6	-5.04	114.48	117.00
54	BA	2798	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	641	U	C5-C6-N1	-5.04	120.18	122.70
54	BA	865	C	N3-C4-C5	5.04	123.92	121.90
54	BA	2354	C	N3-C2-O2	-5.04	118.37	121.90
21	AA	1132	C	N1-C2-O2	5.04	121.92	118.90
21	AA	184	G	N3-C4-C5	-5.04	126.08	128.60
22	A1	8	U	N3-C2-O2	-5.04	118.67	122.20
54	BA	1119	U	O4'-C1'-N1	5.04	112.23	108.20
21	AA	188	C	N1-C2-O2	5.03	121.92	118.90
21	AA	426	U	O4'-C1'-N1	5.03	112.23	108.20
21	AA	1034	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	207	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	1573	G	O4'-C1'-N9	5.03	112.23	108.20
54	BA	2394	C	O4'-C1'-N1	5.03	112.23	108.20
54	BA	2528	U	C5-C6-N1	-5.03	120.18	122.70
54	BA	1463	C	N3-C4-N4	-5.03	114.48	118.00
54	BA	1760	C	O4'-C4'-C3'	5.03	110.12	106.10
21	AA	124	C	N1-C2-O2	5.03	121.92	118.90
21	AA	139	A	O4'-C1'-N9	5.03	112.22	108.20
21	AA	244	U	N3-C2-O2	-5.03	118.68	122.20
21	AA	344	A	C6-C5-N7	5.03	135.82	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BC	211	ARG	NE-CZ-NH1	5.03	122.81	120.30
54	BA	244	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	264	C	N1-C2-O2	5.03	121.92	118.90
54	BA	2291	U	N3-C2-O2	-5.03	118.68	122.20
54	BA	2705	A	C4-C5-C6	-5.03	114.48	117.00
54	BA	2801	G	N1-C6-O6	-5.03	116.88	119.90
21	AA	953	G	N1-C6-O6	-5.03	116.88	119.90
54	BA	2052	A	C5'-C4'-C3'	-5.03	107.95	116.00
54	BA	2078	C	O4'-C1'-N1	5.03	112.22	108.20
21	AA	399	G	C5'-C4'-O4'	5.03	115.13	109.10
23	A2	91	A	C6-C5-N7	5.03	135.82	132.30
54	BA	362	A	C6-C5-N7	5.03	135.82	132.30
54	BA	2354	C	O4'-C1'-N1	5.03	112.22	108.20
55	BB	43	C	N3-C2-O2	-5.03	118.38	121.90
13	AN	85	ARG	NE-CZ-NH1	5.03	122.81	120.30
21	AA	1435	G	N7-C8-N9	5.03	115.61	113.10
54	BA	539	G	O4'-C1'-N9	5.03	112.22	108.20
54	BA	1056	G	O4'-C1'-N9	5.03	112.22	108.20
54	BA	2434	A	C4-C5-C6	-5.03	114.49	117.00
54	BA	2465	C	O4'-C1'-N1	5.03	112.22	108.20
54	BA	2706	A	O4'-C1'-N9	5.03	112.22	108.20
21	AA	1224	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1612	C	O4'-C1'-N1	5.02	112.22	108.20
54	BA	1657	U	O4'-C1'-N1	5.02	112.22	108.20
54	BA	2726	A	C6-C5-N7	5.02	135.82	132.30
54	BA	2838	G	N3-C2-N2	-5.02	116.38	119.90
21	AA	372	C	N3-C2-O2	-5.02	118.38	121.90
54	BA	54	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	905	A	C6-C5-N7	5.02	135.82	132.30
54	BA	980	A	C4-C5-C6	-5.02	114.49	117.00
54	BA	1086	A	O4'-C1'-N9	5.02	112.22	108.20
54	BA	1902	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2047	C	C4'-C3'-C2'	-5.02	97.58	102.60
54	BA	12	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	2089	C	N1-C2-O2	5.02	121.91	118.90
54	BA	2545	G	N1-C6-O6	-5.02	116.89	119.90
54	BA	2598	A	C4-C5-C6	-5.02	114.49	117.00
23	A2	92	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	823	C	N1-C2-O2	5.02	121.91	118.90
54	BA	1088	A	C5'-C4'-O4'	5.02	115.12	109.10
54	BA	1692	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	1872	A	C6-C5-N7	5.02	135.81	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	2512	C	N1-C2-O2	5.02	121.91	118.90
55	BB	47	C	O4'-C1'-N1	5.02	112.22	108.20
20	AU	6	ARG	NE-CZ-NH1	-5.02	117.79	120.30
54	BA	141	G	C5-C6-N1	5.02	114.01	111.50
54	BA	228	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	985	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	1057	A	C6-C5-N7	5.02	135.81	132.30
54	BA	2023	C	O4'-C1'-N1	5.02	112.21	108.20
21	AA	1208	C	C5'-C4'-C3'	-5.02	107.97	116.00
21	AA	1235	U	O4'-C1'-N1	5.02	112.21	108.20
54	BA	639	U	N3-C2-O2	-5.02	118.69	122.20
54	BA	2050	C	O4'-C1'-N1	5.02	112.21	108.20
54	BA	2364	C	C4'-C3'-C2'	-5.02	97.58	102.60
54	BA	2591	C	O4'-C1'-N1	5.02	112.21	108.20
32	BJ	24	THR	C-N-CA	5.01	134.24	121.70
36	BN	30	ARG	NE-CZ-NH1	5.01	122.81	120.30
54	BA	1258	U	C5'-C4'-O4'	5.01	115.12	109.10
54	BA	1318	U	C5-C6-N1	-5.01	120.19	122.70
54	BA	2442	C	N1-C2-O2	5.01	121.91	118.90
54	BA	2790	U	O4'-C1'-N1	5.01	112.21	108.20
55	BB	46	A	C6-C5-N7	5.01	135.81	132.30
54	BA	855	G	O4'-C1'-N9	5.01	112.21	108.20
54	BA	160	A	C4-C5-C6	-5.01	114.50	117.00
54	BA	277	G	N3-C4-C5	-5.01	126.09	128.60
21	AA	268	U	O4'-C1'-N1	5.01	112.21	108.20
21	AA	376	G	C8-N9-C4	-5.01	104.40	106.40
21	AA	974	A	O4'-C1'-N9	5.01	112.21	108.20
21	AA	996	A	C6-C5-N7	5.01	135.81	132.30
54	BA	205	G	C8-N9-C4	-5.01	104.40	106.40
54	BA	970	U	N3-C2-O2	-5.01	118.69	122.20
54	BA	1560	G	C8-N9-C4	-5.01	104.40	106.40
54	BA	1675	C	N1-C2-O2	5.01	121.91	118.90
54	BA	2683	C	N3-C2-O2	-5.01	118.39	121.90
21	AA	1008	U	O4'-C1'-N1	5.01	112.21	108.20
54	BA	1511	G	N1-C6-O6	-5.01	116.89	119.90
21	AA	862	C	N3-C2-O2	-5.01	118.39	121.90
21	AA	899	C	N1-C2-O2	5.01	121.90	118.90
54	BA	1815	A	C6-C5-N7	5.01	135.80	132.30
54	BA	2814	A	C6-C5-N7	5.01	135.80	132.30
55	BB	78	A	O4'-C1'-N9	5.01	112.20	108.20
21	AA	16	A	N1-C6-N6	-5.00	115.60	118.60
21	AA	1094	G	N1-C6-O6	-5.00	116.90	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	BA	484	C	N3-C2-O2	-5.00	118.40	121.90
54	BA	1775	U	N3-C2-O2	-5.00	118.70	122.20
54	BA	2370	G	N1-C6-O6	-5.00	116.90	119.90
21	AA	816	A	C6-C5-N7	5.00	135.80	132.30
26	BD	46	ARG	NE-CZ-NH2	-5.00	117.80	120.30
22	A1	52	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	220	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	956	G	O4'-C1'-N9	5.00	112.20	108.20
54	BA	1452	G	N1-C6-O6	-5.00	116.90	119.90
54	BA	1574	C	N1-C2-O2	5.00	121.90	118.90
54	BA	2563	U	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (1122) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	A1	11	C	Sidechain
22	A1	14	A	Sidechain
22	A1	15	G	Sidechain
22	A1	17	U	Sidechain
22	A1	2	G	Sidechain
22	A1	24	G	Sidechain
22	A1	30	C	Sidechain
22	A1	33	U	Sidechain
22	A1	45	G	Sidechain
22	A1	57	G	Sidechain
22	A1	59	U	Sidechain
22	A1	60	C	Sidechain
22	A1	66	A	Sidechain
22	A1	72	C	Sidechain
22	A1	73	A	Sidechain
22	A1	9	A	Sidechain
23	A2	80	C	Sidechain
23	A2	83	U	Sidechain
23	A2	89	U	Sidechain
23	A2	90	U	Sidechain
23	A2	91	A	Sidechain
24	A3	16	C	Sidechain
24	A3	19	G	Sidechain
24	A3	20	G	Sidechain
24	A3	24	C	Sidechain
24	A3	3	C	Sidechain

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Mol	Chain	Res	Type	Group
24	A3	30	G	Sidechain
24	A3	31	G	Sidechain
24	A3	34	U	Sidechain
24	A3	37	U	Sidechain
24	A3	44	A	Sidechain
24	A3	61	U	Sidechain
24	A3	65	G	Sidechain
24	A3	68	C	Sidechain
24	A3	69	C	Sidechain
24	A3	7	G	Sidechain
24	A3	73	A	Sidechain
24	A3	77	A	Sidechain
21	AA	100	G	Sidechain
21	AA	1008	U	Sidechain
21	AA	1010	U	Sidechain
21	AA	1013	G	Sidechain
21	AA	1015	G	Sidechain
21	AA	102	G	Sidechain
21	AA	1025	U	Sidechain
21	AA	1026	G	Sidechain
21	AA	1028	C	Sidechain
21	AA	1029	U	Sidechain
21	AA	1030	U	Sidechain
21	AA	1033	G	Sidechain
21	AA	1036	A	Sidechain
21	AA	1039	G	Sidechain
21	AA	1044	A	Sidechain
21	AA	1045	C	Sidechain
21	AA	1046	A	Sidechain
21	AA	1048	G	Sidechain
21	AA	1049	U	Sidechain
21	AA	106	C	Sidechain
21	AA	1060	U	Sidechain
21	AA	1061	G	Sidechain
21	AA	1073	U	Sidechain
21	AA	1077	G	Sidechain
21	AA	108	G	Sidechain
21	AA	1090	U	Sidechain
21	AA	1092	A	Sidechain
21	AA	1098	C	Sidechain
21	AA	1099	G	Sidechain
21	AA	1101	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1107	C	Sidechain
21	AA	1108	G	Sidechain
21	AA	111	G	Sidechain
21	AA	1112	C	Sidechain
21	AA	1114	C	Sidechain
21	AA	1116	U	Sidechain
21	AA	1119	C	Sidechain
21	AA	112	G	Sidechain
21	AA	1125	U	Sidechain
21	AA	1128	C	Sidechain
21	AA	1130	A	Sidechain
21	AA	1131	G	Sidechain
21	AA	1142	G	Sidechain
21	AA	1144	G	Sidechain
21	AA	1153	G	Sidechain
21	AA	1167	A	Sidechain
21	AA	1172	C	Sidechain
21	AA	1176	A	Sidechain
21	AA	1178	G	Sidechain
21	AA	1179	A	Sidechain
21	AA	118	U	Sidechain
21	AA	1190	G	Sidechain
21	AA	1192	C	Sidechain
21	AA	1198	G	Sidechain
21	AA	1199	U	Sidechain
21	AA	12	U	Sidechain
21	AA	1205	U	Sidechain
21	AA	1206	G	Sidechain
21	AA	1207	G	Sidechain
21	AA	1208	C	Sidechain
21	AA	1211	U	Sidechain
21	AA	1216	A	Sidechain
21	AA	1224	U	Sidechain
21	AA	1230	C	Sidechain
21	AA	1238	A	Sidechain
21	AA	1239	A	Sidechain
21	AA	1240	U	Sidechain
21	AA	1246	A	Sidechain
21	AA	1248	A	Sidechain
21	AA	1261	A	Sidechain
21	AA	1268	G	Sidechain
21	AA	1271	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	1276	G	Sidechain
21	AA	1279	G	Sidechain
21	AA	129	A	Sidechain
21	AA	1290	G	Sidechain
21	AA	1294	G	Sidechain
21	AA	1297	G	Sidechain
21	AA	1301	U	Sidechain
21	AA	1302	C	Sidechain
21	AA	1305	G	Sidechain
21	AA	1308	U	Sidechain
21	AA	1316	G	Sidechain
21	AA	1317	C	Sidechain
21	AA	1326	U	Sidechain
21	AA	1329	A	Sidechain
21	AA	1330	U	Sidechain
21	AA	1338	G	Sidechain
21	AA	134	G	Sidechain
21	AA	1343	G	Sidechain
21	AA	1345	U	Sidechain
21	AA	1349	A	Sidechain
21	AA	1360	A	Sidechain
21	AA	1363	A	Sidechain
21	AA	137	U	Sidechain
21	AA	1370	G	Sidechain
21	AA	1376	U	Sidechain
21	AA	1378	C	Sidechain
21	AA	1381	U	Sidechain
21	AA	1382	C	Sidechain
21	AA	1384	C	Sidechain
21	AA	1385	G	Sidechain
21	AA	1397	C	Sidechain
21	AA	1398	A	Sidechain
21	AA	1412	C	Sidechain
21	AA	1413	A	Sidechain
21	AA	1414	U	Sidechain
21	AA	1417	G	Sidechain
21	AA	143	A	Sidechain
21	AA	1431	A	Sidechain
21	AA	1435	G	Sidechain
21	AA	1442	G	Sidechain
21	AA	1460	C	Sidechain
21	AA	1464	U	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	147	G	Sidechain
21	AA	1485	U	Sidechain
21	AA	1494	G	Sidechain
21	AA	1502	A	Sidechain
21	AA	1503	A	Sidechain
21	AA	1506	U	Sidechain
21	AA	1514	G	Sidechain
21	AA	1515	G	Sidechain
21	AA	1517	G	Sidechain
21	AA	1525	G	Sidechain
21	AA	1527	U	Sidechain
21	AA	159	G	Sidechain
21	AA	161	A	Sidechain
21	AA	181	A	Sidechain
21	AA	182	A	Sidechain
21	AA	185	U	Sidechain
21	AA	187	G	Sidechain
21	AA	197	A	Sidechain
21	AA	200	G	Sidechain
21	AA	204	G	Sidechain
21	AA	208	U	Sidechain
21	AA	210	C	Sidechain
21	AA	211	G	Sidechain
21	AA	212	G	Sidechain
21	AA	213	G	Sidechain
21	AA	221	C	Sidechain
21	AA	229	U	Sidechain
21	AA	236	A	Sidechain
21	AA	239	U	Sidechain
21	AA	243	A	Sidechain
21	AA	25	C	Sidechain
21	AA	252	U	Sidechain
21	AA	255	G	Sidechain
21	AA	258	G	Sidechain
21	AA	26	A	Sidechain
21	AA	260	G	Sidechain
21	AA	261	U	Sidechain
21	AA	264	C	Sidechain
21	AA	269	C	Sidechain
21	AA	27	G	Sidechain
21	AA	275	G	Sidechain
21	AA	279	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	281	G	Sidechain
21	AA	284	C	Sidechain
21	AA	291	U	Sidechain
21	AA	294	U	Sidechain
21	AA	297	G	Sidechain
21	AA	299	G	Sidechain
21	AA	30	U	Sidechain
21	AA	31	G	Sidechain
21	AA	310	G	Sidechain
21	AA	315	A	Sidechain
21	AA	318	G	Sidechain
21	AA	32	A	Sidechain
21	AA	321	A	Sidechain
21	AA	323	U	Sidechain
21	AA	324	G	Sidechain
21	AA	326	G	Sidechain
21	AA	327	A	Sidechain
21	AA	328	C	Sidechain
21	AA	336	A	Sidechain
21	AA	339	C	Sidechain
21	AA	341	C	Sidechain
21	AA	348	G	Sidechain
21	AA	351	G	Sidechain
21	AA	354	G	Sidechain
21	AA	356	A	Sidechain
21	AA	360	G	Sidechain
21	AA	362	G	Sidechain
21	AA	363	A	Sidechain
21	AA	367	U	Sidechain
21	AA	376	G	Sidechain
21	AA	38	G	Sidechain
21	AA	380	G	Sidechain
21	AA	383	A	Sidechain
21	AA	387	U	Sidechain
21	AA	391	G	Sidechain
21	AA	395	C	Sidechain
21	AA	402	G	Sidechain
21	AA	404	G	Sidechain
21	AA	405	U	Sidechain
21	AA	408	A	Sidechain
21	AA	409	U	Sidechain
21	AA	414	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	421	U	Sidechain
21	AA	423	G	Sidechain
21	AA	428	G	Sidechain
21	AA	429	U	Sidechain
21	AA	432	A	Sidechain
21	AA	433	G	Sidechain
21	AA	439	U	Sidechain
21	AA	44	A	Sidechain
21	AA	448	A	Sidechain
21	AA	453	G	Sidechain
21	AA	456	A	Sidechain
21	AA	457	G	Sidechain
21	AA	468	A	Sidechain
21	AA	471	U	Sidechain
21	AA	474	G	Sidechain
21	AA	475	C	Sidechain
21	AA	476	U	Sidechain
21	AA	48	C	Sidechain
21	AA	480	U	Sidechain
21	AA	485	U	Sidechain
21	AA	492	C	Sidechain
21	AA	493	A	Sidechain
21	AA	494	G	Sidechain
21	AA	499	A	Sidechain
21	AA	5	U	Sidechain
21	AA	507	C	Sidechain
21	AA	51	A	Sidechain
21	AA	510	A	Sidechain
21	AA	515	G	Sidechain
21	AA	519	C	Sidechain
21	AA	525	C	Sidechain
21	AA	528	C	Sidechain
21	AA	529	G	Sidechain
21	AA	533	A	Sidechain
21	AA	537	G	Sidechain
21	AA	553	A	Sidechain
21	AA	557	G	Sidechain
21	AA	566	G	Sidechain
21	AA	573	A	Sidechain
21	AA	575	G	Sidechain
21	AA	577	G	Sidechain
21	AA	583	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	592	G	Sidechain
21	AA	593	U	Sidechain
21	AA	6	G	Sidechain
21	AA	606	G	Sidechain
21	AA	612	C	Sidechain
21	AA	622	A	Sidechain
21	AA	624	C	Sidechain
21	AA	632	U	Sidechain
21	AA	641	U	Sidechain
21	AA	642	A	Sidechain
21	AA	651	C	Sidechain
21	AA	653	U	Sidechain
21	AA	663	A	Sidechain
21	AA	664	G	Sidechain
21	AA	68	G	Sidechain
21	AA	680	C	Sidechain
21	AA	682	G	Sidechain
21	AA	686	U	Sidechain
21	AA	687	A	Sidechain
21	AA	688	G	Sidechain
21	AA	69	G	Sidechain
21	AA	694	A	Sidechain
21	AA	698	G	Sidechain
21	AA	702	A	Sidechain
21	AA	707	U	Sidechain
21	AA	708	C	Sidechain
21	AA	715	A	Sidechain
21	AA	721	G	Sidechain
21	AA	722	G	Sidechain
21	AA	724	G	Sidechain
21	AA	727	G	Sidechain
21	AA	73	C	Sidechain
21	AA	731	G	Sidechain
21	AA	733	G	Sidechain
21	AA	736	C	Sidechain
21	AA	737	C	Sidechain
21	AA	738	C	Sidechain
21	AA	739	C	Sidechain
21	AA	741	G	Sidechain
21	AA	742	G	Sidechain
21	AA	743	A	Sidechain
21	AA	752	G	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	754	C	Sidechain
21	AA	76	G	Sidechain
21	AA	761	G	Sidechain
21	AA	775	G	Sidechain
21	AA	781	A	Sidechain
21	AA	788	U	Sidechain
21	AA	789	U	Sidechain
21	AA	79	G	Sidechain
21	AA	8	A	Sidechain
21	AA	800	G	Sidechain
21	AA	804	U	Sidechain
21	AA	809	G	Sidechain
21	AA	812	G	Sidechain
21	AA	817	C	Sidechain
21	AA	818	G	Sidechain
21	AA	819	A	Sidechain
21	AA	826	C	Sidechain
21	AA	838	G	Sidechain
21	AA	840	C	Sidechain
21	AA	855	U	Sidechain
21	AA	859	G	Sidechain
21	AA	86	G	Sidechain
21	AA	864	A	Sidechain
21	AA	868	C	Sidechain
21	AA	869	G	Sidechain
21	AA	87	C	Sidechain
21	AA	871	U	Sidechain
21	AA	872	A	Sidechain
21	AA	873	A	Sidechain
21	AA	875	U	Sidechain
21	AA	882	C	Sidechain
21	AA	884	U	Sidechain
21	AA	886	G	Sidechain
21	AA	890	G	Sidechain
21	AA	891	U	Sidechain
21	AA	892	A	Sidechain
21	AA	898	G	Sidechain
21	AA	899	C	Sidechain
21	AA	905	U	Sidechain
21	AA	906	A	Sidechain
21	AA	91	U	Sidechain
21	AA	914	A	Sidechain

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Mol	Chain	Res	Type	Group
21	AA	915	A	Sidechain
21	AA	916	U	Sidechain
21	AA	919	A	Sidechain
21	AA	922	G	Sidechain
21	AA	925	G	Sidechain
21	AA	932	C	Sidechain
21	AA	933	G	Sidechain
21	AA	939	G	Sidechain
21	AA	941	G	Sidechain
21	AA	946	A	Sidechain
21	AA	948	C	Sidechain
21	AA	95	C	Sidechain
21	AA	953	G	Sidechain
21	AA	954	G	Sidechain
21	AA	955	U	Sidechain
21	AA	957	U	Sidechain
21	AA	958	A	Sidechain
21	AA	962	C	Sidechain
21	AA	966	G	Sidechain
21	AA	973	G	Sidechain
21	AA	979	C	Sidechain
21	AA	980	C	Sidechain
21	AA	983	A	Sidechain
21	AA	987	G	Sidechain
21	AA	99	C	Sidechain
21	AA	995	C	Sidechain
1	AB	20	ARG	Sidechain
2	AC	178	ARG	Sidechain
5	AF	4	TYR	Sidechain
10	AK	121	ARG	Peptide
14	AO	43	ALA	Peptide
54	BA	10	A	Sidechain
54	BA	1006	C	Sidechain
54	BA	1012	U	Sidechain
54	BA	1013	C	Sidechain
54	BA	1019	U	Sidechain
54	BA	102	U	Sidechain
54	BA	1023	U	Sidechain
54	BA	103	A	Sidechain
54	BA	1034	G	Sidechain
54	BA	1042	G	Sidechain
54	BA	1044	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1046	A	Sidechain
54	BA	1047	G	Sidechain
54	BA	105	C	Sidechain
54	BA	1054	A	Sidechain
54	BA	1055	G	Sidechain
54	BA	1059	G	Sidechain
54	BA	1062	G	Sidechain
54	BA	1068	G	Sidechain
54	BA	1071	G	Sidechain
54	BA	1072	C	Sidechain
54	BA	1073	A	Sidechain
54	BA	1077	A	Sidechain
54	BA	108	G	Sidechain
54	BA	1089	A	Sidechain
54	BA	1092	C	Sidechain
54	BA	1093	G	Sidechain
54	BA	1099	G	Sidechain
54	BA	11	C	Sidechain
54	BA	1101	U	Sidechain
54	BA	1103	A	Sidechain
54	BA	1106	G	Sidechain
54	BA	1107	G	Sidechain
54	BA	1108	U	Sidechain
54	BA	1113	U	Sidechain
54	BA	1125	G	Sidechain
54	BA	1130	U	Sidechain
54	BA	1136	G	Sidechain
54	BA	1137	G	Sidechain
54	BA	114	U	Sidechain
54	BA	1141	U	Sidechain
54	BA	1143	A	Sidechain
54	BA	1145	C	Sidechain
54	BA	1146	C	Sidechain
54	BA	1147	A	Sidechain
54	BA	1150	C	Sidechain
54	BA	1154	G	Sidechain
54	BA	1160	G	Sidechain
54	BA	1162	G	Sidechain
54	BA	1167	C	Sidechain
54	BA	1182	G	Sidechain
54	BA	1185	G	Sidechain
54	BA	1186	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1187	G	Sidechain
54	BA	1190	G	Sidechain
54	BA	1191	G	Sidechain
54	BA	1192	G	Sidechain
54	BA	1197	G	Sidechain
54	BA	1199	U	Sidechain
54	BA	12	U	Sidechain
54	BA	1206	G	Sidechain
54	BA	1208	C	Sidechain
54	BA	1215	G	Sidechain
54	BA	1219	U	Sidechain
54	BA	1220	G	Sidechain
54	BA	1221	C	Sidechain
54	BA	1223	G	Sidechain
54	BA	1235	G	Sidechain
54	BA	1240	U	Sidechain
54	BA	1244	A	Sidechain
54	BA	1245	G	Sidechain
54	BA	1255	U	Sidechain
54	BA	1257	C	Sidechain
54	BA	1258	U	Sidechain
54	BA	1261	C	Sidechain
54	BA	1266	G	Sidechain
54	BA	1268	A	Sidechain
54	BA	127	A	Sidechain
54	BA	1275	A	Sidechain
54	BA	1276	A	Sidechain
54	BA	1280	G	Sidechain
54	BA	1283	G	Sidechain
54	BA	1284	A	Sidechain
54	BA	1285	A	Sidechain
54	BA	1291	C	Sidechain
54	BA	1293	C	Sidechain
54	BA	1299	G	Sidechain
54	BA	1301	A	Sidechain
54	BA	1309	G	Sidechain
54	BA	1311	G	Sidechain
54	BA	1314	C	Sidechain
54	BA	1315	C	Sidechain
54	BA	1319	C	Sidechain
54	BA	132	G	Sidechain
54	BA	1320	C	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1323	C	Sidechain
54	BA	1325	U	Sidechain
54	BA	1328	A	Sidechain
54	BA	1330	C	Sidechain
54	BA	1332	G	Sidechain
54	BA	1333	G	Sidechain
54	BA	1336	A	Sidechain
54	BA	1337	G	Sidechain
54	BA	1340	U	Sidechain
54	BA	1343	G	Sidechain
54	BA	1355	G	Sidechain
54	BA	1359	A	Sidechain
54	BA	1364	G	Sidechain
54	BA	1365	A	Sidechain
54	BA	1366	A	Sidechain
54	BA	1368	G	Sidechain
54	BA	1373	A	Sidechain
54	BA	1376	C	Sidechain
54	BA	1378	A	Sidechain
54	BA	1379	U	Sidechain
54	BA	138	U	Sidechain
54	BA	1380	G	Sidechain
54	BA	1382	G	Sidechain
54	BA	1386	C	Sidechain
54	BA	1388	G	Sidechain
54	BA	1391	U	Sidechain
54	BA	1396	U	Sidechain
54	BA	1397	U	Sidechain
54	BA	1401	G	Sidechain
54	BA	1407	G	Sidechain
54	BA	142	A	Sidechain
54	BA	1420	A	Sidechain
54	BA	1424	G	Sidechain
54	BA	1425	G	Sidechain
54	BA	1431	A	Sidechain
54	BA	1435	G	Sidechain
54	BA	1439	A	Sidechain
54	BA	1441	G	Sidechain
54	BA	1445	G	Sidechain
54	BA	1452	G	Sidechain
54	BA	1454	C	Sidechain
54	BA	1455	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1456	G	Sidechain
54	BA	1459	G	Sidechain
54	BA	146	A	Sidechain
54	BA	1461	C	Sidechain
54	BA	1464	G	Sidechain
54	BA	1469	A	Sidechain
54	BA	1476	U	Sidechain
54	BA	148	U	Sidechain
54	BA	1493	C	Sidechain
54	BA	1495	A	Sidechain
54	BA	1497	U	Sidechain
54	BA	1509	A	Sidechain
54	BA	1515	A	Sidechain
54	BA	1517	G	Sidechain
54	BA	1519	G	Sidechain
54	BA	1526	C	Sidechain
54	BA	1529	G	Sidechain
54	BA	1531	C	Sidechain
54	BA	1534	U	Sidechain
54	BA	1539	U	Sidechain
54	BA	1540	G	Sidechain
54	BA	1541	C	Sidechain
54	BA	1543	G	Sidechain
54	BA	1550	C	Sidechain
54	BA	1552	A	Sidechain
54	BA	1555	G	Sidechain
54	BA	1560	G	Sidechain
54	BA	1561	C	Sidechain
54	BA	1565	C	Sidechain
54	BA	1575	C	Sidechain
54	BA	1580	A	Sidechain
54	BA	1581	G	Sidechain
54	BA	1584	U	Sidechain
54	BA	1585	C	Sidechain
54	BA	1588	G	Sidechain
54	BA	1589	U	Sidechain
54	BA	1594	U	Sidechain
54	BA	1595	C	Sidechain
54	BA	1602	U	Sidechain
54	BA	1603	A	Sidechain
54	BA	1604	C	Sidechain
54	BA	161	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1611	C	Sidechain
54	BA	1616	A	Sidechain
54	BA	162	U	Sidechain
54	BA	1620	G	Sidechain
54	BA	1626	A	Sidechain
54	BA	1632	A	Sidechain
54	BA	1633	G	Sidechain
54	BA	1637	A	Sidechain
54	BA	164	C	Sidechain
54	BA	1641	A	Sidechain
54	BA	1644	C	Sidechain
54	BA	1653	G	Sidechain
54	BA	1655	A	Sidechain
54	BA	1670	C	Sidechain
54	BA	1671	U	Sidechain
54	BA	1672	A	Sidechain
54	BA	1673	G	Sidechain
54	BA	168	G	Sidechain
54	BA	1681	G	Sidechain
54	BA	1682	G	Sidechain
54	BA	1683	U	Sidechain
54	BA	1684	G	Sidechain
54	BA	1687	G	Sidechain
54	BA	1695	G	Sidechain
54	BA	1699	G	Sidechain
54	BA	170	U	Sidechain
54	BA	1708	C	Sidechain
54	BA	1710	G	Sidechain
54	BA	1711	A	Sidechain
54	BA	1713	A	Sidechain
54	BA	1721	G	Sidechain
54	BA	1725	U	Sidechain
54	BA	1731	G	Sidechain
54	BA	1741	C	Sidechain
54	BA	1743	G	Sidechain
54	BA	1747	U	Sidechain
54	BA	1753	G	Sidechain
54	BA	1758	U	Sidechain
54	BA	176	A	Sidechain
54	BA	1762	A	Sidechain
54	BA	1763	G	Sidechain
54	BA	177	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1775	U	Sidechain
54	BA	1782	U	Sidechain
54	BA	1784	A	Sidechain
54	BA	1785	A	Sidechain
54	BA	1796	U	Sidechain
54	BA	1802	A	Sidechain
54	BA	1804	C	Sidechain
54	BA	1807	G	Sidechain
54	BA	1819	A	Sidechain
54	BA	182	A	Sidechain
54	BA	1820	U	Sidechain
54	BA	1822	C	Sidechain
54	BA	1830	C	Sidechain
54	BA	1834	U	Sidechain
54	BA	1835	G	Sidechain
54	BA	1844	C	Sidechain
54	BA	1852	U	Sidechain
54	BA	1854	A	Sidechain
54	BA	1857	G	Sidechain
54	BA	1860	G	Sidechain
54	BA	1865	U	Sidechain
54	BA	1870	C	Sidechain
54	BA	1883	U	Sidechain
54	BA	1884	G	Sidechain
54	BA	1885	A	Sidechain
54	BA	1888	G	Sidechain
54	BA	189	G	Sidechain
54	BA	1891	G	Sidechain
54	BA	1892	C	Sidechain
54	BA	1893	C	Sidechain
54	BA	1895	C	Sidechain
54	BA	19	A	Sidechain
54	BA	190	A	Sidechain
54	BA	1908	C	Sidechain
54	BA	191	A	Sidechain
54	BA	1910	G	Sidechain
54	BA	1914	C	Sidechain
54	BA	1915	U	Sidechain
54	BA	1918	A	Sidechain
54	BA	1919	A	Sidechain
54	BA	1929	G	Sidechain
54	BA	1931	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	1932	A	Sidechain
54	BA	1938	A	Sidechain
54	BA	1946	U	Sidechain
54	BA	1947	C	Sidechain
54	BA	1954	G	Sidechain
54	BA	1955	U	Sidechain
54	BA	1959	G	Sidechain
54	BA	1963	U	Sidechain
54	BA	1964	G	Sidechain
54	BA	1968	G	Sidechain
54	BA	197	A	Sidechain
54	BA	1972	G	Sidechain
54	BA	1974	C	Sidechain
54	BA	1976	U	Sidechain
54	BA	198	C	Sidechain
54	BA	1982	U	Sidechain
54	BA	1993	U	Sidechain
54	BA	1997	C	Sidechain
54	BA	200	U	Sidechain
54	BA	2006	C	Sidechain
54	BA	2014	A	Sidechain
54	BA	2017	U	Sidechain
54	BA	2018	G	Sidechain
54	BA	2019	A	Sidechain
54	BA	202	U	Sidechain
54	BA	2020	A	Sidechain
54	BA	2022	U	Sidechain
54	BA	2023	C	Sidechain
54	BA	2024	G	Sidechain
54	BA	2027	G	Sidechain
54	BA	2030	A	Sidechain
54	BA	2034	U	Sidechain
54	BA	2035	G	Sidechain
54	BA	2037	A	Sidechain
54	BA	2044	C	Sidechain
54	BA	2046	G	Sidechain
54	BA	2057	G	Sidechain
54	BA	2060	A	Sidechain
54	BA	2061	G	Sidechain
54	BA	2062	A	Sidechain
54	BA	2074	U	Sidechain
54	BA	2076	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2077	A	Sidechain
54	BA	2078	C	Sidechain
54	BA	2082	A	Sidechain
54	BA	2086	U	Sidechain
54	BA	2088	A	Sidechain
54	BA	209	C	Sidechain
54	BA	2095	A	Sidechain
54	BA	2097	A	Sidechain
54	BA	2099	U	Sidechain
54	BA	2100	G	Sidechain
54	BA	2104	C	Sidechain
54	BA	2112	G	Sidechain
54	BA	2117	A	Sidechain
54	BA	2119	A	Sidechain
54	BA	2120	G	Sidechain
54	BA	2133	G	Sidechain
54	BA	2135	A	Sidechain
54	BA	2138	G	Sidechain
54	BA	214	G	Sidechain
54	BA	2141	G	Sidechain
54	BA	2145	C	Sidechain
54	BA	2147	A	Sidechain
54	BA	2148	G	Sidechain
54	BA	215	G	Sidechain
54	BA	2150	C	Sidechain
54	BA	2156	G	Sidechain
54	BA	2158	A	Sidechain
54	BA	2163	A	Sidechain
54	BA	2168	G	Sidechain
54	BA	2178	C	Sidechain
54	BA	2180	U	Sidechain
54	BA	2183	A	Sidechain
54	BA	2186	G	Sidechain
54	BA	2187	U	Sidechain
54	BA	219	A	Sidechain
54	BA	2197	U	Sidechain
54	BA	22	C	Sidechain
54	BA	2202	U	Sidechain
54	BA	2208	C	Sidechain
54	BA	2212	A	Sidechain
54	BA	2213	U	Sidechain
54	BA	2216	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2226	C	Sidechain
54	BA	2229	U	Sidechain
54	BA	2240	U	Sidechain
54	BA	2242	G	Sidechain
54	BA	2244	U	Sidechain
54	BA	2247	A	Sidechain
54	BA	2254	C	Sidechain
54	BA	2257	U	Sidechain
54	BA	2264	C	Sidechain
54	BA	2268	A	Sidechain
54	BA	2273	A	Sidechain
54	BA	2275	C	Sidechain
54	BA	2281	A	Sidechain
54	BA	2282	G	Sidechain
54	BA	2288	A	Sidechain
54	BA	2294	G	Sidechain
54	BA	2296	U	Sidechain
54	BA	23	G	Sidechain
54	BA	2301	C	Sidechain
54	BA	2303	G	Sidechain
54	BA	2305	U	Sidechain
54	BA	232	G	Sidechain
54	BA	2323	G	Sidechain
54	BA	2324	U	Sidechain
54	BA	2326	C	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	2340	A	Sidechain
54	BA	2352	A	Sidechain
54	BA	2357	G	Sidechain
54	BA	2365	G	Sidechain
54	BA	2366	A	Sidechain
54	BA	237	C	Sidechain
54	BA	2371	G	Sidechain
54	BA	2375	G	Sidechain
54	BA	2377	A	Sidechain
54	BA	2378	A	Sidechain
54	BA	2382	G	Sidechain
54	BA	2384	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2385	C	Sidechain
54	BA	2389	G	Sidechain
54	BA	2390	U	Sidechain
54	BA	2391	G	Sidechain
54	BA	2401	U	Sidechain
54	BA	2402	U	Sidechain
54	BA	2403	C	Sidechain
54	BA	2418	A	Sidechain
54	BA	2421	G	Sidechain
54	BA	2424	C	Sidechain
54	BA	2425	A	Sidechain
54	BA	2429	G	Sidechain
54	BA	2431	U	Sidechain
54	BA	2433	A	Sidechain
54	BA	2434	A	Sidechain
54	BA	2437	G	Sidechain
54	BA	2439	A	Sidechain
54	BA	2444	G	Sidechain
54	BA	2447	G	Sidechain
54	BA	2448	A	Sidechain
54	BA	2452	C	Sidechain
54	BA	2453	A	Sidechain
54	BA	2458	G	Sidechain
54	BA	2460	U	Sidechain
54	BA	2469	A	Sidechain
54	BA	247	G	Sidechain
54	BA	2472	G	Sidechain
54	BA	2475	C	Sidechain
54	BA	2477	U	Sidechain
54	BA	248	G	Sidechain
54	BA	2481	G	Sidechain
54	BA	2483	C	Sidechain
54	BA	2485	G	Sidechain
54	BA	2489	U	Sidechain
54	BA	249	C	Sidechain
54	BA	2491	U	Sidechain
54	BA	2494	G	Sidechain
54	BA	2495	G	Sidechain
54	BA	2497	A	Sidechain
54	BA	2498	C	Sidechain
54	BA	250	G	Sidechain
54	BA	2504	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2512	C	Sidechain
54	BA	2513	A	Sidechain
54	BA	2517	C	Sidechain
54	BA	2518	A	Sidechain
54	BA	2529	G	Sidechain
54	BA	2531	A	Sidechain
54	BA	2559	C	Sidechain
54	BA	2563	U	Sidechain
54	BA	2571	U	Sidechain
54	BA	2576	G	Sidechain
54	BA	2577	A	Sidechain
54	BA	2580	U	Sidechain
54	BA	2581	G	Sidechain
54	BA	2582	G	Sidechain
54	BA	2595	G	Sidechain
54	BA	2596	U	Sidechain
54	BA	26	G	Sidechain
54	BA	2601	C	Sidechain
54	BA	2602	A	Sidechain
54	BA	2608	G	Sidechain
54	BA	2615	U	Sidechain
54	BA	2620	C	Sidechain
54	BA	2621	G	Sidechain
54	BA	2624	G	Sidechain
54	BA	2625	G	Sidechain
54	BA	2626	C	Sidechain
54	BA	2627	G	Sidechain
54	BA	2635	A	Sidechain
54	BA	2644	G	Sidechain
54	BA	2645	G	Sidechain
54	BA	2647	U	Sidechain
54	BA	2651	C	Sidechain
54	BA	2653	U	Sidechain
54	BA	2656	U	Sidechain
54	BA	2657	A	Sidechain
54	BA	2659	G	Sidechain
54	BA	2661	G	Sidechain
54	BA	2662	A	Sidechain
54	BA	2669	G	Sidechain
54	BA	2674	G	Sidechain
54	BA	2679	A	Sidechain
54	BA	2680	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2682	A	Sidechain
54	BA	2696	U	Sidechain
54	BA	27	G	Sidechain
54	BA	2703	C	Sidechain
54	BA	271	G	Sidechain
54	BA	2718	G	Sidechain
54	BA	2719	G	Sidechain
54	BA	2722	G	Sidechain
54	BA	2723	C	Sidechain
54	BA	2727	A	Sidechain
54	BA	2732	G	Sidechain
54	BA	2735	G	Sidechain
54	BA	2741	A	Sidechain
54	BA	2747	G	Sidechain
54	BA	2751	G	Sidechain
54	BA	2752	C	Sidechain
54	BA	276	U	Sidechain
54	BA	2763	G	Sidechain
54	BA	277	G	Sidechain
54	BA	2770	G	Sidechain
54	BA	2771	C	Sidechain
54	BA	2780	G	Sidechain
54	BA	2781	A	Sidechain
54	BA	2784	U	Sidechain
54	BA	279	A	Sidechain
54	BA	2799	A	Sidechain
54	BA	28	A	Sidechain
54	BA	2806	C	Sidechain
54	BA	2814	A	Sidechain
54	BA	2816	G	Sidechain
54	BA	2817	U	Sidechain
54	BA	2818	U	Sidechain
54	BA	2822	G	Sidechain
54	BA	283	G	Sidechain
54	BA	2831	G	Sidechain
54	BA	2835	A	Sidechain
54	BA	2842	G	Sidechain
54	BA	2847	U	Sidechain
54	BA	2854	G	Sidechain
54	BA	2857	G	Sidechain
54	BA	2864	G	Sidechain
54	BA	2868	A	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	2881	U	Sidechain
54	BA	2883	A	Sidechain
54	BA	2885	G	Sidechain
54	BA	2889	C	Sidechain
54	BA	289	G	Sidechain
54	BA	291	G	Sidechain
54	BA	30	G	Sidechain
54	BA	301	G	Sidechain
54	BA	307	G	Sidechain
54	BA	310	A	Sidechain
54	BA	313	G	Sidechain
54	BA	316	C	Sidechain
54	BA	321	U	Sidechain
54	BA	325	G	Sidechain
54	BA	327	G	Sidechain
54	BA	33	C	Sidechain
54	BA	338	G	Sidechain
54	BA	339	U	Sidechain
54	BA	341	C	Sidechain
54	BA	345	A	Sidechain
54	BA	347	A	Sidechain
54	BA	352	A	Sidechain
54	BA	361	G	Sidechain
54	BA	362	A	Sidechain
54	BA	363	G	Sidechain
54	BA	365	U	Sidechain
54	BA	372	G	Sidechain
54	BA	378	C	Sidechain
54	BA	381	G	Sidechain
54	BA	383	C	Sidechain
54	BA	385	C	Sidechain
54	BA	389	G	Sidechain
54	BA	392	U	Sidechain
54	BA	393	C	Sidechain
54	BA	394	C	Sidechain
54	BA	395	U	Sidechain
54	BA	400	G	Sidechain
54	BA	403	U	Sidechain
54	BA	404	A	Sidechain
54	BA	405	U	Sidechain
54	BA	415	A	Sidechain
54	BA	416	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	417	C	Sidechain
54	BA	420	C	Sidechain
54	BA	426	C	Sidechain
54	BA	428	A	Sidechain
54	BA	43	G	Sidechain
54	BA	430	A	Sidechain
54	BA	437	U	Sidechain
54	BA	44	A	Sidechain
54	BA	444	C	Sidechain
54	BA	447	A	Sidechain
54	BA	458	G	Sidechain
54	BA	463	G	Sidechain
54	BA	464	U	Sidechain
54	BA	470	A	Sidechain
54	BA	473	G	Sidechain
54	BA	476	G	Sidechain
54	BA	479	A	Sidechain
54	BA	481	G	Sidechain
54	BA	483	A	Sidechain
54	BA	484	C	Sidechain
54	BA	488	G	Sidechain
54	BA	491	G	Sidechain
54	BA	500	G	Sidechain
54	BA	505	A	Sidechain
54	BA	507	A	Sidechain
54	BA	515	A	Sidechain
54	BA	520	G	Sidechain
54	BA	526	A	Sidechain
54	BA	530	G	Sidechain
54	BA	531	C	Sidechain
54	BA	533	G	Sidechain
54	BA	535	G	Sidechain
54	BA	537	G	Sidechain
54	BA	545	U	Sidechain
54	BA	546	U	Sidechain
54	BA	547	A	Sidechain
54	BA	551	G	Sidechain
54	BA	554	U	Sidechain
54	BA	584	C	Sidechain
54	BA	586	A	Sidechain
54	BA	587	C	Sidechain
54	BA	597	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	600	G	Sidechain
54	BA	607	U	Sidechain
54	BA	608	A	Sidechain
54	BA	611	C	Sidechain
54	BA	612	G	Sidechain
54	BA	617	G	Sidechain
54	BA	620	G	Sidechain
54	BA	621	A	Sidechain
54	BA	626	A	Sidechain
54	BA	628	G	Sidechain
54	BA	630	G	Sidechain
54	BA	644	A	Sidechain
54	BA	646	U	Sidechain
54	BA	647	G	Sidechain
54	BA	650	C	Sidechain
54	BA	655	A	Sidechain
54	BA	659	G	Sidechain
54	BA	669	G	Sidechain
54	BA	677	A	Sidechain
54	BA	679	C	Sidechain
54	BA	680	C	Sidechain
54	BA	681	G	Sidechain
54	BA	683	U	Sidechain
54	BA	686	U	Sidechain
54	BA	687	C	Sidechain
54	BA	695	G	Sidechain
54	BA	7	G	Sidechain
54	BA	701	G	Sidechain
54	BA	703	U	Sidechain
54	BA	704	G	Sidechain
54	BA	715	A	Sidechain
54	BA	719	C	Sidechain
54	BA	722	A	Sidechain
54	BA	726	G	Sidechain
54	BA	728	G	Sidechain
54	BA	730	A	Sidechain
54	BA	736	C	Sidechain
54	BA	740	C	Sidechain
54	BA	75	G	Sidechain
54	BA	756	A	Sidechain
54	BA	757	G	Sidechain
54	BA	759	G	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	765	C	Sidechain
54	BA	768	G	Sidechain
54	BA	774	G	Sidechain
54	BA	775	G	Sidechain
54	BA	778	G	Sidechain
54	BA	78	U	Sidechain
54	BA	780	G	Sidechain
54	BA	783	A	Sidechain
54	BA	784	G	Sidechain
54	BA	795	C	Sidechain
54	BA	799	G	Sidechain
54	BA	801	G	Sidechain
54	BA	807	U	Sidechain
54	BA	808	G	Sidechain
54	BA	811	U	Sidechain
54	BA	812	C	Sidechain
54	BA	827	U	Sidechain
54	BA	830	G	Sidechain
54	BA	834	G	Sidechain
54	BA	845	A	Sidechain
54	BA	846	U	Sidechain
54	BA	85	G	Sidechain
54	BA	852	U	Sidechain
54	BA	856	G	Sidechain
54	BA	858	G	Sidechain
54	BA	860	U	Sidechain
54	BA	862	G	Sidechain
54	BA	872	U	Sidechain
54	BA	879	G	Sidechain
54	BA	883	G	Sidechain
54	BA	890	C	Sidechain
54	BA	909	A	Sidechain
54	BA	912	C	Sidechain
54	BA	913	U	Sidechain
54	BA	914	G	Sidechain
54	BA	921	C	Sidechain
54	BA	922	C	Sidechain
54	BA	923	G	Sidechain
54	BA	924	G	Sidechain
54	BA	929	U	Sidechain
54	BA	930	G	Sidechain
54	BA	934	U	Sidechain

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Mol	Chain	Res	Type	Group
54	BA	937	C	Sidechain
54	BA	938	G	Sidechain
54	BA	939	G	Sidechain
54	BA	945	A	Sidechain
54	BA	946	C	Sidechain
54	BA	947	A	Sidechain
54	BA	948	C	Sidechain
54	BA	949	G	Sidechain
54	BA	95	A	Sidechain
54	BA	955	U	Sidechain
54	BA	956	G	Sidechain
54	BA	961	C	Sidechain
54	BA	962	G	Sidechain
54	BA	969	G	Sidechain
54	BA	979	A	Sidechain
54	BA	982	C	Sidechain
54	BA	986	C	Sidechain
54	BA	988	A	Sidechain
54	BA	989	G	Sidechain
54	BA	99	U	Sidechain
54	BA	990	A	Sidechain
54	BA	995	C	Sidechain
55	BB	102	G	Sidechain
55	BB	105	G	Sidechain
55	BB	106	G	Sidechain
55	BB	12	C	Sidechain
55	BB	13	G	Sidechain
55	BB	16	G	Sidechain
55	BB	24	G	Sidechain
55	BB	27	C	Sidechain
55	BB	28	C	Sidechain
55	BB	3	C	Sidechain
55	BB	35	C	Sidechain
55	BB	40	U	Sidechain
55	BB	41	G	Sidechain
55	BB	50	A	Sidechain
55	BB	51	G	Sidechain
55	BB	57	A	Sidechain
55	BB	61	G	Sidechain
55	BB	64	G	Sidechain
55	BB	67	G	Sidechain
55	BB	73	A	Sidechain

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Mol	Chain	Res	Type	Group
55	BB	88	C	Sidechain
26	BD	141	ARG	Sidechain
27	BE	49	ARG	Sidechain
37	BO	102	ARG	Sidechain

5.2 Too-close contacts

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	0	0
6	AG	1178	0	1234	0	0
7	AH	979	0	1034	0	0
8	AI	1025	0	1074	0	0
9	AJ	790	0	832	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	1	0
17	AR	459	0	482	0	0
18	AS	641	0	669	0	0
19	AT	668	0	718	0	0
20	AU	429	0	453	0	0
21	AA	32828	0	16520	1	0
22	A1	1627	0	832	0	0
23	A2	309	0	158	0	0
24	A3	1642	0	843	0	0
25	BC	2083	0	2157	2	0
26	BD	1565	0	1616	0	0
27	BE	1552	0	1619	0	0
28	BF	1420	0	1460	0	0
29	BG	1323	0	1374	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
38	BP	917	0	965	0	0
39	BQ	947	0	1022	0	0
40	BR	816	0	839	0	0
41	BS	857	0	922	0	0
42	BT	739	0	807	1	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	1	0
53	B4	302	0	343	0	0
54	BA	62317	0	31345	4	0
55	BB	2504	0	1271	0	0
56	B5	1658	0	1751	0	0
57	A1	7	0	8	0	0
58	BA	10	0	10	0	0
All	All	147653	0	99663	14	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 (14) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BA:889:C:H1'	54:BA:890:C:C6	2.44	0.52
42:BT:19:LYS:HA	42:BT:23:ALA:HB3	1.92	0.52
21:AA:577:G:H1'	21:AA:816:A:C4	2.49	0.47
2:AC:149:LYS:HE3	2:AC:200:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:BA:680:C:H2'	54:BA:681:G:C8	2.52	0.44
52:B3:25:HIS:CG	52:B3:26:ALA:H	2.36	0.44
54:BA:1130:U:H2'	54:BA:1131:G:H2'	2.00	0.43
9:AJ:56:HIS:CG	9:AJ:57:VAL:H	2.36	0.43
35:BM:62:LYS:HE3	35:BM:64:TRP:CZ2	2.54	0.42
25:BC:70:LYS:HE3	25:BC:95:TYR:CZ	2.54	0.42
54:BA:1737:G:H2'	54:BA:1738:G:C2	2.56	0.41
16:AQ:30:HIS:CE1	16:AQ:33:TYR:CD2	3.09	0.41
37:BO:85:LYS:HE2	37:BO:85:LYS:HA	2.03	0.41
25:BC:264:LYS:HE3	25:BC:265:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	202 (93%)	16 (7%)	0	100	100
2	AC	205/208 (99%)	190 (93%)	13 (6%)	2 (1%)	19	65
3	AD	203/206 (98%)	191 (94%)	10 (5%)	2 (1%)	19	65
4	AE	150/152 (99%)	135 (90%)	10 (7%)	5 (3%)	5	40
5	AF	99/101 (98%)	87 (88%)	8 (8%)	4 (4%)	4	35
6	AG	150/152 (99%)	134 (89%)	14 (9%)	2 (1%)	15	60
7	AH	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
8	AI	126/128 (98%)	119 (94%)	4 (3%)	3 (2%)	7	47
9	AJ	98/100 (98%)	93 (95%)	3 (3%)	2 (2%)	9	51
10	AK	116/118 (98%)	105 (90%)	8 (7%)	3 (3%)	7	45
11	AL	121/124 (98%)	106 (88%)	10 (8%)	5 (4%)	3	35
12	AM	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	4	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	AN	98/101 (97%)	88 (90%)	8 (8%)	2 (2%)	9	51
14	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	4	39
15	AP	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
16	AQ	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	7	46
17	AR	55/57 (96%)	53 (96%)	1 (2%)	1 (2%)	11	53
18	AS	79/81 (98%)	69 (87%)	10 (13%)	0	100	100
19	AT	84/86 (98%)	72 (86%)	10 (12%)	2 (2%)	7	47
20	AU	51/53 (96%)	36 (71%)	11 (22%)	4 (8%)	1	20
25	BC	270/273 (99%)	244 (90%)	22 (8%)	4 (2%)	13	57
26	BD	207/209 (99%)	182 (88%)	19 (9%)	6 (3%)	6	43
27	BE	199/201 (99%)	185 (93%)	7 (4%)	7 (4%)	4	39
28	BF	176/179 (98%)	149 (85%)	16 (9%)	11 (6%)	2	25
29	BG	174/177 (98%)	154 (88%)	18 (10%)	2 (1%)	17	63
30	BH	147/149 (99%)	135 (92%)	11 (8%)	1 (1%)	26	71
31	BI	139/142 (98%)	125 (90%)	14 (10%)	0	100	100
32	BJ	140/142 (99%)	125 (89%)	10 (7%)	5 (4%)	4	38
33	BK	121/123 (98%)	106 (88%)	9 (7%)	6 (5%)	3	31
34	BL	141/144 (98%)	118 (84%)	15 (11%)	8 (6%)	2	28
35	BM	134/136 (98%)	128 (96%)	2 (2%)	4 (3%)	5	42
36	BN	119/121 (98%)	105 (88%)	13 (11%)	1 (1%)	24	69
37	BO	114/117 (97%)	109 (96%)	4 (4%)	1 (1%)	21	67
38	BP	112/115 (97%)	95 (85%)	13 (12%)	4 (4%)	4	38
39	BQ	115/118 (98%)	102 (89%)	13 (11%)	0	100	100
40	BR	101/103 (98%)	88 (87%)	11 (11%)	2 (2%)	9	51
41	BS	108/110 (98%)	100 (93%)	6 (6%)	2 (2%)	10	52
42	BT	92/94 (98%)	75 (82%)	13 (14%)	4 (4%)	3	34
43	BU	101/104 (97%)	85 (84%)	9 (9%)	7 (7%)	1	23
44	BV	92/94 (98%)	88 (96%)	3 (3%)	1 (1%)	17	63
45	BW	78/80 (98%)	60 (77%)	13 (17%)	5 (6%)	2	25
46	BX	75/79 (95%)	67 (89%)	7 (9%)	1 (1%)	15	60
47	BY	61/63 (97%)	53 (87%)	8 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BZ	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	2	29
49	B0	54/57 (95%)	47 (87%)	6 (11%)	1 (2%)	10	52
50	B1	50/52 (96%)	46 (92%)	2 (4%)	2 (4%)	4	35
51	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	3	33
52	B3	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	12	56
53	B4	36/38 (95%)	28 (78%)	7 (19%)	1 (3%)	6	44
56	B5	221/234 (94%)	205 (93%)	13 (6%)	3 (1%)	14	58
All	All	5876/6008 (98%)	5257 (90%)	478 (8%)	141 (2%)	12	47

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	AG	5	VAL
11	AL	108	ASP
19	AT	9	ARG
26	BD	2	ILE
27	BE	69	ARG
27	BE	170	ARG
28	BF	12	VAL
28	BF	46	LYS
29	BG	8	VAL
32	BJ	81	ILE
33	BK	103	VAL
34	BL	46	VAL
40	BR	82	HIS
42	BT	81	LYS
43	BU	57	ILE
43	BU	95	PHE
45	BW	70	VAL
45	BW	78	PHE
48	BZ	31	ILE
50	B1	50	GLU
52	B3	3	ILE
56	B5	50	ILE
2	AC	14	VAL
2	AC	163	ARG
4	AE	25	LYS
5	AF	6	ILE
5	AF	63	ASN
5	AF	98	GLU

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Mol	Chain	Res	Type
6	AG	6	ILE
8	AI	12	LYS
9	AJ	77	VAL
13	AN	91	GLY
14	AO	43	ALA
14	AO	44	GLU
14	AO	74	VAL
20	AU	32	ARG
25	BC	142	ASN
25	BC	161	VAL
26	BD	37	VAL
26	BD	49	GLN
26	BD	82	PHE
27	BE	61	ARG
28	BF	87	LYS
28	BF	116	LEU
28	BF	136	ILE
30	BH	83	LYS
32	BJ	2	LYS
33	BK	25	LEU
33	BK	32	TYR
34	BL	15	ALA
34	BL	36	LYS
35	BM	20	LEU
38	BP	113	LEU
41	BS	41	LYS
42	BT	63	VAL
43	BU	45	GLN
43	BU	83	GLY
4	AE	127	TYR
8	AI	55	ASP
10	AK	16	SER
10	AK	121	ARG
11	AL	117	GLY
12	AM	112	ARG
16	AQ	82	VAL
19	AT	8	LYS
20	AU	36	PHE
25	BC	191	LEU
26	BD	77	ARG
27	BE	120	VAL
27	BE	188	MET

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Mol	Chain	Res	Type
28	BF	35	LEU
34	BL	11	GLY
35	BM	58	LYS
38	BP	2	ASN
38	BP	112	ARG
40	BR	80	ARG
42	BT	38	ALA
43	BU	43	LYS
43	BU	51	LEU
44	BV	71	LYS
45	BW	52	CYS
46	BX	27	ARG
48	BZ	34	THR
50	B1	45	HIS
56	B5	217	THR
3	AD	28	ASP
4	AE	43	GLY
4	AE	54	GLU
5	AF	68	GLN
11	AL	33	CYS
11	AL	78	VAL
16	AQ	39	ARG
20	AU	33	ARG
26	BD	40	LEU
28	BF	113	PHE
29	BG	112	VAL
32	BJ	25	LEU
34	BL	10	GLU
34	BL	66	PHE
34	BL	69	ARG
34	BL	86	GLU
41	BS	3	THR
42	BT	75	GLY
43	BU	5	ARG
51	B2	4	THR
53	B4	16	ILE
3	AD	3	TYR
10	AK	126	ARG
12	AM	23	GLY
12	AM	65	GLU
13	AN	41	ARG
28	BF	4	HIS

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Mol	Chain	Res	Type
33	BK	2	ILE
35	BM	134	THR
36	BN	8	ARG
37	BO	23	ALA
38	BP	69	VAL
45	BW	35	ILE
45	BW	74	LYS
56	B5	168	ASN
11	AL	101	LEU
28	BF	133	GLU
32	BJ	45	THR
32	BJ	72	LYS
48	BZ	9	THR
4	AE	93	VAL
17	AR	20	ILE
9	AJ	74	VAL
28	BF	148	VAL
8	AI	57	VAL
25	BC	123	ILE
27	BE	187	VAL
28	BF	43	ILE
33	BK	47	ILE
51	B2	44	VAL
20	AU	27	VAL
27	BE	149	ILE
12	AM	42	VAL
33	BK	71	ARG
35	BM	36	VAL
49	B0	54	ILE

5.3.2 Protein sidechains ⓘ

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%)	60 83
2	AC	170/171 (99%)	167 (98%)	3 (2%)	66 87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	172/173 (99%)	168 (98%)	4 (2%)	58	83
4	AE	113/113 (100%)	113 (100%)	0	100	100
5	AF	87/87 (100%)	84 (97%)	3 (3%)	44	75
6	AG	123/123 (100%)	120 (98%)	3 (2%)	57	82
7	AH	104/105 (99%)	101 (97%)	3 (3%)	50	78
8	AI	105/105 (100%)	103 (98%)	2 (2%)	65	86
9	AJ	86/86 (100%)	86 (100%)	0	100	100
10	AK	90/90 (100%)	86 (96%)	4 (4%)	35	69
11	AL	103/104 (99%)	102 (99%)	1 (1%)	82	92
12	AM	91/92 (99%)	91 (100%)	0	100	100
13	AN	83/84 (99%)	81 (98%)	2 (2%)	57	82
14	AO	76/77 (99%)	74 (97%)	2 (3%)	54	80
15	AP	65/65 (100%)	64 (98%)	1 (2%)	72	88
16	AQ	74/74 (100%)	74 (100%)	0	100	100
17	AR	48/48 (100%)	48 (100%)	0	100	100
18	AS	70/70 (100%)	68 (97%)	2 (3%)	50	78
19	AT	65/65 (100%)	65 (100%)	0	100	100
20	AU	44/44 (100%)	44 (100%)	0	100	100
25	BC	216/217 (100%)	207 (96%)	9 (4%)	36	70
26	BD	164/164 (100%)	161 (98%)	3 (2%)	66	87
27	BE	165/165 (100%)	163 (99%)	2 (1%)	78	90
28	BF	149/150 (99%)	147 (99%)	2 (1%)	76	89
29	BG	137/138 (99%)	135 (98%)	2 (2%)	72	88
30	BH	114/114 (100%)	114 (100%)	0	100	100
31	BI	109/110 (99%)	108 (99%)	1 (1%)	84	93
32	BJ	116/116 (100%)	113 (97%)	3 (3%)	54	80
33	BK	103/103 (100%)	100 (97%)	3 (3%)	50	78
34	BL	102/103 (99%)	99 (97%)	3 (3%)	50	78
35	BM	109/109 (100%)	107 (98%)	2 (2%)	66	87
36	BN	100/100 (100%)	99 (99%)	1 (1%)	82	92
37	BO	86/87 (99%)	85 (99%)	1 (1%)	78	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BP	99/100 (99%)	97 (98%)	2 (2%)	63	85
39	BQ	89/90 (99%)	87 (98%)	2 (2%)	60	83
40	BR	84/84 (100%)	83 (99%)	1 (1%)	78	90
41	BS	93/93 (100%)	93 (100%)	0	100	100
42	BT	80/80 (100%)	78 (98%)	2 (2%)	55	81
43	BU	83/84 (99%)	81 (98%)	2 (2%)	57	82
44	BV	78/78 (100%)	76 (97%)	2 (3%)	54	80
45	BW	59/59 (100%)	57 (97%)	2 (3%)	44	75
46	BX	67/68 (98%)	67 (100%)	0	100	100
47	BY	55/55 (100%)	55 (100%)	0	100	100
48	BZ	48/49 (98%)	48 (100%)	0	100	100
49	B0	47/48 (98%)	45 (96%)	2 (4%)	35	70
50	B1	45/45 (100%)	45 (100%)	0	100	100
51	B2	38/38 (100%)	38 (100%)	0	100	100
52	B3	51/52 (98%)	50 (98%)	1 (2%)	63	85
53	B4	34/34 (100%)	34 (100%)	0	100	100
56	B5	173/181 (96%)	170 (98%)	3 (2%)	68	87
All	All	4842/4870 (99%)	4757 (98%)	85 (2%)	69	87

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

Mol	Chain	Res	Type
1	AB	38	HIS
1	AB	88	GLN
1	AB	168	GLU
1	AB	189	ASN
2	AC	2	GLN
2	AC	5	HIS
2	AC	128	MET
3	AD	56	GLU
3	AD	139	ASN
3	AD	160	LEU
3	AD	201	GLU
5	AF	1	MET
5	AF	5	GLU
5	AF	13	ASP

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Mol	Chain	Res	Type
6	AG	25	PHE
6	AG	58	LEU
6	AG	100	MET
7	AH	12	ARG
7	AH	112	ASP
7	AH	120	LEU
8	AI	33	SER
8	AI	112	ARG
10	AK	52	ARG
10	AK	56	LYS
10	AK	57	SER
10	AK	128	VAL
11	AL	113	ARG
13	AN	38	ASP
13	AN	62	ASN
14	AO	41	HIS
14	AO	60	SER
15	AP	1	MET
18	AS	2	ARG
18	AS	4	LEU
25	BC	45	ASN
25	BC	73	ILE
25	BC	100	ARG
25	BC	128	THR
25	BC	173	LEU
25	BC	188	ARG
25	BC	200	MET
25	BC	261	ARG
25	BC	270	ARG
26	BD	16	THR
26	BD	58	ASN
26	BD	136	ASN
27	BE	122	GLU
27	BE	171	ASP
28	BF	112	ASP
28	BF	127	TYR
29	BG	127	GLN
29	BG	166	GLU
31	BI	42	ASN
32	BJ	43	GLU
32	BJ	44	TYR
32	BJ	135	GLN

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Mol	Chain	Res	Type
33	BK	1	MET
33	BK	30	ARG
33	BK	64	ARG
34	BL	36	LYS
34	BL	66	PHE
34	BL	76	GLU
35	BM	97	GLN
35	BM	126	ILE
36	BN	59	SER
37	BO	2	ASP
38	BP	29	VAL
38	BP	67	GLU
39	BQ	46	TYR
39	BQ	54	ARG
40	BR	39	LEU
42	BT	2	ILE
42	BT	36	LYS
43	BU	44	HIS
43	BU	61	GLU
44	BV	24	ASN
44	BV	51	GLN
45	BW	13	ARG
45	BW	49	ASN
49	B0	5	ASN
49	B0	37	HIS
52	B3	61	LEU
56	B5	33	LEU
56	B5	97	MET
56	B5	167	LYS

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

Mol	Chain	Res	Type
13	AN	62	ASN
26	BD	134	HIS
34	BL	99	ASN
38	BP	55	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1530/1533 (99%)	240 (15%)	90 (5%)
22	A1	73/76 (96%)	9 (12%)	2 (2%)
23	A2	14/15 (93%)	7 (50%)	2 (14%)
24	A3	76/77 (98%)	9 (11%)	5 (6%)
54	BA	2902/2903 (99%)	458 (15%)	137 (4%)
55	BB	116/118 (98%)	12 (10%)	3 (2%)
All	All	4711/4722 (99%)	735 (15%)	239 (5%)

All (735) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	51	A
21	AA	69	G
21	AA	70	U
21	AA	84	U
21	AA	85	U
21	AA	86	G
21	AA	96	U
21	AA	109	A
21	AA	110	C
21	AA	111	G
21	AA	120	A
21	AA	121	U
21	AA	122	G
21	AA	131	A
21	AA	133	U
21	AA	144	G
21	AA	153	C
21	AA	173	U
21	AA	174	A
21	AA	183	C
21	AA	187	G
21	AA	191	G
21	AA	198	G
21	AA	212	G
21	AA	213	G

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Mol	Chain	Res	Type
21	AA	235	C
21	AA	240	G
21	AA	243	A
21	AA	244	U
21	AA	247	G
21	AA	250	A
21	AA	252	U
21	AA	266	G
21	AA	289	G
21	AA	299	G
21	AA	306	A
21	AA	324	G
21	AA	328	C
21	AA	329	A
21	AA	330	C
21	AA	346	G
21	AA	347	G
21	AA	350	G
21	AA	351	G
21	AA	352	C
21	AA	354	G
21	AA	356	A
21	AA	357	G
21	AA	358	U
21	AA	367	U
21	AA	373	A
21	AA	381	C
21	AA	384	G
21	AA	388	G
21	AA	389	A
21	AA	397	A
21	AA	398	U
21	AA	406	G
21	AA	409	U
21	AA	412	A
21	AA	415	A
21	AA	424	G
21	AA	429	U
21	AA	461	A
21	AA	462	G
21	AA	465	A
21	AA	467	U

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Mol	Chain	Res	Type
21	AA	468	A
21	AA	472	U
21	AA	476	U
21	AA	477	C
21	AA	481	G
21	AA	482	A
21	AA	486	U
21	AA	510	A
21	AA	511	C
21	AA	518	C
21	AA	527	G
21	AA	532	A
21	AA	533	A
21	AA	547	A
21	AA	548	G
21	AA	550	G
21	AA	562	U
21	AA	567	G
21	AA	572	A
21	AA	573	A
21	AA	575	G
21	AA	576	C
21	AA	619	U
21	AA	625	U
21	AA	632	U
21	AA	633	G
21	AA	653	U
21	AA	654	G
21	AA	665	A
21	AA	676	A
21	AA	688	G
21	AA	693	G
21	AA	703	G
21	AA	704	A
21	AA	717	U
21	AA	718	A
21	AA	719	C
21	AA	720	C
21	AA	721	G
21	AA	724	G
21	AA	734	G
21	AA	755	G

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Mol	Chain	Res	Type
21	AA	777	A
21	AA	778	G
21	AA	794	A
21	AA	828	U
21	AA	841	C
21	AA	843	U
21	AA	846	G
21	AA	859	G
21	AA	870	U
21	AA	882	C
21	AA	887	G
21	AA	889	A
21	AA	890	G
21	AA	913	A
21	AA	914	A
21	AA	920	U
21	AA	926	G
21	AA	927	G
21	AA	934	C
21	AA	935	A
21	AA	945	G
21	AA	946	A
21	AA	958	A
21	AA	959	A
21	AA	960	U
21	AA	963	G
21	AA	966	G
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	972	C
21	AA	975	A
21	AA	977	A
21	AA	978	A
21	AA	979	C
21	AA	983	A
21	AA	984	C
21	AA	992	U
21	AA	993	G
21	AA	998	C
21	AA	999	C
21	AA	1004	A

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Mol	Chain	Res	Type
21	AA	1015	G
21	AA	1026	G
21	AA	1031	C
21	AA	1032	G
21	AA	1037	C
21	AA	1043	G
21	AA	1050	G
21	AA	1051	C
21	AA	1052	U
21	AA	1053	G
21	AA	1054	C
21	AA	1055	A
21	AA	1058	G
21	AA	1064	G
21	AA	1065	U
21	AA	1066	C
21	AA	1067	A
21	AA	1068	G
21	AA	1086	U
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1112	C
21	AA	1125	U
21	AA	1129	C
21	AA	1130	A
21	AA	1133	G
21	AA	1137	C
21	AA	1139	G
21	AA	1146	A
21	AA	1147	C
21	AA	1159	U
21	AA	1172	C
21	AA	1183	U
21	AA	1184	G
21	AA	1185	G
21	AA	1189	U
21	AA	1191	A
21	AA	1192	C
21	AA	1196	A
21	AA	1198	G

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Mol	Chain	Res	Type
21	AA	1201	A
21	AA	1222	G
21	AA	1225	A
21	AA	1226	C
21	AA	1227	A
21	AA	1240	U
21	AA	1256	A
21	AA	1257	A
21	AA	1267	C
21	AA	1278	G
21	AA	1279	G
21	AA	1280	A
21	AA	1285	A
21	AA	1286	U
21	AA	1298	U
21	AA	1299	A
21	AA	1300	G
21	AA	1301	U
21	AA	1302	C
21	AA	1303	C
21	AA	1305	G
21	AA	1320	C
21	AA	1323	G
21	AA	1331	G
21	AA	1337	G
21	AA	1338	G
21	AA	1347	G
21	AA	1379	G
21	AA	1380	U
21	AA	1381	U
21	AA	1446	A
21	AA	1447	A
21	AA	1453	G
21	AA	1491	G
21	AA	1493	A
21	AA	1494	G
21	AA	1503	A
21	AA	1504	G
21	AA	1506	U
21	AA	1533	C
22	A1	16	C
22	A1	17	U

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Mol	Chain	Res	Type
22	A1	18	G
22	A1	20	G
22	A1	39	G
22	A1	47	U
22	A1	48	C
22	A1	59	U
22	A1	74	C
23	A2	80	C
23	A2	81	U
23	A2	84	G
23	A2	86	U
23	A2	88	U
23	A2	89	U
23	A2	90	U
24	A3	9	G
24	A3	10	G
24	A3	18	U
24	A3	21	H2U
24	A3	32	G
24	A3	35	C
24	A3	48	U
24	A3	74	A
24	A3	76	C
54	BA	12	U
54	BA	28	A
54	BA	29	U
54	BA	34	U
54	BA	45	G
54	BA	71	A
54	BA	72	U
54	BA	74	A
54	BA	75	G
54	BA	77	G
54	BA	85	G
54	BA	86	G
54	BA	91	A
54	BA	92	U
54	BA	98	G
54	BA	100	U
54	BA	103	A
54	BA	118	A
54	BA	119	A

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Mol	Chain	Res	Type
54	BA	120	U
54	BA	121	G
54	BA	142	A
54	BA	143	C
54	BA	144	A
54	BA	145	C
54	BA	148	U
54	BA	181	A
54	BA	196	A
54	BA	199	A
54	BA	204	A
54	BA	205	G
54	BA	216	A
54	BA	222	A
54	BA	223	A
54	BA	224	U
54	BA	233	A
54	BA	242	G
54	BA	248	G
54	BA	249	C
54	BA	252	G
54	BA	265	A
54	BA	266	G
54	BA	278	A
54	BA	279	A
54	BA	280	U
54	BA	294	A
54	BA	301	G
54	BA	321	U
54	BA	330	A
54	BA	331	C
54	BA	332	A
54	BA	333	G
54	BA	335	C
54	BA	338	G
54	BA	346	A
54	BA	347	A
54	BA	370	G
54	BA	386	G
54	BA	389	G
54	BA	411	G
54	BA	412	A

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Mol	Chain	Res	Type
54	BA	428	A
54	BA	429	A
54	BA	443	A
54	BA	455	C
54	BA	457	A
54	BA	467	G
54	BA	477	A
54	BA	478	A
54	BA	479	A
54	BA	481	G
54	BA	504	A
54	BA	505	A
54	BA	508	A
54	BA	512	G
54	BA	527	C
54	BA	529	A
54	BA	531	C
54	BA	532	A
54	BA	533	G
54	BA	546	U
54	BA	548	G
54	BA	549	G
54	BA	550	C
54	BA	555	G
54	BA	556	A
54	BA	569	U
54	BA	570	G
54	BA	573	U
54	BA	575	A
54	BA	587	C
54	BA	589	U
54	BA	603	A
54	BA	613	A
54	BA	614	A
54	BA	615	U
54	BA	617	G
54	BA	620	G
54	BA	631	A
54	BA	632	A
54	BA	634	C
54	BA	637	A
54	BA	653	U

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Mol	Chain	Res	Type
54	BA	662	G
54	BA	671	C
54	BA	672	C
54	BA	675	A
54	BA	680	C
54	BA	686	U
54	BA	687	C
54	BA	695	G
54	BA	719	C
54	BA	724	U
54	BA	725	G
54	BA	728	G
54	BA	730	A
54	BA	736	C
54	BA	747	U
54	BA	762	U
54	BA	763	G
54	BA	764	A
54	BA	775	G
54	BA	776	G
54	BA	782	A
54	BA	784	G
54	BA	789	A
54	BA	790	U
54	BA	792	A
54	BA	793	A
54	BA	794	A
54	BA	805	G
54	BA	809	G
54	BA	814	C
54	BA	815	C
54	BA	827	U
54	BA	846	U
54	BA	855	G
54	BA	857	G
54	BA	858	G
54	BA	888	C
54	BA	889	C
54	BA	890	C
54	BA	896	A
54	BA	910	A
54	BA	914	G

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Mol	Chain	Res	Type
54	BA	915	C
54	BA	924	G
54	BA	932	U
54	BA	934	U
54	BA	941	A
54	BA	946	C
54	BA	957	C
54	BA	958	U
54	BA	959	A
54	BA	961	C
54	BA	974	G
54	BA	975	A
54	BA	982	C
54	BA	983	A
54	BA	995	C
54	BA	1008	A
54	BA	1011	G
54	BA	1012	U
54	BA	1013	C
54	BA	1014	A
54	BA	1022	G
54	BA	1025	G
54	BA	1026	G
54	BA	1033	U
54	BA	1044	C
54	BA	1056	G
54	BA	1058	U
54	BA	1063	G
54	BA	1070	A
54	BA	1071	G
54	BA	1073	A
54	BA	1088	A
54	BA	1089	A
54	BA	1090	A
54	BA	1095	A
54	BA	1096	A
54	BA	1100	C
54	BA	1112	G
54	BA	1128	G
54	BA	1129	A
54	BA	1130	U
54	BA	1133	A

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Mol	Chain	Res	Type
54	BA	1134	A
54	BA	1135	C
54	BA	1136	G
54	BA	1142	A
54	BA	1143	A
54	BA	1155	A
54	BA	1175	A
54	BA	1176	U
54	BA	1189	A
54	BA	1204	A
54	BA	1211	C
54	BA	1220	G
54	BA	1237	A
54	BA	1238	G
54	BA	1254	A
54	BA	1255	U
54	BA	1256	G
54	BA	1265	A
54	BA	1271	G
54	BA	1272	A
54	BA	1276	A
54	BA	1287	A
54	BA	1291	C
54	BA	1292	G
54	BA	1300	G
54	BA	1301	A
54	BA	1307	A
54	BA	1308	A
54	BA	1313	U
54	BA	1314	C
54	BA	1315	C
54	BA	1317	G
54	BA	1318	U
54	BA	1325	U
54	BA	1336	A
54	BA	1341	G
54	BA	1345	C
54	BA	1349	C
54	BA	1350	C
54	BA	1379	U
54	BA	1380	G
54	BA	1388	G

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Mol	Chain	Res	Type
54	BA	1397	U
54	BA	1416	G
54	BA	1417	C
54	BA	1420	A
54	BA	1429	G
54	BA	1458	U
54	BA	1459	G
54	BA	1460	U
54	BA	1482	G
54	BA	1490	A
54	BA	1493	C
54	BA	1508	A
54	BA	1509	A
54	BA	1510	G
54	BA	1523	U
54	BA	1524	G
54	BA	1537	G
54	BA	1539	U
54	BA	1540	G
54	BA	1566	A
54	BA	1568	G
54	BA	1569	A
54	BA	1584	U
54	BA	1598	A
54	BA	1610	A
54	BA	1615	C
54	BA	1616	A
54	BA	1622	G
54	BA	1625	C
54	BA	1627	G
54	BA	1634	A
54	BA	1635	A
54	BA	1645	G
54	BA	1646	C
54	BA	1647	U
54	BA	1648	U
54	BA	1668	A
54	BA	1669	A
54	BA	1674	G
54	BA	1703	G
54	BA	1713	A
54	BA	1715	G

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Mol	Chain	Res	Type
54	BA	1729	U
54	BA	1761	C
54	BA	1764	C
54	BA	1773	A
54	BA	1783	A
54	BA	1791	A
54	BA	1799	G
54	BA	1800	C
54	BA	1802	A
54	BA	1808	A
54	BA	1815	A
54	BA	1816	C
54	BA	1847	A
54	BA	1848	A
54	BA	1870	C
54	BA	1871	A
54	BA	1888	G
54	BA	1900	A
54	BA	1901	A
54	BA	1906	G
54	BA	1913	A
54	BA	1914	C
54	BA	1919	A
54	BA	1920	C
54	BA	1928	A
54	BA	1930	G
54	BA	1937	A
54	BA	1940	U
54	BA	1942	C
54	BA	1953	A
54	BA	1954	G
54	BA	1955	U
54	BA	1956	U
54	BA	1962	C
54	BA	1963	U
54	BA	1965	C
54	BA	1966	A
54	BA	1971	U
54	BA	1972	G
54	BA	1980	G
54	BA	1981	A
54	BA	1993	U

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Mol	Chain	Res	Type
54	BA	1997	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	2044	C
54	BA	2051	A
54	BA	2052	A
54	BA	2056	G
54	BA	2060	A
54	BA	2061	G
54	BA	2062	A
54	BA	2076	U
54	BA	2077	A
54	BA	2078	C
54	BA	2092	U
54	BA	2110	G
54	BA	2112	G
54	BA	2113	U
54	BA	2116	G
54	BA	2117	A
54	BA	2118	U
54	BA	2119	A
54	BA	2126	A
54	BA	2127	G
54	BA	2155	U
54	BA	2158	A
54	BA	2159	G
54	BA	2160	C
54	BA	2172	U
54	BA	2173	A
54	BA	2177	C
54	BA	2181	U
54	BA	2198	A
54	BA	2199	A
54	BA	2203	U
54	BA	2208	C
54	BA	2211	A
54	BA	2212	A
54	BA	2238	G

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Mol	Chain	Res	Type
54	BA	2239	G
54	BA	2269	G
54	BA	2274	A
54	BA	2276	G
54	BA	2283	C
54	BA	2286	G
54	BA	2287	A
54	BA	2306	C
54	BA	2307	G
54	BA	2308	G
54	BA	2309	A
54	BA	2312	U
54	BA	2313	C
54	BA	2320	U
54	BA	2321	U
54	BA	2325	G
54	BA	2334	U
54	BA	2335	A
54	BA	2339	C
54	BA	2345	G
54	BA	2347	C
54	BA	2383	G
54	BA	2385	C
54	BA	2390	U
54	BA	2391	G
54	BA	2392	A
54	BA	2394	C
54	BA	2401	U
54	BA	2402	U
54	BA	2403	C
54	BA	2406	A
54	BA	2425	A
54	BA	2426	A
54	BA	2427	C
54	BA	2428	G
54	BA	2429	G
54	BA	2430	A
54	BA	2431	U
54	BA	2432	A
54	BA	2433	A
54	BA	2439	A
54	BA	2440	C

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Mol	Chain	Res	Type
54	BA	2441	U
54	BA	2445	G
54	BA	2448	A
54	BA	2470	G
54	BA	2474	U
54	BA	2475	C
54	BA	2486	C
54	BA	2491	U
54	BA	2498	C
54	BA	2499	C
54	BA	2501	C
54	BA	2502	G
54	BA	2503	A
54	BA	2504	U
54	BA	2505	G
54	BA	2518	A
54	BA	2532	G
54	BA	2533	U
54	BA	2540	C
54	BA	2543	G
54	BA	2544	G
54	BA	2554	U
54	BA	2565	A
54	BA	2566	A
54	BA	2573	C
54	BA	2602	A
54	BA	2613	U
54	BA	2614	A
54	BA	2629	U
54	BA	2654	A
54	BA	2655	G
54	BA	2660	A
54	BA	2661	G
54	BA	2666	C
54	BA	2668	G
54	BA	2669	G
54	BA	2689	U
54	BA	2690	U
54	BA	2714	G
54	BA	2732	G
54	BA	2733	A
54	BA	2739	U

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Mol	Chain	Res	Type
54	BA	2751	G
54	BA	2752	C
54	BA	2757	A
54	BA	2764	A
54	BA	2778	A
54	BA	2780	G
54	BA	2791	G
54	BA	2797	U
54	BA	2799	A
54	BA	2816	G
54	BA	2817	U
54	BA	2821	A
54	BA	2850	A
54	BA	2858	C
54	BA	2867	G
54	BA	2884	U
54	BA	2886	A
54	BA	2892	G
54	BA	2893	A
55	BB	13	G
55	BB	14	U
55	BB	15	A
55	BB	35	C
55	BB	42	C
55	BB	44	G
55	BB	45	A
55	BB	48	U
55	BB	74	U
55	BB	88	C
55	BB	89	U
55	BB	109	A

All (239) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	13	U
21	AA	32	A
21	AA	49	U
21	AA	69	G
21	AA	110	C

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Mol	Chain	Res	Type
21	AA	120	A
21	AA	128	G
21	AA	173	U
21	AA	212	G
21	AA	243	A
21	AA	251	G
21	AA	306	A
21	AA	307	C
21	AA	327	A
21	AA	328	C
21	AA	346	G
21	AA	350	G
21	AA	351	G
21	AA	357	G
21	AA	372	C
21	AA	388	G
21	AA	408	A
21	AA	412	A
21	AA	421	U
21	AA	422	C
21	AA	461	A
21	AA	476	U
21	AA	480	U
21	AA	482	A
21	AA	494	G
21	AA	509	A
21	AA	530	G
21	AA	532	A
21	AA	573	A
21	AA	575	G
21	AA	577	G
21	AA	624	C
21	AA	632	U
21	AA	703	G
21	AA	717	U
21	AA	719	C
21	AA	722	G
21	AA	731	G
21	AA	761	G
21	AA	777	A
21	AA	787	A
21	AA	827	U

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Mol	Chain	Res	Type
21	AA	869	G
21	AA	886	G
21	AA	888	G
21	AA	890	G
21	AA	913	A
21	AA	945	G
21	AA	962	C
21	AA	965	U
21	AA	977	A
21	AA	978	A
21	AA	982	U
21	AA	983	A
21	AA	992	U
21	AA	998	C
21	AA	1030	U
21	AA	1042	A
21	AA	1050	G
21	AA	1054	C
21	AA	1065	U
21	AA	1066	C
21	AA	1086	U
21	AA	1101	A
21	AA	1129	C
21	AA	1139	G
21	AA	1146	A
21	AA	1159	U
21	AA	1171	A
21	AA	1182	G
21	AA	1184	G
21	AA	1190	G
21	AA	1191	A
21	AA	1225	A
21	AA	1278	G
21	AA	1279	G
21	AA	1298	U
21	AA	1299	A
21	AA	1336	C
21	AA	1380	U
21	AA	1396	A
21	AA	1452	C
21	AA	1492	A
22	A1	16	C

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Mol	Chain	Res	Type
22	A1	47	U
23	A2	85	G
23	A2	89	U
24	A3	9	G
24	A3	31	G
24	A3	34	U
24	A3	73	A
24	A3	76	C
54	BA	34	U
54	BA	71	A
54	BA	101	A
54	BA	142	A
54	BA	199	A
54	BA	215	G
54	BA	223	A
54	BA	278	A
54	BA	279	A
54	BA	322	A
54	BA	330	A
54	BA	388	G
54	BA	428	A
54	BA	446	G
54	BA	529	A
54	BA	531	C
54	BA	549	G
54	BA	555	G
54	BA	613	A
54	BA	631	A
54	BA	645	C
54	BA	661	A
54	BA	670	A
54	BA	685	A
54	BA	724	U
54	BA	752	A
54	BA	762	U
54	BA	776	G
54	BA	793	A
54	BA	805	G
54	BA	808	G
54	BA	888	C
54	BA	896	A
54	BA	914	G

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Mol	Chain	Res	Type
54	BA	931	U
54	BA	933	A
54	BA	957	C
54	BA	981	A
54	BA	984	A
54	BA	992	C
54	BA	1013	C
54	BA	1022	G
54	BA	1056	G
54	BA	1069	A
54	BA	1071	G
54	BA	1078	U
54	BA	1087	G
54	BA	1089	A
54	BA	1128	G
54	BA	1132	U
54	BA	1185	G
54	BA	1210	G
54	BA	1252	G
54	BA	1254	A
54	BA	1255	U
54	BA	1287	A
54	BA	1289	C
54	BA	1290	C
54	BA	1291	C
54	BA	1300	G
54	BA	1307	A
54	BA	1312	U
54	BA	1314	C
54	BA	1317	G
54	BA	1324	G
54	BA	1340	U
54	BA	1349	C
54	BA	1385	A
54	BA	1419	A
54	BA	1451	C
54	BA	1508	A
54	BA	1509	A
54	BA	1523	U
54	BA	1535	A
54	BA	1539	U
54	BA	1568	G

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Mol	Chain	Res	Type
54	BA	1610	A
54	BA	1615	C
54	BA	1634	A
54	BA	1668	A
54	BA	1760	C
54	BA	1779	U
54	BA	1783	A
54	BA	1799	G
54	BA	1863	G
54	BA	1918	A
54	BA	1919	A
54	BA	1927	A
54	BA	1929	G
54	BA	1936	A
54	BA	1945	G
54	BA	1952	A
54	BA	1954	G
54	BA	1955	U
54	BA	1962	C
54	BA	1980	G
54	BA	2022	U
54	BA	2032	G
54	BA	2035	G
54	BA	2043	C
54	BA	2062	A
54	BA	2076	U
54	BA	2077	A
54	BA	2116	G
54	BA	2117	A
54	BA	2126	A
54	BA	2162	G
54	BA	2198	A
54	BA	2212	A
54	BA	2286	G
54	BA	2288	A
54	BA	2306	C
54	BA	2308	G
54	BA	2351	G
54	BA	2389	G
54	BA	2391	G
54	BA	2401	U
54	BA	2425	A

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Mol	Chain	Res	Type
54	BA	2427	C
54	BA	2430	A
54	BA	2431	U
54	BA	2439	A
54	BA	2442	C
54	BA	2474	U
54	BA	2485	G
54	BA	2503	A
54	BA	2504	U
54	BA	2542	A
54	BA	2543	G
54	BA	2613	U
54	BA	2644	G
54	BA	2666	C
54	BA	2689	U
54	BA	2732	G
54	BA	2751	G
54	BA	2756	U
54	BA	2892	G
55	BB	14	U
55	BB	15	A
55	BB	73	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CM0	A1	34	22,23	15,26,27	1.94	3 (20%)	18,37,40	3.08	3 (16%)
22	6MZ	A1	37	22	17,25,26	0.85	0	15,36,39	1.58	1 (6%)
22	7MG	A1	46	22	20,26,27	2.21	3 (15%)	23,39,42	2.17	2 (8%)
22	5MU	A1	54	22	13,22,23	1.26	2 (15%)	16,32,35	4.43	2 (12%)
22	PSU	A1	55	22	15,21,22	1.07	1 (6%)	16,30,33	3.31	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	4SU	A1	7	22	12,21,22	0.95	0	15,30,33	2.18	2 (13%)
24	H2U	A3	21	24	17,21,22	1.39	2 (11%)	23,30,33	1.46	4 (17%)
24	OMC	A3	33	24	15,22,23	1.09	0	20,31,34	0.89	0
24	5MU	A3	55	24	13,22,23	1.06	1 (7%)	16,32,35	4.69	2 (12%)
24	PSU	A3	56	24	15,21,22	1.15	1 (6%)	16,30,33	3.50	5 (31%)
24	4SU	A3	8	24	12,21,22	1.16	1 (8%)	15,30,33	2.23	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CM0	A1	34	22,23	-	0/6/30/31	0/2/2/2
22	6MZ	A1	37	22	-	0/5/27/28	0/3/3/3
22	7MG	A1	46	22	-	0/7/37/38	0/3/3/3
22	5MU	A1	54	22	-	0/3/25/26	0/2/2/2
22	PSU	A1	55	22	-	0/7/25/26	0/2/2/2
22	4SU	A1	7	22	-	0/3/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
24	OMC	A3	33	24	-	0/5/27/28	0/2/2/2
24	5MU	A3	55	24	-	0/3/25/26	0/2/2/2
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/3/25/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	46	7MG	C8-N9	-8.24	1.33	1.45
22	A1	34	CM0	O5-C5	-5.97	1.25	1.37
24	A3	21	H2U	C4-N3	-3.70	1.31	1.37
24	A3	21	H2U	C2-N3	-3.18	1.32	1.38
22	A1	46	7MG	C8-N7	-2.72	1.31	1.43
22	A1	54	5MU	O4'-C1'	2.02	1.44	1.41
24	A3	56	PSU	C4-N3	2.14	1.36	1.33
24	A3	8	4SU	C6-N1	2.31	1.38	1.35
22	A1	55	PSU	C4-N3	2.39	1.37	1.33
24	A3	55	5MU	C4-N3	2.53	1.37	1.33
22	A1	34	CM0	C4-N3	2.69	1.37	1.33
22	A1	34	CM0	C4-C5	2.78	1.47	1.40
22	A1	46	7MG	C6-N1	2.89	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A1	54	5MU	C4-N3	2.93	1.38	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	55	5MU	C5-C4-N3	-12.71	114.68	125.35
22	A1	54	5MU	C5-C4-N3	-12.19	115.12	125.35
24	A3	8	4SU	C5-C4-N3	-7.82	115.27	123.56
22	A1	7	4SU	C5-C4-N3	-7.55	115.56	123.56
22	A1	46	7MG	C5-C6-N1	-6.68	113.44	123.39
22	A1	55	PSU	C5-C1'-C2'	-3.19	110.01	115.44
24	A3	56	PSU	C5-C1'-C2'	-3.10	110.17	115.44
24	A3	56	PSU	C5-C6-N1	-3.09	120.08	124.38
22	A1	55	PSU	C5-C6-N1	-2.81	120.47	124.38
24	A3	21	H2U	O2-C2-N3	-2.21	117.11	121.44
24	A3	56	PSU	C4'-O4'-C1'	-2.04	107.44	109.54
22	A1	7	4SU	O4'-C4'-C3'	2.20	109.61	105.16
24	A3	21	H2U	C5-C6-N1	2.21	113.19	110.76
22	A1	34	CM0	O5-C7-C8	2.33	112.83	108.01
24	A3	21	H2U	C5-C4-N3	2.41	119.17	116.62
22	A1	55	PSU	O4'-C1'-C2'	3.24	108.20	104.69
24	A3	56	PSU	O4'-C1'-C2'	3.55	108.53	104.69
22	A1	34	CM0	O5-C5-C4	3.59	120.06	115.20
24	A3	21	H2U	N3-C2-N1	4.33	120.65	116.64
22	A1	37	6MZ	C2-N1-C6	5.06	120.11	116.47
22	A1	46	7MG	C6-N1-C2	6.68	123.71	115.88
22	A1	55	PSU	C4-N3-C2	11.66	124.89	115.16
22	A1	34	CM0	C4-N3-C2	11.88	125.07	115.16
22	A1	54	5MU	C4-N3-C2	12.23	125.36	115.16
24	A3	56	PSU	C4-N3-C2	12.43	125.53	115.16
24	A3	55	5MU	C4-N3-C2	13.37	126.32	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	VAL	A1	101	58,22	5,6,7	0.55	0	5,7,9	1.37	2 (40%)
58	FME	BA	3001	57	8,9,10	0.78	0	5,9,11	1.33	1 (20%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	FME	O-C-CA	-2.79	118.07	125.69
57	A1	101	VAL	O-C-CA	-2.17	119.76	125.69
57	A1	101	VAL	C-CA-N	2.05	114.48	109.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.