



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 02:22 pm GMT

PDB ID : 7O19
EMDB ID : EMD-12693
Title : Cryo-EM structure of an Escherichia coli TnaC-ribosome complex stalled in response to L-tryptophan
Authors : van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.; Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera, L.R.; Innis, C.A.
Deposited on : 2021-03-29
Resolution : 2.90 Å(reported)
Based on initial model : 6TBV

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

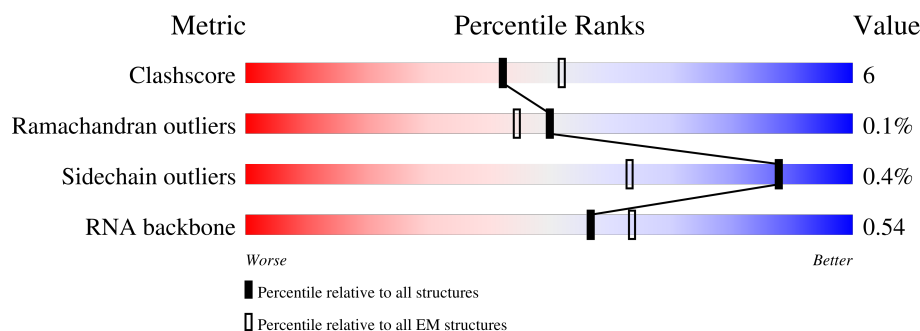
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.











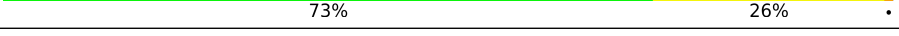

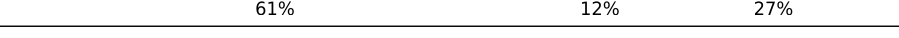
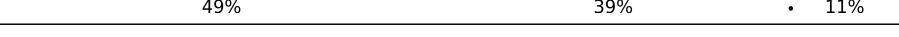
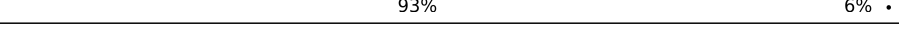
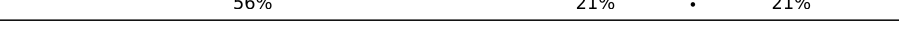


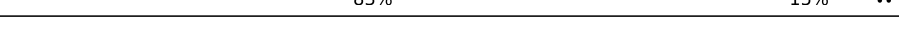

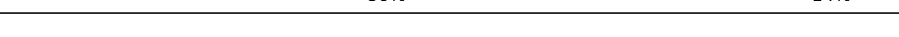






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	AA	1534	<div> <div>47%</div> <div>36%</div> <div>15%</div> <div>.</div> </div>
2	AB	241	<div> <div>66%</div> <div>24%</div> <div>7%</div> <div>.</div> </div>
3	AC	233	<div> <div>62%</div> <div>25%</div> <div>12%</div> <div>.</div> </div>
4	AD	206	<div> <div>71%</div> <div>28%</div> </div>
5	AE	167	<div> <div>70%</div> <div>22%</div> <div>7%</div> <div>.</div> </div>
6	AF	135	<div> <div>50%</div> <div>27%</div> <div>21%</div> <div>.</div> </div>
7	AG	179	<div> <div>59%</div> <div>24%</div> <div>16%</div> <div>.</div> </div>













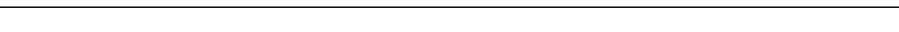



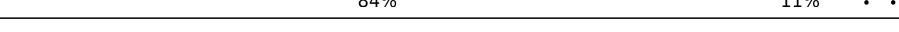






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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2897	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	
28	BG	177	
29	BH	149	
30	BI	70	
31	BJ	142	
32	BK	123	

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Mol	Chain	Length	Quality of chain
33	BL	144	 81% 18% .
34	BM	136	 85% 14% .
35	BN	127	 83% 10% 7%
36	BO	117	 84% 15% .
37	BP	115	 86% 11% ..
38	BQ	118	 89% 10% .
39	BR	103	 83% 17%
40	BS	110	 83% 16% .
41	BT	100	 78% 15% 7%
42	BU	104	 76% 22% .
43	BV	94	 72% 27% .
44	BW	85	 78% 12% 11%
45	BX	78	 90% 9% .
46	BY	63	 86% 13% .
47	BZ	59	 83% 15% .
48	B0	57	 84% 11% . .
49	B1	55	 64% 27% . 7%
50	B2	46	 85% 15%
51	B3	65	 78% 15% . . .
52	B4	38	 87% 13%
53	B5	17	 82% 12% 6%
54	B7	7	 71% 29%
55	B8	77	 55% 29% 14% .

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 145019 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 RNA chain called Ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	82	Total	C	N	O	S	0	0
			656	419	125	110	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called Ribosomal RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

- Molecule 23 is a RNA chain called Ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BI	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BK	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BL	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BN	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BU	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BW	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BY	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	51	Total	C	N	O		0	0
			414	266	76	72			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called Tryptophanase leader peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B5	17	Total	C	N	O	0	0
			146	94	27	25		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B7	7	Total	C	N	O	P	0	0
			146	65	24	50	7		

- Molecule 55 is a RNA chain called P-site tRNA-Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B8	77	Total	C	N	O	P	0	0
			1646	733	295	541	77		

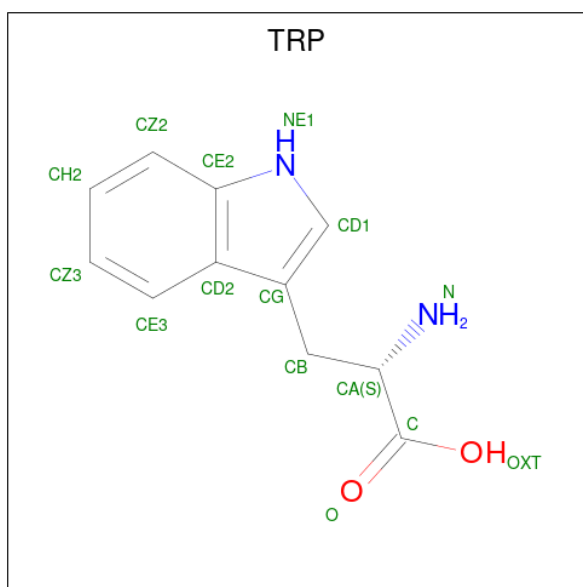
- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	AA	35	Total	Mg	0
			35	35	
56	BA	132	Total	Mg	0
			132	132	
56	BC	1	Total	Mg	0
			1	1	
56	BD	1	Total	Mg	0
			1	1	
56	B8	1	Total	Mg	0
			1	1	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	AB	1	Total	Zn	0
			1	1	
57	BI	1	Total	Zn	0
			1	1	
57	B4	1	Total	Zn	0
			1	1	

- Molecule 58 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				AltConf
58	BA	1	Total	C	N	O	0
			15	11	2	2	

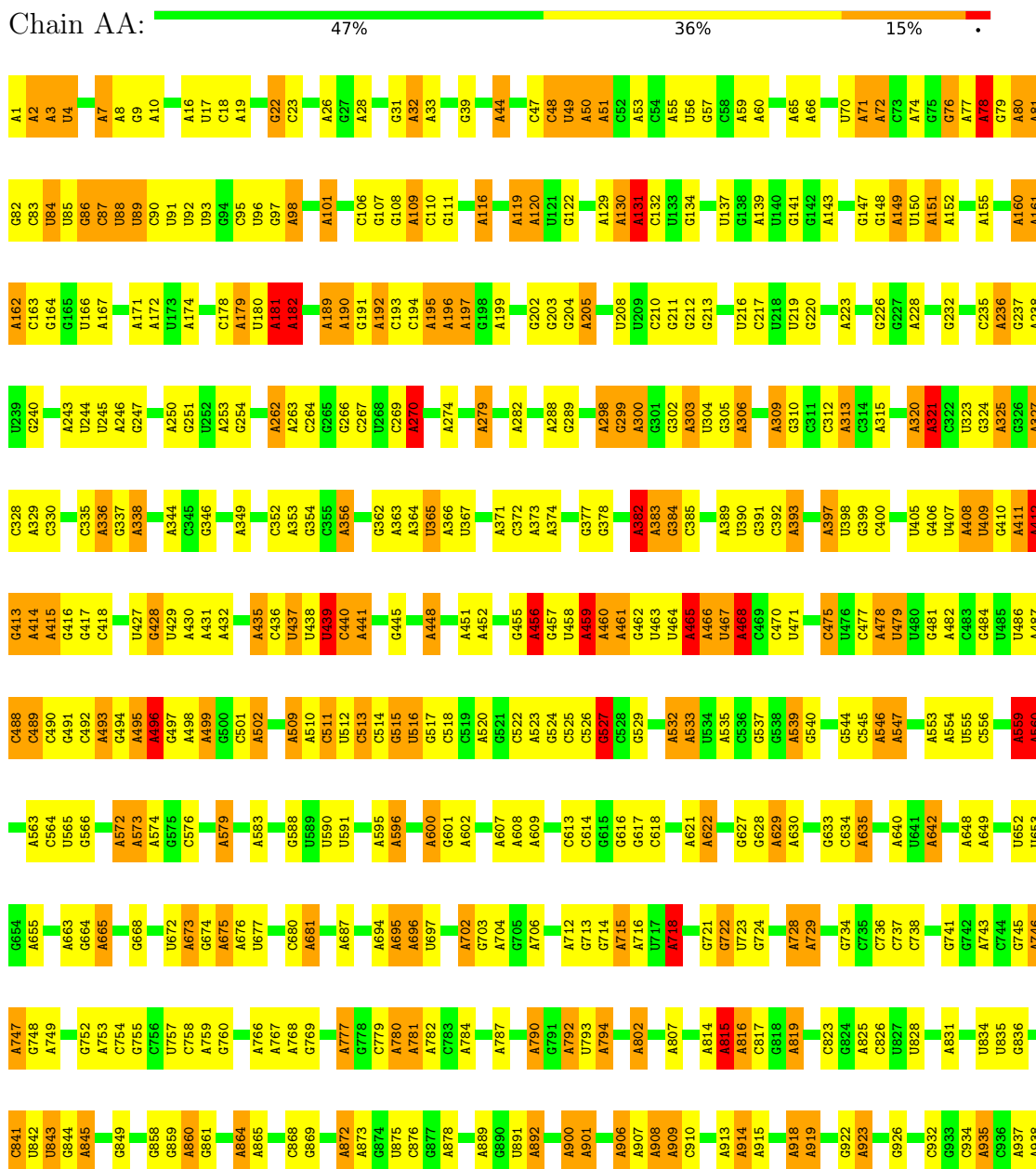
- Molecule 59 is water.

Mol	Chain	Residues	Atoms		AltConf
59	AA	168	Total	O	0
			168	168	
59	AK	1	Total	O	0
			1	1	
59	AM	1	Total	O	0
			1	1	
59	AN	2	Total	O	0
			2	2	
59	BA	608	Total	O	0
			608	608	
59	BC	7	Total	O	0
			7	7	
59	BD	1	Total	O	0
			1	1	
59	BE	1	Total	O	0
			1	1	
59	BL	2	Total	O	0
			2	2	
59	BN	1	Total	O	0
			1	1	
59	B8	1	Total	O	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: Ribosomal RNA 16S





PRO
ALA
ALA
GLN
PRO
PRO
LYS
LYS
GLN
GLN
ARG
LYS
GLY
ARG
LYS

• Molecule 4: 30S ribosomal protein S4

Chain AD:  71% 28%

MET A2 R3 P7 S12 R13 T17 S23 R26 A27 I28 I34 E35 Q36 A37 P38 P46 R56 E57 K58 Q59 K60 V61 R62 Y65 E69 R73 K77 E78 R81 N85 E88 E95 M100 V101 R104 R111 H120 M124

V125 R128 V129 V137 S138 P139 V143 R146 R147 K148 Q152 S153 R154 Q164 P168 R184 K185 P186 R187 R188 L191 D194 I195 N196 E197 H198 L199 I200 V201 E202 K206

• Molecule 5: 30S ribosomal protein S5

Chain AE:  70% 22% 7%

MET ALA HIS ILE GLU LYS GLN ALA GLY E10 E13 K14 L15 T34 T37 K52 P57 K62 A63 M64 E65 K66 N77 Q82 H83 P84 T90 P93 E101 G104 G108 R112 A113 V114 L115 E116 V117 M122 V123 M132 P133 I134 M135 V136

M147 P150 V153 A154 A155 K156 K159 S160 V161 E162 E163 I164 LEU GLY LYS

• Molecule 6: 30S ribosomal protein S6

Chain AF:  50% 27% 21%

M1 R2 H3 Y4 V7 F8 M9 P12 E16 Q17 V18 P19 I22 I26 T26 G34 K35 R38 L39 A40 E40 D41 W42 G43 R44 R45 P50 K56 A57 H58 Y59 Y60 L61 E65 A66 P67 I71 R86 M90 R91 T92 A95 E98 A99 S100 P101 M102

V103 K106 ASP ARG ARG ARG ARG ASP ASP PHE ALA ALA ASN GLU THR ALA ASP ASP ALA ALA ALA ALA GLY SER ASP ASP GLU GLU GLU GLU GLU GLU

• Molecule 7: 30S ribosomal protein S7

Chain AG:  59% 24% 16%

MET P2 R3 R4 P14 D15 P16 F18 K25 F26 I29 S37 E40 Y44 S45 A46 L47 K56 S57 E58 L59 E60 A61 F62 E63 E64 V64 E67 N68 V69 R70 P71 P88 P93 R96 A100 M101 A108 R111 G112 D113 K114 S115 M116 A117 L118

R119 L120 A121 N122 E123 D126 K131 D140 R143 E146 K149 A152 HIS TYR ARG TRP LEU SER LEU ARG SER PHE SER E61 HIS GLN ALA E63 GLY ALA A70 SER SER LYS GLN PRO ALA LEU TYR LEU ASN

• Molecule 8: 30S ribosomal protein S8

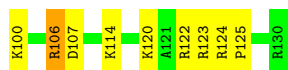
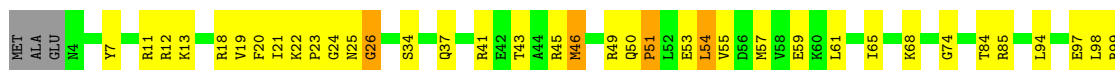
Chain AH:  65% 34% 1%

MET S2 P6 M10 L11 T12 R15 N16 G17 Q18 A24 V25 T26 N27 P28 S29 S30 V34 A35 I36 E52 P57 E58 L59 E60 L63 A70 I75 Q76 R77 V78 S79 R80 P81 I85 Y86 K87 R88 K89 L92 P93 N96 L99 G100 T106



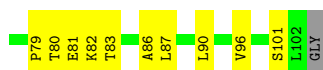
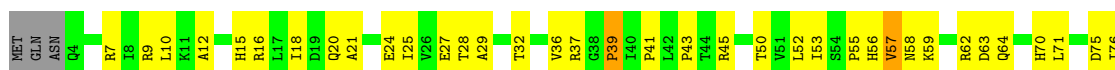
- Molecule 9: 30S ribosomal protein S9

Chain AI: 62% 32%



- Molecule 10: 30S ribosomal protein S10

Chain AJ: 51% 43%



- Molecule 11: 30S ribosomal protein S11

Chain AK: 71% 20% 9%



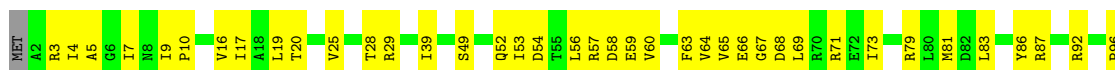
- Molecule 12: 30S ribosomal protein S12

Chain AL: 80% 19%



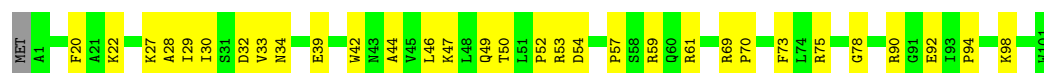
- Molecule 13: 30S ribosomal protein S13

Chain AM: 57% 40%




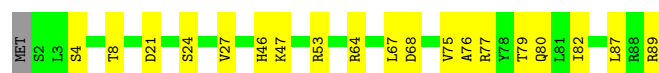
- Molecule 14: 30S ribosomal protein S14

Chain AN:  69% 30%




- Molecule 15: 30S ribosomal protein S15

Chain AO:  78% 21%



- Molecule 16: 30S ribosomal protein S16

Chain AP:  73% 26%



- Molecule 17: 30S ribosomal protein S17

Chain AQ:  70% 24% 5%



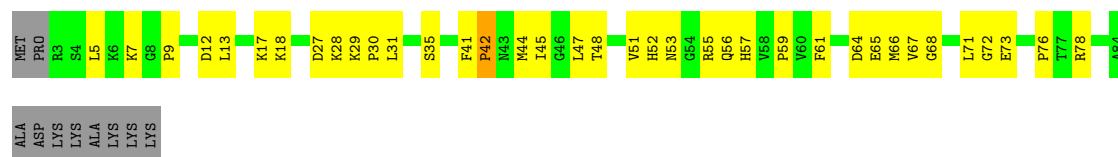
- Molecule 18: 30S ribosomal protein S18

Chain AR:  61% 12% 27%



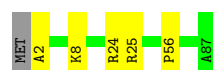
- Molecule 19: 30S ribosomal protein S19

Chain AS:  49% 39% 11%



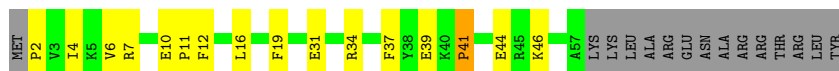
- Molecule 20: 30S ribosomal protein S20

Chain AT:  93% 6%



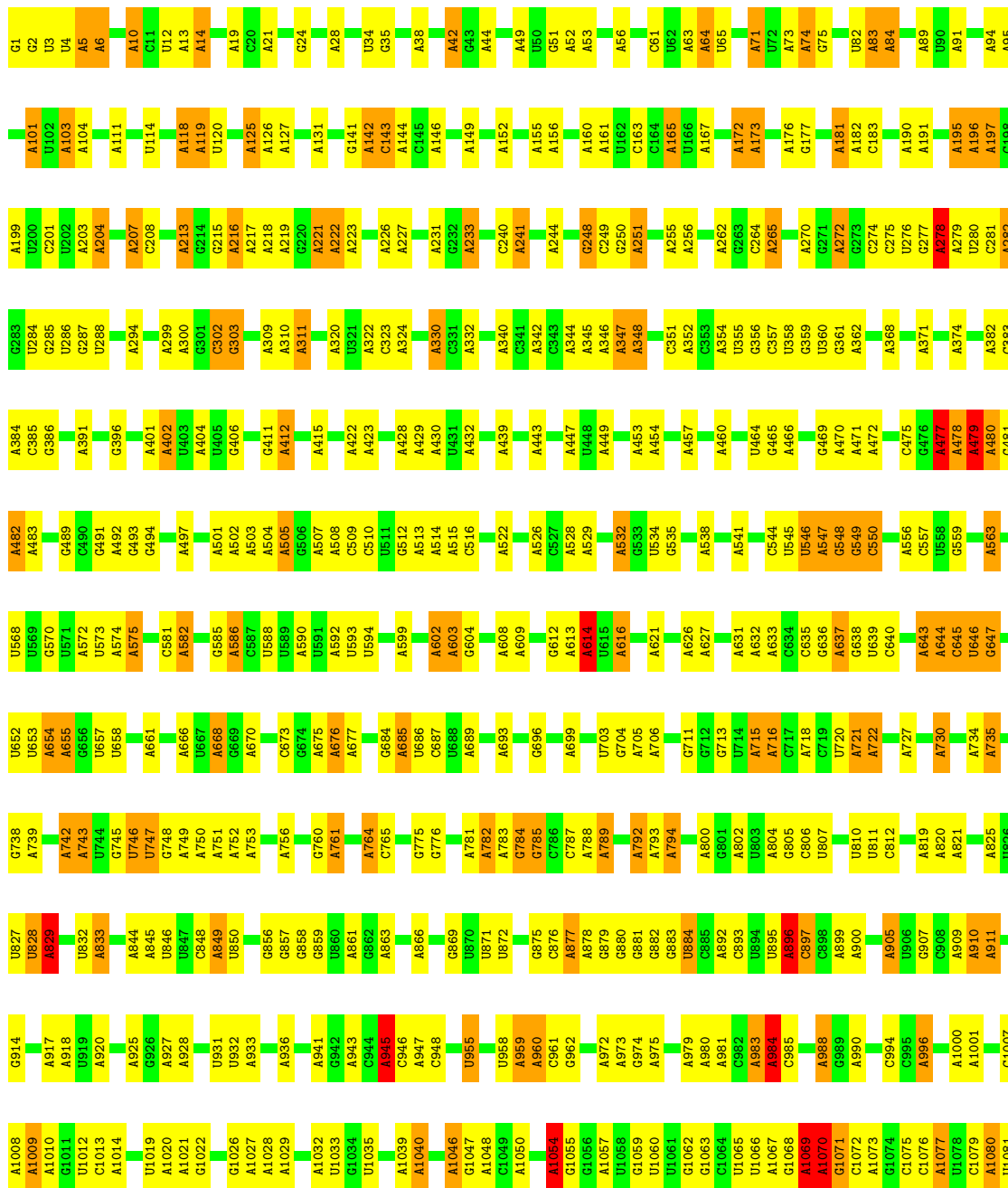
- Molecule 21: 30S ribosomal protein S21

Chain AU:  56% 21% 21%

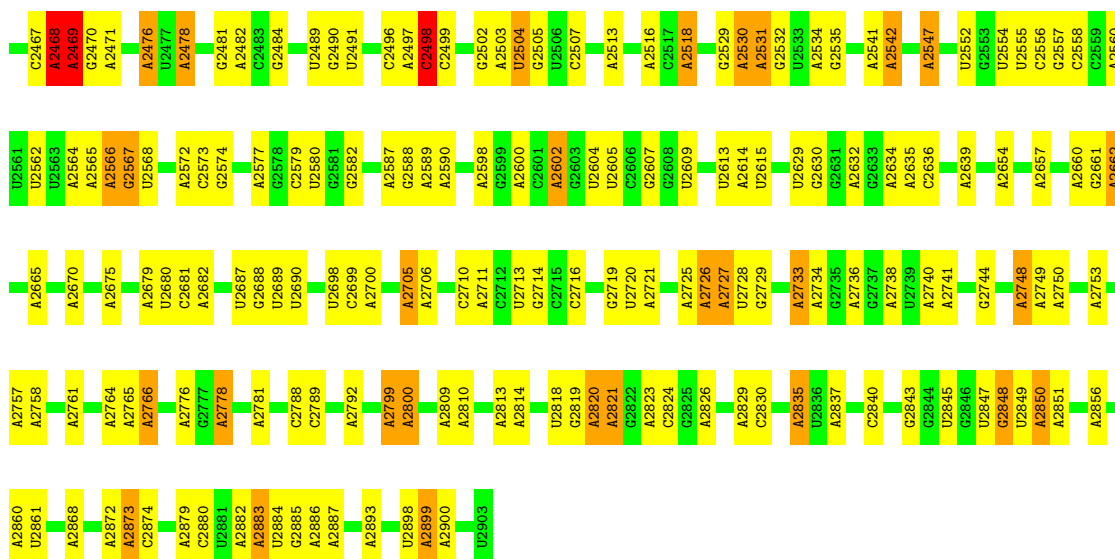


- Molecule 22: Ribosomal RNA 23S

Chain BA:  54% 33% 11%

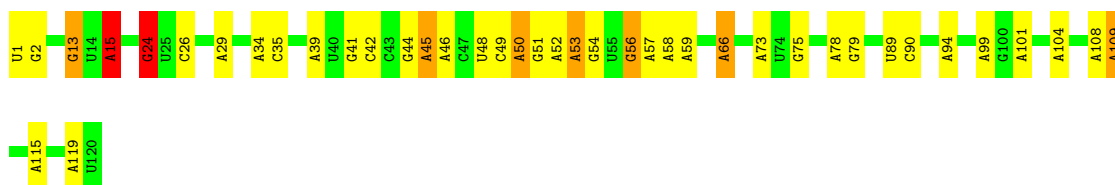






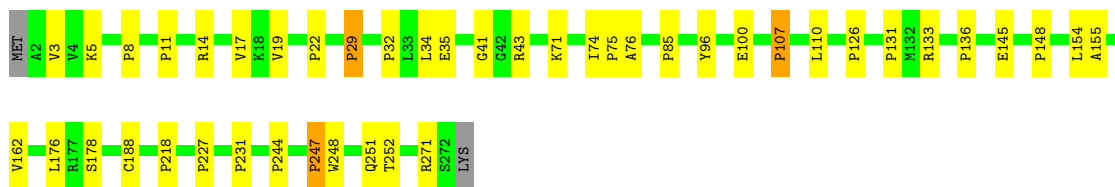
• Molecule 23: Ribosomal RNA 5S

Chain BB: 66% 27% 6% .



• Molecule 24: 50S ribosomal protein L2

Chain BC: 83% 15% ..



• Molecule 25: 50S ribosomal protein L3

Chain BD: 88% 11% .

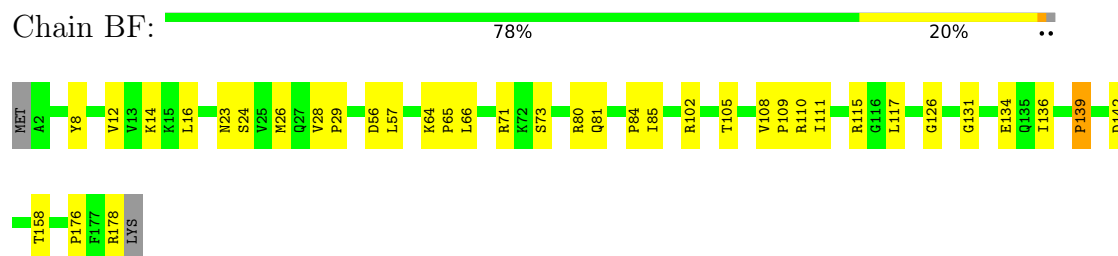


• Molecule 26: 50S ribosomal protein L4

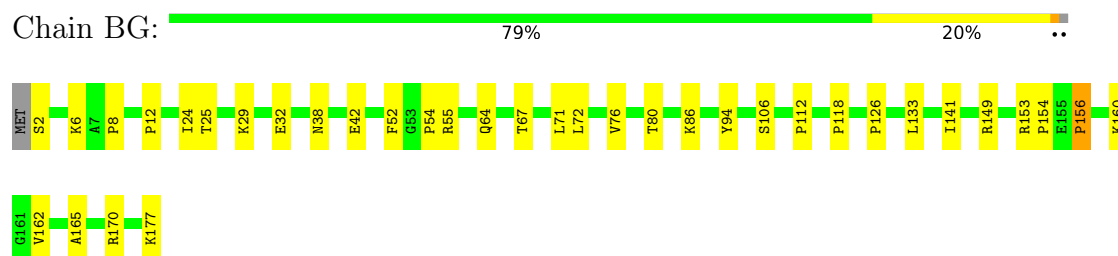
Chain BE: 86% 14%



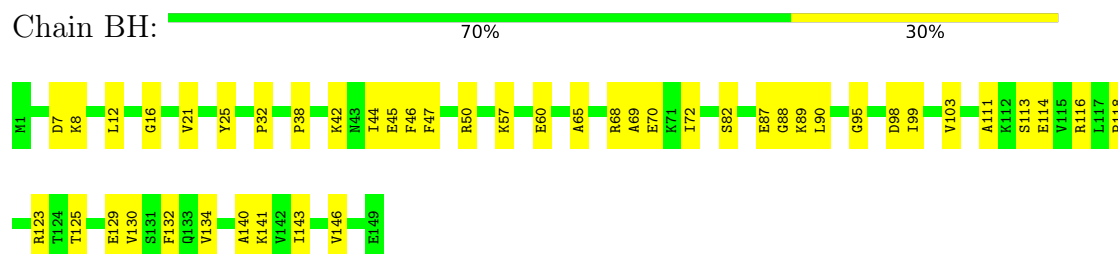
- Molecule 27: 50S ribosomal protein L5



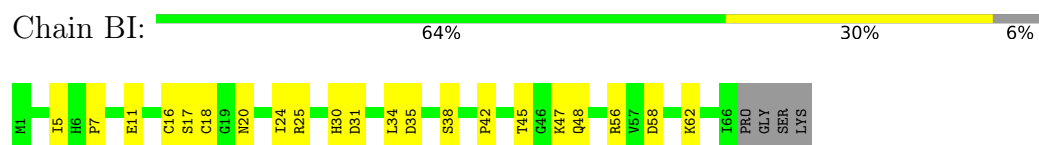
- Molecule 28: 50S ribosomal protein L6



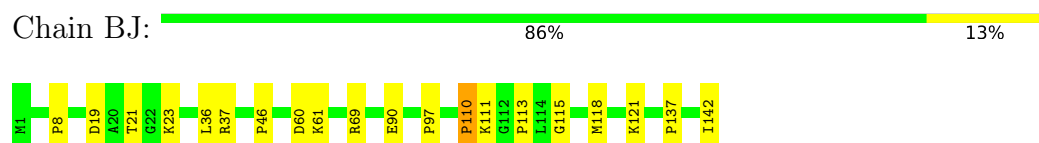
- Molecule 29: 50S ribosomal protein L9



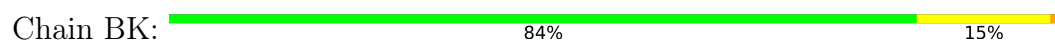
- Molecule 30: 50S ribosomal protein L31



- Molecule 31: 50S ribosomal protein L13

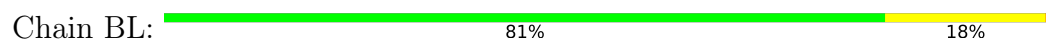


- Molecule 32: 50S ribosomal protein L14





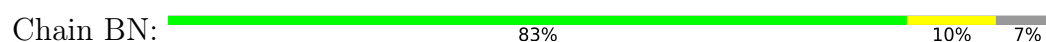
- Molecule 33: 50S ribosomal protein L15



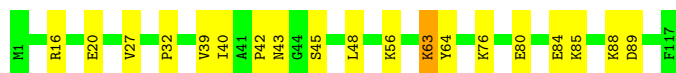
- Molecule 34: 50S ribosomal protein L16



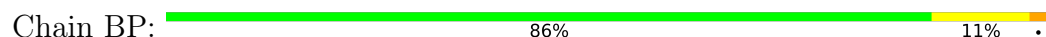
- Molecule 35: 50S ribosomal protein L17



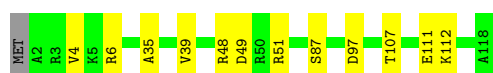
- Molecule 36: 50S ribosomal protein L18



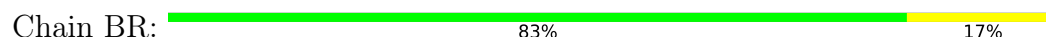
- Molecule 37: 50S ribosomal protein L19



- Molecule 38: 50S ribosomal protein L20



- Molecule 39: 50S ribosomal protein L21





- Molecule 40: 50S ribosomal protein L22

Chain BS: 83% 16%



- Molecule 41: 50S ribosomal protein L23

Chain BT: 78% 15% 7%



- Molecule 42: 50S ribosomal protein L24

Chain BU: 76% 22%



- Molecule 43: 50S ribosomal protein L25

Chain BV: 72% 27%



- Molecule 44: 50S ribosomal protein L27

Chain BW: 78% 12% 11%



- Molecule 45: 50S ribosomal protein L28

Chain BX: 90% 9%



- Molecule 46: 50S ribosomal protein L29

Chain BY: 86% 13%



- Molecule 47: 50S ribosomal protein L30

Chain BZ: 83% 15% .



- Molecule 48: 50S ribosomal protein L32

Chain B0: 84% 11% . .



- Molecule 49: 50S ribosomal protein L33

Chain B1: 64% 27% . 7%



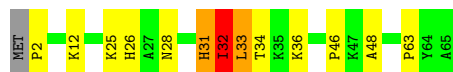
- Molecule 50: 50S ribosomal protein L34

Chain B2: 85% 15%



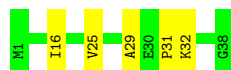
- Molecule 51: 50S ribosomal protein L35

Chain B3: 78% 15% . . .



- Molecule 52: 50S ribosomal protein L36

Chain B4: 87% 13%

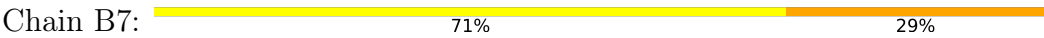


- Molecule 53: Tryptophanase leader peptide

Chain B5: 82% 12% 6%



● Molecule 54: mRNA



● Molecule 55: P-site tRNA-Pro



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	55127	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UR3, OMC, 4D4, PSU, 5MU, 2MG, 3TD, MA6, 2MA, ZN, 6MZ, OMU, 5MC, 1MG, OMG, MEQ, 4OC, G7M, D2T

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	1.49	1045/36593 (2.9%)	3.42	4438/57081 (7.8%)
2	AB	0.81	7/1784 (0.4%)	0.57	1/2403 (0.0%)
3	AC	0.83	7/1651 (0.4%)	0.51	0/2225
4	AD	0.78	6/1665 (0.4%)	0.47	0/2227
5	AE	0.87	5/1157 (0.4%)	0.57	0/1557
6	AF	1.05	7/881 (0.8%)	0.59	0/1189
7	AG	0.93	7/1195 (0.6%)	0.51	0/1602
8	AH	0.90	5/989 (0.5%)	0.55	0/1326
9	AI	0.73	3/1034 (0.3%)	0.66	3/1375 (0.2%)
10	AJ	1.03	6/805 (0.7%)	0.56	0/1089
11	AK	1.09	7/893 (0.8%)	0.57	0/1205
12	AL	1.12	8/960 (0.8%)	0.59	1/1286 (0.1%)
13	AM	0.93	5/892 (0.6%)	0.61	0/1193
14	AN	0.88	4/811 (0.5%)	0.53	0/1081
15	AO	0.36	0/722	0.47	0/964
16	AP	0.76	2/659 (0.3%)	0.54	0/884
17	AQ	0.76	2/657 (0.3%)	0.57	0/881
18	AR	0.87	2/462 (0.4%)	0.54	0/621
19	AS	1.08	5/672 (0.7%)	0.59	0/904
20	AT	0.54	1/676 (0.1%)	0.43	0/895
21	AU	1.08	4/472 (0.8%)	0.56	1/627 (0.2%)
22	BA	1.84	1753/69120 (2.5%)	3.52	8456/107824 (7.8%)
23	BB	1.53	58/2872 (2.0%)	3.02	271/4478 (6.1%)
24	BC	1.20	19/2121 (0.9%)	0.66	0/2852
25	BD	0.95	7/1576 (0.4%)	0.59	0/2119
26	BE	0.85	5/1571 (0.3%)	0.57	0/2113
27	BF	0.85	6/1434 (0.4%)	0.52	0/1926
28	BG	1.00	8/1343 (0.6%)	0.58	0/1816
29	BH	0.70	3/1121 (0.3%)	0.56	0/1515
30	BI	0.80	2/531 (0.4%)	0.60	0/709
31	BJ	1.03	6/1152 (0.5%)	0.56	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BK	1.00	5/955 (0.5%)	0.67	1/1279 (0.1%)
33	BL	0.90	4/1062 (0.4%)	0.64	1/1413 (0.1%)
34	BM	1.09	7/1081 (0.6%)	0.59	0/1443
35	BN	0.98	4/958 (0.4%)	0.59	0/1281
36	BO	0.74	2/910 (0.2%)	0.54	0/1219
37	BP	0.90	3/929 (0.3%)	0.64	2/1242 (0.2%)
38	BQ	0.72	0/960	0.49	0/1278
39	BR	0.81	2/829 (0.2%)	0.56	0/1107
40	BS	0.76	2/864 (0.2%)	0.53	0/1156
41	BT	0.67	1/744 (0.1%)	0.56	0/994
42	BU	0.89	3/787 (0.4%)	0.58	0/1051
43	BV	1.01	4/766 (0.5%)	0.58	0/1025
44	BW	0.80	1/587 (0.2%)	0.57	0/776
45	BX	0.87	2/635 (0.3%)	0.59	0/848
46	BY	0.43	0/502	0.46	0/667
47	BZ	0.91	2/453 (0.4%)	0.57	0/605
48	B0	0.82	1/450 (0.2%)	0.64	1/599 (0.2%)
49	B1	1.19	5/421 (1.2%)	0.76	2/561 (0.4%)
50	B2	0.85	1/380 (0.3%)	0.60	0/498
51	B3	1.12	4/513 (0.8%)	0.74	1/676 (0.1%)
52	B4	0.88	1/303 (0.3%)	0.54	0/397
53	B5	1.51	2/150 (1.3%)	0.71	0/203
54	B7	0.31	0/161	1.06	0/248
55	B8	1.94	66/1839 (3.6%)	2.95	152/2866 (5.3%)
All	All	1.54	3127/155710 (2.0%)	3.00	13331/232950 (5.7%)

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
10	AJ	0	1
27	BF	0	1
51	B3	0	1
All	All	0	3

All (3127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	C2'-C1'	-21.93	1.29	1.53
22	BA	2449	U	C5-C6	20.02	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	B8	14	A	C6-N6	17.45	1.48	1.33
55	B8	59	A	C6-N6	17.43	1.47	1.33
55	B8	76	A	C6-N6	17.33	1.47	1.33
55	B8	58	A	C6-N6	17.28	1.47	1.33
55	B8	66	A	C6-N6	17.23	1.47	1.33
55	B8	73	A	C6-N6	17.19	1.47	1.33
55	B8	6	A	C6-N6	17.17	1.47	1.33
55	B8	38	A	C6-N6	17.14	1.47	1.33
55	B8	26	A	C6-N6	17.13	1.47	1.33
55	B8	51	A	C6-N6	17.03	1.47	1.33
55	B8	42	A	C6-N6	17.01	1.47	1.33
55	B8	21	A	C6-N6	16.96	1.47	1.33
55	B8	69	A	C6-N6	16.94	1.47	1.33
55	B8	41	A	C6-N6	16.81	1.47	1.33
22	BA	892	A	O4'-C1'	16.31	1.62	1.41
53	B5	24	PRO	N-CD	13.55	1.66	1.47
2	AB	48	PRO	N-CD	11.63	1.64	1.47
5	AE	57	PRO	N-CD	11.62	1.64	1.47
13	AM	115	PRO	N-CD	11.60	1.64	1.47
2	AB	193	PRO	N-CD	11.44	1.63	1.47
2	AB	29	PRO	N-CD	11.38	1.63	1.47
10	AJ	39	PRO	N-CD	11.31	1.63	1.47
12	AL	45	PRO	N-CD	11.26	1.63	1.47
9	AI	51	PRO	N-CD	11.25	1.63	1.47
21	AU	2	PRO	N-CD	11.25	1.63	1.47
7	AG	2	PRO	N-CD	11.19	1.63	1.47
28	BG	8	PRO	N-CD	11.19	1.63	1.47
4	AD	46	PRO	N-CD	11.17	1.63	1.47
10	AJ	79	PRO	N-CD	11.14	1.63	1.47
14	AN	52	PRO	N-CD	11.13	1.63	1.47
5	AE	150	PRO	N-CD	11.11	1.63	1.47
3	AC	73	PRO	N-CD	11.10	1.63	1.47
13	AM	10	PRO	N-CD	11.10	1.63	1.47
2	AB	158	PRO	N-CD	11.09	1.63	1.47
12	AL	91	PRO	N-CD	11.08	1.63	1.47
13	AM	112	PRO	N-CD	11.07	1.63	1.47
9	AI	23	PRO	N-CD	11.06	1.63	1.47
30	BI	42	PRO	N-CD	11.06	1.63	1.47
43	BV	84	PRO	N-CD	11.06	1.63	1.47
34	BM	72	PRO	N-CD	11.05	1.63	1.47
27	BF	176	PRO	N-CD	11.02	1.63	1.47
7	AG	88	PRO	N-CD	11.02	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	BU	50	PRO	N-CD	11.01	1.63	1.47
26	BE	129	PRO	N-CD	11.01	1.63	1.47
19	AS	9	PRO	N-CD	11.01	1.63	1.47
19	AS	59	PRO	N-CD	11.01	1.63	1.47
6	AF	19	PRO	N-CD	11.00	1.63	1.47
2	AB	182	PRO	N-CD	10.99	1.63	1.47
7	AG	71	PRO	N-CD	10.99	1.63	1.47
19	AS	76	PRO	N-CD	10.99	1.63	1.47
10	AJ	41	PRO	N-CD	10.99	1.63	1.47
4	AD	186	PRO	N-CD	10.98	1.63	1.47
36	BO	42	PRO	N-CD	10.96	1.63	1.47
4	AD	168	PRO	N-CD	10.96	1.63	1.47
19	AS	42	PRO	N-CD	10.96	1.63	1.47
22	BA	892	A	C4'-O4'	-10.96	1.31	1.45
12	AL	122	PRO	N-CD	10.95	1.63	1.47
28	BG	112	PRO	N-CD	10.93	1.63	1.47
2	AB	201	PRO	N-CD	10.93	1.63	1.47
27	BF	109	PRO	N-CD	10.93	1.63	1.47
3	AC	98	PRO	N-CD	10.91	1.63	1.47
42	BU	48	PRO	N-CD	10.90	1.63	1.47
12	AL	42	PRO	N-CD	10.90	1.63	1.47
3	AC	174	PRO	N-CD	10.89	1.63	1.47
4	AD	38	PRO	N-CD	10.89	1.63	1.47
11	AK	60	PRO	N-CD	10.88	1.63	1.47
2	AB	25	PRO	N-CD	10.88	1.63	1.47
16	AP	41	PRO	N-CD	10.87	1.63	1.47
5	AE	84	PRO	N-CD	10.87	1.63	1.47
11	AK	89	PRO	N-CD	10.86	1.63	1.47
11	AK	91	PRO	N-CD	10.86	1.63	1.47
28	BG	12	PRO	N-CD	10.85	1.63	1.47
26	BE	89	PRO	N-CD	10.85	1.63	1.47
21	AU	11	PRO	N-CD	10.84	1.63	1.47
30	BI	7	PRO	N-CD	10.84	1.63	1.47
7	AG	93	PRO	N-CD	10.83	1.63	1.47
29	BH	38	PRO	N-CD	10.83	1.63	1.47
24	BC	218	PRO	N-CD	10.83	1.63	1.47
18	AR	41	PRO	N-CD	10.83	1.63	1.47
24	BC	8	PRO	N-CD	10.83	1.63	1.47
49	B1	31	PRO	N-CD	10.83	1.63	1.47
9	AI	125	PRO	N-CD	10.82	1.63	1.47
3	AC	109	PRO	N-CD	10.82	1.62	1.47
19	AS	30	PRO	N-CD	10.81	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	BG	118	PRO	N-CD	10.81	1.62	1.47
3	AC	17	PRO	N-CD	10.81	1.62	1.47
45	BX	12	PRO	N-CD	10.81	1.62	1.47
7	AG	14	PRO	N-CD	10.81	1.62	1.47
42	BU	55	PRO	N-CD	10.80	1.62	1.47
14	AN	94	PRO	N-CD	10.80	1.62	1.47
34	BM	109	PRO	N-CD	10.79	1.62	1.47
6	AF	101	PRO	N-CD	10.79	1.62	1.47
43	BV	27	PRO	N-CD	10.79	1.62	1.47
6	AF	67	PRO	N-CD	10.78	1.62	1.47
31	BJ	8	PRO	N-CD	10.78	1.62	1.47
3	AC	60	PRO	N-CD	10.78	1.62	1.47
8	AH	57	PRO	N-CD	10.77	1.62	1.47
17	AQ	66	PRO	N-CD	10.77	1.62	1.47
29	BH	32	PRO	N-CD	10.77	1.62	1.47
24	BC	148	PRO	N-CD	10.77	1.62	1.47
16	AP	15	PRO	N-CD	10.76	1.62	1.47
27	BF	84	PRO	N-CD	10.76	1.62	1.47
11	AK	115	PRO	N-CD	10.75	1.62	1.47
24	BC	32	PRO	N-CD	10.74	1.62	1.47
4	AD	7	PRO	N-CD	10.74	1.62	1.47
43	BV	37	PRO	N-CD	10.74	1.62	1.47
47	BZ	42	PRO	N-CD	10.74	1.62	1.47
6	AF	50	PRO	N-CD	10.73	1.62	1.47
28	BG	126	PRO	N-CD	10.73	1.62	1.47
8	AH	93	PRO	N-CD	10.73	1.62	1.47
33	BL	56	PRO	N-CD	10.72	1.62	1.47
12	AL	22	PRO	N-CD	10.71	1.62	1.47
5	AE	98	PRO	N-CD	10.71	1.62	1.47
10	AJ	43	PRO	N-CD	10.71	1.62	1.47
39	BR	52	PRO	N-CD	10.71	1.62	1.47
12	AL	11	PRO	N-CD	10.70	1.62	1.47
27	BF	65	PRO	N-CD	10.69	1.62	1.47
29	BH	118	PRO	N-CD	10.68	1.62	1.47
44	BW	74	PRO	N-CD	10.68	1.62	1.47
13	AM	96	PRO	N-CD	10.66	1.62	1.47
20	AT	56	PRO	N-CD	10.66	1.62	1.47
14	AN	70	PRO	N-CD	10.65	1.62	1.47
26	BE	177	PRO	N-CD	10.65	1.62	1.47
35	BN	39	PRO	N-CD	10.65	1.62	1.47
4	AD	139	PRO	N-CD	10.64	1.62	1.47
7	AG	16	PRO	N-CD	10.62	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AK	117	PRO	N-CD	10.62	1.62	1.47
14	AN	57	PRO	N-CD	10.62	1.62	1.47
18	AR	69	PRO	N-CD	10.62	1.62	1.47
35	BN	109	PRO	N-CD	10.61	1.62	1.47
51	B3	2	PRO	N-CD	10.61	1.62	1.47
6	AF	12	PRO	N-CD	10.61	1.62	1.47
37	BP	22	PRO	N-CD	10.60	1.62	1.47
35	BN	50	PRO	N-CD	10.60	1.62	1.47
31	BJ	46	PRO	N-CD	10.58	1.62	1.47
32	BK	48	PRO	N-CD	10.58	1.62	1.47
28	BG	154	PRO	N-CD	10.58	1.62	1.47
27	BF	29	PRO	N-CD	10.56	1.62	1.47
28	BG	156	PRO	N-CD	10.56	1.62	1.47
33	BL	119	PRO	N-CD	10.55	1.62	1.47
17	AQ	32	PRO	N-CD	10.54	1.62	1.47
37	BP	18	PRO	N-CD	10.54	1.62	1.47
34	BM	77	PRO	N-CD	10.53	1.62	1.47
8	AH	6	PRO	N-CD	10.53	1.62	1.47
8	AH	28	PRO	N-CD	10.52	1.62	1.47
10	AJ	55	PRO	N-CD	10.52	1.62	1.47
28	BG	54	PRO	N-CD	10.52	1.62	1.47
32	BK	72	PRO	N-CD	10.52	1.62	1.47
41	BT	14	PRO	N-CD	10.51	1.62	1.47
24	BC	29	PRO	N-CD	10.51	1.62	1.47
5	AE	133	PRO	N-CD	10.49	1.62	1.47
11	AK	123	PRO	N-CD	10.49	1.62	1.47
11	AK	124	PRO	N-CD	10.49	1.62	1.47
31	BJ	113	PRO	N-CD	10.49	1.62	1.47
8	AH	81	PRO	N-CD	10.48	1.62	1.47
36	BO	32	PRO	N-CD	10.48	1.62	1.47
24	BC	11	PRO	N-CD	10.47	1.62	1.47
31	BJ	137	PRO	N-CD	10.47	1.62	1.47
12	AL	28	PRO	N-CD	10.47	1.62	1.47
25	BD	23	PRO	N-CD	10.46	1.62	1.47
27	BF	139	PRO	N-CD	10.45	1.62	1.47
37	BP	79	PRO	N-CD	10.45	1.62	1.47
34	BM	4	PRO	N-CD	10.43	1.62	1.47
24	BC	131	PRO	N-CD	10.41	1.62	1.47
52	B4	31	PRO	N-CD	10.41	1.62	1.47
26	BE	59	PRO	N-CD	10.40	1.62	1.47
33	BL	8	PRO	N-CD	10.40	1.62	1.47
25	BD	152	PRO	N-CD	10.40	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BC	22	PRO	N-CD	10.39	1.62	1.47
24	BC	107	PRO	N-CD	10.39	1.62	1.47
51	B3	63	PRO	N-CD	10.37	1.62	1.47
24	BC	227	PRO	N-CD	10.37	1.62	1.47
47	BZ	18	PRO	N-CD	10.36	1.62	1.47
34	BM	69	PRO	N-CD	10.35	1.62	1.47
24	BC	75	PRO	N-CD	10.34	1.62	1.47
31	BJ	97	PRO	N-CD	10.32	1.62	1.47
32	BK	94	PRO	N-CD	10.32	1.62	1.47
32	BK	120	PRO	N-CD	10.29	1.62	1.47
21	AU	41	PRO	N-CD	10.29	1.62	1.47
51	B3	46	PRO	N-CD	10.29	1.62	1.47
24	BC	244	PRO	N-CD	10.28	1.62	1.47
49	B1	41	PRO	N-CD	10.28	1.62	1.47
24	BC	136	PRO	N-CD	10.28	1.62	1.47
25	BD	194	PRO	N-CD	10.28	1.62	1.47
24	BC	126	PRO	N-CD	10.27	1.62	1.47
35	BN	85	PRO	N-CD	10.27	1.62	1.47
25	BD	63	PRO	N-CD	10.27	1.62	1.47
43	BV	81	PRO	N-CD	10.27	1.62	1.47
3	AC	7	PRO	N-CD	10.18	1.62	1.47
25	BD	205	PRO	N-CD	10.11	1.61	1.47
40	BS	87	PRO	N-CD	10.10	1.61	1.47
26	BE	76	PRO	N-CD	10.08	1.61	1.47
25	BD	143	PRO	N-CD	10.07	1.61	1.47
48	B0	8	PRO	N-CD	10.06	1.61	1.47
31	BJ	110	PRO	N-CD	10.05	1.61	1.47
34	BM	125	PRO	N-CD	10.00	1.61	1.47
50	B2	7	PRO	N-CD	9.97	1.61	1.47
24	BC	231	PRO	N-CD	9.97	1.61	1.47
40	BS	80	PRO	N-CD	9.95	1.61	1.47
45	BX	31	PRO	N-CD	9.91	1.61	1.47
22	BA	2542	A	C5-C4	-9.88	1.31	1.38
32	BK	102	PRO	N-CD	9.84	1.61	1.47
34	BM	98	PRO	N-CD	9.79	1.61	1.47
24	BC	85	PRO	N-CD	9.73	1.61	1.47
33	BL	62	PRO	N-CD	9.65	1.61	1.47
6	AF	65	GLU	CB-CG	-9.58	1.33	1.52
22	BA	2052	A	C5-C4	-9.38	1.32	1.38
22	BA	1668	A	C5-C4	-9.30	1.32	1.38
24	BC	247	PRO	N-CD	9.26	1.60	1.47
22	BA	1783	A	C5-C4	-9.20	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2451	A	C8-N7	9.14	1.38	1.31
22	BA	514	A	C5-C4	-9.05	1.32	1.38
22	BA	1265	A	C5-C4	-9.00	1.32	1.38
22	BA	466	A	C5-C4	-8.99	1.32	1.38
22	BA	2711	A	C5-C4	-8.99	1.32	1.38
22	BA	522	A	C5-C4	-8.97	1.32	1.38
22	BA	2740	A	C5-C4	-8.96	1.32	1.38
22	BA	204	A	C5-C4	-8.96	1.32	1.38
22	BA	1652	A	C5-C4	-8.94	1.32	1.38
22	BA	2009	A	C5-C4	-8.93	1.32	1.38
22	BA	742	A	C5-C4	-8.92	1.32	1.38
22	BA	756	A	C5-C4	-8.92	1.32	1.38
22	BA	2741	A	C5-C4	-8.87	1.32	1.38
22	BA	2020	A	C5-C4	-8.86	1.32	1.38
22	BA	1569	A	C5-C4	-8.82	1.32	1.38
22	BA	761	A	C5-C4	-8.80	1.32	1.38
22	BA	1427	A	C5-C4	-8.77	1.32	1.38
1	AA	412	A	C8-N7	8.76	1.37	1.31
22	BA	693	A	C5-C4	-8.73	1.32	1.38
22	BA	1000	A	C5-C4	-8.72	1.32	1.38
25	BD	152	PRO	N-CA	-8.72	1.32	1.47
22	BA	1431	A	C5-C4	-8.70	1.32	1.38
22	BA	119	A	C5-C4	-8.69	1.32	1.38
22	BA	526	A	C5-C4	-8.66	1.32	1.38
22	BA	582	A	C5-C4	-8.65	1.32	1.38
51	B3	2	PRO	N-CA	-8.62	1.32	1.47
22	BA	1953	A	C5-C4	-8.61	1.32	1.38
22	BA	49	A	C5-C4	-8.58	1.32	1.38
22	BA	2369	A	C5-C4	-8.58	1.32	1.38
22	BA	909	A	C5-C4	-8.57	1.32	1.38
22	BA	1268	A	C5-C4	-8.57	1.32	1.38
22	BA	2013	A	C5-C4	-8.54	1.32	1.38
22	BA	2090	A	C5-C4	-8.54	1.32	1.38
22	BA	1791	A	C5-C4	-8.54	1.32	1.38
22	BA	1010	A	C5-C4	-8.53	1.32	1.38
22	BA	1254	A	C5-C4	-8.52	1.32	1.38
22	BA	675	A	C5-C4	-8.50	1.32	1.38
22	BA	592	A	C5-C4	-8.49	1.32	1.38
22	BA	2577	A	C5-C4	-8.48	1.32	1.38
22	BA	1899	A	C5-C4	-8.46	1.32	1.38
22	BA	2727	A	C5-C4	-8.46	1.32	1.38
22	BA	457	A	C5-C4	-8.45	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1630	A	C5-C4	-8.44	1.32	1.38
22	BA	2005	A	C5-C4	-8.44	1.32	1.38
22	BA	2518	A	C5-C4	-8.43	1.32	1.38
22	BA	231	A	C5-C4	-8.42	1.32	1.38
22	BA	699	A	C5-C4	-8.40	1.32	1.38
22	BA	2738	A	C5-C4	-8.40	1.32	1.38
22	BA	2051	A	C5-C4	-8.39	1.32	1.38
22	BA	2721	A	C5-C4	-8.38	1.32	1.38
22	BA	972	A	C5-C4	-8.38	1.32	1.38
22	BA	1327	A	C5-C4	-8.37	1.32	1.38
22	BA	2054	A	C5-C4	-8.37	1.32	1.38
22	BA	1378	A	C5-C4	-8.36	1.32	1.38
39	BR	52	PRO	N-CA	-8.36	1.33	1.47
22	BA	821	A	C5-C4	-8.36	1.32	1.38
22	BA	2358	A	C5-C4	-8.35	1.32	1.38
22	BA	1794	A	C5-C4	-8.35	1.32	1.38
22	BA	1142	A	C5-C4	-8.34	1.32	1.38
22	BA	1247	A	C5-C4	-8.34	1.32	1.38
22	BA	685	A	C5-C4	-8.33	1.32	1.38
22	BA	1155	A	C5-C4	-8.33	1.32	1.38
22	BA	191	A	C5-C4	-8.33	1.32	1.38
22	BA	2497	A	C5-C4	-8.31	1.32	1.38
22	BA	750	A	C5-C4	-8.31	1.32	1.38
22	BA	2418	A	C5-C4	-8.30	1.32	1.38
22	BA	1028	A	C5-C4	-8.30	1.32	1.38
22	BA	1354	A	C5-C4	-8.30	1.32	1.38
22	BA	1571	A	C5-C4	-8.29	1.32	1.38
22	BA	449	A	C5-C4	-8.28	1.32	1.38
22	BA	2435	A	C5-C4	-8.27	1.32	1.38
22	BA	599	A	C5-C4	-8.27	1.32	1.38
22	BA	1960	A	C5-C4	-8.27	1.32	1.38
22	BA	984	A	C5-C4	-8.27	1.32	1.38
22	BA	609	A	C5-C4	-8.25	1.32	1.38
22	BA	668	A	C5-C4	-8.25	1.32	1.38
22	BA	1678	A	C5-C4	-8.24	1.32	1.38
22	BA	2077	A	C5-C4	-8.23	1.32	1.38
21	AU	2	PRO	N-CA	-8.22	1.33	1.47
22	BA	374	A	C5-C4	-8.22	1.32	1.38
22	BA	947	A	C5-C4	-8.21	1.33	1.38
22	BA	38	A	C5-C4	-8.20	1.33	1.38
22	BA	2600	A	C5-C4	-8.20	1.33	1.38
22	BA	1342	A	C5-C4	-8.20	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	632	A	C5-C4	-8.19	1.33	1.38
22	BA	2033	A	C5-C4	-8.18	1.33	1.38
22	BA	1754	A	C5-C4	-8.18	1.33	1.38
1	AA	152	A	C8-N7	8.16	1.37	1.31
22	BA	631	A	C5-C4	-8.16	1.33	1.38
22	BA	1129	A	C5-C4	-8.16	1.33	1.38
22	BA	608	A	C5-C4	-8.15	1.33	1.38
22	BA	1264	A	C5-C4	-8.15	1.33	1.38
22	BA	1269	A	C5-C4	-8.14	1.33	1.38
22	BA	2565	A	C5-C4	-8.14	1.33	1.38
22	BA	1805	A	C5-C4	-8.14	1.33	1.38
22	BA	980	A	C5-C4	-8.12	1.33	1.38
22	BA	2014	A	C5-C4	-8.11	1.33	1.38
22	BA	2598	A	C5-C4	-8.10	1.33	1.38
22	BA	1032	A	C5-C4	-8.10	1.33	1.38
22	BA	1937	A	C5-C4	-8.10	1.33	1.38
22	BA	423	A	C5-C4	-8.09	1.33	1.38
22	BA	920	A	C5-C4	-8.09	1.33	1.38
22	BA	1373	A	C5-C4	-8.09	1.33	1.38
22	BA	1809	A	C5-C4	-8.08	1.33	1.38
22	BA	2564	A	C5-C4	-8.07	1.33	1.38
22	BA	197	A	C5-C4	-8.07	1.33	1.38
22	BA	1304	A	C5-C4	-8.07	1.33	1.38
22	BA	1853	A	C5-C4	-8.07	1.33	1.38
22	BA	983	A	C5-C4	-8.05	1.33	1.38
22	BA	586	A	C5-C4	-8.04	1.33	1.38
22	BA	892	A	C8-N7	8.04	1.37	1.31
22	BA	1762	A	C5-C4	-8.04	1.33	1.38
22	BA	2468	A	C5-C4	-8.04	1.33	1.38
22	BA	676	A	C5-C4	-8.04	1.33	1.38
22	BA	2765	A	C5-C4	-8.03	1.33	1.38
22	BA	602	A	C5-C4	-8.03	1.33	1.38
22	BA	792	A	C5-C4	-8.03	1.33	1.38
22	BA	973	A	C5-C4	-8.03	1.33	1.38
22	BA	2541	A	C5-C4	-8.02	1.33	1.38
22	BA	2381	A	C5-C4	-8.01	1.33	1.38
12	AL	45	PRO	N-CA	-8.00	1.33	1.47
22	BA	199	A	C5-C4	-8.00	1.33	1.38
22	BA	2837	A	C5-C4	-8.00	1.33	1.38
22	BA	127	A	C5-C4	-7.99	1.33	1.38
22	BA	2882	A	C5-C4	-7.99	1.33	1.38
22	BA	990	A	C5-C4	-7.98	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1772	A	C5-C4	-7.98	1.33	1.38
22	BA	19	A	C5-C4	-7.97	1.33	1.38
22	BA	1353	A	C5-C4	-7.97	1.33	1.38
22	BA	833	A	C5-C4	-7.97	1.33	1.38
7	AG	2	PRO	N-CA	-7.97	1.33	1.47
22	BA	917	A	C5-C4	-7.96	1.33	1.38
22	BA	735	A	C5-C4	-7.96	1.33	1.38
22	BA	574	A	C5-C4	-7.96	1.33	1.38
22	BA	804	A	C5-C4	-7.95	1.33	1.38
22	BA	53	A	C5-C4	-7.95	1.33	1.38
22	BA	1165	A	C5-C4	-7.95	1.33	1.38
22	BA	2267	A	C5-C4	-7.94	1.33	1.38
22	BA	1810	A	N7-C5	-7.94	1.34	1.39
22	BA	2434	A	C5-C4	-7.93	1.33	1.38
22	BA	2873	A	C5-C4	-7.93	1.33	1.38
22	BA	677	A	C5-C4	-7.93	1.33	1.38
22	BA	2070	A	C5-C4	-7.93	1.33	1.38
22	BA	2602	A	C8-N7	7.93	1.37	1.31
1	AA	622	A	C8-N7	7.93	1.37	1.31
22	BA	262	A	C5-C4	-7.93	1.33	1.38
22	BA	2119	A	C8-N7	7.93	1.37	1.31
22	BA	863	A	C5-C4	-7.92	1.33	1.38
22	BA	2328	A	C5-C4	-7.92	1.33	1.38
22	BA	743	A	C5-C4	-7.90	1.33	1.38
22	BA	2764	A	C5-C4	-7.90	1.33	1.38
22	BA	1755	A	C5-C4	-7.89	1.33	1.38
22	BA	513	A	C5-C4	-7.89	1.33	1.38
22	BA	1952	A	C5-C4	-7.88	1.33	1.38
22	BA	532	A	C5-C4	-7.88	1.33	1.38
22	BA	2281	A	C5-C4	-7.88	1.33	1.38
22	BA	14	A	C5-C4	-7.88	1.33	1.38
22	BA	1029	A	C5-C4	-7.88	1.33	1.38
22	BA	2241	A	C5-C4	-7.87	1.33	1.38
22	BA	1819	A	C5-C4	-7.87	1.33	1.38
22	BA	2412	A	C5-C4	-7.87	1.33	1.38
22	BA	479	A	C5-C4	-7.87	1.33	1.38
22	BA	918	A	C5-C4	-7.86	1.33	1.38
22	BA	195	A	C8-N7	7.86	1.37	1.31
22	BA	1246	A	C5-C4	-7.86	1.33	1.38
22	BA	2088	A	C5-C4	-7.86	1.33	1.38
22	BA	241	A	C5-C4	-7.85	1.33	1.38
22	BA	2725	A	C5-C4	-7.85	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1966	A	C5-C4	-7.84	1.33	1.38
13	AM	115	PRO	N-CA	-7.83	1.33	1.47
22	BA	910	A	C5-C4	-7.83	1.33	1.38
22	BA	2469	A	C5-C4	-7.83	1.33	1.38
22	BA	401	A	C5-C4	-7.83	1.33	1.38
22	BA	2173	A	C8-N7	7.83	1.37	1.31
22	BA	503	A	C5-C4	-7.82	1.33	1.38
22	BA	1001	A	C5-C4	-7.82	1.33	1.38
22	BA	670	A	C5-C4	-7.82	1.33	1.38
22	BA	1085	A	C8-N7	7.82	1.37	1.31
22	BA	223	A	C5-C4	-7.82	1.33	1.38
22	BA	2425	A	C5-C4	-7.82	1.33	1.38
22	BA	422	A	C5-C4	-7.81	1.33	1.38
22	BA	1815	A	C5-C4	-7.81	1.33	1.38
22	BA	1275	A	C5-C4	-7.81	1.33	1.38
22	BA	825	A	C5-C4	-7.80	1.33	1.38
22	BA	749	A	C5-C4	-7.80	1.33	1.38
22	BA	911	A	C5-C4	-7.80	1.33	1.38
22	BA	2266	A	C5-C4	-7.80	1.33	1.38
22	BA	2883	A	C5-C4	-7.80	1.33	1.38
22	BA	2388	A	C5-C4	-7.79	1.33	1.38
1	AA	766	A	C5-C4	-7.79	1.33	1.38
22	BA	1700	A	C5-C4	-7.78	1.33	1.38
22	BA	2134	A	C8-N7	7.78	1.36	1.31
22	BA	1583	A	C8-N7	7.77	1.36	1.31
22	BA	1133	A	C5-C4	-7.77	1.33	1.38
22	BA	1384	A	C5-C4	-7.77	1.33	1.38
22	BA	1597	A	C5-C4	-7.76	1.33	1.38
22	BA	2015	A	C5-C4	-7.76	1.33	1.38
22	BA	2003	A	C5-C4	-7.76	1.33	1.38
55	B8	76	A	C8-N7	7.76	1.36	1.31
22	BA	2346	A	C5-C4	-7.75	1.33	1.38
22	BA	2154	A	C8-N7	7.75	1.36	1.31
22	BA	2278	A	C5-C4	-7.75	1.33	1.38
22	BA	190	A	C5-C4	-7.74	1.33	1.38
49	B1	44	ARG	CG-CD	-7.74	1.32	1.51
22	BA	300	A	C5-C4	-7.74	1.33	1.38
22	BA	310	A	C5-C4	-7.74	1.33	1.38
22	BA	849	A	C5-C4	-7.74	1.33	1.38
22	BA	800	A	C5-C4	-7.73	1.33	1.38
22	BA	637	A	C5-C4	-7.72	1.33	1.38
22	BA	2169	A	C8-N7	7.72	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	195	A	C8-N7	7.72	1.36	1.31
22	BA	118	A	C5-C4	-7.72	1.33	1.38
22	BA	73	A	C5-C4	-7.72	1.33	1.38
22	BA	203	A	C5-C4	-7.72	1.33	1.38
22	BA	222	A	C5-C4	-7.72	1.33	1.38
22	BA	1328	A	C5-C4	-7.72	1.33	1.38
22	BA	2560	A	C5-C4	-7.71	1.33	1.38
22	BA	563	A	C5-C4	-7.71	1.33	1.38
1	AA	996	A	C8-N7	7.71	1.36	1.31
1	AA	1346	A	C8-N7	7.71	1.36	1.31
22	BA	689	A	C5-C4	-7.71	1.33	1.38
22	BA	1244	A	C5-C4	-7.71	1.33	1.38
22	BA	216	A	C5-C4	-7.71	1.33	1.38
22	BA	794	A	C5-C4	-7.70	1.33	1.38
22	BA	2147	A	C8-N7	7.70	1.36	1.31
22	BA	1253	A	C5-C4	-7.70	1.33	1.38
22	BA	412	A	C5-C4	-7.69	1.33	1.38
22	BA	1237	A	C5-C4	-7.69	1.33	1.38
22	BA	1938	A	C5-C4	-7.69	1.33	1.38
22	BA	2411	A	C5-C4	-7.69	1.33	1.38
22	BA	643	A	C5-C4	-7.68	1.33	1.38
22	BA	819	A	C5-C4	-7.68	1.33	1.38
22	BA	1977	A	C5-C4	-7.68	1.33	1.38
22	BA	478	A	C5-C4	-7.67	1.33	1.38
22	BA	2572	A	C5-C4	-7.67	1.33	1.38
22	BA	52	A	C5-C4	-7.66	1.33	1.38
22	BA	1067	A	C8-N7	7.66	1.36	1.31
22	BA	1262	A	C5-C4	-7.66	1.33	1.38
22	BA	2813	A	C5-C4	-7.66	1.33	1.38
22	BA	1932	A	C5-C4	-7.66	1.33	1.38
22	BA	1552	A	C5-C4	-7.66	1.33	1.38
1	AA	1250	A	C8-N7	7.66	1.36	1.31
22	BA	2823	A	C5-C4	-7.66	1.33	1.38
55	B8	73	A	C8-N7	7.66	1.36	1.31
22	BA	627	A	C5-C4	-7.65	1.33	1.38
22	BA	1126	A	C5-C4	-7.65	1.33	1.38
22	BA	501	A	C5-C4	-7.65	1.33	1.38
22	BA	1189	A	C5-C4	-7.65	1.33	1.38
22	BA	1287	A	C5-C4	-7.64	1.33	1.38
1	AA	466	A	C8-N7	7.64	1.36	1.31
22	BA	739	A	C5-C4	-7.63	1.33	1.38
22	BA	896	A	C8-N7	7.63	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1226	A	C5-C4	-7.62	1.33	1.38
23	BB	99	A	C5-C4	-7.62	1.33	1.38
1	AA	1534	A	C8-N7	7.62	1.36	1.31
22	BA	1981	A	C5-C4	-7.61	1.33	1.38
22	BA	2184	A	C8-N7	7.61	1.36	1.31
22	BA	1286	A	C5-C4	-7.61	1.33	1.38
22	BA	1551	A	C5-C4	-7.61	1.33	1.38
22	BA	227	A	C5-C4	-7.60	1.33	1.38
22	BA	1570	A	C5-C4	-7.60	1.33	1.38
22	BA	2037	A	C5-C4	-7.60	1.33	1.38
22	BA	2386	A	C5-C4	-7.60	1.33	1.38
22	BA	2101	A	N3-C4	7.59	1.39	1.34
22	BA	1147	A	C5-C4	-7.59	1.33	1.38
22	BA	1095	A	C8-N7	7.59	1.36	1.31
22	BA	21	A	C5-C4	-7.59	1.33	1.38
22	BA	2682	A	C5-C4	-7.59	1.33	1.38
22	BA	477	A	C5-C4	-7.59	1.33	1.38
22	BA	654	A	C8-N7	7.58	1.36	1.31
1	AA	1150	A	C8-N7	7.58	1.36	1.31
22	BA	196	A	C5-C4	-7.58	1.33	1.38
22	BA	371	A	C5-C4	-7.58	1.33	1.38
22	BA	1214	A	C5-C4	-7.58	1.33	1.38
22	BA	1387	A	C5-C4	-7.58	1.33	1.38
22	BA	2171	A	C8-N7	7.58	1.36	1.31
22	BA	2829	A	C5-C4	-7.58	1.33	1.38
55	B8	6	A	C8-N7	7.57	1.36	1.31
22	BA	945	A	C5-C4	-7.56	1.33	1.38
22	BA	1073	A	C8-N7	7.56	1.36	1.31
22	BA	1213	A	C5-C4	-7.56	1.33	1.38
55	B8	66	A	C8-N7	7.56	1.36	1.31
22	BA	1086	A	C8-N7	7.56	1.36	1.31
1	AA	1092	A	C8-N7	7.55	1.36	1.31
22	BA	1143	A	C5-C4	-7.55	1.33	1.38
22	BA	1810	A	C5-C4	-7.55	1.33	1.38
22	BA	2860	A	C5-C4	-7.55	1.33	1.38
22	BA	782	A	C5-C4	-7.55	1.33	1.38
22	BA	1650	A	C5-C4	-7.55	1.33	1.38
1	AA	845	A	C8-N7	7.55	1.36	1.31
1	AA	1000	A	C8-N7	7.55	1.36	1.31
22	BA	820	A	C5-C4	-7.55	1.33	1.38
22	BA	1057	A	C8-N7	7.55	1.36	1.31
22	BA	1641	A	C5-C4	-7.55	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1928	A	C5-C4	-7.55	1.33	1.38
22	BA	2142	A	C8-N7	7.55	1.36	1.31
22	BA	2450	A	C5-C4	-7.55	1.33	1.38
1	AA	1179	A	C8-N7	7.54	1.36	1.31
22	BA	2158	A	C8-N7	7.54	1.36	1.31
22	BA	415	A	C5-C4	-7.54	1.33	1.38
22	BA	1803	A	C5-C4	-7.54	1.33	1.38
22	BA	505	A	C5-C4	-7.54	1.33	1.38
22	BA	541	A	C5-C4	-7.54	1.33	1.38
22	BA	1365	A	C5-C4	-7.54	1.33	1.38
22	BA	502	A	C5-C4	-7.53	1.33	1.38
22	BA	2071	A	C5-C4	-7.53	1.33	1.38
22	BA	2094	A	C5-C4	-7.53	1.33	1.38
22	BA	2126	A	C8-N7	7.53	1.36	1.31
55	B8	58	A	C8-N7	7.53	1.36	1.31
22	BA	2031	A	C5-C4	-7.53	1.33	1.38
55	B8	69	A	C8-N7	7.52	1.36	1.31
22	BA	661	A	C5-C4	-7.52	1.33	1.38
22	BA	979	A	C5-C4	-7.52	1.33	1.38
22	BA	547	A	C8-N7	7.51	1.36	1.31
22	BA	322	A	C5-C4	-7.51	1.33	1.38
22	BA	727	A	C5-C4	-7.51	1.33	1.38
22	BA	1572	A	C5-C4	-7.51	1.33	1.38
22	BA	309	A	C5-C4	-7.50	1.33	1.38
22	BA	1987	A	C5-C4	-7.50	1.33	1.38
22	BA	2273	A	C5-C4	-7.50	1.33	1.38
22	BA	6	A	C5-C4	-7.50	1.33	1.38
22	BA	941	A	C5-C4	-7.50	1.33	1.38
22	BA	1614	A	C5-C4	-7.50	1.33	1.38
22	BA	2516	A	C5-C4	-7.50	1.33	1.38
22	BA	2872	A	C8-N7	7.50	1.36	1.31
22	BA	1285	A	C5-C4	-7.49	1.33	1.38
22	BA	1626	A	C5-C4	-7.49	1.33	1.38
22	BA	2679	A	C5-C4	-7.49	1.33	1.38
22	BA	430	A	C5-C4	-7.49	1.33	1.38
1	AA	784	A	C5-C4	-7.49	1.33	1.38
10	AJ	39	PRO	N-CA	-7.49	1.34	1.47
1	AA	432	A	C8-N7	7.48	1.36	1.31
22	BA	633	A	C5-C4	-7.48	1.33	1.38
22	BA	943	A	C5-C4	-7.48	1.33	1.38
22	BA	1784	A	C5-C4	-7.48	1.33	1.38
22	BA	2340	A	C5-C4	-7.48	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	988	A	C5-C4	-7.48	1.33	1.38
22	BA	1084	A	C8-N7	7.48	1.36	1.31
22	BA	2322	A	C5-C4	-7.48	1.33	1.38
1	AA	1036	A	C8-N7	7.47	1.36	1.31
1	AA	205	A	C8-N7	7.47	1.36	1.31
22	BA	2750	A	C5-C4	-7.47	1.33	1.38
22	BA	2170	A	C8-N7	7.47	1.36	1.31
22	BA	981	A	C5-C4	-7.47	1.33	1.38
22	BA	2117	A	C8-N7	7.46	1.36	1.31
22	BA	1802	A	C5-C4	-7.46	1.33	1.38
22	BA	332	A	C5-C4	-7.46	1.33	1.38
22	BA	1194	A	C5-C4	-7.46	1.33	1.38
22	BA	1395	A	C5-C4	-7.46	1.33	1.38
22	BA	789	A	C5-C4	-7.46	1.33	1.38
22	BA	1111	A	C8-N7	7.46	1.36	1.31
22	BA	1096	A	C8-N7	7.46	1.36	1.31
1	AA	495	A	C8-N7	7.45	1.36	1.31
1	AA	1035	A	C8-N7	7.45	1.36	1.31
22	BA	613	A	C8-N7	7.45	1.36	1.31
22	BA	1403	A	C5-C4	-7.45	1.33	1.38
22	BA	2758	A	C5-C4	-7.45	1.33	1.38
1	AA	978	A	C8-N7	7.45	1.36	1.31
1	AA	1145	A	C8-N7	7.45	1.36	1.31
1	AA	98	A	C8-N7	7.45	1.36	1.31
22	BA	1336	A	C5-C4	-7.45	1.33	1.38
22	BA	2448	A	C5-C4	-7.45	1.33	1.38
22	BA	877	A	C8-N7	7.44	1.36	1.31
1	AA	1044	A	C8-N7	7.44	1.36	1.31
22	BA	1156	A	C5-C4	-7.44	1.33	1.38
22	BA	1913	A	C8-N7	7.44	1.36	1.31
22	BA	2336	A	C5-C4	-7.44	1.33	1.38
22	BA	1089	A	C8-N7	7.44	1.36	1.31
22	BA	1787	A	C5-C4	-7.44	1.33	1.38
22	BA	1080	A	C8-N7	7.44	1.36	1.31
1	AA	1319	A	C8-N7	7.43	1.36	1.31
22	BA	621	A	C5-C4	-7.43	1.33	1.38
22	BA	1420	A	C8-N7	7.43	1.36	1.31
22	BA	959	A	C5-C4	-7.43	1.33	1.38
22	BA	1308	A	C5-C4	-7.43	1.33	1.38
22	BA	2270	A	C5-C4	-7.43	1.33	1.38
55	B8	21	A	C8-N7	7.42	1.36	1.31
1	AA	74	A	C8-N7	7.42	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	89	A	C5-C4	-7.42	1.33	1.38
22	BA	207	A	C5-C4	-7.42	1.33	1.38
22	BA	362	A	C8-N7	7.42	1.36	1.31
22	BA	2675	A	C5-C4	-7.42	1.33	1.38
22	BA	861	A	C5-C4	-7.42	1.33	1.38
22	BA	195	A	C5-C4	-7.42	1.33	1.38
1	AA	554	A	C8-N7	7.41	1.36	1.31
55	B8	14	A	C8-N7	7.41	1.36	1.31
22	BA	2211	A	C8-N7	7.40	1.36	1.31
22	BA	2309	A	C8-N7	7.40	1.36	1.31
22	BA	1522	A	C5-C4	-7.40	1.33	1.38
22	BA	2433	A	C5-C4	-7.40	1.33	1.38
22	BA	1596	A	C5-C4	-7.40	1.33	1.38
1	AA	1280	A	C8-N7	7.39	1.36	1.31
22	BA	1347	A	C5-C4	-7.39	1.33	1.38
1	AA	81	A	C8-N7	7.39	1.36	1.31
22	BA	764	A	C5-C4	-7.39	1.33	1.38
22	BA	2019	A	C5-C4	-7.39	1.33	1.38
22	BA	2080	A	C5-C4	-7.39	1.33	1.38
22	BA	1090	A	C8-N7	7.39	1.36	1.31
22	BA	1900	A	C5-C4	-7.39	1.33	1.38
22	BA	2432	A	C5-C4	-7.38	1.33	1.38
22	BA	176	A	C5-C4	-7.38	1.33	1.38
22	BA	1307	A	C5-C4	-7.38	1.33	1.38
55	B8	42	A	C8-N7	7.38	1.36	1.31
1	AA	1441	A	C8-N7	7.38	1.36	1.31
1	AA	767	A	C5-C4	-7.38	1.33	1.38
49	B1	44	ARG	CD-NE	-7.37	1.33	1.46
1	AA	1493	A	C8-N7	7.37	1.36	1.31
22	BA	960	A	C5-C4	-7.37	1.33	1.38
22	BA	1677	A	C5-C4	-7.37	1.33	1.38
1	AA	1274	A	C8-N7	7.37	1.36	1.31
22	BA	1260	A	C5-C4	-7.37	1.33	1.38
22	BA	1098	A	C8-N7	7.37	1.36	1.31
22	BA	1393	A	C5-C4	-7.37	1.33	1.38
22	BA	1272	A	C5-C4	-7.36	1.33	1.38
22	BA	2706	A	C5-C4	-7.36	1.33	1.38
22	BA	529	A	C5-C4	-7.36	1.33	1.38
55	B8	38	A	C8-N7	7.36	1.36	1.31
22	BA	126	A	C5-C4	-7.36	1.33	1.38
22	BA	2530	A	C5-C4	-7.36	1.33	1.38
22	BA	460	A	C5-C4	-7.36	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1067	A	C8-N7	7.35	1.36	1.31
22	BA	1515	A	C8-N7	7.35	1.36	1.31
1	AA	1285	A	C8-N7	7.34	1.36	1.31
22	BA	1890	A	C5-C4	-7.34	1.33	1.38
22	BA	515	A	C5-C4	-7.34	1.33	1.38
22	BA	1566	A	C5-C4	-7.34	1.33	1.38
55	B8	51	A	C8-N7	7.34	1.36	1.31
22	BA	1609	A	C5-C4	-7.34	1.33	1.38
22	BA	2590	A	C5-C4	-7.33	1.33	1.38
1	AA	1005	A	C8-N7	7.33	1.36	1.31
22	BA	340	A	C5-C4	-7.33	1.33	1.38
22	BA	1871	A	C8-N7	7.33	1.36	1.31
1	AA	431	A	C8-N7	7.33	1.36	1.31
1	AA	468	A	C8-N7	7.33	1.36	1.31
22	BA	590	A	C5-C4	-7.33	1.33	1.38
22	BA	1672	A	C5-C4	-7.33	1.33	1.38
22	BA	2566	A	C5-C4	-7.33	1.33	1.38
22	BA	255	A	C5-C4	-7.33	1.33	1.38
22	BA	1069	A	C8-N7	7.33	1.36	1.31
22	BA	2726	A	C5-C4	-7.32	1.33	1.38
22	BA	454	A	C5-C4	-7.32	1.33	1.38
22	BA	1786	A	C5-C4	-7.32	1.33	1.38
22	BA	2333	A	C5-C4	-7.32	1.33	1.38
22	BA	2614	A	C5-C4	-7.32	1.33	1.38
55	B8	75	C	P-O5'	-7.31	1.52	1.59
1	AA	1151	A	C8-N7	7.31	1.36	1.31
22	BA	1889	A	C5-C4	-7.31	1.33	1.38
22	BA	2366	A	C5-C4	-7.31	1.33	1.38
22	BA	2736	A	C5-C4	-7.31	1.33	1.38
1	AA	1117	A	C8-N7	7.31	1.36	1.31
22	BA	1046	A	C8-N7	7.30	1.36	1.31
22	BA	2183	A	C8-N7	7.30	1.36	1.31
22	BA	152	A	C5-C4	-7.30	1.33	1.38
22	BA	453	A	C5-C4	-7.30	1.33	1.38
22	BA	899	A	C8-N7	7.30	1.36	1.31
22	BA	1634	A	C5-C4	-7.30	1.33	1.38
1	AA	1155	A	C8-N7	7.30	1.36	1.31
23	BB	78	A	C5-C4	-7.29	1.33	1.38
1	AA	814	A	C5-C4	-7.29	1.33	1.38
22	BA	1366	A	C5-C4	-7.29	1.33	1.38
22	BA	2268	A	C5-C4	-7.29	1.33	1.38
1	AA	1363	A	C8-N7	7.29	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2776	A	C5-C4	-7.29	1.33	1.38
1	AA	1101	A	C8-N7	7.29	1.36	1.31
22	BA	1144	A	C5-C4	-7.29	1.33	1.38
22	BA	2176	A	C8-N7	7.29	1.36	1.31
22	BA	354	A	C8-N7	7.28	1.36	1.31
22	BA	2459	A	C5-C4	-7.28	1.33	1.38
1	AA	1246	A	C8-N7	7.28	1.36	1.31
22	BA	1070	A	C8-N7	7.28	1.36	1.31
22	BA	2748	A	C5-C4	-7.28	1.33	1.38
22	BA	2042	A	C5-C4	-7.28	1.33	1.38
22	BA	382	A	C5-C4	-7.28	1.33	1.38
22	BA	1419	A	C5-C4	-7.27	1.33	1.38
22	BA	1385	A	C5-C4	-7.27	1.33	1.38
1	AA	167	A	C8-N7	7.27	1.36	1.31
22	BA	219	A	C5-C4	-7.27	1.33	1.38
1	AA	120	A	C8-N7	7.27	1.36	1.31
1	AA	1019	A	C8-N7	7.26	1.36	1.31
22	BA	1676	A	C5-C4	-7.26	1.33	1.38
1	AA	648	A	C8-N7	7.26	1.36	1.31
22	BA	788	A	C5-C4	-7.26	1.33	1.38
22	BA	1785	A	C5-C4	-7.26	1.33	1.38
1	AA	1289	A	C8-N7	7.26	1.36	1.31
1	AA	1229	A	C8-N7	7.25	1.36	1.31
1	AA	1299	A	C8-N7	7.25	1.36	1.31
22	BA	2589	A	C5-C4	-7.25	1.33	1.38
22	BA	2660	A	C8-N7	7.25	1.36	1.31
1	AA	456	A	C8-N7	7.25	1.36	1.31
1	AA	1042	A	C8-N7	7.25	1.36	1.31
1	AA	1429	A	C5-C4	-7.25	1.33	1.38
1	AA	1447	A	C8-N7	7.25	1.36	1.31
1	AA	1213	A	C8-N7	7.25	1.36	1.31
22	BA	2632	A	C5-C4	-7.25	1.33	1.38
1	AA	1357	A	C8-N7	7.24	1.36	1.31
22	BA	1077	A	C8-N7	7.24	1.36	1.31
22	BA	1632	A	C5-C4	-7.24	1.33	1.38
22	BA	2225	A	C5-C4	-7.24	1.33	1.38
22	BA	402	A	C5-C4	-7.24	1.33	1.38
22	BA	2513	A	C5-C4	-7.24	1.33	1.38
22	BA	432	A	C5-C4	-7.24	1.33	1.38
22	BA	1829	A	C5-C4	-7.24	1.33	1.38
22	BA	2761	A	C5-C4	-7.24	1.33	1.38
1	AA	478	A	C8-N7	7.23	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2247	A	C5-C4	-7.23	1.33	1.38
55	B8	41	A	C8-N7	7.23	1.36	1.31
22	BA	1532	A	C8-N7	7.22	1.36	1.31
22	BA	1535	A	C8-N7	7.22	1.36	1.31
22	BA	2439	A	C5-C4	-7.22	1.33	1.38
1	AA	1014	A	C8-N7	7.22	1.36	1.31
22	BA	1616	A	C5-C4	-7.22	1.33	1.38
22	BA	1773	A	C5-C4	-7.22	1.33	1.38
1	AA	901	A	C5-C4	-7.22	1.33	1.38
1	AA	1332	A	C8-N7	7.22	1.36	1.31
1	AA	1022	A	C8-N7	7.22	1.36	1.31
22	BA	103	A	C5-C4	-7.21	1.33	1.38
22	BA	1912	A	C5-C4	-7.21	1.33	1.38
22	BA	2809	A	C5-C4	-7.21	1.33	1.38
22	BA	42	A	C5-C4	-7.21	1.33	1.38
1	AA	250	A	C8-N7	7.21	1.36	1.31
1	AA	1021	A	C8-N7	7.21	1.36	1.31
22	BA	1509	A	C8-N7	7.21	1.36	1.31
1	AA	1256	A	C8-N7	7.21	1.36	1.31
1	AA	72	A	C8-N7	7.21	1.36	1.31
55	B8	26	A	C8-N7	7.21	1.36	1.31
22	BA	2826	A	C5-C4	-7.20	1.33	1.38
22	BA	471	A	C5-C4	-7.20	1.33	1.38
22	BA	878	A	C8-N7	7.20	1.36	1.31
55	B8	76	A	C5-C4	-7.20	1.33	1.38
1	AA	149	A	C8-N7	7.20	1.36	1.31
1	AA	196	A	C8-N7	7.20	1.36	1.31
22	BA	1009	A	C5-C4	-7.20	1.33	1.38
22	BA	1175	A	N3-C4	7.20	1.39	1.34
1	AA	1257	A	C8-N7	7.20	1.36	1.31
1	AA	520	A	C8-N7	7.20	1.36	1.31
22	BA	508	A	C8-N7	7.20	1.36	1.31
22	BA	330	A	C5-C4	-7.19	1.33	1.38
1	AA	1216	A	C8-N7	7.19	1.36	1.31
22	BA	131	A	C5-C4	-7.19	1.33	1.38
53	B5	24	PRO	N-CA	-7.19	1.35	1.47
22	BA	2227	A	C5-C4	-7.19	1.33	1.38
1	AA	532	A	C8-N7	7.18	1.36	1.31
22	BA	44	A	C5-C4	-7.18	1.33	1.38
22	BA	251	A	C5-C4	-7.18	1.33	1.38
22	BA	1503	A	C8-N7	7.18	1.36	1.31
1	AA	1428	A	C5-C4	-7.18	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1008	A	C5-C4	-7.18	1.33	1.38
1	AA	815	A	C5-C4	-7.18	1.33	1.38
22	BA	2134	A	N3-C4	7.18	1.39	1.34
22	BA	2135	A	C8-N7	7.17	1.36	1.31
22	BA	2461	A	C5-C4	-7.17	1.33	1.38
1	AA	753	A	C8-N7	7.17	1.36	1.31
1	AA	816	A	C5-C4	-7.17	1.33	1.38
1	AA	1093	A	C8-N7	7.17	1.36	1.31
1	AA	649	A	C8-N7	7.17	1.36	1.31
22	BA	1665	A	C5-C4	-7.17	1.33	1.38
22	BA	181	A	C8-N7	7.16	1.36	1.31
22	BA	2766	A	C5-C4	-7.16	1.33	1.38
1	AA	715	A	C5-C4	-7.16	1.33	1.38
22	BA	1549	A	C5-C4	-7.15	1.33	1.38
22	BA	1276	A	C5-C4	-7.15	1.33	1.38
22	BA	1701	A	C5-C4	-7.15	1.33	1.38
22	BA	2665	A	C5-C4	-7.15	1.33	1.38
1	AA	1269	A	C8-N7	7.15	1.36	1.31
22	BA	1359	A	C5-C4	-7.15	1.33	1.38
1	AA	65	A	C8-N7	7.15	1.36	1.31
22	BA	1383	A	C5-C4	-7.14	1.33	1.38
22	BA	279	A	C8-N7	7.14	1.36	1.31
1	AA	408	A	C8-N7	7.14	1.36	1.31
1	AA	547	A	C8-N7	7.14	1.36	1.31
22	BA	1919	A	C5-C4	-7.13	1.33	1.38
22	BA	1470	A	C5-C4	-7.13	1.33	1.38
22	BA	504	A	C8-N7	7.13	1.36	1.31
22	BA	753	A	C5-C4	-7.13	1.33	1.38
1	AA	2	A	C8-N7	7.12	1.36	1.31
1	AA	461	A	C8-N7	7.12	1.36	1.31
1	AA	16	A	C5-C4	-7.12	1.33	1.38
22	BA	265	A	C5-C4	-7.12	1.33	1.38
1	AA	1146	A	C8-N7	7.12	1.36	1.31
22	BA	575	A	C5-C4	-7.12	1.33	1.38
1	AA	1196	A	C8-N7	7.12	1.36	1.31
22	BA	975	A	C5-C4	-7.12	1.33	1.38
22	BA	2635	A	C5-C4	-7.12	1.33	1.38
1	AA	704	A	C8-N7	7.11	1.36	1.31
1	AA	1251	A	C8-N7	7.11	1.36	1.31
1	AA	1329	A	C8-N7	7.11	1.36	1.31
22	BA	1854	A	C5-C4	-7.11	1.33	1.38
22	BA	706	A	C5-C4	-7.11	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1127	A	C5-C4	-7.11	1.33	1.38
22	BA	1698	A	C5-C4	-7.11	1.33	1.38
1	AA	181	A	C8-N7	7.11	1.36	1.31
22	BA	829	A	C5-C4	-7.11	1.33	1.38
1	AA	1012	A	C8-N7	7.11	1.36	1.31
1	AA	172	A	C8-N7	7.10	1.36	1.31
22	BA	2327	A	C5-C4	-7.10	1.33	1.38
22	BA	2335	A	C5-C4	-7.10	1.33	1.38
1	AA	629	A	C8-N7	7.10	1.36	1.31
1	AA	1169	A	C8-N7	7.10	1.36	1.31
22	BA	1151	A	C5-C4	-7.10	1.33	1.38
1	AA	77	A	C8-N7	7.10	1.36	1.31
22	BA	1927	A	C5-C4	-7.10	1.33	1.38
22	BA	2274	A	C5-C4	-7.10	1.33	1.38
1	AA	441	A	C8-N7	7.09	1.36	1.31
1	AA	452	A	C8-N7	7.09	1.36	1.31
1	AA	958	A	C8-N7	7.09	1.36	1.31
22	BA	447	A	C5-C4	-7.09	1.33	1.38
22	BA	1284	A	C5-C4	-7.09	1.33	1.38
22	BA	1490	A	C8-N7	7.09	1.36	1.31
1	AA	1252	A	C8-N7	7.09	1.36	1.31
1	AA	448	A	C8-N7	7.09	1.36	1.31
1	AA	1287	A	C8-N7	7.09	1.36	1.31
22	BA	1175	A	C8-N7	7.09	1.36	1.31
22	BA	2471	A	C5-C4	-7.09	1.33	1.38
1	AA	78	A	C8-N7	7.09	1.36	1.31
1	AA	435	A	C8-N7	7.09	1.36	1.31
1	AA	1275	A	C8-N7	7.09	1.36	1.31
22	BA	1998	A	C5-C4	-7.09	1.33	1.38
22	BA	2376	A	C5-C4	-7.08	1.33	1.38
1	AA	913	A	C5-C4	-7.08	1.33	1.38
22	BA	1505	A	C8-N7	7.08	1.36	1.31
1	AA	665	A	C8-N7	7.08	1.36	1.31
22	BA	443	A	C5-C4	-7.08	1.33	1.38
22	BA	2288	A	C5-C4	-7.08	1.33	1.38
1	AA	900	A	C5-C4	-7.08	1.33	1.38
22	BA	2453	A	C5-C4	-7.08	1.33	1.38
1	AA	71	A	C8-N7	7.08	1.36	1.31
22	BA	161	A	C8-N7	7.08	1.36	1.31
22	BA	1711	A	C5-C4	-7.07	1.33	1.38
1	AA	182	A	C8-N7	7.07	1.36	1.31
1	AA	825	A	C5-C4	-7.07	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1664	A	C5-C4	-7.07	1.33	1.38
22	BA	2639	A	C5-C4	-7.07	1.33	1.38
1	AA	1340	A	C8-N7	7.06	1.36	1.31
1	AA	189	A	C8-N7	7.06	1.36	1.31
1	AA	371	A	C8-N7	7.06	1.36	1.31
1	AA	411	A	C8-N7	7.06	1.36	1.31
1	AA	572	A	C5-C4	-7.06	1.33	1.38
1	AA	749	A	C8-N7	7.06	1.36	1.31
1	AA	1311	A	C8-N7	7.06	1.36	1.31
22	BA	1496	A	C5-C4	-7.06	1.33	1.38
22	BA	1088	A	C8-N7	7.06	1.36	1.31
22	BA	2478	A	C5-C4	-7.06	1.33	1.38
22	BA	391	A	C5-C4	-7.05	1.33	1.38
1	AA	356	A	C5-C4	-7.05	1.33	1.38
22	BA	1274	A	C5-C4	-7.05	1.33	1.38
22	BA	1433	A	C5-C4	-7.05	1.33	1.38
22	BA	1970	A	C5-C4	-7.05	1.33	1.38
22	BA	925	A	C5-C4	-7.05	1.33	1.38
1	AA	1492	A	C8-N7	7.04	1.36	1.31
22	BA	2810	A	C5-C4	-7.04	1.33	1.38
1	AA	768	A	C5-C4	-7.04	1.33	1.38
22	BA	2058	A	C5-C4	-7.04	1.33	1.38
22	BA	2114	A	C8-N7	7.04	1.36	1.31
1	AA	155	A	C8-N7	7.03	1.36	1.31
1	AA	974	A	C8-N7	7.03	1.36	1.31
1	AA	1167	A	C8-N7	7.03	1.36	1.31
1	AA	3	A	C8-N7	7.03	1.36	1.31
1	AA	223	A	C8-N7	7.03	1.36	1.31
1	AA	1219	A	C8-N7	7.03	1.36	1.31
22	BA	278	A	C8-N7	7.03	1.36	1.31
22	BA	1392	A	C5-C4	-7.03	1.33	1.38
22	BA	1637	A	C5-C4	-7.03	1.33	1.38
1	AA	621	A	C8-N7	7.02	1.36	1.31
1	AA	1349	A	C8-N7	7.02	1.36	1.31
22	BA	1580	A	C8-N7	7.02	1.36	1.31
22	BA	1969	A	C5-C4	-7.02	1.33	1.38
1	AA	1333	A	C8-N7	7.02	1.36	1.31
22	BA	497	A	C5-C4	-7.02	1.33	1.38
1	AA	523	A	C8-N7	7.02	1.36	1.31
1	AA	975	A	C8-N7	7.02	1.36	1.31
22	BA	2097	A	C8-N7	7.02	1.36	1.31
22	BA	2705	A	C5-C4	-7.02	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1610	A	C5-C4	-7.01	1.33	1.38
22	BA	2850	A	C5-C4	-7.01	1.33	1.38
1	AA	1004	A	C8-N7	7.01	1.36	1.31
22	BA	347	A	C8-N7	7.01	1.36	1.31
22	BA	2119	A	N3-C4	7.01	1.39	1.34
22	BA	282	A	C8-N7	7.01	1.36	1.31
22	BA	83	A	C5-C4	-7.00	1.33	1.38
22	BA	1679	A	C5-C4	-7.00	1.33	1.38
22	BA	173	A	C5-C4	-7.00	1.33	1.38
22	BA	1603	A	C5-C4	-7.00	1.33	1.38
1	AA	171	A	C8-N7	7.00	1.36	1.31
22	BA	311	A	C5-C4	-7.00	1.33	1.38
1	AA	60	A	C8-N7	7.00	1.36	1.31
22	BA	1640	A	C5-C4	-7.00	1.33	1.38
22	BA	1453	A	C8-N7	6.99	1.36	1.31
22	BA	1749	A	C5-C4	-6.99	1.33	1.38
22	BA	84	A	C8-N7	6.99	1.36	1.31
22	BA	1050	A	C8-N7	6.99	1.36	1.31
1	AA	7	A	C8-N7	6.99	1.36	1.31
22	BA	2108	A	C8-N7	6.99	1.36	1.31
22	BA	892	A	N3-C4	6.99	1.39	1.34
22	BA	2781	A	C5-C4	-6.99	1.33	1.38
1	AA	1130	A	C8-N7	6.98	1.36	1.31
22	BA	1508	A	C8-N7	6.98	1.36	1.31
1	AA	253	A	C8-N7	6.98	1.36	1.31
22	BA	644	A	C5-C4	-6.98	1.33	1.38
1	AA	192	A	C8-N7	6.98	1.36	1.31
22	BA	734	A	C5-C4	-6.97	1.33	1.38
22	BA	1103	A	C8-N7	6.97	1.36	1.31
22	BA	752	A	C5-C4	-6.97	1.33	1.38
1	AA	44	A	C8-N7	6.97	1.36	1.31
22	BA	1525	A	C5-C4	-6.97	1.33	1.38
22	BA	213	A	C5-C4	-6.96	1.33	1.38
1	AA	131	A	C8-N7	6.96	1.36	1.31
1	AA	1248	A	C8-N7	6.96	1.36	1.31
22	BA	900	A	C8-N7	6.96	1.36	1.31
22	BA	1469	A	C5-C4	-6.96	1.33	1.38
1	AA	1350	A	C8-N7	6.96	1.36	1.31
1	AA	1111	A	C8-N7	6.96	1.36	1.31
22	BA	1690	A	C5-C4	-6.95	1.33	1.38
22	BA	1978	A	C5-C4	-6.95	1.33	1.38
22	BA	2163	A	C8-N7	6.95	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	104	A	C5-C4	-6.95	1.33	1.38
22	BA	221	A	C5-C4	-6.95	1.33	1.38
22	BA	1095	A	N3-C4	6.95	1.39	1.34
22	BA	1608	A	C5-C4	-6.95	1.33	1.38
22	BA	167	A	C5-C4	-6.95	1.33	1.38
22	BA	2212	A	C5-C4	-6.95	1.33	1.38
22	BA	1802	A	N7-C5	-6.95	1.35	1.39
22	BA	2095	A	C5-C4	-6.95	1.33	1.38
1	AA	336	A	C5-C4	-6.95	1.33	1.38
22	BA	384	A	C5-C4	-6.95	1.33	1.38
1	AA	139	A	C8-N7	6.94	1.36	1.31
22	BA	1413	A	C8-N7	6.94	1.36	1.31
1	AA	1225	A	C8-N7	6.93	1.36	1.31
22	BA	2060	A	C5-C4	-6.93	1.33	1.38
22	BA	2082	A	C5-C4	-6.93	1.33	1.38
1	AA	8	A	C8-N7	6.93	1.36	1.31
1	AA	459	A	C8-N7	6.93	1.36	1.31
1	AA	1288	A	C8-N7	6.93	1.36	1.31
1	AA	1531	A	C8-N7	6.93	1.36	1.31
1	AA	872	A	C8-N7	6.93	1.36	1.31
22	BA	614	A	C8-N7	6.93	1.36	1.31
1	AA	393	A	C8-N7	6.93	1.36	1.31
22	BA	538	A	C5-C4	-6.93	1.33	1.38
22	BA	2311	A	C8-N7	6.92	1.36	1.31
1	AA	1261	A	C8-N7	6.92	1.36	1.31
1	AA	493	A	C8-N7	6.92	1.36	1.31
1	AA	143	A	C8-N7	6.92	1.36	1.31
1	AA	1152	A	C8-N7	6.92	1.36	1.31
22	BA	2900	A	C8-N7	6.92	1.36	1.31
22	BA	56	A	C5-C4	-6.91	1.33	1.38
22	BA	845	A	C5-C4	-6.91	1.33	1.38
23	BB	59	A	C5-C4	-6.91	1.33	1.38
1	AA	179	A	C8-N7	6.90	1.36	1.31
1	AA	694	A	C8-N7	6.90	1.36	1.31
22	BA	2198	A	C5-C4	-6.90	1.33	1.38
1	AA	496	A	C8-N7	6.90	1.36	1.31
1	AA	906	A	C5-C4	-6.90	1.33	1.38
22	BA	2792	A	C8-N7	6.90	1.36	1.31
1	AA	915	A	C8-N7	6.89	1.36	1.31
1	AA	1204	A	C8-N7	6.89	1.36	1.31
22	BA	470	A	C5-C4	-6.89	1.33	1.38
22	BA	1901	A	C5-C4	-6.89	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1362	A	C8-N7	6.89	1.36	1.31
1	AA	1446	A	C8-N7	6.89	1.36	1.31
22	BA	2287	A	C5-C4	-6.89	1.33	1.38
22	BA	2297	A	C5-C4	-6.89	1.33	1.38
1	AA	119	A	C8-N7	6.89	1.36	1.31
22	BA	905	A	C5-C4	-6.89	1.33	1.38
1	AA	460	A	C8-N7	6.89	1.36	1.31
1	AA	1180	A	C8-N7	6.89	1.36	1.31
1	AA	1502	A	C5-C4	-6.89	1.33	1.38
22	BA	2534	A	C5-C4	-6.89	1.33	1.38
1	AA	889	A	C5-C4	-6.88	1.33	1.38
1	AA	949	A	C8-N7	6.88	1.36	1.31
22	BA	2634	A	C5-C4	-6.88	1.33	1.38
1	AA	807	A	C5-C4	-6.88	1.33	1.38
1	AA	415	A	C8-N7	6.88	1.36	1.31
1	AA	129	A	C8-N7	6.88	1.36	1.31
1	AA	1176	A	C8-N7	6.88	1.36	1.31
1	AA	1513	A	C5-C4	-6.88	1.33	1.38
22	BA	13	A	C5-C4	-6.88	1.33	1.38
1	AA	747	A	C8-N7	6.88	1.36	1.31
1	AA	313	A	C5-C4	-6.87	1.33	1.38
1	AA	596	A	C8-N7	6.87	1.36	1.31
1	AA	681	A	C5-C4	-6.87	1.33	1.38
1	AA	1377	A	C8-N7	6.87	1.36	1.31
22	BA	165	A	C8-N7	6.87	1.36	1.31
22	BA	1301	A	C5-C4	-6.87	1.33	1.38
1	AA	1324	A	C8-N7	6.87	1.36	1.31
22	BA	2101	A	C8-N7	6.87	1.36	1.31
22	BA	2407	A	C5-C4	-6.87	1.33	1.38
1	AA	356	A	C8-N7	6.86	1.36	1.31
1	AA	968	A	C8-N7	6.86	1.36	1.31
22	BA	352	A	C8-N7	6.86	1.36	1.31
22	BA	2587	A	C5-C4	-6.86	1.33	1.38
22	BA	2314	A	C8-N7	6.86	1.36	1.31
22	BA	1918	A	C8-N7	6.86	1.36	1.31
55	B8	59	A	C8-N7	6.86	1.36	1.31
1	AA	1360	A	C8-N7	6.85	1.36	1.31
22	BA	1039	A	C5-C4	-6.85	1.33	1.38
22	BA	1439	A	C5-C4	-6.85	1.33	1.38
23	BB	108	A	C5-C4	-6.85	1.33	1.38
22	BA	2734	A	C5-C4	-6.84	1.33	1.38
1	AA	451	A	C8-N7	6.84	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	716	A	C5-C4	-6.84	1.33	1.38
22	BA	2191	A	C8-N7	6.84	1.36	1.31
1	AA	101	A	C8-N7	6.84	1.36	1.31
1	AA	243	A	C8-N7	6.84	1.36	1.31
1	AA	1306	A	C8-N7	6.83	1.36	1.31
22	BA	155	A	C5-C4	-6.83	1.33	1.38
22	BA	2171	A	N3-C4	6.83	1.39	1.34
23	BB	101	A	C5-C4	-6.83	1.33	1.38
1	AA	1157	A	C8-N7	6.83	1.36	1.31
1	AA	1431	A	C5-C4	-6.83	1.33	1.38
22	BA	705	A	C5-C4	-6.83	1.33	1.38
22	BA	439	A	C5-C4	-6.83	1.33	1.38
1	AA	116	A	C5-C4	-6.83	1.33	1.38
1	AA	583	A	C5-C4	-6.83	1.33	1.38
1	AA	831	A	C8-N7	6.83	1.36	1.31
1	AA	1396	A	C5-C4	-6.83	1.33	1.38
22	BA	1635	A	C5-C4	-6.83	1.33	1.38
1	AA	389	A	C8-N7	6.82	1.36	1.31
22	BA	1858	A	C5-C4	-6.82	1.33	1.38
22	BA	2426	A	C5-C4	-6.82	1.33	1.38
1	AA	344	A	C8-N7	6.82	1.36	1.31
1	AA	1410	A	C8-N7	6.82	1.36	1.31
22	BA	10	A	C5-C4	-6.82	1.33	1.38
1	AA	1254	A	C8-N7	6.82	1.36	1.31
1	AA	1188	A	C8-N7	6.82	1.36	1.31
22	BA	844	A	C5-C4	-6.82	1.33	1.38
22	BA	721	A	C8-N7	6.81	1.36	1.31
22	BA	613	A	N3-C4	6.81	1.39	1.34
22	BA	2851	A	C5-C4	-6.81	1.33	1.38
1	AA	938	A	C8-N7	6.81	1.36	1.31
1	AA	873	A	C5-C4	-6.81	1.33	1.38
1	AA	1368	A	C8-N7	6.81	1.36	1.31
1	AA	320	A	C8-N7	6.80	1.36	1.31
22	BA	1419	A	C8-N7	6.80	1.36	1.31
1	AA	1163	A	C8-N7	6.80	1.36	1.31
22	BA	1548	A	C5-C4	-6.80	1.33	1.38
22	BA	2734	A	C8-N7	6.80	1.36	1.31
1	AA	243	A	C5-C4	-6.80	1.33	1.38
1	AA	465	A	C8-N7	6.80	1.36	1.31
22	BA	2753	A	C5-C4	-6.80	1.33	1.38
1	AA	777	A	C5-C4	-6.80	1.33	1.38
23	BB	119	A	C8-N7	6.80	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1055	A	C8-N7	6.80	1.36	1.31
22	BA	28	A	C5-C4	-6.79	1.33	1.38
22	BA	74	A	C5-C4	-6.79	1.33	1.38
22	BA	84	A	C5-C4	-6.79	1.33	1.38
22	BA	781	A	C5-C4	-6.79	1.33	1.38
22	BA	1789	A	C5-C4	-6.79	1.33	1.38
22	BA	2670	A	C5-C4	-6.79	1.33	1.38
1	AA	673	A	C5-C4	-6.79	1.33	1.38
1	AA	573	A	C5-C4	-6.79	1.33	1.38
22	BA	1876	A	C8-N7	6.79	1.36	1.31
1	AA	246	A	C8-N7	6.79	1.36	1.31
22	BA	218	A	C5-C4	-6.79	1.33	1.38
22	BA	2547	A	C5-C4	-6.79	1.33	1.38
1	AA	602	A	C8-N7	6.78	1.36	1.31
1	AA	640	A	C8-N7	6.78	1.36	1.31
1	AA	174	A	C8-N7	6.78	1.36	1.31
22	BA	472	A	C5-C4	-6.78	1.34	1.38
1	AA	1239	A	C8-N7	6.78	1.36	1.31
22	BA	1502	A	C8-N7	6.78	1.36	1.31
22	BA	547	A	N3-C4	6.77	1.39	1.34
1	AA	1413	A	C8-N7	6.77	1.36	1.31
22	BA	2749	A	C5-C4	-6.77	1.34	1.38
1	AA	1105	A	C8-N7	6.77	1.36	1.31
22	BA	1302	A	C5-C4	-6.77	1.34	1.38
1	AA	1	A	C8-N7	6.77	1.36	1.31
1	AA	130	A	C8-N7	6.76	1.36	1.31
1	AA	535	A	C8-N7	6.76	1.36	1.31
22	BA	936	A	C5-C4	-6.76	1.34	1.38
1	AA	309	A	C5-C4	-6.76	1.34	1.38
1	AA	1016	A	C8-N7	6.76	1.36	1.31
1	AA	919	A	C8-N7	6.76	1.36	1.31
22	BA	2800	A	C8-N7	6.76	1.36	1.31
1	AA	274	A	C8-N7	6.75	1.36	1.31
22	BA	1759	A	C5-C4	-6.75	1.34	1.38
1	AA	478	A	N3-C4	6.75	1.39	1.34
1	AA	1433	A	C8-N7	6.75	1.36	1.31
1	AA	1483	A	C5-C4	-6.75	1.34	1.38
22	BA	1780	A	C5-C4	-6.75	1.34	1.38
1	AA	865	A	C5-C4	-6.75	1.34	1.38
1	AA	1227	A	C8-N7	6.75	1.36	1.31
1	AA	994	A	C8-N7	6.75	1.36	1.31
1	AA	655	A	C5-C4	-6.74	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	52	A	C5-C4	-6.74	1.34	1.38
23	BB	34	A	C8-N7	6.74	1.36	1.31
22	BA	793	A	C5-C4	-6.74	1.34	1.38
22	BA	1169	A	C5-C4	-6.74	1.34	1.38
22	BA	1544	A	C5-C4	-6.74	1.34	1.38
1	AA	663	A	C8-N7	6.73	1.36	1.31
22	BA	1705	A	C5-C4	-6.73	1.34	1.38
1	AA	1318	A	C8-N7	6.73	1.36	1.31
1	AA	935	A	C8-N7	6.73	1.36	1.31
22	BA	1717	A	C8-N7	6.72	1.36	1.31
1	AA	579	A	C5-C4	-6.72	1.34	1.38
22	BA	655	A	C5-C4	-6.72	1.34	1.38
22	BA	2135	A	N3-C4	6.72	1.38	1.34
22	BA	1069	A	N3-C4	6.72	1.38	1.34
1	AA	228	A	C8-N7	6.72	1.36	1.31
1	AA	499	A	C8-N7	6.72	1.36	1.31
1	AA	794	A	C5-C4	-6.72	1.34	1.38
1	AA	119	A	C5-C4	-6.71	1.34	1.38
22	BA	1504	A	C8-N7	6.71	1.36	1.31
1	AA	160	A	C8-N7	6.71	1.36	1.31
22	BA	172	A	C5-C4	-6.71	1.34	1.38
1	AA	532	A	N3-C4	6.71	1.38	1.34
22	BA	716	A	C8-N7	6.71	1.36	1.31
22	BA	718	A	C8-N7	6.71	1.36	1.31
22	BA	1014	A	C5-C4	-6.71	1.34	1.38
1	AA	1171	A	C8-N7	6.71	1.36	1.31
22	BA	1535	A	N3-C4	6.71	1.38	1.34
1	AA	845	A	N3-C4	6.70	1.38	1.34
1	AA	676	A	C5-C4	-6.70	1.34	1.38
1	AA	59	A	C8-N7	6.70	1.36	1.31
1	AA	969	A	C8-N7	6.70	1.36	1.31
22	BA	996	A	C5-C4	-6.70	1.34	1.38
1	AA	364	A	C8-N7	6.70	1.36	1.31
22	BA	2388	A	N7-C5	-6.70	1.35	1.39
1	AA	26	A	C5-C4	-6.69	1.34	1.38
22	BA	244	A	C5-C4	-6.69	1.34	1.38
22	BA	2406	A	C5-C4	-6.69	1.34	1.38
1	AA	675	A	C5-C4	-6.69	1.34	1.38
22	BA	614	A	C5-C4	-6.69	1.34	1.38
22	BA	1453	A	C5-C4	-6.69	1.34	1.38
1	AA	539	A	C8-N7	6.69	1.36	1.31
22	BA	1057	A	N3-C4	6.69	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1916	A	C8-N7	6.69	1.36	1.31
22	BA	2142	A	N3-C4	6.69	1.38	1.34
22	BA	161	A	C5-C4	-6.69	1.34	1.38
22	BA	507	A	C8-N7	6.69	1.36	1.31
1	AA	1534	A	N3-C4	6.69	1.38	1.34
1	AA	1456	A	C8-N7	6.68	1.36	1.31
22	BA	226	A	C5-C4	-6.68	1.34	1.38
1	AA	642	A	C8-N7	6.68	1.36	1.31
1	AA	983	A	C8-N7	6.68	1.36	1.31
23	BB	115	A	C5-C4	-6.68	1.34	1.38
1	AA	802	A	C5-C4	-6.68	1.34	1.38
22	BA	1717	A	C5-C4	-6.68	1.34	1.38
22	BA	125	A	C5-C4	-6.68	1.34	1.38
1	AA	729	A	C8-N7	6.68	1.36	1.31
1	AA	1110	A	C8-N7	6.68	1.36	1.31
22	BA	1590	A	C8-N7	6.68	1.36	1.31
1	AA	309	A	C8-N7	6.67	1.36	1.31
1	AA	946	A	C8-N7	6.67	1.36	1.31
1	AA	349	A	C5-C4	-6.67	1.34	1.38
1	AA	374	A	C8-N7	6.67	1.36	1.31
22	BA	345	A	C5-C4	-6.67	1.34	1.38
23	BB	53	A	C8-N7	6.67	1.36	1.31
1	AA	918	A	C8-N7	6.67	1.36	1.31
22	BA	928	A	C5-C4	-6.67	1.34	1.38
1	AA	782	A	C5-C4	-6.67	1.34	1.38
1	AA	371	A	C5-C4	-6.66	1.34	1.38
1	AA	50	A	C8-N7	6.66	1.36	1.31
1	AA	1465	A	C5-C4	-6.66	1.34	1.38
22	BA	2887	A	C5-C4	-6.66	1.34	1.38
1	AA	600	A	C8-N7	6.66	1.36	1.31
22	BA	1021	A	C5-C4	-6.66	1.34	1.38
22	BA	1040	A	C5-C4	-6.66	1.34	1.38
22	BA	324	A	C5-C4	-6.65	1.34	1.38
1	AA	792	A	C5-C4	-6.65	1.34	1.38
1	AA	1394	A	C8-N7	6.65	1.36	1.31
22	BA	142	A	C5-C4	-6.65	1.34	1.38
22	BA	2170	A	N3-C4	6.65	1.38	1.34
22	BA	1070	A	N3-C4	6.65	1.38	1.34
22	BA	2126	A	N3-C4	6.65	1.38	1.34
23	BB	29	A	C5-C4	-6.65	1.34	1.38
1	AA	487	A	C8-N7	6.64	1.36	1.31
1	AA	498	A	N3-C4	6.64	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	595	A	C8-N7	6.64	1.36	1.31
1	AA	695	A	C8-N7	6.64	1.36	1.31
22	BA	1821	A	C5-C4	-6.64	1.34	1.38
22	BA	2117	A	N3-C4	6.64	1.38	1.34
22	BA	2700	A	C5-C4	-6.64	1.34	1.38
1	AA	1271	A	C8-N7	6.64	1.36	1.31
1	AA	1503	A	C8-N7	6.64	1.36	1.31
22	BA	5	A	C5-C4	-6.64	1.34	1.38
22	BA	2154	A	N3-C4	6.64	1.38	1.34
1	AA	792	A	C8-N7	6.63	1.36	1.31
22	BA	320	A	C5-C4	-6.63	1.34	1.38
22	BA	751	A	C5-C4	-6.63	1.34	1.38
1	AA	78	A	N3-C4	6.63	1.38	1.34
22	BA	2749	A	C8-N7	6.63	1.36	1.31
1	AA	1480	A	C8-N7	6.63	1.36	1.31
22	BA	603	A	C8-N7	6.63	1.36	1.31
22	BA	933	A	C5-C4	-6.63	1.34	1.38
1	AA	825	A	C8-N7	6.62	1.36	1.31
1	AA	1418	A	C5-C4	-6.62	1.34	1.38
22	BA	616	A	C5-C4	-6.62	1.34	1.38
1	AA	19	A	C5-C4	-6.62	1.34	1.38
1	AA	1434	A	C5-C4	-6.62	1.34	1.38
22	BA	95	A	C5-C4	-6.62	1.34	1.38
1	AA	572	A	C8-N7	6.62	1.36	1.31
1	AA	19	A	C8-N7	6.61	1.36	1.31
1	AA	1238	A	C8-N7	6.61	1.36	1.31
22	BA	2392	A	C5-C4	-6.61	1.34	1.38
1	AA	607	A	C8-N7	6.61	1.36	1.31
1	AA	1434	A	C8-N7	6.61	1.36	1.31
1	AA	1502	A	C8-N7	6.61	1.36	1.31
22	BA	182	A	C5-C4	-6.61	1.34	1.38
22	BA	655	A	C8-N7	6.61	1.36	1.31
1	AA	865	A	C8-N7	6.61	1.36	1.31
1	AA	909	A	C8-N7	6.61	1.36	1.31
1	AA	197	A	C8-N7	6.61	1.36	1.31
1	AA	482	A	C8-N7	6.61	1.36	1.31
22	BA	10	A	C8-N7	6.61	1.36	1.31
22	BA	1088	A	N3-C4	6.61	1.38	1.34
22	BA	1713	A	C8-N7	6.61	1.36	1.31
1	AA	819	A	C8-N7	6.60	1.36	1.31
22	BA	160	A	C8-N7	6.60	1.36	1.31
22	BA	1801	A	C5-C4	-6.60	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2451	A	C5-C4	-6.60	1.34	1.38
1	AA	892	A	C5-C4	-6.60	1.34	1.38
22	BA	2733	A	C5-C4	-6.59	1.34	1.38
23	BB	15	A	C8-N7	6.59	1.36	1.31
1	AA	199	A	C8-N7	6.59	1.36	1.31
1	AA	510	A	C8-N7	6.59	1.36	1.31
1	AA	533	A	C8-N7	6.59	1.36	1.31
22	BA	2062	A	C8-N7	6.59	1.36	1.31
22	BA	2377	A	C5-C4	-6.59	1.34	1.38
1	AA	630	A	C8-N7	6.59	1.36	1.31
1	AA	959	A	C8-N7	6.58	1.36	1.31
22	BA	866	A	C5-C4	-6.58	1.34	1.38
1	AA	728	A	C8-N7	6.58	1.36	1.31
1	AA	780	A	C5-C4	-6.58	1.34	1.38
22	BA	722	A	C8-N7	6.58	1.36	1.31
22	BA	1553	A	C5-C4	-6.58	1.34	1.38
1	AA	338	A	C5-C4	-6.58	1.34	1.38
22	BA	2778	A	C5-C4	-6.58	1.34	1.38
1	AA	10	A	C5-C4	-6.57	1.34	1.38
1	AA	635	A	C8-N7	6.57	1.36	1.31
22	BA	2284	A	C5-C4	-6.57	1.34	1.38
1	AA	1179	A	N3-C4	6.57	1.38	1.34
22	BA	1359	A	C8-N7	6.57	1.36	1.31
1	AA	236	A	C8-N7	6.57	1.36	1.31
1	AA	306	A	C8-N7	6.56	1.36	1.31
1	AA	151	A	C8-N7	6.56	1.36	1.31
1	AA	553	A	C8-N7	6.56	1.36	1.31
1	AA	26	A	C8-N7	6.56	1.36	1.31
1	AA	1408	A	C5-C4	-6.56	1.34	1.38
1	AA	1468	A	C5-C4	-6.56	1.34	1.38
22	BA	2821	A	C5-C4	-6.56	1.34	1.38
1	AA	935	A	C5-C4	-6.56	1.34	1.38
1	AA	665	A	C5-C4	-6.56	1.34	1.38
22	BA	146	A	C8-N7	6.56	1.36	1.31
1	AA	1046	A	C8-N7	6.55	1.36	1.31
1	AA	1170	A	C8-N7	6.55	1.36	1.31
1	AA	366	A	C8-N7	6.55	1.36	1.31
1	AA	509	A	C8-N7	6.55	1.36	1.31
1	AA	560	A	C8-N7	6.55	1.36	1.31
22	BA	1586	A	C8-N7	6.55	1.36	1.31
1	AA	303	A	C8-N7	6.55	1.36	1.31
22	BA	802	A	C5-C4	-6.55	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	608	A	C5-C4	-6.55	1.34	1.38
1	AA	1500	A	C5-C4	-6.55	1.34	1.38
22	BA	1591	A	C8-N7	6.55	1.36	1.31
22	BA	2205	A	C5-C4	-6.55	1.34	1.38
1	AA	363	A	C5-C4	-6.55	1.34	1.38
22	BA	1169	A	C8-N7	6.55	1.36	1.31
22	BA	896	A	N3-C4	6.54	1.38	1.34
1	AA	964	A	C8-N7	6.54	1.36	1.31
1	AA	1476	A	C8-N7	6.54	1.36	1.31
22	BA	144	A	C5-C4	-6.54	1.34	1.38
1	AA	1021	A	N3-C4	6.54	1.38	1.34
22	BA	2059	A	C5-C4	-6.54	1.34	1.38
22	BA	344	A	C8-N7	6.54	1.36	1.31
1	AA	1339	A	C8-N7	6.54	1.36	1.31
22	BA	342	A	C8-N7	6.54	1.36	1.31
22	BA	1744	A	C8-N7	6.54	1.36	1.31
23	BB	29	A	C8-N7	6.54	1.36	1.31
22	BA	2298	A	C8-N7	6.54	1.36	1.31
23	BB	73	A	C5-C4	-6.54	1.34	1.38
1	AA	919	A	C5-C4	-6.53	1.34	1.38
1	AA	1004	A	N3-C4	6.53	1.38	1.34
22	BA	1050	A	C5-C4	-6.53	1.34	1.38
22	BA	64	A	C5-C4	-6.53	1.34	1.38
22	BA	428	A	C5-C4	-6.53	1.34	1.38
22	BA	1669	A	C5-C4	-6.53	1.34	1.38
22	BA	1746	A	C8-N7	6.53	1.36	1.31
22	BA	342	A	C5-C4	-6.53	1.34	1.38
22	BA	404	A	C8-N7	6.53	1.36	1.31
23	BB	108	A	C8-N7	6.53	1.36	1.31
1	AA	414	A	C8-N7	6.52	1.36	1.31
22	BA	1000	A	N7-C5	-6.52	1.35	1.39
22	BA	2602	A	N3-C4	6.52	1.38	1.34
1	AA	238	A	C8-N7	6.52	1.36	1.31
1	AA	430	A	C8-N7	6.52	1.36	1.31
1	AA	914	A	C5-C4	-6.52	1.34	1.38
1	AA	246	A	C5-C4	-6.52	1.34	1.38
1	AA	1499	A	C5-C4	-6.51	1.34	1.38
22	BA	191	A	N7-C5	-6.51	1.35	1.39
1	AA	574	A	C8-N7	6.51	1.36	1.31
22	BA	513	A	N7-C5	-6.51	1.35	1.39
22	BA	2184	A	N3-C4	6.51	1.38	1.34
1	AA	32	A	C5-C4	-6.51	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	315	A	C8-N7	6.51	1.36	1.31
22	BA	2095	A	C8-N7	6.51	1.36	1.31
1	AA	373	A	C8-N7	6.51	1.36	1.31
22	BA	2856	A	C5-C4	-6.51	1.34	1.38
23	BB	57	A	C8-N7	6.51	1.36	1.31
1	AA	563	A	C8-N7	6.51	1.36	1.31
22	BA	666	A	C5-C4	-6.51	1.34	1.38
22	BA	1054	A	C8-N7	6.51	1.36	1.31
22	BA	1204	A	C5-C4	-6.51	1.34	1.38
1	AA	777	A	C8-N7	6.50	1.36	1.31
22	BA	1039	A	C8-N7	6.50	1.36	1.31
22	BA	1434	A	C8-N7	6.50	1.36	1.31
22	BA	52	A	N7-C5	-6.50	1.35	1.39
22	BA	1477	A	C5-C4	-6.50	1.34	1.38
1	AA	16	A	C8-N7	6.50	1.36	1.31
1	AA	28	A	C8-N7	6.50	1.36	1.31
22	BA	217	A	C5-C4	-6.50	1.34	1.38
22	BA	1321	A	C5-C4	-6.50	1.34	1.38
1	AA	315	A	C5-C4	-6.50	1.34	1.38
1	AA	759	A	C8-N7	6.50	1.36	1.31
22	BA	1032	A	C8-N7	6.50	1.36	1.31
22	BA	2476	A	C5-C4	-6.50	1.34	1.38
1	AA	1437	A	C5-C4	-6.49	1.34	1.38
1	AA	288	A	C5-C4	-6.49	1.34	1.38
1	AA	687	A	C8-N7	6.49	1.36	1.31
22	BA	866	A	C8-N7	6.49	1.36	1.31
22	BA	2352	A	C5-C4	-6.49	1.34	1.38
1	AA	161	A	C8-N7	6.48	1.36	1.31
1	AA	1042	A	N3-C4	6.48	1.38	1.34
1	AA	1507	A	C8-N7	6.48	1.36	1.31
1	AA	81	A	N3-C4	6.48	1.38	1.34
1	AA	1480	A	C5-C4	-6.48	1.34	1.38
22	BA	1757	A	C5-C4	-6.48	1.34	1.38
1	AA	80	A	C8-N7	6.48	1.36	1.31
1	AA	262	A	C8-N7	6.48	1.36	1.31
1	AA	349	A	C8-N7	6.48	1.36	1.31
1	AA	353	A	C8-N7	6.47	1.36	1.31
1	AA	1225	A	N3-C4	6.47	1.38	1.34
1	AA	1236	A	C8-N7	6.47	1.36	1.31
22	BA	1103	A	N3-C4	6.47	1.38	1.34
22	BA	1936	A	C5-C4	-6.47	1.34	1.38
1	AA	298	A	C8-N7	6.47	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	156	A	C8-N7	6.47	1.36	1.31
22	BA	1713	A	C5-C4	-6.47	1.34	1.38
1	AA	382	A	C8-N7	6.47	1.36	1.31
1	AA	787	A	C5-C4	-6.47	1.34	1.38
22	BA	1321	A	C8-N7	6.47	1.36	1.31
22	BA	2406	A	C8-N7	6.47	1.36	1.31
1	AA	353	A	C5-C4	-6.47	1.34	1.38
1	AA	819	A	C5-C4	-6.46	1.34	1.38
1	AA	1022	A	N3-C4	6.46	1.38	1.34
1	AA	1408	A	C8-N7	6.46	1.36	1.31
22	BA	104	A	C5-C4	-6.46	1.34	1.38
1	AA	546	A	C8-N7	6.46	1.36	1.31
22	BA	1322	A	C5-C4	-6.46	1.34	1.38
22	BA	2879	A	C5-C4	-6.46	1.34	1.38
1	AA	250	A	N3-C4	6.46	1.38	1.34
22	BA	685	A	N7-C5	-6.46	1.35	1.39
22	BA	1593	A	C8-N7	6.46	1.36	1.31
22	BA	1877	A	C5-C4	-6.46	1.34	1.38
22	BA	2814	A	C5-C4	-6.46	1.34	1.38
22	BA	715	A	C8-N7	6.46	1.36	1.31
22	BA	2059	A	C8-N7	6.46	1.36	1.31
1	AA	496	A	N3-C4	6.46	1.38	1.34
1	AA	559	A	C8-N7	6.45	1.36	1.31
1	AA	743	A	C5-C4	-6.45	1.34	1.38
22	BA	1089	A	N3-C4	6.45	1.38	1.34
22	BA	1515	A	C5-C4	-6.45	1.34	1.38
1	AA	702	A	C5-C4	-6.44	1.34	1.38
1	AA	499	A	N3-C4	6.44	1.38	1.34
1	AA	1102	A	C8-N7	6.44	1.36	1.31
22	BA	1054	A	N3-C4	6.44	1.38	1.34
22	BA	2657	A	C5-C4	-6.44	1.34	1.38
22	BA	528	A	C5-C4	-6.44	1.34	1.38
22	BA	927	A	C8-N7	6.44	1.36	1.31
1	AA	676	A	C8-N7	6.44	1.36	1.31
22	BA	2163	A	N3-C4	6.43	1.38	1.34
1	AA	1271	A	N3-C4	6.43	1.38	1.34
22	BA	270	A	C5-C4	-6.43	1.34	1.38
22	BA	556	A	C8-N7	6.43	1.36	1.31
22	BA	1490	A	N3-C4	6.43	1.38	1.34
1	AA	889	A	C8-N7	6.43	1.36	1.31
22	BA	1866	A	C5-C4	-6.43	1.34	1.38
1	AA	171	A	C5-C4	-6.42	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1689	A	C5-C4	-6.42	1.34	1.38
1	AA	1375	A	C8-N7	6.42	1.36	1.31
1	AA	977	A	C8-N7	6.42	1.36	1.31
22	BA	155	A	C8-N7	6.42	1.36	1.31
1	AA	746	A	C8-N7	6.42	1.36	1.31
1	AA	66	A	C8-N7	6.42	1.36	1.31
1	AA	1261	A	N3-C4	6.42	1.38	1.34
22	BA	2886	A	C8-N7	6.42	1.36	1.31
1	AA	1398	A	C5-C4	-6.41	1.34	1.38
22	BA	2434	A	C8-N7	6.41	1.36	1.31
1	AA	1081	A	C5-C4	-6.41	1.34	1.38
1	AA	1201	A	C8-N7	6.41	1.36	1.31
22	BA	1495	A	C5-C4	-6.41	1.34	1.38
1	AA	864	A	C8-N7	6.41	1.36	1.31
1	AA	1082	A	C8-N7	6.40	1.36	1.31
22	BA	483	A	C5-C4	-6.40	1.34	1.38
22	BA	730	A	C5-C4	-6.40	1.34	1.38
22	BA	1503	A	C5-C4	-6.40	1.34	1.38
22	BA	1745	A	C8-N7	6.40	1.36	1.31
1	AA	205	A	N3-C4	6.40	1.38	1.34
1	AA	53	A	C8-N7	6.40	1.36	1.31
23	BB	50	A	C8-N7	6.40	1.36	1.31
22	BA	345	A	C8-N7	6.40	1.36	1.31
1	AA	282	A	C8-N7	6.40	1.36	1.31
1	AA	1430	A	C5-C4	-6.40	1.34	1.38
23	BB	94	A	C5-C4	-6.40	1.34	1.38
22	BA	1545	A	C5-C4	-6.39	1.34	1.38
22	BA	2757	A	C5-C4	-6.39	1.34	1.38
22	BA	1020	A	C5-C4	-6.39	1.34	1.38
22	BA	2114	A	N3-C4	6.39	1.38	1.34
1	AA	66	A	C5-C4	-6.39	1.34	1.38
1	AA	1507	A	C5-C4	-6.39	1.34	1.38
22	BA	2835	A	C8-N7	6.38	1.36	1.31
1	AA	77	A	N3-C4	6.38	1.38	1.34
1	AA	435	A	N3-C4	6.38	1.38	1.34
22	BA	2670	A	C8-N7	6.38	1.36	1.31
22	BA	2471	A	C8-N7	6.38	1.36	1.31
22	BA	2309	A	N3-C4	6.38	1.38	1.34
22	BA	2317	A	C8-N7	6.38	1.36	1.31
23	BB	109	A	C8-N7	6.38	1.36	1.31
1	AA	583	A	C8-N7	6.37	1.36	1.31
22	BA	146	A	C5-C4	-6.37	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1257	A	N3-C4	6.37	1.38	1.34
22	BA	782	A	N7-C5	-6.37	1.35	1.39
6	AF	65	GLU	CG-CD	-6.37	1.42	1.51
22	BA	2430	A	C8-N7	6.37	1.36	1.31
22	BA	368	A	C8-N7	6.36	1.36	1.31
22	BA	2657	A	C8-N7	6.36	1.36	1.31
1	AA	759	A	C5-C4	-6.36	1.34	1.38
22	BA	2872	A	C5-C4	-6.36	1.34	1.38
1	AA	913	A	C8-N7	6.36	1.36	1.31
22	BA	125	A	C8-N7	6.36	1.36	1.31
22	BA	2531	A	C5-C4	-6.36	1.34	1.38
22	BA	2534	A	C8-N7	6.36	1.36	1.31
23	BB	34	A	C5-C4	-6.35	1.34	1.38
1	AA	915	A	C5-C4	-6.35	1.34	1.38
23	BB	66	A	C8-N7	6.35	1.35	1.31
1	AA	706	A	C8-N7	6.35	1.35	1.31
1	AA	609	A	C8-N7	6.35	1.35	1.31
22	BA	101	A	C5-C4	-6.35	1.34	1.38
1	AA	288	A	C8-N7	6.35	1.35	1.31
1	AA	1081	A	C8-N7	6.35	1.35	1.31
1	AA	456	A	N3-C4	6.34	1.38	1.34
22	BA	1522	A	C8-N7	6.34	1.35	1.31
22	BA	2899	A	C5-C4	-6.34	1.34	1.38
22	BA	2899	A	C8-N7	6.34	1.35	1.31
49	B1	44	ARG	CB-CG	-6.34	1.35	1.52
1	AA	190	A	N3-C4	6.34	1.38	1.34
22	BA	1876	A	C5-C4	-6.34	1.34	1.38
22	BA	1590	A	C5-C4	-6.34	1.34	1.38
22	BA	2298	A	C5-C4	-6.34	1.34	1.38
22	BA	933	A	C8-N7	6.34	1.35	1.31
22	BA	1241	A	C5-C4	-6.33	1.34	1.38
1	AA	704	A	C5-C4	-6.33	1.34	1.38
22	BA	111	A	C8-N7	6.33	1.35	1.31
22	BA	213	A	C8-N7	6.33	1.35	1.31
22	BA	255	A	N7-C5	-6.33	1.35	1.39
22	BA	404	A	C5-C4	-6.33	1.34	1.38
22	BA	1073	A	N3-C4	6.33	1.38	1.34
1	AA	909	A	C5-C4	-6.33	1.34	1.38
22	BA	2753	A	C8-N7	6.33	1.35	1.31
1	AA	546	A	C5-C4	-6.33	1.34	1.38
1	AA	1410	A	C5-C4	-6.33	1.34	1.38
22	BA	1230	A	C5-C4	-6.33	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	51	A	C8-N7	6.32	1.35	1.31
22	BA	270	A	C8-N7	6.32	1.35	1.31
22	BA	905	A	C8-N7	6.32	1.35	1.31
1	AA	263	A	C8-N7	6.32	1.35	1.31
22	BA	1525	A	C8-N7	6.32	1.35	1.31
22	BA	1912	A	C8-N7	6.32	1.35	1.31
22	BA	346	A	C5-C4	-6.32	1.34	1.38
22	BA	845	A	C8-N7	6.32	1.35	1.31
1	AA	784	A	C8-N7	6.32	1.35	1.31
22	BA	160	A	C5-C4	-6.32	1.34	1.38
22	BA	2173	A	N3-C4	6.32	1.38	1.34
1	AA	498	A	C8-N7	6.31	1.35	1.31
22	BA	294	A	C5-C4	-6.31	1.34	1.38
22	BA	2033	A	C8-N7	6.31	1.35	1.31
1	AA	702	A	C8-N7	6.31	1.35	1.31
1	AA	1152	A	N3-C4	6.31	1.38	1.34
22	BA	2654	A	C8-N7	6.31	1.35	1.31
22	BA	2482	A	C8-N7	6.31	1.35	1.31
22	BA	2893	A	C5-C4	-6.31	1.34	1.38
1	AA	687	A	C5-C4	-6.31	1.34	1.38
22	BA	233	A	C5-C4	-6.31	1.34	1.38
22	BA	979	A	C8-N7	6.31	1.35	1.31
1	AA	1	A	N3-C4	6.31	1.38	1.34
22	BA	1096	A	N3-C4	6.31	1.38	1.34
22	BA	1579	A	C8-N7	6.31	1.35	1.31
22	BA	344	A	C5-C4	-6.31	1.34	1.38
1	AA	1000	A	N3-C4	6.30	1.38	1.34
1	AA	461	A	N3-C4	6.30	1.38	1.34
22	BA	1858	A	C8-N7	6.30	1.35	1.31
22	BA	2497	A	N7-C5	-6.30	1.35	1.39
22	BA	2727	A	N7-C5	-6.30	1.35	1.39
22	BA	1477	A	C8-N7	6.30	1.35	1.31
1	AA	51	A	C5-C4	-6.30	1.34	1.38
22	BA	482	A	C5-C4	-6.30	1.34	1.38
1	AA	1476	A	C5-C4	-6.29	1.34	1.38
22	BA	2158	A	N3-C4	6.29	1.38	1.34
22	BA	2191	A	N3-C4	6.29	1.38	1.34
22	BA	2758	A	C8-N7	6.29	1.35	1.31
1	AA	718	A	C8-N7	6.29	1.35	1.31
1	AA	781	A	C5-C4	-6.29	1.34	1.38
1	AA	1275	A	N3-C4	6.29	1.38	1.34
22	BA	1253	A	C8-N7	6.29	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1544	A	C8-N7	6.29	1.35	1.31
22	BA	1640	A	C8-N7	6.29	1.35	1.31
23	BB	39	A	C5-C4	-6.29	1.34	1.38
1	AA	10	A	C8-N7	6.29	1.35	1.31
22	BA	1098	A	N3-C4	6.29	1.38	1.34
22	BA	788	A	N7-C5	-6.28	1.35	1.39
22	BA	1847	A	C8-N7	6.28	1.35	1.31
22	BA	927	A	C5-C4	-6.28	1.34	1.38
22	BA	936	A	C8-N7	6.28	1.35	1.31
22	BA	1111	A	C5-C4	-6.28	1.34	1.38
22	BA	556	A	C5-C4	-6.28	1.34	1.38
22	BA	2108	A	N3-C4	6.28	1.38	1.34
22	BA	2665	A	C8-N7	6.28	1.35	1.31
1	AA	1105	A	C5-C4	-6.28	1.34	1.38
22	BA	1010	A	N7-C5	-6.28	1.35	1.39
22	BA	1090	A	N3-C4	6.28	1.38	1.34
22	BA	64	A	C8-N7	6.27	1.35	1.31
22	BA	2820	A	C8-N7	6.27	1.35	1.31
22	BA	483	A	C8-N7	6.27	1.35	1.31
22	BA	492	A	C5-C4	-6.27	1.34	1.38
23	BB	115	A	C8-N7	6.27	1.35	1.31
55	B8	69	A	N3-C4	6.27	1.38	1.34
1	AA	7	A	C5-C4	-6.27	1.34	1.38
1	AA	608	A	C8-N7	6.26	1.35	1.31
22	BA	1134	A	C8-N7	6.26	1.35	1.31
22	BA	2449	U	N1-C6	6.26	1.43	1.38
1	AA	279	A	C8-N7	6.26	1.35	1.31
1	AA	1191	A	C8-N7	6.26	1.35	1.31
1	AA	1441	A	N3-C4	6.26	1.38	1.34
1	AA	397	A	C5-C4	-6.26	1.34	1.38
1	AA	878	A	C5-C4	-6.26	1.34	1.38
22	BA	348	A	C8-N7	6.26	1.35	1.31
22	BA	1872	A	C8-N7	6.26	1.35	1.31
55	B8	26	A	N3-C4	6.25	1.38	1.34
1	AA	298	A	C5-C4	-6.25	1.34	1.38
1	AA	712	A	C5-C4	-6.25	1.34	1.38
22	BA	504	A	N3-C4	6.25	1.38	1.34
22	BA	2632	A	C8-N7	6.25	1.35	1.31
22	BA	2750	A	C8-N7	6.25	1.35	1.31
1	AA	1493	A	N3-C4	6.25	1.38	1.34
22	BA	149	A	C5-C4	-6.25	1.34	1.38
1	AA	681	A	C8-N7	6.25	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	15	A	C5-C4	-6.25	1.34	1.38
1	AA	1433	A	C5-C4	-6.25	1.34	1.38
22	BA	479	A	C8-N7	6.25	1.35	1.31
22	BA	1579	A	C5-C4	-6.25	1.34	1.38
23	BB	109	A	C5-C4	-6.25	1.34	1.38
1	AA	33	A	C8-N7	6.24	1.35	1.31
1	AA	560	A	C5-C4	-6.24	1.34	1.38
22	BA	2566	A	C8-N7	6.24	1.35	1.31
22	BA	2800	A	C5-C4	-6.24	1.34	1.38
22	BA	2887	A	C8-N7	6.24	1.35	1.31
22	BA	172	A	C8-N7	6.24	1.35	1.31
23	BB	45	A	C8-N7	6.23	1.35	1.31
22	BA	111	A	C5-C4	-6.23	1.34	1.38
23	BB	66	A	C5-C4	-6.23	1.34	1.38
1	AA	1396	A	C8-N7	6.23	1.35	1.31
22	BA	119	A	C8-N7	6.23	1.35	1.31
22	BA	1505	A	N3-C4	6.23	1.38	1.34
1	AA	236	A	C5-C4	-6.23	1.34	1.38
22	BA	63	A	C8-N7	6.23	1.35	1.31
1	AA	8	A	C5-C4	-6.22	1.34	1.38
22	BA	2176	A	N3-C4	6.22	1.38	1.34
1	AA	263	A	C5-C4	-6.22	1.34	1.38
1	AA	1374	A	C8-N7	6.22	1.35	1.31
1	AA	1437	A	C8-N7	6.22	1.35	1.31
22	BA	1918	A	C5-C4	-6.22	1.34	1.38
1	AA	336	A	C8-N7	6.22	1.35	1.31
1	AA	162	A	C5-C4	-6.22	1.34	1.38
1	AA	1080	A	C8-N7	6.22	1.35	1.31
22	BA	1134	A	C5-C4	-6.22	1.34	1.38
23	BB	39	A	C8-N7	6.22	1.35	1.31
1	AA	553	A	C5-C4	-6.21	1.34	1.38
22	BA	2654	A	C5-C4	-6.21	1.34	1.38
1	AA	695	A	C5-C4	-6.21	1.34	1.38
22	BA	89	A	C8-N7	6.21	1.35	1.31
22	BA	2205	A	C8-N7	6.21	1.35	1.31
1	AA	1428	A	C8-N7	6.21	1.35	1.31
1	AA	466	A	N3-C4	6.21	1.38	1.34
22	BA	2809	A	C8-N7	6.21	1.35	1.31
1	AA	411	A	C5-C4	-6.21	1.34	1.38
22	BA	1084	A	N3-C4	6.21	1.38	1.34
22	BA	1528	A	C5-C4	-6.21	1.34	1.38
1	AA	510	A	C5-C4	-6.20	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	574	A	C5-C4	-6.20	1.34	1.38
1	AA	1429	A	C8-N7	6.20	1.35	1.31
1	AA	1492	A	N3-C4	6.20	1.38	1.34
22	BA	439	A	C8-N7	6.20	1.35	1.31
22	BA	1655	A	C5-C4	-6.20	1.34	1.38
22	BA	346	A	C8-N7	6.20	1.35	1.31
22	BA	2317	A	C5-C4	-6.20	1.34	1.38
22	BA	2634	A	C8-N7	6.20	1.35	1.31
22	BA	1165	A	C8-N7	6.20	1.35	1.31
1	AA	728	A	C5-C4	-6.20	1.34	1.38
1	AA	729	A	C5-C4	-6.20	1.34	1.38
22	BA	2565	A	N7-C5	-6.20	1.35	1.39
1	AA	1080	A	C5-C4	-6.19	1.34	1.38
1	AA	1236	A	N3-C4	6.19	1.38	1.34
1	AA	55	A	C8-N7	6.19	1.35	1.31
1	AA	274	A	C5-C4	-6.19	1.34	1.38
1	AA	1201	A	N3-C4	6.19	1.38	1.34
22	BA	1230	A	C8-N7	6.19	1.35	1.31
22	BA	1735	A	C8-N7	6.19	1.35	1.31
22	BA	272	A	C5-C4	-6.19	1.34	1.38
22	BA	144	A	C8-N7	6.18	1.35	1.31
22	BA	1848	A	C8-N7	6.18	1.35	1.31
22	BA	1854	A	N7-C5	-6.18	1.35	1.39
1	AA	109	A	C8-N7	6.18	1.35	1.31
22	BA	91	A	C5-C4	-6.18	1.34	1.38
22	BA	217	A	C8-N7	6.18	1.35	1.31
22	BA	94	A	C8-N7	6.18	1.35	1.31
22	BA	749	A	C8-N7	6.18	1.35	1.31
1	AA	270	A	C5-C4	-6.18	1.34	1.38
1	AA	977	A	C5-C4	-6.18	1.34	1.38
1	AA	306	A	N3-C4	6.18	1.38	1.34
1	AA	502	A	C8-N7	6.18	1.35	1.31
23	BB	46	A	C8-N7	6.18	1.35	1.31
1	AA	1508	A	C5-C4	-6.17	1.34	1.38
22	BA	142	A	C8-N7	6.17	1.35	1.31
22	BA	2733	A	C8-N7	6.17	1.35	1.31
1	AA	270	A	C8-N7	6.17	1.35	1.31
1	AA	1101	A	C5-C4	-6.17	1.34	1.38
1	AA	411	A	N3-C4	6.17	1.38	1.34
22	BA	2792	A	C5-C4	-6.17	1.34	1.38
23	BB	58	A	C8-N7	6.17	1.35	1.31
22	BA	1302	A	C8-N7	6.17	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	465	A	N3-C4	6.17	1.38	1.34
22	BA	1204	A	C8-N7	6.17	1.35	1.31
23	BB	50	A	C5-C4	-6.17	1.34	1.38
1	AA	327	A	C5-C4	-6.16	1.34	1.38
1	AA	448	A	N3-C4	6.16	1.38	1.34
22	BA	761	A	C8-N7	6.16	1.35	1.31
1	AA	262	A	C5-C4	-6.16	1.34	1.38
22	BA	44	A	C8-N7	6.16	1.35	1.31
1	AA	197	A	C5-C4	-6.16	1.34	1.38
1	AA	766	A	C8-N7	6.16	1.35	1.31
22	BA	616	A	C8-N7	6.16	1.35	1.31
22	BA	1690	A	C8-N7	6.16	1.35	1.31
22	BA	1744	A	C5-C4	-6.16	1.34	1.38
22	BA	2740	A	N7-C5	-6.16	1.35	1.39
1	AA	937	A	C8-N7	6.16	1.35	1.31
1	AA	1197	A	C8-N7	6.16	1.35	1.31
22	BA	156	A	C5-C4	-6.16	1.34	1.38
22	BA	1040	A	C8-N7	6.16	1.35	1.31
22	BA	233	A	C8-N7	6.15	1.35	1.31
23	BB	104	A	C8-N7	6.15	1.35	1.31
22	BA	1494	A	C8-N7	6.15	1.35	1.31
1	AA	790	A	C5-C4	-6.14	1.34	1.38
1	AA	412	A	N3-C4	6.14	1.38	1.34
1	AA	321	A	C5-C4	-6.14	1.34	1.38
22	BA	1385	A	C8-N7	6.14	1.35	1.31
22	BA	256	A	C5-C4	-6.14	1.34	1.38
1	AA	325	A	C8-N7	6.14	1.35	1.31
1	AA	1413	A	C5-C4	-6.14	1.34	1.38
22	BA	2378	A	C8-N7	6.14	1.35	1.31
22	BA	1205	A	C5-C4	-6.13	1.34	1.38
1	AA	363	A	C8-N7	6.13	1.35	1.31
1	AA	1005	A	N3-C4	6.13	1.38	1.34
1	AA	1239	A	C5-C4	-6.13	1.34	1.38
23	BB	58	A	C5-C4	-6.13	1.34	1.38
22	BA	428	A	C8-N7	6.13	1.35	1.31
22	BA	1048	A	C8-N7	6.13	1.35	1.31
22	BA	1749	A	C8-N7	6.12	1.35	1.31
1	AA	397	A	C8-N7	6.12	1.35	1.31
1	AA	663	A	C5-C4	-6.12	1.34	1.38
22	BA	1505	A	C5-C4	-6.12	1.34	1.38
22	BA	1739	A	N3-C4	6.12	1.38	1.34
22	BA	91	A	C8-N7	6.12	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	322	A	C8-N7	6.12	1.35	1.31
1	AA	160	A	C5-C4	-6.12	1.34	1.38
1	AA	303	A	C5-C4	-6.12	1.34	1.38
1	AA	573	A	C8-N7	6.12	1.35	1.31
22	BA	429	A	C5-C4	-6.12	1.34	1.38
22	BA	1937	A	C8-N7	6.12	1.35	1.31
1	AA	923	A	C8-N7	6.11	1.35	1.31
22	BA	5	A	C8-N7	6.11	1.35	1.31
22	BA	104	A	C8-N7	6.11	1.35	1.31
1	AA	1311	A	N3-C4	6.11	1.38	1.34
1	AA	579	A	C8-N7	6.11	1.35	1.31
1	AA	746	A	C5-C4	-6.10	1.34	1.38
1	AA	238	A	C5-C4	-6.10	1.34	1.38
22	BA	1494	A	C5-C4	-6.10	1.34	1.38
22	BA	1981	A	C8-N7	6.10	1.35	1.31
22	BA	2835	A	C5-C4	-6.10	1.34	1.38
22	BA	626	A	C8-N7	6.10	1.35	1.31
1	AA	706	A	C5-C4	-6.10	1.34	1.38
22	BA	71	A	C5-C4	-6.10	1.34	1.38
1	AA	673	A	C8-N7	6.10	1.35	1.31
1	AA	1430	A	C8-N7	6.10	1.35	1.31
1	AA	964	A	C5-C4	-6.10	1.34	1.38
22	BA	2868	A	C5-C4	-6.10	1.34	1.38
1	AA	621	A	C5-C4	-6.09	1.34	1.38
1	AA	1082	A	C5-C4	-6.09	1.34	1.38
22	BA	1286	A	C8-N7	6.09	1.35	1.31
22	BA	2886	A	C5-C4	-6.09	1.34	1.38
1	AA	1145	A	N3-C4	6.09	1.38	1.34
22	BA	2764	A	C8-N7	6.09	1.35	1.31
22	BA	1616	A	C8-N7	6.09	1.35	1.31
1	AA	655	A	C8-N7	6.09	1.35	1.31
1	AA	1035	A	N3-C4	6.09	1.38	1.34
22	BA	960	A	N7-C5	-6.09	1.35	1.39
22	BA	1545	A	C8-N7	6.09	1.35	1.31
1	AA	1513	A	C8-N7	6.09	1.35	1.31
22	BA	892	A	C3'-O3'	-6.09	1.33	1.42
22	BA	1593	A	C5-C4	-6.09	1.34	1.38
1	AA	1499	A	C8-N7	6.08	1.35	1.31
22	BA	348	A	C5-C4	-6.08	1.34	1.38
22	BA	631	A	N7-C5	-6.08	1.35	1.39
22	BA	980	A	N7-C5	-6.08	1.35	1.39
22	BA	1027	A	C5-C4	-6.08	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1591	A	C5-C4	-6.08	1.34	1.38
1	AA	908	A	C5-C4	-6.08	1.34	1.38
22	BA	1502	A	C5-C4	-6.08	1.34	1.38
22	BA	1596	A	C8-N7	6.08	1.35	1.31
22	BA	1383	A	C8-N7	6.08	1.35	1.31
22	BA	2810	A	C8-N7	6.08	1.35	1.31
22	BA	637	A	C8-N7	6.07	1.35	1.31
22	BA	1580	A	C5-C4	-6.07	1.34	1.38
1	AA	1508	A	C8-N7	6.07	1.35	1.31
1	AA	414	A	N3-C4	6.07	1.38	1.34
1	AA	1155	A	N3-C4	6.07	1.38	1.34
1	AA	1036	A	N3-C4	6.07	1.38	1.34
22	BA	429	A	C8-N7	6.07	1.35	1.31
22	BA	272	A	C8-N7	6.06	1.35	1.31
1	AA	907	A	C8-N7	6.06	1.35	1.31
1	AA	787	A	C8-N7	6.06	1.35	1.31
22	BA	722	A	C5-C4	-6.06	1.34	1.38
1	AA	327	A	C8-N7	6.06	1.35	1.31
1	AA	712	A	C8-N7	6.06	1.35	1.31
22	BA	310	A	C8-N7	6.06	1.35	1.31
22	BA	2278	A	C8-N7	6.06	1.35	1.31
22	BA	1367	A	C5-C4	-6.06	1.34	1.38
22	BA	2147	A	N3-C4	6.05	1.38	1.34
1	AA	393	A	C5-C4	-6.05	1.34	1.38
1	AA	50	A	C5-C4	-6.05	1.34	1.38
1	AA	1044	A	N3-C4	6.05	1.38	1.34
55	B8	73	A	N3-C4	6.05	1.38	1.34
22	BA	2478	A	C8-N7	6.05	1.35	1.31
22	BA	2900	A	C5-C4	-6.05	1.34	1.38
22	BA	1635	A	C8-N7	6.04	1.35	1.31
1	AA	101	A	C5-C4	-6.04	1.34	1.38
22	BA	1885	A	C5-C4	-6.04	1.34	1.38
1	AA	1014	A	N3-C4	6.04	1.38	1.34
1	AA	622	A	C5-C4	-6.04	1.34	1.38
1	AA	694	A	C5-C4	-6.04	1.34	1.38
1	AA	878	A	C8-N7	6.04	1.35	1.31
1	AA	1092	A	C5-C4	-6.04	1.34	1.38
55	B8	21	A	N3-C4	6.04	1.38	1.34
22	BA	354	A	N3-C4	6.04	1.38	1.34
1	AA	109	A	C5-C4	-6.03	1.34	1.38
1	AA	1288	A	C5-C4	-6.03	1.34	1.38
1	AA	300	A	C5-C4	-6.03	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	554	A	C5-C4	-6.03	1.34	1.38
1	AA	98	A	C5-C4	-6.03	1.34	1.38
1	AA	430	A	C5-C4	-6.03	1.34	1.38
1	AA	415	A	N3-C4	6.03	1.38	1.34
1	AA	189	A	N3-C4	6.02	1.38	1.34
1	AA	918	A	C5-C4	-6.02	1.34	1.38
22	BA	2378	A	C5-C4	-6.02	1.34	1.38
1	AA	908	A	C8-N7	6.02	1.35	1.31
1	AA	1465	A	C8-N7	6.02	1.35	1.31
22	BA	2813	A	C8-N7	6.02	1.35	1.31
1	AA	460	A	N3-C4	6.02	1.38	1.34
1	AA	794	A	C8-N7	6.02	1.35	1.31
22	BA	1504	A	C5-C4	-6.01	1.34	1.38
22	BA	2587	A	C8-N7	6.01	1.35	1.31
1	AA	329	A	C5-C4	-6.01	1.34	1.38
1	AA	1012	A	N3-C4	6.01	1.38	1.34
1	AA	1151	A	N3-C4	6.01	1.38	1.34
1	AA	1500	A	C8-N7	6.01	1.35	1.31
1	AA	313	A	C8-N7	6.01	1.35	1.31
22	BA	1067	A	N3-C4	6.01	1.38	1.34
1	AA	143	A	N3-C4	6.00	1.38	1.34
1	AA	743	A	C8-N7	6.00	1.35	1.31
22	BA	1919	A	C8-N7	6.00	1.35	1.31
1	AA	596	A	C5-C4	-6.00	1.34	1.38
22	BA	352	A	C5-C4	-6.00	1.34	1.38
22	BA	2199	A	C5-C4	-6.00	1.34	1.38
1	AA	493	A	N3-C4	6.00	1.38	1.34
22	BA	1583	A	N3-C4	6.00	1.38	1.34
22	BA	324	A	C8-N7	6.00	1.35	1.31
22	BA	1885	A	C8-N7	6.00	1.35	1.31
55	B8	66	A	N3-C4	6.00	1.38	1.34
22	BA	1434	A	C5-C4	-6.00	1.34	1.38
1	AA	629	A	N3-C4	5.99	1.38	1.34
22	BA	508	A	N3-C4	5.99	1.38	1.34
1	AA	743	A	N3-C4	5.99	1.38	1.34
22	BA	1085	A	N3-C4	5.99	1.38	1.34
22	BA	95	A	C8-N7	5.99	1.35	1.31
1	AA	600	A	C5-C4	-5.98	1.34	1.38
1	AA	1014	A	C5-C4	-5.98	1.34	1.38
1	AA	1324	A	N3-C4	5.98	1.38	1.34
22	BA	1872	A	N3-C4	5.98	1.38	1.34
1	AA	831	A	C5-C4	-5.98	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1346	A	C5-C4	-5.98	1.34	1.38
22	BA	2376	A	C8-N7	5.98	1.35	1.31
55	B8	41	A	N3-C4	5.98	1.38	1.34
22	BA	278	A	N3-C4	5.98	1.38	1.34
1	AA	325	A	C5-C4	-5.97	1.34	1.38
1	AA	907	A	C5-C4	-5.97	1.34	1.38
1	AA	60	A	C5-C4	-5.97	1.34	1.38
1	AA	1201	A	C5-C4	-5.97	1.34	1.38
1	AA	1398	A	C8-N7	5.97	1.35	1.31
1	AA	607	A	C5-C4	-5.97	1.34	1.38
1	AA	642	A	C5-C4	-5.97	1.34	1.38
1	AA	1191	A	C5-C4	-5.97	1.34	1.38
1	AA	1374	A	N3-C4	5.97	1.38	1.34
22	BA	2297	A	C8-N7	5.97	1.35	1.31
22	BA	2476	A	C8-N7	5.97	1.35	1.31
22	BA	1392	A	C8-N7	5.96	1.35	1.31
1	AA	914	A	C8-N7	5.96	1.35	1.31
1	AA	1170	A	N3-C4	5.96	1.38	1.34
1	AA	1250	A	N3-C4	5.96	1.38	1.34
1	AA	1254	A	N3-C4	5.96	1.38	1.34
22	BA	2388	A	N9-C8	-5.96	1.32	1.37
22	BA	2893	A	C8-N7	5.96	1.35	1.31
1	AA	1171	A	N3-C4	5.96	1.38	1.34
1	AA	1229	A	C5-C4	-5.96	1.34	1.38
22	BA	279	A	N3-C4	5.96	1.38	1.34
22	BA	311	A	C8-N7	5.96	1.35	1.31
22	BA	1821	A	C8-N7	5.96	1.35	1.31
22	BA	2530	A	C8-N7	5.96	1.35	1.31
23	BB	119	A	N3-C4	5.96	1.38	1.34
1	AA	1274	A	N3-C4	5.96	1.38	1.34
22	BA	63	A	C5-C4	-5.96	1.34	1.38
22	BA	231	A	C8-N7	5.96	1.35	1.31
1	AA	1456	A	C5-C4	-5.95	1.34	1.38
22	BA	1808	A	C8-N7	5.95	1.35	1.31
22	BA	2761	A	C8-N7	5.95	1.35	1.31
22	BA	1786	A	C8-N7	5.95	1.35	1.31
22	BA	928	A	C8-N7	5.95	1.35	1.31
22	BA	1347	A	C8-N7	5.95	1.35	1.31
22	BA	1746	A	C5-C4	-5.95	1.34	1.38
22	BA	1701	A	C8-N7	5.94	1.35	1.31
1	AA	958	A	C5-C4	-5.94	1.34	1.38
1	AA	1306	A	N3-C4	5.94	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	279	A	C5-C4	-5.94	1.34	1.38
1	AA	482	A	C5-C4	-5.94	1.34	1.38
1	AA	502	A	C5-C4	-5.94	1.34	1.38
1	AA	781	A	C8-N7	5.94	1.35	1.31
22	BA	2311	A	C5-C4	-5.94	1.34	1.38
22	BA	2856	A	C8-N7	5.94	1.35	1.31
1	AA	389	A	C5-C4	-5.94	1.34	1.38
22	BA	608	A	N7-C5	-5.94	1.35	1.39
1	AA	535	A	C5-C4	-5.94	1.34	1.38
1	AA	320	A	C5-C4	-5.93	1.34	1.38
1	AA	338	A	C8-N7	5.93	1.35	1.31
22	BA	2288	A	C8-N7	5.93	1.35	1.31
22	BA	2814	A	C8-N7	5.93	1.35	1.31
1	AA	181	A	C5-C4	-5.93	1.34	1.38
1	AA	498	A	C5-C4	-5.93	1.34	1.38
22	BA	1745	A	C5-C4	-5.93	1.34	1.38
1	AA	282	A	C5-C4	-5.93	1.34	1.38
1	AA	1251	A	N3-C4	5.93	1.38	1.34
1	AA	129	A	C5-C4	-5.93	1.34	1.38
1	AA	397	A	N3-C4	5.93	1.38	1.34
22	BA	299	A	C5-C4	-5.93	1.34	1.38
22	BA	1609	A	C8-N7	5.93	1.35	1.31
1	AA	1503	A	N3-C4	5.92	1.38	1.34
22	BA	2183	A	N3-C4	5.92	1.38	1.34
1	AA	949	A	C5-C4	-5.92	1.34	1.38
22	BA	603	A	C5-C4	-5.92	1.34	1.38
22	BA	2430	A	C5-C4	-5.92	1.34	1.38
22	BA	1086	A	N3-C4	5.92	1.38	1.34
22	BA	1597	A	C8-N7	5.92	1.35	1.31
22	BA	626	A	C5-C4	-5.91	1.34	1.38
22	BA	1570	A	N7-C5	-5.91	1.35	1.39
22	BA	2560	A	C8-N7	5.91	1.35	1.31
1	AA	329	A	C8-N7	5.91	1.35	1.31
1	AA	1170	A	C5-C4	-5.91	1.34	1.38
1	AA	1176	A	N3-C4	5.91	1.38	1.34
22	BA	2820	A	C5-C4	-5.91	1.34	1.38
22	BA	294	A	C8-N7	5.90	1.35	1.31
22	BA	1265	A	N7-C5	-5.90	1.35	1.39
22	BA	362	A	N3-C4	5.90	1.38	1.34
22	BA	2736	A	C8-N7	5.90	1.35	1.31
1	AA	906	A	C8-N7	5.90	1.35	1.31
1	AA	696	A	C5-C4	-5.90	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	782	A	C8-N7	5.90	1.35	1.31
22	BA	1304	A	C8-N7	5.90	1.35	1.31
22	BA	1508	A	N3-C4	5.90	1.38	1.34
22	BA	2336	A	C8-N7	5.90	1.35	1.31
22	BA	2820	A	N3-C4	5.90	1.38	1.34
1	AA	1360	A	C5-C4	-5.89	1.34	1.38
22	BA	1913	A	C5-C4	-5.89	1.34	1.38
22	BA	2850	A	N7-C5	-5.89	1.35	1.39
1	AA	414	A	C5-C4	-5.89	1.34	1.38
1	AA	959	A	N3-C4	5.89	1.38	1.34
22	BA	1373	A	N7-C5	-5.89	1.35	1.39
22	BA	2060	A	N3-C4	5.89	1.38	1.34
1	AA	1418	A	C8-N7	5.89	1.35	1.31
22	BA	332	A	C8-N7	5.89	1.35	1.31
22	BA	1877	A	C8-N7	5.89	1.35	1.31
22	BA	2799	A	C8-N7	5.89	1.35	1.31
1	AA	431	A	N3-C4	5.88	1.38	1.34
1	AA	1163	A	N3-C4	5.88	1.38	1.34
1	AA	648	A	C5-C4	-5.88	1.34	1.38
22	BA	2459	A	N7-C5	-5.88	1.35	1.39
1	AA	675	A	C8-N7	5.88	1.35	1.31
1	AA	327	A	N3-C4	5.88	1.38	1.34
1	AA	1196	A	N3-C4	5.88	1.38	1.34
22	BA	83	A	C8-N7	5.88	1.35	1.31
22	BA	1571	A	N7-C5	-5.88	1.35	1.39
22	BA	2482	A	C5-C4	-5.88	1.34	1.38
1	AA	65	A	C5-C4	-5.87	1.34	1.38
22	BA	497	A	C8-N7	5.87	1.35	1.31
1	AA	182	A	N3-C4	5.87	1.38	1.34
22	BA	1785	A	C8-N7	5.87	1.35	1.31
22	BA	2031	A	C8-N7	5.87	1.35	1.31
22	BA	402	A	C8-N7	5.87	1.35	1.31
1	AA	892	A	C8-N7	5.87	1.35	1.31
1	AA	1285	A	N3-C4	5.87	1.38	1.34
22	BA	1395	A	C8-N7	5.87	1.35	1.31
1	AA	860	A	C8-N7	5.87	1.35	1.31
1	AA	1236	A	C5-C4	-5.87	1.34	1.38
22	BA	706	A	C8-N7	5.87	1.35	1.31
1	AA	1046	A	N3-C4	5.86	1.38	1.34
1	AA	1157	A	N3-C4	5.86	1.38	1.34
22	BA	1274	A	C8-N7	5.86	1.35	1.31
22	BA	602	A	C8-N7	5.86	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1722	A	C5-C4	-5.86	1.34	1.38
1	AA	149	A	C5-C4	-5.86	1.34	1.38
1	AA	602	A	C5-C4	-5.86	1.34	1.38
22	BA	391	A	C8-N7	5.86	1.35	1.31
1	AA	1368	A	C5-C4	-5.86	1.34	1.38
22	BA	1928	A	C8-N7	5.86	1.35	1.31
22	BA	2101	A	C2-N3	5.86	1.38	1.33
1	AA	533	A	N3-C4	5.85	1.38	1.34
1	AA	1503	A	C5-C4	-5.85	1.34	1.38
1	AA	468	A	N3-C4	5.85	1.38	1.34
1	AA	609	A	C5-C4	-5.85	1.34	1.38
22	BA	94	A	C5-C4	-5.85	1.34	1.38
23	BB	46	A	C5-C4	-5.85	1.34	1.38
1	AA	155	A	N3-C4	5.85	1.38	1.34
22	BA	1413	A	C5-C4	-5.85	1.34	1.38
1	AA	32	A	C8-N7	5.85	1.35	1.31
1	AA	923	A	C5-C4	-5.85	1.34	1.38
1	AA	151	A	N3-C4	5.85	1.38	1.34
1	AA	780	A	C8-N7	5.85	1.35	1.31
1	AA	1431	A	C8-N7	5.84	1.35	1.31
22	BA	1654	A	C5-C4	-5.84	1.34	1.38
1	AA	1362	A	N3-C4	5.84	1.38	1.34
22	BA	654	A	N3-C4	5.84	1.38	1.34
1	AA	130	A	C5-C4	-5.84	1.34	1.38
1	AA	901	A	N7-C5	-5.84	1.35	1.39
22	BA	14	A	N7-C5	-5.84	1.35	1.39
1	AA	630	A	N3-C4	5.84	1.38	1.34
1	AA	1167	A	C5-C4	-5.84	1.34	1.38
22	BA	71	A	C8-N7	5.84	1.35	1.31
22	BA	789	A	C8-N7	5.84	1.35	1.31
55	B8	51	A	N3-C4	5.84	1.38	1.34
1	AA	1110	A	C5-C4	-5.83	1.34	1.38
1	AA	1269	A	N3-C4	5.83	1.38	1.34
1	AA	1229	A	N3-C4	5.83	1.38	1.34
22	BA	2721	A	N7-C5	-5.83	1.35	1.39
1	AA	195	A	C5-C4	-5.83	1.34	1.38
55	B8	6	A	C5-C4	-5.83	1.34	1.38
22	BA	223	A	C8-N7	5.83	1.35	1.31
1	AA	1155	A	C5-C4	-5.83	1.34	1.38
22	BA	152	A	C8-N7	5.83	1.35	1.31
22	BA	2662	A	C5-C4	-5.83	1.34	1.38
1	AA	675	A	N3-C4	5.82	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1225	A	C5-C4	-5.82	1.34	1.38
22	BA	2407	A	N7-C5	-5.82	1.35	1.39
22	BA	131	A	C8-N7	5.82	1.35	1.31
22	BA	541	A	C8-N7	5.82	1.35	1.31
22	BA	844	A	C8-N7	5.82	1.35	1.31
22	BA	1866	A	C8-N7	5.82	1.35	1.31
22	BA	1393	A	C8-N7	5.82	1.35	1.31
22	BA	1722	A	C8-N7	5.82	1.35	1.31
1	AA	321	A	C8-N7	5.82	1.35	1.31
22	BA	2042	A	C8-N7	5.82	1.35	1.31
22	BA	2268	A	N7-C5	-5.82	1.35	1.39
23	BB	119	A	C5-C4	-5.82	1.34	1.38
1	AA	72	A	C5-C4	-5.82	1.34	1.38
1	AA	864	A	C5-C4	-5.82	1.34	1.38
1	AA	547	A	N3-C4	5.81	1.38	1.34
23	BB	53	A	C5-C4	-5.81	1.34	1.38
1	AA	364	A	C5-C4	-5.81	1.34	1.38
22	BA	1509	A	C5-C4	-5.81	1.34	1.38
22	BA	1549	A	C8-N7	5.81	1.35	1.31
22	BA	1678	A	C8-N7	5.81	1.35	1.31
22	BA	1755	A	C8-N7	5.81	1.35	1.31
1	AA	167	A	C5-C4	-5.81	1.34	1.38
1	AA	1340	A	C5-C4	-5.81	1.34	1.38
22	BA	721	A	C5-C4	-5.81	1.34	1.38
1	AA	382	A	C5-C4	-5.80	1.34	1.38
22	BA	783	A	C8-N7	5.80	1.35	1.31
22	BA	2015	A	N7-C5	-5.80	1.35	1.39
1	AA	1102	A	C5-C4	-5.80	1.34	1.38
22	BA	466	A	N7-C5	-5.80	1.35	1.39
22	BA	1626	A	C8-N7	5.80	1.35	1.31
22	BA	1739	A	C8-N7	5.80	1.35	1.31
22	BA	2766	A	C8-N7	5.80	1.35	1.31
22	BA	42	A	C8-N7	5.80	1.35	1.31
22	BA	764	A	C8-N7	5.80	1.35	1.31
1	AA	563	A	C5-C4	-5.80	1.34	1.38
1	AA	1374	A	C5-C4	-5.80	1.34	1.38
1	AA	131	A	C5-C4	-5.80	1.34	1.38
22	BA	173	A	C8-N7	5.80	1.35	1.31
1	AA	649	A	C5-C4	-5.79	1.34	1.38
1	AA	1117	A	N3-C4	5.79	1.38	1.34
22	BA	1966	A	C8-N7	5.79	1.35	1.31
1	AA	746	A	N3-C4	5.79	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1548	A	C8-N7	5.79	1.35	1.31
22	BA	1077	A	N3-C4	5.79	1.38	1.34
22	BA	1272	A	C8-N7	5.79	1.35	1.31
1	AA	116	A	C8-N7	5.79	1.35	1.31
22	BA	1889	A	C8-N7	5.79	1.35	1.31
22	BA	1495	A	C8-N7	5.79	1.35	1.31
22	BA	2211	A	N3-C4	5.78	1.38	1.34
1	AA	983	A	N3-C4	5.78	1.38	1.34
22	BA	730	A	C8-N7	5.78	1.35	1.31
22	BA	2314	A	N3-C4	5.78	1.38	1.34
22	BA	2614	A	C8-N7	5.78	1.35	1.31
1	AA	1318	A	N3-C4	5.78	1.38	1.34
1	AA	1287	A	N3-C4	5.78	1.38	1.34
22	BA	1420	A	N3-C4	5.78	1.38	1.34
1	AA	1377	A	N3-C4	5.78	1.38	1.34
22	BA	1048	A	C5-C4	-5.78	1.34	1.38
1	AA	1252	A	N3-C4	5.77	1.38	1.34
1	AA	716	A	C8-N7	5.77	1.35	1.31
22	BA	221	A	C8-N7	5.77	1.35	1.31
22	BA	1275	A	C8-N7	5.77	1.35	1.31
22	BA	1433	A	C8-N7	5.77	1.35	1.31
55	B8	38	A	N3-C4	5.77	1.38	1.34
22	BA	165	A	C5-C4	-5.77	1.34	1.38
1	AA	696	A	C8-N7	5.77	1.35	1.31
22	BA	1490	A	C5-C4	-5.77	1.34	1.38
22	BA	1676	A	N7-C5	-5.77	1.35	1.39
22	BA	2169	A	N3-C4	5.77	1.38	1.34
55	B8	59	A	N3-C4	5.76	1.38	1.34
22	BA	1133	A	C8-N7	5.76	1.35	1.31
22	BA	1496	A	C8-N7	5.76	1.35	1.31
1	AA	1446	A	C5-C4	-5.76	1.34	1.38
22	BA	984	A	N7-C5	-5.76	1.35	1.39
22	BA	1938	A	C8-N7	5.76	1.35	1.31
1	AA	1329	A	C5-C4	-5.76	1.34	1.38
22	BA	750	A	N7-C5	-5.76	1.35	1.39
22	BA	2411	A	C8-N7	5.76	1.35	1.31
22	BA	2598	A	N7-C5	-5.76	1.35	1.39
1	AA	816	A	C8-N7	5.76	1.35	1.31
22	BA	1916	A	C5-C4	-5.76	1.34	1.38
1	AA	807	A	C8-N7	5.76	1.35	1.31
1	AA	1019	A	N3-C4	5.76	1.38	1.34
1	AA	155	A	C5-C4	-5.75	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	182	A	C5-C4	-5.75	1.34	1.38
1	AA	978	A	C5-C4	-5.75	1.34	1.38
22	BA	996	A	C8-N7	5.75	1.35	1.31
22	BA	1987	A	C8-N7	5.75	1.35	1.31
1	AA	179	A	N3-C4	5.75	1.38	1.34
1	AA	1016	A	C5-C4	-5.75	1.34	1.38
22	BA	2062	A	N3-C4	5.75	1.38	1.34
22	BA	1665	A	C8-N7	5.75	1.35	1.31
1	AA	1271	A	C5-C4	-5.75	1.34	1.38
22	BA	1000	A	N9-C8	-5.75	1.33	1.37
22	BA	1020	A	C8-N7	5.75	1.35	1.31
22	BA	599	A	C8-N7	5.75	1.35	1.31
1	AA	559	A	C5-C4	-5.74	1.34	1.38
1	AA	802	A	C8-N7	5.74	1.35	1.31
1	AA	974	A	C5-C4	-5.74	1.34	1.38
22	BA	2340	A	C8-N7	5.74	1.35	1.31
55	B8	42	A	N3-C4	5.74	1.38	1.34
1	AA	1188	A	C5-C4	-5.74	1.34	1.38
22	BA	1504	A	N3-C4	5.74	1.38	1.34
22	BA	199	A	C8-N7	5.74	1.35	1.31
22	BA	820	A	N7-C5	-5.74	1.35	1.39
22	BA	2799	A	N3-C4	5.74	1.38	1.34
1	AA	873	A	C8-N7	5.74	1.35	1.31
1	AA	949	A	N3-C4	5.74	1.38	1.34
22	BA	2070	A	C8-N7	5.73	1.35	1.31
1	AA	718	A	C5-C4	-5.73	1.34	1.38
1	AA	872	A	C5-C4	-5.73	1.34	1.38
22	BA	299	A	C8-N7	5.73	1.35	1.31
22	BA	715	A	N3-C4	5.73	1.38	1.34
1	AA	344	A	N3-C4	5.73	1.38	1.34
1	AA	815	A	N7-C5	-5.73	1.35	1.39
22	BA	2778	A	C8-N7	5.73	1.35	1.31
1	AA	139	A	C5-C4	-5.73	1.34	1.38
1	AA	303	A	N3-C4	5.73	1.38	1.34
22	BA	1739	A	C5-C4	-5.73	1.34	1.38
22	BA	2328	A	N7-C5	-5.73	1.35	1.39
1	AA	602	A	N3-C4	5.72	1.38	1.34
22	BA	265	A	C8-N7	5.72	1.35	1.31
22	BA	1307	A	N7-C5	-5.72	1.35	1.39
22	BA	1847	A	C5-C4	-5.72	1.34	1.38
22	BA	2776	A	C8-N7	5.72	1.35	1.31
1	AA	44	A	C5-C4	-5.72	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	938	A	C5-C4	-5.72	1.34	1.38
22	BA	126	A	C8-N7	5.72	1.35	1.31
22	BA	1780	A	C8-N7	5.72	1.35	1.31
1	AA	459	A	N3-C4	5.72	1.38	1.34
22	BA	1384	A	C8-N7	5.72	1.35	1.31
22	BA	2469	A	C8-N7	5.72	1.35	1.31
22	BA	2564	A	N7-C5	-5.72	1.35	1.39
22	BA	572	A	N7-C5	-5.72	1.35	1.39
1	AA	253	A	C5-C4	-5.72	1.34	1.38
1	AA	1117	A	C5-C4	-5.72	1.34	1.38
22	BA	582	A	N9-C8	-5.72	1.33	1.37
1	AA	498	A	C2-N3	5.71	1.38	1.33
1	AA	1213	A	C5-C4	-5.71	1.34	1.38
1	AA	1362	A	C5-C4	-5.71	1.34	1.38
22	BA	878	A	N3-C4	5.71	1.38	1.34
1	AA	33	A	C5-C4	-5.71	1.34	1.38
1	AA	923	A	N3-C4	5.71	1.38	1.34
1	AA	1333	A	C5-C4	-5.71	1.34	1.38
1	AA	1456	A	N3-C4	5.71	1.38	1.34
22	BA	508	A	C5-C4	-5.71	1.34	1.38
22	BA	1276	A	C8-N7	5.71	1.35	1.31
55	B8	14	A	N3-C4	5.71	1.38	1.34
1	AA	143	A	C5-C4	-5.71	1.34	1.38
1	AA	1447	A	C5-C4	-5.71	1.34	1.38
22	BA	340	A	C8-N7	5.71	1.35	1.31
22	BA	447	A	N3-C4	5.71	1.38	1.34
22	BA	1147	A	C8-N7	5.71	1.35	1.31
22	BA	2058	A	C8-N7	5.71	1.35	1.31
1	AA	33	A	N3-C4	5.71	1.38	1.34
1	AA	196	A	C5-C4	-5.71	1.34	1.38
1	AA	539	A	C5-C4	-5.71	1.34	1.38
1	AA	753	A	C5-C4	-5.71	1.34	1.38
1	AA	790	A	C8-N7	5.71	1.35	1.31
22	BA	2531	A	C8-N7	5.71	1.35	1.31
1	AA	938	A	N3-C4	5.71	1.38	1.34
1	AA	1055	A	N3-C4	5.71	1.38	1.34
22	BA	1328	A	C8-N7	5.70	1.35	1.31
22	BA	1969	A	N7-C5	-5.70	1.35	1.39
22	BA	480	A	C5-C4	-5.70	1.34	1.38
22	BA	1155	A	C8-N7	5.70	1.35	1.31
22	BA	1308	A	C8-N7	5.70	1.35	1.31
1	AA	635	A	C5-C4	-5.70	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2461	A	C8-N7	5.70	1.35	1.31
22	BA	2635	A	C8-N7	5.70	1.35	1.31
22	BA	2851	A	C8-N7	5.70	1.35	1.31
22	BA	734	A	N3-C4	5.69	1.38	1.34
1	AA	172	A	C5-C4	-5.69	1.34	1.38
1	AA	815	A	C8-N7	5.69	1.35	1.31
1	AA	1363	A	C5-C4	-5.69	1.34	1.38
22	BA	947	A	C8-N7	5.69	1.35	1.31
22	BA	63	A	N3-C4	5.69	1.38	1.34
22	BA	1735	A	C5-C4	-5.69	1.34	1.38
23	BB	52	A	C8-N7	5.69	1.35	1.31
1	AA	715	A	C8-N7	5.69	1.35	1.31
22	BA	1773	A	N7-C5	-5.69	1.35	1.39
22	BA	2333	A	C8-N7	5.69	1.35	1.31
1	AA	306	A	C5-C4	-5.69	1.34	1.38
1	AA	468	A	C5-C4	-5.69	1.34	1.38
1	AA	968	A	C5-C4	-5.68	1.34	1.38
1	AA	1252	A	C5-C4	-5.68	1.34	1.38
1	AA	1349	A	C5-C4	-5.68	1.34	1.38
1	AA	994	A	N3-C4	5.68	1.38	1.34
1	AA	1299	A	C5-C4	-5.68	1.34	1.38
22	BA	227	A	C8-N7	5.68	1.35	1.31
1	AA	782	A	N3-C4	5.68	1.38	1.34
1	AA	946	A	C5-C4	-5.68	1.34	1.38
1	AA	1531	A	N3-C4	5.68	1.38	1.34
22	BA	925	A	C8-N7	5.68	1.35	1.31
1	AA	432	A	C5-C4	-5.68	1.34	1.38
1	AA	1151	A	C5-C4	-5.68	1.34	1.38
1	AA	223	A	N3-C4	5.68	1.38	1.34
22	BA	2381	A	C8-N7	5.68	1.35	1.31
1	AA	749	A	N3-C4	5.67	1.38	1.34
22	BA	1353	A	N7-C5	-5.67	1.35	1.39
22	BA	2829	A	C8-N7	5.67	1.35	1.31
22	BA	1735	A	N3-C4	5.67	1.38	1.34
1	AA	1180	A	N3-C4	5.67	1.38	1.34
1	AA	1377	A	C5-C4	-5.67	1.34	1.38
22	BA	38	A	C8-N7	5.67	1.35	1.31
22	BA	2748	A	C8-N7	5.67	1.35	1.31
23	BB	94	A	C8-N7	5.67	1.35	1.31
22	BA	1598	A	C5-C4	-5.67	1.34	1.38
22	BA	1791	A	N7-C5	-5.67	1.35	1.39
23	BB	57	A	C5-C4	-5.67	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1354	A	N7-C5	-5.67	1.35	1.39
22	BA	730	A	N3-C4	5.66	1.38	1.34
1	AA	509	A	C5-C4	-5.66	1.34	1.38
22	BA	272	A	N3-C4	5.66	1.38	1.34
1	AA	749	A	C5-C4	-5.66	1.34	1.38
22	BA	1336	A	C8-N7	5.66	1.35	1.31
22	BA	1711	A	C8-N7	5.66	1.35	1.31
22	BA	2377	A	C8-N7	5.66	1.35	1.31
22	BA	1014	A	C8-N7	5.66	1.35	1.31
22	BA	2060	A	C8-N7	5.66	1.35	1.31
1	AA	1167	A	N3-C4	5.65	1.38	1.34
22	BA	346	A	N3-C4	5.65	1.38	1.34
22	BA	2883	A	C8-N7	5.65	1.35	1.31
1	AA	937	A	N3-C4	5.65	1.38	1.34
1	AA	55	A	N3-C4	5.65	1.38	1.34
22	BA	1008	A	C8-N7	5.65	1.35	1.31
22	BA	1787	A	N7-C5	-5.65	1.35	1.39
22	BA	368	A	C5-C4	-5.65	1.34	1.38
55	B8	58	A	N3-C4	5.65	1.38	1.34
22	BA	382	A	C8-N7	5.65	1.35	1.31
1	AA	872	A	N3-C4	5.64	1.38	1.34
1	AA	1197	A	N3-C4	5.64	1.38	1.34
1	AA	1289	A	C5-C4	-5.64	1.34	1.38
22	BA	432	A	C8-N7	5.64	1.35	1.31
22	BA	877	A	N3-C4	5.64	1.38	1.34
22	BA	2199	A	C8-N7	5.64	1.35	1.31
23	BB	59	A	N3-C4	5.64	1.38	1.34
1	AA	74	A	N3-C4	5.64	1.38	1.34
1	AA	937	A	C5-C4	-5.64	1.34	1.38
22	BA	1801	A	C8-N7	5.64	1.35	1.31
22	BA	2322	A	C8-N7	5.64	1.35	1.31
1	AA	958	A	N3-C4	5.64	1.38	1.34
1	AA	1394	A	C5-C4	-5.64	1.34	1.38
22	BA	1900	A	N7-C5	-5.64	1.35	1.39
22	BA	320	A	C8-N7	5.64	1.35	1.31
1	AA	228	A	C5-C4	-5.64	1.34	1.38
1	AA	1171	A	C5-C4	-5.64	1.34	1.38
22	BA	1205	A	C8-N7	5.64	1.35	1.31
22	BA	2366	A	N7-C5	-5.63	1.35	1.39
1	AA	860	A	C5-C4	-5.63	1.34	1.38
22	BA	526	A	N7-C5	-5.63	1.35	1.39
22	BA	1532	A	N3-C4	5.63	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1357	A	C5-C4	-5.63	1.34	1.38
22	BA	1307	A	N3-C4	5.63	1.38	1.34
1	AA	996	A	N3-C4	5.63	1.38	1.34
1	AA	1130	A	N3-C4	5.63	1.38	1.34
1	AA	1246	A	C5-C4	-5.63	1.34	1.38
22	BA	1301	A	C8-N7	5.63	1.35	1.31
1	AA	329	A	N3-C4	5.63	1.38	1.34
1	AA	1180	A	C5-C4	-5.63	1.34	1.38
22	BA	1901	A	C8-N7	5.63	1.35	1.31
22	BA	2247	A	N7-C5	-5.63	1.35	1.39
22	BA	190	A	N7-C5	-5.62	1.35	1.39
1	AA	1363	A	N3-C4	5.62	1.38	1.34
22	BA	262	A	C8-N7	5.62	1.35	1.31
1	AA	151	A	C5-C4	-5.62	1.34	1.38
22	BA	1848	A	C5-C4	-5.62	1.34	1.38
22	BA	2052	A	N7-C5	-5.62	1.35	1.39
22	BA	716	A	C5-C4	-5.62	1.34	1.38
1	AA	199	A	C5-C4	-5.62	1.34	1.38
22	BA	528	A	C8-N7	5.62	1.35	1.31
22	BA	1927	A	C8-N7	5.62	1.35	1.31
22	BA	627	A	C8-N7	5.62	1.35	1.31
22	BA	103	A	C8-N7	5.62	1.35	1.31
23	BB	73	A	N3-C4	5.62	1.38	1.34
55	B8	51	A	C5-C4	-5.62	1.34	1.38
1	AA	161	A	N3-C4	5.61	1.38	1.34
1	AA	1082	A	N3-C4	5.61	1.38	1.34
22	BA	1420	A	C5-C4	-5.61	1.34	1.38
22	BA	2721	A	N9-C8	-5.61	1.33	1.37
22	BA	941	A	C8-N7	5.61	1.35	1.31
22	BA	1046	A	N3-C4	5.61	1.38	1.34
22	BA	2020	A	N7-C5	-5.61	1.35	1.39
22	BA	752	A	C8-N7	5.61	1.35	1.31
22	BA	1143	A	N7-C5	-5.61	1.35	1.39
1	AA	383	A	C5-C4	-5.61	1.34	1.38
1	AA	969	A	C5-C4	-5.61	1.34	1.38
1	AA	408	A	N3-C4	5.61	1.38	1.34
22	BA	526	A	C8-N7	5.61	1.35	1.31
22	BA	1133	A	N7-C5	-5.61	1.35	1.39
22	BA	2882	A	C8-N7	5.61	1.35	1.31
55	B8	6	A	N3-C4	5.61	1.38	1.34
1	AA	1204	A	N3-C4	5.60	1.38	1.34
22	BA	19	A	N7-C5	-5.60	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	2	A	C5-C4	-5.60	1.34	1.38
22	BA	472	A	C8-N7	5.60	1.35	1.31
22	BA	2448	A	N7-C5	-5.60	1.35	1.39
1	AA	768	A	C8-N7	5.60	1.35	1.31
22	BA	74	A	C8-N7	5.60	1.35	1.31
22	BA	443	A	N3-C4	5.60	1.38	1.34
1	AA	864	A	N3-C4	5.60	1.38	1.34
22	BA	149	A	C8-N7	5.60	1.35	1.31
22	BA	1264	A	N7-C5	-5.60	1.35	1.39
22	BA	1528	A	C8-N7	5.60	1.35	1.31
22	BA	2542	A	N9-C8	-5.60	1.33	1.37
22	BA	2346	A	C8-N7	5.60	1.35	1.31
22	BA	675	A	N7-C5	-5.59	1.35	1.39
22	BA	1127	A	C8-N7	5.59	1.35	1.31
22	BA	1285	A	C8-N7	5.59	1.35	1.31
1	AA	1256	A	N3-C4	5.59	1.38	1.34
22	BA	718	A	C5-C4	-5.59	1.34	1.38
22	BA	2726	A	C8-N7	5.59	1.35	1.31
1	AA	1204	A	C5-C4	-5.59	1.34	1.38
1	AA	1213	A	N3-C4	5.59	1.38	1.34
22	BA	529	A	C8-N7	5.59	1.35	1.31
22	BA	1808	A	C5-C4	-5.59	1.34	1.38
1	AA	338	A	N3-C4	5.59	1.38	1.34
1	AA	487	A	N3-C4	5.59	1.38	1.34
1	AA	1092	A	N3-C4	5.59	1.38	1.34
1	AA	595	A	N3-C4	5.58	1.38	1.34
1	AA	900	A	C8-N7	5.58	1.35	1.31
1	AA	1067	A	C5-C4	-5.58	1.34	1.38
22	BA	167	A	C8-N7	5.58	1.35	1.31
22	BA	1552	A	C8-N7	5.58	1.35	1.31
22	BA	1632	A	C8-N7	5.58	1.35	1.31
1	AA	167	A	N3-C4	5.58	1.38	1.34
1	AA	344	A	C5-C4	-5.58	1.34	1.38
22	BA	2682	A	C8-N7	5.58	1.35	1.31
22	BA	2639	A	C8-N7	5.58	1.35	1.31
1	AA	65	A	N3-C4	5.58	1.38	1.34
22	BA	374	A	N7-C5	-5.58	1.35	1.39
22	BA	1829	A	C8-N7	5.58	1.35	1.31
1	AA	1275	A	C5-C4	-5.58	1.34	1.38
22	BA	300	A	C8-N7	5.58	1.35	1.31
22	BA	2014	A	N7-C5	-5.58	1.35	1.39
23	BB	59	A	C2-N3	5.58	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	152	A	C5-C4	-5.57	1.34	1.38
22	BA	1669	A	C8-N7	5.57	1.35	1.31
1	AA	199	A	N3-C4	5.57	1.38	1.34
22	BA	621	A	C8-N7	5.57	1.35	1.31
22	BA	900	A	N3-C4	5.57	1.38	1.34
22	BA	1403	A	C8-N7	5.57	1.35	1.31
1	AA	535	A	N3-C4	5.57	1.38	1.34
1	AA	1016	A	N3-C4	5.57	1.38	1.34
22	BA	2059	A	N3-C4	5.57	1.38	1.34
1	AA	190	A	C8-N7	5.57	1.35	1.31
1	AA	1289	A	N3-C4	5.57	1.38	1.34
22	BA	586	A	N7-C5	-5.57	1.35	1.39
22	BA	2314	A	C5-C4	-5.57	1.34	1.38
1	AA	152	A	N3-C4	5.56	1.38	1.34
1	AA	547	A	C5-C4	-5.56	1.34	1.38
1	AA	975	A	C5-C4	-5.56	1.34	1.38
22	BA	590	A	C8-N7	5.56	1.35	1.31
22	BA	899	A	N3-C4	5.56	1.38	1.34
1	AA	71	A	N3-C4	5.56	1.38	1.34
22	BA	2587	A	N3-C4	5.56	1.38	1.34
1	AA	174	A	C5-C4	-5.56	1.34	1.38
22	BA	454	A	C8-N7	5.56	1.35	1.31
1	AA	195	A	N3-C4	5.56	1.38	1.34
22	BA	1509	A	N3-C4	5.56	1.38	1.34
22	BA	1953	A	N7-C5	-5.56	1.35	1.39
22	BA	2757	A	C8-N7	5.56	1.35	1.31
22	BA	825	A	N9-C8	-5.56	1.33	1.37
1	AA	373	A	C5-C4	-5.55	1.34	1.38
22	BA	877	A	C5-C4	-5.55	1.34	1.38
22	BA	2860	A	C8-N7	5.55	1.35	1.31
22	BA	756	A	C8-N7	5.55	1.35	1.31
22	BA	1808	A	N3-C4	5.55	1.38	1.34
1	AA	382	A	N3-C4	5.55	1.38	1.34
22	BA	507	A	C5-C4	-5.55	1.34	1.38
22	BA	1654	A	C8-N7	5.55	1.35	1.31
22	BA	1759	A	N7-C5	-5.55	1.35	1.39
1	AA	747	A	C5-C4	-5.55	1.34	1.38
22	BA	575	A	C8-N7	5.55	1.35	1.31
22	BA	1254	A	N7-C5	-5.55	1.35	1.39
22	BA	2281	A	C8-N7	5.55	1.35	1.31
1	AA	983	A	C5-C4	-5.55	1.34	1.38
22	BA	49	A	N7-C5	-5.55	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	222	A	C8-N7	5.55	1.35	1.31
1	AA	1197	A	C5-C4	-5.54	1.34	1.38
22	BA	1757	A	C8-N7	5.54	1.35	1.31
1	AA	228	A	N3-C4	5.54	1.38	1.34
1	AA	1299	A	N3-C4	5.54	1.38	1.34
22	BA	718	A	N3-C4	5.54	1.38	1.34
22	BA	2564	A	C8-N7	5.54	1.35	1.31
1	AA	1248	A	N3-C4	5.54	1.38	1.34
1	AA	1280	A	C5-C4	-5.54	1.34	1.38
1	AA	1306	A	C5-C4	-5.54	1.34	1.38
1	AA	1340	A	N3-C4	5.54	1.38	1.34
22	BA	2191	A	C5-C4	-5.54	1.34	1.38
22	BA	1913	A	N3-C4	5.54	1.38	1.34
23	BB	45	A	C5-C4	-5.54	1.34	1.38
1	AA	364	A	N3-C4	5.54	1.38	1.34
22	BA	118	A	C8-N7	5.54	1.35	1.31
1	AA	3	A	C5-C4	-5.53	1.34	1.38
1	AA	523	A	C5-C4	-5.53	1.34	1.38
22	BA	1378	A	N9-C8	-5.53	1.33	1.37
1	AA	635	A	N3-C4	5.53	1.38	1.34
1	AA	1044	A	C5-C4	-5.53	1.34	1.38
1	AA	1105	A	N3-C4	5.53	1.38	1.34
22	BA	2476	A	N3-C4	5.53	1.38	1.34
22	BA	21	A	C8-N7	5.53	1.35	1.31
22	BA	2094	A	C8-N7	5.53	1.35	1.31
1	AA	968	A	N3-C4	5.52	1.38	1.34
1	AA	1349	A	N3-C4	5.52	1.38	1.34
22	BA	800	A	N9-C4	-5.52	1.34	1.37
22	BA	1810	A	N9-C8	-5.52	1.33	1.37
1	AA	366	A	C5-C4	-5.52	1.34	1.38
22	BA	981	A	N7-C5	-5.52	1.35	1.39
22	BA	1936	A	N3-C4	5.52	1.38	1.34
1	AA	298	A	N3-C4	5.52	1.38	1.34
1	AA	451	A	C5-C4	-5.52	1.34	1.38
22	BA	502	A	N7-C5	-5.52	1.35	1.39
22	BA	1366	A	C8-N7	5.52	1.35	1.31
22	BA	1803	A	N7-C5	-5.52	1.35	1.39
1	AA	282	A	N3-C4	5.51	1.38	1.34
1	AA	487	A	C5-C4	-5.51	1.34	1.38
1	AA	1150	A	N3-C4	5.51	1.38	1.34
22	BA	572	A	C5-C4	-5.51	1.34	1.38
22	BA	2212	A	C8-N7	5.51	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1157	A	C5-C4	-5.51	1.34	1.38
22	BA	668	A	N7-C5	-5.51	1.35	1.39
22	BA	1960	A	C8-N7	5.51	1.35	1.31
22	BA	2430	A	N7-C5	-5.51	1.35	1.39
22	BA	2873	A	C8-N7	5.51	1.35	1.31
22	BA	1213	A	N7-C5	-5.51	1.35	1.39
1	AA	71	A	C5-C4	-5.51	1.34	1.38
1	AA	161	A	C5-C4	-5.51	1.34	1.38
22	BA	670	A	C8-N7	5.51	1.35	1.31
22	BA	1322	A	C8-N7	5.51	1.35	1.31
22	BA	1871	A	C5-C4	-5.51	1.34	1.38
22	BA	2435	A	C8-N7	5.50	1.35	1.31
22	BA	2541	A	C8-N7	5.50	1.35	1.31
22	BA	1008	A	N7-C5	-5.50	1.35	1.39
22	BA	1809	A	N7-C5	-5.50	1.35	1.39
1	AA	179	A	C5-C4	-5.50	1.34	1.38
1	AA	1319	A	N3-C4	5.50	1.38	1.34
22	BA	282	A	C5-C4	-5.50	1.34	1.38
22	BA	1503	A	N3-C4	5.50	1.38	1.34
1	AA	3	A	N3-C4	5.49	1.38	1.34
1	AA	129	A	N3-C4	5.49	1.38	1.34
1	AA	374	A	N3-C4	5.49	1.38	1.34
1	AA	1368	A	N3-C4	5.49	1.38	1.34
1	AA	1499	A	N3-C4	5.49	1.38	1.34
22	BA	1652	A	N9-C8	-5.49	1.33	1.37
22	BA	2051	A	N7-C5	-5.49	1.35	1.39
23	BB	59	A	C8-N7	5.49	1.35	1.31
1	AA	595	A	C5-C4	-5.49	1.34	1.38
22	BA	802	A	N7-C5	-5.49	1.35	1.39
22	BA	2369	A	C8-N7	5.49	1.35	1.31
1	AA	8	A	N3-C4	5.49	1.38	1.34
1	AA	28	A	N3-C4	5.49	1.38	1.34
22	BA	1246	A	C8-N7	5.49	1.35	1.31
22	BA	197	A	N7-C5	-5.48	1.35	1.39
22	BA	371	A	C8-N7	5.48	1.35	1.31
22	BA	1021	A	C8-N7	5.48	1.35	1.31
22	BA	156	A	N3-C4	5.48	1.38	1.34
22	BA	829	A	C8-N7	5.48	1.35	1.31
22	BA	2274	A	C8-N7	5.48	1.35	1.31
1	AA	964	A	N3-C4	5.48	1.38	1.34
1	AA	1285	A	C5-C4	-5.48	1.34	1.38
22	BA	1586	A	C5-C4	-5.48	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2227	A	C8-N7	5.48	1.35	1.31
1	AA	1288	A	N3-C4	5.47	1.38	1.34
22	BA	990	A	N7-C5	-5.47	1.35	1.39
22	BA	1871	A	N3-C4	5.47	1.38	1.34
1	AA	907	A	N3-C4	5.47	1.38	1.34
22	BA	181	A	C5-C4	-5.47	1.34	1.38
1	AA	1169	A	N3-C4	5.47	1.38	1.34
22	BA	384	A	N7-C5	-5.47	1.35	1.39
22	BA	2433	A	N7-C5	-5.47	1.35	1.39
22	BA	666	A	C8-N7	5.47	1.35	1.31
1	AA	1531	A	C5-C4	-5.46	1.34	1.38
22	BA	282	A	N3-C4	5.46	1.38	1.34
22	BA	480	A	C8-N7	5.46	1.35	1.31
22	BA	735	A	N7-C5	-5.46	1.35	1.39
22	BA	980	A	N9-C8	-5.46	1.33	1.37
22	BA	1189	A	N7-C5	-5.46	1.35	1.39
22	BA	1819	A	N7-C5	-5.46	1.35	1.39
1	AA	181	A	N3-C4	5.46	1.38	1.34
22	BA	1327	A	N7-C5	-5.46	1.35	1.39
22	BA	2662	A	C8-N7	5.46	1.35	1.31
1	AA	192	A	N3-C4	5.46	1.38	1.34
1	AA	959	A	C5-C4	-5.46	1.34	1.38
1	AA	1251	A	C5-C4	-5.46	1.34	1.38
1	AA	1246	A	N3-C4	5.46	1.38	1.34
1	AA	1375	A	C5-C4	-5.46	1.34	1.38
22	BA	503	A	C8-N7	5.46	1.35	1.31
1	AA	53	A	C5-C4	-5.46	1.34	1.38
22	BA	347	A	C5-C4	-5.46	1.34	1.38
1	AA	174	A	N3-C4	5.45	1.38	1.34
1	AA	1468	A	C8-N7	5.45	1.35	1.31
22	BA	422	A	C8-N7	5.45	1.35	1.31
22	BA	2660	A	C5-C4	-5.45	1.34	1.38
1	AA	7	A	N3-C4	5.45	1.38	1.34
1	AA	2	A	N3-C4	5.45	1.38	1.34
1	AA	430	A	N3-C4	5.45	1.38	1.34
1	AA	441	A	N3-C4	5.45	1.38	1.34
1	AA	1176	A	C5-C4	-5.45	1.34	1.38
22	BA	705	A	N7-C5	-5.45	1.35	1.39
22	BA	368	A	N3-C4	5.45	1.38	1.34
1	AA	80	A	N3-C4	5.45	1.38	1.34
22	BA	56	A	N3-C4	5.45	1.38	1.34
22	BA	1569	A	N7-C5	-5.44	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	642	A	N3-C4	5.44	1.38	1.34
22	BA	2868	A	C8-N7	5.44	1.35	1.31
22	BA	727	A	N7-C5	-5.44	1.35	1.39
22	BA	819	A	N7-C5	-5.44	1.35	1.39
1	AA	523	A	N3-C4	5.44	1.38	1.34
1	AA	781	A	N3-C4	5.44	1.38	1.34
22	BA	2352	A	N7-C5	-5.44	1.35	1.39
22	BA	53	A	C8-N7	5.44	1.35	1.31
22	BA	1469	A	N7-C5	-5.44	1.35	1.39
22	BA	182	A	C8-N7	5.43	1.35	1.31
22	BA	849	A	C8-N7	5.43	1.35	1.31
22	BA	1469	A	C8-N7	5.43	1.35	1.31
1	AA	139	A	N3-C4	5.43	1.38	1.34
1	AA	1238	A	C5-C4	-5.43	1.34	1.38
1	AA	1269	A	C5-C4	-5.43	1.34	1.38
1	AA	1163	A	C5-C4	-5.43	1.34	1.38
22	BA	927	A	N3-C4	5.43	1.38	1.34
1	AA	32	A	N3-C4	5.43	1.38	1.34
22	BA	2058	A	N7-C5	-5.43	1.35	1.39
22	BA	2062	A	C5-C4	-5.43	1.34	1.38
1	AA	383	A	N3-C4	5.42	1.38	1.34
22	BA	515	A	C8-N7	5.42	1.35	1.31
1	AA	461	A	C5-C4	-5.42	1.34	1.38
22	BA	676	A	C8-N7	5.42	1.35	1.31
22	BA	1932	A	C8-N7	5.42	1.35	1.31
22	BA	294	A	N3-C4	5.42	1.38	1.34
22	BA	981	A	N9-C8	-5.42	1.33	1.37
1	AA	130	A	N3-C4	5.42	1.38	1.34
22	BA	412	A	C8-N7	5.42	1.35	1.31
22	BA	492	A	C8-N7	5.41	1.35	1.31
22	BA	1226	A	C8-N7	5.41	1.35	1.31
22	BA	1378	A	C8-N7	5.41	1.35	1.31
22	BA	1598	A	N7-C5	-5.41	1.36	1.39
1	AA	1019	A	C5-C4	-5.41	1.34	1.38
1	AA	1216	A	C5-C4	-5.41	1.34	1.38
22	BA	2317	A	N3-C4	5.41	1.38	1.34
1	AA	1188	A	N3-C4	5.41	1.38	1.34
22	BA	1247	A	C8-N7	5.41	1.35	1.31
22	BA	213	A	N3-C4	5.40	1.38	1.34
22	BA	526	A	N9-C8	-5.40	1.33	1.37
1	AA	1196	A	C5-C4	-5.40	1.34	1.38
1	AA	408	A	C5-C4	-5.40	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1311	A	C5-C4	-5.40	1.34	1.38
22	BA	892	A	P-O5'	-5.40	1.54	1.59
22	BA	1265	A	N9-C8	-5.40	1.33	1.37
1	AA	1333	A	N3-C4	5.40	1.38	1.34
22	BA	1586	A	N3-C4	5.40	1.38	1.34
22	BA	1630	A	C8-N7	5.40	1.35	1.31
1	AA	499	A	C5-C4	-5.39	1.34	1.38
22	BA	715	A	C5-C4	-5.39	1.34	1.38
1	AA	59	A	C5-C4	-5.39	1.34	1.38
1	AA	533	A	C5-C4	-5.39	1.34	1.38
22	BA	1244	A	C8-N7	5.39	1.35	1.31
22	BA	1998	A	N9-C8	-5.39	1.33	1.37
1	AA	1493	A	C5-C4	-5.39	1.34	1.38
22	BA	2516	A	N7-C5	-5.39	1.36	1.39
22	BA	1664	A	N3-C4	5.39	1.38	1.34
22	BA	101	A	C8-N7	5.39	1.35	1.31
22	BA	1641	A	C8-N7	5.39	1.35	1.31
1	AA	640	A	C5-C4	-5.38	1.34	1.38
22	BA	910	A	N3-C4	5.38	1.38	1.34
22	BA	1144	A	C8-N7	5.38	1.35	1.31
1	AA	814	A	C8-N7	5.38	1.35	1.31
1	AA	1046	A	C5-C4	-5.38	1.34	1.38
1	AA	1227	A	N3-C4	5.38	1.38	1.34
22	BA	2198	A	C8-N7	5.38	1.35	1.31
22	BA	1054	A	C5-C4	-5.38	1.34	1.38
22	BA	1142	A	C8-N7	5.38	1.35	1.31
22	BA	1551	A	C8-N7	5.38	1.35	1.31
22	BA	1890	A	C8-N7	5.38	1.35	1.31
1	AA	563	A	N3-C4	5.38	1.38	1.34
1	AA	1219	A	C5-C4	-5.38	1.34	1.38
1	AA	1329	A	N3-C4	5.38	1.38	1.34
1	AA	1434	A	N3-C4	5.38	1.38	1.34
1	AA	120	A	C5-C4	-5.38	1.34	1.38
22	BA	899	A	C5-C4	-5.38	1.34	1.38
1	AA	1280	A	N3-C4	5.37	1.38	1.34
22	BA	1591	A	N3-C4	5.37	1.38	1.34
22	BA	2433	A	C8-N7	5.37	1.35	1.31
1	AA	702	A	N3-C4	5.37	1.38	1.34
1	AA	1248	A	C5-C4	-5.37	1.34	1.38
22	BA	609	A	C8-N7	5.37	1.35	1.31
22	BA	1009	A	C8-N7	5.37	1.35	1.31
1	AA	1000	A	C2-N3	5.37	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2097	A	C5-C4	-5.37	1.34	1.38
22	BA	2097	A	N3-C4	5.37	1.38	1.34
22	BA	2439	A	C8-N7	5.37	1.35	1.31
22	BA	2547	A	C8-N7	5.37	1.35	1.31
22	BA	73	A	C8-N7	5.37	1.35	1.31
22	BA	821	A	N9-C8	-5.37	1.33	1.37
22	BA	1872	A	C2-N3	5.37	1.38	1.33
1	AA	373	A	N3-C4	5.36	1.38	1.34
22	BA	13	A	C8-N7	5.36	1.35	1.31
22	BA	792	A	C8-N7	5.36	1.35	1.31
22	BA	1413	A	N3-C4	5.36	1.38	1.34
1	AA	1339	A	N3-C4	5.36	1.38	1.34
22	BA	127	A	C8-N7	5.36	1.35	1.31
22	BA	910	A	N7-C5	-5.36	1.36	1.39
22	BA	1635	A	N3-C4	5.36	1.38	1.34
22	BA	1129	A	C8-N7	5.36	1.35	1.31
22	BA	1194	A	C8-N7	5.36	1.35	1.31
22	BA	1027	A	C8-N7	5.36	1.35	1.31
23	BB	45	A	N3-C4	5.35	1.38	1.34
1	AA	560	A	N3-C4	5.35	1.38	1.34
1	AA	1256	A	C5-C4	-5.35	1.35	1.38
22	BA	244	A	C8-N7	5.35	1.35	1.31
22	BA	2287	A	C8-N7	5.35	1.35	1.31
22	BA	2706	A	C8-N7	5.35	1.35	1.31
22	BA	2572	A	C8-N7	5.35	1.35	1.31
22	BA	2199	A	N3-C4	5.35	1.38	1.34
55	B8	26	A	C5-C4	-5.35	1.35	1.38
22	BA	721	A	N3-C4	5.35	1.38	1.34
55	B8	41	A	C5-C4	-5.34	1.35	1.38
22	BA	1262	A	C8-N7	5.34	1.35	1.31
22	BA	1608	A	N7-C5	-5.34	1.36	1.39
1	AA	389	A	N3-C4	5.34	1.38	1.34
1	AA	753	A	N3-C4	5.34	1.38	1.34
1	AA	1339	A	C5-C4	-5.34	1.35	1.38
22	BA	2453	A	C8-N7	5.34	1.35	1.31
22	BA	1978	A	N3-C4	5.34	1.38	1.34
1	AA	59	A	N3-C4	5.34	1.38	1.34
1	AA	223	A	C5-C4	-5.34	1.35	1.38
22	BA	203	A	N7-C5	-5.33	1.36	1.39
22	BA	1080	A	N3-C4	5.33	1.38	1.34
22	BA	563	A	C8-N7	5.33	1.35	1.31
22	BA	2273	A	N7-C5	-5.33	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2741	A	C8-N7	5.33	1.35	1.31
22	BA	196	A	C8-N7	5.33	1.35	1.31
22	BA	547	A	C2-N3	5.33	1.38	1.33
22	BA	1754	A	N7-C5	-5.33	1.36	1.39
22	BA	2071	A	N7-C5	-5.33	1.36	1.39
1	AA	1111	A	N3-C4	5.33	1.38	1.34
1	AA	1287	A	C5-C4	-5.33	1.35	1.38
22	BA	125	A	N3-C4	5.33	1.38	1.34
22	BA	1689	A	C8-N7	5.33	1.35	1.31
22	BA	1367	A	N7-C5	-5.33	1.36	1.39
22	BA	1583	A	C5-C4	-5.33	1.35	1.38
22	BA	1759	A	C8-N7	5.33	1.35	1.31
22	BA	2327	A	C8-N7	5.33	1.35	1.31
22	BA	2388	A	C8-N7	5.33	1.35	1.31
1	AA	1468	A	N3-C4	5.33	1.38	1.34
22	BA	515	A	N9-C8	-5.33	1.33	1.37
1	AA	495	A	C5-C4	-5.32	1.35	1.38
1	AA	640	A	N3-C4	5.32	1.38	1.34
22	BA	1762	A	C8-N7	5.32	1.35	1.31
1	AA	171	A	N3-C4	5.32	1.38	1.34
22	BA	1085	A	C5-C4	-5.32	1.35	1.38
22	BA	2602	A	C5-C4	-5.32	1.35	1.38
22	BA	1847	A	N3-C4	5.32	1.38	1.34
1	AA	10	A	N3-C4	5.32	1.38	1.34
1	AA	790	A	N3-C4	5.32	1.38	1.34
1	AA	994	A	C5-C4	-5.32	1.35	1.38
22	BA	1226	A	N7-C5	-5.31	1.36	1.39
55	B8	21	A	C5-C4	-5.31	1.35	1.38
55	B8	42	A	C5-C4	-5.31	1.35	1.38
22	BA	1321	A	N3-C4	5.31	1.38	1.34
22	BA	878	A	C5-C4	-5.31	1.35	1.38
22	BA	1244	A	N7-C5	-5.31	1.36	1.39
22	BA	1700	A	C8-N7	5.31	1.35	1.31
22	BA	1978	A	C8-N7	5.31	1.35	1.31
22	BA	2019	A	C8-N7	5.31	1.35	1.31
55	B8	73	A	C2-N3	5.31	1.38	1.33
1	AA	77	A	C2-N3	5.31	1.38	1.33
1	AA	1318	A	C5-C4	-5.31	1.35	1.38
22	BA	943	A	N9-C8	-5.31	1.33	1.37
22	BA	1268	A	N9-C8	-5.31	1.33	1.37
22	BA	1439	A	C8-N7	5.31	1.35	1.31
22	BA	1916	A	N3-C4	5.31	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1998	A	N7-C5	-5.31	1.36	1.39
1	AA	253	A	N3-C4	5.30	1.38	1.34
1	AA	935	A	N3-C4	5.30	1.38	1.34
1	AA	1110	A	N3-C4	5.30	1.38	1.34
22	BA	2065	C	N1-C6	-5.30	1.33	1.37
1	AA	906	A	N3-C4	5.30	1.38	1.34
1	AA	1004	A	C5-C4	-5.30	1.35	1.38
1	AA	1169	A	C5-C4	-5.30	1.35	1.38
1	AA	98	A	N3-C4	5.30	1.38	1.34
1	AA	274	A	N3-C4	5.30	1.38	1.34
22	BA	1009	A	N7-C5	-5.30	1.36	1.39
1	AA	460	A	C5-C4	-5.29	1.35	1.38
1	AA	648	A	N3-C4	5.29	1.38	1.34
22	BA	532	A	N7-C5	-5.29	1.36	1.39
1	AA	162	A	N3-C4	5.29	1.38	1.34
1	AA	746	A	C2-N3	5.29	1.38	1.33
22	BA	739	A	C8-N7	5.29	1.35	1.31
22	BA	1073	A	C5-C4	-5.29	1.35	1.38
1	AA	55	A	C5-C4	-5.29	1.35	1.38
1	AA	1238	A	N3-C4	5.29	1.38	1.34
22	BA	988	A	C8-N7	5.29	1.35	1.31
22	BA	1608	A	N3-C4	5.29	1.38	1.34
22	BA	1977	A	N3-C4	5.29	1.38	1.34
1	AA	1046	A	C2-N3	5.29	1.38	1.33
22	BA	56	A	C8-N7	5.29	1.35	1.31
1	AA	451	A	N3-C4	5.29	1.38	1.34
22	BA	1287	A	N7-C5	-5.29	1.36	1.39
1	AA	502	A	N3-C4	5.29	1.38	1.34
22	BA	482	A	N7-C5	-5.29	1.36	1.39
22	BA	632	A	C8-N7	5.29	1.35	1.31
22	BA	1757	A	N3-C4	5.29	1.38	1.34
55	B8	58	A	C5-C4	-5.29	1.35	1.38
1	AA	706	A	N3-C4	5.28	1.38	1.34
22	BA	354	A	C5-C4	-5.28	1.35	1.38
22	BA	1593	A	N3-C4	5.28	1.38	1.34
23	BB	34	A	N3-C4	5.28	1.38	1.34
22	BA	900	A	C5-C4	-5.28	1.35	1.38
22	BA	430	A	C8-N7	5.28	1.35	1.31
22	BA	666	A	N3-C4	5.28	1.38	1.34
1	AA	53	A	N3-C4	5.28	1.38	1.34
1	AA	393	A	N3-C4	5.28	1.38	1.34
1	AA	493	A	C5-C4	-5.28	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	218	A	C8-N7	5.28	1.35	1.31
22	BA	1553	A	C8-N7	5.28	1.35	1.31
22	BA	2267	A	C8-N7	5.28	1.35	1.31
22	BA	2738	A	C8-N7	5.28	1.35	1.31
1	AA	465	A	C5-C4	-5.28	1.35	1.38
22	BA	251	A	N9-C8	-5.28	1.33	1.37
23	BB	78	A	C8-N7	5.28	1.35	1.31
22	BA	415	A	C8-N7	5.27	1.35	1.31
22	BA	1046	A	C5-C4	-5.27	1.35	1.38
1	AA	431	A	C5-C4	-5.27	1.35	1.38
1	AA	914	A	N3-C4	5.27	1.38	1.34
1	AA	974	A	N3-C4	5.27	1.38	1.34
22	BA	1900	A	C8-N7	5.27	1.35	1.31
22	BA	2311	A	N3-C4	5.27	1.38	1.34
22	BA	2418	A	N3-C4	5.27	1.38	1.34
1	AA	1093	A	N3-C4	5.27	1.38	1.34
22	BA	309	A	C8-N7	5.27	1.35	1.31
22	BA	1069	A	C5-C4	-5.27	1.35	1.38
22	BA	1367	A	C8-N7	5.27	1.35	1.31
22	BA	2560	A	N7-C5	-5.27	1.36	1.39
22	BA	2577	A	N9-C8	-5.27	1.33	1.37
55	B8	69	A	C2-N3	5.27	1.38	1.33
1	AA	977	A	N3-C4	5.27	1.38	1.34
1	AA	1201	A	C2-N3	5.26	1.38	1.33
22	BA	204	A	N7-C5	-5.26	1.36	1.39
22	BA	470	A	N7-C5	-5.26	1.36	1.39
22	BA	983	A	N7-C5	-5.26	1.36	1.39
1	AA	205	A	C5-C4	-5.26	1.35	1.38
22	BA	1789	A	C8-N7	5.26	1.35	1.31
22	BA	2799	A	C5-C4	-5.26	1.35	1.38
1	AA	1219	A	N3-C4	5.26	1.38	1.34
22	BA	219	A	C8-N7	5.26	1.35	1.31
22	BA	2005	A	N7-C5	-5.26	1.36	1.39
22	BA	2516	A	C8-N7	5.26	1.35	1.31
22	BA	1936	A	N7-C5	-5.26	1.36	1.39
1	AA	482	A	N3-C4	5.26	1.38	1.34
22	BA	1151	A	N7-C5	-5.25	1.36	1.39
22	BA	1254	A	N9-C8	-5.25	1.33	1.37
1	AA	579	A	N3-C4	5.25	1.38	1.34
22	BA	2170	A	C2-N3	5.25	1.38	1.33
22	BA	2799	A	C2-N3	5.25	1.38	1.33
1	AA	383	A	C2-N3	5.25	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	501	A	C8-N7	5.25	1.35	1.31
22	BA	1532	A	C5-C4	-5.25	1.35	1.38
22	BA	2241	A	C8-N7	5.25	1.35	1.31
1	AA	1227	A	C5-C4	-5.25	1.35	1.38
1	AA	546	A	N3-C4	5.25	1.38	1.34
22	BA	1387	A	C8-N7	5.25	1.35	1.31
1	AA	366	A	N3-C4	5.25	1.38	1.34
22	BA	2725	A	N3-C4	5.25	1.38	1.34
1	AA	520	A	N3-C4	5.25	1.38	1.34
22	BA	207	A	C8-N7	5.25	1.35	1.31
22	BA	1241	A	C8-N7	5.24	1.35	1.31
23	BB	73	A	C8-N7	5.24	1.35	1.31
22	BA	1431	A	N7-C5	-5.24	1.36	1.39
22	BA	2426	A	C8-N7	5.24	1.35	1.31
1	AA	1171	A	C2-N3	5.24	1.38	1.33
22	BA	2082	A	N7-C5	-5.24	1.36	1.39
1	AA	767	A	C8-N7	5.24	1.35	1.31
22	BA	1899	A	N7-C5	-5.24	1.36	1.39
22	BA	2211	A	C5-C4	-5.24	1.35	1.38
22	BA	1722	A	N3-C4	5.24	1.38	1.34
22	BA	1354	A	N9-C8	-5.24	1.33	1.37
22	BA	2183	A	C5-C4	-5.24	1.35	1.38
1	AA	1375	A	N3-C4	5.23	1.38	1.34
1	AA	192	A	C5-C4	-5.23	1.35	1.38
22	BA	1502	A	N3-C4	5.23	1.38	1.34
22	BA	1772	A	C8-N7	5.23	1.35	1.31
1	AA	533	A	C2-N3	5.23	1.38	1.33
22	BA	226	A	C8-N7	5.23	1.35	1.31
22	BA	1705	A	C8-N7	5.23	1.35	1.31
1	AA	1350	A	N3-C4	5.23	1.38	1.34
22	BA	2020	A	C8-N7	5.23	1.35	1.31
22	BA	2837	A	C8-N7	5.23	1.35	1.31
1	AA	172	A	N3-C4	5.23	1.38	1.34
1	AA	1012	A	C2-N3	5.23	1.38	1.33
22	BA	1353	A	N9-C8	-5.23	1.33	1.37
1	AA	72	A	N3-C4	5.22	1.38	1.34
1	AA	900	A	N7-C5	-5.22	1.36	1.39
22	BA	574	A	C8-N7	5.22	1.35	1.31
22	BA	920	A	N9-C8	-5.22	1.33	1.37
1	AA	1398	A	N3-C4	5.22	1.38	1.34
22	BA	1237	A	C8-N7	5.22	1.35	1.31
22	BA	2765	A	N7-C5	-5.22	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	495	A	N3-C4	5.22	1.38	1.34
22	BA	845	A	N3-C4	5.22	1.38	1.34
1	AA	74	A	C5-C4	-5.22	1.35	1.38
22	BA	522	A	N7-C5	-5.22	1.36	1.39
22	BA	2117	A	C2-N3	5.22	1.38	1.33
1	AA	1012	A	C5-C4	-5.21	1.35	1.38
1	AA	1080	A	N3-C4	5.21	1.38	1.34
55	B8	26	A	C2-N3	5.21	1.38	1.33
1	AA	1408	A	N3-C4	5.21	1.38	1.34
22	BA	460	A	C8-N7	5.21	1.35	1.31
22	BA	570	G	N1-C2	-5.21	1.33	1.37
22	BA	2432	A	N3-C4	5.21	1.38	1.34
1	AA	452	A	C5-C4	-5.21	1.35	1.38
22	BA	1746	A	N3-C4	5.21	1.38	1.34
22	BA	1759	A	N3-C4	5.21	1.38	1.34
22	BA	2052	A	N9-C8	-5.21	1.33	1.37
24	BC	247	PRO	CG-CD	-5.21	1.33	1.50
22	BA	1809	A	C8-N7	5.21	1.35	1.31
55	B8	41	A	C2-N3	5.21	1.38	1.33
23	BB	39	A	N3-C4	5.21	1.38	1.34
22	BA	1689	A	N7-C5	-5.20	1.36	1.39
22	BA	1794	A	N9-C8	-5.20	1.33	1.37
22	BA	2247	A	N9-C8	-5.20	1.33	1.37
1	AA	878	A	N3-C4	5.20	1.38	1.34
22	BA	1853	A	C8-N7	5.20	1.35	1.31
1	AA	539	A	N3-C4	5.20	1.38	1.34
1	AA	1261	A	C5-C4	-5.20	1.35	1.38
22	BA	352	A	N3-C4	5.20	1.38	1.34
22	BA	505	A	C8-N7	5.20	1.35	1.31
22	BA	522	A	N9-C8	-5.20	1.33	1.37
22	BA	582	A	N7-C5	-5.20	1.36	1.39
22	BA	675	A	N9-C8	-5.20	1.33	1.37
22	BA	734	A	C8-N7	5.20	1.35	1.31
22	BA	1010	A	N9-C8	-5.20	1.33	1.37
22	BA	1393	A	N9-C8	-5.20	1.33	1.37
55	B8	58	A	C2-N3	5.20	1.38	1.33
1	AA	196	A	N3-C4	5.19	1.38	1.34
1	AA	1055	A	C5-C4	-5.19	1.35	1.38
22	BA	2014	A	N9-C8	-5.19	1.33	1.37
22	BA	2053	G	C5-C4	-5.19	1.34	1.38
23	BB	15	A	N3-C4	5.19	1.38	1.34
22	BA	2199	A	N7-C5	-5.19	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	300	A	N7-C5	-5.19	1.36	1.39
22	BA	556	A	N3-C4	5.19	1.38	1.34
23	BB	50	A	N3-C4	5.19	1.38	1.34
1	AA	694	A	N3-C4	5.19	1.38	1.34
1	AA	718	A	N3-C4	5.19	1.38	1.34
1	AA	792	A	N3-C4	5.19	1.38	1.34
22	BA	1155	A	N7-C5	-5.19	1.36	1.39
22	BA	1655	A	C8-N7	5.19	1.35	1.31
1	AA	978	A	N3-C4	5.18	1.38	1.34
1	AA	16	A	N3-C4	5.18	1.38	1.34
1	AA	160	A	N3-C4	5.18	1.38	1.34
22	BA	2212	A	N7-C5	-5.18	1.36	1.39
22	BA	2378	A	N3-C4	5.18	1.38	1.34
22	BA	2733	A	N3-C4	5.18	1.38	1.34
22	BA	1284	A	C8-N7	5.18	1.35	1.31
22	BA	2710	C	N3-C4	-5.18	1.30	1.33
22	BA	668	A	C8-N7	5.18	1.35	1.31
22	BA	1535	A	C2-N3	5.18	1.38	1.33
1	AA	28	A	C5-C4	-5.18	1.35	1.38
22	BA	196	A	N7-C5	-5.18	1.36	1.39
22	BA	1966	A	N7-C5	-5.18	1.36	1.39
1	AA	1324	A	C5-C4	-5.17	1.35	1.38
22	BA	14	A	C8-N7	5.17	1.35	1.31
22	BA	637	A	N3-C4	5.17	1.38	1.34
22	BA	1169	A	N3-C4	5.17	1.38	1.34
22	BA	1614	A	C8-N7	5.17	1.35	1.31
22	BA	2425	A	N7-C5	-5.17	1.36	1.39
22	BA	2513	A	C8-N7	5.17	1.35	1.31
22	BA	592	A	N7-C5	-5.17	1.36	1.39
22	BA	689	A	C8-N7	5.17	1.35	1.31
22	BA	1952	A	C8-N7	5.17	1.35	1.31
1	AA	969	A	N3-C4	5.17	1.38	1.34
22	BA	374	A	C8-N7	5.17	1.35	1.31
22	BA	2386	A	N9-C8	-5.17	1.33	1.37
22	BA	2497	A	N9-C8	-5.17	1.33	1.37
1	AA	630	A	C5-C4	-5.17	1.35	1.38
22	BA	401	A	C8-N7	5.17	1.35	1.31
22	BA	1815	A	C8-N7	5.17	1.35	1.31
22	BA	626	A	N3-C4	5.16	1.38	1.34
22	BA	1866	A	N3-C4	5.16	1.38	1.34
22	BA	2298	A	N3-C4	5.16	1.38	1.34
22	BA	644	A	C8-N7	5.16	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	227	A	N7-C5	-5.16	1.36	1.39
22	BA	716	A	N3-C4	5.16	1.38	1.34
22	BA	1084	A	C5-C4	-5.16	1.35	1.38
22	BA	2781	A	C8-N7	5.16	1.35	1.31
55	B8	69	A	C5-C4	-5.16	1.35	1.38
22	BA	176	A	C8-N7	5.16	1.35	1.31
22	BA	1678	A	N7-C5	-5.16	1.36	1.39
55	B8	66	A	C2-N3	5.16	1.38	1.33
1	AA	263	A	N3-C4	5.16	1.38	1.34
22	BA	2071	A	N9-C8	-5.16	1.33	1.37
1	AA	1446	A	N3-C4	5.16	1.38	1.34
22	BA	783	A	C5-C4	-5.16	1.35	1.38
22	BA	800	A	C8-N7	5.16	1.35	1.31
22	BA	1677	A	N3-C4	5.16	1.38	1.34
1	AA	66	A	N3-C4	5.15	1.38	1.34
22	BA	1095	A	C2-N3	5.15	1.38	1.33
22	BA	1677	A	C8-N7	5.15	1.35	1.31
22	BA	2542	A	C8-N7	5.15	1.35	1.31
1	AA	300	A	N3-C4	5.15	1.38	1.34
1	AA	432	A	N3-C4	5.15	1.38	1.34
22	BA	251	A	N7-C5	-5.15	1.36	1.39
22	BA	477	A	N7-C5	-5.15	1.36	1.39
22	BA	1569	A	N9-C8	-5.15	1.33	1.37
22	BA	972	A	C8-N7	5.15	1.35	1.31
1	AA	901	A	N3-C4	5.14	1.38	1.34
22	BA	981	A	C8-N7	5.14	1.35	1.31
1	AA	1102	A	N3-C4	5.14	1.38	1.34
22	BA	1322	A	N3-C4	5.14	1.38	1.34
22	BA	1508	A	C5-C4	-5.14	1.35	1.38
22	BA	1745	A	N3-C4	5.14	1.38	1.34
22	BA	2171	A	C2-N3	5.14	1.38	1.33
22	BA	1762	A	N7-C5	-5.14	1.36	1.39
55	B8	51	A	C2-N3	5.14	1.38	1.33
1	AA	363	A	N3-C4	5.14	1.38	1.34
1	AA	78	A	C2-N3	5.14	1.38	1.33
22	BA	256	A	C8-N7	5.14	1.35	1.31
22	BA	443	A	C8-N7	5.14	1.35	1.31
22	BA	794	A	N7-C5	-5.14	1.36	1.39
22	BA	1590	A	N3-C4	5.14	1.38	1.34
22	BA	2450	A	C8-N7	5.14	1.35	1.31
23	BB	109	A	N3-C4	5.14	1.38	1.34
1	AA	1239	A	N3-C4	5.13	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1089	A	C2-N3	5.13	1.38	1.33
22	BA	1652	A	N7-C5	-5.13	1.36	1.39
1	AA	250	A	C2-N3	5.13	1.38	1.33
22	BA	538	A	C8-N7	5.13	1.35	1.31
22	BA	905	A	N3-C4	5.13	1.38	1.34
22	BA	1021	A	N7-C5	-5.13	1.36	1.39
22	BA	1269	A	C8-N7	5.13	1.35	1.31
22	BA	1528	A	N3-C4	5.13	1.38	1.34
22	BA	2679	A	N7-C5	-5.13	1.36	1.39
22	BA	447	A	N7-C5	-5.13	1.36	1.39
22	BA	833	A	C8-N7	5.13	1.35	1.31
22	BA	1151	A	C8-N7	5.13	1.35	1.31
22	BA	1672	A	N7-C5	-5.13	1.36	1.39
23	BB	94	A	N3-C4	5.13	1.38	1.34
22	BA	821	A	N7-C5	-5.12	1.36	1.39
1	AA	831	A	N3-C4	5.12	1.38	1.34
1	AA	1005	A	C2-N3	5.12	1.38	1.33
22	BA	457	A	C8-N7	5.12	1.35	1.31
22	BA	1077	A	C5-C4	-5.12	1.35	1.38
22	BA	1977	A	C8-N7	5.12	1.35	1.31
1	AA	1250	A	C5-C4	-5.12	1.35	1.38
22	BA	1551	A	N7-C5	-5.12	1.36	1.39
22	BA	1598	A	C8-N7	5.12	1.35	1.31
22	BA	2270	A	C8-N7	5.12	1.35	1.31
22	BA	21	A	N7-C5	-5.12	1.36	1.39
22	BA	514	A	C8-N7	5.12	1.35	1.31
22	BA	2176	A	C2-N3	5.12	1.38	1.33
22	BA	661	A	N9-C8	-5.12	1.33	1.37
22	BA	739	A	N7-C5	-5.12	1.36	1.39
22	BA	1668	A	C8-N7	5.12	1.35	1.31
22	BA	2459	A	C8-N7	5.12	1.35	1.31
1	AA	649	A	N3-C4	5.11	1.38	1.34
22	BA	586	A	C8-N7	5.11	1.35	1.31
22	BA	6	A	C8-N7	5.11	1.35	1.31
22	BA	925	A	N3-C4	5.11	1.38	1.34
1	AA	1146	A	N3-C4	5.11	1.38	1.34
22	BA	1151	A	N9-C8	-5.11	1.33	1.37
22	BA	1773	A	C8-N7	5.11	1.35	1.31
55	B8	38	A	C2-N3	5.11	1.38	1.33
22	BA	800	A	N9-C8	-5.11	1.33	1.37
1	AA	435	A	C5-C4	-5.11	1.35	1.38
22	BA	203	A	C8-N7	5.11	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	959	A	C8-N7	5.11	1.35	1.31
1	AA	747	A	N3-C4	5.11	1.38	1.34
1	AA	1350	A	C5-C4	-5.11	1.35	1.38
22	BA	478	A	C8-N7	5.11	1.35	1.31
22	BA	1155	A	N9-C8	-5.11	1.33	1.37
22	BA	2547	A	N7-C5	-5.11	1.36	1.39
22	BA	1854	A	N9-C8	-5.10	1.33	1.37
1	AA	1150	A	C5-C4	-5.10	1.35	1.38
22	BA	2142	A	C2-N3	5.10	1.38	1.33
22	BA	2448	A	C8-N7	5.10	1.35	1.31
1	AA	452	A	N3-C4	5.10	1.38	1.34
22	BA	735	A	C8-N7	5.10	1.35	1.31
22	BA	2542	A	N7-C5	-5.10	1.36	1.39
55	B8	73	A	C5-C4	-5.10	1.35	1.38
1	AA	397	A	C2-N3	5.10	1.38	1.33
22	BA	1247	A	N9-C8	-5.10	1.33	1.37
22	BA	1353	A	C8-N7	5.10	1.35	1.31
22	BA	917	A	N7-C5	-5.10	1.36	1.39
1	AA	915	A	N3-C4	5.09	1.38	1.34
22	BA	866	A	N3-C4	5.09	1.38	1.34
22	BA	2705	A	C8-N7	5.09	1.35	1.31
22	BA	2020	A	N9-C8	-5.09	1.33	1.37
22	BA	2163	A	C2-N3	5.09	1.38	1.33
55	B8	66	A	C5-C4	-5.09	1.35	1.38
1	AA	780	A	N7-C5	-5.09	1.36	1.39
1	AA	1441	A	C2-N3	5.09	1.38	1.33
22	BA	199	A	N7-C5	-5.09	1.36	1.39
22	BA	401	A	N7-C5	-5.09	1.36	1.39
22	BA	502	A	C8-N7	5.09	1.35	1.31
1	AA	1437	A	N3-C4	5.09	1.38	1.34
22	BA	471	A	C8-N7	5.09	1.35	1.31
22	BA	1890	A	N3-C4	5.09	1.38	1.34
1	AA	1152	A	C2-N3	5.09	1.38	1.33
1	AA	1413	A	N3-C4	5.09	1.38	1.34
22	BA	28	A	N9-C8	-5.09	1.33	1.37
22	BA	781	A	N7-C5	-5.09	1.36	1.39
1	AA	696	A	N3-C4	5.08	1.38	1.34
1	AA	1146	A	C5-C4	-5.08	1.35	1.38
22	BA	613	A	C2-N3	5.08	1.38	1.33
22	BA	241	A	N7-C5	-5.08	1.36	1.39
22	BA	990	A	C8-N7	5.08	1.35	1.31
22	BA	1126	A	N7-C5	-5.08	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2266	A	N9-C8	-5.08	1.33	1.37
22	BA	104	A	N3-C4	5.08	1.37	1.34
22	BA	241	A	C8-N7	5.08	1.35	1.31
22	BA	2119	A	C2-N3	5.08	1.38	1.33
1	AA	116	A	N3-C4	5.08	1.37	1.34
22	BA	920	A	C8-N7	5.08	1.35	1.31
1	AA	238	A	N3-C4	5.08	1.37	1.34
22	BA	2009	A	N9-C8	-5.08	1.33	1.37
22	BA	2757	A	N3-C4	5.08	1.37	1.34
55	B8	14	A	C5-C4	-5.08	1.35	1.38
22	BA	1268	A	N7-C5	-5.07	1.36	1.39
1	AA	1000	A	C5-C4	-5.07	1.35	1.38
22	BA	231	A	N7-C5	-5.07	1.36	1.39
55	B8	38	A	C5-C4	-5.07	1.35	1.38
1	AA	1219	A	C2-N3	5.07	1.38	1.33
1	AA	1274	A	C5-C4	-5.07	1.35	1.38
22	BA	384	A	C8-N7	5.07	1.35	1.31
22	BA	1970	A	N3-C4	5.07	1.37	1.34
22	BA	2412	A	N9-C8	-5.07	1.33	1.37
1	AA	1254	A	C5-C4	-5.07	1.35	1.38
22	BA	2154	A	C2-N3	5.07	1.38	1.33
22	BA	207	A	N7-C5	-5.07	1.36	1.39
22	BA	362	A	C5-C4	-5.07	1.35	1.38
22	BA	1269	A	N7-C5	-5.07	1.36	1.39
22	BA	1676	A	N9-C8	-5.07	1.33	1.37
22	BA	2835	A	N3-C4	5.07	1.37	1.34
23	BB	57	A	N3-C4	5.07	1.37	1.34
1	AA	609	A	N3-C4	5.07	1.37	1.34
22	BA	750	A	N9-C8	-5.07	1.33	1.37
22	BA	1392	A	N3-C4	5.07	1.37	1.34
22	BA	1789	A	N7-C5	-5.07	1.36	1.39
22	BA	348	A	N3-C4	5.06	1.37	1.34
1	AA	190	A	C5-C4	-5.06	1.35	1.38
1	AA	300	A	C8-N7	5.06	1.35	1.31
22	BA	412	A	N7-C5	-5.06	1.36	1.39
22	BA	1655	A	N3-C4	5.06	1.37	1.34
1	AA	819	A	N3-C4	5.06	1.37	1.34
1	AA	1500	A	N3-C4	5.06	1.37	1.34
1	AA	131	A	N3-C4	5.06	1.37	1.34
1	AA	320	A	N3-C4	5.06	1.37	1.34
22	BA	2009	A	N7-C5	-5.06	1.36	1.39
22	BA	2037	A	N7-C5	-5.06	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2358	A	N9-C8	-5.06	1.33	1.37
1	AA	26	A	N3-C4	5.06	1.37	1.34
1	AA	1093	A	C5-C4	-5.06	1.35	1.38
1	AA	1197	A	C2-N3	5.06	1.38	1.33
22	BA	270	A	N3-C4	5.06	1.37	1.34
22	BA	959	A	N7-C5	-5.06	1.36	1.39
22	BA	1787	A	N9-C8	-5.06	1.33	1.37
22	BA	1969	A	N9-C8	-5.06	1.33	1.37
22	BA	2589	A	N3-C4	5.06	1.37	1.34
22	BA	52	A	N9-C8	-5.06	1.33	1.37
1	AA	1350	A	C2-N3	5.05	1.38	1.33
22	BA	1876	A	N3-C4	5.05	1.37	1.34
22	BA	1877	A	N3-C4	5.05	1.37	1.34
22	BA	2757	A	N7-C5	-5.05	1.36	1.39
1	AA	1394	A	N3-C4	5.05	1.37	1.34
22	BA	1090	A	C5-C4	-5.05	1.35	1.38
1	AA	120	A	N3-C4	5.05	1.37	1.34
1	AA	502	A	C2-N3	5.05	1.38	1.33
22	BA	1098	A	C2-N3	5.05	1.38	1.33
22	BA	1175	A	C2-N3	5.05	1.38	1.33
55	B8	21	A	C2-N3	5.05	1.38	1.33
22	BA	918	A	C8-N7	5.05	1.35	1.31
23	BB	52	A	N3-C4	5.05	1.37	1.34
22	BA	1805	A	C8-N7	5.05	1.35	1.31
22	BA	2879	A	C8-N7	5.04	1.35	1.31
22	BA	943	A	N7-C5	-5.04	1.36	1.39
22	BA	1664	A	C8-N7	5.04	1.35	1.31
22	BA	1672	A	N3-C4	5.04	1.37	1.34
22	BA	2101	A	N1-C2	5.04	1.38	1.34
22	BA	2590	A	C8-N7	5.04	1.35	1.31
1	AA	28	A	C2-N3	5.04	1.38	1.33
24	BC	218	PRO	CG-CD	-5.04	1.34	1.50
22	BA	1548	A	N3-C4	5.04	1.37	1.34
23	BB	99	A	C8-N7	5.04	1.35	1.31
1	AA	583	A	N3-C4	5.04	1.37	1.34
22	BA	216	A	N7-C5	-5.04	1.36	1.39
22	BA	1854	A	N3-C4	5.04	1.37	1.34
1	AA	189	A	C2-N3	5.04	1.38	1.33
1	AA	374	A	C5-C4	-5.04	1.35	1.38
22	BA	911	A	C8-N7	5.04	1.35	1.31
22	BA	1009	A	N9-C8	-5.04	1.33	1.37
22	BA	1637	A	N3-C4	5.04	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	665	A	N3-C4	5.03	1.37	1.34
1	AA	1022	A	C2-N3	5.03	1.38	1.33
22	BA	2184	A	C2-N3	5.03	1.38	1.33
1	AA	1111	A	C5-C4	-5.03	1.35	1.38
22	BA	344	A	N3-C4	5.03	1.37	1.34
22	BA	216	A	C8-N7	5.03	1.35	1.31
22	BA	532	A	C8-N7	5.03	1.35	1.31
22	BA	538	A	N7-C5	-5.03	1.36	1.39
22	BA	804	A	N7-C5	-5.03	1.36	1.39
22	BA	1088	A	C2-N3	5.03	1.38	1.33
22	BA	1260	A	N9-C8	-5.03	1.33	1.37
22	BA	2335	A	C8-N7	5.03	1.35	1.31
22	BA	1477	A	N3-C4	5.03	1.37	1.34
1	AA	101	A	N3-C4	5.03	1.37	1.34
1	AA	816	A	N3-C4	5.03	1.37	1.34
1	AA	1151	A	C2-N3	5.03	1.38	1.33
22	BA	453	A	N7-C5	-5.03	1.36	1.39
22	BA	1393	A	N7-C5	-5.03	1.36	1.39
55	B8	42	A	C2-N3	5.02	1.38	1.33
1	AA	996	A	C5-C4	-5.02	1.35	1.38
22	BA	1698	A	C8-N7	5.02	1.35	1.31
22	BA	1784	A	C8-N7	5.02	1.35	1.31
22	BA	2893	A	N3-C4	5.02	1.37	1.34
22	BA	1001	A	N7-C5	-5.02	1.36	1.39
22	BA	1365	A	N7-C5	-5.02	1.36	1.39
22	BA	1936	A	C2-N3	5.02	1.38	1.33
22	BA	2675	A	C8-N7	5.02	1.35	1.31
22	BA	825	A	C8-N7	5.02	1.35	1.31
22	BA	2241	A	N7-C5	-5.02	1.36	1.39
1	AA	55	A	C2-N3	5.01	1.38	1.33
22	BA	477	A	C8-N7	5.01	1.35	1.31
22	BA	1610	A	C8-N7	5.01	1.35	1.31
22	BA	2169	A	C2-N3	5.01	1.38	1.33
22	BA	2577	A	N7-C5	-5.01	1.36	1.39
1	AA	1042	A	C5-C4	-5.01	1.35	1.38
22	BA	1808	A	C2-N3	5.01	1.38	1.33
22	BA	172	A	N3-C4	5.01	1.37	1.34
22	BA	960	A	N9-C8	-5.01	1.33	1.37
22	BA	1580	A	N3-C4	5.01	1.37	1.34
22	BA	1998	A	N3-C4	5.01	1.37	1.34
22	BA	101	A	N7-C5	-5.01	1.36	1.39
22	BA	661	A	C8-N7	5.01	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	685	A	N9-C8	-5.01	1.33	1.37
22	BA	2471	A	N3-C4	5.01	1.37	1.34
22	BA	1821	A	N7-C5	-5.01	1.36	1.39
22	BA	2418	A	N7-C5	-5.01	1.36	1.39
22	BA	2660	A	N3-C4	5.01	1.37	1.34
22	BA	2826	A	N3-C4	5.01	1.37	1.34
1	AA	465	A	C2-N3	5.00	1.38	1.33
22	BA	1214	A	C8-N7	5.00	1.35	1.31
22	BA	2366	A	C8-N7	5.00	1.35	1.31
22	BA	1090	A	C2-N3	5.00	1.38	1.33
22	BA	1342	A	N9-C8	-5.00	1.33	1.37
55	B8	14	A	C2-N3	5.00	1.38	1.33
1	AA	860	A	N3-C4	5.00	1.37	1.34
22	BA	892	A	C2'-O2'	5.00	1.48	1.41
22	BA	1598	A	N3-C4	5.00	1.37	1.34
22	BA	1634	A	C8-N7	5.00	1.35	1.31
22	BA	2407	A	C8-N7	5.00	1.35	1.31

All (13331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2451	A	N1-C6-N6	-24.52	103.89	118.60
22	BA	2872	A	N1-C6-N6	-23.89	104.27	118.60
22	BA	1668	A	N1-C6-N6	-23.68	104.39	118.60
22	BA	1668	A	C2-N3-C4	23.56	122.38	110.60
22	BA	1668	A	N1-C2-N3	-23.30	117.65	129.30
22	BA	1328	A	N1-C6-N6	-22.77	104.94	118.60
22	BA	1937	A	N1-C6-N6	-22.49	105.11	118.60
22	BA	119	A	N1-C6-N6	-22.10	105.34	118.60
22	BA	821	A	N1-C6-N6	-22.10	105.34	118.60
22	BA	1378	A	N1-C6-N6	-22.05	105.37	118.60
22	BA	1815	A	N1-C6-N6	-22.01	105.39	118.60
22	BA	1308	A	N1-C6-N6	-21.98	105.41	118.60
22	BA	2327	A	N1-C6-N6	-21.97	105.42	118.60
22	BA	2346	A	N1-C6-N6	-21.95	105.43	118.60
22	BA	1133	A	N1-C6-N6	-21.95	105.43	118.60
22	BA	84	A	N1-C6-N6	-21.93	105.44	118.60
22	BA	2542	A	N1-C2-N3	-21.90	118.35	129.30
22	BA	2765	A	N1-C6-N6	-21.75	105.55	118.60
22	BA	2052	A	C2-N3-C4	21.67	121.43	110.60
22	BA	941	A	N1-C2-N3	-21.56	118.52	129.30
22	BA	575	A	N1-C6-N6	-21.54	105.68	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1789	A	N1-C6-N6	-21.48	105.71	118.60
22	BA	126	A	N1-C6-N6	-21.47	105.72	118.60
22	BA	1652	A	N1-C6-N6	-21.47	105.72	118.60
22	BA	526	A	N1-C6-N6	-21.45	105.73	118.60
22	BA	582	A	N1-C6-N6	-21.44	105.73	118.60
22	BA	1515	A	N1-C6-N6	-21.43	105.74	118.60
22	BA	1698	A	N1-C6-N6	-21.42	105.75	118.60
22	BA	2764	A	N1-C6-N6	-21.40	105.76	118.60
22	BA	1803	A	N1-C6-N6	-21.39	105.77	118.60
22	BA	825	A	N1-C6-N6	-21.36	105.79	118.60
22	BA	199	A	N1-C6-N6	-21.31	105.82	118.60
1	AA	119	A	N1-C6-N6	-21.30	105.82	118.60
22	BA	2766	A	C2-N3-C4	21.29	121.24	110.60
22	BA	503	A	C2-N3-C4	21.27	121.24	110.60
22	BA	764	A	N1-C2-N3	-21.26	118.67	129.30
22	BA	783	A	N1-C6-N6	-21.23	105.86	118.60
22	BA	1821	A	N1-C6-N6	-21.21	105.87	118.60
22	BA	1936	A	C2-N3-C4	21.18	121.19	110.60
22	BA	1937	A	N1-C2-N3	-21.17	118.72	129.30
22	BA	792	A	C2-N3-C4	21.14	121.17	110.60
22	BA	2766	A	N1-C2-N3	-21.11	118.74	129.30
1	AA	915	A	N1-C6-N6	-21.11	105.94	118.60
1	AA	243	A	N1-C6-N6	-21.10	105.94	118.60
22	BA	1669	A	N1-C6-N6	-21.09	105.94	118.60
1	AA	729	A	N1-C6-N6	-21.09	105.95	118.60
1	AA	412	A	N1-C6-N6	-21.08	105.95	118.60
22	BA	2077	A	C2-N3-C4	21.07	121.14	110.60
1	AA	498	A	C2-N3-C4	21.07	121.14	110.60
1	AA	1225	A	C2-N3-C4	21.05	121.13	110.60
22	BA	1262	A	N1-C6-N6	-21.05	105.97	118.60
22	BA	53	A	N1-C6-N6	-21.05	105.97	118.60
1	AA	431	A	N1-C6-N6	-21.04	105.97	118.60
1	AA	1433	A	N1-C6-N6	-21.02	105.98	118.60
22	BA	1669	A	C2-N3-C4	21.02	121.11	110.60
22	BA	1286	A	N1-C2-N3	-21.00	118.80	129.30
1	AA	152	A	N1-C6-N6	-21.00	106.00	118.60
22	BA	2753	A	N1-C6-N6	-20.99	106.01	118.60
22	BA	2070	A	C2-N3-C4	20.98	121.09	110.60
22	BA	911	A	C2-N3-C4	20.95	121.08	110.60
22	BA	1253	A	N1-C6-N6	-20.95	106.03	118.60
22	BA	345	A	N1-C6-N6	-20.95	106.03	118.60
22	BA	1254	A	N1-C2-N3	-20.92	118.84	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1815	A	N1-C2-N3	-20.91	118.85	129.30
1	AA	1213	A	N1-C6-N6	-20.90	106.06	118.60
22	BA	1021	A	N1-C6-N6	-20.89	106.07	118.60
22	BA	1032	A	N1-C6-N6	-20.87	106.08	118.60
22	BA	2829	A	N1-C6-N6	-20.87	106.08	118.60
22	BA	2070	A	N1-C6-N6	-20.86	106.09	118.60
22	BA	241	A	N1-C6-N6	-20.85	106.09	118.60
22	BA	756	A	C2-N3-C4	20.85	121.03	110.60
55	B8	76	A	N1-C2-N3	-20.85	118.88	129.30
1	AA	1480	A	N1-C6-N6	-20.83	106.10	118.60
22	BA	603	A	N1-C6-N6	-20.83	106.10	118.60
22	BA	146	A	N1-C6-N6	-20.82	106.11	118.60
22	BA	1932	A	N1-C6-N6	-20.82	106.11	118.60
22	BA	161	A	N1-C6-N6	-20.82	106.11	118.60
22	BA	219	A	C2-N3-C4	20.80	121.00	110.60
1	AA	665	A	N1-C6-N6	-20.80	106.12	118.60
22	BA	984	A	C2-N3-C4	20.80	121.00	110.60
22	BA	2435	A	N1-C6-N6	-20.80	106.12	118.60
1	AA	977	A	C2-N3-C4	20.80	121.00	110.60
22	BA	2513	A	N1-C6-N6	-20.78	106.13	118.60
1	AA	397	A	C2-N3-C4	20.78	120.99	110.60
22	BA	219	A	N1-C6-N6	-20.77	106.14	118.60
22	BA	783	A	C2-N3-C4	20.77	120.98	110.60
22	BA	2369	A	C2-N3-C4	20.77	120.98	110.60
22	BA	1937	A	C2-N3-C4	20.75	120.97	110.60
22	BA	1204	A	N1-C6-N6	-20.75	106.15	118.60
22	BA	1690	A	N1-C6-N6	-20.75	106.15	118.60
22	BA	2227	A	N1-C6-N6	-20.72	106.17	118.60
22	BA	1395	A	N1-C6-N6	-20.72	106.17	118.60
22	BA	756	A	N1-C2-N3	-20.72	118.94	129.30
22	BA	1359	A	N1-C6-N6	-20.70	106.18	118.60
1	AA	695	A	N1-C6-N6	-20.69	106.18	118.60
22	BA	195	A	N1-C2-N3	-20.69	118.95	129.30
22	BA	2453	A	N1-C6-N6	-20.68	106.19	118.60
22	BA	38	A	C2-N3-C4	20.66	120.93	110.60
22	BA	2267	A	C2-N3-C4	20.66	120.93	110.60
22	BA	2726	A	N1-C2-N3	-20.66	118.97	129.30
22	BA	2660	A	N1-C6-N6	-20.66	106.21	118.60
22	BA	2054	A	C2-N3-C4	20.65	120.92	110.60
22	BA	1354	A	N1-C6-N6	-20.65	106.21	118.60
22	BA	1809	A	C2-N3-C4	20.64	120.92	110.60
1	AA	704	A	N1-C6-N6	-20.64	106.21	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	71	A	N1-C6-N6	-20.63	106.22	118.60
22	BA	1142	A	N1-C6-N6	-20.63	106.22	118.60
22	BA	2352	A	N1-C6-N6	-20.61	106.23	118.60
22	BA	2267	A	N1-C6-N6	-20.61	106.24	118.60
22	BA	1021	A	C2-N3-C4	20.60	120.90	110.60
22	BA	1237	A	N1-C6-N6	-20.60	106.24	118.60
22	BA	443	A	N1-C2-N3	-20.59	119.00	129.30
22	BA	1085	A	N1-C6-N6	-20.59	106.24	118.60
22	BA	1385	A	N1-C6-N6	-20.59	106.24	118.60
22	BA	2060	A	N1-C2-N3	-20.59	119.00	129.30
22	BA	2766	A	N1-C6-N6	-20.59	106.25	118.60
22	BA	1165	A	N1-C6-N6	-20.59	106.25	118.60
22	BA	1264	A	N1-C2-N3	-20.57	119.01	129.30
22	BA	2518	A	C2-N3-C4	20.57	120.89	110.60
22	BA	2761	A	N1-C2-N3	-20.57	119.02	129.30
22	BA	756	A	N1-C6-N6	-20.56	106.26	118.60
22	BA	2679	A	N1-C6-N6	-20.56	106.26	118.60
22	BA	2273	A	C2-N3-C4	20.55	120.88	110.60
22	BA	2726	A	C2-N3-C4	20.55	120.87	110.60
1	AA	1229	A	N1-C6-N6	-20.55	106.27	118.60
22	BA	13	A	N1-C6-N6	-20.54	106.28	118.60
22	BA	973	A	N1-C6-N6	-20.52	106.28	118.60
1	AA	938	A	C2-N3-C4	20.52	120.86	110.60
22	BA	2169	A	C2-N3-C4	20.52	120.86	110.60
1	AA	919	A	N1-C6-N6	-20.50	106.30	118.60
22	BA	449	A	N1-C6-N6	-20.50	106.30	118.60
22	BA	1260	A	N1-C6-N6	-20.49	106.31	118.60
22	BA	1544	A	C2-N3-C4	20.49	120.84	110.60
22	BA	1970	A	N1-C2-N3	-20.48	119.06	129.30
1	AA	195	A	C2-N3-C4	20.48	120.84	110.60
22	BA	752	A	N1-C6-N6	-20.47	106.32	118.60
22	BA	2418	A	N1-C2-N3	-20.46	119.07	129.30
22	BA	310	A	C2-N3-C4	20.45	120.83	110.60
22	BA	764	A	N1-C6-N6	-20.45	106.33	118.60
22	BA	699	A	N1-C6-N6	-20.43	106.34	118.60
22	BA	2765	A	C2-N3-C4	20.43	120.82	110.60
22	BA	637	A	N1-C2-N3	-20.43	119.08	129.30
22	BA	2052	A	N1-C2-N3	-20.43	119.09	129.30
22	BA	2564	A	N1-C2-N3	-20.42	119.09	129.30
22	BA	2741	A	N1-C6-N6	-20.41	106.35	118.60
22	BA	1803	A	C2-N3-C4	20.41	120.81	110.60
1	AA	149	A	N1-C6-N6	-20.41	106.36	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	199	A	C2-N3-C4	20.39	120.80	110.60
22	BA	2835	A	N1-C6-N6	-20.39	106.37	118.60
22	BA	833	A	N1-C2-N3	-20.39	119.11	129.30
22	BA	911	A	N1-C2-N3	-20.38	119.11	129.30
22	BA	1772	A	N1-C6-N6	-20.38	106.37	118.60
1	AA	1319	A	N1-C6-N6	-20.38	106.38	118.60
22	BA	1583	A	N1-C6-N6	-20.38	106.38	118.60
1	AA	716	A	C2-N3-C4	20.37	120.79	110.60
22	BA	1701	A	N1-C6-N6	-20.37	106.38	118.60
1	AA	356	A	C2-N3-C4	20.37	120.78	110.60
22	BA	627	A	N1-C2-N3	-20.37	119.12	129.30
22	BA	699	A	N1-C2-N3	-20.37	119.12	129.30
22	BA	347	A	N1-C6-N6	-20.36	106.38	118.60
22	BA	910	A	N1-C2-N3	-20.35	119.12	129.30
22	BA	2882	A	N1-C2-N3	-20.34	119.13	129.30
22	BA	514	A	C2-N3-C4	20.33	120.77	110.60
22	BA	262	A	N1-C6-N6	-20.33	106.40	118.60
1	AA	195	A	N1-C6-N6	-20.33	106.40	118.60
22	BA	196	A	C2-N3-C4	20.32	120.76	110.60
22	BA	1919	A	N1-C2-N3	-20.32	119.14	129.30
22	BA	1928	A	N1-C6-N6	-20.32	106.41	118.60
22	BA	1970	A	C2-N3-C4	20.32	120.76	110.60
22	BA	627	A	C2-N3-C4	20.31	120.76	110.60
22	BA	742	A	C2-N3-C4	20.31	120.75	110.60
22	BA	1088	A	C2-N3-C4	20.31	120.75	110.60
1	AA	313	A	C2-N3-C4	20.31	120.75	110.60
1	AA	1179	A	N1-C6-N6	-20.30	106.42	118.60
22	BA	563	A	N1-C2-N3	-20.30	119.15	129.30
22	BA	2518	A	N1-C2-N3	-20.30	119.15	129.30
22	BA	689	A	N1-C2-N3	-20.29	119.16	129.30
22	BA	1569	A	N1-C2-N3	-20.29	119.16	129.30
22	BA	2632	A	N1-C6-N6	-20.29	106.42	118.60
22	BA	800	A	N1-C6-N6	-20.29	106.43	118.60
22	BA	84	A	N1-C2-N3	-20.28	119.16	129.30
22	BA	402	A	N1-C6-N6	-20.28	106.43	118.60
22	BA	1392	A	C2-N3-C4	20.27	120.73	110.60
22	BA	1664	A	C2-N3-C4	20.27	120.73	110.60
22	BA	2435	A	N1-C2-N3	-20.27	119.17	129.30
22	BA	637	A	N1-C6-N6	-20.26	106.44	118.60
22	BA	1366	A	N1-C2-N3	-20.26	119.17	129.30
1	AA	1101	A	N1-C6-N6	-20.26	106.44	118.60
22	BA	1129	A	N1-C6-N6	-20.25	106.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	53	A	N1-C2-N3	-20.25	119.18	129.30
22	BA	892	A	N1-C6-N6	-20.25	106.45	118.60
1	AA	1434	A	N1-C6-N6	-20.24	106.45	118.60
22	BA	1522	A	N1-C6-N6	-20.24	106.45	118.60
22	BA	1307	A	N1-C2-N3	-20.24	119.18	129.30
1	AA	195	A	N1-C2-N3	-20.23	119.18	129.30
22	BA	2042	A	N1-C6-N6	-20.23	106.46	118.60
22	BA	2450	A	N1-C2-N3	-20.23	119.18	129.30
1	AA	16	A	N1-C2-N3	-20.23	119.19	129.30
1	AA	563	A	N1-C6-N6	-20.23	106.46	118.60
22	BA	845	A	C2-N3-C4	20.23	120.71	110.60
1	AA	313	A	N1-C6-N6	-20.23	106.46	118.60
22	BA	825	A	C2-N3-C4	20.23	120.71	110.60
22	BA	1641	A	N1-C6-N6	-20.23	106.47	118.60
22	BA	1762	A	N1-C6-N6	-20.22	106.47	118.60
22	BA	556	A	C2-N3-C4	20.22	120.71	110.60
1	AA	288	A	N1-C6-N6	-20.21	106.47	118.60
22	BA	2013	A	C2-N3-C4	20.21	120.70	110.60
22	BA	1641	A	C2-N3-C4	20.21	120.70	110.60
22	BA	990	A	N1-C2-N3	-20.20	119.20	129.30
22	BA	1805	A	C2-N3-C4	20.20	120.70	110.60
22	BA	792	A	N1-C2-N3	-20.20	119.20	129.30
22	BA	1269	A	N1-C6-N6	-20.20	106.48	118.60
22	BA	532	A	C2-N3-C4	20.19	120.70	110.60
22	BA	119	A	N1-C2-N3	-20.19	119.21	129.30
1	AA	1434	A	C2-N3-C4	20.18	120.69	110.60
22	BA	599	A	N1-C6-N6	-20.18	106.49	118.60
1	AA	160	A	N1-C6-N6	-20.17	106.50	118.60
1	AA	1333	A	N1-C6-N6	-20.17	106.50	118.60
22	BA	278	A	C2-N3-C4	20.17	120.69	110.60
1	AA	171	A	N1-C2-N3	-20.17	119.22	129.30
1	AA	152	A	N1-C2-N3	-20.17	119.22	129.30
22	BA	2736	A	N1-C2-N3	-20.16	119.22	129.30
22	BA	1755	A	N1-C6-N6	-20.15	106.51	118.60
22	BA	309	A	C2-N3-C4	20.15	120.67	110.60
22	BA	1544	A	N1-C6-N6	-20.14	106.51	118.60
22	BA	478	A	C2-N3-C4	20.14	120.67	110.60
22	BA	2328	A	C2-N3-C4	20.14	120.67	110.60
1	AA	782	A	N1-C2-N3	-20.14	119.23	129.30
23	BB	108	A	N1-C6-N6	-20.14	106.52	118.60
22	BA	1789	A	C2-N3-C4	20.13	120.67	110.60
23	BB	59	A	C2-N3-C4	20.13	120.67	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1302	A	N1-C2-N3	-20.13	119.24	129.30
22	BA	1755	A	N1-C2-N3	-20.13	119.23	129.30
22	BA	979	A	N1-C6-N6	-20.13	106.52	118.60
22	BA	1427	A	N1-C2-N3	-20.11	119.25	129.30
22	BA	1678	A	N1-C6-N6	-20.11	106.54	118.60
22	BA	2003	A	N1-C6-N6	-20.10	106.54	118.60
22	BA	412	A	C2-N3-C4	20.09	120.65	110.60
22	BA	972	A	N1-C2-N3	-20.09	119.25	129.30
22	BA	2212	A	N1-C6-N6	-20.09	106.54	118.60
22	BA	541	A	N1-C6-N6	-20.09	106.55	118.60
22	BA	479	A	N1-C2-N3	-20.09	119.25	129.30
22	BA	1630	A	C2-N3-C4	20.09	120.64	110.60
22	BA	2471	A	N1-C6-N6	-20.08	106.55	118.60
1	AA	766	A	C2-N3-C4	20.08	120.64	110.60
22	BA	2426	A	N1-C2-N3	-20.08	119.26	129.30
22	BA	1262	A	N1-C2-N3	-20.08	119.26	129.30
22	BA	802	A	N1-C6-N6	-20.07	106.56	118.60
22	BA	2003	A	C2-N3-C4	20.07	120.64	110.60
22	BA	478	A	N1-C2-N3	-20.07	119.26	129.30
22	BA	2542	A	N1-C6-N6	-20.07	106.56	118.60
22	BA	2589	A	N1-C2-N3	-20.07	119.27	129.30
22	BA	2706	A	N1-C6-N6	-20.07	106.56	118.60
23	BB	52	A	N1-C2-N3	-20.07	119.27	129.30
22	BA	56	A	C2-N3-C4	20.07	120.63	110.60
22	BA	502	A	C2-N3-C4	20.06	120.63	110.60
22	BA	1262	A	C2-N3-C4	20.06	120.63	110.60
22	BA	322	A	N1-C2-N3	-20.06	119.27	129.30
22	BA	2013	A	N1-C6-N6	-20.06	106.56	118.60
1	AA	889	A	N1-C6-N6	-20.06	106.56	118.60
22	BA	195	A	C2-N3-C4	20.06	120.63	110.60
22	BA	2005	A	N1-C2-N3	-20.06	119.27	129.30
22	BA	501	A	N1-C2-N3	-20.05	119.27	129.30
1	AA	432	A	N1-C6-N6	-20.05	106.57	118.60
22	BA	563	A	C2-N3-C4	20.05	120.62	110.60
1	AA	816	A	N1-C2-N3	-20.05	119.28	129.30
1	AA	915	A	N1-C2-N3	-20.05	119.28	129.30
22	BA	1829	A	C2-N3-C4	20.04	120.62	110.60
22	BA	2471	A	C2-N3-C4	20.04	120.62	110.60
22	BA	1700	A	N1-C6-N6	-20.04	106.58	118.60
22	BA	1665	A	C2-N3-C4	20.03	120.61	110.60
22	BA	1378	A	C2-N3-C4	20.03	120.61	110.60
1	AA	1287	A	N1-C6-N6	-20.03	106.58	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	749	A	N1-C6-N6	-20.02	106.58	118.60
22	BA	1630	A	N1-C6-N6	-20.02	106.58	118.60
22	BA	2088	A	C2-N3-C4	20.02	120.61	110.60
1	AA	753	A	N1-C6-N6	-20.02	106.59	118.60
22	BA	676	A	N1-C2-N3	-20.02	119.29	129.30
22	BA	574	A	C2-N3-C4	20.02	120.61	110.60
22	BA	670	A	N1-C6-N6	-20.02	106.59	118.60
22	BA	1032	A	C2-N3-C4	20.01	120.61	110.60
22	BA	1156	A	C2-N3-C4	20.01	120.61	110.60
22	BA	782	A	N1-C6-N6	-20.01	106.59	118.60
22	BA	1525	A	N1-C6-N6	-20.01	106.60	118.60
22	BA	1635	A	N1-C6-N6	-20.00	106.60	118.60
22	BA	412	A	N1-C2-N3	-20.00	119.30	129.30
22	BA	2461	A	C2-N3-C4	20.00	120.60	110.60
22	BA	2813	A	N1-C2-N3	-19.99	119.31	129.30
1	AA	825	A	N1-C6-N6	-19.99	106.61	118.60
22	BA	2451	A	C2-N3-C4	19.99	120.59	110.60
1	AA	461	A	N1-C2-N3	-19.99	119.31	129.30
1	AA	766	A	N1-C6-N6	-19.99	106.61	118.60
1	AA	431	A	N1-C2-N3	-19.98	119.31	129.30
1	AA	622	A	N1-C6-N6	-19.97	106.62	118.60
22	BA	2882	A	N1-C6-N6	-19.97	106.62	118.60
22	BA	764	A	C2-N3-C4	19.97	120.58	110.60
1	AA	496	A	N1-C2-N3	-19.97	119.32	129.30
22	BA	792	A	N1-C6-N6	-19.97	106.62	118.60
22	BA	1142	A	C2-N3-C4	19.96	120.58	110.60
22	BA	1247	A	C2-N3-C4	19.96	120.58	110.60
1	AA	1346	A	N1-C6-N6	-19.96	106.62	118.60
22	BA	1805	A	N1-C2-N3	-19.96	119.32	129.30
1	AA	26	A	C2-N3-C4	19.96	120.58	110.60
22	BA	2020	A	N1-C2-N3	-19.96	119.32	129.30
22	BA	207	A	N1-C2-N3	-19.95	119.32	129.30
22	BA	197	A	C2-N3-C4	19.95	120.58	110.60
22	BA	443	A	C2-N3-C4	19.95	120.58	110.60
22	BA	1253	A	N1-C2-N3	-19.95	119.32	129.30
22	BA	2278	A	N1-C2-N3	-19.95	119.32	129.30
22	BA	972	A	N1-C6-N6	-19.95	106.63	118.60
22	BA	528	A	N1-C6-N6	-19.94	106.64	118.60
23	BB	73	A	N1-C2-N3	-19.94	119.33	129.30
1	AA	1362	A	N1-C2-N3	-19.94	119.33	129.30
1	AA	1413	A	N1-C2-N3	-19.94	119.33	129.30
22	BA	322	A	N1-C6-N6	-19.94	106.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1032	A	N1-C2-N3	-19.94	119.33	129.30
1	AA	1150	A	N1-C6-N6	-19.93	106.64	118.60
22	BA	2432	A	N1-C2-N3	-19.93	119.33	129.30
22	BA	2033	A	N1-C2-N3	-19.93	119.33	129.30
22	BA	2706	A	C2-N3-C4	19.93	120.57	110.60
22	BA	2572	A	N1-C6-N6	-19.93	106.64	118.60
22	BA	310	A	N1-C2-N3	-19.93	119.34	129.30
22	BA	513	A	C2-N3-C4	19.92	120.56	110.60
22	BA	1597	A	C2-N3-C4	19.92	120.56	110.60
1	AA	845	A	C2-N3-C4	19.92	120.56	110.60
22	BA	1809	A	N1-C6-N6	-19.92	106.65	118.60
1	AA	1357	A	N1-C6-N6	-19.92	106.65	118.60
1	AA	174	A	N1-C6-N6	-19.92	106.65	118.60
1	AA	777	A	N1-C2-N3	-19.91	119.34	129.30
22	BA	1786	A	C2-N3-C4	19.91	120.56	110.60
22	BA	2758	A	N1-C6-N6	-19.91	106.65	118.60
22	BA	2560	A	N1-C6-N6	-19.90	106.66	118.60
23	BB	78	A	N1-C2-N3	-19.90	119.35	129.30
22	BA	2602	A	N1-C6-N6	-19.89	106.66	118.60
22	BA	2560	A	C2-N3-C4	19.89	120.55	110.60
22	BA	322	A	C2-N3-C4	19.88	120.54	110.60
22	BA	423	A	N1-C2-N3	-19.88	119.36	129.30
22	BA	374	A	C2-N3-C4	19.88	120.54	110.60
22	BA	676	A	N1-C6-N6	-19.88	106.67	118.60
22	BA	1308	A	C2-N3-C4	19.88	120.54	110.60
22	BA	311	A	C2-N3-C4	19.87	120.54	110.60
22	BA	2572	A	N1-C2-N3	-19.87	119.36	129.30
22	BA	374	A	N1-C2-N3	-19.87	119.37	129.30
22	BA	1858	A	N1-C6-N6	-19.87	106.68	118.60
22	BA	866	A	N1-C2-N3	-19.86	119.37	129.30
22	BA	1086	A	N1-C6-N6	-19.86	106.68	118.60
1	AA	563	A	C2-N3-C4	19.86	120.53	110.60
22	BA	2311	A	C2-N3-C4	19.86	120.53	110.60
22	BA	2820	A	N1-C2-N3	-19.86	119.37	129.30
22	BA	402	A	C2-N3-C4	19.86	120.53	110.60
22	BA	2711	A	N1-C2-N3	-19.86	119.37	129.30
22	BA	1084	A	N1-C6-N6	-19.86	106.69	118.60
22	BA	1757	A	N1-C2-N3	-19.86	119.37	129.30
22	BA	217	A	N1-C6-N6	-19.85	106.69	118.60
22	BA	689	A	C2-N3-C4	19.85	120.53	110.60
22	BA	2009	A	N1-C6-N6	-19.85	106.69	118.60
22	BA	2560	A	N1-C2-N3	-19.85	119.37	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1229	A	C2-N3-C4	19.85	120.52	110.60
22	BA	866	A	N1-C6-N6	-19.85	106.69	118.60
22	BA	1665	A	N1-C6-N6	-19.85	106.69	118.60
22	BA	5	A	N1-C6-N6	-19.84	106.69	118.60
22	BA	2516	A	N1-C2-N3	-19.84	119.38	129.30
1	AA	1447	A	N1-C6-N6	-19.84	106.69	118.60
22	BA	941	A	C2-N3-C4	19.84	120.52	110.60
1	AA	1179	A	N1-C2-N3	-19.84	119.38	129.30
22	BA	2516	A	C2-N3-C4	19.84	120.52	110.60
22	BA	223	A	N1-C6-N6	-19.83	106.70	118.60
22	BA	2750	A	N1-C2-N3	-19.83	119.38	129.30
22	BA	2823	A	N1-C2-N3	-19.83	119.38	129.30
22	BA	402	A	N1-C2-N3	-19.83	119.38	129.30
22	BA	896	A	N1-C6-N6	-19.83	106.70	118.60
22	BA	74	A	N1-C2-N3	-19.82	119.39	129.30
22	BA	1566	A	N1-C2-N3	-19.82	119.39	129.30
22	BA	2425	A	C2-N3-C4	19.82	120.51	110.60
22	BA	217	A	N1-C2-N3	-19.82	119.39	129.30
22	BA	1901	A	C2-N3-C4	19.82	120.51	110.60
22	BA	347	A	C2-N3-C4	19.82	120.51	110.60
1	AA	321	A	N1-C6-N6	-19.82	106.71	118.60
22	BA	2587	A	C2-N3-C4	19.82	120.51	110.60
22	BA	89	A	N1-C2-N3	-19.81	119.40	129.30
22	BA	216	A	N1-C2-N3	-19.81	119.39	129.30
1	AA	913	A	N1-C2-N3	-19.80	119.40	129.30
22	BA	2541	A	N1-C6-N6	-19.80	106.72	118.60
22	BA	2711	A	C2-N3-C4	19.80	120.50	110.60
1	AA	675	A	N1-C2-N3	-19.80	119.40	129.30
22	BA	332	A	C2-N3-C4	19.80	120.50	110.60
22	BA	2809	A	C2-N3-C4	19.80	120.50	110.60
22	BA	2764	A	C2-N3-C4	19.80	120.50	110.60
1	AA	1225	A	N1-C2-N3	-19.80	119.40	129.30
1	AA	777	A	C2-N3-C4	19.79	120.50	110.60
22	BA	1522	A	N1-C2-N3	-19.79	119.40	129.30
22	BA	126	A	C2-N3-C4	19.79	120.49	110.60
22	BA	739	A	C2-N3-C4	19.79	120.49	110.60
22	BA	1596	A	N1-C6-N6	-19.79	106.73	118.60
22	BA	1551	A	N1-C6-N6	-19.79	106.73	118.60
1	AA	32	A	C2-N3-C4	19.78	120.49	110.60
22	BA	1439	A	N1-C6-N6	-19.78	106.73	118.60
22	BA	1490	A	C2-N3-C4	19.78	120.49	110.60
22	BA	972	A	C2-N3-C4	19.78	120.49	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2033	A	N1-C6-N6	-19.78	106.73	118.60
1	AA	1287	A	C2-N3-C4	19.78	120.49	110.60
1	AA	411	A	N1-C2-N3	-19.77	119.41	129.30
22	BA	621	A	N1-C6-N6	-19.77	106.74	118.60
1	AA	282	A	C2-N3-C4	19.77	120.48	110.60
22	BA	89	A	N1-C6-N6	-19.77	106.74	118.60
22	BA	1759	A	N1-C2-N3	-19.77	119.42	129.30
22	BA	470	A	C2-N3-C4	19.77	120.48	110.60
22	BA	44	A	C2-N3-C4	19.76	120.48	110.60
22	BA	1780	A	N1-C6-N6	-19.76	106.74	118.60
22	BA	2761	A	C2-N3-C4	19.76	120.48	110.60
22	BA	1717	A	N1-C2-N3	-19.76	119.42	129.30
23	BB	94	A	N1-C6-N6	-19.76	106.74	118.60
1	AA	665	A	N1-C2-N3	-19.75	119.42	129.30
1	AA	815	A	C2-N3-C4	19.75	120.47	110.60
22	BA	199	A	N1-C2-N3	-19.75	119.43	129.30
22	BA	910	A	C2-N3-C4	19.75	120.47	110.60
22	BA	1626	A	N1-C2-N3	-19.75	119.43	129.30
22	BA	1321	A	C2-N3-C4	19.75	120.47	110.60
1	AA	448	A	C2-N3-C4	19.74	120.47	110.60
22	BA	1496	A	N1-C2-N3	-19.74	119.43	129.30
22	BA	119	A	C2-N3-C4	19.74	120.47	110.60
1	AA	336	A	N1-C6-N6	-19.74	106.76	118.60
22	BA	592	A	C2-N3-C4	19.74	120.47	110.60
1	AA	729	A	C2-N3-C4	19.73	120.47	110.60
22	BA	330	A	N1-C6-N6	-19.73	106.76	118.60
22	BA	905	A	N1-C2-N3	-19.73	119.44	129.30
22	BA	1654	A	N1-C2-N3	-19.72	119.44	129.30
22	BA	1247	A	N1-C2-N3	-19.72	119.44	129.30
22	BA	1614	A	N1-C2-N3	-19.72	119.44	129.30
1	AA	1	A	C2-N3-C4	19.72	120.46	110.60
22	BA	613	A	C2-N3-C4	19.72	120.46	110.60
22	BA	1214	A	N1-C2-N3	-19.72	119.44	129.30
22	BA	1889	A	N1-C2-N3	-19.72	119.44	129.30
22	BA	2134	A	N1-C6-N6	-19.72	106.77	118.60
1	AA	389	A	C2-N3-C4	19.71	120.46	110.60
22	BA	2003	A	N1-C2-N3	-19.71	119.44	129.30
22	BA	2119	A	C2-N3-C4	19.71	120.46	110.60
22	BA	575	A	N1-C2-N3	-19.71	119.44	129.30
22	BA	706	A	N1-C6-N6	-19.71	106.77	118.60
1	AA	1433	A	C2-N3-C4	19.71	120.45	110.60
22	BA	1505	A	C2-N3-C4	19.71	120.45	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2274	A	N1-C6-N6	-19.71	106.78	118.60
22	BA	1549	A	C2-N3-C4	19.71	120.45	110.60
22	BA	602	A	C2-N3-C4	19.70	120.45	110.60
22	BA	1342	A	N1-C2-N3	-19.70	119.45	129.30
22	BA	1384	A	N1-C6-N6	-19.70	106.78	118.60
1	AA	766	A	N1-C2-N3	-19.70	119.45	129.30
22	BA	819	A	C2-N3-C4	19.70	120.45	110.60
22	BA	1677	A	N1-C2-N3	-19.70	119.45	129.30
22	BA	2388	A	N1-C6-N6	-19.70	106.78	118.60
22	BA	2740	A	N1-C2-N3	-19.70	119.45	129.30
22	BA	2270	A	N1-C6-N6	-19.69	106.78	118.60
22	BA	1129	A	N1-C2-N3	-19.69	119.45	129.30
1	AA	236	A	N1-C6-N6	-19.69	106.79	118.60
22	BA	1977	A	N1-C2-N3	-19.69	119.46	129.30
22	BA	2278	A	C2-N3-C4	19.69	120.44	110.60
22	BA	1490	A	N1-C2-N3	-19.68	119.46	129.30
22	BA	2281	A	N1-C2-N3	-19.68	119.46	129.30
22	BA	217	A	C2-N3-C4	19.68	120.44	110.60
22	BA	1635	A	C2-N3-C4	19.68	120.44	110.60
22	BA	1583	A	C2-N3-C4	19.68	120.44	110.60
22	BA	1801	A	N1-C6-N6	-19.68	106.79	118.60
22	BA	2135	A	C2-N3-C4	19.68	120.44	110.60
1	AA	298	A	N1-C2-N3	-19.68	119.46	129.30
22	BA	299	A	N1-C6-N6	-19.68	106.79	118.60
22	BA	311	A	N1-C6-N6	-19.68	106.79	118.60
22	BA	800	A	N1-C2-N3	-19.68	119.46	129.30
22	BA	2273	A	N1-C2-N3	-19.68	119.46	129.30
22	BA	1571	A	N1-C2-N3	-19.67	119.46	129.30
22	BA	1155	A	N1-C6-N6	-19.67	106.80	118.60
1	AA	892	A	C2-N3-C4	19.67	120.44	110.60
1	AA	746	A	C2-N3-C4	19.67	120.43	110.60
22	BA	514	A	N1-C6-N6	-19.67	106.80	118.60
22	BA	861	A	N1-C2-N3	-19.67	119.47	129.30
22	BA	1387	A	C2-N3-C4	19.67	120.43	110.60
22	BA	2369	A	N1-C6-N6	-19.67	106.80	118.60
1	AA	1250	A	C2-N3-C4	19.66	120.43	110.60
1	AA	1092	A	N1-C2-N3	-19.66	119.47	129.30
22	BA	1111	A	N1-C6-N6	-19.66	106.80	118.60
1	AA	1213	A	N1-C2-N3	-19.66	119.47	129.30
22	BA	2386	A	N1-C6-N6	-19.66	106.81	118.60
55	B8	76	A	N1-C6-N6	-19.66	106.80	118.60
22	BA	2542	A	C2-N3-C4	19.66	120.43	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	789	A	C2-N3-C4	19.66	120.43	110.60
22	BA	2080	A	N1-C6-N6	-19.66	106.81	118.60
22	BA	502	A	N1-C2-N3	-19.65	119.47	129.30
22	BA	1805	A	N1-C6-N6	-19.65	106.81	118.60
22	BA	1784	A	N1-C6-N6	-19.65	106.81	118.60
22	BA	2406	A	N1-C2-N3	-19.65	119.47	129.30
23	BB	34	A	C2-N3-C4	19.65	120.43	110.60
1	AA	119	A	C2-N3-C4	19.65	120.42	110.60
22	BA	345	A	C2-N3-C4	19.65	120.42	110.60
22	BA	374	A	N1-C6-N6	-19.65	106.81	118.60
22	BA	2657	A	N1-C6-N6	-19.65	106.81	118.60
22	BA	947	A	N1-C2-N3	-19.65	119.48	129.30
22	BA	1552	A	N1-C2-N3	-19.65	119.48	129.30
1	AA	1014	A	N1-C2-N3	-19.65	119.48	129.30
22	BA	1194	A	N1-C6-N6	-19.64	106.81	118.60
22	BA	1226	A	N1-C2-N3	-19.64	119.48	129.30
22	BA	2336	A	N1-C6-N6	-19.64	106.81	118.60
1	AA	825	A	C2-N3-C4	19.64	120.42	110.60
22	BA	1889	A	C2-N3-C4	19.64	120.42	110.60
1	AA	815	A	N1-C2-N3	-19.64	119.48	129.30
1	AA	1251	A	N1-C6-N6	-19.64	106.82	118.60
1	AA	872	A	C2-N3-C4	19.63	120.42	110.60
22	BA	2566	A	N1-C6-N6	-19.63	106.82	118.60
1	AA	1398	A	C2-N3-C4	19.63	120.41	110.60
22	BA	1434	A	N1-C6-N6	-19.63	106.83	118.60
22	BA	89	A	C2-N3-C4	19.62	120.41	110.60
22	BA	1809	A	N1-C2-N3	-19.62	119.49	129.30
1	AA	1250	A	N1-C6-N6	-19.62	106.83	118.60
1	AA	913	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	1393	A	N1-C6-N6	-19.62	106.83	118.60
1	AA	179	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	2749	A	N1-C2-N3	-19.62	119.49	129.30
1	AA	495	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	928	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	1977	A	C2-N3-C4	19.62	120.41	110.60
22	BA	2587	A	N1-C2-N3	-19.61	119.49	129.30
55	B8	69	A	C2-N3-C4	19.61	120.41	110.60
22	BA	1978	A	N1-C6-N6	-19.61	106.83	118.60
1	AA	509	A	C2-N3-C4	19.61	120.41	110.60
22	BA	693	A	C2-N3-C4	19.61	120.40	110.60
22	BA	1640	A	N1-C6-N6	-19.61	106.83	118.60
22	BA	1745	A	N1-C2-N3	-19.61	119.50	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	807	A	N1-C2-N3	-19.61	119.50	129.30
1	AA	949	A	C2-N3-C4	19.61	120.40	110.60
1	AA	816	A	C2-N3-C4	19.60	120.40	110.60
22	BA	1069	A	N1-C2-N3	-19.60	119.50	129.30
22	BA	1088	A	N1-C6-N6	-19.60	106.84	118.60
1	AA	171	A	N1-C6-N6	-19.60	106.84	118.60
22	BA	1307	A	C2-N3-C4	19.60	120.40	110.60
22	BA	1495	A	C2-N3-C4	19.60	120.40	110.60
22	BA	1269	A	C2-N3-C4	19.60	120.40	110.60
1	AA	171	A	C2-N3-C4	19.60	120.40	110.60
22	BA	1327	A	N1-C2-N3	-19.60	119.50	129.30
22	BA	1998	A	C2-N3-C4	19.60	120.40	110.60
22	BA	1000	A	N1-C2-N3	-19.60	119.50	129.30
1	AA	1275	A	N1-C2-N3	-19.59	119.50	129.30
22	BA	984	A	N1-C2-N3	-19.59	119.50	129.30
23	BB	101	A	C2-N3-C4	19.59	120.40	110.60
22	BA	2598	A	N1-C2-N3	-19.59	119.50	129.30
22	BA	196	A	N1-C2-N3	-19.59	119.50	129.30
22	BA	2333	A	N1-C2-N3	-19.59	119.51	129.30
23	BB	99	A	N1-C6-N6	-19.59	106.85	118.60
22	BA	1966	A	C2-N3-C4	19.58	120.39	110.60
22	BA	2634	A	C2-N3-C4	19.58	120.39	110.60
1	AA	642	A	N1-C6-N6	-19.58	106.85	118.60
1	AA	579	A	C2-N3-C4	19.57	120.39	110.60
1	AA	958	A	N1-C2-N3	-19.57	119.52	129.30
22	BA	1689	A	N1-C6-N6	-19.57	106.86	118.60
22	BA	1762	A	N1-C2-N3	-19.57	119.51	129.30
22	BA	2721	A	C2-N3-C4	19.57	120.38	110.60
1	AA	468	A	N1-C6-N6	-19.56	106.86	118.60
22	BA	820	A	N1-C2-N3	-19.56	119.52	129.30
22	BA	1111	A	C2-N3-C4	19.56	120.38	110.60
22	BA	2634	A	N1-C6-N6	-19.56	106.86	118.60
22	BA	2826	A	C2-N3-C4	19.56	120.38	110.60
1	AA	320	A	N1-C6-N6	-19.56	106.87	118.60
22	BA	739	A	N1-C6-N6	-19.56	106.87	118.60
22	BA	1020	A	N1-C6-N6	-19.56	106.87	118.60
22	BA	2411	A	N1-C6-N6	-19.56	106.87	118.60
22	BA	522	A	N1-C6-N6	-19.55	106.87	118.60
22	BA	1544	A	N1-C2-N3	-19.55	119.52	129.30
1	AA	51	A	N1-C6-N6	-19.55	106.87	118.60
1	AA	246	A	N1-C6-N6	-19.55	106.87	118.60
22	BA	947	A	N1-C6-N6	-19.55	106.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	777	A	N1-C6-N6	-19.55	106.87	118.60
22	BA	207	A	N1-C6-N6	-19.55	106.87	118.60
1	AA	978	A	N1-C6-N6	-19.54	106.88	118.60
1	AA	151	A	C2-N3-C4	19.54	120.37	110.60
1	AA	559	A	N1-C6-N6	-19.54	106.88	118.60
22	BA	2266	A	C2-N3-C4	19.53	120.37	110.60
22	BA	2054	A	N1-C2-N3	-19.53	119.53	129.30
1	AA	1092	A	N1-C6-N6	-19.53	106.88	118.60
22	BA	223	A	N1-C2-N3	-19.53	119.53	129.30
22	BA	1522	A	C2-N3-C4	19.53	120.37	110.60
1	AA	1176	A	C2-N3-C4	19.53	120.36	110.60
22	BA	2191	A	C2-N3-C4	19.53	120.36	110.60
22	BA	863	A	N1-C2-N3	-19.52	119.54	129.30
22	BA	2564	A	C2-N3-C4	19.52	120.36	110.60
22	BA	1744	A	N1-C6-N6	-19.52	106.89	118.60
1	AA	167	A	C2-N3-C4	19.52	120.36	110.60
1	AA	412	A	N1-C2-N3	-19.52	119.54	129.30
22	BA	532	A	N1-C6-N6	-19.52	106.89	118.60
22	BA	752	A	C2-N3-C4	19.52	120.36	110.60
22	BA	845	A	N1-C6-N6	-19.52	106.89	118.60
22	BA	861	A	C2-N3-C4	19.52	120.36	110.60
22	BA	2873	A	N1-C2-N3	-19.52	119.54	129.30
22	BA	53	A	C2-N3-C4	19.52	120.36	110.60
22	BA	1285	A	N1-C2-N3	-19.52	119.54	129.30
1	AA	306	A	C2-N3-C4	19.52	120.36	110.60
22	BA	1927	A	N1-C2-N3	-19.52	119.54	129.30
22	BA	311	A	N1-C2-N3	-19.51	119.54	129.30
22	BA	614	A	N1-C2-N3	-19.51	119.54	129.30
22	BA	2386	A	C2-N3-C4	19.51	120.36	110.60
22	BA	2749	A	N1-C6-N6	-19.51	106.89	118.60
1	AA	978	A	N1-C2-N3	-19.51	119.55	129.30
22	BA	575	A	C2-N3-C4	19.51	120.36	110.60
22	BA	165	A	N1-C6-N6	-19.51	106.89	118.60
1	AA	282	A	N1-C6-N6	-19.50	106.90	118.60
22	BA	1322	A	N1-C6-N6	-19.50	106.90	118.60
22	BA	1545	A	N1-C6-N6	-19.50	106.90	118.60
22	BA	529	A	N1-C6-N6	-19.50	106.90	118.60
22	BA	56	A	N1-C6-N6	-19.50	106.90	118.60
22	BA	829	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	2534	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	83	A	C2-N3-C4	19.50	120.35	110.60
22	BA	1265	A	C2-N3-C4	19.50	120.35	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	502	A	C2-N3-C4	19.49	120.35	110.60
22	BA	401	A	N1-C2-N3	-19.49	119.55	129.30
1	AA	1280	A	N1-C6-N6	-19.49	106.91	118.60
22	BA	74	A	N1-C6-N6	-19.49	106.91	118.60
22	BA	590	A	C2-N3-C4	19.49	120.34	110.60
22	BA	2665	A	C2-N3-C4	19.49	120.34	110.60
22	BA	2741	A	N1-C2-N3	-19.49	119.56	129.30
22	BA	195	A	N1-C6-N6	-19.48	106.91	118.60
55	B8	73	A	N1-C6-N6	-19.48	106.91	118.60
1	AA	864	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	2033	A	C2-N3-C4	19.48	120.34	110.60
1	AA	918	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	13	A	C2-N3-C4	19.48	120.34	110.60
22	BA	74	A	C2-N3-C4	19.48	120.34	110.60
22	BA	231	A	C2-N3-C4	19.48	120.34	110.60
22	BA	2005	A	C2-N3-C4	19.48	120.34	110.60
22	BA	2169	A	N1-C6-N6	-19.48	106.91	118.60
23	BB	34	A	N1-C6-N6	-19.48	106.91	118.60
1	AA	373	A	C2-N3-C4	19.48	120.34	110.60
1	AA	872	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	449	A	C2-N3-C4	19.48	120.34	110.60
22	BA	1086	A	C2-N3-C4	19.48	120.34	110.60
22	BA	1654	A	N1-C6-N6	-19.48	106.91	118.60
1	AA	28	A	C2-N3-C4	19.48	120.34	110.60
22	BA	6	A	C2-N3-C4	19.48	120.34	110.60
22	BA	742	A	N1-C2-N3	-19.48	119.56	129.30
22	BA	2317	A	C2-N3-C4	19.48	120.34	110.60
22	BA	1287	A	C2-N3-C4	19.47	120.34	110.60
22	BA	2336	A	C2-N3-C4	19.47	120.34	110.60
1	AA	665	A	C2-N3-C4	19.47	120.34	110.60
1	AA	787	A	N1-C2-N3	-19.47	119.56	129.30
22	BA	10	A	N1-C2-N3	-19.47	119.56	129.30
22	BA	1551	A	C2-N3-C4	19.47	120.34	110.60
23	BB	104	A	N1-C2-N3	-19.47	119.56	129.30
1	AA	574	A	N1-C6-N6	-19.47	106.92	118.60
1	AA	152	A	C2-N3-C4	19.47	120.33	110.60
22	BA	1635	A	N1-C2-N3	-19.47	119.57	129.30
22	BA	125	A	N1-C2-N3	-19.47	119.57	129.30
22	BA	637	A	C2-N3-C4	19.47	120.33	110.60
22	BA	1265	A	N1-C2-N3	-19.46	119.57	129.30
22	BA	241	A	N1-C2-N3	-19.46	119.57	129.30
1	AA	50	A	N1-C6-N6	-19.46	106.93	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2173	A	C2-N3-C4	19.46	120.33	110.60
1	AA	10	A	C2-N3-C4	19.45	120.33	110.60
22	BA	1901	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	1936	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	2080	A	C2-N3-C4	19.45	120.33	110.60
22	BA	2814	A	N1-C6-N6	-19.45	106.93	118.60
1	AA	382	A	C2-N3-C4	19.45	120.33	110.60
22	BA	980	A	C2-N3-C4	19.45	120.33	110.60
22	BA	1077	A	N1-C2-N3	-19.45	119.57	129.30
22	BA	1785	A	C2-N3-C4	19.45	120.33	110.60
22	BA	2163	A	N1-C6-N6	-19.45	106.93	118.60
55	B8	26	A	C2-N3-C4	19.45	120.33	110.60
1	AA	1413	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	1780	A	C2-N3-C4	19.45	120.32	110.60
22	BA	2191	A	N1-C2-N3	-19.45	119.58	129.30
1	AA	906	A	N1-C2-N3	-19.45	119.58	129.30
22	BA	2013	A	N1-C2-N3	-19.45	119.58	129.30
22	BA	2176	A	C2-N3-C4	19.45	120.32	110.60
22	BA	2298	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	2851	A	N1-C6-N6	-19.45	106.93	118.60
1	AA	363	A	C2-N3-C4	19.44	120.32	110.60
1	AA	1101	A	C2-N3-C4	19.44	120.32	110.60
22	BA	2020	A	C2-N3-C4	19.44	120.32	110.60
22	BA	1772	A	C2-N3-C4	19.44	120.32	110.60
22	BA	2095	A	N1-C2-N3	-19.44	119.58	129.30
22	BA	2453	A	C2-N3-C4	19.44	120.32	110.60
1	AA	977	A	N1-C2-N3	-19.43	119.58	129.30
22	BA	1155	A	N1-C2-N3	-19.43	119.58	129.30
22	BA	2657	A	N1-C2-N3	-19.43	119.58	129.30
22	BA	2705	A	N1-C6-N6	-19.43	106.94	118.60
1	AA	393	A	C2-N3-C4	19.43	120.32	110.60
1	AA	914	A	N1-C2-N3	-19.43	119.58	129.30
1	AA	1236	A	C2-N3-C4	19.43	120.31	110.60
22	BA	362	A	N1-C2-N3	-19.43	119.58	129.30
22	BA	2778	A	N1-C6-N6	-19.43	106.94	118.60
1	AA	161	A	N1-C2-N3	-19.43	119.58	129.30
22	BA	2336	A	N1-C2-N3	-19.43	119.59	129.30
22	BA	1899	A	N1-C2-N3	-19.43	119.59	129.30
22	BA	1515	A	C2-N3-C4	19.42	120.31	110.60
22	BA	2059	A	N1-C2-N3	-19.42	119.59	129.30
1	AA	533	A	C2-N3-C4	19.42	120.31	110.60
22	BA	2741	A	C2-N3-C4	19.42	120.31	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	917	A	N1-C2-N3	-19.42	119.59	129.30
22	BA	309	A	N1-C6-N6	-19.41	106.95	118.60
22	BA	631	A	N1-C2-N3	-19.41	119.59	129.30
22	BA	749	A	N1-C2-N3	-19.41	119.59	129.30
55	B8	76	A	C2-N3-C4	19.41	120.31	110.60
22	BA	1392	A	N1-C2-N3	-19.41	119.59	129.30
1	AA	1229	A	N1-C2-N3	-19.41	119.60	129.30
1	AA	1333	A	C2-N3-C4	19.41	120.31	110.60
22	BA	10	A	C2-N3-C4	19.41	120.30	110.60
22	BA	829	A	N1-C6-N6	-19.41	106.95	118.60
22	BA	2764	A	N1-C2-N3	-19.41	119.59	129.30
1	AA	1261	A	N1-C2-N3	-19.41	119.60	129.30
22	BA	1057	A	C2-N3-C4	19.41	120.30	110.60
1	AA	411	A	C2-N3-C4	19.41	120.30	110.60
1	AA	872	A	N1-C2-N3	-19.41	119.60	129.30
22	BA	945	A	N1-C6-N6	-19.41	106.96	118.60
22	BA	1253	A	C2-N3-C4	19.41	120.30	110.60
1	AA	546	A	C2-N3-C4	19.40	120.30	110.60
1	AA	246	A	N1-C2-N3	-19.40	119.60	129.30
1	AA	81	A	C2-N3-C4	19.40	120.30	110.60
1	AA	964	A	N1-C6-N6	-19.40	106.96	118.60
22	BA	1189	A	N1-C2-N3	-19.40	119.60	129.30
1	AA	26	A	N1-C2-N3	-19.40	119.60	129.30
22	BA	1566	A	C2-N3-C4	19.40	120.30	110.60
22	BA	1632	A	N1-C2-N3	-19.40	119.60	129.30
1	AA	167	A	N1-C6-N6	-19.39	106.96	118.60
22	BA	1749	A	N1-C2-N3	-19.39	119.60	129.30
22	BA	2435	A	C2-N3-C4	19.39	120.30	110.60
22	BA	918	A	N1-C6-N6	-19.39	106.97	118.60
23	BB	15	A	C2-N3-C4	19.39	120.30	110.60
22	BA	693	A	N1-C6-N6	-19.39	106.97	118.60
22	BA	1630	A	N1-C2-N3	-19.39	119.61	129.30
1	AA	579	A	N1-C2-N3	-19.39	119.61	129.30
22	BA	918	A	N1-C2-N3	-19.39	119.61	129.30
22	BA	1403	A	C2-N3-C4	19.39	120.29	110.60
22	BA	1583	A	N1-C2-N3	-19.39	119.61	129.30
22	BA	2388	A	C2-N3-C4	19.39	120.29	110.60
1	AA	572	A	N1-C2-N3	-19.38	119.61	129.30
1	AA	468	A	C2-N3-C4	19.38	120.29	110.60
1	AA	743	A	C2-N3-C4	19.38	120.29	110.60
22	BA	10	A	N1-C6-N6	-19.38	106.97	118.60
22	BA	64	A	C2-N3-C4	19.38	120.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2513	A	C2-N3-C4	19.38	120.29	110.60
22	BA	1189	A	N1-C6-N6	-19.38	106.97	118.60
22	BA	299	A	C2-N3-C4	19.38	120.29	110.60
22	BA	825	A	N1-C2-N3	-19.38	119.61	129.30
22	BA	1147	A	N1-C6-N6	-19.38	106.97	118.60
22	BA	2733	A	N1-C6-N6	-19.38	106.97	118.60
22	BA	508	A	N1-C2-N3	-19.37	119.61	129.30
22	BA	1641	A	N1-C2-N3	-19.37	119.61	129.30
22	BA	2471	A	N1-C2-N3	-19.37	119.61	129.30
1	AA	864	A	C2-N3-C4	19.37	120.28	110.60
22	BA	196	A	N1-C6-N6	-19.37	106.98	118.60
22	BA	2322	A	C2-N3-C4	19.37	120.28	110.60
22	BA	1918	A	N1-C6-N6	-19.37	106.98	118.60
22	BA	2135	A	N1-C2-N3	-19.37	119.62	129.30
1	AA	1285	A	N1-C6-N6	-19.37	106.98	118.60
22	BA	2314	A	N1-C6-N6	-19.37	106.98	118.60
22	BA	2837	A	N1-C6-N6	-19.36	106.98	118.60
23	BB	15	A	N1-C6-N6	-19.36	106.98	118.60
22	BA	849	A	N1-C6-N6	-19.36	106.98	118.60
22	BA	2051	A	C2-N3-C4	19.36	120.28	110.60
22	BA	2311	A	N1-C2-N3	-19.36	119.62	129.30
22	BA	532	A	N1-C2-N3	-19.36	119.62	129.30
22	BA	1204	A	C2-N3-C4	19.36	120.28	110.60
22	BA	1419	A	N1-C2-N3	-19.36	119.62	129.30
1	AA	715	A	N1-C2-N3	-19.36	119.62	129.30
22	BA	920	A	N1-C2-N3	-19.36	119.62	129.30
22	BA	1214	A	N1-C6-N6	-19.36	106.99	118.60
22	BA	42	A	N1-C2-N3	-19.36	119.62	129.30
22	BA	2009	A	N1-C2-N3	-19.35	119.62	129.30
22	BA	2088	A	N1-C6-N6	-19.35	106.99	118.60
22	BA	1515	A	N1-C2-N3	-19.35	119.62	129.30
22	BA	1705	A	N1-C6-N6	-19.35	106.99	118.60
22	BA	1785	A	N1-C6-N6	-19.35	106.99	118.60
22	BA	1872	A	C2-N3-C4	19.35	120.28	110.60
22	BA	2015	A	N1-C2-N3	-19.35	119.62	129.30
22	BA	2883	A	N1-C2-N3	-19.35	119.63	129.30
1	AA	306	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	2434	A	N1-C6-N6	-19.34	107.00	118.60
1	AA	101	A	C2-N3-C4	19.34	120.27	110.60
22	BA	270	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	2288	A	N1-C2-N3	-19.34	119.63	129.30
1	AA	478	A	C2-N3-C4	19.34	120.27	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1201	A	C2-N3-C4	19.34	120.27	110.60
22	BA	896	A	C2-N3-C4	19.34	120.27	110.60
22	BA	191	A	C2-N3-C4	19.34	120.27	110.60
22	BA	2781	A	C2-N3-C4	19.34	120.27	110.60
1	AA	546	A	N1-C2-N3	-19.33	119.63	129.30
1	AA	909	A	N1-C6-N6	-19.33	107.00	118.60
1	AA	1311	A	C2-N3-C4	19.33	120.27	110.60
1	AA	596	A	N1-C6-N6	-19.33	107.00	118.60
1	AA	1269	A	N1-C2-N3	-19.33	119.63	129.30
22	BA	64	A	N1-C6-N6	-19.33	107.00	118.60
22	BA	2031	A	N1-C6-N6	-19.33	107.00	118.60
22	BA	2327	A	C2-N3-C4	19.33	120.27	110.60
22	BA	2381	A	N1-C2-N3	-19.33	119.63	129.30
22	BA	1276	A	N1-C6-N6	-19.33	107.00	118.60
22	BA	2823	A	C2-N3-C4	19.33	120.27	110.60
1	AA	496	A	N1-C6-N6	-19.33	107.00	118.60
1	AA	728	A	C2-N3-C4	19.33	120.26	110.60
22	BA	340	A	C2-N3-C4	19.33	120.26	110.60
22	BA	616	A	C2-N3-C4	19.33	120.26	110.60
22	BA	2675	A	N1-C2-N3	-19.32	119.64	129.30
22	BA	2761	A	N1-C6-N6	-19.32	107.01	118.60
22	BA	590	A	N1-C2-N3	-19.32	119.64	129.30
22	BA	2241	A	N1-C6-N6	-19.32	107.01	118.60
22	BA	2837	A	C2-N3-C4	19.32	120.26	110.60
22	BA	943	A	C2-N3-C4	19.32	120.26	110.60
22	BA	1008	A	N1-C6-N6	-19.32	107.01	118.60
22	BA	1322	A	N1-C2-N3	-19.32	119.64	129.30
22	BA	213	A	N1-C2-N3	-19.32	119.64	129.30
22	BA	670	A	C2-N3-C4	19.32	120.26	110.60
1	AA	983	A	C2-N3-C4	19.32	120.26	110.60
22	BA	160	A	C2-N3-C4	19.32	120.26	110.60
22	BA	173	A	C2-N3-C4	19.31	120.26	110.60
1	AA	466	A	C2-N3-C4	19.31	120.26	110.60
22	BA	2750	A	C2-N3-C4	19.31	120.25	110.60
22	BA	1014	A	N1-C6-N6	-19.31	107.02	118.60
1	AA	1014	A	C2-N3-C4	19.31	120.25	110.60
22	BA	1786	A	N1-C2-N3	-19.30	119.65	129.30
1	AA	1067	A	N1-C6-N6	-19.30	107.02	118.60
1	AA	1324	A	C2-N3-C4	19.30	120.25	110.60
1	AA	1434	A	N1-C2-N3	-19.30	119.65	129.30
1	AA	782	A	C2-N3-C4	19.30	120.25	110.60
22	BA	2758	A	N1-C2-N3	-19.30	119.65	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	99	A	C2-N3-C4	19.30	120.25	110.60
22	BA	730	A	C2-N3-C4	19.30	120.25	110.60
22	BA	2468	A	C2-N3-C4	19.30	120.25	110.60
22	BA	320	A	C2-N3-C4	19.29	120.25	110.60
22	BA	233	A	N1-C6-N6	-19.29	107.03	118.60
1	AA	243	A	C2-N3-C4	19.29	120.24	110.60
22	BA	1786	A	N1-C6-N6	-19.29	107.03	118.60
22	BA	586	A	N1-C6-N6	-19.28	107.03	118.60
22	BA	2418	A	C2-N3-C4	19.28	120.24	110.60
1	AA	583	A	N1-C2-N3	-19.28	119.66	129.30
1	AA	642	A	C2-N3-C4	19.28	120.24	110.60
1	AA	1368	A	N1-C6-N6	-19.28	107.03	118.60
22	BA	833	A	C2-N3-C4	19.28	120.24	110.60
22	BA	439	A	C2-N3-C4	19.28	120.24	110.60
22	BA	460	A	C2-N3-C4	19.28	120.24	110.60
22	BA	538	A	N1-C6-N6	-19.27	107.03	118.60
22	BA	1001	A	N1-C2-N3	-19.27	119.66	129.30
1	AA	1110	A	C2-N3-C4	19.27	120.24	110.60
1	AA	353	A	N1-C6-N6	-19.27	107.04	118.60
1	AA	1349	A	N1-C6-N6	-19.27	107.04	118.60
22	BA	1650	A	C2-N3-C4	19.27	120.23	110.60
22	BA	2114	A	C2-N3-C4	19.27	120.24	110.60
1	AA	622	A	N1-C2-N3	-19.27	119.67	129.30
1	AA	74	A	N1-C6-N6	-19.27	107.04	118.60
1	AA	1499	A	N1-C2-N3	-19.27	119.67	129.30
22	BA	2327	A	N1-C2-N3	-19.27	119.67	129.30
1	AA	807	A	C2-N3-C4	19.27	120.23	110.60
22	BA	1871	A	N1-C6-N6	-19.27	107.04	118.60
22	BA	1953	A	N1-C2-N3	-19.27	119.67	129.30
22	BA	1966	A	N1-C6-N6	-19.27	107.04	118.60
22	BA	2577	A	C2-N3-C4	19.27	120.23	110.60
1	AA	1288	A	C2-N3-C4	19.26	120.23	110.60
23	BB	57	A	N1-C6-N6	-19.26	107.04	118.60
22	BA	1287	A	N1-C2-N3	-19.26	119.67	129.30
1	AA	1285	A	N1-C2-N3	-19.26	119.67	129.30
22	BA	1165	A	C2-N3-C4	19.26	120.23	110.60
23	BB	45	A	N1-C6-N6	-19.26	107.04	118.60
1	AA	602	A	C2-N3-C4	19.26	120.23	110.60
22	BA	1328	A	N1-C2-N3	-19.26	119.67	129.30
1	AA	149	A	C2-N3-C4	19.26	120.23	110.60
1	AA	327	A	C2-N3-C4	19.26	120.23	110.60
1	AA	336	A	N1-C2-N3	-19.26	119.67	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	959	A	C2-N3-C4	19.26	120.23	110.60
1	AA	1350	A	C2-N3-C4	19.26	120.23	110.60
22	BA	917	A	C2-N3-C4	19.26	120.23	110.60
22	BA	979	A	C2-N3-C4	19.26	120.23	110.60
22	BA	877	A	N1-C2-N3	-19.25	119.67	129.30
22	BA	2227	A	C2-N3-C4	19.25	120.23	110.60
22	BA	2748	A	N1-C6-N6	-19.25	107.05	118.60
1	AA	1476	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	959	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	1142	A	N1-C2-N3	-19.25	119.67	129.30
22	BA	1669	A	N1-C2-N3	-19.25	119.67	129.30
22	BA	1773	A	C2-N3-C4	19.25	120.22	110.60
22	BA	2727	A	C2-N3-C4	19.25	120.22	110.60
1	AA	329	A	C2-N3-C4	19.25	120.22	110.60
22	BA	1085	A	C2-N3-C4	19.25	120.22	110.60
22	BA	2101	A	C2-N3-C4	19.25	120.22	110.60
22	BA	2516	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	2850	A	C2-N3-C4	19.25	120.22	110.60
22	BA	878	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	1070	A	C2-N3-C4	19.25	120.22	110.60
55	B8	38	A	C2-N3-C4	19.25	120.22	110.60
22	BA	1040	A	C2-N3-C4	19.24	120.22	110.60
1	AA	59	A	N1-C6-N6	-19.24	107.05	118.60
22	BA	2635	A	C2-N3-C4	19.24	120.22	110.60
1	AA	60	A	N1-C6-N6	-19.24	107.06	118.60
1	AA	918	A	C2-N3-C4	19.24	120.22	110.60
22	BA	563	A	N1-C6-N6	-19.24	107.06	118.60
22	BA	2705	A	C2-N3-C4	19.24	120.22	110.60
22	BA	1246	A	C2-N3-C4	19.24	120.22	110.60
1	AA	1004	A	C2-N3-C4	19.24	120.22	110.60
22	BA	181	A	N1-C6-N6	-19.24	107.06	118.60
1	AA	119	A	N1-C2-N3	-19.23	119.68	129.30
1	AA	1261	A	C2-N3-C4	19.23	120.22	110.60
22	BA	743	A	C2-N3-C4	19.23	120.22	110.60
22	BA	1762	A	C2-N3-C4	19.23	120.22	110.60
22	BA	1783	A	N1-C6-N6	-19.23	107.06	118.60
22	BA	2482	A	N1-C2-N3	-19.23	119.68	129.30
22	BA	1616	A	N1-C2-N3	-19.23	119.69	129.30
22	BA	1677	A	N1-C6-N6	-19.23	107.06	118.60
22	BA	1938	A	N1-C2-N3	-19.23	119.69	129.30
22	BA	2281	A	C2-N3-C4	19.23	120.22	110.60
22	BA	2311	A	N1-C6-N6	-19.23	107.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1239	A	N1-C2-N3	-19.23	119.69	129.30
22	BA	633	A	N1-C2-N3	-19.23	119.69	129.30
1	AA	702	A	N1-C2-N3	-19.23	119.69	129.30
22	BA	1901	A	N1-C2-N3	-19.23	119.69	129.30
1	AA	716	A	N1-C2-N3	-19.23	119.69	129.30
1	AA	792	A	C2-N3-C4	19.23	120.21	110.60
1	AA	1004	A	N1-C2-N3	-19.23	119.69	129.30
1	AA	1499	A	C2-N3-C4	19.23	120.21	110.60
1	AA	1513	A	N1-C6-N6	-19.23	107.06	118.60
22	BA	457	A	N1-C2-N3	-19.23	119.69	129.30
22	BA	1204	A	N1-C2-N3	-19.23	119.69	129.30
22	BA	2566	A	N1-C2-N3	-19.23	119.69	129.30
22	BA	2810	A	N1-C2-N3	-19.23	119.69	129.30
55	B8	66	A	C2-N3-C4	19.23	120.21	110.60
1	AA	151	A	N1-C2-N3	-19.22	119.69	129.30
22	BA	118	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	221	A	N1-C6-N6	-19.22	107.07	118.60
1	AA	1287	A	N1-C2-N3	-19.22	119.69	129.30
22	BA	2266	A	N1-C6-N6	-19.22	107.07	118.60
1	AA	181	A	C2-N3-C4	19.22	120.21	110.60
1	AA	560	A	N1-C2-N3	-19.22	119.69	129.30
22	BA	149	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	2020	A	N1-C6-N6	-19.22	107.07	118.60
1	AA	768	A	N1-C6-N6	-19.22	107.07	118.60
1	AA	994	A	C2-N3-C4	19.22	120.21	110.60
1	AA	1238	A	C2-N3-C4	19.22	120.21	110.60
22	BA	556	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	1095	A	C2-N3-C4	19.22	120.21	110.60
1	AA	1105	A	N1-C2-N3	-19.22	119.69	129.30
22	BA	2700	A	N1-C6-N6	-19.22	107.07	118.60
1	AA	373	A	N1-C2-N3	-19.22	119.69	129.30
22	BA	28	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	1847	A	C2-N3-C4	19.22	120.21	110.60
22	BA	2497	A	C2-N3-C4	19.22	120.21	110.60
22	BA	2163	A	C2-N3-C4	19.21	120.21	110.60
1	AA	478	A	N1-C6-N6	-19.21	107.07	118.60
22	BA	2287	A	N1-C2-N3	-19.21	119.69	129.30
22	BA	2225	A	N1-C2-N3	-19.21	119.69	129.30
22	BA	428	A	N1-C2-N3	-19.21	119.69	129.30
22	BA	1960	A	C2-N3-C4	19.21	120.20	110.60
22	BA	2433	A	C2-N3-C4	19.21	120.20	110.60
1	AA	189	A	C2-N3-C4	19.20	120.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	560	A	C2-N3-C4	19.20	120.20	110.60
1	AA	673	A	C2-N3-C4	19.20	120.20	110.60
22	BA	644	A	N1-C6-N6	-19.20	107.08	118.60
22	BA	1640	A	C2-N3-C4	19.20	120.20	110.60
22	BA	432	A	N1-C2-N3	-19.20	119.70	129.30
22	BA	454	A	N1-C2-N3	-19.20	119.70	129.30
22	BA	947	A	C2-N3-C4	19.20	120.20	110.60
22	BA	1126	A	C2-N3-C4	19.20	120.20	110.60
22	BA	111	A	N1-C6-N6	-19.20	107.08	118.60
22	BA	176	A	C2-N3-C4	19.20	120.20	110.60
22	BA	1913	A	N1-C2-N3	-19.20	119.70	129.30
1	AA	547	A	N1-C2-N3	-19.20	119.70	129.30
1	AA	583	A	C2-N3-C4	19.20	120.20	110.60
22	BA	428	A	N1-C6-N6	-19.20	107.08	118.60
22	BA	892	A	C2-N3-C4	19.20	120.20	110.60
22	BA	1237	A	C2-N3-C4	19.20	120.20	110.60
22	BA	1803	A	N1-C2-N3	-19.20	119.70	129.30
22	BA	2198	A	N1-C2-N3	-19.20	119.70	129.30
22	BA	2781	A	N1-C2-N3	-19.20	119.70	129.30
22	BA	522	A	C2-N3-C4	19.20	120.20	110.60
22	BA	1913	A	N1-C6-N6	-19.20	107.08	118.60
22	BA	38	A	N1-C6-N6	-19.19	107.08	118.60
22	BA	1916	A	C2-N3-C4	19.19	120.20	110.60
22	BA	2736	A	N1-C6-N6	-19.19	107.08	118.60
1	AA	1046	A	C2-N3-C4	19.19	120.20	110.60
22	BA	470	A	N1-C2-N3	-19.19	119.70	129.30
22	BA	1889	A	N1-C6-N6	-19.19	107.08	118.60
22	BA	2497	A	N1-C2-N3	-19.19	119.70	129.30
1	AA	649	A	N1-C6-N6	-19.19	107.09	118.60
1	AA	964	A	N1-C2-N3	-19.19	119.71	129.30
22	BA	197	A	N1-C6-N6	-19.19	107.09	118.60
22	BA	2184	A	C2-N3-C4	19.19	120.19	110.60
22	BA	2765	A	N1-C2-N3	-19.19	119.71	129.30
22	BA	1858	A	C2-N3-C4	19.19	120.19	110.60
22	BA	2809	A	N1-C2-N3	-19.19	119.71	129.30
22	BA	1744	A	C2-N3-C4	19.18	120.19	110.60
22	BA	2094	A	N1-C2-N3	-19.18	119.71	129.30
22	BA	2469	A	N1-C2-N3	-19.18	119.71	129.30
22	BA	1632	A	C2-N3-C4	19.18	120.19	110.60
22	BA	1593	A	C2-N3-C4	19.18	120.19	110.60
1	AA	160	A	N1-C2-N3	-19.18	119.71	129.30
22	BA	1503	A	C2-N3-C4	19.18	120.19	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1288	A	N1-C6-N6	-19.18	107.09	118.60
1	AA	621	A	C2-N3-C4	19.18	120.19	110.60
22	BA	1276	A	C2-N3-C4	19.18	120.19	110.60
22	BA	2829	A	C2-N3-C4	19.18	120.19	110.60
23	BB	52	A	C2-N3-C4	19.18	120.19	110.60
1	AA	327	A	N1-C2-N3	-19.17	119.71	129.30
1	AA	782	A	N1-C6-N6	-19.17	107.10	118.60
1	AA	1044	A	N1-C2-N3	-19.17	119.71	129.30
22	BA	1821	A	C2-N3-C4	19.17	120.19	110.60
22	BA	1821	A	N1-C2-N3	-19.17	119.71	129.30
22	BA	2856	A	N1-C6-N6	-19.17	107.10	118.60
1	AA	496	A	C2-N3-C4	19.17	120.19	110.60
22	BA	522	A	N1-C2-N3	-19.17	119.72	129.30
22	BA	556	A	N1-C2-N3	-19.17	119.71	129.30
22	BA	2837	A	N1-C2-N3	-19.17	119.72	129.30
1	AA	1167	A	N1-C2-N3	-19.17	119.72	129.30
1	AA	8	A	N1-C2-N3	-19.17	119.72	129.30
1	AA	451	A	N1-C6-N6	-19.17	107.10	118.60
22	BA	1175	A	C2-N3-C4	19.17	120.18	110.60
22	BA	1890	A	C2-N3-C4	19.17	120.18	110.60
1	AA	825	A	N1-C2-N3	-19.16	119.72	129.30
22	BA	103	A	N1-C2-N3	-19.16	119.72	129.30
22	BA	2482	A	N1-C6-N6	-19.16	107.10	118.60
22	BA	2314	A	N1-C2-N3	-19.16	119.72	129.30
22	BA	2432	A	C2-N3-C4	19.16	120.18	110.60
1	AA	583	A	N1-C6-N6	-19.16	107.10	118.60
1	AA	892	A	N1-C6-N6	-19.16	107.10	118.60
22	BA	2119	A	N1-C6-N6	-19.16	107.10	118.60
22	BA	125	A	C2-N3-C4	19.16	120.18	110.60
1	AA	1493	A	N1-C2-N3	-19.16	119.72	129.30
22	BA	1268	A	N1-C2-N3	-19.16	119.72	129.30
22	BA	1596	A	C2-N3-C4	19.16	120.18	110.60
22	BA	699	A	C2-N3-C4	19.16	120.18	110.60
22	BA	2328	A	N1-C6-N6	-19.16	107.11	118.60
22	BA	447	A	N1-C2-N3	-19.15	119.72	129.30
1	AA	1035	A	N1-C6-N6	-19.15	107.11	118.60
22	BA	226	A	C2-N3-C4	19.15	120.18	110.60
23	BB	101	A	N1-C6-N6	-19.15	107.11	118.60
22	BA	422	A	C2-N3-C4	19.15	120.18	110.60
1	AA	172	A	N1-C6-N6	-19.15	107.11	118.60
22	BA	877	A	N1-C6-N6	-19.15	107.11	118.60
22	BA	1383	A	N1-C6-N6	-19.15	107.11	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1419	A	N1-C6-N6	-19.15	107.11	118.60
1	AA	574	A	C2-N3-C4	19.15	120.17	110.60
1	AA	1213	A	C2-N3-C4	19.15	120.17	110.60
22	BA	1938	A	C2-N3-C4	19.14	120.17	110.60
22	BA	753	A	C2-N3-C4	19.14	120.17	110.60
22	BA	1070	A	N1-C2-N3	-19.14	119.73	129.30
22	BA	2071	A	C2-N3-C4	19.14	120.17	110.60
1	AA	167	A	N1-C2-N3	-19.14	119.73	129.30
23	BB	119	A	N1-C2-N3	-19.14	119.73	129.30
1	AA	364	A	N1-C6-N6	-19.14	107.12	118.60
1	AA	728	A	N1-C6-N6	-19.14	107.12	118.60
1	AA	1157	A	C2-N3-C4	19.14	120.17	110.60
22	BA	592	A	N1-C2-N3	-19.14	119.73	129.30
22	BA	104	A	N1-C6-N6	-19.14	107.12	118.60
22	BA	1194	A	N1-C2-N3	-19.14	119.73	129.30
22	BA	909	A	C2-N3-C4	19.14	120.17	110.60
22	BA	2851	A	C2-N3-C4	19.14	120.17	110.60
1	AA	532	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	309	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	920	A	C2-N3-C4	19.13	120.17	110.60
22	BA	1672	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	1749	A	N1-C6-N6	-19.13	107.12	118.60
22	BA	1858	A	N1-C2-N3	-19.13	119.73	129.30
23	BB	50	A	N1-C6-N6	-19.13	107.12	118.60
22	BA	1347	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	1960	A	N1-C6-N6	-19.13	107.12	118.60
22	BA	330	A	C2-N3-C4	19.13	120.16	110.60
22	BA	1453	A	N1-C2-N3	-19.13	119.74	129.30
22	BA	447	A	N1-C6-N6	-19.13	107.12	118.60
22	BA	1230	A	N1-C6-N6	-19.13	107.12	118.60
22	BA	1385	A	C2-N3-C4	19.13	120.16	110.60
22	BA	1927	A	N1-C6-N6	-19.13	107.12	118.60
22	BA	2173	A	N1-C6-N6	-19.13	107.12	118.60
1	AA	1271	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	1469	A	C2-N3-C4	19.12	120.16	110.60
1	AA	1280	A	C2-N3-C4	19.12	120.16	110.60
22	BA	2119	A	N1-C2-N3	-19.12	119.74	129.30
1	AA	968	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	1919	A	C2-N3-C4	19.12	120.16	110.60
22	BA	1010	A	N1-C2-N3	-19.12	119.74	129.30
1	AA	205	A	C2-N3-C4	19.12	120.16	110.60
1	AA	262	A	C2-N3-C4	19.12	120.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	983	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	1987	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	103	A	N1-C6-N6	-19.12	107.13	118.60
22	BA	715	A	N1-C6-N6	-19.12	107.13	118.60
1	AA	1350	A	N1-C6-N6	-19.11	107.13	118.60
22	BA	2614	A	N1-C6-N6	-19.11	107.13	118.60
22	BA	631	A	N1-C6-N6	-19.11	107.13	118.60
22	BA	2882	A	C2-N3-C4	19.11	120.16	110.60
55	B8	58	A	C2-N3-C4	19.11	120.16	110.60
22	BA	221	A	N1-C2-N3	-19.11	119.75	129.30
22	BA	1890	A	N1-C2-N3	-19.11	119.75	129.30
1	AA	1431	A	N1-C6-N6	-19.11	107.14	118.60
22	BA	2019	A	N1-C2-N3	-19.11	119.75	129.30
1	AA	915	A	C2-N3-C4	19.11	120.15	110.60
22	BA	2433	A	N1-C6-N6	-19.11	107.14	118.60
22	BA	2821	A	N1-C2-N3	-19.10	119.75	129.30
1	AA	282	A	N1-C2-N3	-19.10	119.75	129.30
1	AA	949	A	N1-C6-N6	-19.10	107.14	118.60
22	BA	632	A	C2-N3-C4	19.10	120.15	110.60
22	BA	1532	A	N1-C2-N3	-19.10	119.75	129.30
22	BA	2126	A	C2-N3-C4	19.10	120.15	110.60
1	AA	794	A	C2-N3-C4	19.10	120.15	110.60
1	AA	320	A	C2-N3-C4	19.10	120.15	110.60
22	BA	1393	A	N1-C2-N3	-19.10	119.75	129.30
23	BB	57	A	N1-C2-N3	-19.10	119.75	129.30
22	BA	863	A	C2-N3-C4	19.10	120.15	110.60
22	BA	1927	A	C2-N3-C4	19.10	120.15	110.60
1	AA	1534	A	N1-C2-N3	-19.09	119.75	129.30
22	BA	340	A	N1-C6-N6	-19.09	107.14	118.60
22	BA	514	A	N1-C2-N3	-19.09	119.75	129.30
1	AA	768	A	C2-N3-C4	19.09	120.15	110.60
22	BA	1919	A	N1-C6-N6	-19.09	107.14	118.60
22	BA	2778	A	C2-N3-C4	19.09	120.14	110.60
1	AA	1145	A	N1-C2-N3	-19.09	119.75	129.30
22	BA	1998	A	N1-C6-N6	-19.09	107.15	118.60
22	BA	2154	A	N1-C2-N3	-19.09	119.75	129.30
22	BA	83	A	N1-C2-N3	-19.09	119.75	129.30
22	BA	1365	A	C2-N3-C4	19.09	120.14	110.60
22	BA	2468	A	N1-C2-N3	-19.09	119.75	129.30
1	AA	414	A	N1-C2-N3	-19.09	119.76	129.30
1	AA	1080	A	N1-C2-N3	-19.09	119.76	129.30
1	AA	1225	A	N1-C6-N6	-19.09	107.15	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1306	A	N1-C2-N3	-19.09	119.76	129.30
1	AA	1429	A	N1-C2-N3	-19.09	119.76	129.30
22	BA	2873	A	N1-C6-N6	-19.09	107.15	118.60
22	BA	19	A	C2-N3-C4	19.08	120.14	110.60
1	AA	460	A	N1-C2-N3	-19.08	119.76	129.30
1	AA	629	A	C2-N3-C4	19.08	120.14	110.60
1	AA	1171	A	C2-N3-C4	19.08	120.14	110.60
22	BA	911	A	N1-C6-N6	-19.08	107.15	118.60
22	BA	1593	A	N1-C2-N3	-19.08	119.76	129.30
1	AA	1151	A	C2-N3-C4	19.08	120.14	110.60
22	BA	529	A	N1-C2-N3	-19.08	119.76	129.30
22	BA	933	A	C2-N3-C4	19.08	120.14	110.60
22	BA	2358	A	N1-C6-N6	-19.08	107.15	118.60
22	BA	2835	A	N1-C2-N3	-19.08	119.76	129.30
22	BA	1237	A	N1-C2-N3	-19.08	119.76	129.30
22	BA	1354	A	N1-C2-N3	-19.08	119.76	129.30
22	BA	1936	A	N1-C2-N3	-19.08	119.76	129.30
22	BA	1637	A	C2-N3-C4	19.08	120.14	110.60
22	BA	2810	A	N1-C6-N6	-19.08	107.15	118.60
22	BA	2868	A	C2-N3-C4	19.08	120.14	110.60
1	AA	414	A	C2-N3-C4	19.07	120.14	110.60
22	BA	2227	A	N1-C2-N3	-19.07	119.76	129.30
1	AA	1082	A	C2-N3-C4	19.07	120.14	110.60
22	BA	1597	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	1794	A	N1-C6-N6	-19.07	107.16	118.60
1	AA	816	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	182	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	981	A	N1-C2-N3	-19.07	119.76	129.30
22	BA	1705	A	C2-N3-C4	19.07	120.14	110.60
1	AA	712	A	C2-N3-C4	19.07	120.14	110.60
22	BA	2199	A	N1-C2-N3	-19.07	119.77	129.30
1	AA	1016	A	C2-N3-C4	19.07	120.13	110.60
22	BA	262	A	C2-N3-C4	19.07	120.13	110.60
22	BA	1815	A	C2-N3-C4	19.07	120.13	110.60
1	AA	1155	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	244	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	1328	A	C2-N3-C4	19.07	120.13	110.60
1	AA	1362	A	C2-N3-C4	19.06	120.13	110.60
1	AA	1176	A	N1-C2-N3	-19.06	119.77	129.30
1	AA	1503	A	N1-C2-N3	-19.06	119.77	129.30
22	BA	1552	A	C2-N3-C4	19.06	120.13	110.60
22	BA	2590	A	N1-C2-N3	-19.06	119.77	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2451	A	N1-C2-N3	-19.06	119.77	129.30
1	AA	1531	A	N1-C2-N3	-19.06	119.77	129.30
22	BA	1876	A	N1-C2-N3	-19.06	119.77	129.30
1	AA	1428	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	845	A	N1-C2-N3	-19.05	119.77	129.30
1	AA	1251	A	C2-N3-C4	19.05	120.13	110.60
1	AA	1311	A	N1-C2-N3	-19.05	119.77	129.30
22	BA	529	A	C2-N3-C4	19.05	120.13	110.60
1	AA	179	A	C2-N3-C4	19.05	120.13	110.60
22	BA	528	A	C2-N3-C4	19.05	120.13	110.60
22	BA	905	A	C2-N3-C4	19.05	120.12	110.60
22	BA	1913	A	C2-N3-C4	19.05	120.12	110.60
1	AA	253	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	219	A	N1-C2-N3	-19.05	119.78	129.30
22	BA	1000	A	C2-N3-C4	19.05	120.12	110.60
22	BA	1420	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	1783	A	C2-N3-C4	19.05	120.12	110.60
22	BA	2173	A	N1-C2-N3	-19.05	119.78	129.30
1	AA	1374	A	C2-N3-C4	19.05	120.12	110.60
22	BA	2241	A	C2-N3-C4	19.05	120.12	110.60
22	BA	661	A	C2-N3-C4	19.04	120.12	110.60
1	AA	306	A	N1-C6-N6	-19.04	107.17	118.60
1	AA	468	A	N1-C2-N3	-19.04	119.78	129.30
22	BA	2309	A	N1-C2-N3	-19.04	119.78	129.30
22	BA	2740	A	C2-N3-C4	19.04	120.12	110.60
1	AA	655	A	C2-N3-C4	19.04	120.12	110.60
22	BA	1829	A	N1-C2-N3	-19.04	119.78	129.30
1	AA	706	A	C2-N3-C4	19.04	120.12	110.60
22	BA	1385	A	N1-C2-N3	-19.04	119.78	129.30
22	BA	2381	A	N1-C6-N6	-19.04	107.18	118.60
22	BA	2476	A	N1-C2-N3	-19.04	119.78	129.30
1	AA	8	A	N1-C6-N6	-19.04	107.18	118.60
1	AA	131	A	C2-N3-C4	19.04	120.12	110.60
1	AA	452	A	N1-C6-N6	-19.04	107.18	118.60
1	AA	595	A	C2-N3-C4	19.04	120.12	110.60
22	BA	1077	A	N1-C6-N6	-19.04	107.18	118.60
22	BA	1916	A	N1-C2-N3	-19.04	119.78	129.30
1	AA	182	A	N1-C2-N3	-19.03	119.78	129.30
1	AA	802	A	N1-C6-N6	-19.03	107.18	118.60
22	BA	310	A	N1-C6-N6	-19.03	107.18	118.60
22	BA	655	A	N1-C6-N6	-19.03	107.18	118.60
22	BA	2547	A	N1-C6-N6	-19.03	107.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	51	A	N1-C2-N3	-19.03	119.78	129.30
22	BA	131	A	N1-C2-N3	-19.03	119.78	129.30
22	BA	1189	A	C2-N3-C4	19.03	120.11	110.60
22	BA	1420	A	C2-N3-C4	19.03	120.11	110.60
22	BA	1569	A	N1-C6-N6	-19.03	107.18	118.60
1	AA	1019	A	N1-C2-N3	-19.03	119.79	129.30
1	AA	1155	A	N1-C2-N3	-19.03	119.79	129.30
22	BA	613	A	N1-C6-N6	-19.03	107.18	118.60
1	AA	1021	A	N1-C2-N3	-19.03	119.79	129.30
22	BA	1876	A	C2-N3-C4	19.02	120.11	110.60
22	BA	1570	A	N1-C6-N6	-19.02	107.19	118.60
22	BA	1509	A	N1-C6-N6	-19.02	107.19	118.60
1	AA	74	A	C2-N3-C4	19.02	120.11	110.60
1	AA	629	A	N1-C6-N6	-19.02	107.19	118.60
1	AA	1299	A	N1-C2-N3	-19.02	119.79	129.30
22	BA	975	A	C2-N3-C4	19.02	120.11	110.60
22	BA	2097	A	N1-C6-N6	-19.02	107.19	118.60
22	BA	2665	A	N1-C6-N6	-19.02	107.19	118.60
22	BA	1759	A	C2-N3-C4	19.02	120.11	110.60
55	B8	41	A	C2-N3-C4	19.02	120.11	110.60
22	BA	2014	A	N1-C6-N6	-19.01	107.19	118.60
22	BA	2169	A	N1-C2-N3	-19.01	119.79	129.30
22	BA	505	A	N1-C6-N6	-19.01	107.19	118.60
22	BA	899	A	C2-N3-C4	19.01	120.11	110.60
22	BA	1784	A	N1-C2-N3	-19.01	119.80	129.30
22	BA	1981	A	N1-C6-N6	-19.01	107.19	118.60
22	BA	541	A	C2-N3-C4	19.01	120.11	110.60
1	AA	1363	A	C2-N3-C4	19.01	120.10	110.60
22	BA	1347	A	C2-N3-C4	19.01	120.10	110.60
22	BA	2358	A	N1-C2-N3	-19.00	119.80	129.30
1	AA	819	A	N1-C2-N3	-19.00	119.80	129.30
1	AA	74	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	371	A	N1-C6-N6	-19.00	107.20	118.60
1	AA	182	A	N1-C6-N6	-19.00	107.20	118.60
1	AA	1441	A	N1-C6-N6	-19.00	107.20	118.60
22	BA	1453	A	C2-N3-C4	19.00	120.10	110.60
1	AA	1500	A	C2-N3-C4	19.00	120.10	110.60
22	BA	2377	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	2753	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	2813	A	C2-N3-C4	19.00	120.10	110.60
55	B8	51	A	C2-N3-C4	19.00	120.10	110.60
1	AA	143	A	N1-C2-N3	-19.00	119.80	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1005	A	C2-N3-C4	19.00	120.10	110.60
22	BA	1089	A	N1-C6-N6	-19.00	107.20	118.60
1	AA	10	A	N1-C2-N3	-18.99	119.80	129.30
1	AA	1022	A	C2-N3-C4	18.99	120.10	110.60
22	BA	144	A	N1-C6-N6	-18.99	107.20	118.60
22	BA	453	A	C2-N3-C4	18.99	120.09	110.60
1	AA	130	A	C2-N3-C4	18.99	120.09	110.60
1	AA	298	A	C2-N3-C4	18.99	120.09	110.60
1	AA	1180	A	C2-N3-C4	18.99	120.09	110.60
22	BA	693	A	N1-C2-N3	-18.99	119.81	129.30
22	BA	1690	A	C2-N3-C4	18.99	120.09	110.60
22	BA	2577	A	N1-C2-N3	-18.99	119.81	129.30
1	AA	160	A	C2-N3-C4	18.99	120.09	110.60
22	BA	945	A	C2-N3-C4	18.99	120.09	110.60
22	BA	1365	A	N1-C2-N3	-18.99	119.81	129.30
1	AA	288	A	C2-N3-C4	18.98	120.09	110.60
22	BA	2070	A	N1-C2-N3	-18.98	119.81	129.30
1	AA	263	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	5	A	C2-N3-C4	18.98	120.09	110.60
1	AA	72	A	N1-C6-N6	-18.98	107.21	118.60
22	BA	1535	A	C2-N3-C4	18.98	120.09	110.60
22	BA	2738	A	N1-C6-N6	-18.98	107.21	118.60
22	BA	422	A	N1-C2-N3	-18.98	119.81	129.30
1	AA	1152	A	C2-N3-C4	18.98	120.09	110.60
1	AA	1329	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	346	A	N1-C6-N6	-18.98	107.21	118.60
22	BA	1654	A	C2-N3-C4	18.98	120.09	110.60
22	BA	2051	A	N1-C2-N3	-18.98	119.81	129.30
1	AA	1248	A	C2-N3-C4	18.97	120.09	110.60
22	BA	984	A	N1-C6-N6	-18.97	107.22	118.60
1	AA	958	A	C2-N3-C4	18.97	120.08	110.60
1	AA	1044	A	C2-N3-C4	18.97	120.09	110.60
22	BA	1413	A	N1-C2-N3	-18.97	119.81	129.30
1	AA	523	A	C2-N3-C4	18.97	120.08	110.60
23	BB	73	A	C2-N3-C4	18.97	120.08	110.60
1	AA	344	A	N1-C2-N3	-18.96	119.82	129.30
22	BA	2378	A	N1-C2-N3	-18.96	119.82	129.30
22	BA	1039	A	N1-C2-N3	-18.96	119.82	129.30
1	AA	1534	A	C2-N3-C4	18.96	120.08	110.60
22	BA	1597	A	N1-C2-N3	-18.96	119.82	129.30
22	BA	2425	A	N1-C2-N3	-18.96	119.82	129.30
1	AA	784	A	C2-N3-C4	18.96	120.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	226	A	N1-C6-N6	-18.96	107.22	118.60
22	BA	504	A	N1-C6-N6	-18.96	107.22	118.60
1	AA	8	A	C2-N3-C4	18.96	120.08	110.60
22	BA	2541	A	C2-N3-C4	18.96	120.08	110.60
22	BA	2810	A	C2-N3-C4	18.96	120.08	110.60
22	BA	676	A	C2-N3-C4	18.95	120.08	110.60
22	BA	2369	A	N1-C2-N3	-18.95	119.82	129.30
22	BA	643	A	N1-C2-N3	-18.95	119.82	129.30
22	BA	936	A	C2-N3-C4	18.95	120.08	110.60
22	BA	1754	A	N1-C2-N3	-18.95	119.83	129.30
22	BA	2134	A	N1-C2-N3	-18.95	119.83	129.30
22	BA	2602	A	N1-C2-N3	-18.95	119.83	129.30
23	BB	78	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	980	A	N1-C2-N3	-18.95	119.83	129.30
22	BA	1918	A	C2-N3-C4	18.95	120.07	110.60
22	BA	2809	A	N1-C6-N6	-18.95	107.23	118.60
1	AA	621	A	N1-C2-N3	-18.95	119.83	129.30
1	AA	889	A	N1-C2-N3	-18.95	119.83	129.30
22	BA	2706	A	N1-C2-N3	-18.95	119.83	129.30
23	BB	99	A	N1-C2-N3	-18.95	119.83	129.30
22	BA	1046	A	N1-C2-N3	-18.94	119.83	129.30
22	BA	2042	A	C2-N3-C4	18.94	120.07	110.60
1	AA	1492	A	N1-C2-N3	-18.94	119.83	129.30
22	BA	1966	A	N1-C2-N3	-18.94	119.83	129.30
1	AA	1042	A	C2-N3-C4	18.94	120.07	110.60
1	AA	1289	A	N1-C6-N6	-18.94	107.24	118.60
22	BA	1655	A	N1-C6-N6	-18.94	107.24	118.60
22	BA	1912	A	N1-C6-N6	-18.94	107.24	118.60
22	BA	2126	A	N1-C2-N3	-18.94	119.83	129.30
22	BA	190	A	N1-C2-N3	-18.93	119.83	129.30
22	BA	866	A	C2-N3-C4	18.93	120.07	110.60
22	BA	896	A	N1-C2-N3	-18.93	119.83	129.30
22	BA	1698	A	C2-N3-C4	18.93	120.07	110.60
22	BA	2757	A	C2-N3-C4	18.93	120.07	110.60
23	BB	15	A	N1-C2-N3	-18.93	119.83	129.30
22	BA	670	A	N1-C2-N3	-18.93	119.83	129.30
22	BA	2883	A	N1-C6-N6	-18.93	107.24	118.60
1	AA	371	A	C2-N3-C4	18.93	120.07	110.60
1	AA	1005	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	1156	A	N1-C2-N3	-18.93	119.83	129.30
1	AA	1446	A	C2-N3-C4	18.93	120.06	110.60
1	AA	1446	A	N1-C6-N6	-18.93	107.24	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	694	A	C2-N3-C4	18.93	120.06	110.60
22	BA	44	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	443	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	501	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	2135	A	N1-C6-N6	-18.93	107.24	118.60
23	BB	115	A	N1-C2-N3	-18.93	119.84	129.30
1	AA	781	A	C2-N3-C4	18.93	120.06	110.60
22	BA	415	A	C2-N3-C4	18.93	120.06	110.60
22	BA	899	A	N1-C2-N3	-18.93	119.84	129.30
22	BA	2418	A	N1-C6-N6	-18.93	107.24	118.60
1	AA	969	A	C2-N3-C4	18.93	120.06	110.60
22	BA	244	A	N1-C2-N3	-18.93	119.84	129.30
22	BA	1978	A	C2-N3-C4	18.93	120.06	110.60
55	B8	14	A	C2-N3-C4	18.93	120.06	110.60
55	B8	21	A	C2-N3-C4	18.93	120.06	110.60
22	BA	56	A	N1-C2-N3	-18.92	119.84	129.30
22	BA	1665	A	N1-C2-N3	-18.92	119.84	129.30
1	AA	174	A	C2-N3-C4	18.92	120.06	110.60
1	AA	364	A	C2-N3-C4	18.92	120.06	110.60
1	AA	728	A	N1-C2-N3	-18.92	119.84	129.30
22	BA	354	A	N1-C6-N6	-18.92	107.25	118.60
22	BA	685	A	C2-N3-C4	18.92	120.06	110.60
22	BA	1321	A	N1-C2-N3	-18.92	119.84	129.30
22	BA	1427	A	C2-N3-C4	18.92	120.06	110.60
22	BA	2014	A	N1-C2-N3	-18.92	119.84	129.30
1	AA	19	A	N1-C6-N6	-18.92	107.25	118.60
1	AA	1408	A	N1-C2-N3	-18.92	119.84	129.30
22	BA	346	A	C2-N3-C4	18.92	120.06	110.60
22	BA	2670	A	N1-C2-N3	-18.92	119.84	129.30
1	AA	393	A	N1-C6-N6	-18.92	107.25	118.60
1	AA	441	A	N1-C6-N6	-18.92	107.25	118.60
22	BA	644	A	C2-N3-C4	18.92	120.06	110.60
1	AA	532	A	C2-N3-C4	18.92	120.06	110.60
1	AA	116	A	N1-C2-N3	-18.91	119.84	129.30
22	BA	1050	A	C2-N3-C4	18.91	120.06	110.60
22	BA	2800	A	N1-C6-N6	-18.91	107.25	118.60
55	B8	21	A	N1-C2-N3	-18.91	119.84	129.30
1	AA	520	A	N1-C6-N6	-18.91	107.25	118.60
1	AA	1500	A	N1-C6-N6	-18.91	107.25	118.60
22	BA	608	A	C2-N3-C4	18.91	120.06	110.60
1	AA	51	A	C2-N3-C4	18.91	120.06	110.60
22	BA	933	A	N1-C6-N6	-18.91	107.25	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1244	A	C2-N3-C4	18.91	120.06	110.60
1	AA	313	A	N1-C2-N3	-18.91	119.84	129.30
1	AA	1456	A	N1-C2-N3	-18.91	119.85	129.30
22	BA	526	A	N1-C2-N3	-18.91	119.85	129.30
22	BA	781	A	N1-C6-N6	-18.91	107.25	118.60
22	BA	1098	A	C2-N3-C4	18.91	120.06	110.60
22	BA	2564	A	N1-C6-N6	-18.91	107.25	118.60
1	AA	487	A	C2-N3-C4	18.91	120.05	110.60
22	BA	155	A	N1-C2-N3	-18.91	119.85	129.30
22	BA	2097	A	C2-N3-C4	18.91	120.05	110.60
1	AA	595	A	N1-C6-N6	-18.91	107.26	118.60
22	BA	1535	A	N1-C2-N3	-18.91	119.85	129.30
1	AA	1000	A	C2-N3-C4	18.90	120.05	110.60
1	AA	1239	A	N1-C6-N6	-18.90	107.26	118.60
22	BA	111	A	N1-C2-N3	-18.90	119.85	129.30
1	AA	1021	A	C2-N3-C4	18.90	120.05	110.60
22	BA	294	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	1509	A	C2-N3-C4	18.90	120.05	110.60
1	AA	573	A	N1-C2-N3	-18.90	119.85	129.30
1	AA	1117	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	2602	A	C2-N3-C4	18.90	120.05	110.60
1	AA	263	A	C2-N3-C4	18.90	120.05	110.60
22	BA	979	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	1403	A	N1-C6-N6	-18.90	107.26	118.60
22	BA	2682	A	C2-N3-C4	18.90	120.05	110.60
1	AA	432	A	C2-N3-C4	18.90	120.05	110.60
22	BA	471	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	1783	A	N1-C2-N3	-18.90	119.85	129.30
1	AA	72	A	N1-C2-N3	-18.90	119.85	129.30
1	AA	535	A	C2-N3-C4	18.90	120.05	110.60
22	BA	1147	A	C2-N3-C4	18.90	120.05	110.60
1	AA	2	A	C2-N3-C4	18.89	120.05	110.60
1	AA	205	A	N1-C6-N6	-18.89	107.26	118.60
1	AA	1092	A	C2-N3-C4	18.89	120.05	110.60
22	BA	2060	A	C2-N3-C4	18.89	120.05	110.60
1	AA	412	A	C2-N3-C4	18.89	120.05	110.60
1	AA	1534	A	N1-C6-N6	-18.89	107.27	118.60
22	BA	980	A	N1-C6-N6	-18.89	107.27	118.60
22	BA	1090	A	N1-C2-N3	-18.89	119.86	129.30
22	BA	1155	A	C2-N3-C4	18.89	120.05	110.60
22	BA	2406	A	N1-C6-N6	-18.89	107.27	118.60
1	AA	1204	A	C2-N3-C4	18.89	120.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	155	A	C2-N3-C4	18.89	120.04	110.60
22	BA	216	A	C2-N3-C4	18.89	120.04	110.60
22	BA	1126	A	N1-C6-N6	-18.89	107.27	118.60
1	AA	205	A	N1-C2-N3	-18.89	119.86	129.30
22	BA	354	A	C2-N3-C4	18.89	120.04	110.60
22	BA	466	A	N1-C2-N3	-18.89	119.86	129.30
22	BA	1570	A	N1-C2-N3	-18.89	119.86	129.30
22	BA	1650	A	N1-C2-N3	-18.89	119.86	129.30
1	AA	1035	A	C2-N3-C4	18.88	120.04	110.60
1	AA	482	A	C2-N3-C4	18.88	120.04	110.60
22	BA	190	A	C2-N3-C4	18.88	120.04	110.60
22	BA	479	A	N1-C6-N6	-18.88	107.27	118.60
22	BA	609	A	N1-C6-N6	-18.88	107.27	118.60
22	BA	1505	A	N1-C2-N3	-18.88	119.86	129.30
22	BA	1819	A	C2-N3-C4	18.88	120.04	110.60
22	BA	2682	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	792	A	N1-C6-N6	-18.88	107.27	118.60
55	B8	38	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	199	A	C2-N3-C4	18.88	120.04	110.60
22	BA	144	A	C2-N3-C4	18.88	120.04	110.60
22	BA	1067	A	C2-N3-C4	18.88	120.04	110.60
55	B8	73	A	C2-N3-C4	18.88	120.04	110.60
1	AA	196	A	N1-C6-N6	-18.88	107.27	118.60
1	AA	923	A	C2-N3-C4	18.88	120.04	110.60
22	BA	118	A	C2-N3-C4	18.88	120.04	110.60
22	BA	1129	A	C2-N3-C4	18.88	120.04	110.60
22	BA	1133	A	C2-N3-C4	18.88	120.04	110.60
22	BA	2868	A	N1-C2-N3	-18.88	119.86	129.30
22	BA	1090	A	N1-C6-N6	-18.87	107.28	118.60
1	AA	1101	A	N1-C2-N3	-18.87	119.86	129.30
22	BA	1755	A	C2-N3-C4	18.87	120.03	110.60
22	BA	2309	A	C2-N3-C4	18.87	120.03	110.60
22	BA	2705	A	N1-C2-N3	-18.87	119.86	129.30
1	AA	3	A	N1-C2-N3	-18.87	119.86	129.30
1	AA	607	A	N1-C2-N3	-18.87	119.86	129.30
1	AA	1408	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	631	A	C2-N3-C4	18.87	120.03	110.60
22	BA	1477	A	N1-C2-N3	-18.87	119.87	129.30
23	BB	104	A	C2-N3-C4	18.87	120.03	110.60
22	BA	1046	A	C2-N3-C4	18.87	120.03	110.60
1	AA	553	A	N1-C6-N6	-18.86	107.28	118.60
1	AA	845	A	N1-C2-N3	-18.86	119.87	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1306	A	C2-N3-C4	18.86	120.03	110.60
22	BA	743	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	2750	A	N1-C6-N6	-18.86	107.28	118.60
1	AA	1368	A	C2-N3-C4	18.86	120.03	110.60
22	BA	802	A	C2-N3-C4	18.86	120.03	110.60
22	BA	1784	A	C2-N3-C4	18.86	120.03	110.60
1	AA	781	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	1048	A	C2-N3-C4	18.86	120.03	110.60
22	BA	2298	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	2386	A	N1-C2-N3	-18.86	119.87	129.30
55	B8	42	A	C2-N3-C4	18.86	120.03	110.60
1	AA	478	A	N1-C2-N3	-18.86	119.87	129.30
1	AA	1180	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	191	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	2211	A	N1-C6-N6	-18.86	107.28	118.60
22	BA	2850	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	1431	A	C2-N3-C4	18.86	120.03	110.60
22	BA	1987	A	N1-C6-N6	-18.86	107.29	118.60
22	BA	1928	A	N1-C2-N3	-18.85	119.87	129.30
22	BA	1932	A	C2-N3-C4	18.85	120.03	110.60
22	BA	1069	A	N1-C6-N6	-18.85	107.29	118.60
22	BA	1877	A	C2-N3-C4	18.85	120.03	110.60
22	BA	1260	A	C2-N3-C4	18.85	120.03	110.60
22	BA	1336	A	C2-N3-C4	18.85	120.03	110.60
22	BA	1354	A	C2-N3-C4	18.85	120.03	110.60
22	BA	2142	A	C2-N3-C4	18.85	120.03	110.60
1	AA	572	A	N1-C6-N6	-18.85	107.29	118.60
22	BA	2335	A	N1-C6-N6	-18.85	107.29	118.60
1	AA	155	A	C2-N3-C4	18.85	120.02	110.60
1	AA	1110	A	N1-C6-N6	-18.85	107.29	118.60
1	AA	397	A	N1-C6-N6	-18.84	107.29	118.60
22	BA	794	A	N1-C6-N6	-18.84	107.29	118.60
22	BA	1431	A	N1-C2-N3	-18.84	119.88	129.30
22	BA	1009	A	C2-N3-C4	18.84	120.02	110.60
22	BA	1213	A	N1-C2-N3	-18.84	119.88	129.30
22	BA	1509	A	N1-C2-N3	-18.84	119.88	129.30
22	BA	925	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	466	A	N1-C6-N6	-18.84	107.30	118.60
22	BA	423	A	C2-N3-C4	18.84	120.02	110.60
22	BA	384	A	C2-N3-C4	18.84	120.02	110.60
22	BA	172	A	N1-C2-N3	-18.84	119.88	129.30
22	BA	2094	A	N1-C6-N6	-18.84	107.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2725	A	N1-C2-N3	-18.84	119.88	129.30
1	AA	1431	A	N1-C2-N3	-18.83	119.88	129.30
22	BA	104	A	N1-C2-N3	-18.83	119.88	129.30
22	BA	730	A	N1-C2-N3	-18.83	119.88	129.30
1	AA	865	A	C2-N3-C4	18.83	120.02	110.60
1	AA	1289	A	N1-C2-N3	-18.83	119.88	129.30
22	BA	981	A	N1-C6-N6	-18.83	107.30	118.60
1	AA	681	A	N1-C6-N6	-18.83	107.30	118.60
22	BA	320	A	N1-C2-N3	-18.83	119.89	129.30
22	BA	453	A	N1-C6-N6	-18.83	107.30	118.60
22	BA	1978	A	N1-C2-N3	-18.83	119.89	129.30
22	BA	2288	A	C2-N3-C4	18.83	120.01	110.60
22	BA	2670	A	C2-N3-C4	18.83	120.02	110.60
1	AA	366	A	N1-C6-N6	-18.83	107.30	118.60
1	AA	676	A	N1-C6-N6	-18.83	107.30	118.60
1	AA	1196	A	N1-C2-N3	-18.83	119.89	129.30
22	BA	71	A	C2-N3-C4	18.83	120.01	110.60
22	BA	899	A	N1-C6-N6	-18.83	107.30	118.60
23	BB	119	A	C2-N3-C4	18.83	120.01	110.60
1	AA	431	A	C2-N3-C4	18.83	120.01	110.60
1	AA	1250	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	788	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	2725	A	C2-N3-C4	18.82	120.01	110.60
23	BB	108	A	N1-C2-N3	-18.82	119.89	129.30
1	AA	19	A	C2-N3-C4	18.82	120.01	110.60
1	AA	303	A	C2-N3-C4	18.82	120.01	110.60
1	AA	1431	A	C2-N3-C4	18.82	120.01	110.60
1	AA	129	A	N1-C6-N6	-18.82	107.31	118.60
22	BA	182	A	C2-N3-C4	18.82	120.01	110.60
22	BA	479	A	C2-N3-C4	18.82	120.01	110.60
22	BA	936	A	N1-C6-N6	-18.82	107.31	118.60
22	BA	1095	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	1366	A	C2-N3-C4	18.82	120.01	110.60
22	BA	2734	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	362	A	C2-N3-C4	18.82	120.01	110.60
22	BA	1477	A	N1-C6-N6	-18.82	107.31	118.60
1	AA	892	A	N1-C2-N3	-18.81	119.89	129.30
1	AA	959	A	C2-N3-C4	18.81	120.01	110.60
22	BA	231	A	N1-C2-N3	-18.81	119.89	129.30
1	AA	7	A	N1-C2-N3	-18.81	119.89	129.30
22	BA	472	A	N1-C6-N6	-18.81	107.31	118.60
1	AA	1441	A	N1-C2-N3	-18.81	119.90	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	613	A	N1-C2-N3	-18.81	119.90	129.30
1	AA	320	A	N1-C2-N3	-18.81	119.90	129.30
1	AA	994	A	N1-C2-N3	-18.81	119.90	129.30
1	AA	1319	A	N1-C2-N3	-18.81	119.90	129.30
1	AA	253	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	1256	A	N1-C6-N6	-18.80	107.32	118.60
22	BA	2682	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	366	A	C2-N3-C4	18.80	120.00	110.60
22	BA	391	A	C2-N3-C4	18.80	120.00	110.60
1	AA	130	A	N1-C2-N3	-18.80	119.90	129.30
1	AA	461	A	C2-N3-C4	18.80	120.00	110.60
1	AA	448	A	N1-C6-N6	-18.80	107.32	118.60
22	BA	423	A	N1-C6-N6	-18.80	107.32	118.60
1	AA	1398	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	892	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	504	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	1434	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	1596	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	1785	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	2478	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	2733	A	C2-N3-C4	18.80	120.00	110.60
22	BA	1322	A	C2-N3-C4	18.79	120.00	110.60
1	AA	129	A	C2-N3-C4	18.79	120.00	110.60
22	BA	1496	A	C2-N3-C4	18.79	120.00	110.60
1	AA	338	A	N1-C2-N3	-18.79	119.90	129.30
1	AA	1105	A	C2-N3-C4	18.79	120.00	110.60
1	AA	1179	A	C2-N3-C4	18.79	119.99	110.60
22	BA	1711	A	N1-C2-N3	-18.79	119.91	129.30
22	BA	2241	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	1021	A	N1-C6-N6	-18.79	107.33	118.60
22	BA	528	A	N1-C2-N3	-18.79	119.91	129.30
22	BA	1169	A	N1-C2-N3	-18.79	119.91	129.30
1	AA	1042	A	N1-C6-N6	-18.78	107.33	118.60
22	BA	918	A	C2-N3-C4	18.78	119.99	110.60
22	BA	2476	A	N1-C6-N6	-18.78	107.33	118.60
1	AA	1468	A	C2-N3-C4	18.78	119.99	110.60
22	BA	1169	A	C2-N3-C4	18.78	119.99	110.60
22	BA	2037	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	2781	A	N1-C6-N6	-18.78	107.33	118.60
1	AA	1507	A	C2-N3-C4	18.78	119.99	110.60
22	BA	2654	A	N1-C2-N3	-18.78	119.91	129.30
1	AA	873	A	C2-N3-C4	18.78	119.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	602	A	N1-C6-N6	-18.78	107.33	118.60
1	AA	510	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	1477	A	C2-N3-C4	18.78	119.99	110.60
22	BA	1772	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	2776	A	N1-C6-N6	-18.77	107.33	118.60
1	AA	223	A	N1-C6-N6	-18.77	107.34	118.60
22	BA	677	A	C2-N3-C4	18.77	119.99	110.60
22	BA	1336	A	N1-C6-N6	-18.77	107.34	118.60
22	BA	1353	A	N1-C6-N6	-18.77	107.34	118.60
22	BA	2675	A	N1-C6-N6	-18.77	107.34	118.60
1	AA	460	A	C2-N3-C4	18.77	119.98	110.60
1	AA	1188	A	N1-C2-N3	-18.77	119.92	129.30
22	BA	1535	A	N1-C6-N6	-18.77	107.34	118.60
1	AA	935	A	C2-N3-C4	18.77	119.98	110.60
22	BA	1133	A	N1-C2-N3	-18.77	119.92	129.30
22	BA	2147	A	C2-N3-C4	18.77	119.98	110.60
22	BA	160	A	N1-C6-N6	-18.76	107.34	118.60
1	AA	687	A	N1-C6-N6	-18.76	107.34	118.60
1	AA	1531	A	C2-N3-C4	18.76	119.98	110.60
22	BA	2090	A	C2-N3-C4	18.76	119.98	110.60
22	BA	231	A	N1-C6-N6	-18.76	107.34	118.60
22	BA	1739	A	N1-C2-N3	-18.76	119.92	129.30
22	BA	1953	A	C2-N3-C4	18.76	119.98	110.60
23	BB	104	A	N1-C6-N6	-18.76	107.34	118.60
22	BA	1247	A	N1-C6-N6	-18.76	107.34	118.60
22	BA	1664	A	N1-C2-N3	-18.76	119.92	129.30
1	AA	327	A	N1-C6-N6	-18.75	107.35	118.60
22	BA	1433	A	N1-C6-N6	-18.75	107.35	118.60
22	BA	2530	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	906	A	N1-C6-N6	-18.75	107.35	118.60
1	AA	44	A	N1-C6-N6	-18.75	107.35	118.60
1	AA	523	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	937	A	C2-N3-C4	18.75	119.98	110.60
22	BA	2314	A	C2-N3-C4	18.75	119.98	110.60
22	BA	2872	A	N1-C2-N3	-18.75	119.92	129.30
1	AA	315	A	N1-C2-N3	-18.75	119.93	129.30
22	BA	1700	A	C2-N3-C4	18.75	119.97	110.60
22	BA	1701	A	N1-C2-N3	-18.75	119.93	129.30
22	BA	2052	A	N1-C6-N6	-18.75	107.35	118.60
22	BA	2134	A	C2-N3-C4	18.75	119.97	110.60
22	BA	2267	A	N1-C2-N3	-18.75	119.92	129.30
23	BB	29	A	N1-C6-N6	-18.75	107.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1430	A	N1-C2-N3	-18.75	119.93	129.30
22	BA	1147	A	N1-C2-N3	-18.75	119.93	129.30
22	BA	2176	A	N1-C2-N3	-18.75	119.93	129.30
22	BA	2284	A	C2-N3-C4	18.75	119.97	110.60
22	BA	2058	A	N1-C2-N3	-18.75	119.93	129.30
22	BA	207	A	C2-N3-C4	18.74	119.97	110.60
22	BA	1854	A	C2-N3-C4	18.74	119.97	110.60
1	AA	28	A	N1-C6-N6	-18.74	107.35	118.60
1	AA	1428	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	265	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	340	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	1096	A	C2-N3-C4	18.74	119.97	110.60
22	BA	2900	A	C2-N3-C4	18.74	119.97	110.60
23	BB	57	A	C2-N3-C4	18.74	119.97	110.60
22	BA	789	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	1548	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	2117	A	C2-N3-C4	18.74	119.97	110.60
22	BA	2388	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	547	A	C2-N3-C4	18.74	119.97	110.60
1	AA	681	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	1446	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	2534	A	C2-N3-C4	18.74	119.97	110.60
22	BA	2726	A	N1-C6-N6	-18.74	107.36	118.60
1	AA	262	A	N1-C2-N3	-18.74	119.93	129.30
1	AA	270	A	C2-N3-C4	18.74	119.97	110.60
1	AA	681	A	C2-N3-C4	18.74	119.97	110.60
1	AA	559	A	C2-N3-C4	18.73	119.97	110.60
22	BA	415	A	N1-C2-N3	-18.73	119.93	129.30
22	BA	504	A	C2-N3-C4	18.73	119.97	110.60
22	BA	1787	A	C2-N3-C4	18.73	119.97	110.60
1	AA	596	A	C2-N3-C4	18.73	119.97	110.60
22	BA	1001	A	N1-C6-N6	-18.73	107.36	118.60
22	BA	1214	A	C2-N3-C4	18.73	119.96	110.60
22	BA	1304	A	C2-N3-C4	18.73	119.96	110.60
22	BA	1899	A	C2-N3-C4	18.73	119.96	110.60
23	BB	108	A	C2-N3-C4	18.73	119.96	110.60
1	AA	607	A	C2-N3-C4	18.73	119.96	110.60
1	AA	1044	A	N1-C6-N6	-18.73	107.36	118.60
22	BA	1048	A	N1-C6-N6	-18.72	107.36	118.60
22	BA	2328	A	N1-C2-N3	-18.72	119.94	129.30
22	BA	181	A	N1-C2-N3	-18.72	119.94	129.30
22	BA	721	A	N1-C6-N6	-18.72	107.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1652	A	C2-N3-C4	18.72	119.96	110.60
22	BA	1853	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	909	A	C2-N3-C4	18.72	119.96	110.60
1	AA	344	A	N1-C6-N6	-18.72	107.37	118.60
1	AA	649	A	C2-N3-C4	18.72	119.96	110.60
1	AA	935	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	1363	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	103	A	C2-N3-C4	18.72	119.96	110.60
22	BA	820	A	C2-N3-C4	18.72	119.96	110.60
22	BA	975	A	N1-C2-N3	-18.72	119.94	129.30
55	B8	66	A	N1-C2-N3	-18.72	119.94	129.30
1	AA	1191	A	C2-N3-C4	18.71	119.96	110.60
1	AA	1227	A	N1-C2-N3	-18.71	119.94	129.30
1	AA	1377	A	C2-N3-C4	18.71	119.96	110.60
22	BA	342	A	N1-C2-N3	-18.71	119.94	129.30
22	BA	655	A	N1-C2-N3	-18.71	119.94	129.30
22	BA	2147	A	N1-C6-N6	-18.71	107.37	118.60
22	BA	270	A	C2-N3-C4	18.71	119.96	110.60
22	BA	863	A	N1-C6-N6	-18.71	107.37	118.60
1	AA	1288	A	N1-C2-N3	-18.71	119.95	129.30
22	BA	160	A	N1-C2-N3	-18.71	119.95	129.30
22	BA	2376	A	N1-C2-N3	-18.71	119.95	129.30
22	BA	2572	A	C2-N3-C4	18.71	119.95	110.60
1	AA	72	A	C2-N3-C4	18.71	119.95	110.60
1	AA	329	A	N1-C2-N3	-18.71	119.95	129.30
22	BA	849	A	C2-N3-C4	18.71	119.95	110.60
22	BA	1780	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	466	A	N1-C2-N3	-18.70	119.95	129.30
22	BA	538	A	C2-N3-C4	18.70	119.95	110.60
22	BA	2095	A	N1-C6-N6	-18.70	107.38	118.60
1	AA	382	A	N1-C6-N6	-18.70	107.38	118.60
55	B8	42	A	N1-C2-N3	-18.70	119.95	129.30
1	AA	338	A	C2-N3-C4	18.70	119.95	110.60
1	AA	1246	A	N1-C6-N6	-18.70	107.38	118.60
1	AA	1441	A	C2-N3-C4	18.70	119.95	110.60
1	AA	197	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	819	A	C2-N3-C4	18.69	119.95	110.60
1	AA	1150	A	C2-N3-C4	18.69	119.95	110.60
22	BA	943	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	1271	A	C2-N3-C4	18.69	119.95	110.60
1	AA	1360	A	N1-C6-N6	-18.69	107.39	118.60
1	AA	65	A	N1-C2-N3	-18.69	119.95	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	608	A	N1-C2-N3	-18.69	119.95	129.30
22	BA	1829	A	N1-C6-N6	-18.69	107.39	118.60
22	BA	2142	A	N1-C2-N3	-18.69	119.95	129.30
1	AA	50	A	C2-N3-C4	18.69	119.94	110.60
1	AA	131	A	N1-C2-N3	-18.69	119.96	129.30
1	AA	523	A	N1-C6-N6	-18.69	107.39	118.60
1	AA	535	A	N1-C6-N6	-18.69	107.39	118.60
1	AA	1180	A	N1-C6-N6	-18.69	107.39	118.60
22	BA	616	A	N1-C6-N6	-18.69	107.39	118.60
22	BA	2748	A	N1-C2-N3	-18.69	119.96	129.30
1	AA	535	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	702	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1169	A	N1-C6-N6	-18.68	107.39	118.60
22	BA	152	A	C2-N3-C4	18.68	119.94	110.60
22	BA	959	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	1413	A	N1-C6-N6	-18.68	107.39	118.60
1	AA	382	A	N1-C2-N3	-18.68	119.96	129.30
1	AA	228	A	N1-C6-N6	-18.68	107.39	118.60
1	AA	325	A	N1-C6-N6	-18.68	107.39	118.60
1	AA	363	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	471	A	C2-N3-C4	18.68	119.94	110.60
22	BA	1365	A	N1-C6-N6	-18.68	107.39	118.60
22	BA	1419	A	C2-N3-C4	18.68	119.94	110.60
22	BA	2335	A	C2-N3-C4	18.68	119.94	110.60
1	AA	753	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1019	A	C2-N3-C4	18.68	119.94	110.60
22	BA	127	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	2476	A	C2-N3-C4	18.68	119.94	110.60
22	BA	1039	A	N1-C6-N6	-18.68	107.39	118.60
22	BA	1900	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	2309	A	N1-C6-N6	-18.68	107.39	118.60
1	AA	1012	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1016	A	N1-C6-N6	-18.68	107.39	118.60
22	BA	2657	A	C2-N3-C4	18.68	119.94	110.60
1	AA	190	A	C2-N3-C4	18.68	119.94	110.60
22	BA	1254	A	C2-N3-C4	18.68	119.94	110.60
1	AA	1167	A	N1-C6-N6	-18.67	107.40	118.60
22	BA	429	A	N1-C6-N6	-18.67	107.39	118.60
22	BA	1591	A	C2-N3-C4	18.67	119.94	110.60
1	AA	630	A	N1-C2-N3	-18.67	119.96	129.30
22	BA	1579	A	N1-C6-N6	-18.67	107.40	118.60
22	BA	1609	A	N1-C2-N3	-18.67	119.96	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2665	A	N1-C2-N3	-18.67	119.96	129.30
1	AA	694	A	N1-C6-N6	-18.67	107.40	118.60
1	AA	845	A	N1-C6-N6	-18.67	107.40	118.60
1	AA	1500	A	N1-C2-N3	-18.67	119.97	129.30
22	BA	877	A	C2-N3-C4	18.67	119.93	110.60
22	BA	256	A	N1-C6-N6	-18.67	107.40	118.60
22	BA	1420	A	N1-C2-N3	-18.67	119.97	129.30
1	AA	1252	A	N1-C6-N6	-18.66	107.40	118.60
22	BA	345	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	2080	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	2758	A	C2-N3-C4	18.66	119.93	110.60
1	AA	1248	A	N1-C6-N6	-18.66	107.40	118.60
22	BA	1572	A	N1-C2-N3	-18.66	119.97	129.30
1	AA	704	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	1165	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	632	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	272	A	C2-N3-C4	18.66	119.93	110.60
22	BA	1609	A	C2-N3-C4	18.66	119.93	110.60
22	BA	2835	A	C2-N3-C4	18.66	119.93	110.60
1	AA	250	A	N1-C2-N3	-18.65	119.97	129.30
1	AA	901	A	C2-N3-C4	18.65	119.93	110.60
1	AA	189	A	N1-C6-N6	-18.65	107.41	118.60
1	AA	1465	A	C2-N3-C4	18.65	119.93	110.60
22	BA	49	A	C2-N3-C4	18.65	119.93	110.60
22	BA	344	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	1268	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	2082	A	C2-N3-C4	18.65	119.93	110.60
1	AA	608	A	C2-N3-C4	18.65	119.92	110.60
1	AA	415	A	C2-N3-C4	18.65	119.92	110.60
1	AA	649	A	N1-C2-N3	-18.65	119.98	129.30
1	AA	71	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	91	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	197	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	1040	A	N1-C6-N6	-18.64	107.41	118.60
22	BA	1439	A	C2-N3-C4	18.64	119.92	110.60
22	BA	1616	A	N1-C6-N6	-18.64	107.41	118.60
1	AA	172	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	448	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	330	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	1175	A	N1-C2-N3	-18.64	119.98	129.30
1	AA	1146	A	N1-C6-N6	-18.64	107.42	118.60
1	AA	1280	A	N1-C2-N3	-18.64	119.98	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	332	A	N1-C6-N6	-18.64	107.42	118.60
22	BA	1090	A	C2-N3-C4	18.64	119.92	110.60
1	AA	1429	A	C2-N3-C4	18.64	119.92	110.60
22	BA	515	A	N1-C6-N6	-18.64	107.42	118.60
1	AA	1014	A	N1-C6-N6	-18.64	107.42	118.60
22	BA	1285	A	N1-C6-N6	-18.64	107.42	118.60
22	BA	2059	A	C2-N3-C4	18.64	119.92	110.60
1	AA	974	A	N1-C2-N3	-18.63	119.98	129.30
22	BA	716	A	N1-C2-N3	-18.63	119.98	129.30
1	AA	1204	A	N1-C6-N6	-18.63	107.42	118.60
22	BA	1395	A	C2-N3-C4	18.63	119.92	110.60
1	AA	819	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	1036	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	1285	A	C2-N3-C4	18.63	119.91	110.60
22	BA	73	A	N1-C6-N6	-18.63	107.42	118.60
22	BA	1787	A	N1-C6-N6	-18.63	107.42	118.60
22	BA	2587	A	N1-C6-N6	-18.63	107.42	118.60
1	AA	223	A	C2-N3-C4	18.62	119.91	110.60
1	AA	349	A	N1-C2-N3	-18.62	119.99	129.30
22	BA	63	A	C2-N3-C4	18.62	119.91	110.60
22	BA	142	A	C2-N3-C4	18.62	119.91	110.60
22	BA	2062	A	N1-C6-N6	-18.62	107.42	118.60
22	BA	1548	A	C2-N3-C4	18.62	119.91	110.60
1	AA	363	A	N1-C6-N6	-18.62	107.43	118.60
22	BA	401	A	C2-N3-C4	18.62	119.91	110.60
1	AA	374	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	1022	A	N1-C2-N3	-18.62	119.99	129.30
22	BA	900	A	C2-N3-C4	18.62	119.91	110.60
22	BA	2184	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	7	A	N1-C6-N6	-18.62	107.43	118.60
1	AA	236	A	C2-N3-C4	18.62	119.91	110.60
1	AA	675	A	C2-N3-C4	18.62	119.91	110.60
1	AA	1499	A	N1-C6-N6	-18.62	107.43	118.60
22	BA	1342	A	C2-N3-C4	18.62	119.91	110.60
1	AA	315	A	N1-C6-N6	-18.61	107.43	118.60
1	AA	1254	A	C2-N3-C4	18.61	119.91	110.60
22	BA	176	A	N1-C2-N3	-18.61	119.99	129.30
22	BA	1127	A	C2-N3-C4	18.61	119.91	110.60
22	BA	2823	A	N1-C6-N6	-18.61	107.43	118.60
1	AA	430	A	C2-N3-C4	18.61	119.91	110.60
1	AA	1110	A	N1-C2-N3	-18.61	120.00	129.30
22	BA	2071	A	N1-C6-N6	-18.61	107.43	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2776	A	N1-C2-N3	-18.61	119.99	129.30
1	AA	130	A	N1-C6-N6	-18.61	107.43	118.60
22	BA	2088	A	N1-C2-N3	-18.61	120.00	129.30
22	BA	2154	A	C2-N3-C4	18.61	119.91	110.60
22	BA	586	A	N1-C2-N3	-18.61	120.00	129.30
22	BA	1264	A	N1-C6-N6	-18.61	107.44	118.60
1	AA	498	A	N1-C6-N6	-18.61	107.44	118.60
22	BA	1287	A	N1-C6-N6	-18.61	107.44	118.60
1	AA	1410	A	C2-N3-C4	18.61	119.90	110.60
22	BA	324	A	N1-C2-N3	-18.61	120.00	129.30
22	BA	480	A	C2-N3-C4	18.61	119.90	110.60
1	AA	864	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	38	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	382	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	1490	A	N1-C6-N6	-18.60	107.44	118.60
22	BA	1701	A	C2-N3-C4	18.60	119.90	110.60
1	AA	50	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	546	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	1152	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	941	A	N1-C6-N6	-18.60	107.44	118.60
22	BA	2748	A	C2-N3-C4	18.60	119.90	110.60
1	AA	196	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	1495	A	N1-C2-N3	-18.60	120.00	129.30
23	BB	109	A	C2-N3-C4	18.60	119.90	110.60
1	AA	116	A	C2-N3-C4	18.60	119.90	110.60
1	AA	1145	A	C2-N3-C4	18.60	119.90	110.60
1	AA	1251	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	1549	A	N1-C2-N3	-18.60	120.00	129.30
1	AA	101	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	1492	A	C2-N3-C4	18.60	119.90	110.60
22	BA	371	A	C2-N3-C4	18.60	119.90	110.60
22	BA	722	A	C2-N3-C4	18.60	119.90	110.60
22	BA	1637	A	N1-C6-N6	-18.60	107.44	118.60
1	AA	1238	A	N1-C6-N6	-18.59	107.44	118.60
22	BA	104	A	C2-N3-C4	18.59	119.90	110.60
22	BA	300	A	N1-C6-N6	-18.59	107.44	118.60
22	BA	905	A	N1-C6-N6	-18.59	107.44	118.60
22	BA	2288	A	N1-C6-N6	-18.59	107.44	118.60
22	BA	2639	A	N1-C6-N6	-18.59	107.44	118.60
55	B8	51	A	N1-C2-N3	-18.59	120.00	129.30
22	BA	354	A	N1-C2-N3	-18.59	120.00	129.30
1	AA	1000	A	N1-C2-N3	-18.59	120.00	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	156	A	C2-N3-C4	18.59	119.89	110.60
1	AA	790	A	N1-C2-N3	-18.59	120.00	129.30
22	BA	2366	A	C2-N3-C4	18.59	119.89	110.60
1	AA	172	A	C2-N3-C4	18.59	119.89	110.60
1	AA	609	A	N1-C2-N3	-18.59	120.01	129.30
22	BA	218	A	C2-N3-C4	18.59	119.89	110.60
22	BA	621	A	N1-C2-N3	-18.59	120.01	129.30
22	BA	608	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	749	A	C2-N3-C4	18.58	119.89	110.60
1	AA	1016	A	N1-C2-N3	-18.58	120.01	129.30
22	BA	472	A	N1-C2-N3	-18.58	120.01	129.30
22	BA	1244	A	N1-C2-N3	-18.58	120.01	129.30
22	BA	1213	A	C2-N3-C4	18.58	119.89	110.60
55	B8	41	A	N1-C2-N3	-18.58	120.01	129.30
1	AA	238	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	131	A	C2-N3-C4	18.58	119.89	110.60
22	BA	1308	A	N1-C2-N3	-18.58	120.01	129.30
22	BA	1453	A	N1-C6-N6	-18.58	107.45	118.60
55	B8	59	A	C2-N3-C4	18.58	119.89	110.60
22	BA	1285	A	C2-N3-C4	18.58	119.89	110.60
1	AA	98	A	C2-N3-C4	18.57	119.89	110.60
1	AA	602	A	N1-C2-N3	-18.57	120.01	129.30
22	BA	849	A	N1-C2-N3	-18.57	120.01	129.30
22	BA	1268	A	C2-N3-C4	18.57	119.89	110.60
1	AA	465	A	C2-N3-C4	18.57	119.89	110.60
22	BA	223	A	C2-N3-C4	18.57	119.89	110.60
22	BA	384	A	N1-C6-N6	-18.57	107.46	118.60
1	AA	814	A	C2-N3-C4	18.57	119.89	110.60
22	BA	614	A	C2-N3-C4	18.57	119.88	110.60
22	BA	1508	A	N1-C2-N3	-18.57	120.02	129.30
22	BA	1791	A	N1-C2-N3	-18.57	120.02	129.30
22	BA	2184	A	N1-C2-N3	-18.57	120.02	129.30
1	AA	1394	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	503	A	N1-C2-N3	-18.57	120.02	129.30
22	BA	716	A	C2-N3-C4	18.56	119.88	110.60
22	BA	878	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	408	A	N1-C6-N6	-18.56	107.46	118.60
1	AA	1145	A	N1-C6-N6	-18.56	107.46	118.60
22	BA	1067	A	N1-C6-N6	-18.56	107.46	118.60
22	BA	1096	A	N1-C2-N3	-18.56	120.02	129.30
22	BA	1301	A	N1-C6-N6	-18.56	107.46	118.60
22	BA	118	A	N1-C2-N3	-18.56	120.02	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1093	A	C2-N3-C4	18.56	119.88	110.60
1	AA	1081	A	C2-N3-C4	18.56	119.88	110.60
1	AA	1219	A	C2-N3-C4	18.56	119.88	110.60
22	BA	1095	A	N1-C6-N6	-18.56	107.47	118.60
22	BA	1103	A	N1-C2-N3	-18.56	120.02	129.30
1	AA	630	A	C2-N3-C4	18.55	119.88	110.60
1	AA	1102	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	1204	A	N1-C2-N3	-18.55	120.02	129.30
22	BA	1952	A	C2-N3-C4	18.55	119.88	110.60
1	AA	393	A	N1-C2-N3	-18.55	120.02	129.30
1	AA	600	A	N1-C6-N6	-18.55	107.47	118.60
22	BA	632	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	2	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	1082	A	N1-C2-N3	-18.55	120.03	129.30
1	AA	1102	A	C2-N3-C4	18.55	119.87	110.60
1	AA	1346	A	N1-C2-N3	-18.55	120.03	129.30
22	BA	6	A	N1-C2-N3	-18.55	120.03	129.30
22	BA	2198	A	C2-N3-C4	18.55	119.87	110.60
22	BA	2426	A	C2-N3-C4	18.55	119.87	110.60
1	AA	349	A	N1-C6-N6	-18.55	107.47	118.60
1	AA	908	A	C2-N3-C4	18.55	119.87	110.60
22	BA	925	A	C2-N3-C4	18.55	119.87	110.60
22	BA	1144	A	C2-N3-C4	18.55	119.87	110.60
22	BA	1987	A	C2-N3-C4	18.55	119.87	110.60
22	BA	2478	A	N1-C6-N6	-18.55	107.47	118.60
23	BB	45	A	C2-N3-C4	18.55	119.87	110.60
1	AA	199	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1248	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	1374	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	415	A	N1-C6-N6	-18.54	107.47	118.60
1	AA	1275	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1353	A	C2-N3-C4	18.54	119.87	110.60
22	BA	2158	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	131	A	N1-C6-N6	-18.54	107.47	118.60
1	AA	900	A	C2-N3-C4	18.54	119.87	110.60
22	BA	861	A	N1-C6-N6	-18.54	107.47	118.60
1	AA	794	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	900	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	2094	A	C2-N3-C4	18.54	119.87	110.60
1	AA	344	A	C2-N3-C4	18.54	119.87	110.60
22	BA	278	A	N1-C6-N6	-18.54	107.48	118.60
22	BA	503	A	N1-C6-N6	-18.54	107.48	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1084	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1572	A	C2-N3-C4	18.54	119.87	110.60
22	BA	2740	A	N1-C6-N6	-18.54	107.48	118.60
23	BB	109	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	1127	A	N1-C2-N3	-18.54	120.03	129.30
1	AA	753	A	N1-C2-N3	-18.53	120.03	129.30
22	BA	666	A	N1-C2-N3	-18.53	120.03	129.30
23	BB	39	A	N1-C6-N6	-18.53	107.48	118.60
55	B8	58	A	N1-C2-N3	-18.53	120.03	129.30
1	AA	1274	A	C2-N3-C4	18.53	119.86	110.60
22	BA	1960	A	N1-C2-N3	-18.53	120.03	129.30
22	BA	2147	A	N1-C2-N3	-18.53	120.03	129.30
22	BA	2407	A	C2-N3-C4	18.53	119.86	110.60
22	BA	222	A	N1-C2-N3	-18.53	120.04	129.30
1	AA	65	A	C2-N3-C4	18.53	119.86	110.60
22	BA	1028	A	N1-C6-N6	-18.53	107.48	118.60
22	BA	1029	A	C2-N3-C4	18.53	119.86	110.60
22	BA	1791	A	C2-N3-C4	18.53	119.86	110.60
22	BA	2614	A	N1-C2-N3	-18.53	120.04	129.30
1	AA	759	A	C2-N3-C4	18.52	119.86	110.60
1	AA	1157	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	603	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	988	A	N1-C6-N6	-18.52	107.48	118.60
22	BA	2042	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	101	A	C2-N3-C4	18.52	119.86	110.60
1	AA	109	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	969	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	1456	A	C2-N3-C4	18.52	119.86	110.60
22	BA	2886	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	1236	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	582	A	C2-N3-C4	18.52	119.86	110.60
22	BA	1384	A	C2-N3-C4	18.52	119.86	110.60
22	BA	251	A	C2-N3-C4	18.52	119.86	110.60
22	BA	715	A	C2-N3-C4	18.52	119.86	110.60
22	BA	1272	A	N1-C6-N6	-18.52	107.49	118.60
22	BA	1393	A	C2-N3-C4	18.52	119.86	110.60
23	BB	39	A	C2-N3-C4	18.52	119.86	110.60
22	BA	1246	A	N1-C6-N6	-18.52	107.49	118.60
1	AA	959	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	1028	A	C2-N3-C4	18.52	119.86	110.60
22	BA	2205	A	N1-C2-N3	-18.52	120.04	129.30
1	AA	120	A	N1-C6-N6	-18.51	107.49	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	533	A	N1-C6-N6	-18.51	107.49	118.60
22	BA	161	A	C2-N3-C4	18.51	119.86	110.60
22	BA	666	A	N1-C6-N6	-18.51	107.49	118.60
1	AA	1169	A	C2-N3-C4	18.51	119.86	110.60
1	AA	1428	A	C2-N3-C4	18.51	119.86	110.60
22	BA	1054	A	C2-N3-C4	18.51	119.86	110.60
22	BA	1900	A	C2-N3-C4	18.51	119.86	110.60
55	B8	58	A	N1-C6-N6	-18.51	107.50	118.60
1	AA	456	A	C2-N3-C4	18.51	119.85	110.60
1	AA	1256	A	C2-N3-C4	18.51	119.85	110.60
22	BA	213	A	C2-N3-C4	18.51	119.85	110.60
22	BA	2199	A	N1-C6-N6	-18.51	107.50	118.60
22	BA	920	A	N1-C6-N6	-18.51	107.50	118.60
22	BA	1470	A	C2-N3-C4	18.51	119.85	110.60
23	BB	119	A	N1-C6-N6	-18.51	107.50	118.60
1	AA	325	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	408	A	C2-N3-C4	18.50	119.85	110.60
1	AA	1377	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	1745	A	C2-N3-C4	18.50	119.85	110.60
22	BA	844	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	435	A	C2-N3-C4	18.50	119.85	110.60
1	AA	622	A	C2-N3-C4	18.50	119.85	110.60
22	BA	1650	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	1847	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	382	A	C2-N3-C4	18.50	119.85	110.60
22	BA	538	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	487	A	N1-C2-N3	-18.50	120.05	129.30
1	AA	978	A	C2-N3-C4	18.50	119.85	110.60
22	BA	927	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	1579	A	C2-N3-C4	18.50	119.85	110.60
22	BA	1057	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	384	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	602	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	751	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	1900	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	299	A	N1-C2-N3	-18.49	120.05	129.30
22	BA	2377	A	C2-N3-C4	18.49	119.85	110.60
22	BA	1504	A	C2-N3-C4	18.49	119.85	110.60
1	AA	1261	A	N1-C6-N6	-18.49	107.50	118.60
22	BA	1057	A	N1-C6-N6	-18.49	107.50	118.60
1	AA	3	A	C2-N3-C4	18.49	119.84	110.60
22	BA	592	A	N1-C6-N6	-18.49	107.51	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1819	A	N1-C6-N6	-18.49	107.51	118.60
1	AA	432	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	767	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	139	A	C2-N3-C4	18.49	119.84	110.60
1	AA	695	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	996	A	N1-C2-N3	-18.49	120.06	129.30
22	BA	1802	A	N1-C2-N3	-18.49	120.06	129.30
1	AA	1170	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	1340	A	C2-N3-C4	18.48	119.84	110.60
1	AA	1340	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	1413	A	C2-N3-C4	18.48	119.84	110.60
22	BA	346	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	2887	A	C2-N3-C4	18.48	119.84	110.60
23	BB	50	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	1274	A	N1-C2-N3	-18.48	120.06	129.30
1	AA	374	A	C2-N3-C4	18.48	119.84	110.60
22	BA	1284	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	2171	A	C2-N3-C4	18.48	119.84	110.60
22	BA	2736	A	C2-N3-C4	18.48	119.84	110.60
22	BA	1301	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	483	A	N1-C6-N6	-18.48	107.51	118.60
1	AA	1257	A	C2-N3-C4	18.47	119.84	110.60
22	BA	1698	A	N1-C2-N3	-18.47	120.06	129.30
22	BA	2406	A	C2-N3-C4	18.47	119.84	110.60
1	AA	694	A	N1-C2-N3	-18.47	120.06	129.30
1	AA	889	A	C2-N3-C4	18.47	119.84	110.60
22	BA	111	A	C2-N3-C4	18.47	119.84	110.60
22	BA	95	A	C2-N3-C4	18.47	119.83	110.60
22	BA	127	A	N1-C6-N6	-18.47	107.52	118.60
22	BA	2077	A	N1-C2-N3	-18.47	120.06	129.30
22	BA	282	A	N1-C2-N3	-18.47	120.07	129.30
22	BA	1525	A	C2-N3-C4	18.47	119.83	110.60
22	BA	668	A	N1-C6-N6	-18.47	107.52	118.60
22	BA	804	A	N1-C2-N3	-18.47	120.07	129.30
22	BA	1854	A	N1-C2-N3	-18.47	120.07	129.30
22	BA	2887	A	N1-C2-N3	-18.47	120.07	129.30
1	AA	493	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	348	A	C2-N3-C4	18.46	119.83	110.60
1	AA	946	A	C2-N3-C4	18.46	119.83	110.60
1	AA	1035	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	401	A	N1-C6-N6	-18.46	107.52	118.60
22	BA	1301	A	C2-N3-C4	18.46	119.83	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	574	A	N1-C6-N6	-18.46	107.52	118.60
22	BA	616	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	1073	A	C2-N3-C4	18.46	119.83	110.60
22	BA	1626	A	C2-N3-C4	18.46	119.83	110.60
22	BA	2058	A	C2-N3-C4	18.46	119.83	110.60
22	BA	430	A	N1-C6-N6	-18.46	107.53	118.60
22	BA	1028	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	2662	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	324	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	572	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	900	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	2225	A	C2-N3-C4	18.45	119.83	110.60
22	BA	2433	A	N1-C2-N3	-18.45	120.07	129.30
1	AA	780	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	819	A	N1-C2-N3	-18.45	120.07	129.30
22	BA	1009	A	N1-C6-N6	-18.45	107.53	118.60
1	AA	574	A	N1-C2-N3	-18.45	120.07	129.30
22	BA	783	A	N1-C2-N3	-18.45	120.07	129.30
22	BA	1789	A	N1-C2-N3	-18.45	120.07	129.30
1	AA	629	A	N1-C2-N3	-18.45	120.08	129.30
1	AA	1329	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	1366	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	1794	A	C2-N3-C4	18.45	119.83	110.60
22	BA	1977	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	2662	A	C2-N3-C4	18.45	119.83	110.60
22	BA	1086	A	N1-C2-N3	-18.45	120.08	129.30
22	BA	1503	A	N1-C2-N3	-18.45	120.08	129.30
22	BA	2266	A	N1-C2-N3	-18.45	120.08	129.30
22	BA	2333	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	547	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	167	A	C2-N3-C4	18.44	119.82	110.60
22	BA	1054	A	N1-C2-N3	-18.44	120.08	129.30
22	BA	1899	A	N1-C6-N6	-18.44	107.53	118.60
22	BA	2205	A	N1-C6-N6	-18.44	107.53	118.60
22	BA	2873	A	C2-N3-C4	18.44	119.82	110.60
22	BA	2879	A	N1-C2-N3	-18.44	120.08	129.30
22	BA	1050	A	N1-C2-N3	-18.44	120.08	129.30
22	BA	2733	A	N1-C2-N3	-18.44	120.08	129.30
55	B8	69	A	N1-C2-N3	-18.44	120.08	129.30
1	AA	704	A	C2-N3-C4	18.44	119.82	110.60
1	AA	1155	A	C2-N3-C4	18.44	119.82	110.60
22	BA	2448	A	N1-C6-N6	-18.44	107.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	974	A	N1-C6-N6	-18.43	107.54	118.60
22	BA	2879	A	C2-N3-C4	18.43	119.82	110.60
22	BA	1469	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	129	A	N1-C2-N3	-18.43	120.08	129.30
1	AA	499	A	N1-C2-N3	-18.43	120.08	129.30
22	BA	718	A	C2-N3-C4	18.43	119.82	110.60
22	BA	2211	A	N1-C2-N3	-18.43	120.08	129.30
22	BA	739	A	N1-C2-N3	-18.43	120.08	129.30
22	BA	2037	A	C2-N3-C4	18.43	119.81	110.60
55	B8	14	A	N1-C6-N6	-18.43	107.54	118.60
1	AA	1	A	N1-C6-N6	-18.43	107.54	118.60
1	AA	1468	A	N1-C2-N3	-18.43	120.09	129.30
22	BA	84	A	C2-N3-C4	18.43	119.81	110.60
22	BA	422	A	N1-C6-N6	-18.43	107.54	118.60
22	BA	1089	A	C2-N3-C4	18.43	119.81	110.60
22	BA	2654	A	N1-C6-N6	-18.43	107.54	118.60
22	BA	2826	A	N1-C2-N3	-18.43	120.08	129.30
22	BA	2887	A	N1-C6-N6	-18.43	107.54	118.60
22	BA	2278	A	N1-C6-N6	-18.43	107.54	118.60
22	BA	2753	A	C2-N3-C4	18.43	119.81	110.60
22	BA	173	A	N1-C2-N3	-18.43	120.09	129.30
1	AA	559	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	472	A	C2-N3-C4	18.42	119.81	110.60
22	BA	1353	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	1073	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	1246	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	1549	A	N1-C6-N6	-18.42	107.55	118.60
22	BA	2270	A	C2-N3-C4	18.42	119.81	110.60
22	BA	1040	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	2778	A	N1-C2-N3	-18.41	120.09	129.30
22	BA	2800	A	N1-C2-N3	-18.41	120.09	129.30
1	AA	1340	A	N1-C6-N6	-18.41	107.55	118.60
22	BA	95	A	N1-C2-N3	-18.41	120.09	129.30
22	BA	675	A	N1-C2-N3	-18.41	120.09	129.30
22	BA	1373	A	C2-N3-C4	18.41	119.81	110.60
1	AA	451	A	N1-C2-N3	-18.41	120.09	129.30
1	AA	1004	A	N1-C6-N6	-18.41	107.55	118.60
22	BA	508	A	C2-N3-C4	18.41	119.81	110.60
22	BA	483	A	C2-N3-C4	18.41	119.80	110.60
22	BA	960	A	C2-N3-C4	18.41	119.81	110.60
22	BA	2114	A	N1-C6-N6	-18.41	107.56	118.60
22	BA	453	A	N1-C2-N3	-18.41	120.10	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	654	A	C2-N3-C4	18.41	119.80	110.60
22	BA	1918	A	N1-C2-N3	-18.41	120.10	129.30
22	BA	2590	A	N1-C6-N6	-18.41	107.56	118.60
1	AA	33	A	C2-N3-C4	18.40	119.80	110.60
1	AA	499	A	C2-N3-C4	18.40	119.80	110.60
22	BA	2813	A	N1-C6-N6	-18.40	107.56	118.60
1	AA	663	A	N1-C6-N6	-18.40	107.56	118.60
22	BA	460	A	N1-C6-N6	-18.40	107.56	118.60
22	BA	2734	A	N1-C6-N6	-18.40	107.56	118.60
1	AA	1197	A	C2-N3-C4	18.40	119.80	110.60
1	AA	1349	A	N1-C2-N3	-18.40	120.10	129.30
22	BA	270	A	N1-C6-N6	-18.40	107.56	118.60
22	BA	654	A	N1-C6-N6	-18.40	107.56	118.60
22	BA	1126	A	N1-C2-N3	-18.40	120.10	129.30
22	BA	2005	A	N1-C6-N6	-18.40	107.56	118.60
22	BA	2660	A	C2-N3-C4	18.40	119.80	110.60
1	AA	509	A	N1-C6-N6	-18.40	107.56	118.60
1	AA	1289	A	C2-N3-C4	18.40	119.80	110.60
22	BA	574	A	N1-C2-N3	-18.40	120.10	129.30
22	BA	973	A	N1-C2-N3	-18.40	120.10	129.30
22	BA	404	A	N1-C2-N3	-18.39	120.10	129.30
22	BA	2821	A	C2-N3-C4	18.39	119.80	110.60
1	AA	1319	A	C2-N3-C4	18.39	119.80	110.60
22	BA	44	A	N1-C2-N3	-18.39	120.10	129.30
22	BA	609	A	C2-N3-C4	18.39	119.80	110.60
22	BA	749	A	C2-N3-C4	18.39	119.80	110.60
22	BA	1127	A	N1-C6-N6	-18.39	107.56	118.60
22	BA	1553	A	N1-C6-N6	-18.39	107.56	118.60
1	AA	787	A	C2-N3-C4	18.39	119.80	110.60
22	BA	2378	A	C2-N3-C4	18.39	119.80	110.60
1	AA	1408	A	C2-N3-C4	18.39	119.80	110.60
22	BA	2860	A	N1-C6-N6	-18.39	107.57	118.60
1	AA	181	A	N1-C2-N3	-18.39	120.11	129.30
1	AA	554	A	N1-C6-N6	-18.39	107.57	118.60
22	BA	685	A	N1-C6-N6	-18.39	107.57	118.60
22	BA	203	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	243	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	451	A	C2-N3-C4	18.38	119.79	110.60
1	AA	547	A	N1-C6-N6	-18.38	107.57	118.60
1	AA	1502	A	N1-C6-N6	-18.38	107.57	118.60
22	BA	1241	A	C2-N3-C4	18.38	119.79	110.60
1	AA	553	A	C2-N3-C4	18.38	119.79	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1528	A	C2-N3-C4	18.38	119.79	110.60
22	BA	1678	A	N1-C2-N3	-18.38	120.11	129.30
1	AA	802	A	C2-N3-C4	18.38	119.79	110.60
1	AA	1236	A	N1-C6-N6	-18.38	107.57	118.60
22	BA	1048	A	N1-C2-N3	-18.37	120.11	129.30
22	BA	1603	A	C2-N3-C4	18.37	119.79	110.60
22	BA	2411	A	C2-N3-C4	18.37	119.79	110.60
1	AA	262	A	N1-C6-N6	-18.37	107.58	118.60
1	AA	336	A	C2-N3-C4	18.37	119.78	110.60
1	AA	1151	A	N1-C6-N6	-18.37	107.58	118.60
22	BA	643	A	N1-C6-N6	-18.37	107.58	118.60
1	AA	1507	A	N1-C6-N6	-18.37	107.58	118.60
22	BA	2205	A	C2-N3-C4	18.37	119.78	110.60
1	AA	908	A	N1-C6-N6	-18.37	107.58	118.60
1	AA	1196	A	C2-N3-C4	18.37	119.78	110.60
22	BA	1713	A	N1-C2-N3	-18.37	120.12	129.30
22	BA	1877	A	N1-C6-N6	-18.37	107.58	118.60
22	BA	2439	A	N1-C2-N3	-18.37	120.12	129.30
1	AA	435	A	N1-C2-N3	-18.37	120.12	129.30
22	BA	722	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	2247	A	N1-C6-N6	-18.36	107.58	118.60
23	BB	52	A	N1-C6-N6	-18.36	107.58	118.60
1	AA	1513	A	C2-N3-C4	18.36	119.78	110.60
1	AA	996	A	N1-C6-N6	-18.36	107.58	118.60
1	AA	1346	A	C2-N3-C4	18.36	119.78	110.60
22	BA	63	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	878	A	C2-N3-C4	18.36	119.78	110.60
22	BA	1367	A	N1-C6-N6	-18.36	107.58	118.60
1	AA	635	A	C2-N3-C4	18.36	119.78	110.60
1	AA	1508	A	C2-N3-C4	18.36	119.78	110.60
22	BA	460	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	1952	A	N1-C6-N6	-18.36	107.58	118.60
1	AA	977	A	N1-C6-N6	-18.36	107.59	118.60
22	BA	2566	A	C2-N3-C4	18.36	119.78	110.60
1	AA	338	A	N1-C6-N6	-18.35	107.59	118.60
22	BA	282	A	C2-N3-C4	18.35	119.78	110.60
22	BA	1690	A	N1-C2-N3	-18.35	120.12	129.30
22	BA	342	A	N1-C6-N6	-18.35	107.59	118.60
1	AA	675	A	N1-C6-N6	-18.35	107.59	118.60
1	AA	1269	A	N1-C6-N6	-18.35	107.59	118.60
22	BA	497	A	N1-C6-N6	-18.35	107.59	118.60
22	BA	1069	A	C2-N3-C4	18.35	119.78	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2439	A	C2-N3-C4	18.35	119.78	110.60
1	AA	747	A	N1-C6-N6	-18.35	107.59	118.60
1	AA	865	A	N1-C6-N6	-18.35	107.59	118.60
22	BA	1503	A	N1-C6-N6	-18.35	107.59	118.60
23	BB	34	A	N1-C2-N3	-18.35	120.13	129.30
22	BA	988	A	N1-C2-N3	-18.34	120.13	129.30
1	AA	600	A	C2-N3-C4	18.34	119.77	110.60
1	AA	906	A	C2-N3-C4	18.34	119.77	110.60
1	AA	1093	A	N1-C2-N3	-18.34	120.13	129.30
1	AA	1219	A	N1-C6-N6	-18.34	107.59	118.60
22	BA	146	A	C2-N3-C4	18.34	119.77	110.60
22	BA	727	A	N1-C2-N3	-18.34	120.13	129.30
22	BA	1103	A	C2-N3-C4	18.34	119.77	110.60
22	BA	2868	A	N1-C6-N6	-18.34	107.59	118.60
22	BA	320	A	N1-C6-N6	-18.34	107.60	118.60
22	BA	621	A	C2-N3-C4	18.34	119.77	110.60
22	BA	1378	A	N1-C2-N3	-18.34	120.13	129.30
22	BA	2851	A	N1-C2-N3	-18.34	120.13	129.30
1	AA	493	A	N1-C6-N6	-18.34	107.60	118.60
1	AA	1036	A	N1-C2-N3	-18.34	120.13	129.30
22	BA	2298	A	C2-N3-C4	18.34	119.77	110.60
1	AA	1437	A	C2-N3-C4	18.34	119.77	110.60
22	BA	1470	A	N1-C2-N3	-18.34	120.13	129.30
22	BA	1569	A	C2-N3-C4	18.33	119.77	110.60
1	AA	1157	A	N1-C6-N6	-18.33	107.60	118.60
1	AA	1191	A	N1-C2-N3	-18.33	120.13	129.30
22	BA	1431	A	N1-C6-N6	-18.33	107.60	118.60
22	BA	1640	A	N1-C2-N3	-18.33	120.13	129.30
1	AA	16	A	N1-C6-N6	-18.33	107.60	118.60
1	AA	1170	A	C2-N3-C4	18.33	119.77	110.60
22	BA	204	A	N1-C2-N3	-18.33	120.14	129.30
22	BA	1508	A	C2-N3-C4	18.33	119.77	110.60
1	AA	155	A	N1-C2-N3	-18.33	120.14	129.30
1	AA	228	A	C2-N3-C4	18.33	119.77	110.60
1	AA	718	A	N1-C6-N6	-18.33	107.60	118.60
22	BA	2095	A	C2-N3-C4	18.33	119.77	110.60
1	AA	1531	A	N1-C6-N6	-18.33	107.60	118.60
22	BA	829	A	C2-N3-C4	18.33	119.76	110.60
22	BA	1590	A	N1-C2-N3	-18.33	120.14	129.30
22	BA	2199	A	C2-N3-C4	18.33	119.76	110.60
22	BA	368	A	N1-C6-N6	-18.33	107.61	118.60
22	BA	1532	A	C2-N3-C4	18.33	119.76	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2274	A	C2-N3-C4	18.33	119.76	110.60
1	AA	325	A	C2-N3-C4	18.32	119.76	110.60
1	AA	1171	A	N1-C6-N6	-18.32	107.61	118.60
22	BA	222	A	C2-N3-C4	18.32	119.76	110.60
22	BA	2163	A	N1-C2-N3	-18.32	120.14	129.30
22	BA	2725	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	1093	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	1257	A	N1-C2-N3	-18.32	120.14	129.30
1	AA	1368	A	N1-C2-N3	-18.32	120.14	129.30
1	AA	1357	A	C2-N3-C4	18.32	119.76	110.60
1	AA	1410	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	909	A	N1-C2-N3	-18.32	120.14	129.30
1	AA	964	A	C2-N3-C4	18.32	119.76	110.60
1	AA	1117	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	456	A	N1-C6-N6	-18.32	107.61	118.60
1	AA	640	A	N1-C2-N3	-18.32	120.14	129.30
22	BA	927	A	C2-N3-C4	18.32	119.76	110.60
22	BA	282	A	N1-C6-N6	-18.31	107.61	118.60
1	AA	579	A	N1-C6-N6	-18.31	107.61	118.60
22	BA	218	A	N1-C2-N3	-18.31	120.14	129.30
22	BA	1579	A	N1-C2-N3	-18.31	120.14	129.30
22	BA	2776	A	C2-N3-C4	18.31	119.76	110.60
22	BA	2886	A	C2-N3-C4	18.31	119.75	110.60
1	AA	59	A	C2-N3-C4	18.31	119.75	110.60
22	BA	181	A	C2-N3-C4	18.31	119.75	110.60
22	BA	1134	A	N1-C6-N6	-18.31	107.61	118.60
1	AA	1012	A	N1-C6-N6	-18.31	107.62	118.60
23	BB	53	A	C2-N3-C4	18.31	119.75	110.60
1	AA	718	A	N1-C2-N3	-18.30	120.15	129.30
1	AA	946	A	N1-C2-N3	-18.30	120.15	129.30
22	BA	1275	A	C2-N3-C4	18.30	119.75	110.60
1	AA	321	A	C2-N3-C4	18.30	119.75	110.60
1	AA	1	A	N1-C2-N3	-18.30	120.15	129.30
22	BA	241	A	C2-N3-C4	18.30	119.75	110.60
22	BA	483	A	N1-C2-N3	-18.30	120.15	129.30
22	BA	1070	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	1570	A	C2-N3-C4	18.30	119.75	110.60
22	BA	1676	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	2381	A	C2-N3-C4	18.30	119.75	110.60
22	BA	454	A	C2-N3-C4	18.30	119.75	110.60
22	BA	1302	A	C2-N3-C4	18.30	119.75	110.60
1	AA	238	A	C2-N3-C4	18.30	119.75	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	303	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	5	A	N1-C2-N3	-18.30	120.15	129.30
1	AA	197	A	C2-N3-C4	18.30	119.75	110.60
1	AA	975	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	734	A	N1-C2-N3	-18.30	120.15	129.30
22	BA	2037	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	1274	A	C2-N3-C4	18.29	119.75	110.60
22	BA	501	A	C2-N3-C4	18.29	119.75	110.60
22	BA	2062	A	N1-C2-N3	-18.29	120.15	129.30
22	BA	1717	A	C2-N3-C4	18.29	119.75	110.60
1	AA	55	A	C2-N3-C4	18.29	119.75	110.60
1	AA	482	A	N1-C2-N3	-18.29	120.16	129.30
1	AA	673	A	N1-C6-N6	-18.29	107.63	118.60
22	BA	925	A	N1-C6-N6	-18.29	107.63	118.60
22	BA	2317	A	N1-C6-N6	-18.29	107.63	118.60
23	BB	46	A	C2-N3-C4	18.29	119.75	110.60
22	BA	156	A	N1-C2-N3	-18.29	120.16	129.30
22	BA	654	A	N1-C2-N3	-18.29	120.16	129.30
1	AA	790	A	C2-N3-C4	18.29	119.74	110.60
22	BA	1085	A	N1-C2-N3	-18.29	120.16	129.30
1	AA	71	A	N1-C6-N6	-18.28	107.63	118.60
1	AA	349	A	C2-N3-C4	18.28	119.74	110.60
23	BB	115	A	C2-N3-C4	18.28	119.74	110.60
1	AA	1410	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	626	A	N1-C2-N3	-18.28	120.16	129.30
1	AA	602	A	N1-C6-N6	-18.28	107.63	118.60
1	AA	968	A	N1-C6-N6	-18.28	107.63	118.60
1	AA	1042	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	1757	A	C2-N3-C4	18.28	119.74	110.60
22	BA	2541	A	N1-C2-N3	-18.28	120.16	129.30
1	AA	907	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	161	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	1275	A	N1-C6-N6	-18.28	107.63	118.60
22	BA	1413	A	C2-N3-C4	18.28	119.74	110.60
1	AA	270	A	N1-C6-N6	-18.28	107.64	118.60
22	BA	735	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	793	A	C2-N3-C4	18.27	119.74	110.60
22	BA	927	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	2176	A	N1-C6-N6	-18.27	107.64	118.60
1	AA	1169	A	N1-C2-N3	-18.27	120.16	129.30
22	BA	572	A	C2-N3-C4	18.27	119.73	110.60
22	BA	1532	A	N1-C6-N6	-18.27	107.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	46	A	N1-C2-N3	-18.27	120.17	129.30
1	AA	2	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	1632	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	2019	A	C2-N3-C4	18.27	119.73	110.60
22	BA	2108	A	C2-N3-C4	18.27	119.73	110.60
23	BB	115	A	N1-C6-N6	-18.27	107.64	118.60
1	AA	1105	A	N1-C6-N6	-18.26	107.64	118.60
22	BA	1046	A	N1-C6-N6	-18.26	107.64	118.60
22	BA	1551	A	N1-C2-N3	-18.26	120.17	129.30
22	BA	2346	A	N1-C2-N3	-18.26	120.17	129.30
1	AA	968	A	C2-N3-C4	18.26	119.73	110.60
22	BA	165	A	C2-N3-C4	18.26	119.73	110.60
22	BA	272	A	N1-C2-N3	-18.26	120.17	129.30
22	BA	582	A	N1-C2-N3	-18.26	120.17	129.30
22	BA	2727	A	N1-C2-N3	-18.26	120.17	129.30
1	AA	1332	A	N1-C6-N6	-18.26	107.64	118.60
22	BA	300	A	N1-C2-N3	-18.26	120.17	129.30
22	BA	344	A	N1-C2-N3	-18.26	120.17	129.30
1	AA	456	A	N1-C2-N3	-18.26	120.17	129.30
22	BA	2019	A	N1-C6-N6	-18.26	107.65	118.60
1	AA	161	A	C2-N3-C4	18.25	119.73	110.60
22	BA	945	A	N1-C2-N3	-18.25	120.17	129.30
22	BA	1439	A	N1-C2-N3	-18.25	120.17	129.30
22	BA	1626	A	N1-C6-N6	-18.25	107.65	118.60
22	BA	1801	A	C2-N3-C4	18.25	119.73	110.60
22	BA	2632	A	C2-N3-C4	18.25	119.73	110.60
22	BA	2738	A	N1-C2-N3	-18.25	120.17	129.30
1	AA	648	A	C2-N3-C4	18.25	119.72	110.60
1	AA	759	A	N1-C6-N6	-18.25	107.65	118.60
22	BA	1151	A	N1-C6-N6	-18.25	107.65	118.60
22	BA	1746	A	N1-C6-N6	-18.25	107.65	118.60
55	B8	21	A	N1-C6-N6	-18.25	107.65	118.60
22	BA	1502	A	N1-C2-N3	-18.25	120.17	129.30
22	BA	1586	A	C2-N3-C4	18.25	119.72	110.60
22	BA	457	A	C2-N3-C4	18.25	119.72	110.60
22	BA	599	A	C2-N3-C4	18.25	119.72	110.60
22	BA	1571	A	C2-N3-C4	18.25	119.72	110.60
1	AA	743	A	N1-C2-N3	-18.24	120.18	129.30
1	AA	161	A	N1-C6-N6	-18.24	107.66	118.60
22	BA	2031	A	C2-N3-C4	18.24	119.72	110.60
1	AA	78	A	C2-N3-C4	18.24	119.72	110.60
1	AA	676	A	N1-C2-N3	-18.24	120.18	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	718	A	C2-N3-C4	18.24	119.72	110.60
22	BA	21	A	N1-C6-N6	-18.24	107.66	118.60
22	BA	1871	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	2009	A	C2-N3-C4	18.24	119.72	110.60
22	BA	2482	A	C2-N3-C4	18.24	119.72	110.60
22	BA	2893	A	N1-C2-N3	-18.24	120.18	129.30
1	AA	759	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	1876	A	N1-C6-N6	-18.24	107.66	118.60
1	AA	182	A	C2-N3-C4	18.24	119.72	110.60
1	AA	1163	A	C2-N3-C4	18.24	119.72	110.60
22	BA	1580	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	1794	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	721	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	804	A	N1-C6-N6	-18.23	107.66	118.60
22	BA	1359	A	C2-N3-C4	18.23	119.72	110.60
22	BA	1664	A	N1-C6-N6	-18.23	107.66	118.60
22	BA	1672	A	C2-N3-C4	18.23	119.72	110.60
1	AA	814	A	N1-C2-N3	-18.23	120.18	129.30
22	BA	2273	A	N1-C6-N6	-18.23	107.66	118.60
23	BB	50	A	C2-N3-C4	18.23	119.72	110.60
1	AA	461	A	N1-C6-N6	-18.23	107.66	118.60
1	AA	1019	A	N1-C6-N6	-18.23	107.66	118.60
1	AA	1176	A	N1-C6-N6	-18.23	107.66	118.60
22	BA	457	A	N1-C6-N6	-18.23	107.66	118.60
22	BA	675	A	C2-N3-C4	18.23	119.72	110.60
22	BA	2211	A	C2-N3-C4	18.23	119.71	110.60
1	AA	1005	A	N1-C2-N3	-18.23	120.19	129.30
1	AA	1333	A	N1-C2-N3	-18.23	120.19	129.30
1	AA	181	A	N1-C6-N6	-18.23	107.67	118.60
22	BA	466	A	C2-N3-C4	18.23	119.71	110.60
22	BA	1717	A	N1-C6-N6	-18.22	107.67	118.60
1	AA	1318	A	N1-C6-N6	-18.22	107.67	118.60
22	BA	1014	A	N1-C2-N3	-18.22	120.19	129.30
1	AA	149	A	N1-C2-N3	-18.22	120.19	129.30
1	AA	1437	A	N1-C2-N3	-18.22	120.19	129.30
22	BA	661	A	N1-C6-N6	-18.22	107.67	118.60
22	BA	2734	A	C2-N3-C4	18.22	119.71	110.60
1	AA	768	A	N1-C2-N3	-18.22	120.19	129.30
1	AA	10	A	N1-C6-N6	-18.22	107.67	118.60
1	AA	366	A	N1-C2-N3	-18.22	120.19	129.30
1	AA	493	A	C2-N3-C4	18.22	119.71	110.60
1	AA	1483	A	N1-C2-N3	-18.22	120.19	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1342	A	N1-C6-N6	-18.22	107.67	118.60
22	BA	750	A	C2-N3-C4	18.21	119.71	110.60
22	BA	1286	A	N1-C6-N6	-18.21	107.67	118.60
22	BA	1711	A	N1-C6-N6	-18.21	107.67	118.60
22	BA	2117	A	N1-C6-N6	-18.21	107.67	118.60
1	AA	441	A	C2-N3-C4	18.21	119.70	110.60
22	BA	1039	A	C2-N3-C4	18.21	119.70	110.60
22	BA	1553	A	C2-N3-C4	18.21	119.70	110.60
22	BA	1276	A	N1-C2-N3	-18.21	120.20	129.30
22	BA	2478	A	C2-N3-C4	18.21	119.70	110.60
1	AA	1102	A	N1-C2-N3	-18.21	120.20	129.30
22	BA	95	A	N1-C6-N6	-18.21	107.68	118.60
22	BA	706	A	C2-N3-C4	18.21	119.70	110.60
1	AA	595	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	94	A	C2-N3-C4	18.20	119.70	110.60
22	BA	1050	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	1610	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	2469	A	C2-N3-C4	18.20	119.70	110.60
1	AA	1036	A	C2-N3-C4	18.20	119.70	110.60
22	BA	996	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	614	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	1853	A	C2-N3-C4	18.20	119.70	110.60
23	BB	46	A	N1-C6-N6	-18.20	107.68	118.60
1	AA	919	A	C2-N3-C4	18.20	119.70	110.60
22	BA	513	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	1952	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	2335	A	N1-C2-N3	-18.20	120.20	129.30
1	AA	621	A	N1-C6-N6	-18.19	107.68	118.60
1	AA	781	A	N1-C6-N6	-18.19	107.68	118.60
1	AA	949	A	N1-C2-N3	-18.19	120.20	129.30
22	BA	677	A	N1-C2-N3	-18.19	120.20	129.30
22	BA	1496	A	N1-C6-N6	-18.19	107.68	118.60
22	BA	172	A	C2-N3-C4	18.19	119.70	110.60
1	AA	502	A	N1-C6-N6	-18.19	107.69	118.60
22	BA	1866	A	N1-C2-N3	-18.19	120.20	129.30
1	AA	192	A	C2-N3-C4	18.19	119.69	110.60
22	BA	94	A	N1-C6-N6	-18.19	107.69	118.60
22	BA	1194	A	C2-N3-C4	18.19	119.69	110.60
23	BB	53	A	N1-C2-N3	-18.19	120.21	129.30
1	AA	309	A	C2-N3-C4	18.19	119.69	110.60
22	BA	2426	A	N1-C6-N6	-18.19	107.69	118.60
22	BA	497	A	N1-C2-N3	-18.18	120.21	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2434	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	1749	A	C2-N3-C4	18.18	119.69	110.60
22	BA	2287	A	C2-N3-C4	18.18	119.69	110.60
1	AA	228	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	146	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	751	A	C2-N3-C4	18.18	119.69	110.60
22	BA	753	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	1890	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	1134	A	C2-N3-C4	18.18	119.69	110.60
22	BA	2448	A	C2-N3-C4	18.18	119.69	110.60
1	AA	65	A	N1-C6-N6	-18.18	107.69	118.60
1	AA	274	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	1067	A	N1-C2-N3	-18.18	120.21	129.30
1	AA	913	A	C2-N3-C4	18.17	119.69	110.60
22	BA	730	A	N1-C6-N6	-18.17	107.70	118.60
22	BA	2826	A	N1-C6-N6	-18.17	107.70	118.60
1	AA	353	A	C2-N3-C4	18.17	119.69	110.60
23	BB	29	A	C2-N3-C4	18.17	119.69	110.60
22	BA	1494	A	N1-C6-N6	-18.17	107.70	118.60
1	AA	77	A	C2-N3-C4	18.17	119.68	110.60
22	BA	2513	A	N1-C2-N3	-18.17	120.22	129.30
22	BA	626	A	C2-N3-C4	18.16	119.68	110.60
1	AA	460	A	N1-C6-N6	-18.16	107.70	118.60
55	B8	69	A	N1-C6-N6	-18.16	107.70	118.60
1	AA	572	A	C2-N3-C4	18.16	119.68	110.60
1	AA	1117	A	C2-N3-C4	18.16	119.68	110.60
22	BA	19	A	N1-C6-N6	-18.16	107.70	118.60
22	BA	1347	A	N1-C6-N6	-18.16	107.70	118.60
22	BA	2412	A	C2-N3-C4	18.16	119.68	110.60
22	BA	2531	A	N1-C6-N6	-18.16	107.70	118.60
22	BA	1077	A	C2-N3-C4	18.16	119.68	110.60
1	AA	878	A	N1-C2-N3	-18.16	120.22	129.30
1	AA	1349	A	C2-N3-C4	18.16	119.68	110.60
22	BA	1928	A	C2-N3-C4	18.16	119.68	110.60
22	BA	2453	A	N1-C2-N3	-18.16	120.22	129.30
22	BA	2577	A	N1-C6-N6	-18.16	107.70	118.60
1	AA	1480	A	C2-N3-C4	18.16	119.68	110.60
22	BA	547	A	C2-N3-C4	18.16	119.68	110.60
22	BA	1020	A	N1-C2-N3	-18.16	120.22	129.30
22	BA	2856	A	C2-N3-C4	18.16	119.68	110.60
1	AA	274	A	C2-N3-C4	18.15	119.67	110.60
22	BA	1912	A	N1-C2-N3	-18.15	120.22	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1430	A	N1-C6-N6	-18.15	107.71	118.60
22	BA	1434	A	C2-N3-C4	18.15	119.67	110.60
22	BA	2565	A	N1-C2-N3	-18.15	120.22	129.30
22	BA	1590	A	N1-C6-N6	-18.15	107.71	118.60
22	BA	1877	A	N1-C2-N3	-18.15	120.23	129.30
22	BA	2411	A	N1-C2-N3	-18.15	120.23	129.30
1	AA	539	A	C2-N3-C4	18.14	119.67	110.60
1	AA	78	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	324	A	C2-N3-C4	18.14	119.67	110.60
22	BA	1274	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	1711	A	C2-N3-C4	18.14	119.67	110.60
1	AA	81	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	718	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	722	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	1586	A	N1-C6-N6	-18.14	107.72	118.60
1	AA	509	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	2212	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	2346	A	C2-N3-C4	18.14	119.67	110.60
1	AA	702	A	N1-C6-N6	-18.14	107.72	118.60
1	AA	747	A	C2-N3-C4	18.14	119.67	110.60
1	AA	983	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	1096	A	N1-C6-N6	-18.14	107.72	118.60
1	AA	465	A	N1-C2-N3	-18.13	120.23	129.30
1	AA	1493	A	C2-N3-C4	18.13	119.67	110.60
22	BA	2183	A	C2-N3-C4	18.13	119.67	110.60
1	AA	26	A	N1-C6-N6	-18.13	107.72	118.60
1	AA	695	A	C2-N3-C4	18.13	119.67	110.60
1	AA	1398	A	N1-C6-N6	-18.13	107.72	118.60
22	BA	173	A	N1-C6-N6	-18.13	107.72	118.60
22	BA	2600	A	C2-N3-C4	18.13	119.67	110.60
1	AA	1465	A	N1-C6-N6	-18.13	107.72	118.60
1	AA	802	A	N1-C2-N3	-18.13	120.24	129.30
1	AA	1513	A	N1-C2-N3	-18.13	120.24	129.30
22	BA	515	A	N1-C2-N3	-18.13	120.24	129.30
22	BA	1226	A	C2-N3-C4	18.13	119.66	110.60
22	BA	721	A	C2-N3-C4	18.12	119.66	110.60
1	AA	162	A	C2-N3-C4	18.12	119.66	110.60
1	AA	1362	A	N1-C6-N6	-18.12	107.73	118.60
1	AA	640	A	C2-N3-C4	18.12	119.66	110.60
22	BA	1021	A	N1-C2-N3	-18.12	120.24	129.30
1	AA	430	A	N1-C2-N3	-18.12	120.24	129.30
1	AA	502	A	N1-C2-N3	-18.12	120.24	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1456	A	N1-C6-N6	-18.12	107.73	118.60
22	BA	300	A	C2-N3-C4	18.12	119.66	110.60
22	BA	782	A	C2-N3-C4	18.12	119.66	110.60
22	BA	2051	A	N1-C6-N6	-18.12	107.73	118.60
22	BA	900	A	N1-C2-N3	-18.12	120.24	129.30
1	AA	937	A	N1-C2-N3	-18.12	120.24	129.30
22	BA	2639	A	C2-N3-C4	18.12	119.66	110.60
1	AA	397	A	N1-C2-N3	-18.11	120.24	129.30
22	BA	794	A	C2-N3-C4	18.11	119.66	110.60
22	BA	1010	A	C2-N3-C4	18.11	119.66	110.60
22	BA	1655	A	C2-N3-C4	18.11	119.66	110.60
22	BA	332	A	N1-C2-N3	-18.11	120.24	129.30
22	BA	1508	A	N1-C6-N6	-18.11	107.73	118.60
1	AA	1167	A	C2-N3-C4	18.11	119.66	110.60
22	BA	2700	A	N1-C2-N3	-18.11	120.24	129.30
1	AA	996	A	C2-N3-C4	18.11	119.66	110.60
1	AA	1256	A	N1-C2-N3	-18.11	120.25	129.30
1	AA	1329	A	C2-N3-C4	18.11	119.66	110.60
22	BA	1637	A	N1-C2-N3	-18.11	120.25	129.30
22	BA	2183	A	N1-C2-N3	-18.11	120.25	129.30
22	BA	2534	A	N1-C6-N6	-18.11	107.73	118.60
1	AA	860	A	C2-N3-C4	18.11	119.65	110.60
1	AA	1080	A	C2-N3-C4	18.11	119.65	110.60
1	AA	918	A	N1-C2-N3	-18.11	120.25	129.30
1	AA	938	A	N1-C2-N3	-18.11	120.25	129.30
22	BA	2171	A	N1-C6-N6	-18.10	107.74	118.60
22	BA	2461	A	N1-C2-N3	-18.10	120.25	129.30
1	AA	246	A	C2-N3-C4	18.10	119.65	110.60
1	AA	935	A	N1-C6-N6	-18.10	107.74	118.60
22	BA	1545	A	N1-C2-N3	-18.10	120.25	129.30
1	AA	958	A	N1-C6-N6	-18.10	107.74	118.60
1	AA	1396	A	C2-N3-C4	18.10	119.65	110.60
22	BA	599	A	N1-C2-N3	-18.10	120.25	129.30
1	AA	553	A	N1-C2-N3	-18.09	120.25	129.30
1	AA	1430	A	C2-N3-C4	18.09	119.65	110.60
22	BA	1603	A	N1-C6-N6	-18.09	107.74	118.60
22	BA	348	A	N1-C6-N6	-18.09	107.74	118.60
22	BA	2799	A	C2-N3-C4	18.09	119.65	110.60
1	AA	7	A	C2-N3-C4	18.09	119.65	110.60
1	AA	250	A	C2-N3-C4	18.09	119.65	110.60
22	BA	1746	A	C2-N3-C4	18.09	119.64	110.60
1	AA	274	A	N1-C6-N6	-18.09	107.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	73	A	N1-C2-N3	-18.09	120.26	129.30
22	BA	742	A	N1-C6-N6	-18.08	107.75	118.60
22	BA	609	A	N1-C2-N3	-18.08	120.26	129.30
22	BA	1304	A	N1-C6-N6	-18.08	107.75	118.60
22	BA	2158	A	C2-N3-C4	18.08	119.64	110.60
22	BA	14	A	N1-C6-N6	-18.08	107.75	118.60
22	BA	2639	A	N1-C2-N3	-18.08	120.26	129.30
22	BA	256	A	N1-C2-N3	-18.08	120.26	129.30
1	AA	1502	A	N1-C2-N3	-18.08	120.26	129.30
1	AA	1055	A	C2-N3-C4	18.07	119.64	110.60
22	BA	917	A	N1-C6-N6	-18.07	107.76	118.60
22	BA	1739	A	C2-N3-C4	18.07	119.64	110.60
1	AA	3	A	N1-C6-N6	-18.07	107.76	118.60
1	AA	120	A	N1-C2-N3	-18.07	120.27	129.30
1	AA	1433	A	N1-C2-N3	-18.07	120.27	129.30
22	BA	368	A	C2-N3-C4	18.07	119.63	110.60
22	BA	909	A	N1-C2-N3	-18.07	120.27	129.30
22	BA	1383	A	C2-N3-C4	18.07	119.63	110.60
1	AA	303	A	N1-C2-N3	-18.06	120.27	129.30
1	AA	329	A	N1-C6-N6	-18.06	107.76	118.60
1	AA	749	A	N1-C2-N3	-18.06	120.27	129.30
55	B8	38	A	N1-C2-N3	-18.06	120.27	129.30
1	AA	321	A	N1-C2-N3	-18.06	120.27	129.30
22	BA	279	A	C2-N3-C4	18.06	119.63	110.60
22	BA	344	A	C2-N3-C4	18.06	119.63	110.60
22	BA	6	A	N1-C6-N6	-18.06	107.77	118.60
22	BA	1027	A	N1-C2-N3	-18.06	120.27	129.30
22	BA	348	A	N1-C2-N3	-18.05	120.27	129.30
22	BA	1073	A	N1-C6-N6	-18.05	107.77	118.60
22	BA	1098	A	N1-C2-N3	-18.05	120.27	129.30
22	BA	2170	A	N1-C2-N3	-18.05	120.27	129.30
1	AA	495	A	N1-C2-N3	-18.05	120.28	129.30
1	AA	792	A	N1-C2-N3	-18.05	120.28	129.30
22	BA	2792	A	C2-N3-C4	18.05	119.62	110.60
22	BA	788	A	N1-C6-N6	-18.05	107.77	118.60
1	AA	189	A	N1-C2-N3	-18.04	120.28	129.30
1	AA	408	A	N1-C2-N3	-18.04	120.28	129.30
1	AA	162	A	N1-C2-N3	-18.04	120.28	129.30
1	AA	1252	A	C2-N3-C4	18.04	119.62	110.60
1	AA	1318	A	N1-C2-N3	-18.04	120.28	129.30
22	BA	1677	A	C2-N3-C4	18.04	119.62	110.60
22	BA	265	A	C2-N3-C4	18.04	119.62	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	19	A	N1-C2-N3	-18.04	120.28	129.30
22	BA	1494	A	C2-N3-C4	18.04	119.62	110.60
1	AA	174	A	N1-C2-N3	-18.03	120.28	129.30
1	AA	452	A	C2-N3-C4	18.03	119.62	110.60
1	AA	807	A	N1-C6-N6	-18.03	107.78	118.60
22	BA	1008	A	N1-C2-N3	-18.03	120.29	129.30
1	AA	878	A	C2-N3-C4	18.02	119.61	110.60
22	BA	382	A	N1-C6-N6	-18.02	107.78	118.60
55	B8	66	A	N1-C6-N6	-18.02	107.78	118.60
22	BA	655	A	C2-N3-C4	18.02	119.61	110.60
22	BA	1938	A	N1-C6-N6	-18.02	107.79	118.60
1	AA	101	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	64	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	2757	A	N1-C6-N6	-18.02	107.79	118.60
1	AA	959	A	N1-C6-N6	-18.02	107.79	118.60
22	BA	1286	A	C2-N3-C4	18.02	119.61	110.60
22	BA	1504	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	1598	A	N1-C6-N6	-18.02	107.79	118.60
22	BA	2281	A	N1-C6-N6	-18.02	107.79	118.60
22	BA	125	A	N1-C6-N6	-18.01	107.79	118.60
22	BA	492	A	N1-C6-N6	-18.01	107.79	118.60
22	BA	2270	A	N1-C2-N3	-18.01	120.29	129.30
1	AA	907	A	C2-N3-C4	18.01	119.61	110.60
22	BA	507	A	N1-C2-N3	-18.01	120.30	129.30
1	AA	873	A	N1-C2-N3	-18.01	120.30	129.30
1	AA	937	A	N1-C6-N6	-18.01	107.80	118.60
22	BA	1590	A	C2-N3-C4	18.01	119.60	110.60
22	BA	2274	A	N1-C2-N3	-18.01	120.30	129.30
22	BA	2675	A	C2-N3-C4	18.01	119.60	110.60
1	AA	109	A	C2-N3-C4	18.01	119.60	110.60
1	AA	253	A	C2-N3-C4	18.01	119.60	110.60
1	AA	1146	A	C2-N3-C4	18.00	119.60	110.60
22	BA	144	A	N1-C2-N3	-18.00	120.30	129.30
22	BA	14	A	C2-N3-C4	18.00	119.60	110.60
22	BA	1610	A	C2-N3-C4	18.00	119.60	110.60
1	AA	1503	A	C2-N3-C4	18.00	119.60	110.60
22	BA	204	A	N1-C6-N6	-18.00	107.80	118.60
1	AA	696	A	C2-N3-C4	18.00	119.60	110.60
1	AA	1252	A	N1-C2-N3	-18.00	120.30	129.30
22	BA	928	A	N1-C2-N3	-18.00	120.30	129.30
22	BA	973	A	C2-N3-C4	18.00	119.60	110.60
23	BB	45	A	N1-C2-N3	-18.00	120.30	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	197	A	N1-C6-N6	-18.00	107.80	118.60
22	BA	1241	A	N1-C2-N3	-18.00	120.30	129.30
1	AA	1012	A	N1-C2-N3	-18.00	120.30	129.30
1	AA	1447	A	C2-N3-C4	18.00	119.60	110.60
22	BA	928	A	C2-N3-C4	17.99	119.60	110.60
22	BA	1848	A	C2-N3-C4	17.99	119.60	110.60
22	BA	2412	A	N1-C6-N6	-17.99	107.80	118.60
1	AA	815	A	N1-C6-N6	-17.99	107.81	118.60
22	BA	2660	A	N1-C2-N3	-17.99	120.30	129.30
1	AA	66	A	C2-N3-C4	17.99	119.59	110.60
22	BA	52	A	C2-N3-C4	17.99	119.59	110.60
1	AA	223	A	N1-C2-N3	-17.99	120.31	129.30
22	BA	1244	A	N1-C6-N6	-17.99	107.81	118.60
22	BA	1427	A	N1-C6-N6	-17.98	107.81	118.60
22	BA	1505	A	N1-C6-N6	-17.98	107.81	118.60
23	BB	78	A	C2-N3-C4	17.98	119.59	110.60
1	AA	1299	A	C2-N3-C4	17.98	119.59	110.60
22	BA	1916	A	N1-C6-N6	-17.98	107.81	118.60
1	AA	199	A	N1-C6-N6	-17.98	107.81	118.60
22	BA	255	A	N1-C2-N3	-17.98	120.31	129.30
22	BA	2170	A	C2-N3-C4	17.98	119.59	110.60
1	AA	729	A	N1-C2-N3	-17.98	120.31	129.30
1	AA	1394	A	C2-N3-C4	17.98	119.59	110.60
22	BA	2117	A	N1-C2-N3	-17.98	120.31	129.30
1	AA	900	A	N1-C6-N6	-17.98	107.81	118.60
22	BA	1871	A	C2-N3-C4	17.98	119.59	110.60
1	AA	687	A	N1-C2-N3	-17.97	120.31	129.30
1	AA	1246	A	N1-C2-N3	-17.97	120.31	129.30
22	BA	2530	A	C2-N3-C4	17.97	119.59	110.60
1	AA	969	A	N1-C6-N6	-17.97	107.82	118.60
22	BA	278	A	N1-C2-N3	-17.97	120.31	129.30
22	BA	1754	A	C2-N3-C4	17.97	119.59	110.60
1	AA	1503	A	N1-C6-N6	-17.97	107.82	118.60
22	BA	430	A	C2-N3-C4	17.97	119.58	110.60
23	BB	53	A	N1-C6-N6	-17.97	107.82	118.60
55	B8	41	A	N1-C6-N6	-17.97	107.82	118.60
22	BA	2635	A	N1-C6-N6	-17.97	107.82	118.60
55	B8	6	A	C2-N3-C4	17.96	119.58	110.60
22	BA	1745	A	N1-C6-N6	-17.96	107.82	118.60
1	AA	1377	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	751	A	N1-C6-N6	-17.96	107.82	118.60
1	AA	364	A	N1-C2-N3	-17.96	120.32	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1492	A	N1-C6-N6	-17.96	107.82	118.60
22	BA	1009	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	1089	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	233	A	C2-N3-C4	17.96	119.58	110.60
1	AA	179	A	N1-C2-N3	-17.96	120.32	129.30
1	AA	1246	A	C2-N3-C4	17.96	119.58	110.60
1	AA	1447	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	391	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	1134	A	N1-C2-N3	-17.95	120.32	129.30
22	BA	2287	A	N1-C6-N6	-17.95	107.83	118.60
22	BA	1634	A	C2-N3-C4	17.95	119.57	110.60
22	BA	1885	A	N1-C2-N3	-17.95	120.33	129.30
1	AA	1311	A	N1-C6-N6	-17.95	107.83	118.60
1	AA	1374	A	N1-C6-N6	-17.95	107.83	118.60
22	BA	42	A	C2-N3-C4	17.95	119.57	110.60
22	BA	1098	A	N1-C6-N6	-17.95	107.83	118.60
22	BA	1254	A	N1-C6-N6	-17.95	107.83	118.60
22	BA	1275	A	N1-C2-N3	-17.95	120.33	129.30
22	BA	590	A	N1-C6-N6	-17.95	107.83	118.60
1	AA	16	A	C2-N3-C4	17.94	119.57	110.60
22	BA	155	A	N1-C6-N6	-17.94	107.83	118.60
22	BA	983	A	C2-N3-C4	17.94	119.57	110.60
22	BA	2031	A	N1-C2-N3	-17.94	120.33	129.30
23	BB	39	A	N1-C2-N3	-17.94	120.33	129.30
1	AA	923	A	N1-C6-N6	-17.94	107.83	118.60
22	BA	1912	A	C2-N3-C4	17.94	119.57	110.60
1	AA	143	A	C2-N3-C4	17.94	119.57	110.60
1	AA	263	A	N1-C6-N6	-17.94	107.84	118.60
1	AA	532	A	N1-C6-N6	-17.94	107.83	118.60
22	BA	1705	A	N1-C2-N3	-17.94	120.33	129.30
22	BA	1359	A	N1-C2-N3	-17.94	120.33	129.30
1	AA	1274	A	N1-C6-N6	-17.94	107.84	118.60
22	BA	2700	A	C2-N3-C4	17.94	119.57	110.60
22	BA	1603	A	N1-C2-N3	-17.93	120.33	129.30
22	BA	2082	A	N1-C2-N3	-17.93	120.33	129.30
22	BA	2468	A	N1-C6-N6	-17.93	107.84	118.60
22	BA	454	A	N1-C6-N6	-17.93	107.84	118.60
22	BA	2358	A	C2-N3-C4	17.93	119.57	110.60
55	B8	59	A	N1-C6-N6	-17.93	107.84	118.60
22	BA	1616	A	C2-N3-C4	17.93	119.57	110.60
22	BA	1111	A	N1-C2-N3	-17.93	120.34	129.30
22	BA	1981	A	N1-C2-N3	-17.93	120.34	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	975	A	N1-C2-N3	-17.93	120.34	129.30
1	AA	1000	A	N1-C6-N6	-17.93	107.84	118.60
1	AA	642	A	N1-C2-N3	-17.92	120.34	129.30
1	AA	712	A	N1-C6-N6	-17.92	107.85	118.60
1	AA	1130	A	C2-N3-C4	17.92	119.56	110.60
22	BA	2757	A	N1-C2-N3	-17.92	120.34	129.30
22	BA	1819	A	N1-C2-N3	-17.92	120.34	129.30
22	BA	2114	A	N1-C2-N3	-17.92	120.34	129.30
22	BA	2860	A	N1-C2-N3	-17.92	120.34	129.30
22	BA	2547	A	N1-C2-N3	-17.92	120.34	129.30
1	AA	298	A	N1-C6-N6	-17.91	107.85	118.60
22	BA	2654	A	C2-N3-C4	17.91	119.56	110.60
22	BA	1029	A	N1-C2-N3	-17.91	120.34	129.30
1	AA	143	A	N1-C6-N6	-17.91	107.85	118.60
1	AA	495	A	C2-N3-C4	17.91	119.56	110.60
22	BA	603	A	C2-N3-C4	17.91	119.55	110.60
1	AA	749	A	N1-C6-N6	-17.91	107.86	118.60
22	BA	2821	A	N1-C6-N6	-17.91	107.86	118.60
22	BA	1383	A	N1-C2-N3	-17.90	120.35	129.30
1	AA	300	A	C2-N3-C4	17.90	119.55	110.60
1	AA	1146	A	N1-C2-N3	-17.90	120.35	129.30
22	BA	844	A	C2-N3-C4	17.90	119.55	110.60
22	BA	2860	A	C2-N3-C4	17.90	119.55	110.60
22	BA	668	A	C2-N3-C4	17.90	119.55	110.60
22	BA	2614	A	C2-N3-C4	17.90	119.55	110.60
22	BA	2883	A	C2-N3-C4	17.90	119.55	110.60
1	AA	55	A	N1-C6-N6	-17.90	107.86	118.60
22	BA	936	A	N1-C2-N3	-17.90	120.35	129.30
1	AA	706	A	N1-C6-N6	-17.89	107.86	118.60
1	AA	196	A	C2-N3-C4	17.89	119.55	110.60
1	AA	914	A	C2-N3-C4	17.89	119.55	110.60
1	AA	1375	A	C2-N3-C4	17.89	119.55	110.60
22	BA	221	A	C2-N3-C4	17.89	119.54	110.60
22	BA	371	A	N1-C2-N3	-17.89	120.36	129.30
22	BA	2212	A	C2-N3-C4	17.89	119.54	110.60
1	AA	44	A	C2-N3-C4	17.89	119.54	110.60
22	BA	526	A	C2-N3-C4	17.89	119.54	110.60
23	BB	94	A	C2-N3-C4	17.89	119.54	110.60
1	AA	77	A	N1-C2-N3	-17.88	120.36	129.30
22	BA	265	A	N1-C6-N6	-17.88	107.87	118.60
22	BA	608	A	N1-C6-N6	-17.88	107.87	118.60
1	AA	435	A	N1-C6-N6	-17.88	107.87	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1476	A	N1-C2-N3	-17.88	120.36	129.30
22	BA	2856	A	N1-C2-N3	-17.88	120.36	129.30
1	AA	908	A	N1-C2-N3	-17.88	120.36	129.30
22	BA	1969	A	N1-C2-N3	-17.88	120.36	129.30
22	BA	781	A	C2-N3-C4	17.88	119.54	110.60
22	BA	127	A	C2-N3-C4	17.87	119.54	110.60
1	AA	573	A	C2-N3-C4	17.87	119.53	110.60
1	AA	60	A	C2-N3-C4	17.87	119.53	110.60
22	BA	1553	A	N1-C2-N3	-17.87	120.37	129.30
22	BA	1676	A	C2-N3-C4	17.86	119.53	110.60
1	AA	71	A	C2-N3-C4	17.86	119.53	110.60
22	BA	1008	A	C2-N3-C4	17.86	119.53	110.60
22	BA	1801	A	N1-C2-N3	-17.86	120.37	129.30
1	AA	716	A	N1-C6-N6	-17.86	107.89	118.60
22	BA	1495	A	N1-C6-N6	-17.86	107.89	118.60
22	BA	432	A	C2-N3-C4	17.85	119.53	110.60
22	BA	788	A	C2-N3-C4	17.85	119.53	110.60
22	BA	1848	A	N1-C2-N3	-17.85	120.37	129.30
1	AA	520	A	C2-N3-C4	17.85	119.53	110.60
22	BA	256	A	C2-N3-C4	17.85	119.53	110.60
22	BA	1932	A	N1-C2-N3	-17.85	120.38	129.30
1	AA	60	A	N1-C2-N3	-17.85	120.38	129.30
22	BA	715	A	N1-C2-N3	-17.85	120.38	129.30
22	BA	1084	A	N1-C2-N3	-17.85	120.38	129.30
22	BA	661	A	N1-C2-N3	-17.84	120.38	129.30
1	AA	1130	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	1151	A	C2-N3-C4	17.84	119.52	110.60
22	BA	244	A	C2-N3-C4	17.84	119.52	110.60
22	BA	1744	A	N1-C2-N3	-17.84	120.38	129.30
1	AA	975	A	C2-N3-C4	17.84	119.52	110.60
1	AA	1332	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	1713	A	N1-C6-N6	-17.83	107.90	118.60
22	BA	2800	A	C2-N3-C4	17.83	119.52	110.60
1	AA	640	A	N1-C6-N6	-17.83	107.90	118.60
1	AA	1227	A	C2-N3-C4	17.83	119.52	110.60
1	AA	1269	A	C2-N3-C4	17.83	119.52	110.60
22	BA	447	A	C2-N3-C4	17.83	119.52	110.60
22	BA	2600	A	N1-C2-N3	-17.83	120.39	129.30
1	AA	1275	A	N1-C6-N6	-17.83	107.90	118.60
22	BA	1525	A	N1-C2-N3	-17.83	120.39	129.30
1	AA	983	A	N1-C6-N6	-17.83	107.91	118.60
1	AA	1418	A	N1-C2-N3	-17.83	120.39	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1678	A	C2-N3-C4	17.83	119.51	110.60
22	BA	227	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	1088	A	N1-C2-N3	-17.82	120.39	129.30
1	AA	1150	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	218	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	227	A	C2-N3-C4	17.82	119.51	110.60
22	BA	412	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	1494	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	1802	A	C2-N3-C4	17.82	119.51	110.60
22	BA	716	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	2158	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	279	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	1634	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	1773	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	2711	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	83	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	352	A	C2-N3-C4	17.82	119.51	110.60
22	BA	1791	A	N1-C6-N6	-17.82	107.91	118.60
1	AA	1306	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	1175	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	432	A	N1-C6-N6	-17.81	107.91	118.60
1	AA	1191	A	N1-C6-N6	-17.81	107.91	118.60
22	BA	804	A	C2-N3-C4	17.81	119.51	110.60
1	AA	482	A	N1-C6-N6	-17.81	107.91	118.60
22	BA	2392	A	C2-N3-C4	17.81	119.51	110.60
55	B8	26	A	N1-C2-N3	-17.81	120.40	129.30
22	BA	1614	A	C2-N3-C4	17.81	119.50	110.60
1	AA	1151	A	N1-C2-N3	-17.80	120.40	129.30
22	BA	262	A	N1-C2-N3	-17.80	120.40	129.30
22	BA	2531	A	C2-N3-C4	17.80	119.50	110.60
1	AA	53	A	N1-C6-N6	-17.80	107.92	118.60
55	B8	26	A	N1-C6-N6	-17.80	107.92	118.60
1	AA	1196	A	N1-C6-N6	-17.80	107.92	118.60
1	AA	1239	A	C2-N3-C4	17.80	119.50	110.60
1	AA	767	A	C2-N3-C4	17.80	119.50	110.60
1	AA	441	A	N1-C2-N3	-17.80	120.40	129.30
22	BA	1609	A	N1-C6-N6	-17.80	107.92	118.60
1	AA	1055	A	N1-C2-N3	-17.79	120.40	129.30
1	AA	1324	A	N1-C2-N3	-17.79	120.40	129.30
22	BA	910	A	N1-C6-N6	-17.79	107.92	118.60
22	BA	1387	A	N1-C2-N3	-17.79	120.40	129.30
1	AA	1254	A	N1-C6-N6	-17.79	107.92	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	541	A	N1-C2-N3	-17.79	120.41	129.30
1	AA	236	A	N1-C2-N3	-17.79	120.41	129.30
1	AA	1201	A	N1-C2-N3	-17.79	120.41	129.30
22	BA	2439	A	N1-C6-N6	-17.79	107.93	118.60
1	AA	831	A	C2-N3-C4	17.79	119.49	110.60
22	BA	182	A	N1-C2-N3	-17.79	120.41	129.30
22	BA	821	A	C2-N3-C4	17.79	119.49	110.60
22	BA	165	A	N1-C2-N3	-17.78	120.41	129.30
22	BA	1866	A	C2-N3-C4	17.78	119.49	110.60
1	AA	901	A	N1-C2-N3	-17.78	120.41	129.30
1	AA	1394	A	N1-C2-N3	-17.78	120.41	129.30
22	BA	2738	A	C2-N3-C4	17.78	119.49	110.60
22	BA	1571	A	N1-C6-N6	-17.78	107.93	118.60
22	BA	515	A	C2-N3-C4	17.78	119.49	110.60
22	BA	2872	A	C2-N3-C4	17.78	119.49	110.60
1	AA	635	A	N1-C2-N3	-17.77	120.41	129.30
22	BA	1502	A	N1-C6-N6	-17.77	107.94	118.60
1	AA	1363	A	N1-C2-N3	-17.77	120.41	129.30
22	BA	1080	A	N1-C6-N6	-17.77	107.94	118.60
22	BA	2317	A	N1-C2-N3	-17.77	120.42	129.30
1	AA	288	A	N1-C2-N3	-17.77	120.42	129.30
1	AA	353	A	N1-C2-N3	-17.77	120.42	129.30
1	AA	607	A	N1-C6-N6	-17.77	107.94	118.60
22	BA	2191	A	N1-C6-N6	-17.77	107.94	118.60
22	BA	821	A	N1-C2-N3	-17.76	120.42	129.30
22	BA	2376	A	N1-C6-N6	-17.76	107.94	118.60
1	AA	415	A	N1-C2-N3	-17.76	120.42	129.30
22	BA	547	A	N1-C2-N3	-17.76	120.42	129.30
22	BA	1264	A	C2-N3-C4	17.76	119.48	110.60
22	BA	1735	A	N1-C2-N3	-17.76	120.42	129.30
22	BA	1392	A	N1-C6-N6	-17.76	107.95	118.60
1	AA	635	A	N1-C6-N6	-17.75	107.95	118.60
1	AA	1216	A	C2-N3-C4	17.75	119.47	110.60
22	BA	28	A	C2-N3-C4	17.75	119.47	110.60
22	BA	1689	A	C2-N3-C4	17.75	119.47	110.60
22	BA	2459	A	N1-C2-N3	-17.75	120.42	129.30
22	BA	428	A	C2-N3-C4	17.75	119.47	110.60
22	BA	1754	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	789	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	2225	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	1808	A	C2-N3-C4	17.74	119.47	110.60
22	BA	2171	A	N1-C2-N3	-17.74	120.43	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	21	A	N1-C2-N3	-17.74	120.43	129.30
22	BA	2333	A	C2-N3-C4	17.74	119.47	110.60
22	BA	502	A	N1-C6-N6	-17.74	107.96	118.60
22	BA	718	A	N1-C6-N6	-17.74	107.96	118.60
22	BA	734	A	C2-N3-C4	17.74	119.47	110.60
22	BA	1395	A	N1-C2-N3	-17.74	120.43	129.30
1	AA	1022	A	N1-C6-N6	-17.73	107.96	118.60
1	AA	1360	A	C2-N3-C4	17.73	119.47	110.60
22	BA	793	A	N1-C6-N6	-17.73	107.96	118.60
22	BA	1652	A	N1-C2-N3	-17.73	120.43	129.30
22	BA	1998	A	N1-C2-N3	-17.73	120.43	129.30
22	BA	391	A	N1-C6-N6	-17.73	107.96	118.60
22	BA	2530	A	N1-C6-N6	-17.73	107.96	118.60
22	BA	294	A	C2-N3-C4	17.73	119.46	110.60
22	BA	480	A	N1-C6-N6	-17.73	107.97	118.60
22	BA	1014	A	C2-N3-C4	17.73	119.46	110.60
22	BA	1321	A	N1-C6-N6	-17.73	107.97	118.60
1	AA	78	A	N1-C6-N6	-17.72	107.97	118.60
1	AA	554	A	C2-N3-C4	17.72	119.46	110.60
22	BA	190	A	N1-C6-N6	-17.72	107.97	118.60
22	BA	1302	A	N1-C6-N6	-17.72	107.97	118.60
22	BA	2814	A	C2-N3-C4	17.72	119.46	110.60
1	AA	411	A	N1-C6-N6	-17.71	107.97	118.60
1	AA	608	A	N1-C6-N6	-17.71	107.97	118.60
22	BA	1591	A	N1-C2-N3	-17.71	120.44	129.30
22	BA	1502	A	C2-N3-C4	17.71	119.45	110.60
22	BA	478	A	N1-C6-N6	-17.71	107.98	118.60
22	BA	705	A	C2-N3-C4	17.71	119.45	110.60
22	BA	2015	A	C2-N3-C4	17.71	119.45	110.60
1	AA	53	A	C2-N3-C4	17.70	119.45	110.60
1	AA	81	A	N1-C2-N3	-17.70	120.45	129.30
1	AA	1476	A	C2-N3-C4	17.70	119.45	110.60
22	BA	2886	A	N1-C6-N6	-17.70	107.98	118.60
1	AA	315	A	C2-N3-C4	17.70	119.45	110.60
1	AA	510	A	C2-N3-C4	17.70	119.45	110.60
1	AA	663	A	N1-C2-N3	-17.70	120.45	129.30
1	AA	1429	A	N1-C6-N6	-17.70	107.98	118.60
1	AA	1227	A	N1-C6-N6	-17.70	107.98	118.60
1	AA	1163	A	N1-C2-N3	-17.70	120.45	129.30
22	BA	2054	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	71	A	N1-C2-N3	-17.69	120.45	129.30
22	BA	1103	A	N1-C6-N6	-17.69	107.98	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1566	A	N1-C6-N6	-17.69	107.98	118.60
1	AA	1081	A	N1-C2-N3	-17.69	120.45	129.30
22	BA	2322	A	N1-C2-N3	-17.69	120.45	129.30
22	BA	2814	A	N1-C2-N3	-17.69	120.45	129.30
22	BA	2126	A	N1-C6-N6	-17.69	107.99	118.60
1	AA	1502	A	C2-N3-C4	17.69	119.44	110.60
22	BA	1433	A	N1-C2-N3	-17.68	120.46	129.30
22	BA	203	A	C2-N3-C4	17.68	119.44	110.60
22	BA	689	A	N1-C6-N6	-17.68	107.99	118.60
22	BA	449	A	N1-C2-N3	-17.68	120.46	129.30
22	BA	1808	A	N1-C2-N3	-17.68	120.46	129.30
22	BA	191	A	N1-C6-N6	-17.67	108.00	118.60
22	BA	706	A	N1-C2-N3	-17.67	120.46	129.30
22	BA	13	A	N1-C2-N3	-17.67	120.46	129.30
22	BA	2060	A	N1-C6-N6	-17.66	108.00	118.60
22	BA	1608	A	N1-C2-N3	-17.66	120.47	129.30
55	B8	6	A	N1-C2-N3	-17.66	120.47	129.30
1	AA	696	A	N1-C2-N3	-17.66	120.47	129.30
22	BA	750	A	N1-C2-N3	-17.66	120.47	129.30
22	BA	1759	A	N1-C6-N6	-17.66	108.00	118.60
55	B8	42	A	N1-C6-N6	-17.66	108.00	118.60
1	AA	109	A	N1-C2-N3	-17.66	120.47	129.30
22	BA	14	A	N1-C2-N3	-17.66	120.47	129.30
22	BA	2679	A	C2-N3-C4	17.66	119.43	110.60
1	AA	787	A	N1-C6-N6	-17.66	108.01	118.60
22	BA	1001	A	C2-N3-C4	17.66	119.43	110.60
22	BA	1433	A	C2-N3-C4	17.65	119.43	110.60
22	BA	505	A	C2-N3-C4	17.65	119.43	110.60
22	BA	347	A	N1-C2-N3	-17.65	120.47	129.30
22	BA	477	A	C2-N3-C4	17.65	119.42	110.60
22	BA	1373	A	N1-C2-N3	-17.64	120.48	129.30
23	BB	58	A	N1-C2-N3	-17.64	120.48	129.30
22	BA	1265	A	N1-C6-N6	-17.64	108.02	118.60
22	BA	1387	A	N1-C6-N6	-17.64	108.02	118.60
22	BA	352	A	N1-C2-N3	-17.64	120.48	129.30
23	BB	58	A	N1-C6-N6	-17.64	108.02	118.60
1	AA	938	A	N1-C6-N6	-17.64	108.02	118.60
22	BA	1169	A	N1-C6-N6	-17.64	108.02	118.60
22	BA	1586	A	N1-C2-N3	-17.64	120.48	129.30
1	AA	1081	A	N1-C6-N6	-17.64	108.02	118.60
22	BA	1272	A	N1-C2-N3	-17.64	120.48	129.30
22	BA	2432	A	N1-C6-N6	-17.64	108.02	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	780	A	C2-N3-C4	17.63	119.42	110.60
22	BA	1143	A	C2-N3-C4	17.63	119.42	110.60
22	BA	1953	A	N1-C6-N6	-17.63	108.02	118.60
22	BA	2598	A	C2-N3-C4	17.63	119.42	110.60
22	BA	2721	A	N1-C2-N3	-17.62	120.49	129.30
22	BA	1735	A	C2-N3-C4	17.62	119.41	110.60
1	AA	1299	A	N1-C6-N6	-17.62	108.03	118.60
22	BA	1384	A	N1-C2-N3	-17.62	120.49	129.30
1	AA	878	A	N1-C6-N6	-17.61	108.03	118.60
1	AA	1188	A	C2-N3-C4	17.61	119.41	110.60
22	BA	2090	A	N1-C6-N6	-17.61	108.03	118.60
1	AA	250	A	N1-C6-N6	-17.61	108.03	118.60
1	AA	1216	A	N1-C6-N6	-17.61	108.03	118.60
1	AA	1483	A	C2-N3-C4	17.61	119.40	110.60
1	AA	1111	A	N1-C6-N6	-17.61	108.03	118.60
22	BA	1156	A	N1-C6-N6	-17.61	108.03	118.60
22	BA	909	A	N1-C6-N6	-17.61	108.04	118.60
1	AA	563	A	N1-C2-N3	-17.61	120.50	129.30
1	AA	539	A	N1-C6-N6	-17.60	108.04	118.60
1	AA	1171	A	N1-C2-N3	-17.60	120.50	129.30
22	BA	2879	A	N1-C6-N6	-17.60	108.04	118.60
1	AA	560	A	N1-C6-N6	-17.60	108.04	118.60
22	BA	49	A	N1-C2-N3	-17.60	120.50	129.30
22	BA	988	A	C2-N3-C4	17.60	119.40	110.60
1	AA	784	A	N1-C6-N6	-17.59	108.04	118.60
22	BA	477	A	N1-C6-N6	-17.59	108.04	118.60
22	BA	279	A	N1-C6-N6	-17.59	108.05	118.60
22	BA	2014	A	C2-N3-C4	17.59	119.39	110.60
1	AA	459	A	C2-N3-C4	17.58	119.39	110.60
1	AA	1238	A	N1-C2-N3	-17.58	120.51	129.30
22	BA	233	A	N1-C2-N3	-17.58	120.51	129.30
1	AA	1197	A	N1-C6-N6	-17.58	108.05	118.60
22	BA	1548	A	N1-C6-N6	-17.58	108.05	118.60
22	BA	2799	A	N1-C2-N3	-17.58	120.51	129.30
1	AA	573	A	N1-C6-N6	-17.58	108.05	118.60
1	AA	487	A	N1-C6-N6	-17.57	108.06	118.60
1	AA	510	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	222	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	227	A	N1-C2-N3	-17.57	120.51	129.30
22	BA	251	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	2108	A	N1-C2-N3	-17.57	120.52	129.30
22	BA	176	A	N1-C6-N6	-17.57	108.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1610	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	2059	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	2392	A	N1-C2-N3	-17.57	120.52	129.30
1	AA	1318	A	C2-N3-C4	17.56	119.38	110.60
22	BA	633	A	C2-N3-C4	17.56	119.38	110.60
1	AA	831	A	N1-C2-N3	-17.56	120.52	129.30
22	BA	1143	A	N1-C2-N3	-17.56	120.52	129.30
22	BA	1634	A	N1-C6-N6	-17.56	108.06	118.60
1	AA	155	A	N1-C6-N6	-17.56	108.06	118.60
1	AA	279	A	C2-N3-C4	17.56	119.38	110.60
22	BA	1230	A	N1-C2-N3	-17.56	120.52	129.30
1	AA	80	A	C2-N3-C4	17.56	119.38	110.60
22	BA	1722	A	C2-N3-C4	17.56	119.38	110.60
1	AA	356	A	N1-C6-N6	-17.56	108.07	118.60
1	AA	994	A	N1-C6-N6	-17.55	108.07	118.60
22	BA	1284	A	C2-N3-C4	17.55	119.38	110.60
1	AA	780	A	N1-C2-N3	-17.55	120.52	129.30
1	AA	1465	A	N1-C2-N3	-17.55	120.53	129.30
1	AA	1493	A	N1-C6-N6	-17.55	108.07	118.60
22	BA	1872	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	2434	A	C2-N3-C4	17.54	119.37	110.60
1	AA	151	A	N1-C6-N6	-17.54	108.07	118.60
22	BA	2378	A	N1-C6-N6	-17.54	108.08	118.60
1	AA	663	A	C2-N3-C4	17.54	119.37	110.60
1	AA	59	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	52	A	N1-C2-N3	-17.54	120.53	129.30
22	BA	94	A	N1-C2-N3	-17.53	120.53	129.30
22	BA	2058	A	N1-C6-N6	-17.53	108.08	118.60
1	AA	1332	A	C2-N3-C4	17.53	119.36	110.60
22	BA	2412	A	N1-C2-N3	-17.53	120.53	129.30
1	AA	974	A	C2-N3-C4	17.53	119.36	110.60
1	AA	1418	A	N1-C6-N6	-17.53	108.08	118.60
22	BA	2097	A	N1-C2-N3	-17.53	120.54	129.30
22	BA	1853	A	N1-C6-N6	-17.53	108.08	118.60
22	BA	429	A	C2-N3-C4	17.52	119.36	110.60
22	BA	1757	A	N1-C6-N6	-17.52	108.08	118.60
55	B8	14	A	N1-C2-N3	-17.52	120.54	129.30
22	BA	833	A	N1-C6-N6	-17.52	108.09	118.60
22	BA	2461	A	N1-C6-N6	-17.52	108.09	118.60
22	BA	2820	A	C2-N3-C4	17.52	119.36	110.60
1	AA	192	A	N1-C6-N6	-17.52	108.09	118.60
23	BB	58	A	C2-N3-C4	17.52	119.36	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2377	A	N1-C6-N6	-17.51	108.09	118.60
1	AA	1111	A	C2-N3-C4	17.51	119.36	110.60
1	AA	279	A	N1-C6-N6	-17.51	108.09	118.60
1	AA	1339	A	N1-C2-N3	-17.51	120.55	129.30
22	BA	996	A	N1-C2-N3	-17.51	120.55	129.30
1	AA	139	A	N1-C2-N3	-17.51	120.55	129.30
22	BA	1746	A	N1-C2-N3	-17.51	120.55	129.30
1	AA	1082	A	N1-C6-N6	-17.51	108.10	118.60
22	BA	750	A	N1-C6-N6	-17.50	108.10	118.60
22	BA	1593	A	N1-C6-N6	-17.50	108.10	118.60
1	AA	1046	A	N1-C2-N3	-17.50	120.55	129.30
22	BA	497	A	C2-N3-C4	17.50	119.35	110.60
22	BA	156	A	N1-C6-N6	-17.50	108.10	118.60
22	BA	2893	A	C2-N3-C4	17.50	119.35	110.60
22	BA	1700	A	N1-C2-N3	-17.49	120.55	129.30
1	AA	116	A	N1-C6-N6	-17.49	108.11	118.60
22	BA	167	A	N1-C2-N3	-17.49	120.55	129.30
1	AA	190	A	N1-C2-N3	-17.49	120.56	129.30
22	BA	2154	A	N1-C6-N6	-17.49	108.11	118.60
22	BA	2340	A	N1-C2-N3	-17.49	120.56	129.30
22	BA	2850	A	N1-C6-N6	-17.49	108.11	118.60
22	BA	430	A	N1-C2-N3	-17.49	120.56	129.30
22	BA	1144	A	N1-C6-N6	-17.48	108.11	118.60
22	BA	1230	A	C2-N3-C4	17.48	119.34	110.60
22	BA	1773	A	N1-C6-N6	-17.48	108.11	118.60
55	B8	51	A	N1-C6-N6	-17.48	108.11	118.60
1	AA	1257	A	N1-C6-N6	-17.48	108.11	118.60
1	AA	630	A	N1-C6-N6	-17.48	108.11	118.60
1	AA	831	A	N1-C6-N6	-17.48	108.11	118.60
22	BA	1403	A	N1-C2-N3	-17.48	120.56	129.30
22	BA	1545	A	C2-N3-C4	17.48	119.34	110.60
22	BA	2634	A	N1-C2-N3	-17.48	120.56	129.30
22	BA	2590	A	C2-N3-C4	17.47	119.34	110.60
22	BA	2062	A	C2-N3-C4	17.47	119.33	110.60
1	AA	371	A	N1-C6-N6	-17.47	108.12	118.60
22	BA	1580	A	C2-N3-C4	17.46	119.33	110.60
1	AA	238	A	N1-C2-N3	-17.46	120.57	129.30
1	AA	746	A	N1-C2-N3	-17.46	120.57	129.30
1	AA	860	A	N1-C2-N3	-17.45	120.57	129.30
1	AA	1357	A	N1-C2-N3	-17.45	120.57	129.30
22	BA	761	A	C2-N3-C4	17.45	119.33	110.60
1	AA	356	A	N1-C2-N3	-17.45	120.57	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1480	A	N1-C2-N3	-17.45	120.57	129.30
1	AA	1339	A	C2-N3-C4	17.45	119.33	110.60
1	AA	371	A	N1-C2-N3	-17.45	120.58	129.30
22	BA	342	A	C2-N3-C4	17.45	119.33	110.60
22	BA	1151	A	N1-C2-N3	-17.45	120.58	129.30
22	BA	439	A	N1-C6-N6	-17.45	108.13	118.60
22	BA	21	A	C2-N3-C4	17.44	119.32	110.60
1	AA	33	A	N1-C6-N6	-17.44	108.14	118.60
22	BA	1470	A	N1-C6-N6	-17.44	108.14	118.60
1	AA	655	A	N1-C2-N3	-17.44	120.58	129.30
1	AA	1507	A	N1-C2-N3	-17.44	120.58	129.30
1	AA	120	A	C2-N3-C4	17.44	119.32	110.60
1	AA	687	A	C2-N3-C4	17.44	119.32	110.60
1	AA	374	A	N1-C2-N3	-17.43	120.58	129.30
22	BA	2366	A	N1-C2-N3	-17.43	120.59	129.30
22	BA	362	A	N1-C6-N6	-17.42	108.15	118.60
22	BA	1885	A	C2-N3-C4	17.42	119.31	110.60
1	AA	389	A	N1-C6-N6	-17.42	108.15	118.60
55	B8	59	A	N1-C2-N3	-17.42	120.59	129.30
22	BA	1272	A	C2-N3-C4	17.42	119.31	110.60
22	BA	1274	A	N1-C6-N6	-17.42	108.15	118.60
22	BA	643	A	C2-N3-C4	17.42	119.31	110.60
22	BA	996	A	C2-N3-C4	17.42	119.31	110.60
22	BA	1284	A	N1-C6-N6	-17.41	108.15	118.60
1	AA	520	A	N1-C2-N3	-17.41	120.59	129.30
22	BA	2247	A	C2-N3-C4	17.41	119.31	110.60
22	BA	2459	A	C2-N3-C4	17.41	119.31	110.60
22	BA	1336	A	N1-C2-N3	-17.41	120.60	129.30
1	AA	1067	A	C2-N3-C4	17.40	119.30	110.60
1	AA	1339	A	N1-C6-N6	-17.40	108.16	118.60
22	BA	753	A	N1-C6-N6	-17.40	108.16	118.60
22	BA	2170	A	N1-C6-N6	-17.40	108.16	118.60
1	AA	53	A	N1-C2-N3	-17.40	120.60	129.30
1	AA	648	A	N1-C2-N3	-17.40	120.60	129.30
23	BB	66	A	N1-C2-N3	-17.39	120.60	129.30
1	AA	1418	A	C2-N3-C4	17.39	119.29	110.60
22	BA	226	A	N1-C2-N3	-17.38	120.61	129.30
22	BA	586	A	C2-N3-C4	17.38	119.29	110.60
22	BA	794	A	N1-C2-N3	-17.38	120.61	129.30
1	AA	383	A	C2-N3-C4	17.38	119.29	110.60
1	AA	279	A	N1-C2-N3	-17.37	120.61	129.30
22	BA	404	A	N1-C6-N6	-17.37	108.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1679	A	N1-C6-N6	-17.37	108.18	118.60
1	AA	648	A	N1-C6-N6	-17.36	108.18	118.60
22	BA	2071	A	N1-C2-N3	-17.36	120.62	129.30
22	BA	149	A	C2-N3-C4	17.36	119.28	110.60
22	BA	1970	A	N1-C6-N6	-17.36	108.19	118.60
22	BA	294	A	N1-C6-N6	-17.36	108.19	118.60
22	BA	149	A	N1-C2-N3	-17.35	120.62	129.30
22	BA	819	A	N1-C6-N6	-17.35	108.19	118.60
22	BA	1591	A	N1-C6-N6	-17.35	108.19	118.60
1	AA	609	A	N1-C6-N6	-17.35	108.19	118.60
22	BA	49	A	N1-C6-N6	-17.35	108.19	118.60
22	BA	1504	A	N1-C6-N6	-17.35	108.19	118.60
1	AA	270	A	N1-C2-N3	-17.34	120.63	129.30
1	AA	919	A	N1-C2-N3	-17.34	120.63	129.30
22	BA	2268	A	N1-C6-N6	-17.34	108.19	118.60
22	BA	644	A	N1-C2-N3	-17.34	120.63	129.30
1	AA	655	A	N1-C6-N6	-17.34	108.19	118.60
22	BA	752	A	N1-C2-N3	-17.34	120.63	129.30
1	AA	77	A	N1-C6-N6	-17.33	108.20	118.60
1	AA	794	A	N1-C6-N6	-17.33	108.20	118.60
22	BA	1327	A	C2-N3-C4	17.33	119.26	110.60
22	BA	1144	A	N1-C2-N3	-17.32	120.64	129.30
22	BA	1614	A	N1-C6-N6	-17.32	108.20	118.60
1	AA	414	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	2749	A	C2-N3-C4	17.32	119.26	110.60
1	AA	66	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	2297	A	C2-N3-C4	17.32	119.26	110.60
22	BA	2297	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	1598	A	C2-N3-C4	17.32	119.26	110.60
22	BA	1655	A	N1-C2-N3	-17.32	120.64	129.30
22	BA	2082	A	N1-C6-N6	-17.31	108.21	118.60
22	BA	2872	A	C5-C6-N6	17.31	137.54	123.70
22	BA	1226	A	N1-C6-N6	-17.30	108.22	118.60
22	BA	255	A	C2-N3-C4	17.30	119.25	110.60
22	BA	152	A	N1-C2-N3	-17.30	120.65	129.30
22	BA	204	A	C2-N3-C4	17.30	119.25	110.60
22	BA	1205	A	N1-C2-N3	-17.30	120.65	129.30
1	AA	33	A	N1-C2-N3	-17.29	120.65	129.30
22	BA	1469	A	N1-C6-N6	-17.29	108.22	118.60
23	BB	94	A	N1-C2-N3	-17.29	120.65	129.30
1	AA	673	A	N1-C2-N3	-17.29	120.66	129.30
22	BA	101	A	N1-C2-N3	-17.28	120.66	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	802	A	N1-C2-N3	-17.28	120.66	129.30
1	AA	715	A	C2-N3-C4	17.28	119.24	110.60
22	BA	1205	A	N1-C6-N6	-17.27	108.24	118.60
22	BA	368	A	N1-C2-N3	-17.27	120.67	129.30
22	BA	1528	A	N1-C2-N3	-17.27	120.67	129.30
1	AA	609	A	C2-N3-C4	17.26	119.23	110.60
22	BA	705	A	N1-C6-N6	-17.26	108.24	118.60
22	BA	272	A	N1-C6-N6	-17.26	108.24	118.60
22	BA	492	A	C2-N3-C4	17.26	119.23	110.60
22	BA	1373	A	N1-C6-N6	-17.26	108.25	118.60
22	BA	1608	A	C2-N3-C4	17.26	119.23	110.60
22	BA	2077	A	N1-C6-N6	-17.25	108.25	118.60
22	BA	943	A	N1-C6-N6	-17.25	108.25	118.60
22	BA	2632	A	N1-C2-N3	-17.25	120.68	129.30
1	AA	790	A	N1-C6-N6	-17.23	108.26	118.60
1	AA	1375	A	N1-C2-N3	-17.23	120.69	129.30
22	BA	1304	A	N1-C2-N3	-17.23	120.69	129.30
22	BA	626	A	N1-C6-N6	-17.22	108.27	118.60
22	BA	1808	A	N1-C6-N6	-17.22	108.27	118.60
22	BA	2407	A	N1-C2-N3	-17.22	120.69	129.30
1	AA	1437	A	N1-C6-N6	-17.22	108.27	118.60
22	BA	981	A	C2-N3-C4	17.22	119.21	110.60
22	BA	685	A	N1-C2-N3	-17.21	120.69	129.30
22	BA	1679	A	N1-C2-N3	-17.21	120.69	129.30
22	BA	2448	A	N1-C2-N3	-17.21	120.69	129.30
22	BA	2015	A	N1-C6-N6	-17.21	108.27	118.60
22	BA	73	A	C2-N3-C4	17.21	119.20	110.60
22	BA	167	A	N1-C6-N6	-17.21	108.27	118.60
1	AA	32	A	N1-C6-N6	-17.21	108.28	118.60
22	BA	126	A	N1-C2-N3	-17.21	120.70	129.30
1	AA	415	A	N1-C6-N6	-17.20	108.28	118.60
1	AA	452	A	N1-C2-N3	-17.20	120.70	129.30
22	BA	152	A	N1-C6-N6	-17.20	108.28	118.60
22	BA	735	A	C2-N3-C4	17.20	119.20	110.60
22	BA	2430	A	N1-C6-N6	-17.20	108.28	118.60
22	BA	131	A	N1-C6-N6	-17.19	108.28	118.60
22	BA	933	A	N1-C2-N3	-17.19	120.70	129.30
22	BA	2450	A	C2-N3-C4	17.19	119.19	110.60
1	AA	32	A	N1-C2-N3	-17.19	120.71	129.30
1	AA	600	A	N1-C2-N3	-17.18	120.71	129.30
22	BA	2565	A	N1-C6-N6	-17.18	108.29	118.60
1	AA	907	A	N1-C6-N6	-17.17	108.30	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1722	A	N1-C2-N3	-17.17	120.72	129.30
22	BA	2547	A	C2-N3-C4	17.17	119.18	110.60
22	BA	2322	A	N1-C6-N6	-17.17	108.30	118.60
22	BA	2425	A	N1-C6-N6	-17.17	108.30	118.60
22	BA	727	A	C2-N3-C4	17.17	119.18	110.60
22	BA	960	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	91	A	C2-N3-C4	17.16	119.18	110.60
1	AA	676	A	C2-N3-C4	17.16	119.18	110.60
1	AA	946	A	N1-C6-N6	-17.16	108.31	118.60
22	BA	2518	A	N1-C6-N6	-17.16	108.31	118.60
22	BA	429	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	705	A	N1-C2-N3	-17.15	120.73	129.30
55	B8	73	A	N1-C2-N3	-17.14	120.73	129.30
22	BA	2899	A	C2-N3-C4	17.14	119.17	110.60
22	BA	761	A	N1-C6-N6	-17.13	108.32	118.60
22	BA	1689	A	N1-C2-N3	-17.13	120.74	129.30
1	AA	28	A	N1-C2-N3	-17.12	120.74	129.30
22	BA	2198	A	N1-C6-N6	-17.12	108.33	118.60
1	AA	860	A	N1-C6-N6	-17.11	108.33	118.60
1	AA	1111	A	N1-C2-N3	-17.11	120.74	129.30
22	BA	2376	A	C2-N3-C4	17.11	119.16	110.60
22	BA	477	A	N1-C2-N3	-17.11	120.75	129.30
22	BA	91	A	N1-C6-N6	-17.11	108.33	118.60
22	BA	1872	A	N1-C6-N6	-17.10	108.34	118.60
22	BA	727	A	N1-C6-N6	-17.10	108.34	118.60
1	AA	300	A	N1-C2-N3	-17.09	120.75	129.30
22	BA	471	A	N1-C6-N6	-17.09	108.34	118.60
22	BA	2352	A	C2-N3-C4	17.09	119.14	110.60
22	BA	2497	A	N1-C6-N6	-17.09	108.35	118.60
22	BA	2183	A	N1-C6-N6	-17.07	108.36	118.60
22	BA	975	A	N1-C6-N6	-17.07	108.36	118.60
22	BA	1269	A	N1-C2-N3	-17.07	120.76	129.30
22	BA	2635	A	N1-C2-N3	-17.07	120.76	129.30
1	AA	430	A	N1-C6-N6	-17.07	108.36	118.60
22	BA	2284	A	N1-C2-N3	-17.06	120.77	129.30
22	BA	2101	A	N1-C2-N3	-17.06	120.77	129.30
22	BA	1672	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	2893	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	2829	A	N1-C2-N3	-17.05	120.77	129.30
22	BA	1713	A	C2-N3-C4	17.05	119.12	110.60
23	BB	109	A	N1-C6-N6	-17.05	108.37	118.60
1	AA	1170	A	N1-C6-N6	-17.05	108.37	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	746	A	N1-C6-N6	-17.05	108.37	118.60
1	AA	1375	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	1029	A	N1-C6-N6	-17.04	108.38	118.60
1	AA	923	A	N1-C2-N3	-17.03	120.79	129.30
22	BA	1080	A	C2-N3-C4	17.03	119.11	110.60
22	BA	2340	A	C2-N3-C4	17.02	119.11	110.60
1	AA	1055	A	N1-C6-N6	-17.01	108.39	118.60
22	BA	1608	A	N1-C6-N6	-17.01	108.39	118.60
22	BA	2721	A	N1-C6-N6	-17.00	108.40	118.60
1	AA	44	A	N1-C2-N3	-17.00	120.80	129.30
1	AA	1350	A	N1-C2-N3	-17.00	120.80	129.30
22	BA	2268	A	N1-C2-N3	-17.00	120.80	129.30
22	BA	1307	A	N1-C6-N6	-16.99	108.41	118.60
22	BA	203	A	N1-C6-N6	-16.99	108.41	118.60
22	BA	480	A	N1-C2-N3	-16.99	120.81	129.30
1	AA	465	A	N1-C6-N6	-16.99	108.41	118.60
22	BA	1000	A	N1-C6-N6	-16.99	108.41	118.60
22	BA	2284	A	N1-C6-N6	-16.99	108.41	118.60
22	BA	1885	A	N1-C6-N6	-16.98	108.41	118.60
1	AA	309	A	N1-C6-N6	-16.98	108.41	118.60
22	BA	1010	A	N1-C6-N6	-16.98	108.41	118.60
22	BA	1676	A	N1-C2-N3	-16.98	120.81	129.30
22	BA	1981	A	C2-N3-C4	16.97	119.08	110.60
1	AA	784	A	N1-C2-N3	-16.96	120.82	129.30
1	AA	1508	A	N1-C6-N6	-16.96	108.42	118.60
1	AA	373	A	N1-C6-N6	-16.96	108.42	118.60
22	BA	668	A	N1-C2-N3	-16.96	120.82	129.30
22	BA	2268	A	C2-N3-C4	16.95	119.08	110.60
1	AA	1254	A	N1-C2-N3	-16.95	120.82	129.30
22	BA	2090	A	N1-C2-N3	-16.95	120.83	129.30
1	AA	767	A	N1-C6-N6	-16.93	108.44	118.60
22	BA	743	A	N1-C6-N6	-16.93	108.44	118.60
22	BA	2679	A	N1-C2-N3	-16.92	120.84	129.30
1	AA	1468	A	N1-C6-N6	-16.92	108.45	118.60
1	AA	66	A	N1-C2-N3	-16.91	120.84	129.30
22	BA	800	A	C2-N3-C4	16.91	119.05	110.60
1	AA	383	A	N1-C2-N3	-16.91	120.85	129.30
1	AA	80	A	N1-C2-N3	-16.90	120.85	129.30
1	AA	706	A	N1-C2-N3	-16.90	120.85	129.30
22	BA	677	A	N1-C6-N6	-16.90	108.46	118.60
1	AA	98	A	N1-C6-N6	-16.89	108.46	118.60
22	BA	28	A	N1-C2-N3	-16.89	120.85	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	533	A	N1-C2-N3	-16.89	120.86	129.30
1	AA	1271	A	N1-C6-N6	-16.89	108.47	118.60
1	AA	1360	A	N1-C2-N3	-16.88	120.86	129.30
23	BB	73	A	N1-C6-N6	-16.88	108.47	118.60
1	AA	1508	A	N1-C2-N3	-16.88	120.86	129.30
1	AA	1130	A	N1-C6-N6	-16.87	108.48	118.60
1	AA	696	A	N1-C6-N6	-16.86	108.49	118.60
22	BA	1367	A	C2-N3-C4	16.85	119.03	110.60
22	BA	1866	A	N1-C6-N6	-16.85	108.49	118.60
22	BA	2352	A	N1-C2-N3	-16.84	120.88	129.30
22	BA	2792	A	N1-C2-N3	-16.84	120.88	129.30
22	BA	2589	A	C2-N3-C4	16.84	119.02	110.60
22	BA	507	A	N1-C6-N6	-16.83	108.50	118.60
22	BA	793	A	N1-C2-N3	-16.83	120.89	129.30
22	BA	2407	A	N1-C6-N6	-16.83	108.50	118.60
1	AA	1219	A	N1-C2-N3	-16.82	120.89	129.30
22	BA	2108	A	N1-C6-N6	-16.82	108.51	118.60
1	AA	139	A	N1-C6-N6	-16.81	108.51	118.60
1	AA	389	A	N1-C2-N3	-16.81	120.89	129.30
22	BA	2670	A	N1-C6-N6	-16.81	108.51	118.60
22	BA	666	A	C2-N3-C4	16.80	119.00	110.60
22	BA	142	A	N1-C6-N6	-16.79	108.53	118.60
22	BA	2366	A	N1-C6-N6	-16.78	108.53	118.60
1	AA	539	A	N1-C2-N3	-16.78	120.91	129.30
22	BA	1367	A	N1-C2-N3	-16.78	120.91	129.30
22	BA	172	A	N1-C6-N6	-16.78	108.53	118.60
22	BA	1969	A	C2-N3-C4	16.78	118.99	110.60
1	AA	814	A	N1-C6-N6	-16.77	108.53	118.60
22	BA	2450	A	N1-C6-N6	-16.77	108.54	118.60
1	AA	1216	A	N1-C2-N3	-16.77	120.92	129.30
22	BA	482	A	N1-C2-N3	-16.76	120.92	129.30
22	BA	2565	A	C2-N3-C4	16.76	118.98	110.60
1	AA	499	A	N1-C6-N6	-16.76	108.54	118.60
22	BA	1027	A	C2-N3-C4	16.76	118.98	110.60
22	BA	781	A	N1-C2-N3	-16.76	120.92	129.30
22	BA	1598	A	N1-C2-N3	-16.75	120.92	129.30
22	BA	1847	A	N1-C6-N6	-16.75	108.55	118.60
22	BA	2531	A	N1-C2-N3	-16.75	120.92	129.30
22	BA	1327	A	N1-C6-N6	-16.74	108.56	118.60
22	BA	2247	A	N1-C2-N3	-16.74	120.93	129.30
22	BA	2900	A	N1-C2-N3	-16.73	120.93	129.30
1	AA	712	A	N1-C2-N3	-16.72	120.94	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1067	A	N1-C2-N3	-16.72	120.94	129.30
22	BA	1580	A	N1-C6-N6	-16.72	108.57	118.60
1	AA	309	A	N1-C2-N3	-16.72	120.94	129.30
1	AA	1197	A	N1-C2-N3	-16.72	120.94	129.30
55	B8	6	A	N1-C6-N6	-16.69	108.58	118.60
1	AA	715	A	N1-C6-N6	-16.69	108.59	118.60
22	BA	470	A	N1-C6-N6	-16.68	108.59	118.60
22	BA	1143	A	N1-C6-N6	-16.68	108.59	118.60
22	BA	1241	A	N1-C6-N6	-16.68	108.59	118.60
22	BA	63	A	N1-C6-N6	-16.67	108.59	118.60
22	BA	1552	A	N1-C6-N6	-16.67	108.60	118.60
22	BA	142	A	N1-C2-N3	-16.67	120.97	129.30
22	BA	1848	A	N1-C6-N6	-16.66	108.60	118.60
22	BA	735	A	N1-C2-N3	-16.66	120.97	129.30
22	BA	2600	A	N1-C6-N6	-16.66	108.61	118.60
1	AA	914	A	N1-C6-N6	-16.64	108.61	118.60
22	BA	2662	A	N1-C6-N6	-16.64	108.61	118.60
22	BA	492	A	N1-C2-N3	-16.63	120.99	129.30
22	BA	1679	A	C2-N3-C4	16.63	118.91	110.60
22	BA	52	A	N1-C6-N6	-16.62	108.63	118.60
22	BA	505	A	N1-C2-N3	-16.60	121.00	129.30
1	AA	1188	A	N1-C6-N6	-16.59	108.64	118.60
22	BA	1205	A	C2-N3-C4	16.58	118.89	110.60
22	BA	2900	A	N1-C6-N6	-16.56	108.67	118.60
22	BA	844	A	N1-C6-N6	-16.55	108.67	118.60
22	BA	42	A	N1-C6-N6	-16.54	108.67	118.60
22	BA	1787	A	N1-C2-N3	-16.54	121.03	129.30
23	BB	29	A	N1-C2-N3	-16.54	121.03	129.30
1	AA	1152	A	N1-C6-N6	-16.51	108.70	118.60
22	BA	2469	A	N1-C6-N6	-16.49	108.70	118.60
1	AA	459	A	N1-C2-N3	-16.48	121.06	129.30
22	BA	213	A	N1-C6-N6	-16.48	108.71	118.60
22	BA	2297	A	N1-C2-N3	-16.48	121.06	129.30
22	BA	508	A	N1-C6-N6	-16.46	108.72	118.60
1	AA	1324	A	N1-C6-N6	-16.42	108.75	118.60
1	AA	1163	A	N1-C6-N6	-16.41	108.75	118.60
22	BA	507	A	C2-N3-C4	16.40	118.80	110.60
1	AA	1396	A	N1-C2-N3	-16.40	121.10	129.30
22	BA	675	A	N1-C6-N6	-16.40	108.76	118.60
22	BA	2899	A	N1-C2-N3	-16.37	121.11	129.30
1	AA	1080	A	N1-C6-N6	-16.37	108.78	118.60
1	AA	554	A	N1-C2-N3	-16.36	121.12	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	983	A	N1-C6-N6	-16.36	108.78	118.60
22	BA	990	A	C2-N3-C4	16.35	118.78	110.60
1	AA	55	A	N1-C2-N3	-16.34	121.13	129.30
22	BA	2598	A	N1-C6-N6	-16.33	108.80	118.60
22	BA	1080	A	N1-C2-N3	-16.32	121.14	129.30
22	BA	1260	A	N1-C2-N3	-16.31	121.14	129.30
22	BA	439	A	N1-C2-N3	-16.31	121.14	129.30
22	BA	1810	A	C2-N3-C4	16.30	118.75	110.60
22	BA	2589	A	N1-C6-N6	-16.30	108.82	118.60
22	BA	761	A	N1-C2-N3	-16.30	121.15	129.30
22	BA	2792	A	N1-C6-N6	-16.28	108.83	118.60
22	BA	2392	A	N1-C6-N6	-16.28	108.83	118.60
1	AA	865	A	N1-C2-N3	-16.27	121.17	129.30
1	AA	98	A	N1-C2-N3	-16.26	121.17	129.30
22	BA	990	A	N1-C6-N6	-16.26	108.84	118.60
1	AA	192	A	N1-C2-N3	-16.25	121.17	129.30
22	BA	216	A	N1-C6-N6	-16.25	108.85	118.60
22	BA	1213	A	N1-C6-N6	-16.25	108.85	118.60
22	BA	1739	A	N1-C6-N6	-16.24	108.86	118.60
22	BA	2142	A	N1-C6-N6	-16.23	108.86	118.60
1	AA	596	A	N1-C2-N3	-16.21	121.19	129.30
22	BA	572	A	N1-C2-N3	-16.19	121.20	129.30
22	BA	1722	A	N1-C6-N6	-16.19	108.88	118.60
1	AA	1201	A	N1-C6-N6	-16.17	108.90	118.60
22	BA	1854	A	N1-C6-N6	-16.16	108.90	118.60
22	BA	251	A	N1-C2-N3	-16.15	121.22	129.30
22	BA	627	A	N1-C6-N6	-16.14	108.91	118.60
1	AA	747	A	N1-C2-N3	-16.12	121.24	129.30
23	BB	66	A	C2-N3-C4	16.11	118.66	110.60
1	AA	873	A	N1-C6-N6	-16.10	108.94	118.60
22	BA	782	A	N1-C2-N3	-16.04	121.28	129.30
22	BA	352	A	N1-C6-N6	-16.00	109.00	118.60
1	AA	1046	A	N1-C6-N6	-15.99	109.00	118.60
22	BA	2459	A	N1-C6-N6	-15.97	109.02	118.60
22	BA	513	A	N1-C6-N6	-15.96	109.02	118.60
22	BA	1572	A	N1-C6-N6	-15.96	109.02	118.60
22	BA	2727	A	N1-C6-N6	-15.94	109.04	118.60
22	BA	2899	A	N1-C6-N6	-15.91	109.05	118.60
1	AA	1396	A	N1-C6-N6	-15.90	109.06	118.60
22	BA	255	A	N1-C6-N6	-15.89	109.06	118.60
22	BA	633	A	N1-C6-N6	-15.86	109.08	118.60
22	BA	1528	A	N1-C6-N6	-15.84	109.10	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2340	A	N1-C6-N6	-15.81	109.11	118.60
1	AA	19	A	N1-C2-N3	-15.79	121.41	129.30
22	BA	404	A	C2-N3-C4	15.76	118.48	110.60
22	BA	482	A	C2-N3-C4	15.75	118.47	110.60
22	BA	960	A	N1-C6-N6	-15.72	109.17	118.60
22	BA	1810	A	N1-C2-N3	-15.69	121.45	129.30
22	BA	1020	A	C2-N3-C4	15.67	118.44	110.60
1	AA	459	A	N1-C6-N6	-15.66	109.20	118.60
22	BA	734	A	N1-C6-N6	-15.62	109.23	118.60
1	AA	743	A	N1-C6-N6	-15.61	109.23	118.60
1	AA	498	A	N1-C2-N3	-15.60	121.50	129.30
22	BA	1735	A	N1-C6-N6	-15.58	109.25	118.60
23	BB	66	A	N1-C6-N6	-15.55	109.27	118.60
22	BA	101	A	N1-C6-N6	-15.54	109.28	118.60
22	BA	2820	A	N1-C6-N6	-15.52	109.29	118.60
22	BA	1027	A	N1-C6-N6	-15.50	109.30	118.60
23	BB	59	A	N1-C2-N3	-15.45	121.58	129.30
22	BA	1054	A	N1-C6-N6	-15.30	109.42	118.60
22	BA	820	A	N1-C6-N6	-15.30	109.42	118.60
1	AA	1483	A	N1-C6-N6	-15.27	109.44	118.60
22	BA	1969	A	N1-C6-N6	-15.21	109.48	118.60
1	AA	190	A	N1-C6-N6	-15.17	109.50	118.60
23	BB	59	A	N1-C6-N6	-15.04	109.58	118.60
22	BA	466	A	N1-C6-N6	-14.90	109.66	118.60
1	AA	80	A	N1-C6-N6	-14.78	109.73	118.60
1	AA	162	A	N1-C6-N6	-14.47	109.92	118.60
22	BA	1802	A	N1-C6-N6	-14.38	109.97	118.60
1	AA	901	A	N1-C6-N6	-14.27	110.04	118.60
22	BA	2101	A	N1-C6-N6	-14.23	110.06	118.60
22	BA	2542	A	N7-C8-N9	-14.16	106.72	113.80
22	BA	2799	A	N1-C6-N6	-14.11	110.13	118.60
22	BA	800	A	C5-C6-N6	13.95	134.86	123.70
22	BA	1328	A	C5-C6-N6	13.94	134.85	123.70
22	BA	1937	A	C5-C6-N6	13.91	134.83	123.70
1	AA	300	A	N1-C6-N6	-13.85	110.29	118.60
1	AA	431	A	C5-C6-N6	13.81	134.75	123.70
22	BA	84	A	C5-C6-N6	13.68	134.64	123.70
22	BA	2430	A	C2-N3-C4	13.66	117.43	110.60
22	BA	1032	A	N7-C8-N9	-13.66	106.97	113.80
1	AA	1239	A	N7-C8-N9	-13.65	106.97	113.80
55	B8	76	A	C5-C6-N6	13.57	134.55	123.70
22	BA	1936	A	N3-C4-C5	-13.54	117.32	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	101	A	N3-C4-C5	-13.49	117.36	126.80
22	BA	1050	A	N7-C8-N9	-13.36	107.12	113.80
22	BA	1133	A	C5-C6-N6	13.36	134.39	123.70
1	AA	1502	A	N7-C8-N9	-13.34	107.13	113.80
1	AA	498	A	N3-C4-C5	-13.34	117.46	126.80
22	BA	783	A	C5-C6-N6	13.34	134.37	123.70
1	AA	1105	A	N7-C8-N9	-13.27	107.16	113.80
22	BA	2346	A	C5-C6-N6	13.26	134.31	123.70
22	BA	1810	A	N1-C6-N6	-13.20	110.68	118.60
22	BA	2009	A	N7-C8-N9	-13.19	107.20	113.80
1	AA	766	A	N7-C8-N9	-13.16	107.22	113.80
22	BA	2020	A	N7-C8-N9	-13.14	107.23	113.80
22	BA	2753	A	C5-C6-N6	13.13	134.21	123.70
22	BA	1789	A	C5-C6-N6	13.12	134.19	123.70
22	BA	526	A	N7-C8-N9	-13.09	107.25	113.80
22	BA	825	A	C5-C6-N6	13.08	134.16	123.70
22	BA	522	A	N7-C8-N9	-13.07	107.26	113.80
1	AA	1117	A	N7-C8-N9	-13.07	107.27	113.80
22	BA	575	A	C5-C6-N6	13.07	134.16	123.70
22	BA	2518	A	N7-C8-N9	-13.06	107.27	113.80
22	BA	1427	A	N7-C8-N9	-13.03	107.28	113.80
1	AA	1275	A	N7-C8-N9	-13.03	107.29	113.80
22	BA	693	A	N7-C8-N9	-12.99	107.31	113.80
22	BA	1668	A	C5-C6-N6	12.97	134.08	123.70
22	BA	979	A	N7-C8-N9	-12.96	107.32	113.80
1	AA	935	A	N7-C8-N9	-12.93	107.33	113.80
22	BA	603	A	C5-C6-N6	12.93	134.05	123.70
22	BA	1419	A	N7-C8-N9	-12.92	107.34	113.80
22	BA	2430	A	N1-C2-N3	-12.92	122.84	129.30
22	BA	2439	A	N7-C8-N9	-12.92	107.34	113.80
22	BA	526	A	C5-C6-N6	12.89	134.01	123.70
22	BA	821	A	C5-C6-N6	12.89	134.01	123.70
1	AA	1155	A	N7-C8-N9	-12.85	107.38	113.80
1	AA	1340	A	N7-C8-N9	-12.85	107.37	113.80
22	BA	614	A	N7-C8-N9	-12.85	107.38	113.80
22	BA	2471	A	N7-C8-N9	-12.84	107.38	113.80
22	BA	1503	A	N7-C8-N9	-12.83	107.39	113.80
22	BA	734	A	N7-C8-N9	-12.81	107.39	113.80
1	AA	974	A	N7-C8-N9	-12.81	107.40	113.80
22	BA	2327	A	C5-C6-N6	12.80	133.94	123.70
22	BA	1247	A	N7-C8-N9	-12.79	107.40	113.80
23	BB	59	A	N3-C4-C5	-12.79	117.84	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	468	A	N7-C8-N9	-12.79	107.40	113.80
22	BA	2418	A	N7-C8-N9	-12.79	107.41	113.80
22	BA	627	A	N7-C8-N9	-12.78	107.41	113.80
22	BA	1069	A	N7-C8-N9	-12.78	107.41	113.80
22	BA	1669	A	C5-C6-N6	12.78	133.92	123.70
22	BA	1821	A	C5-C6-N6	12.78	133.92	123.70
22	BA	676	A	N7-C8-N9	-12.78	107.41	113.80
22	BA	2412	A	N7-C8-N9	-12.77	107.41	113.80
22	BA	749	A	N7-C8-N9	-12.77	107.42	113.80
22	BA	1308	A	C5-C6-N6	12.76	133.91	123.70
1	AA	1213	A	C5-C6-N6	12.76	133.91	123.70
22	BA	637	A	N7-C8-N9	-12.75	107.42	113.80
23	BB	101	A	N1-C2-N3	-12.75	122.92	129.30
22	BA	2340	A	N7-C8-N9	-12.74	107.43	113.80
22	BA	262	A	N7-C8-N9	-12.74	107.43	113.80
22	BA	1652	A	N7-C8-N9	-12.73	107.44	113.80
1	AA	1319	A	C5-C6-N6	12.72	133.88	123.70
1	AA	913	A	N7-C8-N9	-12.71	107.44	113.80
22	BA	479	A	N7-C8-N9	-12.71	107.44	113.80
22	BA	1981	A	N7-C8-N9	-12.71	107.45	113.80
22	BA	2665	A	N7-C8-N9	-12.70	107.45	113.80
22	BA	2750	A	N7-C8-N9	-12.70	107.45	113.80
1	AA	430	A	N7-C8-N9	-12.68	107.46	113.80
1	AA	1179	A	C5-C6-N6	12.65	133.82	123.70
1	AA	1081	A	N7-C8-N9	-12.65	107.48	113.80
22	BA	1630	A	N7-C8-N9	-12.64	107.48	113.80
22	BA	1937	A	N7-C8-N9	-12.64	107.48	113.80
22	BA	1020	A	C5-C6-N6	12.64	133.81	123.70
22	BA	2031	A	N7-C8-N9	-12.63	107.48	113.80
1	AA	414	A	N7-C8-N9	-12.63	107.49	113.80
22	BA	2352	A	C5-C6-N6	12.63	133.80	123.70
22	BA	352	A	N7-C8-N9	-12.62	107.49	113.80
22	BA	1652	A	C5-C6-N6	12.62	133.79	123.70
22	BA	2741	A	N7-C8-N9	-12.62	107.49	113.80
22	BA	1783	A	N7-C8-N9	-12.61	107.49	113.80
1	AA	8	A	N7-C8-N9	-12.60	107.50	113.80
22	BA	2281	A	N7-C8-N9	-12.60	107.50	113.80
1	AA	119	A	C5-C6-N6	12.60	133.78	123.70
22	BA	514	A	N7-C8-N9	-12.60	107.50	113.80
22	BA	161	A	C5-C6-N6	12.59	133.78	123.70
1	AA	825	A	N7-C8-N9	-12.59	107.51	113.80
22	BA	1378	A	C5-C6-N6	12.58	133.77	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	915	A	C5-C6-N6	12.57	133.76	123.70
22	BA	1700	A	N7-C8-N9	-12.57	107.51	113.80
22	BA	1815	A	C5-C6-N6	12.57	133.76	123.70
22	BA	1913	A	N7-C8-N9	-12.57	107.52	113.80
22	BA	71	A	C5-C6-N6	12.56	133.75	123.70
22	BA	2052	A	N7-C8-N9	-12.56	107.52	113.80
22	BA	2227	A	C5-C6-N6	12.54	133.73	123.70
22	BA	2534	A	N7-C8-N9	-12.54	107.53	113.80
1	AA	1503	A	N7-C8-N9	-12.54	107.53	113.80
22	BA	1169	A	N7-C8-N9	-12.53	107.53	113.80
1	AA	1408	A	N7-C8-N9	-12.52	107.54	113.80
1	AA	7	A	N7-C8-N9	-12.52	107.54	113.80
1	AA	383	A	N1-C6-N6	-12.52	111.09	118.60
22	BA	789	A	N7-C8-N9	-12.52	107.54	113.80
22	BA	2765	A	C5-C6-N6	12.51	133.71	123.70
1	AA	1285	A	N7-C8-N9	-12.51	107.55	113.80
22	BA	2758	A	N7-C8-N9	-12.51	107.55	113.80
1	AA	1101	A	N7-C8-N9	-12.49	107.55	113.80
22	BA	1384	A	N7-C8-N9	-12.49	107.56	113.80
22	BA	920	A	N7-C8-N9	-12.48	107.56	113.80
1	AA	1434	A	N7-C8-N9	-12.48	107.56	113.80
22	BA	699	A	C5-C6-N6	12.48	133.69	123.70
22	BA	2530	A	N7-C8-N9	-12.47	107.56	113.80
22	BA	213	A	N7-C8-N9	-12.46	107.57	113.80
1	AA	784	A	N7-C8-N9	-12.46	107.57	113.80
22	BA	222	A	N7-C8-N9	-12.46	107.57	113.80
22	BA	2451	A	C5-C6-N6	12.45	133.66	123.70
1	AA	16	A	N7-C8-N9	-12.44	107.58	113.80
22	BA	756	A	N7-C8-N9	-12.45	107.58	113.80
22	BA	1515	A	C5-C6-N6	12.44	133.65	123.70
22	BA	2449	U	C5-C6-N1	-12.44	116.48	122.70
22	BA	1597	A	N7-C8-N9	-12.44	107.58	113.80
22	BA	602	A	N7-C8-N9	-12.43	107.58	113.80
22	BA	374	A	N7-C8-N9	-12.43	107.58	113.80
22	BA	1453	A	N7-C8-N9	-12.43	107.58	113.80
1	AA	919	A	C5-C6-N6	12.43	133.64	123.70
22	BA	2733	A	N7-C8-N9	-12.43	107.59	113.80
1	AA	1167	A	N7-C8-N9	-12.42	107.59	113.80
22	BA	2333	A	N7-C8-N9	-12.42	107.59	113.80
1	AA	60	A	N7-C8-N9	-12.42	107.59	113.80
23	BB	119	A	N7-C8-N9	-12.41	107.59	113.80
22	BA	1928	A	C5-C6-N6	12.41	133.63	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	528	A	C5-C6-N6	12.41	133.62	123.70
1	AA	1346	A	N7-C8-N9	-12.39	107.60	113.80
22	BA	2434	A	N7-C8-N9	-12.39	107.60	113.80
22	BA	1569	A	N7-C8-N9	-12.39	107.61	113.80
1	AA	349	A	N7-C8-N9	-12.38	107.61	113.80
22	BA	2660	A	C5-C6-N6	12.38	133.61	123.70
22	BA	2154	A	N7-C8-N9	-12.38	107.61	113.80
1	AA	10	A	N7-C8-N9	-12.38	107.61	113.80
22	BA	2077	A	N3-C4-C5	-12.37	118.14	126.80
1	AA	432	A	N7-C8-N9	-12.37	107.61	113.80
1	AA	695	A	C5-C6-N6	12.37	133.60	123.70
22	BA	2435	A	C5-C6-N6	12.37	133.60	123.70
22	BA	2469	A	N7-C8-N9	-12.37	107.61	113.80
22	BA	497	A	N7-C8-N9	-12.37	107.61	113.80
22	BA	1590	A	N7-C8-N9	-12.37	107.61	113.80
1	AA	1019	A	N7-C8-N9	-12.37	107.62	113.80
22	BA	2602	A	N7-C8-N9	-12.37	107.62	113.80
1	AA	572	A	N7-C8-N9	-12.36	107.62	113.80
1	AA	55	A	N7-C8-N9	-12.36	107.62	113.80
1	AA	1374	A	N7-C8-N9	-12.36	107.62	113.80
1	AA	1329	A	N7-C8-N9	-12.36	107.62	113.80
22	BA	2670	A	N7-C8-N9	-12.35	107.62	113.80
22	BA	1165	A	N7-C8-N9	-12.35	107.62	113.80
22	BA	1359	A	C5-C6-N6	12.35	133.58	123.70
22	BA	1213	A	N7-C8-N9	-12.34	107.63	113.80
1	AA	309	A	N7-C8-N9	-12.33	107.63	113.80
22	BA	1794	A	N7-C8-N9	-12.33	107.64	113.80
22	BA	1690	A	C5-C6-N6	12.33	133.56	123.70
1	AA	246	A	N7-C8-N9	-12.32	107.64	113.80
22	BA	1204	A	C5-C6-N6	12.32	133.56	123.70
22	BA	655	A	N7-C8-N9	-12.31	107.64	113.80
22	BA	2738	A	N7-C8-N9	-12.31	107.64	113.80
22	BA	905	A	N7-C8-N9	-12.31	107.64	113.80
22	BA	2792	A	N7-C8-N9	-12.31	107.65	113.80
23	BB	104	A	N7-C8-N9	-12.31	107.65	113.80
1	AA	1447	A	C5-C6-N6	12.31	133.54	123.70
1	AA	583	A	N7-C8-N9	-12.30	107.65	113.80
22	BA	1262	A	C5-C6-N6	12.30	133.54	123.70
1	AA	1429	A	N7-C8-N9	-12.29	107.65	113.80
22	BA	2042	A	C5-C6-N6	12.29	133.53	123.70
22	BA	241	A	C5-C6-N6	12.29	133.53	123.70
22	BA	749	A	C5-C6-N6	12.28	133.53	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1275	A	N7-C8-N9	-12.28	107.66	113.80
1	AA	356	A	N7-C8-N9	-12.28	107.66	113.80
22	BA	1021	A	N3-C4-C5	-12.28	118.20	126.80
1	AA	978	A	C5-C6-N6	12.28	133.52	123.70
1	AA	1493	A	N7-C8-N9	-12.28	107.66	113.80
22	BA	1420	A	N7-C8-N9	-12.28	107.66	113.80
22	BA	2211	A	N7-C8-N9	-12.28	107.66	113.80
1	AA	819	A	N7-C8-N9	-12.27	107.66	113.80
22	BA	1039	A	N7-C8-N9	-12.27	107.66	113.80
22	BA	216	A	N7-C8-N9	-12.27	107.67	113.80
22	BA	2212	A	C5-C6-N6	12.27	133.51	123.70
22	BA	2873	A	N7-C8-N9	-12.26	107.67	113.80
1	AA	554	A	N7-C8-N9	-12.26	107.67	113.80
22	BA	2734	A	N7-C8-N9	-12.26	107.67	113.80
1	AA	274	A	N7-C8-N9	-12.26	107.67	113.80
22	BA	910	A	N7-C8-N9	-12.26	107.67	113.80
22	BA	1678	A	N7-C8-N9	-12.26	107.67	113.80
22	BA	1385	A	C5-C6-N6	12.25	133.50	123.70
1	AA	143	A	N7-C8-N9	-12.24	107.68	113.80
22	BA	1111	A	N7-C8-N9	-12.24	107.68	113.80
22	BA	1393	A	C5-C6-N6	12.22	133.48	123.70
1	AA	1480	A	C5-C6-N6	12.22	133.47	123.70
22	BA	699	A	N7-C8-N9	-12.22	107.69	113.80
1	AA	539	A	N7-C8-N9	-12.22	107.69	113.80
22	BA	1803	A	C5-C6-N6	12.21	133.47	123.70
1	AA	397	A	N3-C4-C5	-12.21	118.25	126.80
1	AA	1456	A	N7-C8-N9	-12.21	107.70	113.80
22	BA	2183	A	N7-C8-N9	-12.21	107.70	113.80
1	AA	1360	A	N7-C8-N9	-12.20	107.70	113.80
1	AA	243	A	C5-C6-N6	12.20	133.46	123.70
22	BA	925	A	N7-C8-N9	-12.20	107.70	113.80
22	BA	126	A	C5-C6-N6	12.20	133.46	123.70
22	BA	2541	A	N7-C8-N9	-12.19	107.70	113.80
1	AA	681	A	N7-C8-N9	-12.18	107.71	113.80
23	BB	34	A	N7-C8-N9	-12.18	107.71	113.80
22	BA	1919	A	N7-C8-N9	-12.18	107.71	113.80
1	AA	814	A	N7-C8-N9	-12.18	107.71	113.80
22	BA	1912	A	N7-C8-N9	-12.18	107.71	113.80
1	AA	1044	A	N7-C8-N9	-12.17	107.71	113.80
1	AA	412	A	C5-C6-N6	12.17	133.44	123.70
22	BA	49	A	N7-C8-N9	-12.17	107.71	113.80
22	BA	877	A	N7-C8-N9	-12.17	107.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	253	A	N7-C8-N9	-12.17	107.72	113.80
22	BA	742	A	N7-C8-N9	-12.17	107.72	113.80
22	BA	155	A	N7-C8-N9	-12.16	107.72	113.80
22	BA	482	A	N1-C6-N6	-12.16	111.30	118.60
1	AA	792	A	N7-C8-N9	-12.16	107.72	113.80
22	BA	282	A	N7-C8-N9	-12.15	107.73	113.80
1	AA	906	A	N7-C8-N9	-12.14	107.73	113.80
22	BA	1342	A	N7-C8-N9	-12.14	107.73	113.80
23	BB	52	A	N7-C8-N9	-12.13	107.73	113.80
1	AA	71	A	N7-C8-N9	-12.13	107.74	113.80
1	AA	622	A	C5-C6-N6	12.13	133.40	123.70
22	BA	251	A	N3-C4-C5	-12.13	118.31	126.80
22	BA	2435	A	N7-C8-N9	-12.12	107.74	113.80
1	AA	197	A	N7-C8-N9	-12.12	107.74	113.80
22	BA	1522	A	N7-C8-N9	-12.12	107.74	113.80
22	BA	146	A	N7-C8-N9	-12.12	107.74	113.80
22	BA	1689	A	C5-C6-N6	12.12	133.40	123.70
1	AA	1101	A	C5-C6-N6	12.12	133.39	123.70
22	BA	1698	A	C5-C6-N6	12.12	133.39	123.70
22	BA	2094	A	N7-C8-N9	-12.12	107.74	113.80
22	BA	1609	A	N7-C8-N9	-12.11	107.74	113.80
1	AA	461	A	N7-C8-N9	-12.11	107.75	113.80
22	BA	2482	A	C5-C6-N6	12.11	133.39	123.70
1	AA	306	A	N7-C8-N9	-12.11	107.75	113.80
1	AA	1213	A	N7-C8-N9	-12.11	107.75	113.80
22	BA	401	A	N7-C8-N9	-12.11	107.75	113.80
23	BB	108	A	N7-C8-N9	-12.10	107.75	113.80
22	BA	706	A	N7-C8-N9	-12.10	107.75	113.80
1	AA	149	A	C5-C6-N6	12.10	133.38	123.70
1	AA	171	A	N7-C8-N9	-12.10	107.75	113.80
1	AA	478	A	N7-C8-N9	-12.10	107.75	113.80
22	BA	127	A	N7-C8-N9	-12.09	107.75	113.80
22	BA	2336	A	N7-C8-N9	-12.09	107.75	113.80
22	BA	1413	A	N7-C8-N9	-12.09	107.75	113.80
1	AA	432	A	C5-C6-N6	12.09	133.37	123.70
22	BA	196	A	C5-C6-N6	12.08	133.37	123.70
1	AA	246	A	C5-C6-N6	12.08	133.36	123.70
55	B8	76	A	N7-C8-N9	-12.08	107.76	113.80
1	AA	978	A	N7-C8-N9	-12.07	107.76	113.80
22	BA	1086	A	C5-C6-N6	12.07	133.36	123.70
22	BA	1304	A	N7-C8-N9	-12.07	107.76	113.80
22	BA	231	A	N7-C8-N9	-12.06	107.77	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1780	A	C5-C6-N6	12.06	133.35	123.70
1	AA	729	A	C5-C6-N6	12.06	133.34	123.70
22	BA	1254	A	N7-C8-N9	-12.05	107.77	113.80
1	AA	152	A	C5-C6-N6	12.04	133.34	123.70
1	AA	174	A	C5-C6-N6	12.04	133.33	123.70
22	BA	718	A	N7-C8-N9	-12.04	107.78	113.80
22	BA	2062	A	N7-C8-N9	-12.04	107.78	113.80
22	BA	125	A	N7-C8-N9	-12.04	107.78	113.80
1	AA	1014	A	N7-C8-N9	-12.03	107.78	113.80
22	BA	2013	A	N7-C8-N9	-12.03	107.78	113.80
1	AA	205	A	N7-C8-N9	-12.03	107.79	113.80
1	AA	958	A	N7-C8-N9	-12.02	107.79	113.80
1	AA	802	A	N7-C8-N9	-12.02	107.79	113.80
1	AA	889	A	N7-C8-N9	-12.02	107.79	113.80
22	BA	1858	A	N7-C8-N9	-12.02	107.79	113.80
1	AA	665	A	C5-C6-N6	12.02	133.31	123.70
1	AA	1377	A	N7-C8-N9	-12.02	107.79	113.80
22	BA	1545	A	C5-C6-N6	12.02	133.31	123.70
1	AA	1016	A	N7-C8-N9	-12.01	107.79	113.80
22	BA	2829	A	N7-C8-N9	-12.01	107.79	113.80
22	BA	2478	A	N7-C8-N9	-12.01	107.79	113.80
1	AA	782	A	N7-C8-N9	-12.01	107.80	113.80
1	AA	1163	A	N7-C8-N9	-12.01	107.80	113.80
22	BA	223	A	C5-C6-N6	12.01	133.31	123.70
1	AA	1180	A	N7-C8-N9	-12.01	107.80	113.80
22	BA	721	A	N7-C8-N9	-12.01	107.80	113.80
22	BA	2513	A	C5-C6-N6	12.01	133.31	123.70
22	BA	2860	A	N7-C8-N9	-12.01	107.80	113.80
22	BA	345	A	C5-C6-N6	12.00	133.30	123.70
1	AA	753	A	N7-C8-N9	-12.00	107.80	113.80
22	BA	457	A	N7-C8-N9	-12.00	107.80	113.80
22	BA	1354	A	C5-C6-N6	12.00	133.30	123.70
1	AA	579	A	N7-C8-N9	-12.00	107.80	113.80
22	BA	13	A	C5-C6-N6	12.00	133.30	123.70
22	BA	1987	A	N7-C8-N9	-12.00	107.80	113.80
1	AA	1170	A	N7-C8-N9	-12.00	107.80	113.80
1	AA	1188	A	N7-C8-N9	-12.00	107.80	113.80
22	BA	10	A	N7-C8-N9	-12.00	107.80	113.80
22	BA	2297	A	N7-C8-N9	-12.00	107.80	113.80
22	BA	2835	A	C5-C6-N6	12.00	133.30	123.70
22	BA	2776	A	N7-C8-N9	-11.99	107.80	113.80
1	AA	411	A	N7-C8-N9	-11.99	107.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2736	A	N7-C8-N9	-11.99	107.80	113.80
1	AA	704	A	C5-C6-N6	11.99	133.29	123.70
22	BA	1749	A	N7-C8-N9	-11.99	107.81	113.80
22	BA	1395	A	C5-C6-N6	11.98	133.29	123.70
22	BA	1580	A	N7-C8-N9	-11.98	107.81	113.80
22	BA	1755	A	C5-C6-N6	11.98	133.29	123.70
22	BA	1755	A	N7-C8-N9	-11.98	107.81	113.80
22	BA	119	A	C5-C6-N6	11.98	133.28	123.70
22	BA	244	A	C5-C6-N6	11.98	133.28	123.70
22	BA	783	A	N3-C4-C5	-11.98	118.42	126.80
22	BA	2009	A	C5-C6-N6	11.98	133.28	123.70
22	BA	1713	A	N7-C8-N9	-11.97	107.81	113.80
22	BA	1509	A	N7-C8-N9	-11.97	107.81	113.80
22	BA	1020	A	N7-C8-N9	-11.96	107.82	113.80
1	AA	60	A	C5-C6-N6	11.96	133.27	123.70
55	B8	73	A	C5-C6-N6	11.96	133.27	123.70
22	BA	909	A	N7-C8-N9	-11.96	107.82	113.80
22	BA	1272	A	N7-C8-N9	-11.95	107.82	113.80
1	AA	787	A	N7-C8-N9	-11.95	107.82	113.80
22	BA	1286	A	N7-C8-N9	-11.95	107.82	113.80
23	BB	29	A	N7-C8-N9	-11.95	107.82	113.80
22	BA	1431	A	N7-C8-N9	-11.95	107.83	113.80
1	AA	196	A	N7-C8-N9	-11.95	107.83	113.80
1	AA	371	A	N7-C8-N9	-11.95	107.83	113.80
1	AA	649	A	N7-C8-N9	-11.95	107.83	113.80
22	BA	1253	A	C5-C6-N6	11.95	133.26	123.70
22	BA	1434	A	C5-C6-N6	11.95	133.26	123.70
1	AA	336	A	N7-C8-N9	-11.95	107.83	113.80
22	BA	947	A	N7-C8-N9	-11.94	107.83	113.80
1	AA	621	A	N7-C8-N9	-11.94	107.83	113.80
22	BA	2095	A	N7-C8-N9	-11.94	107.83	113.80
1	AA	1287	A	C5-C6-N6	11.94	133.25	123.70
1	AA	1150	A	N7-C8-N9	-11.94	107.83	113.80
1	AA	321	A	C5-C6-N6	11.94	133.25	123.70
22	BA	599	A	N7-C8-N9	-11.93	107.83	113.80
22	BA	1088	A	N3-C4-C5	-11.93	118.45	126.80
22	BA	207	A	C5-C6-N6	11.93	133.25	123.70
1	AA	336	A	C5-C6-N6	11.93	133.24	123.70
1	AA	1480	A	N7-C8-N9	-11.93	107.84	113.80
22	BA	892	A	C5-C6-N6	11.93	133.24	123.70
22	BA	1046	A	N7-C8-N9	-11.93	107.84	113.80
22	BA	1147	A	N7-C8-N9	-11.93	107.84	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2033	A	C5-C6-N6	11.93	133.24	123.70
22	BA	896	A	C5-C6-N6	11.92	133.24	123.70
22	BA	1583	A	N7-C8-N9	-11.92	107.84	113.80
1	AA	499	A	N7-C8-N9	-11.92	107.84	113.80
22	BA	181	A	C5-C6-N6	11.92	133.24	123.70
22	BA	802	A	C5-C6-N6	11.92	133.23	123.70
1	AA	1431	A	N7-C8-N9	-11.92	107.84	113.80
22	BA	505	A	N7-C8-N9	-11.91	107.84	113.80
22	BA	1938	A	N7-C8-N9	-11.91	107.84	113.80
22	BA	1073	A	N7-C8-N9	-11.91	107.84	113.80
1	AA	1021	A	N7-C8-N9	-11.91	107.84	113.80
1	AA	913	A	C5-C6-N6	11.91	133.23	123.70
1	AA	1000	A	N7-C8-N9	-11.91	107.85	113.80
22	BA	146	A	C5-C6-N6	11.91	133.23	123.70
1	AA	243	A	N7-C8-N9	-11.90	107.85	113.80
1	AA	546	A	N7-C8-N9	-11.90	107.85	113.80
1	AA	572	A	C5-C6-N6	11.90	133.22	123.70
55	B8	73	A	N7-C8-N9	-11.90	107.85	113.80
1	AA	199	A	N7-C8-N9	-11.90	107.85	113.80
1	AA	600	A	N7-C8-N9	-11.89	107.85	113.80
22	BA	501	A	N7-C8-N9	-11.89	107.85	113.80
22	BA	2461	A	N7-C8-N9	-11.89	107.85	113.80
1	AA	753	A	C5-C6-N6	11.89	133.21	123.70
22	BA	2411	A	N7-C8-N9	-11.89	107.85	113.80
1	AA	915	A	N7-C8-N9	-11.89	107.86	113.80
1	AA	1201	A	N7-C8-N9	-11.88	107.86	113.80
22	BA	1142	A	C5-C6-N6	11.88	133.21	123.70
1	AA	1433	A	C5-C6-N6	11.88	133.21	123.70
22	BA	829	A	N7-C8-N9	-11.88	107.86	113.80
1	AA	236	A	N7-C8-N9	-11.88	107.86	113.80
1	AA	315	A	N7-C8-N9	-11.88	107.86	113.80
22	BA	278	A	N3-C4-C5	-11.88	118.48	126.80
1	AA	1171	A	N7-C8-N9	-11.88	107.86	113.80
22	BA	2142	A	N7-C8-N9	-11.88	107.86	113.80
1	AA	32	A	N3-C4-C5	-11.88	118.49	126.80
1	AA	160	A	C5-C6-N6	11.88	133.20	123.70
1	AA	1269	A	N7-C8-N9	-11.88	107.86	113.80
22	BA	2711	A	N7-C8-N9	-11.87	107.86	113.80
1	AA	181	A	N7-C8-N9	-11.87	107.86	113.80
1	AA	1229	A	N7-C8-N9	-11.87	107.86	113.80
1	AA	1067	A	N7-C8-N9	-11.87	107.86	113.80
22	BA	586	A	C5-C6-N6	11.87	133.20	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	238	A	N7-C8-N9	-11.87	107.86	113.80
22	BA	2090	A	N7-C8-N9	-11.87	107.86	113.80
22	BA	2298	A	N7-C8-N9	-11.87	107.87	113.80
22	BA	73	A	N7-C8-N9	-11.87	107.87	113.80
22	BA	2101	A	N7-C8-N9	-11.87	107.87	113.80
22	BA	1591	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	371	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	2381	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	223	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	1701	A	C5-C6-N6	11.86	133.19	123.70
1	AA	431	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	310	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	354	A	N7-C8-N9	-11.85	107.87	113.80
22	BA	1142	A	N7-C8-N9	-11.85	107.88	113.80
22	BA	2800	A	N7-C8-N9	-11.85	107.87	113.80
22	BA	2572	A	C5-C6-N6	11.85	133.18	123.70
22	BA	2660	A	N7-C8-N9	-11.85	107.88	113.80
1	AA	182	A	N7-C8-N9	-11.85	107.88	113.80
22	BA	1678	A	C5-C6-N6	11.85	133.18	123.70
22	BA	2003	A	N7-C8-N9	-11.85	107.88	113.80
22	BA	340	A	N7-C8-N9	-11.84	107.88	113.80
22	BA	2453	A	C5-C6-N6	11.84	133.17	123.70
22	BA	2632	A	N7-C8-N9	-11.84	107.88	113.80
1	AA	520	A	C5-C6-N6	11.84	133.17	123.70
22	BA	1871	A	N7-C8-N9	-11.84	107.88	113.80
23	BB	59	A	N7-C8-N9	-11.84	107.88	113.80
22	BA	2632	A	C5-C6-N6	11.84	133.17	123.70
1	AA	1229	A	C5-C6-N6	11.83	133.17	123.70
22	BA	1981	A	C5-C6-N6	11.83	133.16	123.70
22	BA	2406	A	N7-C8-N9	-11.83	107.88	113.80
22	BA	2657	A	C5-C6-N6	11.83	133.17	123.70
22	BA	2199	A	C5-C6-N6	11.83	133.16	123.70
1	AA	1035	A	N7-C8-N9	-11.83	107.89	113.80
1	AA	1413	A	C5-C6-N6	11.83	133.16	123.70
22	BA	2288	A	N7-C8-N9	-11.83	107.89	113.80
22	BA	1385	A	N7-C8-N9	-11.82	107.89	113.80
22	BA	1640	A	N7-C8-N9	-11.82	107.89	113.80
1	AA	1067	A	C5-C6-N6	11.82	133.15	123.70
22	BA	233	A	C5-C6-N6	11.82	133.15	123.70
22	BA	503	A	N3-C4-C5	-11.82	118.53	126.80
22	BA	2134	A	N7-C8-N9	-11.82	107.89	113.80
22	BA	2758	A	C5-C6-N6	11.82	133.15	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1439	A	C5-C6-N6	11.81	133.15	123.70
22	BA	1085	A	C5-C6-N6	11.81	133.15	123.70
22	BA	917	A	N7-C8-N9	-11.81	107.89	113.80
22	BA	2358	A	N7-C8-N9	-11.81	107.89	113.80
1	AA	648	A	N7-C8-N9	-11.81	107.90	113.80
22	BA	2778	A	C5-C6-N6	11.81	133.15	123.70
22	BA	973	A	C5-C6-N6	11.80	133.14	123.70
22	BA	1057	A	N7-C8-N9	-11.80	107.90	113.80
22	BA	1819	A	N7-C8-N9	-11.80	107.90	113.80
22	BA	668	A	N7-C8-N9	-11.80	107.90	113.80
22	BA	764	A	C5-C6-N6	11.80	133.14	123.70
1	AA	1196	A	N7-C8-N9	-11.80	107.90	113.80
1	AA	1271	A	N7-C8-N9	-11.80	107.90	113.80
22	BA	165	A	C5-C6-N6	11.80	133.14	123.70
22	BA	1383	A	N7-C8-N9	-11.80	107.90	113.80
1	AA	975	A	N7-C8-N9	-11.80	107.90	113.80
22	BA	167	A	N7-C8-N9	-11.79	107.90	113.80
22	BA	344	A	N7-C8-N9	-11.79	107.90	113.80
22	BA	1378	A	N7-C8-N9	-11.79	107.90	113.80
1	AA	715	A	N7-C8-N9	-11.79	107.90	113.80
1	AA	1004	A	N7-C8-N9	-11.79	107.90	113.80
1	AA	1257	A	N7-C8-N9	-11.79	107.90	113.80
22	BA	1084	A	C5-C6-N6	11.79	133.13	123.70
22	BA	2309	A	N7-C8-N9	-11.79	107.91	113.80
22	BA	2369	A	N7-C8-N9	-11.79	107.90	113.80
22	BA	899	A	N7-C8-N9	-11.79	107.91	113.80
22	BA	1129	A	C5-C6-N6	11.79	133.13	123.70
1	AA	964	A	N7-C8-N9	-11.79	107.91	113.80
22	BA	1393	A	N7-C8-N9	-11.79	107.91	113.80
22	BA	1635	A	C5-C6-N6	11.78	133.13	123.70
1	AA	1110	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	572	A	N3-C4-C5	-11.78	118.55	126.80
22	BA	103	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	1353	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	89	A	N7-C8-N9	-11.77	107.91	113.80
1	AA	573	A	N7-C8-N9	-11.77	107.92	113.80
22	BA	1744	A	N7-C8-N9	-11.77	107.92	113.80
22	BA	503	A	N7-C8-N9	-11.76	107.92	113.80
22	BA	2311	A	N7-C8-N9	-11.76	107.92	113.80
22	BA	1505	A	N7-C8-N9	-11.76	107.92	113.80
22	BA	2764	A	C5-C6-N6	11.76	133.11	123.70
1	AA	1437	A	N7-C8-N9	-11.76	107.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	204	A	N7-C8-N9	-11.75	107.92	113.80
1	AA	553	A	N7-C8-N9	-11.75	107.92	113.80
1	AA	687	A	N7-C8-N9	-11.75	107.92	113.80
22	BA	429	A	C5-C6-N6	11.75	133.10	123.70
22	BA	2590	A	C5-C6-N6	11.75	133.10	123.70
1	AA	130	A	N7-C8-N9	-11.75	107.93	113.80
1	AA	1246	A	N7-C8-N9	-11.75	107.93	113.80
1	AA	901	A	N3-C4-C5	-11.74	118.58	126.80
1	AA	1476	A	N7-C8-N9	-11.74	107.93	113.80
22	BA	1194	A	C5-C6-N6	11.74	133.10	123.70
22	BA	1552	A	N7-C8-N9	-11.74	107.93	113.80
22	BA	2602	A	C5-C6-N6	11.74	133.09	123.70
1	AA	1150	A	C5-C6-N6	11.74	133.09	123.70
1	AA	119	A	N7-C8-N9	-11.74	107.93	113.80
22	BA	1365	A	N7-C8-N9	-11.74	107.93	113.80
22	BA	2541	A	C5-C6-N6	11.74	133.09	123.70
22	BA	466	A	N7-C8-N9	-11.73	107.93	113.80
1	AA	74	A	C5-C6-N6	11.73	133.09	123.70
1	AA	596	A	N7-C8-N9	-11.73	107.94	113.80
1	AA	1368	A	N7-C8-N9	-11.73	107.94	113.80
1	AA	149	A	N7-C8-N9	-11.73	107.94	113.80
22	BA	849	A	N7-C8-N9	-11.73	107.94	113.80
22	BA	1237	A	C5-C6-N6	11.73	133.08	123.70
1	AA	77	A	N7-C8-N9	-11.72	107.94	113.80
22	BA	1553	A	N7-C8-N9	-11.72	107.94	113.80
1	AA	172	A	N7-C8-N9	-11.72	107.94	113.80
1	AA	493	A	N7-C8-N9	-11.72	107.94	113.80
22	BA	91	A	N7-C8-N9	-11.72	107.94	113.80
22	BA	1960	A	N7-C8-N9	-11.72	107.94	113.80
22	BA	402	A	C5-C6-N6	11.72	133.07	123.70
22	BA	1230	A	C5-C6-N6	11.72	133.07	123.70
1	AA	1413	A	N7-C8-N9	-11.71	107.94	113.80
23	BB	39	A	N7-C8-N9	-11.71	107.94	113.80
1	AA	228	A	N7-C8-N9	-11.71	107.94	113.80
22	BA	1095	A	N7-C8-N9	-11.71	107.94	113.80
22	BA	14	A	N7-C8-N9	-11.71	107.95	113.80
22	BA	2577	A	N7-C8-N9	-11.71	107.94	113.80
1	AA	1285	A	C5-C6-N6	11.71	133.06	123.70
22	BA	1155	A	N7-C8-N9	-11.70	107.95	113.80
1	AA	313	A	C5-C6-N6	11.70	133.06	123.70
1	AA	547	A	N7-C8-N9	-11.70	107.95	113.80
22	BA	845	A	N7-C8-N9	-11.70	107.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2542	A	C5-C6-N6	11.70	133.06	123.70
1	AA	129	A	N7-C8-N9	-11.70	107.95	113.80
1	AA	495	A	C5-C6-N6	11.70	133.06	123.70
1	AA	1151	A	N7-C8-N9	-11.70	107.95	113.80
22	BA	1969	A	N7-C8-N9	-11.70	107.95	113.80
23	BB	115	A	N7-C8-N9	-11.70	107.95	113.80
22	BA	221	A	C5-C6-N6	11.70	133.06	123.70
22	BA	2119	A	N7-C8-N9	-11.70	107.95	113.80
1	AA	533	A	N3-C4-C5	-11.70	118.61	126.80
22	BA	1596	A	N7-C8-N9	-11.70	107.95	113.80
22	BA	2829	A	C5-C6-N6	11.70	133.06	123.70
22	BA	199	A	C5-C6-N6	11.69	133.05	123.70
22	BA	322	A	N7-C8-N9	-11.69	107.95	113.80
22	BA	959	A	C5-C6-N6	11.69	133.05	123.70
22	BA	1387	A	N7-C8-N9	-11.69	107.95	113.80
22	BA	1525	A	N7-C8-N9	-11.69	107.95	113.80
22	BA	1717	A	N7-C8-N9	-11.69	107.95	113.80
22	BA	1953	A	N7-C8-N9	-11.69	107.95	113.80
1	AA	563	A	N3-C4-C5	-11.69	118.62	126.80
1	AA	777	A	C5-C6-N6	11.69	133.05	123.70
22	BA	2590	A	N7-C8-N9	-11.69	107.96	113.80
22	BA	538	A	C5-C6-N6	11.69	133.05	123.70
22	BA	1490	A	N7-C8-N9	-11.69	107.96	113.80
22	BA	2376	A	N7-C8-N9	-11.69	107.96	113.80
1	AA	1534	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	167	A	N7-C8-N9	-11.68	107.96	113.80
1	AA	344	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	1932	A	C5-C6-N6	11.68	133.04	123.70
22	BA	1302	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	324	A	N7-C8-N9	-11.67	107.96	113.80
22	BA	1269	A	N3-C4-C5	-11.67	118.63	126.80
1	AA	98	A	N7-C8-N9	-11.67	107.96	113.80
22	BA	1085	A	N7-C8-N9	-11.67	107.97	113.80
22	BA	1276	A	N7-C8-N9	-11.67	107.96	113.80
22	BA	44	A	N7-C8-N9	-11.67	107.97	113.80
1	AA	767	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	1346	A	C5-C6-N6	11.66	133.03	123.70
22	BA	172	A	N7-C8-N9	-11.66	107.97	113.80
22	BA	574	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	78	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	574	A	C5-C6-N6	11.66	133.03	123.70
1	AA	675	A	N7-C8-N9	-11.66	107.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	752	A	C5-C6-N6	11.66	133.03	123.70
1	AA	195	A	C5-C6-N6	11.66	133.03	123.70
22	BA	1735	A	N7-C8-N9	-11.66	107.97	113.80
1	AA	635	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	2468	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	496	A	C5-C6-N6	11.65	133.02	123.70
1	AA	794	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	311	A	C5-C6-N6	11.65	133.02	123.70
22	BA	1040	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	2765	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	510	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	983	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	821	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	1508	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	1513	A	N7-C8-N9	-11.65	107.97	113.80
1	AA	1363	A	N7-C8-N9	-11.65	107.98	113.80
22	BA	2158	A	N7-C8-N9	-11.65	107.98	113.80
22	BA	2721	A	N3-C4-C5	-11.65	118.65	126.80
22	BA	960	A	N3-C4-C5	-11.64	118.65	126.80
22	BA	685	A	N3-C4-C5	-11.64	118.65	126.80
22	BA	1787	A	N3-C4-C5	-11.64	118.65	126.80
22	BA	1872	A	N3-C4-C5	-11.64	118.65	126.80
1	AA	559	A	C5-C6-N6	11.64	133.01	123.70
22	BA	219	A	C5-C6-N6	11.64	133.01	123.70
22	BA	927	A	N7-C8-N9	-11.64	107.98	113.80
1	AA	495	A	N7-C8-N9	-11.63	107.98	113.80
22	BA	156	A	N7-C8-N9	-11.64	107.98	113.80
22	BA	2547	A	C5-C6-N6	11.63	133.01	123.70
1	AA	695	A	N7-C8-N9	-11.63	107.98	113.80
1	AA	889	A	C5-C6-N6	11.63	133.01	123.70
22	BA	804	A	N7-C8-N9	-11.63	107.98	113.80
22	BA	391	A	N7-C8-N9	-11.63	107.99	113.80
22	BA	2600	A	N7-C8-N9	-11.63	107.99	113.80
1	AA	1252	A	N7-C8-N9	-11.63	107.99	113.80
22	BA	1668	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	72	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	363	A	N7-C8-N9	-11.62	107.99	113.80
1	AA	831	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	1773	A	N3-C4-C5	-11.62	118.67	126.80
22	BA	2872	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	1522	A	C5-C6-N6	11.62	132.99	123.70
22	BA	2893	A	N7-C8-N9	-11.61	107.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2761	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	1483	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	749	A	N7-C8-N9	-11.61	108.00	113.80
22	BA	572	A	C5-C6-N6	11.61	132.98	123.70
22	BA	2813	A	N7-C8-N9	-11.61	108.00	113.80
1	AA	1236	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	1289	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	226	A	N3-C4-C5	-11.60	118.68	126.80
22	BA	654	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	1021	A	C5-C6-N6	11.60	132.98	123.70
22	BA	1762	A	C5-C6-N6	11.60	132.98	123.70
22	BA	2278	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	2566	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	83	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	1654	A	C5-C6-N6	11.60	132.98	123.70
22	BA	1789	A	N3-C4-C5	-11.60	118.68	126.80
22	BA	782	A	C5-C6-N6	11.60	132.98	123.70
22	BA	878	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	1504	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	936	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	2117	A	N7-C8-N9	-11.60	108.00	113.80
1	AA	640	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	1433	A	N7-C8-N9	-11.59	108.00	113.80
22	BA	529	A	C5-C6-N6	11.59	132.97	123.70
22	BA	750	A	N7-C8-N9	-11.59	108.00	113.80
22	BA	981	A	C5-C6-N6	11.59	132.97	123.70
22	BA	2388	A	C5-C6-N6	11.59	132.97	123.70
22	BA	2883	A	N7-C8-N9	-11.59	108.00	113.80
1	AA	131	A	N7-C8-N9	-11.59	108.01	113.80
22	BA	412	A	N7-C8-N9	-11.59	108.01	113.80
22	BA	2322	A	N7-C8-N9	-11.59	108.01	113.80
1	AA	179	A	C5-C6-N6	11.58	132.97	123.70
1	AA	687	A	C5-C6-N6	11.58	132.97	123.70
22	BA	404	A	N7-C8-N9	-11.58	108.01	113.80
22	BA	621	A	C5-C6-N6	11.58	132.97	123.70
22	BA	1434	A	N7-C8-N9	-11.58	108.01	113.80
1	AA	303	A	N7-C8-N9	-11.58	108.01	113.80
22	BA	221	A	N7-C8-N9	-11.58	108.01	113.80
22	BA	270	A	N7-C8-N9	-11.58	108.01	113.80
22	BA	1165	A	C5-C6-N6	11.58	132.96	123.70
22	BA	2740	A	N7-C8-N9	-11.58	108.01	113.80
22	BA	689	A	N7-C8-N9	-11.58	108.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2614	A	C5-C6-N6	11.58	132.96	123.70
22	BA	1583	A	C5-C6-N6	11.58	132.96	123.70
22	BA	1700	A	C5-C6-N6	11.58	132.96	123.70
1	AA	1357	A	C5-C6-N6	11.57	132.96	123.70
22	BA	1383	A	C5-C6-N6	11.57	132.96	123.70
1	AA	938	A	N3-C4-C5	-11.57	118.70	126.80
22	BA	2749	A	C5-C6-N6	11.57	132.96	123.70
22	BA	1677	A	C5-C6-N6	11.57	132.96	123.70
22	BA	2388	A	N7-C8-N9	-11.57	108.02	113.80
22	BA	582	A	C5-C6-N6	11.56	132.95	123.70
1	AA	288	A	C5-C6-N6	11.56	132.95	123.70
22	BA	1701	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	1333	A	C5-C6-N6	11.56	132.95	123.70
22	BA	152	A	N7-C8-N9	-11.56	108.02	113.80
22	BA	1090	A	N7-C8-N9	-11.56	108.02	113.80
22	BA	2019	A	N7-C8-N9	-11.56	108.02	113.80
1	AA	408	A	N7-C8-N9	-11.55	108.02	113.80
22	BA	1067	A	N7-C8-N9	-11.55	108.02	113.80
1	AA	320	A	C5-C6-N6	11.55	132.94	123.70
1	AA	320	A	N7-C8-N9	-11.55	108.02	113.80
1	AA	816	A	N7-C8-N9	-11.55	108.02	113.80
1	AA	116	A	N7-C8-N9	-11.55	108.03	113.80
1	AA	1410	A	N7-C8-N9	-11.55	108.02	113.80
22	BA	1801	A	N7-C8-N9	-11.55	108.02	113.80
22	BA	1890	A	N7-C8-N9	-11.55	108.03	113.80
22	BA	118	A	N7-C8-N9	-11.55	108.03	113.80
22	BA	1569	A	C5-C6-N6	11.55	132.94	123.70
22	BA	2814	A	C5-C6-N6	11.55	132.94	123.70
1	AA	1299	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1418	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	2749	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1169	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	1321	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	2823	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	5	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	1572	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	353	A	N7-C8-N9	-11.53	108.03	113.80
1	AA	1042	A	N7-C8-N9	-11.54	108.03	113.80
1	AA	1191	A	N7-C8-N9	-11.53	108.03	113.80
22	BA	706	A	C5-C6-N6	11.54	132.93	123.70
22	BA	2736	A	C5-C6-N6	11.54	132.93	123.70
22	BA	1008	A	C5-C6-N6	11.53	132.93	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1010	A	N7-C8-N9	-11.53	108.03	113.80
1	AA	51	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	253	A	C5-C6-N6	11.53	132.92	123.70
1	AA	1035	A	C5-C6-N6	11.53	132.92	123.70
22	BA	330	A	C5-C6-N6	11.53	132.92	123.70
22	BA	508	A	N7-C8-N9	-11.53	108.03	113.80
22	BA	1525	A	C5-C6-N6	11.53	132.92	123.70
22	BA	322	A	C5-C6-N6	11.53	132.92	123.70
1	AA	563	A	N7-C8-N9	-11.53	108.04	113.80
22	BA	1048	A	N7-C8-N9	-11.53	108.04	113.80
1	AA	66	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	265	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1428	A	N7-C8-N9	-11.52	108.04	113.80
1	AA	1476	A	C5-C6-N6	11.52	132.92	123.70
22	BA	262	A	C5-C6-N6	11.52	132.92	123.70
22	BA	332	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	2705	A	C5-C6-N6	11.52	132.92	123.70
22	BA	900	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	1144	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	2031	A	C5-C6-N6	11.52	132.92	123.70
22	BA	896	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	782	A	N3-C4-C5	-11.52	118.74	126.80
22	BA	2170	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	504	A	N7-C8-N9	-11.51	108.04	113.80
1	AA	190	A	N3-C4-C5	-11.51	118.74	126.80
22	BA	541	A	C5-C6-N6	11.51	132.91	123.70
23	BB	57	A	C5-C6-N6	11.51	132.91	123.70
1	AA	172	A	C5-C6-N6	11.51	132.91	123.70
1	AA	263	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	535	A	N7-C8-N9	-11.51	108.05	113.80
22	BA	53	A	C5-C6-N6	11.51	132.91	123.70
22	BA	866	A	C5-C6-N6	11.51	132.91	123.70
22	BA	1096	A	N7-C8-N9	-11.51	108.05	113.80
22	BA	2062	A	C5-C6-N6	11.51	132.91	123.70
1	AA	1239	A	C5-C6-N6	11.51	132.91	123.70
1	AA	1274	A	N7-C8-N9	-11.51	108.05	113.80
22	BA	2589	A	N7-C8-N9	-11.51	108.05	113.80
1	AA	1398	A	N7-C8-N9	-11.51	108.05	113.80
22	BA	1899	A	C5-C6-N6	11.51	132.91	123.70
1	AA	676	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	2287	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	50	A	N7-C8-N9	-11.50	108.05	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1362	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	1155	A	C5-C6-N6	11.50	132.90	123.70
22	BA	1246	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	1899	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	2682	A	N7-C8-N9	-11.50	108.05	113.80
1	AA	1145	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	1853	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	256	A	C5-C6-N6	11.49	132.90	123.70
1	AA	65	A	N7-C8-N9	-11.49	108.06	113.80
1	AA	918	A	N7-C8-N9	-11.49	108.05	113.80
22	BA	829	A	C5-C6-N6	11.49	132.89	123.70
22	BA	2882	A	C5-C6-N6	11.49	132.89	123.70
1	AA	19	A	N7-C8-N9	-11.49	108.06	113.80
23	BB	45	A	C5-C6-N6	11.48	132.89	123.70
22	BA	6	A	N7-C8-N9	-11.48	108.06	113.80
1	AA	196	A	C5-C6-N6	11.48	132.88	123.70
22	BA	1635	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	1927	A	C5-C6-N6	11.48	132.88	123.70
1	AA	120	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	1876	A	N7-C8-N9	-11.47	108.06	113.80
22	BA	1269	A	N7-C8-N9	-11.47	108.06	113.80
22	BA	1535	A	N7-C8-N9	-11.47	108.06	113.80
22	BA	299	A	C5-C6-N6	11.47	132.88	123.70
22	BA	1268	A	N7-C8-N9	-11.47	108.07	113.80
22	BA	13	A	N3-C4-C5	-11.46	118.78	126.80
22	BA	1634	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	393	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	520	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	294	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	1669	A	N3-C4-C5	-11.46	118.78	126.80
22	BA	28	A	C5-C6-N6	11.46	132.87	123.70
22	BA	1327	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	907	A	N7-C8-N9	-11.46	108.07	113.80
1	AA	937	A	N7-C8-N9	-11.46	108.07	113.80
23	BB	99	A	C5-C6-N6	11.46	132.87	123.70
22	BA	2335	A	C5-C6-N6	11.46	132.87	123.70
1	AA	908	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	2273	A	N3-C4-C5	-11.45	118.78	126.80
22	BA	996	A	N7-C8-N9	-11.45	108.08	113.80
22	BA	2042	A	N7-C8-N9	-11.45	108.08	113.80
1	AA	1280	A	C5-C6-N6	11.45	132.86	123.70
1	AA	1306	A	N7-C8-N9	-11.45	108.08	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1396	A	N7-C8-N9	-11.45	108.08	113.80
22	BA	5	A	C5-C6-N6	11.45	132.86	123.70
22	BA	226	A	C5-C6-N6	11.45	132.86	123.70
22	BA	501	A	C5-C6-N6	11.45	132.86	123.70
22	BA	637	A	C5-C6-N6	11.45	132.86	123.70
22	BA	513	A	N3-C4-C5	-11.45	118.79	126.80
22	BA	272	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	2461	A	N3-C4-C5	-11.44	118.79	126.80
1	AA	451	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1204	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	1032	A	C5-C6-N6	11.44	132.85	123.70
22	BA	1665	A	C5-C6-N6	11.44	132.85	123.70
22	BA	2565	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	642	A	C5-C6-N6	11.44	132.85	123.70
22	BA	1077	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	50	A	C5-C6-N6	11.44	132.85	123.70
1	AA	1080	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	996	A	N7-C8-N9	-11.44	108.08	113.80
1	AA	1269	A	C5-C6-N6	11.44	132.85	123.70
22	BA	2810	A	C5-C6-N6	11.44	132.85	123.70
22	BA	1610	A	N7-C8-N9	-11.43	108.08	113.80
22	BA	2516	A	N7-C8-N9	-11.43	108.08	113.80
22	BA	42	A	N7-C8-N9	-11.43	108.08	113.80
22	BA	149	A	C5-C6-N6	11.43	132.84	123.70
22	BA	165	A	N7-C8-N9	-11.43	108.08	113.80
22	BA	300	A	N7-C8-N9	-11.43	108.08	113.80
1	AA	1350	A	N3-C4-C5	-11.43	118.80	126.80
22	BA	1579	A	N7-C8-N9	-11.43	108.09	113.80
22	BA	2314	A	N7-C8-N9	-11.43	108.09	113.80
22	BA	2882	A	N7-C8-N9	-11.43	108.09	113.80
22	BA	2060	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	2639	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	1005	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	126	A	N3-C4-C5	-11.42	118.81	126.80
22	BA	449	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	2336	A	C5-C6-N6	11.42	132.84	123.70
22	BA	1871	A	C5-C6-N6	11.42	132.83	123.70
22	BA	2241	A	N7-C8-N9	-11.42	108.09	113.80
1	AA	155	A	N7-C8-N9	-11.41	108.09	113.80
22	BA	472	A	C5-C6-N6	11.41	132.83	123.70
22	BA	2274	A	C5-C6-N6	11.41	132.83	123.70
22	BA	2328	A	N3-C4-C5	-11.41	118.81	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1534	A	C5-C6-N6	11.41	132.83	123.70
22	BA	217	A	C5-C6-N6	11.41	132.83	123.70
22	BA	1189	A	C5-C6-N6	11.41	132.83	123.70
22	BA	1757	A	N7-C8-N9	-11.41	108.09	113.80
22	BA	1801	A	C5-C6-N6	11.41	132.83	123.70
1	AA	321	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	1146	A	C5-C6-N6	11.41	132.83	123.70
1	AA	28	A	N3-C4-C5	-11.41	118.81	126.80
22	BA	2198	A	N7-C8-N9	-11.41	108.09	113.80
1	AA	759	A	N7-C8-N9	-11.41	108.10	113.80
22	BA	1156	A	N7-C8-N9	-11.41	108.10	113.80
1	AA	768	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	1092	A	C5-C6-N6	11.40	132.82	123.70
22	BA	1077	A	C5-C6-N6	11.40	132.82	123.70
22	BA	1502	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	1446	A	N7-C8-N9	-11.40	108.10	113.80
1	AA	452	A	N7-C8-N9	-11.39	108.10	113.80
22	BA	101	A	N3-C4-C5	-11.39	118.83	126.80
22	BA	1048	A	C5-C6-N6	11.39	132.81	123.70
22	BA	1772	A	C5-C6-N6	11.39	132.81	123.70
22	BA	2070	A	C5-C6-N6	11.39	132.81	123.70
22	BA	101	A	N7-C8-N9	-11.39	108.10	113.80
22	BA	655	A	C5-C6-N6	11.39	132.81	123.70
22	BA	911	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	1970	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	2225	A	N7-C8-N9	-11.39	108.11	113.80
1	AA	109	A	C5-C6-N6	11.39	132.81	123.70
22	BA	103	A	C5-C6-N6	11.39	132.81	123.70
22	BA	866	A	N7-C8-N9	-11.39	108.11	113.80
1	AA	1394	A	N7-C8-N9	-11.38	108.11	113.80
22	BA	1359	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	432	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	1318	A	N7-C8-N9	-11.38	108.11	113.80
23	BB	53	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	532	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	746	A	N3-C4-C5	-11.38	118.83	126.80
22	BA	2560	A	C5-C6-N6	11.38	132.80	123.70
22	BA	447	A	C5-C6-N6	11.37	132.80	123.70
22	BA	2887	A	N7-C8-N9	-11.38	108.11	113.80
1	AA	288	A	N7-C8-N9	-11.37	108.11	113.80
1	AA	782	A	C5-C6-N6	11.37	132.80	123.70
22	BA	197	A	N7-C8-N9	-11.37	108.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	452	A	C5-C6-N6	11.37	132.79	123.70
22	BA	1014	A	C5-C6-N6	11.37	132.79	123.70
22	BA	2052	A	N3-C4-C5	-11.37	118.84	126.80
22	BA	111	A	N7-C8-N9	-11.37	108.12	113.80
22	BA	428	A	C5-C6-N6	11.37	132.79	123.70
22	BA	1630	A	C5-C6-N6	11.37	132.79	123.70
22	BA	2314	A	C5-C6-N6	11.37	132.79	123.70
22	BA	2346	A	N7-C8-N9	-11.37	108.12	113.80
22	BA	2381	A	C5-C6-N6	11.36	132.79	123.70
22	BA	2766	A	C5-C6-N6	11.36	132.79	123.70
1	AA	1250	A	C5-C6-N6	11.36	132.79	123.70
1	AA	1499	A	N7-C8-N9	-11.36	108.12	113.80
55	B8	38	A	C5-C6-N6	11.36	132.79	123.70
22	BA	608	A	N7-C8-N9	-11.36	108.12	113.80
22	BA	1084	A	N7-C8-N9	-11.36	108.12	113.80
1	AA	441	A	C5-C6-N6	11.36	132.79	123.70
1	AA	712	A	N3-C4-C5	-11.36	118.85	126.80
1	AA	728	A	C5-C6-N6	11.36	132.79	123.70
22	BA	1901	A	C5-C6-N6	11.36	132.79	123.70
23	BB	99	A	N7-C8-N9	-11.36	108.12	113.80
1	AA	51	A	C5-C6-N6	11.36	132.78	123.70
1	AA	1146	A	N7-C8-N9	-11.36	108.12	113.80
22	BA	144	A	N7-C8-N9	-11.36	108.12	113.80
22	BA	529	A	N7-C8-N9	-11.36	108.12	113.80
22	BA	984	A	N3-C4-C5	-11.36	118.85	126.80
22	BA	1614	A	N7-C8-N9	-11.36	108.12	113.80
22	BA	2014	A	C5-C6-N6	11.36	132.78	123.70
1	AA	44	A	N7-C8-N9	-11.35	108.12	113.80
1	AA	909	A	C5-C6-N6	11.35	132.78	123.70
1	AA	1250	A	N7-C8-N9	-11.35	108.12	113.80
1	AA	1441	A	N7-C8-N9	-11.35	108.12	113.80
22	BA	1805	A	N7-C8-N9	-11.35	108.12	113.80
22	BA	2820	A	N7-C8-N9	-11.35	108.12	113.80
55	B8	6	A	N7-C8-N9	-11.35	108.12	113.80
1	AA	1248	A	N7-C8-N9	-11.35	108.12	113.80
22	BA	2163	A	C5-C6-N6	11.35	132.78	123.70
1	AA	1332	A	C5-C6-N6	11.35	132.78	123.70
22	BA	574	A	N3-C4-C5	-11.35	118.86	126.80
22	BA	1387	A	N3-C4-C5	-11.35	118.86	126.80
22	BA	119	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	373	A	N7-C8-N9	-11.34	108.13	113.80
1	AA	270	A	N7-C8-N9	-11.34	108.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	735	A	N7-C8-N9	-11.34	108.13	113.80
22	BA	1928	A	N7-C8-N9	-11.34	108.13	113.80
22	BA	497	A	C5-C6-N6	11.34	132.77	123.70
23	BB	73	A	N7-C8-N9	-11.34	108.13	113.80
22	BA	64	A	N7-C8-N9	-11.33	108.13	113.80
1	AA	780	A	C5-C6-N6	11.33	132.77	123.70
23	BB	94	A	C5-C6-N6	11.33	132.77	123.70
1	AA	1311	A	N7-C8-N9	-11.33	108.13	113.80
1	AA	139	A	N7-C8-N9	-11.33	108.14	113.80
22	BA	2872	A	N9-C4-C5	11.33	110.33	105.80
22	BA	2358	A	C5-C6-N6	11.32	132.76	123.70
1	AA	353	A	C5-C6-N6	11.32	132.76	123.70
22	BA	1515	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	2173	A	C5-C6-N6	11.32	132.76	123.70
22	BA	1598	A	C5-C6-N6	11.32	132.76	123.70
22	BA	1088	A	C5-C6-N6	11.32	132.76	123.70
22	BA	2173	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	315	A	C5-C6-N6	11.32	132.75	123.70
22	BA	347	A	C5-C6-N6	11.32	132.75	123.70
22	BA	988	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	729	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	2856	A	C5-C6-N6	11.32	132.75	123.70
23	BB	101	A	N7-C8-N9	-11.32	108.14	113.80
1	AA	1465	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	236	A	C5-C6-N6	11.31	132.75	123.70
22	BA	666	A	N7-C8-N9	-11.31	108.14	113.80
1	AA	1256	A	N7-C8-N9	-11.31	108.15	113.80
22	BA	1744	A	C5-C6-N6	11.31	132.75	123.70
22	BA	2327	A	N7-C8-N9	-11.31	108.15	113.80
1	AA	2	A	N7-C8-N9	-11.31	108.15	113.80
1	AA	1349	A	C5-C6-N6	11.30	132.74	123.70
22	BA	945	A	C5-C6-N6	11.30	132.74	123.70
22	BA	1272	A	C5-C6-N6	11.30	132.74	123.70
1	AA	366	A	C5-C6-N6	11.30	132.74	123.70
1	AA	702	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	2733	A	C5-C6-N6	11.30	132.74	123.70
1	AA	825	A	C5-C6-N6	11.30	132.74	123.70
22	BA	2826	A	N3-C4-C5	-11.30	118.89	126.80
22	BA	2851	A	C5-C6-N6	11.30	132.74	123.70
1	AA	171	A	C5-C6-N6	11.30	132.74	123.70
1	AA	694	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	1216	A	N7-C8-N9	-11.30	108.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1384	A	C5-C6-N6	11.30	132.74	123.70
22	BA	1711	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	325	A	C5-C6-N6	11.30	132.74	123.70
22	BA	1784	A	N7-C8-N9	-11.30	108.15	113.80
1	AA	59	A	C5-C6-N6	11.30	132.74	123.70
22	BA	670	A	C5-C6-N6	11.30	132.74	123.70
22	BA	792	A	C5-C6-N6	11.29	132.74	123.70
22	BA	1810	A	C4-C5-C6	11.29	122.65	117.00
22	BA	2071	A	N3-C4-C5	-11.29	118.89	126.80
22	BA	2823	A	C5-C6-N6	11.30	132.74	123.70
22	BA	2757	A	N3-C4-C5	-11.29	118.89	126.80
1	AA	109	A	N7-C8-N9	-11.29	108.15	113.80
22	BA	2572	A	N7-C8-N9	-11.29	108.15	113.80
1	AA	1357	A	N7-C8-N9	-11.29	108.15	113.80
22	BA	2837	A	N7-C8-N9	-11.29	108.15	113.80
22	BA	2298	A	C5-C6-N6	11.29	132.73	123.70
1	AA	74	A	N7-C8-N9	-11.28	108.16	113.80
1	AA	364	A	C5-C6-N6	11.28	132.72	123.70
1	AA	478	A	C5-C6-N6	11.28	132.73	123.70
22	BA	1378	A	N3-C4-C5	-11.28	118.90	126.80
1	AA	1130	A	N7-C8-N9	-11.28	108.16	113.80
1	AA	81	A	N7-C8-N9	-11.27	108.16	113.80
22	BA	1749	A	C5-C6-N6	11.27	132.72	123.70
1	AA	1167	A	C5-C6-N6	11.27	132.72	123.70
22	BA	590	A	N7-C8-N9	-11.27	108.16	113.80
22	BA	1544	A	C5-C6-N6	11.27	132.72	123.70
22	BA	613	A	C5-C6-N6	11.27	132.72	123.70
22	BA	2766	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	1069	A	C5-C6-N6	11.27	132.72	123.70
22	BA	505	A	C5-C6-N6	11.27	132.71	123.70
22	BA	863	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	1287	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	2211	A	C5-C6-N6	11.27	132.71	123.70
22	BA	2873	A	C5-C6-N6	11.27	132.71	123.70
22	BA	2738	A	C5-C6-N6	11.26	132.71	123.70
1	AA	860	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	781	A	C5-C6-N6	11.26	132.71	123.70
22	BA	1129	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	1866	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	676	A	C5-C6-N6	11.26	132.70	123.70
22	BA	979	A	C5-C6-N6	11.26	132.71	123.70
22	BA	2267	A	C5-C6-N6	11.26	132.70	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	408	A	C5-C6-N6	11.25	132.70	123.70
22	BA	345	A	N7-C8-N9	-11.25	108.17	113.80
22	BA	739	A	C5-C6-N6	11.25	132.70	123.70
22	BA	1998	A	N3-C4-C5	-11.25	118.92	126.80
22	BA	2134	A	C5-C6-N6	11.25	132.70	123.70
22	BA	661	A	N7-C8-N9	-11.25	108.17	113.80
22	BA	1433	A	C5-C6-N6	11.25	132.70	123.70
1	AA	807	A	N7-C8-N9	-11.25	108.18	113.80
22	BA	2097	A	N7-C8-N9	-11.25	108.18	113.80
1	AA	1036	A	C5-C6-N6	11.24	132.70	123.70
22	BA	2810	A	N7-C8-N9	-11.24	108.18	113.80
1	AA	781	A	N7-C8-N9	-11.24	108.18	113.80
22	BA	449	A	C5-C6-N6	11.24	132.69	123.70
22	BA	1551	A	C5-C6-N6	11.24	132.69	123.70
22	BA	2800	A	C5-C6-N6	11.24	132.69	123.70
23	BB	108	A	C5-C6-N6	11.24	132.70	123.70
1	AA	704	A	N7-C8-N9	-11.24	108.18	113.80
22	BA	1014	A	N7-C8-N9	-11.24	108.18	113.80
22	BA	1784	A	C5-C6-N6	11.24	132.69	123.70
22	BA	1919	A	C5-C6-N6	11.24	132.69	123.70
22	BA	504	A	C5-C6-N6	11.24	132.69	123.70
22	BA	2101	A	N3-C4-C5	-11.24	118.93	126.80
22	BA	2634	A	N3-C4-C5	-11.24	118.93	126.80
1	AA	325	A	N7-C8-N9	-11.23	108.18	113.80
1	AA	860	A	C5-C6-N6	11.23	132.69	123.70
1	AA	1157	A	N7-C8-N9	-11.23	108.18	113.80
1	AA	676	A	C5-C6-N6	11.23	132.69	123.70
22	BA	1089	A	N7-C8-N9	-11.23	108.18	113.80
22	BA	1528	A	N3-C4-C5	-11.23	118.94	126.80
22	BA	1918	A	C5-C6-N6	11.23	132.68	123.70
22	BA	1809	A	C5-C6-N6	11.23	132.68	123.70
1	AA	101	A	N7-C8-N9	-11.23	108.19	113.80
22	BA	614	A	C5-C6-N6	11.23	132.68	123.70
22	BA	792	A	N7-C8-N9	-11.23	108.19	113.80
22	BA	2169	A	C5-C6-N6	11.23	132.68	123.70
23	BB	109	A	N7-C8-N9	-11.23	108.19	113.80
22	BA	877	A	C5-C6-N6	11.22	132.68	123.70
1	AA	435	A	N7-C8-N9	-11.22	108.19	113.80
1	AA	609	A	N7-C8-N9	-11.22	108.19	113.80
1	AA	1531	A	N7-C8-N9	-11.22	108.19	113.80
1	AA	1	A	N3-C4-C5	-11.22	118.95	126.80
22	BA	348	A	N7-C8-N9	-11.22	108.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	633	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	2388	A	N3-C4-C5	-11.22	118.94	126.80
22	BA	2851	A	N7-C8-N9	-11.22	108.19	113.80
1	AA	964	A	C5-C6-N6	11.22	132.68	123.70
22	BA	722	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	1260	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	1640	A	C5-C6-N6	11.22	132.68	123.70
1	AA	3	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	2566	A	C5-C6-N6	11.22	132.67	123.70
22	BA	1885	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	2088	A	N7-C8-N9	-11.21	108.19	113.80
23	BB	50	A	C5-C6-N6	11.21	132.67	123.70
1	AA	26	A	N7-C8-N9	-11.21	108.19	113.80
1	AA	182	A	C5-C6-N6	11.21	132.67	123.70
1	AA	300	A	N3-C4-C5	-11.21	118.95	126.80
1	AA	313	A	N3-C4-C5	-11.21	118.95	126.80
1	AA	996	A	C5-C6-N6	11.21	132.67	123.70
55	B8	14	A	C5-C6-N6	11.21	132.67	123.70
1	AA	1036	A	N7-C8-N9	-11.21	108.20	113.80
1	AA	1238	A	N7-C8-N9	-11.21	108.20	113.80
22	BA	1392	A	N7-C8-N9	-11.21	108.20	113.80
22	BA	2366	A	N3-C4-C5	-11.21	118.95	126.80
1	AA	389	A	N7-C8-N9	-11.21	108.20	113.80
1	AA	468	A	C5-C6-N6	11.21	132.66	123.70
1	AA	487	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	126	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	483	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	479	A	C5-C6-N6	11.20	132.66	123.70
22	BA	1214	A	C5-C6-N6	11.20	132.66	123.70
22	BA	2054	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	2270	A	C5-C6-N6	11.20	132.66	123.70
22	BA	2317	A	N7-C8-N9	-11.20	108.20	113.80
1	AA	1492	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	1262	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	2425	A	N3-C4-C5	-11.20	118.96	126.80
22	BA	2634	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	219	A	N3-C4-C5	-11.19	118.97	126.80
22	BA	347	A	N3-C4-C5	-11.19	118.97	126.80
22	BA	1308	A	N3-C4-C5	-11.19	118.97	126.80
22	BA	1268	A	C5-C6-N6	11.19	132.65	123.70
22	BA	1269	A	C5-C6-N6	11.19	132.65	123.70
1	AA	1225	A	N3-C4-C5	-11.19	118.97	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	111	A	C5-C6-N6	11.18	132.65	123.70
22	BA	430	A	N7-C8-N9	-11.18	108.21	113.80
22	BA	2015	A	N7-C8-N9	-11.18	108.21	113.80
1	AA	768	A	C5-C6-N6	11.18	132.64	123.70
22	BA	63	A	N7-C8-N9	-11.18	108.21	113.80
1	AA	1394	A	C5-C6-N6	11.18	132.64	123.70
22	BA	195	A	C5-C6-N6	11.18	132.64	123.70
22	BA	928	A	C5-C6-N6	11.18	132.64	123.70
22	BA	191	A	N7-C8-N9	-11.18	108.21	113.80
22	BA	742	A	N3-C4-C5	-11.18	118.98	126.80
1	AA	338	A	N7-C8-N9	-11.17	108.21	113.80
1	AA	706	A	N3-C4-C5	-11.17	118.98	126.80
22	BA	2700	A	C5-C6-N6	11.17	132.64	123.70
22	BA	1877	A	N7-C8-N9	-11.17	108.21	113.80
1	AA	1169	A	C5-C6-N6	11.17	132.64	123.70
22	BA	1276	A	C5-C6-N6	11.17	132.64	123.70
22	BA	1593	A	N7-C8-N9	-11.17	108.22	113.80
22	BA	2033	A	N7-C8-N9	-11.17	108.21	113.80
22	BA	2453	A	N7-C8-N9	-11.17	108.22	113.80
1	AA	949	A	N7-C8-N9	-11.17	108.22	113.80
1	AA	1447	A	N7-C8-N9	-11.17	108.22	113.80
1	AA	1500	A	N7-C8-N9	-11.17	108.22	113.80
22	BA	750	A	N3-C4-C5	-11.17	118.98	126.80
22	BA	819	A	N3-C4-C5	-11.17	118.98	126.80
22	BA	2654	A	C5-C6-N6	11.17	132.63	123.70
22	BA	2059	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	2191	A	N7-C8-N9	-11.16	108.22	113.80
1	AA	608	A	N7-C8-N9	-11.16	108.22	113.80
1	AA	649	A	C5-C6-N6	11.16	132.63	123.70
22	BA	1322	A	C5-C6-N6	11.16	132.63	123.70
22	BA	182	A	C5-C6-N6	11.16	132.63	123.70
22	BA	1549	A	N7-C8-N9	-11.16	108.22	113.80
1	AA	1333	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	173	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	654	A	C5-C6-N6	11.15	132.62	123.70
22	BA	2147	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	167	A	C5-C6-N6	11.15	132.62	123.70
1	AA	1092	A	N7-C8-N9	-11.15	108.22	113.80
22	BA	176	A	N7-C8-N9	-11.15	108.22	113.80
22	BA	470	A	N3-C4-C5	-11.15	119.00	126.80
22	BA	1977	A	N7-C8-N9	-11.15	108.22	113.80
1	AA	1145	A	C5-C6-N6	11.15	132.62	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1952	A	N7-C8-N9	-11.15	108.23	113.80
1	AA	451	A	C5-C6-N6	11.15	132.62	123.70
1	AA	1428	A	C5-C6-N6	11.15	132.62	123.70
22	BA	439	A	N3-C4-C5	-11.15	119.00	126.80
22	BA	1301	A	N7-C8-N9	-11.15	108.23	113.80
22	BA	2171	A	N7-C8-N9	-11.15	108.23	113.80
1	AA	179	A	N7-C8-N9	-11.14	108.23	113.80
22	BA	56	A	N3-C4-C5	-11.14	119.00	126.80
22	BA	483	A	C5-C6-N6	11.14	132.62	123.70
22	BA	1810	A	N3-C4-C5	-11.14	119.00	126.80
22	BA	1913	A	C5-C6-N6	11.14	132.62	123.70
22	BA	2883	A	C5-C6-N6	11.14	132.62	123.70
55	B8	58	A	C5-C6-N6	11.14	132.62	123.70
22	BA	371	A	C5-C6-N6	11.14	132.61	123.70
22	BA	2476	A	N7-C8-N9	-11.14	108.23	113.80
1	AA	344	A	C5-C6-N6	11.14	132.61	123.70
1	AA	1012	A	N7-C8-N9	-11.14	108.23	113.80
22	BA	118	A	C5-C6-N6	11.14	132.61	123.70
22	BA	878	A	C5-C6-N6	11.14	132.61	123.70
22	BA	988	A	C5-C6-N6	11.14	132.61	123.70
1	AA	1046	A	N7-C8-N9	-11.13	108.23	113.80
22	BA	1308	A	N7-C8-N9	-11.14	108.23	113.80
1	AA	1360	A	C5-C6-N6	11.13	132.61	123.70
1	AA	1434	A	C5-C6-N6	11.13	132.60	123.70
22	BA	241	A	N7-C8-N9	-11.13	108.23	113.80
22	BA	1354	A	N7-C8-N9	-11.13	108.23	113.80
22	BA	1783	A	C5-C6-N6	11.13	132.61	123.70
1	AA	559	A	N7-C8-N9	-11.13	108.23	113.80
22	BA	2879	A	N7-C8-N9	-11.13	108.23	113.80
22	BA	478	A	N7-C8-N9	-11.13	108.24	113.80
22	BA	1089	A	C5-C6-N6	11.13	132.60	123.70
22	BA	161	A	N7-C8-N9	-11.13	108.24	113.80
1	AA	1251	A	C5-C6-N6	11.12	132.60	123.70
22	BA	282	A	C5-C6-N6	11.12	132.60	123.70
22	BA	1872	A	N7-C8-N9	-11.13	108.24	113.80
23	BB	46	A	C5-C6-N6	11.13	132.60	123.70
22	BA	675	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	1535	A	C5-C6-N6	11.12	132.60	123.70
22	BA	2856	A	N7-C8-N9	-11.12	108.24	113.80
1	AA	465	A	N7-C8-N9	-11.12	108.24	113.80
1	AA	1441	A	C5-C6-N6	11.12	132.59	123.70
22	BA	2430	A	C5-C6-N6	11.12	132.59	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	941	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	2587	A	N7-C8-N9	-11.12	108.24	113.80
1	AA	790	A	N7-C8-N9	-11.12	108.24	113.80
1	AA	1225	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	74	A	C5-C6-N6	11.12	132.59	123.70
22	BA	2411	A	C5-C6-N6	11.12	132.59	123.70
23	BB	50	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	10	A	C5-C6-N6	11.11	132.59	123.70
22	BA	131	A	N7-C8-N9	-11.11	108.24	113.80
1	AA	923	A	N3-C4-C5	-11.11	119.02	126.80
22	BA	2679	A	C5-C6-N6	11.11	132.59	123.70
23	BB	15	A	C5-C6-N6	11.11	132.59	123.70
1	AA	712	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	1001	A	C5-C6-N6	11.11	132.59	123.70
22	BA	693	A	C5-C6-N6	11.11	132.59	123.70
22	BA	1127	A	N7-C8-N9	-11.11	108.25	113.80
1	AA	918	A	C5-C6-N6	11.11	132.59	123.70
22	BA	84	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	2119	A	C5-C6-N6	11.11	132.59	123.70
55	B8	58	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	1237	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	1285	A	C5-C6-N6	11.10	132.58	123.70
22	BA	1403	A	N3-C4-C5	-11.10	119.03	126.80
1	AA	977	A	N3-C4-C5	-11.10	119.03	126.80
1	AA	397	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	739	A	N3-C4-C5	-11.10	119.03	126.80
22	BA	2765	A	N3-C4-C5	-11.10	119.03	126.80
1	AA	120	A	C5-C6-N6	11.10	132.58	123.70
1	AA	642	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	1553	A	C5-C6-N6	11.10	132.58	123.70
1	AA	55	A	N3-C4-C5	-11.09	119.04	126.80
1	AA	642	A	N3-C4-C5	-11.09	119.03	126.80
22	BA	599	A	C5-C6-N6	11.09	132.57	123.70
1	AA	938	A	N7-C8-N9	-11.09	108.26	113.80
22	BA	1966	A	C5-C6-N6	11.09	132.57	123.70
22	BA	1111	A	N3-C4-C5	-11.09	119.04	126.80
1	AA	969	A	N7-C8-N9	-11.08	108.26	113.80
1	AA	1287	A	N7-C8-N9	-11.08	108.26	113.80
1	AA	533	A	N7-C8-N9	-11.08	108.26	113.80
1	AA	1430	A	N7-C8-N9	-11.08	108.26	113.80
22	BA	196	A	N7-C8-N9	-11.08	108.26	113.80
22	BA	52	A	N7-C8-N9	-11.08	108.26	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2741	A	C5-C6-N6	11.08	132.56	123.70
22	BA	1664	A	N3-C4-C5	-11.08	119.05	126.80
1	AA	864	A	C5-C6-N6	11.07	132.56	123.70
1	AA	663	A	N7-C8-N9	-11.07	108.26	113.80
22	BA	415	A	N7-C8-N9	-11.07	108.26	113.80
22	BA	2448	A	N7-C8-N9	-11.07	108.26	113.80
1	AA	466	A	C5-C6-N6	11.07	132.56	123.70
22	BA	346	A	N7-C8-N9	-11.07	108.26	113.80
22	BA	402	A	N7-C8-N9	-11.07	108.26	113.80
22	BA	1786	A	N7-C8-N9	-11.07	108.27	113.80
1	AA	908	A	C5-C6-N6	11.07	132.56	123.70
1	AA	1005	A	C5-C6-N6	11.07	132.56	123.70
22	BA	2014	A	N7-C8-N9	-11.07	108.27	113.80
1	AA	595	A	C5-C6-N6	11.07	132.56	123.70
1	AA	1256	A	C5-C6-N6	11.07	132.56	123.70
22	BA	1420	A	C5-C6-N6	11.07	132.55	123.70
22	BA	1366	A	N7-C8-N9	-11.07	108.27	113.80
1	AA	1176	A	N7-C8-N9	-11.06	108.27	113.80
1	AA	1251	A	N7-C8-N9	-11.06	108.27	113.80
1	AA	1468	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	73	A	C5-C6-N6	11.06	132.55	123.70
22	BA	182	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	1274	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	1403	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	2267	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	2753	A	N7-C8-N9	-11.06	108.27	113.80
1	AA	192	A	N7-C8-N9	-11.06	108.27	113.80
1	AA	728	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	300	A	C5-C6-N6	11.06	132.55	123.70
22	BA	1111	A	C5-C6-N6	11.06	132.55	123.70
1	AA	456	A	N7-C8-N9	-11.06	108.27	113.80
1	AA	994	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	362	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	943	A	N3-C4-C5	-11.06	119.06	126.80
1	AA	382	A	C5-C6-N6	11.05	132.54	123.70
22	BA	609	A	C5-C6-N6	11.06	132.54	123.70
22	BA	2241	A	C5-C6-N6	11.05	132.54	123.70
22	BA	2311	A	C5-C6-N6	11.06	132.54	123.70
1	AA	655	A	N3-C4-C5	-11.05	119.06	126.80
1	AA	919	A	N7-C8-N9	-11.05	108.27	113.80
1	AA	977	A	N7-C8-N9	-11.05	108.27	113.80
22	BA	492	A	N7-C8-N9	-11.05	108.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	541	A	N7-C8-N9	-11.05	108.27	113.80
22	BA	990	A	N7-C8-N9	-11.05	108.27	113.80
22	BA	1641	A	C5-C6-N6	11.05	132.54	123.70
22	BA	2135	A	C5-C6-N6	11.05	132.54	123.70
22	BA	2886	A	N7-C8-N9	-11.05	108.27	113.80
1	AA	816	A	C5-C6-N6	11.05	132.54	123.70
22	BA	1571	A	C5-C6-N6	11.05	132.54	123.70
22	BA	2287	A	C5-C6-N6	11.05	132.54	123.70
1	AA	382	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	1854	A	N3-C4-C5	-11.04	119.07	126.80
1	AA	262	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	342	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	454	A	C5-C6-N6	11.04	132.53	123.70
22	BA	480	A	N3-C4-C5	-11.04	119.07	126.80
22	BA	1151	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	2434	A	C5-C6-N6	11.04	132.53	123.70
1	AA	746	A	N7-C8-N9	-11.04	108.28	113.80
1	AA	718	A	C5-C6-N6	11.04	132.53	123.70
22	BA	1328	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	2284	A	N3-C4-C5	-11.04	119.07	126.80
22	BA	142	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	644	A	N3-C4-C5	-11.04	119.07	126.80
22	BA	2448	A	C5-C6-N6	11.04	132.53	123.70
1	AA	223	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	196	A	N3-C4-C5	-11.03	119.08	126.80
22	BA	2406	A	C5-C6-N6	11.03	132.53	123.70
22	BA	311	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	439	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	1230	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	2163	A	N7-C8-N9	-11.03	108.28	113.80
1	AA	282	A	C5-C6-N6	11.03	132.52	123.70
1	AA	909	A	N7-C8-N9	-11.03	108.29	113.80
1	AA	974	A	C5-C6-N6	11.03	132.52	123.70
22	BA	422	A	N7-C8-N9	-11.03	108.29	113.80
22	BA	2077	A	N7-C8-N9	-11.03	108.29	113.80
1	AA	777	A	N7-C8-N9	-11.02	108.29	113.80
1	AA	845	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	582	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	1544	A	N7-C8-N9	-11.02	108.29	113.80
1	AA	129	A	C5-C6-N6	11.02	132.51	123.70
22	BA	1028	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	1254	A	C5-C6-N6	11.02	132.51	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	596	A	C5-C6-N6	11.02	132.51	123.70
22	BA	2205	A	C5-C6-N6	11.02	132.51	123.70
22	BA	2267	A	N3-C4-C5	-11.02	119.09	126.80
22	BA	2270	A	N7-C8-N9	-11.02	108.29	113.80
1	AA	393	A	C5-C6-N6	11.01	132.51	123.70
22	BA	384	A	C5-C6-N6	11.01	132.51	123.70
22	BA	1987	A	C5-C6-N6	11.01	132.51	123.70
22	BA	2005	A	N7-C8-N9	-11.01	108.29	113.80
22	BA	2309	A	C5-C6-N6	11.01	132.51	123.70
22	BA	2799	A	N3-C4-C5	-11.01	119.09	126.80
1	AA	1093	A	C5-C6-N6	11.01	132.51	123.70
1	AA	306	A	C5-C6-N6	11.01	132.51	123.70
22	BA	1336	A	N7-C8-N9	-11.01	108.30	113.80
22	BA	2425	A	N7-C8-N9	-11.01	108.30	113.80
1	AA	959	A	N7-C8-N9	-11.01	108.30	113.80
22	BA	1433	A	N7-C8-N9	-11.01	108.30	113.80
22	BA	1722	A	N7-C8-N9	-11.01	108.30	113.80
22	BA	2748	A	C5-C6-N6	11.01	132.51	123.70
22	BA	2860	A	C5-C6-N6	11.01	132.51	123.70
55	B8	21	A	C5-C6-N6	11.01	132.50	123.70
55	B8	51	A	N7-C8-N9	-11.01	108.30	113.80
1	AA	389	A	N3-C4-C5	-11.00	119.10	126.80
22	BA	547	A	C5-C6-N6	11.00	132.50	123.70
22	BA	38	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	1912	A	C5-C6-N6	11.00	132.50	123.70
22	BA	2205	A	N7-C8-N9	-11.00	108.30	113.80
1	AA	1055	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	1156	A	N3-C4-C5	-11.00	119.10	126.80
22	BA	2117	A	C5-C6-N6	11.00	132.50	123.70
22	BA	279	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	423	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	1495	A	N3-C4-C5	-11.00	119.10	126.80
22	BA	788	A	C5-C6-N6	11.00	132.50	123.70
22	BA	849	A	C5-C6-N6	11.00	132.50	123.70
22	BA	1260	A	N3-C4-C5	-11.00	119.10	126.80
22	BA	2868	A	C5-C6-N6	11.00	132.50	123.70
22	BA	632	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	2412	A	C5-C6-N6	11.00	132.50	123.70
55	B8	73	A	N3-C4-C5	-11.00	119.10	126.80
1	AA	466	A	N7-C8-N9	-10.99	108.30	113.80
1	AA	949	A	N3-C4-C5	-10.99	119.10	126.80
1	AA	1248	A	C5-C6-N6	10.99	132.50	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1332	A	N7-C8-N9	-10.99	108.30	113.80
1	AA	1368	A	C5-C6-N6	10.99	132.50	123.70
22	BA	332	A	N3-C4-C5	-10.99	119.10	126.80
1	AA	665	A	N7-C8-N9	-10.99	108.30	113.80
22	BA	64	A	C5-C6-N6	10.99	132.49	123.70
22	BA	197	A	N3-C4-C5	-10.99	119.11	126.80
22	BA	1090	A	C5-C6-N6	10.99	132.50	123.70
22	BA	2665	A	C5-C6-N6	10.99	132.50	123.70
1	AA	509	A	N7-C8-N9	-10.99	108.31	113.80
1	AA	1155	A	C5-C6-N6	10.99	132.49	123.70
1	AA	1179	A	N7-C8-N9	-10.99	108.31	113.80
22	BA	1570	A	C5-C6-N6	10.99	132.49	123.70
22	BA	1669	A	N7-C8-N9	-10.99	108.31	113.80
1	AA	130	A	C5-C6-N6	10.99	132.49	123.70
1	AA	298	A	N7-C8-N9	-10.99	108.31	113.80
1	AA	1508	A	N3-C4-C5	-10.99	119.11	126.80
22	BA	1889	A	N7-C8-N9	-10.99	108.31	113.80
1	AA	364	A	N7-C8-N9	-10.98	108.31	113.80
1	AA	1329	A	C5-C6-N6	10.98	132.49	123.70
22	BA	752	A	N3-C4-C5	-10.98	119.11	126.80
22	BA	1791	A	N7-C8-N9	-10.98	108.31	113.80
23	BB	78	A	N7-C8-N9	-10.98	108.31	113.80
1	AA	743	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	2778	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	804	A	C5-C6-N6	10.98	132.48	123.70
22	BA	1000	A	N7-C8-N9	-10.98	108.31	113.80
23	BB	115	A	C5-C6-N6	10.98	132.49	123.70
1	AA	706	A	N7-C8-N9	-10.98	108.31	113.80
23	BB	34	A	C5-C6-N6	10.98	132.48	123.70
1	AA	1046	A	N3-C4-C5	-10.98	119.12	126.80
22	BA	715	A	C5-C6-N6	10.98	132.48	123.70
22	BA	845	A	N3-C4-C5	-10.98	119.12	126.80
1	AA	81	A	N3-C4-C5	-10.97	119.12	126.80
1	AA	622	A	N7-C8-N9	-10.97	108.31	113.80
22	BA	1918	A	N7-C8-N9	-10.97	108.31	113.80
1	AA	1110	A	C5-C6-N6	10.97	132.48	123.70
1	AA	1431	A	C5-C6-N6	10.97	132.48	123.70
22	BA	1889	A	C5-C6-N6	10.97	132.48	123.70
1	AA	502	A	N7-C8-N9	-10.97	108.31	113.80
22	BA	449	A	N3-C4-C5	-10.97	119.12	126.80
22	BA	1103	A	C5-C6-N6	10.97	132.48	123.70
1	AA	602	A	N7-C8-N9	-10.97	108.32	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1446	A	C5-C6-N6	10.97	132.47	123.70
22	BA	1705	A	C5-C6-N6	10.97	132.47	123.70
22	BA	368	A	C5-C6-N6	10.96	132.47	123.70
22	BA	382	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	2781	A	C5-C6-N6	10.96	132.47	123.70
22	BA	1571	A	N7-C8-N9	-10.96	108.32	113.80
1	AA	819	A	C5-C6-N6	10.96	132.47	123.70
22	BA	1744	A	N3-C4-C5	-10.96	119.13	126.80
22	BA	2478	A	C5-C6-N6	10.96	132.47	123.70
22	BA	1927	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	1978	A	C5-C6-N6	10.96	132.47	123.70
22	BA	142	A	N3-C4-C5	-10.96	119.13	126.80
22	BA	1070	A	C5-C6-N6	10.96	132.47	123.70
22	BA	2070	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	2335	A	N7-C8-N9	-10.96	108.32	113.80
1	AA	1197	A	N3-C4-C5	-10.95	119.13	126.80
22	BA	53	A	N7-C8-N9	-10.95	108.32	113.80
22	BA	1080	A	C5-C6-N6	10.95	132.46	123.70
22	BA	547	A	N7-C8-N9	-10.95	108.32	113.80
22	BA	592	A	N7-C8-N9	-10.95	108.32	113.80
22	BA	1858	A	C5-C6-N6	10.95	132.46	123.70
22	BA	2135	A	N7-C8-N9	-10.95	108.32	113.80
22	BA	2727	A	N3-C4-C5	-10.95	119.14	126.80
22	BA	1509	A	C5-C6-N6	10.95	132.46	123.70
22	BA	56	A	N7-C8-N9	-10.95	108.33	113.80
22	BA	2433	A	C5-C6-N6	10.95	132.46	123.70
1	AA	873	A	N7-C8-N9	-10.94	108.33	113.80
1	AA	968	A	N7-C8-N9	-10.94	108.33	113.80
1	AA	1204	A	C5-C6-N6	10.94	132.45	123.70
22	BA	1027	A	N7-C8-N9	-10.94	108.33	113.80
1	AA	975	A	C5-C6-N6	10.94	132.45	123.70
1	AA	1507	A	N7-C8-N9	-10.94	108.33	113.80
22	BA	430	A	C5-C6-N6	10.94	132.45	123.70
22	BA	1650	A	N7-C8-N9	-10.94	108.33	113.80
22	BA	2850	A	N3-C4-C5	-10.94	119.14	126.80
1	AA	131	A	C5-C6-N6	10.94	132.45	123.70
1	AA	161	A	C5-C6-N6	10.94	132.45	123.70
22	BA	899	A	C5-C6-N6	10.94	132.45	123.70
22	BA	933	A	N7-C8-N9	-10.94	108.33	113.80
22	BA	1494	A	C5-C6-N6	10.94	132.45	123.70
22	BA	1829	A	N3-C4-C5	-10.94	119.15	126.80
22	BA	2126	A	N7-C8-N9	-10.94	108.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	747	A	N7-C8-N9	-10.93	108.33	113.80
22	BA	1046	A	C5-C6-N6	10.93	132.44	123.70
1	AA	459	A	N7-C8-N9	-10.93	108.34	113.80
1	AA	595	A	N7-C8-N9	-10.93	108.34	113.80
22	BA	789	A	N3-C4-C5	-10.93	119.15	126.80
22	BA	2426	A	N7-C8-N9	-10.93	108.34	113.80
1	AA	195	A	N7-C8-N9	-10.93	108.34	113.80
1	AA	535	A	C5-C6-N6	10.93	132.44	123.70
1	AA	1340	A	C5-C6-N6	10.93	132.44	123.70
22	BA	1785	A	C5-C6-N6	10.93	132.44	123.70
1	AA	1021	A	C5-C6-N6	10.92	132.44	123.70
22	BA	1134	A	N7-C8-N9	-10.92	108.34	113.80
1	AA	1227	A	C5-C6-N6	10.92	132.44	123.70
22	BA	346	A	C5-C6-N6	10.92	132.44	123.70
22	BA	1264	A	C5-C6-N6	10.92	132.44	123.70
22	BA	2317	A	N3-C4-C5	-10.92	119.15	126.80
22	BA	2899	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	677	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	2095	A	C5-C6-N6	10.92	132.44	123.70
1	AA	718	A	N7-C8-N9	-10.91	108.34	113.80
1	AA	607	A	N7-C8-N9	-10.91	108.34	113.80
1	AA	1350	A	C5-C6-N6	10.91	132.43	123.70
22	BA	616	A	N7-C8-N9	-10.91	108.34	113.80
22	BA	730	A	N3-C4-C5	-10.91	119.16	126.80
22	BA	470	A	N7-C8-N9	-10.91	108.34	113.80
22	BA	1803	A	N3-C4-C5	-10.91	119.16	126.80
22	BA	2003	A	C5-C6-N6	10.91	132.43	123.70
1	AA	44	A	C5-C6-N6	10.91	132.43	123.70
22	BA	1745	A	C5-C6-N6	10.91	132.43	123.70
22	BA	1419	A	C5-C6-N6	10.91	132.43	123.70
22	BA	1532	A	N7-C8-N9	-10.91	108.35	113.80
1	AA	16	A	C5-C6-N6	10.90	132.42	123.70
1	AA	250	A	N7-C8-N9	-10.90	108.35	113.80
1	AA	1042	A	C5-C6-N6	10.90	132.42	123.70
22	BA	1805	A	C5-C6-N6	10.90	132.42	123.70
22	BA	644	A	N7-C8-N9	-10.90	108.35	113.80
22	BA	104	A	N7-C8-N9	-10.90	108.35	113.80
22	BA	1413	A	C5-C6-N6	10.90	132.42	123.70
22	BA	2635	A	N7-C8-N9	-10.90	108.35	113.80
1	AA	1180	A	C5-C6-N6	10.90	132.42	123.70
22	BA	532	A	N7-C8-N9	-10.90	108.35	113.80
1	AA	872	A	C5-C6-N6	10.90	132.42	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	844	A	N7-C8-N9	-10.90	108.35	113.80
22	BA	1632	A	N7-C8-N9	-10.90	108.35	113.80
1	AA	878	A	N7-C8-N9	-10.90	108.35	113.80
22	BA	2386	A	C5-C6-N6	10.90	132.42	123.70
55	B8	59	A	C5-C6-N6	10.90	132.42	123.70
1	AA	356	A	N3-C4-C5	-10.89	119.17	126.80
1	AA	1289	A	C5-C6-N6	10.89	132.42	123.70
22	BA	631	A	C5-C6-N6	10.89	132.42	123.70
22	BA	1745	A	N7-C8-N9	-10.89	108.35	113.80
1	AA	174	A	N7-C8-N9	-10.89	108.35	113.80
1	AA	55	A	C5-C6-N6	10.89	132.41	123.70
1	AA	892	A	C5-C6-N6	10.89	132.41	123.70
22	BA	492	A	C5-C6-N6	10.89	132.41	123.70
22	BA	918	A	C5-C6-N6	10.89	132.41	123.70
22	BA	990	A	C5-C6-N6	10.89	132.41	123.70
1	AA	1280	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	1067	A	C5-C6-N6	10.89	132.41	123.70
22	BA	19	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	1847	A	N3-C4-C5	-10.88	119.18	126.80
1	AA	383	A	N3-C4-C5	-10.88	119.18	126.80
1	AA	412	A	N7-C8-N9	-10.88	108.36	113.80
1	AA	766	A	C5-C6-N6	10.88	132.41	123.70
22	BA	2114	A	C5-C6-N6	10.88	132.41	123.70
1	AA	983	A	N3-C4-C5	-10.88	119.18	126.80
22	BA	975	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	127	A	C5-C6-N6	10.88	132.40	123.70
22	BA	309	A	N7-C8-N9	-10.88	108.36	113.80
1	AA	629	A	C5-C6-N6	10.88	132.40	123.70
22	BA	2675	A	N7-C8-N9	-10.87	108.36	113.80
1	AA	694	A	C5-C6-N6	10.87	132.40	123.70
1	AA	563	A	C5-C6-N6	10.87	132.40	123.70
1	AA	1499	A	C5-C6-N6	10.87	132.40	123.70
22	BA	1916	A	N7-C8-N9	-10.87	108.36	113.80
22	BA	1655	A	C5-C6-N6	10.87	132.40	123.70
22	BA	1809	A	N3-C4-C5	-10.87	119.19	126.80
22	BA	2560	A	N7-C8-N9	-10.87	108.36	113.80
1	AA	151	A	N7-C8-N9	-10.87	108.37	113.80
22	BA	1932	A	N7-C8-N9	-10.87	108.37	113.80
22	BA	2516	A	C5-C6-N6	10.86	132.39	123.70
1	AA	946	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	1070	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	2598	A	N7-C8-N9	-10.86	108.37	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1469	A	N3-C4-C5	-10.86	119.20	126.80
1	AA	1219	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	1496	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	575	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	89	A	C5-C6-N6	10.86	132.39	123.70
22	BA	666	A	C5-C6-N6	10.86	132.39	123.70
22	BA	941	A	C5-C6-N6	10.86	132.38	123.70
22	BA	1819	A	N3-C4-C5	-10.86	119.20	126.80
22	BA	2726	A	C5-C6-N6	10.86	132.38	123.70
55	B8	26	A	N3-C4-C5	-10.86	119.20	126.80
22	BA	1098	A	N7-C8-N9	-10.85	108.37	113.80
22	BA	1287	A	N3-C4-C5	-10.85	119.20	126.80
22	BA	1786	A	C5-C6-N6	10.85	132.38	123.70
1	AA	493	A	C5-C6-N6	10.85	132.38	123.70
22	BA	1095	A	C5-C6-N6	10.85	132.38	123.70
22	BA	1284	A	N7-C8-N9	-10.85	108.38	113.80
1	AA	160	A	N7-C8-N9	-10.85	108.38	113.80
23	BB	45	A	N7-C8-N9	-10.85	108.38	113.80
1	AA	560	A	N7-C8-N9	-10.85	108.38	113.80
22	BA	1690	A	N7-C8-N9	-10.85	108.38	113.80
22	BA	2080	A	C5-C6-N6	10.85	132.38	123.70
1	AA	502	A	N3-C4-C5	-10.85	119.21	126.80
1	AA	1288	A	N7-C8-N9	-10.85	108.38	113.80
22	BA	1287	A	C5-C6-N6	10.85	132.38	123.70
22	BA	1080	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	900	A	C5-C6-N6	10.84	132.37	123.70
22	BA	2147	A	C5-C6-N6	10.84	132.37	123.70
23	BB	39	A	C5-C6-N6	10.84	132.38	123.70
1	AA	892	A	N3-C4-C5	-10.84	119.21	126.80
22	BA	374	A	C5-C6-N6	10.84	132.37	123.70
22	BA	1637	A	N3-C4-C5	-10.84	119.21	126.80
22	BA	453	A	C5-C6-N6	10.84	132.37	123.70
1	AA	574	A	N7-C8-N9	-10.84	108.38	113.80
1	AA	1318	A	C5-C6-N6	10.84	132.37	123.70
22	BA	800	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	2776	A	C5-C6-N6	10.84	132.37	123.70
23	BB	52	A	C5-C6-N6	10.84	132.37	123.70
22	BA	793	A	N3-C4-C5	-10.83	119.22	126.80
22	BA	2070	A	N3-C4-C5	-10.83	119.22	126.80
1	AA	1261	A	C5-C6-N6	10.83	132.36	123.70
22	BA	2266	A	C5-C6-N6	10.83	132.36	123.70
22	BA	2675	A	C5-C6-N6	10.83	132.37	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	460	A	N7-C8-N9	-10.83	108.39	113.80
1	AA	815	A	N7-C8-N9	-10.83	108.39	113.80
1	AA	1082	A	N7-C8-N9	-10.83	108.39	113.80
22	BA	52	A	N3-C4-C5	-10.82	119.22	126.80
22	BA	794	A	C5-C6-N6	10.82	132.36	123.70
22	BA	972	A	C5-C6-N6	10.82	132.36	123.70
55	B8	21	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	144	A	C5-C6-N6	10.82	132.35	123.70
1	AA	313	A	N7-C8-N9	-10.82	108.39	113.80
1	AA	729	A	N3-C4-C5	-10.82	119.23	126.80
1	AA	1004	A	C5-C6-N6	10.82	132.35	123.70
22	BA	2476	A	C5-C6-N6	10.82	132.35	123.70
1	AA	448	A	N3-C4-C5	-10.82	119.23	126.80
1	AA	1014	A	C5-C6-N6	10.82	132.35	123.70
1	AA	1433	A	N3-C4-C5	-10.82	119.23	126.80
22	BA	2407	A	N3-C4-C5	-10.82	119.23	126.80
1	AA	8	A	C5-C6-N6	10.81	132.35	123.70
1	AA	802	A	C5-C6-N6	10.81	132.35	123.70
55	B8	42	A	N7-C8-N9	-10.81	108.39	113.80
1	AA	1377	A	C5-C6-N6	10.81	132.35	123.70
22	BA	443	A	N7-C8-N9	-10.81	108.39	113.80
22	BA	1392	A	N3-C4-C5	-10.81	119.23	126.80
22	BA	2366	A	N7-C8-N9	-10.81	108.39	113.80
1	AA	673	A	N7-C8-N9	-10.81	108.39	113.80
1	AA	780	A	N7-C8-N9	-10.81	108.39	113.80
22	BA	309	A	N3-C4-C5	-10.81	119.23	126.80
22	BA	340	A	C5-C6-N6	10.81	132.35	123.70
22	BA	2328	A	C5-C6-N6	10.81	132.35	123.70
22	BA	2418	A	C5-C6-N6	10.81	132.35	123.70
1	AA	223	A	C5-C6-N6	10.81	132.35	123.70
1	AA	374	A	C5-C6-N6	10.81	132.35	123.70
22	BA	199	A	N7-C8-N9	-10.81	108.40	113.80
22	BA	563	A	N7-C8-N9	-10.81	108.40	113.80
22	BA	781	A	N3-C4-C5	-10.81	119.23	126.80
1	AA	7	A	C5-C6-N6	10.81	132.34	123.70
1	AA	59	A	N7-C8-N9	-10.81	108.40	113.80
1	AA	228	A	C5-C6-N6	10.80	132.34	123.70
1	AA	509	A	N3-C4-C5	-10.80	119.24	126.80
22	BA	1477	A	C5-C6-N6	10.80	132.34	123.70
22	BA	563	A	C5-C6-N6	10.80	132.34	123.70
55	B8	41	A	N7-C8-N9	-10.80	108.40	113.80
1	AA	583	A	C5-C6-N6	10.80	132.34	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	655	A	N7-C8-N9	-10.80	108.40	113.80
1	AA	892	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	104	A	C5-C6-N6	10.80	132.34	123.70
22	BA	345	A	N3-C4-C5	-10.80	119.24	126.80
22	BA	945	A	N3-C4-C5	-10.80	119.24	126.80
22	BA	1367	A	C5-C6-N6	10.80	132.34	123.70
22	BA	2090	A	N3-C4-C5	-10.80	119.24	126.80
22	BA	1705	A	N3-C4-C5	-10.80	119.24	126.80
22	BA	310	A	N3-C4-C5	-10.80	119.24	126.80
22	BA	2322	A	N3-C4-C5	-10.80	119.24	126.80
1	AA	71	A	C5-C6-N6	10.80	132.34	123.70
22	BA	173	A	N3-C4-C5	-10.80	119.24	126.80
22	BA	2288	A	C5-C6-N6	10.80	132.34	123.70
22	BA	2471	A	C5-C6-N6	10.80	132.34	123.70
22	BA	160	A	C5-C6-N6	10.79	132.34	123.70
22	BA	2564	A	C5-C6-N6	10.79	132.34	123.70
23	BB	58	A	N7-C8-N9	-10.79	108.40	113.80
22	BA	2176	A	C5-C6-N6	10.79	132.33	123.70
1	AA	640	A	C5-C6-N6	10.79	132.33	123.70
1	AA	673	A	N3-C4-C5	-10.79	119.25	126.80
22	BA	756	A	C5-C6-N6	10.79	132.33	123.70
22	BA	2060	A	C5-C6-N6	10.79	132.33	123.70
22	BA	2634	A	C5-C6-N6	10.79	132.33	123.70
1	AA	1201	A	N3-C4-C5	-10.79	119.25	126.80
22	BA	342	A	C5-C6-N6	10.79	132.33	123.70
22	BA	95	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	1532	A	C5-C6-N6	10.78	132.33	123.70
1	AA	547	A	C5-C6-N6	10.78	132.33	123.70
1	AA	553	A	C5-C6-N6	10.78	132.33	123.70
22	BA	191	A	N3-C4-C5	-10.78	119.25	126.80
22	BA	2851	A	N3-C4-C5	-10.78	119.25	126.80
1	AA	914	A	N7-C8-N9	-10.78	108.41	113.80
22	BA	735	A	C5-C6-N6	10.78	132.32	123.70
22	BA	2513	A	N7-C8-N9	-10.78	108.41	113.80
22	BA	2426	A	C5-C6-N6	10.78	132.32	123.70
22	BA	996	A	C5-C6-N6	10.78	132.32	123.70
22	BA	91	A	C5-C6-N6	10.78	132.32	123.70
1	AA	205	A	C5-C6-N6	10.77	132.32	123.70
22	BA	1260	A	C5-C6-N6	10.77	132.32	123.70
22	BA	522	A	C5-C6-N6	10.77	132.32	123.70
22	BA	1808	A	N7-C8-N9	-10.77	108.42	113.80
22	BA	1655	A	N3-C4-C5	-10.77	119.26	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1261	A	N7-C8-N9	-10.77	108.42	113.80
1	AA	743	A	N3-C4-C5	-10.77	119.26	126.80
23	BB	78	A	C5-C6-N6	10.77	132.31	123.70
1	AA	1102	A	C5-C6-N6	10.77	132.31	123.70
22	BA	1916	A	C5-C6-N6	10.77	132.31	123.70
55	B8	14	A	N3-C4-C5	-10.77	119.26	126.80
55	B8	66	A	C5-C6-N6	10.76	132.31	123.70
1	AA	845	A	C5-C6-N6	10.76	132.31	123.70
22	BA	38	A	N3-C4-C5	-10.76	119.27	126.80
22	BA	2333	A	C5-C6-N6	10.76	132.31	123.70
1	AA	716	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	644	A	C5-C6-N6	10.76	132.31	123.70
1	AA	189	A	C5-C6-N6	10.76	132.31	123.70
1	AA	262	A	C5-C6-N6	10.76	132.31	123.70
22	BA	1616	A	C5-C6-N6	10.76	132.31	123.70
1	AA	968	A	C5-C6-N6	10.76	132.31	123.70
22	BA	453	A	N3-C4-C5	-10.76	119.27	126.80
22	BA	532	A	N3-C4-C5	-10.76	119.27	126.80
22	BA	532	A	C5-C6-N6	10.76	132.31	123.70
22	BA	602	A	C5-C6-N6	10.76	132.31	123.70
1	AA	1238	A	C5-C6-N6	10.75	132.30	123.70
1	AA	1350	A	N7-C8-N9	-10.75	108.42	113.80
22	BA	64	A	N3-C4-C5	-10.75	119.27	126.80
22	BA	309	A	C5-C6-N6	10.75	132.30	123.70
1	AA	554	A	C5-C6-N6	10.75	132.30	123.70
1	AA	1219	A	N3-C4-C5	-10.75	119.28	126.80
22	BA	1373	A	N3-C4-C5	-10.75	119.28	126.80
23	BB	29	A	C5-C6-N6	10.75	132.30	123.70
1	AA	681	A	C5-C6-N6	10.75	132.30	123.70
22	BA	265	A	C5-C6-N6	10.75	132.30	123.70
22	BA	2212	A	N7-C8-N9	-10.74	108.43	113.80
1	AA	1531	A	C5-C6-N6	10.74	132.29	123.70
22	BA	609	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	2266	A	N3-C4-C5	-10.74	119.28	126.80
22	BA	354	A	C5-C6-N6	10.74	132.29	123.70
22	BA	947	A	C5-C6-N6	10.74	132.29	123.70
22	BA	980	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	1551	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	2565	A	C5-C6-N6	10.74	132.29	123.70
1	AA	65	A	C5-C6-N6	10.74	132.29	123.70
22	BA	1057	A	C5-C6-N6	10.74	132.29	123.70
22	BA	1205	A	N7-C8-N9	-10.74	108.43	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1016	A	C5-C6-N6	10.74	132.29	123.70
22	BA	1147	A	C5-C6-N6	10.74	132.29	123.70
22	BA	2837	A	C5-C6-N6	10.74	132.29	123.70
1	AA	189	A	N7-C8-N9	-10.73	108.43	113.80
1	AA	1324	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	49	A	N3-C4-C5	-10.73	119.28	126.80
22	BA	825	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	2679	A	N7-C8-N9	-10.73	108.43	113.80
1	AA	609	A	C5-C6-N6	10.73	132.28	123.70
22	BA	592	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	661	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	1342	A	C5-C6-N6	10.73	132.28	123.70
1	AA	1	A	C5-C6-N6	10.73	132.28	123.70
22	BA	1932	A	N3-C4-C5	-10.73	119.29	126.80
1	AA	19	A	N3-C4-C5	-10.73	119.29	126.80
1	AA	349	A	C5-C6-N6	10.73	132.28	123.70
22	BA	404	A	C5-C6-N6	10.73	132.28	123.70
22	BA	1672	A	N7-C8-N9	-10.73	108.44	113.80
22	BA	2247	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	2278	A	C5-C6-N6	10.73	132.28	123.70
22	BA	2706	A	C5-C6-N6	10.73	132.28	123.70
1	AA	1468	A	N3-C4-C5	-10.72	119.29	126.80
22	BA	1496	A	C5-C6-N6	10.72	132.28	123.70
22	BA	2082	A	N3-C4-C5	-10.72	119.30	126.80
22	BA	2814	A	N7-C8-N9	-10.72	108.44	113.80
1	AA	143	A	C5-C6-N6	10.72	132.28	123.70
22	BA	727	A	N7-C8-N9	-10.72	108.44	113.80
22	BA	825	A	N7-C8-N9	-10.72	108.44	113.80
22	BA	2114	A	N3-C4-C5	-10.72	119.30	126.80
22	BA	2432	A	N7-C8-N9	-10.72	108.44	113.80
1	AA	873	A	N3-C4-C5	-10.71	119.30	126.80
1	AA	959	A	C5-C6-N6	10.71	132.27	123.70
22	BA	21	A	N7-C8-N9	-10.71	108.44	113.80
22	BA	299	A	N3-C4-C5	-10.71	119.30	126.80
22	BA	1754	A	C5-C6-N6	10.71	132.27	123.70
22	BA	2886	A	C5-C6-N6	10.71	132.27	123.70
22	BA	502	A	N3-C4-C5	-10.71	119.30	126.80
1	AA	179	A	N3-C4-C5	-10.71	119.30	126.80
1	AA	523	A	C5-C6-N6	10.71	132.26	123.70
1	AA	1246	A	C5-C6-N6	10.71	132.26	123.70
22	BA	2657	A	N7-C8-N9	-10.71	108.45	113.80
1	AA	1456	A	C5-C6-N6	10.70	132.26	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	344	A	C5-C6-N6	10.70	132.26	123.70
22	BA	477	A	N7-C8-N9	-10.70	108.45	113.80
1	AA	279	A	C5-C6-N6	10.70	132.26	123.70
22	BA	2705	A	N7-C8-N9	-10.70	108.45	113.80
1	AA	282	A	N7-C8-N9	-10.70	108.45	113.80
22	BA	2274	A	N7-C8-N9	-10.70	108.45	113.80
1	AA	1324	A	N7-C8-N9	-10.70	108.45	113.80
23	BB	15	A	N7-C8-N9	-10.70	108.45	113.80
22	BA	918	A	N7-C8-N9	-10.70	108.45	113.80
22	BA	715	A	N7-C8-N9	-10.70	108.45	113.80
22	BA	1321	A	N3-C4-C5	-10.70	119.31	126.80
22	BA	1494	A	N7-C8-N9	-10.70	108.45	113.80
1	AA	949	A	C5-C6-N6	10.69	132.25	123.70
23	BB	58	A	C5-C6-N6	10.69	132.25	123.70
22	BA	1286	A	C5-C6-N6	10.69	132.25	123.70
22	BA	2564	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	556	A	C5-C6-N6	10.69	132.25	123.70
22	BA	2051	A	N3-C4-C5	-10.69	119.32	126.80
23	BB	66	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	2433	A	N3-C4-C5	-10.69	119.32	126.80
1	AA	393	A	N3-C4-C5	-10.69	119.32	126.80
22	BA	1133	A	N7-C8-N9	-10.69	108.46	113.80
1	AA	983	A	N7-C8-N9	-10.69	108.46	113.80
1	AA	1465	A	N3-C4-C5	-10.68	119.32	126.80
22	BA	1194	A	N7-C8-N9	-10.68	108.46	113.80
22	BA	1829	A	C5-C6-N6	10.68	132.25	123.70
1	AA	1502	A	C5-C6-N6	10.68	132.25	123.70
55	B8	38	A	N3-C4-C5	-10.68	119.32	126.80
1	AA	1492	A	C5-C6-N6	10.68	132.24	123.70
22	BA	480	A	C5-C6-N6	10.68	132.24	123.70
55	B8	26	A	N7-C8-N9	-10.68	108.46	113.80
1	AA	509	A	C5-C6-N6	10.68	132.24	123.70
1	AA	1430	A	C5-C6-N6	10.68	132.24	123.70
22	BA	447	A	N7-C8-N9	-10.68	108.46	113.80
22	BA	905	A	C5-C6-N6	10.68	132.24	123.70
22	BA	1787	A	C5-C6-N6	10.68	132.24	123.70
22	BA	2781	A	N3-C4-C5	-10.68	119.33	126.80
1	AA	845	A	N3-C4-C5	-10.67	119.33	126.80
22	BA	820	A	N3-C4-C5	-10.67	119.33	126.80
22	BA	1244	A	N7-C8-N9	-10.67	108.46	113.80
22	BA	2176	A	N3-C4-C5	-10.67	119.33	126.80
22	BA	2386	A	N3-C4-C5	-10.67	119.33	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	33	A	N3-C4-C5	-10.67	119.33	126.80
22	BA	1528	A	N7-C8-N9	-10.67	108.46	113.80
22	BA	1009	A	C5-C6-N6	10.67	132.24	123.70
22	BA	2887	A	C5-C6-N6	10.67	132.24	123.70
1	AA	546	A	C5-C6-N6	10.67	132.23	123.70
22	BA	861	A	N7-C8-N9	-10.67	108.47	113.80
1	AA	860	A	N3-C4-C5	-10.66	119.33	126.80
1	AA	937	A	N3-C4-C5	-10.66	119.33	126.80
22	BA	752	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	1204	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	1632	A	C5-C6-N6	10.66	132.23	123.70
22	BA	1936	A	C5-C6-N6	10.66	132.23	123.70
22	BA	2665	A	N3-C4-C5	-10.66	119.33	126.80
1	AA	448	A	C5-C6-N6	10.66	132.23	123.70
22	BA	152	A	N3-C4-C5	-10.66	119.34	126.80
1	AA	607	A	C5-C6-N6	10.66	132.23	123.70
1	AA	1111	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	432	A	C5-C6-N6	10.66	132.23	123.70
22	BA	603	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	1054	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	1285	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	1307	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	643	A	C5-C6-N6	10.66	132.23	123.70
22	BA	1365	A	C5-C6-N6	10.66	132.23	123.70
22	BA	454	A	N7-C8-N9	-10.66	108.47	113.80
1	AA	908	A	N3-C4-C5	-10.65	119.34	126.80
22	BA	471	A	N7-C8-N9	-10.65	108.47	113.80
22	BA	1403	A	C5-C6-N6	10.65	132.22	123.70
1	AA	906	A	C5-C6-N6	10.65	132.22	123.70
22	BA	199	A	N3-C4-C5	-10.65	119.35	126.80
22	BA	761	A	N3-C4-C5	-10.65	119.35	126.80
22	BA	2080	A	N3-C4-C5	-10.65	119.35	126.80
22	BA	721	A	C5-C6-N6	10.64	132.22	123.70
22	BA	753	A	N3-C4-C5	-10.64	119.35	126.80
1	AA	456	A	C5-C6-N6	10.64	132.21	123.70
22	BA	423	A	C5-C6-N6	10.64	132.21	123.70
22	BA	1966	A	N7-C8-N9	-10.64	108.48	113.80
1	AA	1349	A	N7-C8-N9	-10.64	108.48	113.80
1	AA	792	A	N3-C4-C5	-10.64	119.35	126.80
22	BA	1134	A	C5-C6-N6	10.64	132.21	123.70
22	BA	833	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	1039	A	C5-C6-N6	10.64	132.21	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	327	A	C5-C6-N6	10.63	132.21	123.70
22	BA	693	A	N3-C4-C5	-10.63	119.36	126.80
1	AA	865	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	556	A	N3-C4-C5	-10.63	119.36	126.80
22	BA	613	A	N3-C4-C5	-10.63	119.36	126.80
22	BA	2169	A	N3-C4-C5	-10.63	119.36	126.80
22	BA	330	A	N3-C4-C5	-10.63	119.36	126.80
22	BA	631	A	N7-C8-N9	-10.63	108.49	113.80
22	BA	911	A	C5-C6-N6	10.63	132.20	123.70
22	BA	1650	A	C5-C6-N6	10.63	132.20	123.70
1	AA	162	A	N7-C8-N9	-10.62	108.49	113.80
1	AA	1252	A	C5-C6-N6	10.63	132.20	123.70
22	BA	920	A	C5-C6-N6	10.62	132.20	123.70
22	BA	1616	A	N7-C8-N9	-10.62	108.49	113.80
1	AA	3	A	C5-C6-N6	10.62	132.20	123.70
1	AA	72	A	C5-C6-N6	10.62	132.20	123.70
1	AA	1254	A	N3-C4-C5	-10.62	119.36	126.80
1	AA	1500	A	C5-C6-N6	10.62	132.20	123.70
55	B8	69	A	N3-C4-C5	-10.62	119.36	126.80
1	AA	270	A	N3-C4-C5	-10.62	119.37	126.80
1	AA	374	A	N3-C4-C5	-10.62	119.37	126.80
1	AA	1171	A	N3-C4-C5	-10.62	119.37	126.80
22	BA	1596	A	C5-C6-N6	10.62	132.20	123.70
1	AA	1363	A	C5-C6-N6	10.62	132.19	123.70
22	BA	2013	A	C5-C6-N6	10.62	132.19	123.70
1	AA	1288	A	C5-C6-N6	10.62	132.19	123.70
22	BA	1151	A	C5-C6-N6	10.62	132.19	123.70
23	BB	104	A	C5-C6-N6	10.62	132.19	123.70
22	BA	1057	A	N3-C4-C5	-10.61	119.37	126.80
22	BA	1508	A	C5-C6-N6	10.61	132.19	123.70
22	BA	2879	A	C5-C6-N6	10.61	132.19	123.70
22	BA	1603	A	C5-C6-N6	10.61	132.19	123.70
22	BA	2376	A	C5-C6-N6	10.61	132.19	123.70
22	BA	71	A	N3-C4-C5	-10.61	119.38	126.80
22	BA	1001	A	N7-C8-N9	-10.61	108.50	113.80
1	AA	33	A	N7-C8-N9	-10.61	108.50	113.80
22	BA	608	A	N3-C4-C5	-10.61	119.38	126.80
22	BA	1205	A	C5-C6-N6	10.61	132.19	123.70
22	BA	1566	A	N7-C8-N9	-10.61	108.50	113.80
22	BA	2750	A	C5-C6-N6	10.61	132.19	123.70
1	AA	2	A	C5-C6-N6	10.60	132.18	123.70
1	AA	98	A	N3-C4-C5	-10.60	119.38	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	368	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	861	A	C5-C6-N6	10.60	132.18	123.70
22	BA	2531	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1586	A	C5-C6-N6	10.60	132.18	123.70
22	BA	56	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1127	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1302	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1901	A	N3-C4-C5	-10.60	119.38	126.80
22	BA	1322	A	N7-C8-N9	-10.59	108.50	113.80
22	BA	1665	A	N7-C8-N9	-10.59	108.50	113.80
1	AA	327	A	N7-C8-N9	-10.59	108.50	113.80
22	BA	2097	A	C5-C6-N6	10.59	132.17	123.70
22	BA	167	A	N3-C4-C5	-10.59	119.39	126.80
22	BA	428	A	N7-C8-N9	-10.59	108.50	113.80
22	BA	2734	A	C5-C6-N6	10.59	132.17	123.70
22	BA	2534	A	C5-C6-N6	10.59	132.17	123.70
22	BA	2654	A	N7-C8-N9	-10.59	108.50	113.80
22	BA	401	A	C5-C6-N6	10.59	132.17	123.70
22	BA	515	A	N7-C8-N9	-10.59	108.51	113.80
22	BA	1029	A	N3-C4-C5	-10.59	119.39	126.80
1	AA	1408	A	C5-C6-N6	10.59	132.17	123.70
22	BA	1009	A	N3-C4-C5	-10.59	119.39	126.80
22	BA	6	A	N3-C4-C5	-10.58	119.39	126.80
22	BA	95	A	C5-C6-N6	10.58	132.17	123.70
1	AA	482	A	N3-C4-C5	-10.58	119.39	126.80
22	BA	1096	A	C5-C6-N6	10.58	132.16	123.70
22	BA	1551	A	N3-C4-C5	-10.58	119.39	126.80
1	AA	630	A	C5-C6-N6	10.58	132.16	123.70
1	AA	794	A	N3-C4-C5	-10.58	119.40	126.80
1	AA	977	A	C5-C6-N6	10.58	132.16	123.70
23	BB	46	A	N7-C8-N9	-10.58	108.51	113.80
22	BA	2497	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	2171	A	C5-C6-N6	10.57	132.16	123.70
22	BA	2412	A	N3-C4-C5	-10.57	119.40	126.80
1	AA	759	A	C5-C6-N6	10.57	132.16	123.70
1	AA	1238	A	N3-C4-C5	-10.57	119.40	126.80
1	AA	1275	A	C5-C6-N6	10.57	132.16	123.70
22	BA	19	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	160	A	N7-C8-N9	-10.57	108.52	113.80
22	BA	2054	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	2158	A	C5-C6-N6	10.57	132.16	123.70
22	BA	2740	A	C5-C6-N6	10.57	132.16	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2809	A	C5-C6-N6	10.57	132.16	123.70
22	BA	782	A	N7-C8-N9	-10.57	108.52	113.80
22	BA	819	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	670	A	N7-C8-N9	-10.56	108.52	113.80
1	AA	600	A	C5-C6-N6	10.56	132.15	123.70
1	AA	1236	A	N3-C4-C5	-10.56	119.41	126.80
22	BA	1787	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	2799	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	616	A	N3-C4-C5	-10.56	119.41	126.80
22	BA	1698	A	N3-C4-C5	-10.56	119.41	126.80
1	AA	498	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	181	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	227	A	N7-C8-N9	-10.56	108.52	113.80
1	AA	415	A	N3-C4-C5	-10.55	119.41	126.80
1	AA	901	A	N7-C8-N9	-10.55	108.52	113.80
22	BA	1549	A	N3-C4-C5	-10.55	119.41	126.80
55	B8	66	A	N7-C8-N9	-10.55	108.52	113.80
1	AA	460	A	C5-C6-N6	10.55	132.14	123.70
1	AA	1339	A	N7-C8-N9	-10.55	108.53	113.80
22	BA	541	A	N3-C4-C5	-10.55	119.42	126.80
22	BA	460	A	N7-C8-N9	-10.55	108.53	113.80
22	BA	515	A	C5-C6-N6	10.55	132.14	123.70
22	BA	602	A	N3-C4-C5	-10.54	119.42	126.80
1	AA	663	A	C5-C6-N6	10.54	132.13	123.70
22	BA	1998	A	C5-C6-N6	10.54	132.13	123.70
22	BA	2518	A	N3-C4-C5	-10.54	119.42	126.80
1	AA	1507	A	N3-C4-C5	-10.54	119.42	126.80
1	AA	1513	A	C5-C6-N6	10.54	132.13	123.70
22	BA	911	A	N3-C4-C5	-10.54	119.42	126.80
55	B8	42	A	C5-C6-N6	10.54	132.13	123.70
1	AA	329	A	N7-C8-N9	-10.54	108.53	113.80
1	AA	539	A	N3-C4-C5	-10.54	119.42	126.80
22	BA	1126	A	N3-C4-C5	-10.54	119.42	126.80
22	BA	2448	A	N3-C4-C5	-10.54	119.42	126.80
22	BA	2813	A	C5-C6-N6	10.54	132.13	123.70
22	BA	1780	A	N3-C4-C5	-10.53	119.43	126.80
1	AA	1102	A	N7-C8-N9	-10.53	108.53	113.80
22	BA	2117	A	N3-C4-C5	-10.53	119.43	126.80
1	AA	792	A	C5-C6-N6	10.53	132.12	123.70
22	BA	673	C	C2-N3-C4	-10.53	114.64	119.90
1	AA	382	A	N3-C4-C5	-10.53	119.43	126.80
1	AA	814	A	N3-C4-C5	-10.53	119.43	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	44	A	N3-C4-C5	-10.53	119.43	126.80
22	BA	1336	A	N3-C4-C5	-10.53	119.43	126.80
22	BA	1900	A	C5-C6-N6	10.53	132.12	123.70
22	BA	2020	A	C5-C6-N6	10.53	132.12	123.70
22	BA	1103	A	N7-C8-N9	-10.52	108.54	113.80
1	AA	1196	A	C5-C6-N6	10.52	132.12	123.70
22	BA	2094	A	C5-C6-N6	10.52	132.12	123.70
1	AA	1197	A	N7-C8-N9	-10.52	108.54	113.80
22	BA	980	A	C5-C6-N6	10.52	132.12	123.70
22	BA	2682	A	C5-C6-N6	10.52	132.12	123.70
1	AA	1257	A	C5-C6-N6	10.52	132.12	123.70
1	AA	1503	A	C5-C6-N6	10.52	132.12	123.70
22	BA	278	A	C5-C6-N6	10.52	132.12	123.70
22	BA	1746	A	N7-C8-N9	-10.52	108.54	113.80
1	AA	807	A	C5-C6-N6	10.52	132.11	123.70
1	AA	1191	A	C5-C6-N6	10.52	132.11	123.70
22	BA	472	A	N7-C8-N9	-10.52	108.54	113.80
22	BA	1490	A	C5-C6-N6	10.52	132.11	123.70
22	BA	362	A	C5-C6-N6	10.51	132.11	123.70
22	BA	514	A	N3-C4-C5	-10.51	119.44	126.80
22	BA	716	A	C5-C6-N6	10.51	132.11	123.70
1	AA	189	A	N3-C4-C5	-10.51	119.44	126.80
22	BA	1126	A	C5-C6-N6	10.51	132.11	123.70
22	BA	1780	A	N7-C8-N9	-10.51	108.55	113.80
22	BA	933	A	N3-C4-C5	-10.51	119.44	126.80
1	AA	1117	A	C5-C6-N6	10.51	132.10	123.70
1	AA	1152	A	N7-C8-N9	-10.51	108.55	113.80
22	BA	936	A	C5-C6-N6	10.51	132.11	123.70
22	BA	2577	A	N3-C4-C5	-10.51	119.45	126.80
1	AA	329	A	N3-C4-C5	-10.50	119.45	126.80
22	BA	310	A	C5-C6-N6	10.50	132.10	123.70
22	BA	705	A	N3-C4-C5	-10.50	119.45	126.80
22	BA	892	A	N7-C8-N9	-10.50	108.55	113.80
22	BA	1029	A	N7-C8-N9	-10.50	108.55	113.80
22	BA	1676	A	C5-C6-N6	10.50	132.10	123.70
22	BA	2761	A	C5-C6-N6	10.50	132.10	123.70
1	AA	19	A	C5-C6-N6	10.50	132.10	123.70
22	BA	1505	A	N3-C4-C5	-10.50	119.45	126.80
1	AA	101	A	N3-C4-C5	-10.50	119.45	126.80
22	BA	1544	A	N3-C4-C5	-10.50	119.45	126.80
22	BA	2482	A	N7-C8-N9	-10.50	108.55	113.80
22	BA	2764	A	N7-C8-N9	-10.50	108.55	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2850	A	N7-C8-N9	-10.50	108.55	113.80
1	AA	238	A	C5-C6-N6	10.49	132.09	123.70
1	AA	441	A	N7-C8-N9	-10.49	108.55	113.80
1	AA	1287	A	N3-C4-C5	-10.49	119.45	126.80
22	BA	94	A	C5-C6-N6	10.49	132.09	123.70
22	BA	1098	A	C5-C6-N6	10.49	132.09	123.70
22	BA	2184	A	N7-C8-N9	-10.49	108.55	113.80
1	AA	415	A	N7-C8-N9	-10.49	108.55	113.80
1	AA	1111	A	C5-C6-N6	10.49	132.09	123.70
22	BA	2114	A	N7-C8-N9	-10.49	108.55	113.80
22	BA	1470	A	N7-C8-N9	-10.49	108.56	113.80
22	BA	1597	A	N3-C4-C5	-10.49	119.46	126.80
22	BA	1679	A	N7-C8-N9	-10.49	108.56	113.80
22	BA	2097	A	N3-C4-C5	-10.49	119.46	126.80
1	AA	1019	A	C5-C6-N6	10.49	132.09	123.70
22	BA	1040	A	C5-C6-N6	10.49	132.09	123.70
22	BA	1275	A	C5-C6-N6	10.48	132.09	123.70
22	BA	1453	A	C5-C6-N6	10.48	132.09	123.70
1	AA	969	A	C5-C6-N6	10.48	132.09	123.70
22	BA	2311	A	N3-C4-C5	-10.48	119.46	126.80
22	BA	1276	A	N3-C4-C5	-10.48	119.46	126.80
22	BA	2835	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	197	A	C5-C6-N6	10.48	132.08	123.70
22	BA	1347	A	C5-C6-N6	10.48	132.09	123.70
22	BA	2268	A	C5-C6-N6	10.48	132.09	123.70
22	BA	2639	A	C5-C6-N6	10.48	132.09	123.70
22	BA	718	A	C5-C6-N6	10.48	132.08	123.70
22	BA	1353	A	C5-C6-N6	10.48	132.08	123.70
22	BA	1630	A	N3-C4-C5	-10.48	119.47	126.80
22	BA	1626	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	2184	A	C5-C6-N6	10.48	132.08	123.70
22	BA	2037	A	C5-C6-N6	10.47	132.08	123.70
22	BA	2450	A	N7-C8-N9	-10.47	108.56	113.80
55	B8	41	A	C5-C6-N6	10.47	132.08	123.70
22	BA	1754	A	N7-C8-N9	-10.47	108.56	113.80
1	AA	787	A	C5-C6-N6	10.47	132.08	123.70
22	BA	412	A	N3-C4-C5	-10.47	119.47	126.80
22	BA	761	A	N7-C8-N9	-10.47	108.56	113.80
22	BA	1175	A	C5-C6-N6	10.47	132.08	123.70
22	BA	2809	A	N7-C8-N9	-10.47	108.56	113.80
23	BB	119	A	C5-C6-N6	10.47	132.08	123.70
22	BA	621	A	N7-C8-N9	-10.47	108.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	99	A	N3-C4-C5	-10.47	119.47	126.80
1	AA	181	A	N3-C4-C5	-10.46	119.47	126.80
1	AA	364	A	N3-C4-C5	-10.47	119.47	126.80
1	AA	629	A	N3-C4-C5	-10.46	119.47	126.80
1	AA	747	A	C5-C6-N6	10.46	132.07	123.70
1	AA	815	A	N3-C4-C5	-10.46	119.47	126.80
22	BA	94	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	528	A	N3-C4-C5	-10.46	119.47	126.80
22	BA	1821	A	N3-C4-C5	-10.46	119.47	126.80
22	BA	2900	A	N7-C8-N9	-10.46	108.57	113.80
55	B8	59	A	N3-C4-C5	-10.47	119.47	126.80
1	AA	596	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	279	A	C5-C6-N6	10.46	132.07	123.70
22	BA	1175	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	320	A	N7-C8-N9	-10.46	108.57	113.80
1	AA	366	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	176	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	1009	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	1366	A	C5-C6-N6	10.46	132.06	123.70
22	BA	1214	A	N7-C8-N9	-10.45	108.57	113.80
22	BA	1598	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	2247	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	2587	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	1395	A	N7-C8-N9	-10.45	108.58	113.80
1	AA	197	A	C5-C6-N6	10.45	132.06	123.70
1	AA	1363	A	N3-C4-C5	-10.45	119.49	126.80
22	BA	1689	A	N3-C4-C5	-10.45	119.49	126.80
22	BA	2227	A	N7-C8-N9	-10.45	108.58	113.80
1	AA	274	A	C5-C6-N6	10.44	132.06	123.70
1	AA	900	A	C5-C6-N6	10.45	132.06	123.70
22	BA	616	A	C5-C6-N6	10.45	132.06	123.70
22	BA	792	A	N3-C4-C5	-10.45	119.49	126.80
22	BA	278	A	N7-C8-N9	-10.44	108.58	113.80
22	BA	346	A	N3-C4-C5	-10.44	119.49	126.80
22	BA	460	A	N3-C4-C5	-10.45	119.49	126.80
22	BA	1665	A	N3-C4-C5	-10.45	119.49	126.80
22	BA	311	A	N3-C4-C5	-10.44	119.49	126.80
22	BA	1676	A	N3-C4-C5	-10.44	119.49	126.80
22	BA	1938	A	C5-C6-N6	10.44	132.05	123.70
1	AA	1082	A	N3-C4-C5	-10.44	119.49	126.80
22	BA	294	A	C5-C6-N6	10.44	132.05	123.70
22	BA	2726	A	N7-C8-N9	-10.44	108.58	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1250	A	N3-C4-C5	-10.44	119.50	126.80
22	BA	685	A	C5-C6-N6	10.44	132.05	123.70
22	BA	1431	A	N3-C4-C5	-10.44	119.50	126.80
22	BA	1722	A	N3-C4-C5	-10.44	119.50	126.80
1	AA	26	A	N3-C4-C5	-10.43	119.50	126.80
1	AA	630	A	N7-C8-N9	-10.43	108.58	113.80
22	BA	368	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	2450	A	C5-C6-N6	10.43	132.04	123.70
1	AA	560	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	1010	A	C5-C6-N6	10.43	132.04	123.70
22	BA	1213	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	1373	A	N7-C8-N9	-10.43	108.58	113.80
22	BA	371	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	2327	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	538	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	677	A	N3-C4-C5	-10.43	119.50	126.80
1	AA	595	A	N3-C4-C5	-10.42	119.50	126.80
22	BA	204	A	C5-C6-N6	10.42	132.04	123.70
1	AA	81	A	C5-C6-N6	10.42	132.04	123.70
1	AA	768	A	N3-C4-C5	-10.42	119.50	126.80
22	BA	1439	A	N7-C8-N9	-10.42	108.59	113.80
22	BA	2531	A	N3-C4-C5	-10.42	119.50	126.80
1	AA	602	A	C5-C6-N6	10.42	132.04	123.70
1	AA	1225	A	C5-C6-N6	10.42	132.04	123.70
23	BB	94	A	N7-C8-N9	-10.42	108.59	113.80
22	BA	2227	A	N3-C4-C5	-10.42	119.51	126.80
1	AA	1012	A	C5-C6-N6	10.42	132.03	123.70
22	BA	1746	A	N3-C4-C5	-10.42	119.51	126.80
1	AA	1398	A	N3-C4-C5	-10.41	119.51	126.80
22	BA	735	A	N3-C4-C5	-10.41	119.51	126.80
22	BA	1960	A	C5-C6-N6	10.41	132.03	123.70
22	BA	2706	A	N3-C4-C5	-10.41	119.51	126.80
1	AA	303	A	N3-C4-C5	-10.41	119.51	126.80
22	BA	2247	A	C5-C6-N6	10.41	132.03	123.70
22	BA	2778	A	N3-C4-C5	-10.41	119.51	126.80
22	BA	959	A	N3-C4-C5	-10.41	119.51	126.80
1	AA	696	A	N3-C4-C5	-10.41	119.52	126.80
1	AA	1022	A	C5-C6-N6	10.41	132.03	123.70
1	AA	1410	A	C5-C6-N6	10.41	132.03	123.70
22	BA	492	A	N3-C4-C5	-10.41	119.52	126.80
22	BA	2170	A	C5-C6-N6	10.41	132.03	123.70
22	BA	207	A	N7-C8-N9	-10.40	108.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	270	A	C5-C6-N6	10.40	132.02	123.70
22	BA	1590	A	C5-C6-N6	10.40	132.02	123.70
22	BA	1705	A	N7-C8-N9	-10.40	108.60	113.80
22	BA	1711	A	C5-C6-N6	10.40	132.02	123.70
1	AA	363	A	C5-C6-N6	10.40	132.02	123.70
1	AA	1333	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	1773	A	N7-C8-N9	-10.40	108.60	113.80
22	BA	1952	A	C5-C6-N6	10.40	132.02	123.70
22	BA	1143	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	1579	A	C5-C6-N6	10.40	132.02	123.70
1	AA	10	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	384	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	2766	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	984	A	C5-C6-N6	10.40	132.02	123.70
22	BA	1284	A	C5-C6-N6	10.40	132.02	123.70
22	BA	2386	A	N7-C8-N9	-10.39	108.60	113.80
22	BA	415	A	C5-C6-N6	10.39	132.01	123.70
1	AA	1274	A	C5-C6-N6	10.39	132.01	123.70
22	BA	190	A	N7-C8-N9	-10.39	108.61	113.80
22	BA	2336	A	N3-C4-C5	-10.39	119.53	126.80
22	BA	2005	A	C5-C6-N6	10.38	132.01	123.70
55	B8	38	A	N7-C8-N9	-10.38	108.61	113.80
1	AA	32	A	N7-C8-N9	-10.38	108.61	113.80
22	BA	945	A	N7-C8-N9	-10.38	108.61	113.80
1	AA	461	A	C5-C6-N6	10.38	132.00	123.70
1	AA	781	A	C5-C6-N6	10.38	132.00	123.70
1	AA	864	A	N3-C4-C5	-10.38	119.54	126.80
22	BA	960	A	N7-C8-N9	-10.38	108.61	113.80
22	BA	1553	A	N3-C4-C5	-10.38	119.54	126.80
22	BA	2587	A	C5-C6-N6	10.38	132.00	123.70
1	AA	250	A	C5-C6-N6	10.38	132.00	123.70
22	BA	391	A	C5-C6-N6	10.38	132.00	123.70
22	BA	2082	A	N7-C8-N9	-10.38	108.61	113.80
1	AA	958	A	C5-C6-N6	10.37	132.00	123.70
22	BA	14	A	C5-C6-N6	10.37	132.00	123.70
22	BA	63	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	1050	A	C5-C6-N6	10.37	132.00	123.70
1	AA	994	A	C5-C6-N6	10.37	131.99	123.70
22	BA	1586	A	N7-C8-N9	-10.37	108.62	113.80
55	B8	69	A	C5-C6-N6	10.37	131.99	123.70
22	BA	1098	A	N3-C4-C5	-10.37	119.54	126.80
1	AA	1306	A	C5-C6-N6	10.36	131.99	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	730	A	N7-C8-N9	-10.37	108.62	113.80
22	BA	1307	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	751	A	C5-C6-N6	10.36	131.99	123.70
22	BA	1802	A	N3-C4-C5	-10.37	119.55	126.80
22	BA	28	A	N7-C8-N9	-10.36	108.62	113.80
22	BA	71	A	N7-C8-N9	-10.36	108.62	113.80
1	AA	969	A	N3-C4-C5	-10.36	119.55	126.80
1	AA	1012	A	N3-C4-C5	-10.36	119.55	126.80
22	BA	1626	A	C5-C6-N6	10.36	131.99	123.70
22	BA	2198	A	C5-C6-N6	10.36	131.99	123.70
22	BA	1241	A	N3-C4-C5	-10.36	119.55	126.80
1	AA	1216	A	C5-C6-N6	10.36	131.99	123.70
22	BA	5	A	N3-C4-C5	-10.36	119.55	126.80
22	BA	149	A	N7-C8-N9	-10.36	108.62	113.80
22	BA	1000	A	C5-C6-N6	10.36	131.99	123.70
22	BA	2273	A	C5-C6-N6	10.36	131.99	123.70
22	BA	2727	A	N7-C8-N9	-10.36	108.62	113.80
1	AA	532	A	C5-C6-N6	10.35	131.98	123.70
22	BA	83	A	N3-C4-C5	-10.35	119.55	126.80
22	BA	764	A	N7-C8-N9	-10.35	108.62	113.80
22	BA	1614	A	C5-C6-N6	10.35	131.98	123.70
1	AA	174	A	N3-C4-C5	-10.35	119.56	126.80
22	BA	1877	A	C5-C6-N6	10.35	131.98	123.70
22	BA	391	A	N3-C4-C5	-10.35	119.56	126.80
1	AA	1176	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	190	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	2809	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	2821	A	C5-C6-N6	10.34	131.97	123.70
1	AA	1105	A	C5-C6-N6	10.34	131.97	123.70
22	BA	743	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	1086	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	2635	A	N3-C4-C5	-10.34	119.56	126.80
1	AA	1151	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	1690	A	N3-C4-C5	-10.34	119.56	126.80
1	AA	298	A	C5-C6-N6	10.34	131.97	123.70
55	B8	14	A	N7-C8-N9	-10.34	108.63	113.80
1	AA	702	A	C5-C6-N6	10.33	131.97	123.70
22	BA	1247	A	C5-C6-N6	10.33	131.97	123.70
22	BA	2459	A	N7-C8-N9	-10.33	108.63	113.80
22	BA	1241	A	N7-C8-N9	-10.33	108.64	113.80
22	BA	613	A	N7-C8-N9	-10.33	108.64	113.80
22	BA	1301	A	C5-C6-N6	10.33	131.96	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2879	A	N3-C4-C5	-10.33	119.57	126.80
22	BA	1469	A	N7-C8-N9	-10.32	108.64	113.80
22	BA	1677	A	N7-C8-N9	-10.32	108.64	113.80
1	AA	28	A	C5-C6-N6	10.32	131.96	123.70
1	AA	937	A	C5-C6-N6	10.32	131.96	123.70
22	BA	1427	A	C5-C6-N6	10.32	131.96	123.70
22	BA	1717	A	C5-C6-N6	10.32	131.96	123.70
1	AA	1374	A	C5-C6-N6	10.32	131.96	123.70
1	AA	716	A	N3-C4-C5	-10.32	119.58	126.80
1	AA	694	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	910	A	N3-C4-C5	-10.31	119.58	126.80
1	AA	935	A	C5-C6-N6	10.31	131.95	123.70
1	AA	1005	A	N3-C4-C5	-10.31	119.58	126.80
1	AA	1362	A	C5-C6-N6	10.31	131.95	123.70
22	BA	227	A	C5-C6-N6	10.31	131.95	123.70
22	BA	685	A	N7-C8-N9	-10.31	108.64	113.80
22	BA	1970	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	2547	A	N7-C8-N9	-10.31	108.64	113.80
22	BA	1591	A	N3-C4-C5	-10.31	119.58	126.80
55	B8	51	A	C5-C6-N6	10.31	131.95	123.70
22	BA	374	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	1347	A	N7-C8-N9	-10.31	108.65	113.80
22	BA	528	A	N7-C8-N9	-10.30	108.65	113.80
22	BA	2241	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	218	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	262	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	586	A	N7-C8-N9	-10.30	108.65	113.80
22	BA	590	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	443	A	C5-C6-N6	10.30	131.94	123.70
22	BA	2088	A	N3-C4-C5	-10.30	119.59	126.80
55	B8	69	A	N7-C8-N9	-10.30	108.65	113.80
1	AA	1042	A	N3-C4-C5	-10.30	119.59	126.80
1	AA	363	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	1088	A	N7-C8-N9	-10.30	108.65	113.80
22	BA	2335	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	1028	A	C5-C6-N6	10.30	131.94	123.70
22	BA	1640	A	N3-C4-C5	-10.29	119.59	126.80
22	BA	2453	A	N3-C4-C5	-10.29	119.59	126.80
1	AA	288	A	N3-C4-C5	-10.29	119.59	126.80
22	BA	1274	A	C5-C6-N6	10.29	131.94	123.70
22	BA	233	A	N7-C8-N9	-10.29	108.66	113.80
22	BA	933	A	C5-C6-N6	10.29	131.93	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1189	A	N3-C4-C5	-10.29	119.60	126.80
22	BA	1265	A	N3-C4-C5	-10.29	119.60	126.80
22	BA	2598	A	C5-C6-N6	10.29	131.93	123.70
1	AA	59	A	N3-C4-C5	-10.29	119.60	126.80
22	BA	802	A	N3-C4-C5	-10.29	119.60	126.80
1	AA	199	A	C5-C6-N6	10.29	131.93	123.70
22	BA	478	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	1477	A	N7-C8-N9	-10.28	108.66	113.80
22	BA	2163	A	N3-C4-C5	-10.28	119.60	126.80
1	AA	1110	A	N3-C4-C5	-10.28	119.61	126.80
22	BA	231	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	1336	A	C5-C6-N6	10.28	131.92	123.70
22	BA	2369	A	N3-C4-C5	-10.28	119.61	126.80
1	AA	715	A	C5-C6-N6	10.28	131.92	123.70
22	BA	928	A	N7-C8-N9	-10.28	108.66	113.80
22	BA	2378	A	C5-C6-N6	10.28	131.92	123.70
1	AA	181	A	C5-C6-N6	10.27	131.92	123.70
1	AA	329	A	C5-C6-N6	10.27	131.92	123.70
1	AA	574	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	1634	A	C5-C6-N6	10.27	131.92	123.70
1	AA	1375	A	N3-C4-C5	-10.27	119.61	126.80
1	AA	510	A	C5-C6-N6	10.27	131.91	123.70
1	AA	675	A	C5-C6-N6	10.27	131.92	123.70
22	BA	1848	A	N3-C4-C5	-10.27	119.61	126.80
23	BB	34	A	N3-C4-C5	-10.27	119.61	126.80
1	AA	1236	A	C5-C6-N6	10.27	131.91	123.70
1	AA	1434	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	2392	A	N3-C4-C5	-10.26	119.61	126.80
1	AA	1374	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	14	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	980	A	N3-C4-C5	-10.26	119.61	126.80
22	BA	2328	A	N7-C8-N9	-10.26	108.67	113.80
1	AA	282	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	1759	A	C5-C6-N6	10.26	131.91	123.70
22	BA	2821	A	N7-C8-N9	-10.26	108.67	113.80
1	AA	435	A	C5-C6-N6	10.26	131.91	123.70
22	BA	2071	A	C5-C6-N6	10.26	131.91	123.70
22	BA	182	A	N3-C4-C5	-10.26	119.62	126.80
1	AA	747	A	N3-C4-C5	-10.25	119.62	126.80
22	BA	324	A	C5-C6-N6	10.25	131.90	123.70
22	BA	936	A	N3-C4-C5	-10.25	119.62	126.80
22	BA	1048	A	N3-C4-C5	-10.25	119.62	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1073	A	C5-C6-N6	10.25	131.90	123.70
1	AA	53	A	N7-C8-N9	-10.25	108.68	113.80
1	AA	523	A	N3-C4-C5	-10.25	119.63	126.80
22	BA	272	A	N3-C4-C5	-10.25	119.63	126.80
22	BA	1641	A	N7-C8-N9	-10.25	108.68	113.80
22	BA	429	A	N7-C8-N9	-10.25	108.68	113.80
22	BA	1679	A	C5-C6-N6	10.25	131.90	123.70
22	BA	1700	A	N3-C4-C5	-10.24	119.63	126.80
1	AA	864	A	N7-C8-N9	-10.24	108.68	113.80
22	BA	332	A	C5-C6-N6	10.24	131.90	123.70
22	BA	1304	A	N3-C4-C5	-10.24	119.63	126.80
1	AA	1093	A	N3-C4-C5	-10.24	119.63	126.80
22	BA	925	A	C5-C6-N6	10.24	131.89	123.70
22	BA	1503	A	N3-C4-C5	-10.24	119.63	126.80
22	BA	2169	A	N7-C8-N9	-10.24	108.68	113.80
23	BB	53	A	C5-C6-N6	10.24	131.89	123.70
1	AA	149	A	N3-C4-C5	-10.24	119.63	126.80
22	BA	1890	A	N3-C4-C5	-10.24	119.63	126.80
1	AA	151	A	N3-C4-C5	-10.23	119.64	126.80
1	AA	192	A	N3-C4-C5	-10.23	119.64	126.80
1	AA	872	A	N3-C4-C5	-10.23	119.64	126.80
1	AA	1339	A	C5-C6-N6	10.23	131.89	123.70
1	AA	1493	A	C5-C6-N6	10.23	131.89	123.70
22	BA	793	A	N7-C8-N9	-10.23	108.68	113.80
22	BA	1650	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	1762	A	N7-C8-N9	-10.23	108.68	113.80
1	AA	162	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	1635	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	1757	A	C5-C6-N6	10.23	131.89	123.70
22	BA	44	A	C5-C6-N6	10.23	131.88	123.70
22	BA	1977	A	C5-C6-N6	10.23	131.88	123.70
22	BA	2439	A	C5-C6-N6	10.23	131.88	123.70
22	BA	52	A	C5-C6-N6	10.23	131.88	123.70
22	BA	538	A	N7-C8-N9	-10.23	108.69	113.80
22	BA	1872	A	C5-C6-N6	10.23	131.88	123.70
22	BA	2377	A	C5-C6-N6	10.23	131.88	123.70
1	AA	448	A	N7-C8-N9	-10.23	108.69	113.80
1	AA	784	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	794	A	N7-C8-N9	-10.23	108.69	113.80
22	BA	900	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	2900	A	N3-C4-C5	-10.23	119.64	126.80
1	AA	1152	A	N3-C4-C5	-10.22	119.64	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	320	A	N3-C4-C5	-10.22	119.64	126.80
22	BA	1008	A	N7-C8-N9	-10.22	108.69	113.80
1	AA	994	A	N3-C4-C5	-10.22	119.64	126.80
22	BA	2171	A	N3-C4-C5	-10.22	119.64	126.80
22	BA	2513	A	N3-C4-C5	-10.22	119.65	126.80
22	BA	2700	A	N7-C8-N9	-10.22	108.69	113.80
1	AA	279	A	N7-C8-N9	-10.22	108.69	113.80
1	AA	1483	A	N3-C4-C5	-10.22	119.65	126.80
22	BA	505	A	N3-C4-C5	-10.22	119.65	126.80
22	BA	626	A	N7-C8-N9	-10.22	108.69	113.80
22	BA	1637	A	C5-C6-N6	10.22	131.87	123.70
22	BA	2019	A	C5-C6-N6	10.22	131.87	123.70
22	BA	2058	A	C5-C6-N6	10.22	131.88	123.70
22	BA	2725	A	N7-C8-N9	-10.22	108.69	113.80
23	BB	57	A	N7-C8-N9	-10.22	108.69	113.80
1	AA	1022	A	N3-C4-C5	-10.22	119.65	126.80
23	BB	39	A	N3-C4-C5	-10.22	119.65	126.80
22	BA	1876	A	C5-C6-N6	10.21	131.87	123.70
1	AA	366	A	N7-C8-N9	-10.21	108.69	113.80
1	AA	865	A	C5-C6-N6	10.21	131.87	123.70
22	BA	1900	A	N7-C8-N9	-10.21	108.69	113.80
1	AA	414	A	N3-C4-C5	-10.21	119.65	126.80
1	AA	959	A	N3-C4-C5	-10.21	119.65	126.80
23	BB	15	A	N3-C4-C5	-10.21	119.65	126.80
1	AA	482	A	N7-C8-N9	-10.21	108.70	113.80
1	AA	1254	A	N7-C8-N9	-10.21	108.70	113.80
22	BA	340	A	N3-C4-C5	-10.21	119.66	126.80
22	BA	422	A	C5-C6-N6	10.21	131.87	123.70
22	BA	715	A	N3-C4-C5	-10.21	119.66	126.80
22	BA	2270	A	N3-C4-C5	-10.21	119.66	126.80
22	BA	125	A	C5-C6-N6	10.20	131.86	123.70
1	AA	262	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	2080	A	N7-C8-N9	-10.20	108.70	113.80
22	BA	2199	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	402	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	1085	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	1490	A	N3-C4-C5	-10.20	119.66	126.80
1	AA	498	A	C5-C6-N1	10.20	122.80	117.70
1	AA	728	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	632	A	C5-C6-N6	10.20	131.86	123.70
22	BA	1794	A	C5-C6-N6	10.20	131.86	123.70
22	BA	1889	A	N3-C4-C5	-10.20	119.66	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	781	A	N3-C4-C5	-10.20	119.66	126.80
1	AA	1507	A	C5-C6-N6	10.20	131.86	123.70
22	BA	1689	A	N7-C8-N9	-10.19	108.70	113.80
22	BA	1877	A	N3-C4-C5	-10.19	119.66	126.80
22	BA	2757	A	C5-C6-N6	10.19	131.85	123.70
22	BA	1773	A	C5-C6-N6	10.19	131.85	123.70
22	BA	1244	A	C5-C6-N6	10.19	131.85	123.70
22	BA	2432	A	N3-C4-C5	-10.19	119.67	126.80
22	BA	2468	A	C5-C6-N6	10.19	131.85	123.70
1	AA	865	A	N3-C4-C5	-10.19	119.67	126.80
1	AA	1418	A	C5-C6-N6	10.19	131.85	123.70
1	AA	44	A	N3-C4-C5	-10.18	119.67	126.80
1	AA	465	A	N3-C4-C5	-10.18	119.67	126.80
1	AA	502	A	C5-C6-N6	10.18	131.85	123.70
1	AA	533	A	C5-C6-N6	10.18	131.85	123.70
22	BA	1040	A	N3-C4-C5	-10.18	119.67	126.80
22	BA	1246	A	N3-C4-C5	-10.18	119.67	126.80
22	BA	1609	A	C5-C6-N6	10.18	131.85	123.70
22	BA	1265	A	N7-C8-N9	-10.18	108.71	113.80
1	AA	1398	A	C5-C6-N6	10.18	131.84	123.70
22	BA	83	A	C5-C6-N6	10.18	131.84	123.70
22	BA	1028	A	N3-C4-C5	-10.18	119.67	126.80
1	AA	466	A	N3-C4-C5	-10.18	119.67	126.80
22	BA	1151	A	N3-C4-C5	-10.18	119.67	126.80
22	BA	1165	A	N3-C4-C5	-10.18	119.67	126.80
1	AA	1288	A	N3-C4-C5	-10.18	119.68	126.80
22	BA	718	A	N3-C4-C5	-10.18	119.68	126.80
22	BA	722	A	C5-C6-N6	10.17	131.84	123.70
1	AA	430	A	N3-C4-C5	-10.17	119.68	126.80
1	AA	1157	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	1050	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	1641	A	N3-C4-C5	-10.17	119.68	126.80
1	AA	815	A	C5-C6-N6	10.17	131.83	123.70
22	BA	502	A	C5-C6-N6	10.17	131.83	123.70
22	BA	668	A	C5-C6-N6	10.17	131.83	123.70
22	BA	1586	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	2516	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	2297	A	C5-C6-N6	10.16	131.83	123.70
1	AA	303	A	C5-C6-N6	10.16	131.83	123.70
22	BA	2126	A	C5-C6-N6	10.16	131.83	123.70
22	BA	348	A	C5-C6-N6	10.16	131.82	123.70
1	AA	1176	A	C5-C6-N6	10.15	131.82	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1377	A	N3-C4-C5	-10.15	119.69	126.80
22	BA	320	A	C5-C6-N6	10.15	131.82	123.70
1	AA	131	A	N3-C4-C5	-10.15	119.69	126.80
22	BA	2284	A	N7-C8-N9	-10.15	108.72	113.80
22	BA	2530	A	C5-C6-N6	10.15	131.82	123.70
1	AA	635	A	C5-C6-N6	10.15	131.82	123.70
22	BA	1365	A	N3-C4-C5	-10.15	119.70	126.80
1	AA	139	A	N3-C4-C5	-10.15	119.70	126.80
22	BA	28	A	N3-C4-C5	-10.15	119.70	126.80
22	BA	330	A	N7-C8-N9	-10.15	108.73	113.80
22	BA	2662	A	C5-C6-N6	10.15	131.82	123.70
1	AA	918	A	N3-C4-C5	-10.14	119.70	126.80
1	AA	1429	A	C5-C6-N6	10.14	131.82	123.70
22	BA	626	A	C5-C6-N6	10.14	131.82	123.70
22	BA	845	A	C5-C6-N6	10.14	131.81	123.70
22	BA	1144	A	N3-C4-C5	-10.14	119.70	126.80
1	AA	1022	A	N7-C8-N9	-10.14	108.73	113.80
22	BA	1244	A	N3-C4-C5	-10.14	119.70	126.80
1	AA	1499	A	N3-C4-C5	-10.14	119.70	126.80
1	AA	499	A	N3-C4-C5	-10.14	119.70	126.80
1	AA	600	A	N3-C4-C5	-10.14	119.70	126.80
1	AA	1102	A	N3-C4-C5	-10.14	119.70	126.80
1	AA	1508	A	N7-C8-N9	-10.14	108.73	113.80
22	BA	144	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	675	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	1819	A	C5-C6-N6	10.14	131.81	123.70
22	BA	2352	A	N3-C4-C5	-10.14	119.70	126.80
1	AA	560	A	C5-C6-N6	10.13	131.81	123.70
1	AA	1368	A	N3-C4-C5	-10.13	119.71	126.80
22	BA	917	A	C5-C6-N6	10.13	131.81	123.70
22	BA	2850	A	C5-C6-N6	10.13	131.81	123.70
22	BA	2893	A	C5-C6-N6	10.13	131.81	123.70
22	BA	1503	A	C5-C6-N6	10.13	131.80	123.70
22	BA	2823	A	N3-C4-C5	-10.13	119.71	126.80
1	AA	1465	A	C5-C6-N6	10.13	131.80	123.70
22	BA	1713	A	C5-C6-N6	10.13	131.80	123.70
1	AA	559	A	N3-C4-C5	-10.12	119.71	126.80
55	B8	26	A	C5-C6-N6	10.12	131.80	123.70
1	AA	1500	A	N3-C4-C5	-10.12	119.72	126.80
22	BA	1086	A	N7-C8-N9	-10.12	108.74	113.80
22	BA	1772	A	N7-C8-N9	-10.12	108.74	113.80
55	B8	51	A	N3-C4-C5	-10.12	119.72	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	374	A	N7-C8-N9	-10.12	108.74	113.80
1	AA	573	A	C5-C6-N6	10.12	131.80	123.70
22	BA	608	A	C5-C6-N6	10.12	131.80	123.70
22	BA	38	A	C5-C6-N6	10.12	131.79	123.70
22	BA	514	A	C5-C6-N6	10.12	131.80	123.70
22	BA	2031	A	N3-C4-C5	-10.12	119.72	126.80
22	BA	2108	A	N3-C4-C5	-10.12	119.72	126.80
22	BA	2432	A	C5-C6-N6	10.12	131.80	123.70
22	BA	1494	A	N3-C4-C5	-10.12	119.72	126.80
22	BA	705	A	N7-C8-N9	-10.11	108.74	113.80
1	AA	1044	A	C5-C6-N6	10.11	131.79	123.70
22	BA	477	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	1570	A	N7-C8-N9	-10.11	108.74	113.80
22	BA	1000	A	N3-C4-C5	-10.11	119.72	126.80
1	AA	1251	A	N3-C4-C5	-10.11	119.72	126.80
1	AA	630	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	256	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	1175	A	N7-C8-N9	-10.11	108.75	113.80
22	BA	1759	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	1502	A	C5-C6-N6	10.11	131.78	123.70
1	AA	263	A	C5-C6-N6	10.10	131.78	123.70
22	BA	1021	A	N7-C8-N9	-10.10	108.75	113.80
22	BA	2748	A	N7-C8-N9	-10.10	108.75	113.80
22	BA	2037	A	N7-C8-N9	-10.10	108.75	113.80
55	B8	66	A	N3-C4-C5	-10.10	119.73	126.80
1	AA	383	A	C4-C5-C6	10.10	122.05	117.00
1	AA	648	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	251	A	C5-C6-N6	10.10	131.78	123.70
22	BA	1966	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	2154	A	C5-C6-N6	10.10	131.78	123.70
22	BA	2191	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	2829	A	N3-C4-C5	-10.10	119.73	126.80
55	B8	41	A	N3-C4-C5	-10.10	119.73	126.80
1	AA	1081	A	N3-C4-C5	-10.10	119.73	126.80
1	AA	1375	A	C5-C6-N6	10.10	131.78	123.70
22	BA	670	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	1247	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	1785	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	2369	A	C5-C6-N6	10.10	131.78	123.70
1	AA	101	A	C5-C6-N6	10.09	131.77	123.70
22	BA	1470	A	N3-C4-C5	-10.09	119.74	126.80
1	AA	629	A	N7-C8-N9	-10.09	108.76	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1143	A	N7-C8-N9	-10.09	108.76	113.80
22	BA	1785	A	N7-C8-N9	-10.09	108.76	113.80
22	BA	430	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	750	A	C5-C6-N6	10.09	131.77	123.70
22	BA	1603	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	1610	A	C5-C6-N6	10.09	131.77	123.70
22	BA	2577	A	C5-C6-N6	10.09	131.77	123.70
1	AA	66	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	1936	A	N3-C4-N9	10.08	135.47	127.40
1	AA	1004	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	1070	A	N3-C4-C5	-10.08	119.74	126.80
1	AA	452	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	1253	A	N7-C8-N9	-10.08	108.76	113.80
22	BA	1470	A	C5-C6-N6	10.08	131.76	123.70
22	BA	1916	A	N3-C4-C5	-10.07	119.75	126.80
1	AA	579	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	2126	A	N3-C4-C5	-10.07	119.75	126.80
1	AA	238	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	910	A	C5-C6-N6	10.07	131.76	123.70
22	BA	2662	A	N3-C4-C5	-10.07	119.75	126.80
1	AA	338	A	C5-C6-N6	10.07	131.75	123.70
22	BA	2377	A	N7-C8-N9	-10.07	108.77	113.80
22	BA	1854	A	N7-C8-N9	-10.07	108.77	113.80
1	AA	1257	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	1978	A	N3-C4-C5	-10.07	119.75	126.80
1	AA	759	A	N3-C4-C5	-10.06	119.75	126.80
1	AA	1093	A	N7-C8-N9	-10.06	108.77	113.80
22	BA	94	A	N3-C4-C5	-10.06	119.75	126.80
22	BA	1885	A	C5-C6-N6	10.06	131.75	123.70
22	BA	471	A	N3-C4-C5	-10.06	119.76	126.80
22	BA	1566	A	C5-C6-N6	10.06	131.75	123.70
22	BA	2733	A	N3-C4-C5	-10.06	119.76	126.80
1	AA	373	A	N3-C4-C5	-10.06	119.76	126.80
22	BA	590	A	C5-C6-N6	10.06	131.75	123.70
22	BA	1918	A	N3-C4-C5	-10.06	119.76	126.80
1	AA	161	A	N7-C8-N9	-10.05	108.77	113.80
22	BA	190	A	C5-C6-N6	10.06	131.74	123.70
22	BA	460	A	C5-C6-N6	10.05	131.74	123.70
22	BA	2108	A	C5-C6-N6	10.05	131.74	123.70
1	AA	119	A	N3-C4-C5	-10.05	119.77	126.80
1	AA	909	A	N3-C4-C5	-10.05	119.77	126.80
22	BA	1495	A	C5-C6-N6	10.05	131.74	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1548	A	C5-C6-N6	10.05	131.74	123.70
1	AA	1375	A	N7-C8-N9	-10.05	108.78	113.80
22	BA	627	A	N3-C4-C5	-10.05	119.77	126.80
22	BA	1746	A	C5-C6-N6	10.05	131.74	123.70
22	BA	2173	A	N3-C4-C5	-10.05	119.77	126.80
1	AA	10	A	C5-C6-N6	10.05	131.74	123.70
22	BA	1876	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	2497	A	N7-C8-N9	-10.04	108.78	113.80
1	AA	1101	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	927	A	C5-C6-N6	10.04	131.73	123.70
22	BA	574	A	C5-C6-N6	10.04	131.73	123.70
22	BA	1095	A	N3-C4-C5	-10.04	119.77	126.80
1	AA	621	A	C5-C6-N6	10.04	131.73	123.70
1	AA	831	A	C5-C6-N6	10.04	131.73	123.70
1	AA	900	A	N3-C4-C5	-10.04	119.77	126.80
1	AA	1000	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	1264	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	1548	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	1664	A	N7-C8-N9	-10.04	108.78	113.80
1	AA	1081	A	C5-C6-N6	10.04	131.73	123.70
1	AA	1130	A	C5-C6-N6	10.03	131.73	123.70
1	AA	1513	A	N3-C4-C5	-10.04	119.78	126.80
22	BA	255	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	743	A	N3-C4-C5	-10.04	119.78	126.80
1	AA	327	A	N3-C4-C5	-10.03	119.78	126.80
1	AA	487	A	N3-C4-C5	-10.03	119.78	126.80
1	AA	520	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	160	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	794	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	1126	A	N7-C8-N9	-10.03	108.78	113.80
22	BA	2042	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	2705	A	N3-C4-C5	-10.03	119.78	126.80
1	AA	825	A	N3-C4-C5	-10.03	119.78	126.80
55	B8	6	A	C5-C6-N6	10.03	131.72	123.70
1	AA	28	A	N7-C8-N9	-10.03	108.79	113.80
22	BA	217	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	1029	A	C5-C6-N6	10.03	131.72	123.70
22	BA	1809	A	N7-C8-N9	-10.03	108.79	113.80
22	BA	2184	A	N3-C4-C5	-10.03	119.78	126.80
1	AA	53	A	C5-C6-N6	10.02	131.72	123.70
1	AA	223	A	N3-C4-C5	-10.02	119.79	126.80
1	AA	1311	A	C5-C6-N6	10.02	131.72	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1698	A	N7-C8-N9	-10.02	108.79	113.80
22	BA	1805	A	N3-C4-C5	-10.02	119.79	126.80
1	AA	1	A	N7-C8-N9	-10.02	108.79	113.80
1	AA	767	A	C5-C6-N6	10.02	131.71	123.70
1	AA	790	A	C5-C6-N6	10.02	131.71	123.70
22	BA	457	A	C5-C6-N6	10.02	131.71	123.70
22	BA	1608	A	N7-C8-N9	-10.02	108.79	113.80
22	BA	2273	A	N7-C8-N9	-10.02	108.79	113.80
22	BA	2725	A	N3-C4-C5	-10.02	119.79	126.80
1	AA	499	A	C5-C6-N6	10.01	131.71	123.70
1	AA	1151	A	C5-C6-N6	10.01	131.71	123.70
22	BA	231	A	C5-C6-N6	10.01	131.71	123.70
22	BA	422	A	N3-C4-C5	-10.01	119.79	126.80
22	BA	1593	A	N3-C4-C5	-10.01	119.79	126.80
55	B8	59	A	N7-C8-N9	-10.01	108.79	113.80
22	BA	661	A	C5-C6-N6	10.01	131.71	123.70
22	BA	917	A	N3-C4-C5	-10.01	119.79	126.80
22	BA	1597	A	C5-C6-N6	10.01	131.71	123.70
22	BA	1133	A	N3-C4-C5	-10.01	119.80	126.80
22	BA	471	A	C5-C6-N6	10.01	131.70	123.70
22	BA	705	A	C5-C6-N6	10.01	131.70	123.70
1	AA	535	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	1127	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	946	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	2868	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	602	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	1067	A	N3-C4-C5	-10.00	119.80	126.80
1	AA	1055	A	C5-C6-N6	9.99	131.69	123.70
22	BA	322	A	N3-C4-C5	-9.99	119.80	126.80
22	BA	1960	A	N3-C4-C5	-9.99	119.81	126.80
22	BA	1439	A	N3-C4-C5	-9.99	119.81	126.80
22	BA	2108	A	N7-C8-N9	-9.99	108.81	113.80
1	AA	167	A	N3-C4-C5	-9.99	119.81	126.80
1	AA	353	A	N3-C4-C5	-9.99	119.81	126.80
1	AA	1311	A	N3-C4-C5	-9.99	119.81	126.80
55	B8	58	A	N3-C4-C5	-9.99	119.81	126.80
22	BA	793	A	C5-C6-N6	9.98	131.69	123.70
23	BB	94	A	N3-C4-C5	-9.98	119.81	126.80
1	AA	243	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	256	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	2135	A	N3-C4-C5	-9.98	119.81	126.80
1	AA	236	A	N3-C4-C5	-9.98	119.82	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	482	A	C5-C6-N6	9.98	131.68	123.70
1	AA	907	A	C5-C6-N6	9.98	131.68	123.70
22	BA	348	A	N3-C4-C5	-9.98	119.82	126.80
22	BA	1054	A	N3-C4-C5	-9.98	119.82	126.80
22	BA	2058	A	N7-C8-N9	-9.98	108.81	113.80
1	AA	946	A	C5-C6-N6	9.97	131.68	123.70
22	BA	49	A	C5-C6-N6	9.97	131.68	123.70
22	BA	547	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	943	A	C5-C6-N6	9.97	131.68	123.70
22	BA	233	A	N3-C4-C5	-9.97	119.82	126.80
1	AA	478	A	N3-C4-C5	-9.96	119.82	126.80
1	AA	790	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	1789	A	N7-C8-N9	-9.97	108.82	113.80
1	AA	1016	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	892	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	2725	A	C5-C6-N6	9.96	131.67	123.70
22	BA	716	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	927	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	2726	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	635	A	N3-C4-C5	-9.96	119.83	126.80
1	AA	415	A	C5-C6-N6	9.96	131.67	123.70
22	BA	2119	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	2433	A	N7-C8-N9	-9.96	108.82	113.80
1	AA	321	A	N3-C4-C5	-9.95	119.83	126.80
1	AA	1150	A	N3-C4-C5	-9.95	119.83	126.80
22	BA	756	A	N3-C4-C5	-9.95	119.83	126.80
22	BA	2013	A	N3-C4-C5	-9.95	119.83	126.80
23	BB	29	A	N3-C4-C5	-9.95	119.83	126.80
1	AA	878	A	C5-C6-N6	9.95	131.66	123.70
1	AA	696	A	C5-C6-N6	9.95	131.66	123.70
1	AA	1410	A	N3-C4-C5	-9.95	119.84	126.80
22	BA	1735	A	N3-C4-C5	-9.95	119.84	126.80
22	BA	1084	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	2826	A	N7-C8-N9	-9.95	108.83	113.80
1	AA	1204	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	2531	A	N7-C8-N9	-9.94	108.83	113.80
23	BB	45	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	263	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	579	A	C5-C6-N6	9.94	131.65	123.70
22	BA	1495	A	N7-C8-N9	-9.94	108.83	113.80
1	AA	151	A	C5-C6-N6	9.94	131.65	123.70
1	AA	408	A	N3-C4-C5	-9.94	119.84	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1157	A	C5-C6-N6	9.94	131.65	123.70
1	AA	1280	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	2632	A	N3-C4-C5	-9.94	119.84	126.80
1	AA	1191	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	2352	A	N7-C8-N9	-9.93	108.83	113.80
1	AA	155	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	190	A	N7-C8-N9	-9.93	108.83	113.80
1	AA	441	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	2411	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	1392	A	C5-C6-N6	9.93	131.65	123.70
22	BA	415	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	1395	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	1477	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	2225	A	C5-C6-N6	9.93	131.64	123.70
1	AA	199	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	270	A	C5-C6-N6	9.93	131.64	123.70
22	BA	1385	A	N3-C4-C5	-9.93	119.85	126.80
1	AA	306	A	N3-C4-C5	-9.92	119.85	126.80
1	AA	907	A	N3-C4-C5	-9.92	119.85	126.80
1	AA	1219	A	C5-C6-N6	9.92	131.64	123.70
1	AA	1248	A	N3-C4-C5	-9.92	119.85	126.80
22	BA	1572	A	N3-C4-C5	-9.92	119.85	126.80
55	B8	21	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	820	A	N7-C8-N9	-9.92	108.84	113.80
22	BA	1431	A	C5-C6-N6	9.92	131.64	123.70
22	BA	2741	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	2826	A	C5-C6-N6	9.92	131.63	123.70
1	AA	414	A	C5-C6-N6	9.92	131.63	123.70
22	BA	219	A	N7-C8-N9	-9.92	108.84	113.80
22	BA	592	A	C5-C6-N6	9.92	131.63	123.70
22	BA	753	A	N7-C8-N9	-9.91	108.84	113.80
1	AA	802	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	1180	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	1256	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	477	A	C5-C6-N6	9.91	131.63	123.70
22	BA	1189	A	N7-C8-N9	-9.91	108.84	113.80
22	BA	632	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	382	A	C5-C6-N6	9.91	131.63	123.70
22	BA	1593	A	C5-C6-N6	9.91	131.63	123.70
1	AA	1111	A	N3-C4-C5	-9.91	119.87	126.80
22	BA	849	A	N3-C4-C5	-9.91	119.86	126.80
1	AA	718	A	N3-C4-C5	-9.90	119.87	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1829	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	2679	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	1437	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	706	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	1469	A	C5-C6-N6	9.90	131.62	123.70
22	BA	2541	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	383	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	507	A	C5-C6-N6	9.90	131.62	123.70
22	BA	1089	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	1786	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	2082	A	C5-C6-N6	9.90	131.62	123.70
1	AA	749	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	863	A	C5-C6-N6	9.90	131.62	123.70
22	BA	1347	A	N3-C4-C5	-9.90	119.87	126.80
1	AA	816	A	N3-C4-C5	-9.89	119.87	126.80
22	BA	943	A	N7-C8-N9	-9.89	108.85	113.80
22	BA	1262	A	N3-C4-C5	-9.89	119.87	126.80
22	BA	1608	A	C5-C6-N6	9.89	131.62	123.70
22	BA	2088	A	C5-C6-N6	9.89	131.62	123.70
22	BA	2468	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	914	A	C5-C6-N6	9.89	131.61	123.70
1	AA	1163	A	N3-C4-C5	-9.89	119.88	126.80
1	AA	1229	A	N3-C4-C5	-9.89	119.88	126.80
22	BA	722	A	N3-C4-C5	-9.88	119.88	126.80
55	B8	42	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	218	A	N7-C8-N9	-9.88	108.86	113.80
22	BA	1634	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	2191	A	C5-C6-N6	9.88	131.60	123.70
22	BA	2497	A	C5-C6-N6	9.88	131.60	123.70
1	AA	74	A	N3-C4-C5	-9.88	119.89	126.80
1	AA	780	A	N3-C4-C5	-9.88	119.89	126.80
22	BA	226	A	N7-C8-N9	-9.88	108.86	113.80
1	AA	777	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	478	A	C5-C6-N6	9.87	131.60	123.70
22	BA	1783	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	1938	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	456	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	354	A	N3-C4-C5	-9.87	119.89	126.80
1	AA	648	A	C5-C6-N6	9.86	131.59	123.70
1	AA	2	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	739	A	N7-C8-N9	-9.86	108.87	113.80
1	AA	1319	A	N7-C8-N9	-9.86	108.87	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	523	A	N7-C8-N9	-9.86	108.87	113.80
1	AA	1394	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	2142	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	522	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	1142	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	216	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	1327	A	C5-C6-N6	9.86	131.59	123.70
1	AA	1306	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	156	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	21	A	C5-C6-N6	9.85	131.58	123.70
22	BA	981	A	N7-C8-N9	-9.85	108.87	113.80
22	BA	1900	A	N3-C4-C5	-9.85	119.90	126.80
1	AA	546	A	N3-C4-C5	-9.85	119.91	126.80
22	BA	1548	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	1468	A	C5-C6-N6	9.85	131.58	123.70
1	AA	681	A	N3-C4-C5	-9.85	119.91	126.80
1	AA	1130	A	N3-C4-C5	-9.85	119.91	126.80
22	BA	384	A	N7-C8-N9	-9.85	108.88	113.80
22	BA	103	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1339	A	N3-C4-C5	-9.84	119.91	126.80
22	BA	1246	A	C5-C6-N6	9.84	131.57	123.70
22	BA	2005	A	N3-C4-C5	-9.84	119.91	126.80
23	BB	58	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	80	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	1254	A	C5-C6-N6	9.84	131.57	123.70
22	BA	1853	A	C5-C6-N6	9.84	131.57	123.70
22	BA	2810	A	N3-C4-C5	-9.84	119.91	126.80
1	AA	300	A	C4-C5-C6	9.84	121.92	117.00
22	BA	118	A	N3-C4-C5	-9.84	119.91	126.80
22	BA	279	A	N3-C4-C5	-9.84	119.91	126.80
22	BA	1637	A	N7-C8-N9	-9.84	108.88	113.80
22	BA	1970	A	C5-C6-N6	9.84	131.57	123.70
1	AA	1456	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	1655	A	N7-C8-N9	-9.83	108.88	113.80
22	BA	2887	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	1384	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	2706	A	N7-C8-N9	-9.83	108.89	113.80
22	BA	191	A	C5-C6-N6	9.83	131.56	123.70
22	BA	255	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	483	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	2476	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	2837	A	N3-C4-C5	-9.83	119.92	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2856	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	1237	A	N3-C4-C5	-9.82	119.92	126.80
22	BA	1808	A	N3-C4-C5	-9.82	119.92	126.80
1	AA	338	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	1000	A	C5-C6-N6	9.82	131.56	123.70
1	AA	1171	A	C5-C6-N6	9.82	131.56	123.70
22	BA	563	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	899	A	N3-C4-C5	-9.82	119.92	126.80
22	BA	1596	A	N3-C4-C5	-9.82	119.92	126.80
23	BB	59	A	N3-C4-N9	9.82	135.26	127.40
22	BA	1204	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	167	A	C5-C6-N6	9.82	131.55	123.70
22	BA	734	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	1977	A	N3-C4-C5	-9.82	119.93	126.80
1	AA	583	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	300	A	N7-C8-N9	-9.81	108.89	113.80
22	BA	1535	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	607	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	983	A	C5-C6-N6	9.81	131.55	123.70
22	BA	1103	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	1147	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	1275	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	2872	A	C5-N7-C8	9.81	108.81	103.90
22	BA	1848	A	C5-C6-N6	9.81	131.55	123.70
22	BA	2052	A	C5-C6-N6	9.81	131.55	123.70
23	BB	109	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	195	A	N3-C4-C5	-9.81	119.93	126.80
1	AA	1271	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	480	A	N7-C8-N9	-9.81	108.89	113.80
1	AA	451	A	N3-C4-C5	-9.81	119.94	126.80
22	BA	730	A	C5-C6-N6	9.81	131.55	123.70
22	BA	973	A	N7-C8-N9	-9.81	108.90	113.80
1	AA	749	A	C5-C6-N6	9.80	131.54	123.70
22	BA	1226	A	C5-C6-N6	9.81	131.54	123.70
22	BA	447	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	1393	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	1664	A	C5-C6-N6	9.80	131.54	123.70
22	BA	2317	A	C5-C6-N6	9.80	131.54	123.70
1	AA	1360	A	N3-C4-C5	-9.80	119.94	126.80
1	AA	621	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	1739	A	N7-C8-N9	-9.80	108.90	113.80
1	AA	78	A	C5-C6-N6	9.80	131.54	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	487	A	C5-C6-N6	9.79	131.54	123.70
22	BA	165	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	863	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	1155	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	1321	A	C5-C6-N6	9.80	131.54	123.70
22	BA	1367	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	1504	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	2471	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	222	A	N3-C4-C5	-9.79	119.94	126.80
1	AA	55	A	C5-N7-C8	9.79	108.80	103.90
1	AA	900	A	N7-C8-N9	-9.79	108.91	113.80
1	AA	1170	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	920	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	325	A	N3-C4-C5	-9.79	119.95	126.80
1	AA	1055	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	1169	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	1304	A	C5-C6-N6	9.79	131.53	123.70
22	BA	1580	A	C5-C6-N6	9.79	131.53	123.70
22	BA	1899	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	1791	A	C5-C6-N6	9.79	131.53	123.70
1	AA	784	A	C5-C6-N6	9.79	131.53	123.70
22	BA	2430	A	N7-C8-N9	-9.79	108.91	113.80
23	BB	46	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	50	A	N3-C4-C5	-9.78	119.95	126.80
22	BA	443	A	N3-C4-C5	-9.78	119.95	126.80
22	BA	1509	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	1274	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	1396	A	N3-C4-C5	-9.78	119.95	126.80
22	BA	761	A	C5-C6-N6	9.78	131.52	123.70
22	BA	1268	A	N3-C4-C5	-9.78	119.95	126.80
1	AA	1035	A	N3-C4-C5	-9.78	119.96	126.80
1	AA	1261	A	N3-C4-C5	-9.78	119.96	126.80
22	BA	1505	A	C5-C6-N6	9.78	131.52	123.70
22	BA	788	A	N7-C8-N9	-9.77	108.91	113.80
22	BA	2015	A	C5-C6-N6	9.77	131.52	123.70
22	BA	1847	A	C5-C6-N6	9.77	131.52	123.70
22	BA	1952	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	192	A	C5-C6-N6	9.77	131.51	123.70
1	AA	1437	A	C5-C6-N6	9.77	131.51	123.70
22	BA	1274	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	2560	A	N3-C4-C5	-9.77	119.96	126.80
1	AA	26	A	C5-C6-N6	9.77	131.51	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	919	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	1265	A	C5-C6-N6	9.77	131.51	123.70
22	BA	1354	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	1810	A	N7-C8-N9	-9.77	108.92	113.80
22	BA	2199	A	N7-C8-N9	-9.77	108.92	113.80
22	BA	1073	A	N3-C4-C5	-9.76	119.97	126.80
22	BA	1672	A	N3-C4-C5	-9.76	119.97	126.80
22	BA	2564	A	N3-C4-C5	-9.76	119.97	126.80
22	BA	2058	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	1480	A	N3-C4-C5	-9.76	119.97	126.80
22	BA	1322	A	N3-C4-C5	-9.76	119.97	126.80
22	BA	203	A	N7-C8-N9	-9.76	108.92	113.80
22	BA	1739	A	N3-C4-C5	-9.76	119.97	126.80
22	BA	1772	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	373	A	C5-C6-N6	9.76	131.51	123.70
22	BA	1525	A	N3-C4-C5	-9.76	119.97	126.80
1	AA	766	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	2071	A	N7-C8-N9	-9.75	108.92	113.80
22	BA	482	A	N7-C8-N9	-9.75	108.92	113.80
22	BA	1791	A	N3-C4-C5	-9.75	119.97	126.80
1	AA	129	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	1937	A	C5-N7-C8	9.75	108.78	103.90
22	BA	218	A	C5-C6-N6	9.75	131.50	123.70
22	BA	716	A	N7-C8-N9	-9.75	108.93	113.80
22	BA	896	A	N3-C4-C5	-9.75	119.98	126.80
22	BA	2278	A	N3-C4-C5	-9.75	119.98	126.80
23	BB	53	A	N3-C4-C5	-9.75	119.98	126.80
22	BA	2378	A	N3-C4-C5	-9.75	119.98	126.80
1	AA	1431	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	1549	A	C5-C6-N6	9.74	131.50	123.70
22	BA	556	A	N7-C8-N9	-9.74	108.93	113.80
22	BA	996	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	727	A	C5-C6-N6	9.74	131.49	123.70
1	AA	1082	A	C5-C6-N6	9.73	131.49	123.70
1	AA	716	A	C5-C6-N6	9.73	131.49	123.70
22	BA	2266	A	N7-C8-N9	-9.73	108.93	113.80
1	AA	532	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	435	A	N3-C4-C5	-9.73	119.99	126.80
22	BA	1890	A	C5-C6-N6	9.73	131.48	123.70
22	BA	2147	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	1319	A	N3-C4-C5	-9.73	119.99	126.80
1	AA	228	A	N3-C4-C5	-9.72	119.99	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1226	A	N7-C8-N9	-9.72	108.94	113.80
22	BA	1583	A	N3-C4-C5	-9.72	119.99	126.80
1	AA	1170	A	C5-C6-N6	9.72	131.48	123.70
22	BA	861	A	N3-C4-C5	-9.72	120.00	126.80
22	BA	10	A	N3-C4-C5	-9.72	120.00	126.80
22	BA	1134	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	130	A	N3-C4-C5	-9.72	120.00	126.80
1	AA	309	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	161	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1169	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	1340	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	412	A	C5-C6-N6	9.71	131.47	123.70
22	BA	751	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	2682	A	N3-C4-C5	-9.71	120.00	126.80
1	AA	673	A	C5-C6-N6	9.71	131.47	123.70
22	BA	2003	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	633	A	C5-C6-N6	9.71	131.47	123.70
22	BA	2740	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	1866	A	C5-C6-N6	9.71	131.46	123.70
1	AA	77	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	78	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	1668	A	N3-C4-C5	-9.71	120.01	126.80
22	BA	2439	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	2459	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	2764	A	N3-C4-C5	-9.71	120.01	126.80
1	AA	109	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	1531	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	2614	A	N7-C8-N9	-9.70	108.95	113.80
1	AA	553	A	N3-C4-C5	-9.70	120.01	126.80
1	AA	901	A	C4-C5-C6	9.70	121.85	117.00
1	AA	1299	A	C5-C6-N6	9.70	131.46	123.70
22	BA	6	A	C5-C6-N6	9.70	131.46	123.70
22	BA	244	A	N7-C8-N9	-9.70	108.95	113.80
22	BA	2814	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	1808	A	C5-C6-N6	9.69	131.46	123.70
22	BA	983	A	C5-C6-N6	9.69	131.45	123.70
22	BA	972	A	N7-C8-N9	-9.69	108.95	113.80
22	BA	1090	A	N3-C4-C5	-9.69	120.02	126.80
22	BA	2700	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	1188	A	C5-C6-N6	9.69	131.45	123.70
22	BA	203	A	C5-C6-N6	9.69	131.45	123.70
22	BA	802	A	N7-C8-N9	-9.69	108.96	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2657	A	N3-C4-C5	-9.69	120.02	126.80
1	AA	152	A	N7-C8-N9	-9.68	108.96	113.80
1	AA	460	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	116	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	468	A	N3-C4-C5	-9.68	120.02	126.80
1	AA	155	A	C5-C6-N6	9.68	131.44	123.70
1	AA	279	A	N3-C4-C5	-9.68	120.03	126.80
22	BA	429	A	N3-C4-C5	-9.68	120.03	126.80
22	BA	2662	A	N7-C8-N9	-9.68	108.96	113.80
1	AA	459	A	N3-C4-C5	-9.68	120.03	126.80
22	BA	1156	A	C5-C6-N6	9.68	131.44	123.70
22	BA	668	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	1545	A	N7-C8-N9	-9.67	108.96	113.80
22	BA	1821	A	N7-C8-N9	-9.67	108.96	113.80
22	BA	2860	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	1021	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	1036	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	689	A	C5-C6-N6	9.67	131.43	123.70
22	BA	959	A	N7-C8-N9	-9.67	108.97	113.80
22	BA	1433	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	2274	A	N3-C4-C5	-9.67	120.03	126.80
1	AA	753	A	N3-C4-C5	-9.66	120.03	126.80
1	AA	397	A	C5-C6-N6	9.66	131.43	123.70
22	BA	1301	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	1858	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	608	A	C5-C6-N6	9.66	131.43	123.70
1	AA	935	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	831	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	1357	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	19	A	C5-C6-N6	9.66	131.43	123.70
22	BA	2268	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	382	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	1784	A	N3-C4-C5	-9.66	120.04	126.80
1	AA	205	A	N3-C4-C5	-9.65	120.04	126.80
1	AA	794	A	C5-C6-N6	9.65	131.42	123.70
22	BA	216	A	C5-C6-N6	9.65	131.42	123.70
22	BA	689	A	N3-C4-C5	-9.65	120.04	126.80
22	BA	2407	A	N7-C8-N9	-9.65	108.97	113.80
22	BA	222	A	C5-C6-N6	9.65	131.42	123.70
1	AA	539	A	C5-C6-N6	9.65	131.42	123.70
22	BA	1603	A	N7-C8-N9	-9.64	108.98	113.80
1	AA	1197	A	C5-C6-N6	9.64	131.41	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1367	A	N7-C8-N9	-9.64	108.98	113.80
22	BA	979	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	53	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	706	A	C5-C6-N6	9.64	131.41	123.70
22	BA	95	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	2792	A	N3-C4-C5	-9.64	120.05	126.80
1	AA	1252	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	975	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	401	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	2037	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	411	A	C5-C6-N6	9.63	131.41	123.70
22	BA	173	A	C5-C6-N6	9.63	131.40	123.70
22	BA	352	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	909	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	1446	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	74	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	1608	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	2639	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	807	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	324	A	N3-C4-C5	-9.63	120.06	126.80
1	AA	1216	A	N3-C4-C5	-9.62	120.06	126.80
22	BA	1579	A	N3-C4-C5	-9.62	120.06	126.80
22	BA	1654	A	N3-C4-C5	-9.62	120.06	126.80
22	BA	1609	A	N3-C4-C5	-9.62	120.06	126.80
1	AA	65	A	N3-C4-C5	-9.62	120.07	126.80
22	BA	472	A	N3-C4-C5	-9.62	120.07	126.80
22	BA	1571	A	N3-C4-C5	-9.62	120.07	126.80
1	AA	702	A	N3-C4-C5	-9.62	120.07	126.80
22	BA	764	A	N3-C4-C5	-9.62	120.07	126.80
22	BA	2288	A	N3-C4-C5	-9.62	120.07	126.80
22	BA	1420	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	1927	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	1953	A	C5-C6-N6	9.61	131.39	123.70
1	AA	60	A	N3-C4-C5	-9.61	120.08	126.80
1	AA	1014	A	N3-C4-C5	-9.61	120.08	126.80
22	BA	1241	A	C5-C6-N6	9.61	131.38	123.70
22	BA	2020	A	N3-C4-C5	-9.60	120.08	126.80
1	AA	782	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	172	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	626	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	925	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	1953	A	N3-C4-C5	-9.60	120.08	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1146	A	N3-C4-C5	-9.59	120.08	126.80
22	BA	104	A	N3-C4-C5	-9.59	120.08	126.80
22	BA	2170	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	2225	A	N3-C4-C5	-9.59	120.08	126.80
22	BA	2614	A	N3-C4-C5	-9.59	120.08	126.80
1	AA	1080	A	C5-C6-N6	9.59	131.37	123.70
22	BA	454	A	N3-C4-C5	-9.59	120.09	126.80
1	AA	432	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	2212	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	2407	A	C5-C6-N6	9.59	131.37	123.70
23	BB	104	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	529	A	N3-C4-C5	-9.58	120.09	126.80
22	BA	1978	A	N7-C8-N9	-9.58	109.01	113.80
23	BB	101	A	C5-N7-C8	9.58	108.69	103.90
1	AA	1418	A	N3-C4-C5	-9.58	120.09	126.80
22	BA	2392	A	C5-C6-N6	9.58	131.37	123.70
22	BA	819	A	C5-C6-N6	9.58	131.36	123.70
1	AA	250	A	N3-C4-C5	-9.58	120.10	126.80
22	BA	654	A	N3-C4-C5	-9.58	120.09	126.80
23	BB	73	A	C5-C6-N6	9.58	131.36	123.70
1	AA	687	A	N3-C4-C5	-9.57	120.10	126.80
1	AA	33	A	C5-C6-N6	9.57	131.36	123.70
1	AA	77	A	C5-C6-N6	9.57	131.36	123.70
22	BA	1672	A	C5-C6-N6	9.57	131.36	123.70
1	AA	1067	A	N3-C4-C5	-9.57	120.10	126.80
22	BA	2835	A	N3-C4-C5	-9.57	120.10	126.80
1	AA	547	A	N3-C4-C5	-9.57	120.10	126.80
22	BA	804	A	N3-C4-C5	-9.57	120.10	126.80
22	BA	362	A	N3-C4-C5	-9.57	120.10	126.80
22	BA	2176	A	N7-C8-N9	-9.56	109.02	113.80
22	BA	2670	A	N3-C4-C5	-9.56	120.11	126.80
1	AA	493	A	N3-C4-C5	-9.56	120.11	126.80
1	AA	496	A	N7-C8-N9	-9.56	109.02	113.80
23	BB	73	A	N3-C4-C5	-9.56	120.11	126.80
22	BA	984	A	N7-C8-N9	-9.56	109.02	113.80
22	BA	1359	A	N3-C4-C5	-9.56	120.11	126.80
22	BA	1937	A	N3-C4-C5	-9.56	120.11	126.80
22	BA	2478	A	N3-C4-C5	-9.56	120.11	126.80
22	BA	227	A	N3-C4-C5	-9.56	120.11	126.80
22	BA	2589	A	C5-C6-N6	9.55	131.34	123.70
1	AA	320	A	N3-C4-C5	-9.55	120.12	126.80
22	BA	504	A	N3-C4-C5	-9.55	120.12	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1610	A	N3-C4-C5	-9.55	120.12	126.80
22	BA	2198	A	N3-C4-C5	-9.55	120.12	126.80
23	BB	101	A	C4-C5-C6	9.55	121.77	117.00
1	AA	1349	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	721	A	N3-C4-C5	-9.54	120.12	126.80
23	BB	57	A	N3-C4-C5	-9.54	120.12	126.80
1	AA	172	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	1096	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	89	A	N3-C4-C5	-9.54	120.12	126.80
1	AA	872	A	N7-C8-N9	-9.53	109.03	113.80
22	BA	2378	A	N7-C8-N9	-9.53	109.03	113.80
22	BA	905	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	1522	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	1230	A	N3-C4-C5	-9.53	120.13	126.80
1	AA	496	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	63	A	C5-C6-N6	9.53	131.32	123.70
22	BA	844	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	1936	A	C4-C5-C6	9.53	121.76	117.00
22	BA	2309	A	N3-C4-C5	-9.53	120.13	126.80
1	AA	66	A	C5-C6-N6	9.53	131.32	123.70
22	BA	2183	A	C5-C6-N6	9.53	131.32	123.70
22	BA	753	A	C5-C6-N6	9.53	131.32	123.70
22	BA	983	A	N3-C4-C5	-9.53	120.13	126.80
1	AA	923	A	C5-C6-N6	9.52	131.32	123.70
22	BA	1632	A	N3-C4-C5	-9.52	120.14	126.80
22	BA	1794	A	N3-C4-C5	-9.52	120.14	126.80
1	AA	298	A	N3-C4-C5	-9.52	120.14	126.80
22	BA	975	A	C5-C6-N6	9.51	131.31	123.70
22	BA	1383	A	N3-C4-C5	-9.51	120.14	126.80
22	BA	1866	A	N3-C4-C5	-9.51	120.14	126.80
1	AA	695	A	N3-C4-C5	-9.51	120.14	126.80
1	AA	814	A	C5-C6-N6	9.51	131.31	123.70
22	BA	1722	A	C5-C6-N6	9.51	131.31	123.70
1	AA	1534	A	N3-C4-C5	-9.51	120.15	126.80
22	BA	2711	A	N3-C4-C5	-9.51	120.15	126.80
22	BA	300	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	1008	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	1342	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	149	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	1353	A	N3-C4-C5	-9.49	120.15	126.80
22	BA	2451	A	C5-C6-N1	9.49	122.45	117.70
1	AA	371	A	C5-C6-N6	9.49	131.29	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	914	A	N3-C4-C5	-9.49	120.16	126.80
22	BA	1552	A	N3-C4-C5	-9.49	120.16	126.80
22	BA	1815	A	N7-C8-N9	-9.49	109.06	113.80
22	BA	1508	A	N3-C4-C5	-9.48	120.16	126.80
1	AA	878	A	N3-C4-C5	-9.48	120.16	126.80
1	AA	1441	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	146	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	1801	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	2377	A	N3-C4-C5	-9.48	120.16	126.80
22	BA	2670	A	C5-C6-N6	9.48	131.28	123.70
1	AA	975	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	131	A	N3-C4-C5	-9.47	120.17	126.80
1	AA	3	A	N3-C4-C5	-9.46	120.18	126.80
1	AA	665	A	N3-C4-C5	-9.46	120.17	126.80
1	AA	430	A	C5-C6-N6	9.46	131.27	123.70
22	BA	272	A	C5-C6-N6	9.46	131.27	123.70
22	BA	470	A	C5-C6-N6	9.46	131.27	123.70
22	BA	2813	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	575	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	2821	A	N3-C4-C5	-9.46	120.18	126.80
1	AA	1447	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	1885	A	N3-C4-C5	-9.45	120.18	126.80
1	AA	1145	A	N3-C4-C5	-9.45	120.18	126.80
22	BA	155	A	C5-C6-N6	9.45	131.26	123.70
22	BA	1745	A	N3-C4-C5	-9.45	120.18	126.80
22	BA	244	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	347	A	N7-C8-N9	-9.45	109.07	113.80
22	BA	2435	A	N3-C4-C5	-9.45	120.18	126.80
22	BA	508	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	609	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	2600	A	N3-C4-C5	-9.45	120.19	126.80
1	AA	51	A	N3-C4-C5	-9.45	120.19	126.80
1	AA	712	A	C5-C6-N6	9.45	131.26	123.70
1	AA	1318	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	1854	A	C5-C6-N6	9.44	131.25	123.70
22	BA	155	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	1590	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	2134	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	2205	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	207	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	2366	A	C5-C6-N6	9.43	131.25	123.70
22	BA	42	A	C5-C6-N6	9.43	131.25	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	265	A	N3-C4-C5	-9.43	120.20	126.80
1	AA	649	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	1652	A	N3-C4-C5	-9.43	120.20	126.80
23	BB	109	A	C5-C6-N6	9.43	131.24	123.70
1	AA	309	A	C5-C6-N6	9.42	131.24	123.70
22	BA	788	A	N3-C4-C5	-9.42	120.20	126.80
23	BB	101	A	N3-C4-N9	9.42	134.94	127.40
22	BA	2757	A	N7-C8-N9	-9.42	109.09	113.80
22	BA	675	A	C5-C6-N6	9.42	131.24	123.70
1	AA	411	A	N3-C4-C5	-9.42	120.21	126.80
22	BA	1566	A	N3-C4-C5	-9.42	120.21	126.80
22	BA	1853	A	N3-C4-C5	-9.42	120.21	126.80
22	BA	2059	A	N3-C4-C5	-9.42	120.21	126.80
22	BA	282	A	N3-C4-C5	-9.41	120.21	126.80
22	BA	101	A	C4-C5-C6	9.41	121.70	117.00
22	BA	2425	A	C5-C6-N6	9.41	131.23	123.70
22	BA	53	A	N3-C4-C5	-9.41	120.22	126.80
22	BA	1504	A	C5-C6-N6	9.41	131.22	123.70
22	BA	21	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	1969	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	631	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	2893	A	N3-C4-C5	-9.40	120.22	126.80
1	AA	608	A	N3-C4-C5	-9.40	120.22	126.80
1	AA	1492	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	2051	A	C5-C6-N6	9.40	131.22	123.70
22	BA	2154	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	2602	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	1515	A	N3-C4-C5	-9.39	120.22	126.80
22	BA	1591	A	C5-C6-N6	9.39	131.22	123.70
22	BA	2211	A	N3-C4-C5	-9.39	120.22	126.80
1	AA	8	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	947	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	1373	A	C5-C6-N6	9.39	131.21	123.70
1	AA	1429	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	344	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	2059	A	C5-C6-N6	9.39	131.21	123.70
1	AA	696	A	N7-C8-N9	-9.39	109.11	113.80
22	BA	1169	A	C5-C6-N6	9.38	131.21	123.70
1	AA	1483	A	C5-C6-N6	9.38	131.21	123.70
22	BA	2748	A	N3-C4-C5	-9.38	120.23	126.80
1	AA	923	A	N7-C8-N9	-9.38	109.11	113.80
22	BA	131	A	C5-C6-N6	9.38	131.20	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	270	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	1913	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	829	A	N3-C4-C5	-9.38	120.24	126.80
22	BA	2033	A	N3-C4-C5	-9.38	120.24	126.80
22	BA	1213	A	C5-C6-N6	9.37	131.20	123.70
22	BA	572	A	C4-C5-C6	9.37	121.68	117.00
22	BA	1046	A	N3-C4-C5	-9.37	120.24	126.80
22	BA	1502	A	N3-C4-C5	-9.37	120.24	126.80
1	AA	139	A	C5-C6-N6	9.37	131.19	123.70
22	BA	1762	A	N3-C4-C5	-9.37	120.24	126.80
22	BA	156	A	C5-C6-N6	9.36	131.19	123.70
1	AA	640	A	N3-C4-C5	-9.36	120.25	126.80
1	AA	1428	A	N3-C4-C5	-9.36	120.25	126.80
1	AA	1408	A	N3-C4-C5	-9.36	120.25	126.80
1	AA	1476	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	497	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	1328	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	1711	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	1998	A	N7-C8-N9	-9.35	109.12	113.80
22	BA	2060	A	N3-C4-C5	-9.35	120.25	126.80
1	AA	1332	A	N3-C4-C5	-9.35	120.26	126.80
1	AA	819	A	N3-C4-C5	-9.35	120.26	126.80
22	BA	176	A	C5-C6-N6	9.35	131.18	123.70
1	AA	1289	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	866	A	N3-C4-C5	-9.34	120.26	126.80
55	B8	73	A	C5-N7-C8	9.34	108.57	103.90
22	BA	2019	A	N3-C4-C5	-9.34	120.27	126.80
22	BA	1434	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	482	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	2872	A	C4-C5-N7	-9.33	106.03	110.70
22	BA	181	A	N3-C4-C5	-9.33	120.27	126.80
1	AA	554	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	582	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	972	A	N3-C4-C5	-9.32	120.27	126.80
22	BA	2660	A	N3-C4-C5	-9.32	120.27	126.80
22	BA	2886	A	N3-C4-C5	-9.32	120.27	126.80
22	BA	1901	A	N7-C8-N9	-9.32	109.14	113.80
22	BA	878	A	N3-C4-C5	-9.32	120.28	126.80
22	BA	2418	A	N3-C4-C5	-9.32	120.28	126.80
22	BA	2094	A	N3-C4-C5	-9.32	120.28	126.80
23	BB	108	A	N3-C4-C5	-9.32	120.28	126.80
22	BA	513	A	N7-C8-N9	-9.31	109.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	515	A	N3-C4-C5	-9.31	120.28	126.80
22	BA	2281	A	C5-C6-N6	9.31	131.15	123.70
22	BA	223	A	N3-C4-C5	-9.31	120.28	126.80
22	BA	960	A	C4-C5-C6	9.31	121.65	117.00
22	BA	1032	A	N3-C4-C5	-9.31	120.28	126.80
23	BB	50	A	N3-C4-C5	-9.31	120.28	126.80
1	AA	1362	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	502	A	N7-C8-N9	-9.30	109.15	113.80
22	BA	1919	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	2412	A	C5-N7-C8	9.30	108.55	103.90
22	BA	203	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	781	A	N7-C8-N9	-9.29	109.15	113.80
22	BA	508	A	C5-C6-N6	9.29	131.13	123.70
22	BA	2287	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	1032	A	C5-N7-C8	9.29	108.54	103.90
22	BA	1453	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	1528	A	C5-C6-N6	9.29	131.13	123.70
22	BA	2314	A	N3-C4-C5	-9.29	120.30	126.80
55	B8	76	A	N9-C4-C5	9.29	109.52	105.80
1	AA	274	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	1496	A	N3-C4-C5	-9.29	120.30	126.80
1	AA	371	A	N3-C4-C5	-9.28	120.30	126.80
1	AA	1227	A	N3-C4-C5	-9.28	120.30	126.80
22	BA	599	A	N3-C4-C5	-9.28	120.30	126.80
22	BA	1144	A	C5-C6-N6	9.28	131.12	123.70
1	AA	1105	A	N3-C4-C5	-9.28	120.31	126.80
22	BA	1987	A	N3-C4-C5	-9.28	120.31	126.80
22	BA	1630	A	C5-N7-C8	9.27	108.54	103.90
22	BA	1754	A	N3-C4-C5	-9.27	120.31	126.80
23	BB	66	A	C5-C6-N6	9.27	131.12	123.70
22	BA	2734	A	N3-C4-C5	-9.27	120.31	126.80
1	AA	72	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	1701	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	251	A	C4-C5-C6	9.27	121.63	117.00
22	BA	2868	A	N7-C8-N9	-9.27	109.17	113.80
22	BA	2800	A	N3-C4-C5	-9.27	120.31	126.80
1	AA	116	A	C5-C6-N6	9.26	131.11	123.70
1	AA	873	A	C5-C6-N6	9.26	131.11	123.70
1	AA	573	A	N3-C4-C5	-9.26	120.32	126.80
1	AA	767	A	N3-C4-C5	-9.26	120.32	126.80
22	BA	2675	A	N3-C4-C5	-9.26	120.32	126.80
1	AA	1246	A	N3-C4-C5	-9.26	120.32	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	101	A	C5-C6-N6	9.26	131.11	123.70
22	BA	2753	A	N3-C4-C5	-9.26	120.32	126.80
1	AA	675	A	N3-C4-C5	-9.26	120.32	126.80
22	BA	172	A	C5-C6-N6	9.26	131.10	123.70
22	BA	213	A	N3-C4-C5	-9.26	120.32	126.80
22	BA	453	A	N7-C8-N9	-9.26	109.17	113.80
22	BA	844	A	C5-C6-N6	9.25	131.10	123.70
1	AA	1196	A	N3-C4-C5	-9.24	120.33	126.80
1	AA	160	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	637	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	2062	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	1027	A	C5-C6-N6	9.24	131.09	123.70
1	AA	655	A	C5-C6-N6	9.23	131.09	123.70
22	BA	1679	A	N3-C4-C5	-9.23	120.34	126.80
22	BA	1739	A	C5-C6-N6	9.23	131.09	123.70
22	BA	2534	A	N3-C4-C5	-9.23	120.34	126.80
1	AA	498	A	N3-C4-N9	9.23	134.78	127.40
22	BA	1143	A	C5-C6-N6	9.23	131.08	123.70
22	BA	2482	A	N3-C4-C5	-9.23	120.34	126.80
1	AA	1503	A	N3-C4-C5	-9.22	120.34	126.80
22	BA	142	A	C5-C6-N6	9.22	131.08	123.70
22	BA	1847	A	N7-C8-N9	-9.22	109.19	113.80
22	BA	2635	A	C5-C6-N6	9.22	131.08	123.70
23	BB	115	A	N3-C4-C5	-9.22	120.34	126.80
55	B8	6	A	N3-C4-C5	-9.22	120.34	126.80
1	AA	663	A	N3-C4-C5	-9.22	120.35	126.80
1	AA	958	A	N3-C4-C5	-9.22	120.35	126.80
1	AA	1155	A	N3-C4-C5	-9.22	120.35	126.80
1	AA	1213	A	N3-C4-C5	-9.22	120.35	126.80
1	AA	996	A	N3-C4-C5	-9.21	120.35	126.80
22	BA	1194	A	N3-C4-C5	-9.22	120.35	126.80
22	BA	1552	A	C5-C6-N6	9.21	131.07	123.70
22	BA	503	A	C5-C6-N6	9.21	131.07	123.70
22	BA	13	A	N7-C8-N9	-9.21	109.19	113.80
22	BA	1532	A	N3-C4-C5	-9.21	120.36	126.80
22	BA	125	A	N3-C4-C5	-9.21	120.36	126.80
22	BA	1616	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	2776	A	N3-C4-C5	-9.20	120.36	126.80
1	AA	1179	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	262	A	C5-N7-C8	9.20	108.50	103.90
22	BA	918	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	2547	A	N3-C4-C5	-9.19	120.36	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	432	A	N3-C4-C5	-9.19	120.37	126.80
22	BA	1010	A	N3-C4-C5	-9.19	120.37	126.80
22	BA	2530	A	N3-C4-C5	-9.19	120.37	126.80
1	AA	349	A	N3-C4-C5	-9.19	120.37	126.80
22	BA	251	A	N7-C8-N9	-9.19	109.21	113.80
23	BB	52	A	N3-C4-C5	-9.18	120.37	126.80
22	BA	821	A	N3-C4-C5	-9.18	120.37	126.80
23	BB	119	A	N3-C4-C5	-9.18	120.37	126.80
22	BA	1080	A	N3-C4-C5	-9.18	120.37	126.80
1	AA	1508	A	C5-C6-N6	9.18	131.04	123.70
22	BA	2322	A	C5-C6-N6	9.18	131.04	123.70
1	AA	197	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	52	A	C4-C5-C6	9.17	121.59	117.00
22	BA	2281	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	2750	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	2459	A	C5-C6-N6	9.17	131.03	123.70
1	AA	190	A	C4-C5-C6	9.17	121.58	117.00
1	AA	253	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	751	A	N7-C8-N9	-9.16	109.22	113.80
22	BA	820	A	C5-C6-N6	9.16	131.03	123.70
22	BA	1014	A	N3-C4-C5	-9.16	120.38	126.80
1	AA	171	A	N3-C4-C5	-9.16	120.39	126.80
1	AA	938	A	C5-C6-N6	9.16	131.03	123.70
1	AA	1101	A	C5-N7-C8	9.16	108.48	103.90
22	BA	1580	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	466	A	N3-C4-C5	-9.16	120.39	126.80
1	AA	465	A	C5-C6-N6	9.15	131.02	123.70
1	AA	1044	A	N3-C4-C5	-9.15	120.39	126.80
1	AA	1285	A	N3-C4-C5	-9.15	120.40	126.80
22	BA	1677	A	N3-C4-C5	-9.15	120.40	126.80
22	BA	1272	A	N3-C4-C5	-9.14	120.40	126.80
1	AA	196	A	N3-C4-C5	-9.14	120.40	126.80
1	AA	344	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	2183	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	526	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	973	A	N3-C4-C5	-9.13	120.41	126.80
22	BA	1050	A	C5-N7-C8	9.14	108.47	103.90
22	BA	2738	A	N3-C4-C5	-9.13	120.41	126.80
22	BA	1871	A	N3-C4-C5	-9.12	120.41	126.80
1	AA	1271	A	C5-C6-N6	9.12	131.00	123.70
22	BA	1214	A	N3-C4-C5	-9.12	120.42	126.80
22	BA	1387	A	C5-C6-N6	9.12	130.99	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	526	A	C5-N7-C8	9.12	108.46	103.90
22	BA	1427	A	N3-C4-C5	-9.12	120.42	126.80
22	BA	2158	A	N3-C4-C5	-9.12	120.42	126.80
22	BA	522	A	C5-N7-C8	9.11	108.46	103.90
22	BA	1928	A	N3-C4-C5	-9.11	120.42	126.80
22	BA	2572	A	N3-C4-C5	-9.11	120.42	126.80
22	BA	2388	A	C5-N7-C8	9.11	108.45	103.90
22	BA	2392	A	N7-C8-N9	-9.11	109.25	113.80
22	BA	74	A	N7-C8-N9	-9.10	109.25	113.80
22	BA	2430	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	1129	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	1669	A	C5-N7-C8	9.10	108.45	103.90
22	BA	2346	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	2451	A	N3-C4-C5	-9.10	120.43	126.80
1	AA	120	A	N3-C4-C5	-9.10	120.43	126.80
1	AA	459	A	C5-C6-N6	9.10	130.98	123.70
22	BA	2142	A	C5-C6-N6	9.10	130.98	123.70
1	AA	1324	A	C5-C6-N6	9.09	130.97	123.70
22	BA	299	A	N7-C8-N9	-9.09	109.25	113.80
22	BA	877	A	N3-C4-C5	-9.09	120.44	126.80
22	BA	1802	A	C5-C6-N6	9.09	130.97	123.70
22	BA	1802	A	N7-C8-N9	-9.09	109.25	113.80
22	BA	2298	A	N3-C4-C5	-9.09	120.44	126.80
22	BA	217	A	N7-C8-N9	-9.09	109.26	113.80
22	BA	2297	A	N3-C4-C5	-9.09	120.44	126.80
22	BA	988	A	N3-C4-C5	-9.08	120.44	126.80
1	AA	1340	A	C5-N7-C8	9.08	108.44	103.90
22	BA	2899	A	N3-C4-C5	-9.08	120.44	126.80
22	BA	2711	A	C5-C6-N6	9.08	130.96	123.70
22	BA	423	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	693	A	C5-N7-C8	9.07	108.44	103.90
1	AA	1092	A	N3-C4-C5	-9.06	120.45	126.80
1	AA	787	A	N3-C4-C5	-9.06	120.46	126.80
1	AA	1227	A	N7-C8-N9	-9.06	109.27	113.80
22	BA	960	A	C5-C6-N6	9.06	130.95	123.70
1	AA	1080	A	N3-C4-C5	-9.06	120.46	126.80
22	BA	1205	A	N3-C4-C5	-9.06	120.46	126.80
23	BB	59	A	C5-C6-N1	9.06	122.23	117.70
22	BA	603	A	N3-C4-C5	-9.05	120.46	126.80
22	BA	2758	A	N3-C4-C5	-9.05	120.46	126.80
22	BA	2518	A	C5-C6-N6	9.05	130.94	123.70
1	AA	495	A	N3-C4-C5	-9.05	120.47	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	111	A	N3-C4-C5	-9.05	120.47	126.80
1	AA	182	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	221	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	655	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	1528	A	C4-C5-C6	9.04	121.52	117.00
22	BA	2430	A	C4-C5-C6	9.04	121.52	117.00
22	BA	2721	A	N7-C8-N9	-9.04	109.28	113.80
1	AA	964	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	1912	A	N3-C4-C5	-9.04	120.47	126.80
1	AA	71	A	N3-C4-C5	-9.03	120.48	126.80
1	AA	461	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	928	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	586	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	743	A	C5-C6-N6	9.03	130.93	123.70
22	BA	1001	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	833	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	1419	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	2461	A	C5-C6-N6	9.03	130.92	123.70
22	BA	2665	A	C5-N7-C8	9.02	108.41	103.90
22	BA	255	A	C5-C6-N6	9.02	130.91	123.70
22	BA	152	A	C5-C6-N6	9.02	130.91	123.70
22	BA	2077	A	C5-C6-N6	9.02	130.91	123.70
1	AA	1502	A	N3-C4-C5	-9.02	120.49	126.80
1	AA	336	A	N3-C4-C5	-9.01	120.49	126.80
22	BA	1749	A	N3-C4-C5	-9.01	120.49	126.80
22	BA	2418	A	C5-N7-C8	9.01	108.40	103.90
22	BA	699	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	783	A	N7-C8-N9	-9.00	109.30	113.80
1	AA	1117	A	N3-C4-C5	-9.00	120.50	126.80
1	AA	431	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	1545	A	N3-C4-C5	-8.99	120.50	126.80
22	BA	119	A	N3-C4-C5	-8.99	120.51	126.80
22	BA	742	A	C5-C6-N6	8.99	130.89	123.70
22	BA	2820	A	C5-C6-N6	8.99	130.89	123.70
1	AA	190	A	C5-C6-N6	8.98	130.89	123.70
22	BA	1759	A	N7-C8-N9	-8.98	109.31	113.80
1	AA	143	A	N3-C4-C5	-8.97	120.52	126.80
22	BA	633	A	N3-C4-C5	-8.97	120.52	126.80
22	BA	727	A	N3-C4-C5	-8.96	120.53	126.80
1	AA	889	A	N3-C4-C5	-8.96	120.53	126.80
1	AA	1299	A	N3-C4-C5	-8.96	120.53	126.80
22	BA	2284	A	C5-C6-N6	8.96	130.87	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	596	A	C5-N7-C8	8.95	108.38	103.90
1	AA	1239	A	C5-N7-C8	8.96	108.38	103.90
1	AA	704	A	N3-C4-C5	-8.95	120.53	126.80
1	AA	1152	A	C5-C6-N6	8.95	130.86	123.70
22	BA	621	A	N3-C4-C5	-8.95	120.53	126.80
1	AA	784	A	C5-N7-C8	8.95	108.37	103.90
22	BA	2542	A	C5-N7-C8	8.95	108.37	103.90
22	BA	2761	A	N3-C4-C5	-8.95	120.54	126.80
22	BA	1413	A	N3-C4-C5	-8.94	120.54	126.80
1	AA	1430	A	N3-C4-C5	-8.94	120.54	126.80
22	BA	1284	A	N3-C4-C5	-8.94	120.54	126.80
22	BA	941	A	N3-C4-C5	-8.94	120.54	126.80
22	BA	1654	A	N7-C8-N9	-8.94	109.33	113.80
22	BA	1969	A	C5-C6-N6	8.93	130.85	123.70
22	BA	2721	A	C5-C6-N6	8.93	130.84	123.70
1	AA	389	A	C5-C6-N6	8.93	130.84	123.70
1	AA	161	A	N3-C4-C5	-8.93	120.55	126.80
1	AA	968	A	N3-C4-C5	-8.92	120.55	126.80
22	BA	1700	A	C5-N7-C8	8.92	108.36	103.90
22	BA	1802	A	C4-C5-C6	8.92	121.46	117.00
22	BA	2733	A	C5-N7-C8	8.91	108.36	103.90
23	BB	59	A	C4-C5-C6	8.91	121.45	117.00
1	AA	978	A	N3-C4-C5	-8.90	120.57	126.80
1	AA	913	A	N3-C4-C5	-8.90	120.57	126.80
22	BA	1570	A	N3-C4-C5	-8.90	120.57	126.80
22	BA	789	A	C5-C6-N6	8.90	130.82	123.70
22	BA	1803	A	N7-C8-N9	-8.90	109.35	113.80
1	AA	152	A	N3-C4-C5	-8.89	120.58	126.80
22	BA	1757	A	N3-C4-C5	-8.89	120.58	126.80
22	BA	2101	A	N3-C4-N9	8.89	134.51	127.40
1	AA	1275	A	N3-C4-C5	-8.89	120.58	126.80
22	BA	1789	A	C5-N7-C8	8.89	108.34	103.90
22	BA	909	A	C5-C6-N6	8.88	130.81	123.70
22	BA	1285	A	N3-C4-C5	-8.88	120.58	126.80
22	BA	1307	A	C5-C6-N6	8.88	130.80	123.70
1	AA	1374	A	C5-N7-C8	8.88	108.34	103.90
22	BA	2471	A	C5-N7-C8	8.88	108.34	103.90
22	BA	294	A	N3-C4-C5	-8.87	120.59	126.80
22	BA	833	A	C5-C6-N6	8.87	130.80	123.70
1	AA	7	A	N3-C4-C5	-8.87	120.59	126.80
22	BA	614	A	N3-C4-C5	-8.87	120.59	126.80
1	AA	1434	A	C5-N7-C8	8.87	108.34	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1039	A	N3-C4-C5	-8.87	120.59	126.80
22	BA	482	A	C4-C5-C6	8.87	121.44	117.00
22	BA	1652	A	C5-N7-C8	8.87	108.33	103.90
22	BA	2654	A	N3-C4-C5	-8.87	120.59	126.80
22	BA	1111	A	C5-N7-C8	8.87	108.33	103.90
22	BA	2882	A	N3-C4-C5	-8.86	120.60	126.80
23	BB	101	A	C5-C6-N1	8.86	122.13	117.70
22	BA	677	A	C5-C6-N6	8.85	130.78	123.70
22	BA	1872	A	C5-N7-C8	8.85	108.33	103.90
1	AA	572	A	N3-C4-C5	-8.85	120.61	126.80
1	AA	860	A	C4-C5-C6	8.85	121.42	117.00
1	AA	478	A	C5-N7-C8	8.84	108.32	103.90
22	BA	2406	A	N3-C4-C5	-8.84	120.61	126.80
1	AA	80	A	N7-C8-N9	-8.83	109.38	113.80
22	BA	718	A	C5-N7-C8	8.83	108.32	103.90
22	BA	2873	A	N3-C4-C5	-8.83	120.62	126.80
22	BA	2340	A	N3-C4-C5	-8.83	120.62	126.80
23	BB	101	A	C5-C6-N6	8.83	130.76	123.70
1	AA	622	A	N3-C4-C5	-8.83	120.62	126.80
22	BA	2340	A	C5-C6-N6	8.83	130.76	123.70
1	AA	246	A	N3-C4-C5	-8.82	120.62	126.80
22	BA	127	A	N3-C4-C5	-8.82	120.62	126.80
22	BA	2015	A	N3-C4-C5	-8.82	120.62	126.80
22	BA	2469	A	N3-C4-C5	-8.82	120.63	126.80
22	BA	2051	A	N7-C8-N9	-8.81	109.39	113.80
1	AA	1493	A	N3-C4-C5	-8.81	120.63	126.80
1	AA	315	A	N3-C4-C5	-8.81	120.63	126.80
22	BA	2117	A	C5-N7-C8	8.81	108.31	103.90
1	AA	906	A	N3-C4-C5	-8.81	120.64	126.80
22	BA	1302	A	N3-C4-C5	-8.81	120.64	126.80
1	AA	1188	A	N3-C4-C5	-8.80	120.64	126.80
1	AA	1495	U	N1-C2-O2	8.80	128.96	122.80
22	BA	1598	A	N7-C8-N9	-8.80	109.40	113.80
22	BA	2095	A	N3-C4-C5	-8.80	120.64	126.80
1	AA	432	A	C5-N7-C8	8.80	108.30	103.90
1	AA	792	A	C5-N7-C8	8.80	108.30	103.90
1	AA	1019	A	N3-C4-C5	-8.80	120.64	126.80
22	BA	1503	A	C5-N7-C8	8.80	108.30	103.90
1	AA	149	A	C5-N7-C8	8.79	108.30	103.90
1	AA	162	A	C5-C6-N6	8.79	130.74	123.70
22	BA	73	A	N3-C4-C5	-8.80	120.64	126.80
22	BA	1254	A	N3-C4-C5	-8.79	120.64	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1226	A	N3-C4-C5	-8.79	120.65	126.80
1	AA	1167	A	N3-C4-C5	-8.79	120.65	126.80
22	BA	1057	A	C5-N7-C8	8.79	108.29	103.90
1	AA	468	A	C5-N7-C8	8.78	108.29	103.90
1	AA	609	A	N3-C4-C5	-8.79	120.65	126.80
22	BA	1872	A	C4-C5-C6	8.79	121.39	117.00
22	BA	1213	A	C5-N7-C8	8.78	108.29	103.90
22	BA	2031	A	C5-N7-C8	8.78	108.29	103.90
22	BA	2542	A	N3-C4-C5	-8.78	120.65	126.80
22	BA	2602	A	C5-N7-C8	8.78	108.29	103.90
1	AA	356	A	C5-N7-C8	8.78	108.29	103.90
1	AA	1329	A	N3-C4-C5	-8.78	120.66	126.80
22	BA	1678	A	N3-C4-C5	-8.78	120.65	126.80
55	B8	76	A	N3-C4-C5	-8.78	120.66	126.80
22	BA	352	A	C5-C6-N6	8.77	130.72	123.70
22	BA	501	A	N3-C4-C5	-8.77	120.66	126.80
22	BA	734	A	C5-C6-N6	8.77	130.71	123.70
22	BA	2899	A	C5-C6-N6	8.76	130.71	123.70
1	AA	1213	A	C5-N7-C8	8.76	108.28	103.90
22	BA	204	A	N3-C4-C5	-8.76	120.67	126.80
22	BA	374	A	C5-N7-C8	8.76	108.28	103.90
22	BA	1276	A	C5-N7-C8	8.75	108.28	103.90
22	BA	1854	A	C4-C5-C6	8.75	121.38	117.00
22	BA	2518	A	C5-N7-C8	8.75	108.28	103.90
1	AA	1163	A	C5-C6-N6	8.74	130.70	123.70
1	AA	1275	A	C5-N7-C8	8.74	108.27	103.90
22	BA	1755	A	N3-C4-C5	-8.74	120.68	126.80
22	BA	2590	A	N3-C4-C5	-8.74	120.68	126.80
1	AA	32	A	C5-C6-N6	8.74	130.69	123.70
1	AA	510	A	N3-C4-C5	-8.74	120.69	126.80
22	BA	749	A	N3-C4-C5	-8.74	120.69	126.80
22	BA	2435	A	C5-N7-C8	8.73	108.27	103.90
22	BA	1676	A	N7-C8-N9	-8.73	109.43	113.80
22	BA	1308	A	C5-N7-C8	8.73	108.27	103.90
23	BB	29	A	C5-N7-C8	8.73	108.26	103.90
1	AA	915	A	N3-C4-C5	-8.72	120.69	126.80
1	AA	1346	A	N3-C4-C5	-8.72	120.69	126.80
1	AA	19	A	C5-N7-C8	8.71	108.26	103.90
22	BA	91	A	N3-C4-C5	-8.71	120.70	126.80
22	BA	2268	A	N7-C8-N9	-8.72	109.44	113.80
23	BB	66	A	N3-C4-C5	-8.72	120.70	126.80
22	BA	2565	A	N3-C4-C5	-8.71	120.70	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	676	A	N3-C4-C5	-8.71	120.71	126.80
22	BA	428	A	N3-C4-C5	-8.70	120.71	126.80
22	BA	2900	A	C5-C6-N6	8.70	130.66	123.70
1	AA	860	A	C5-N7-C8	8.70	108.25	103.90
22	BA	699	A	C5-N7-C8	8.70	108.25	103.90
22	BA	750	A	C4-C5-C6	8.69	121.35	117.00
22	BA	1069	A	N3-C4-C5	-8.69	120.71	126.80
1	AA	1269	A	N3-C4-C5	-8.69	120.72	126.80
22	BA	507	A	N7-C8-N9	-8.69	109.45	113.80
1	AA	430	A	C5-N7-C8	8.69	108.24	103.90
22	BA	2799	A	C4-C5-C6	8.68	121.34	117.00
22	BA	2090	A	C5-C6-N6	8.68	130.64	123.70
1	AA	1285	A	C5-N7-C8	8.68	108.24	103.90
23	BB	34	A	C5-N7-C8	8.67	108.24	103.90
22	BA	1084	A	C5-N7-C8	8.67	108.23	103.90
1	AA	825	A	C5-N7-C8	8.67	108.23	103.90
22	BA	2448	A	C5-N7-C8	8.67	108.23	103.90
1	AA	414	A	C5-N7-C8	8.66	108.23	103.90
1	AA	539	A	C5-N7-C8	8.66	108.23	103.90
22	BA	2799	A	N3-C4-N9	8.65	134.32	127.40
1	AA	243	A	C5-N7-C8	8.65	108.23	103.90
22	BA	213	A	C5-C6-N6	8.65	130.62	123.70
22	BA	2426	A	N3-C4-C5	-8.65	120.75	126.80
1	AA	1046	A	C5-C6-N6	8.64	130.62	123.70
22	BA	981	A	N3-C4-C5	-8.64	120.75	126.80
22	BA	1626	A	N3-C4-C5	-8.64	120.75	126.80
1	AA	1377	A	C5-N7-C8	8.63	108.22	103.90
22	BA	2461	A	C5-N7-C8	8.64	108.22	103.90
22	BA	2781	A	N7-C8-N9	-8.63	109.48	113.80
1	AA	80	A	C5-C6-N6	8.63	130.60	123.70
1	AA	949	A	C5-N7-C8	8.63	108.22	103.90
1	AA	1150	A	C5-N7-C8	8.63	108.22	103.90
22	BA	2358	A	N3-C4-C5	-8.63	120.76	126.80
22	BA	196	A	C5-N7-C8	8.61	108.20	103.90
22	BA	439	A	C5-C6-N6	8.61	130.59	123.70
22	BA	2336	A	C5-N7-C8	8.61	108.20	103.90
1	AA	55	A	C4-C5-C6	8.60	121.30	117.00
22	BA	666	A	N3-C4-C5	-8.60	120.78	126.80
22	BA	1088	A	C5-N7-C8	8.60	108.20	103.90
22	BA	1027	A	N3-C4-C5	-8.60	120.78	126.80
22	BA	457	A	N3-C4-C5	-8.60	120.78	126.80
22	BA	2311	A	C5-N7-C8	8.60	108.20	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	935	A	C5-N7-C8	8.59	108.20	103.90
22	BA	42	A	N3-C4-C5	-8.59	120.79	126.80
22	BA	1717	A	N3-C4-C5	-8.59	120.79	126.80
22	BA	2598	A	N3-C4-C5	-8.58	120.79	126.80
1	AA	1105	A	C5-N7-C8	8.58	108.19	103.90
22	BA	49	A	C5-N7-C8	8.58	108.19	103.90
22	BA	2009	A	N3-C4-C5	-8.57	120.80	126.80
22	BA	2014	A	N3-C4-C5	-8.57	120.80	126.80
22	BA	1553	A	C5-N7-C8	8.57	108.18	103.90
22	BA	2381	A	N3-C4-C5	-8.57	120.80	126.80
22	BA	2211	A	C5-N7-C8	8.56	108.18	103.90
22	BA	734	A	C8-N9-C4	8.56	109.22	105.80
1	AA	60	A	C5-N7-C8	8.56	108.18	103.90
1	AA	431	A	C5-N7-C8	8.55	108.18	103.90
1	AA	309	A	C5-N7-C8	8.55	108.18	103.90
1	AA	1035	A	C5-N7-C8	8.55	108.18	103.90
22	BA	706	A	C5-N7-C8	8.55	108.18	103.90
22	BA	782	A	C4-C5-C6	8.55	121.28	117.00
22	BA	1069	A	C5-N7-C8	8.55	108.18	103.90
1	AA	642	A	C5-N7-C8	8.55	108.18	103.90
1	AA	520	A	C5-N7-C8	8.55	108.17	103.90
22	BA	2736	A	N3-C4-C5	-8.55	120.81	126.80
1	AA	782	A	C5-N7-C8	8.55	108.17	103.90
22	BA	1095	A	C5-N7-C8	8.55	108.17	103.90
22	BA	1783	A	C5-N7-C8	8.55	108.17	103.90
22	BA	1735	A	C5-C6-N6	8.54	130.53	123.70
1	AA	1155	A	C5-N7-C8	8.54	108.17	103.90
22	BA	282	A	C5-N7-C8	8.54	108.17	103.90
22	BA	1378	A	C5-N7-C8	8.54	108.17	103.90
1	AA	412	A	N3-C4-C5	-8.54	120.83	126.80
1	AA	533	A	C5-N7-C8	8.53	108.17	103.90
1	AA	1502	A	C8-N9-C4	8.53	109.21	105.80
22	BA	1981	A	N3-C4-C5	-8.53	120.83	126.80
22	BA	2077	A	C4-C5-C6	8.53	121.27	117.00
22	BA	2765	A	C5-N7-C8	8.53	108.17	103.90
1	AA	1042	A	C5-N7-C8	8.53	108.17	103.90
22	BA	2883	A	N3-C4-C5	-8.53	120.83	126.80
22	BA	1269	A	C5-N7-C8	8.52	108.16	103.90
22	BA	2054	A	C5-C6-N6	8.52	130.52	123.70
22	BA	807	U	C2-N3-C4	-8.52	121.89	127.00
22	BA	2434	A	N3-C4-C5	-8.52	120.84	126.80
1	AA	1229	A	C5-N7-C8	8.51	108.16	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	685	A	C4-C5-C6	8.51	121.26	117.00
22	BA	479	A	N3-C4-C5	-8.51	120.84	126.80
22	BA	1787	A	C4-C5-C6	8.51	121.25	117.00
22	BA	1981	A	C5-N7-C8	8.51	108.16	103.90
22	BA	1304	A	C5-N7-C8	8.51	108.15	103.90
1	AA	397	A	C5-N7-C8	8.50	108.15	103.90
1	AA	563	A	C5-N7-C8	8.50	108.15	103.90
1	AA	908	A	C5-N7-C8	8.50	108.15	103.90
22	BA	1085	A	C5-N7-C8	8.50	108.15	103.90
22	BA	2829	A	C5-N7-C8	8.50	108.15	103.90
1	AA	1433	A	C5-N7-C8	8.50	108.15	103.90
22	BA	195	A	N3-C4-C5	-8.50	120.85	126.80
22	BA	1913	A	C5-N7-C8	8.49	108.15	103.90
22	BA	2412	A	C4-C5-C6	8.49	121.25	117.00
1	AA	167	A	C5-N7-C8	8.49	108.15	103.90
1	AA	676	A	N3-C4-C5	-8.49	120.85	126.80
22	BA	2600	A	C5-C6-N6	8.49	130.50	123.70
1	AA	1067	A	C5-N7-C8	8.49	108.15	103.90
22	BA	1744	A	C5-N7-C8	8.49	108.15	103.90
22	BA	2792	A	C5-C6-N6	8.49	130.49	123.70
1	AA	1456	A	C5-N7-C8	8.48	108.14	103.90
22	BA	195	A	N9-C4-C5	8.48	109.19	105.80
22	BA	979	A	C5-N7-C8	8.48	108.14	103.90
1	AA	162	A	C4-C5-C6	8.48	121.24	117.00
22	BA	655	A	C5-N7-C8	8.47	108.14	103.90
1	AA	715	A	N3-C4-C5	-8.47	120.87	126.80
22	BA	2119	A	C5-N7-C8	8.47	108.13	103.90
1	AA	499	A	C5-N7-C8	8.46	108.13	103.90
22	BA	643	A	N3-C4-C5	-8.46	120.87	126.80
22	BA	742	A	N3-C4-N9	8.47	134.17	127.40
22	BA	1165	A	C5-N7-C8	8.46	108.13	103.90
22	BA	2366	A	C4-C5-C6	8.46	121.23	117.00
22	BA	1247	A	C5-N7-C8	8.46	108.13	103.90
22	BA	322	A	C5-N7-C8	8.46	108.13	103.90
22	BA	1077	A	N3-C4-C5	-8.46	120.88	126.80
1	AA	681	A	C5-N7-C8	8.46	108.13	103.90
1	AA	746	A	C5-C6-N6	8.46	130.47	123.70
1	AA	1368	A	C5-N7-C8	8.45	108.13	103.90
1	AA	1483	A	C4-C5-C6	8.45	121.23	117.00
1	AA	1534	A	C5-N7-C8	8.45	108.12	103.90
22	BA	2851	A	C5-N7-C8	8.45	108.12	103.90
1	AA	1239	A	C8-N9-C4	8.45	109.18	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1597	A	C5-N7-C8	8.45	108.12	103.90
22	BA	761	A	C4-C5-C6	8.44	121.22	117.00
22	BA	825	A	C5-N7-C8	8.44	108.12	103.90
1	AA	1236	A	C5-N7-C8	8.44	108.12	103.90
22	BA	1773	A	C4-C5-C6	8.44	121.22	117.00
1	AA	1360	A	C5-N7-C8	8.44	108.12	103.90
22	BA	470	A	C5-N7-C8	8.44	108.12	103.90
22	BA	910	A	C5-N7-C8	8.44	108.12	103.90
22	BA	2052	A	C5-N7-C8	8.44	108.12	103.90
1	AA	356	A	C5-C6-N6	8.44	130.45	123.70
22	BA	896	A	C5-N7-C8	8.44	108.12	103.90
23	BB	78	A	N3-C4-C5	-8.44	120.89	126.80
1	AA	98	A	C5-C6-N6	8.43	130.44	123.70
22	BA	241	A	N3-C4-C5	-8.43	120.90	126.80
1	AA	81	A	C5-N7-C8	8.43	108.11	103.90
22	BA	1819	A	C5-N7-C8	8.43	108.11	103.90
1	AA	1503	A	C5-N7-C8	8.42	108.11	103.90
1	AA	1396	A	C5-C6-N6	8.42	130.43	123.70
1	AA	1413	A	N3-C4-C5	-8.42	120.91	126.80
22	BA	756	A	C5-N7-C8	8.42	108.11	103.90
22	BA	1366	A	N3-C4-C5	-8.42	120.91	126.80
1	AA	8	A	C5-N7-C8	8.41	108.11	103.90
22	BA	614	A	C5-N7-C8	8.41	108.11	103.90
22	BA	2009	A	C5-N7-C8	8.41	108.11	103.90
22	BA	2820	A	N3-C4-C5	-8.41	120.91	126.80
1	AA	236	A	C5-N7-C8	8.41	108.10	103.90
1	AA	408	A	C5-N7-C8	8.41	108.10	103.90
1	AA	179	A	C5-N7-C8	8.40	108.10	103.90
22	BA	1936	A	N7-C8-N9	-8.40	109.60	113.80
22	BA	2632	A	C5-N7-C8	8.40	108.10	103.90
1	AA	288	A	C5-N7-C8	8.39	108.10	103.90
1	AA	10	A	C5-N7-C8	8.39	108.09	103.90
22	BA	2439	A	C8-N9-C4	8.39	109.16	105.80
22	BA	146	A	C5-N7-C8	8.39	108.09	103.90
22	BA	2542	A	C8-N9-C4	8.39	109.15	105.80
22	BA	1327	A	N3-C4-C5	-8.38	120.93	126.80
1	AA	493	A	C5-N7-C8	8.38	108.09	103.90
22	BA	1614	A	N3-C4-C5	-8.38	120.93	126.80
22	BA	637	A	C5-N7-C8	8.38	108.09	103.90
22	BA	345	A	C5-N7-C8	8.37	108.09	103.90
1	AA	1110	A	C5-N7-C8	8.37	108.09	103.90
22	BA	52	A	C5-N7-C8	8.37	108.09	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2451	A	N9-C4-C5	8.37	109.15	105.80
1	AA	1250	A	C5-N7-C8	8.37	108.08	103.90
1	AA	901	A	N3-C4-N9	8.36	134.09	127.40
22	BA	2850	A	C5-N7-C8	8.36	108.08	103.90
1	AA	1180	A	C5-N7-C8	8.36	108.08	103.90
1	AA	554	A	C5-N7-C8	8.36	108.08	103.90
1	AA	1117	A	C5-N7-C8	8.35	108.08	103.90
1	AA	1167	A	C5-N7-C8	8.35	108.07	103.90
22	BA	371	A	C5-N7-C8	8.35	108.07	103.90
1	AA	1004	A	C5-N7-C8	8.35	108.07	103.90
22	BA	1420	A	C5-N7-C8	8.35	108.07	103.90
1	AA	1363	A	C5-N7-C8	8.34	108.07	103.90
23	BB	59	A	C5-N7-C8	8.34	108.07	103.90
1	AA	974	A	N3-C4-C5	-8.34	120.96	126.80
22	BA	64	A	C5-N7-C8	8.34	108.07	103.90
22	BA	1328	A	N9-C4-C5	8.34	109.14	105.80
22	BA	1384	A	C5-N7-C8	8.34	108.07	103.90
23	BB	39	A	C5-N7-C8	8.34	108.07	103.90
1	AA	119	A	C5-N7-C8	8.34	108.07	103.90
1	AA	766	A	C5-N7-C8	8.34	108.07	103.90
1	AA	913	A	C5-N7-C8	8.34	108.07	103.90
1	AA	1350	A	C5-N7-C8	8.34	108.07	103.90
22	BA	126	A	C5-N7-C8	8.34	108.07	103.90
22	BA	1387	A	C5-N7-C8	8.34	108.07	103.90
22	BA	2376	A	N3-C4-C5	-8.34	120.97	126.80
22	BA	2453	A	C5-N7-C8	8.34	108.07	103.90
1	AA	1287	A	C5-N7-C8	8.33	108.07	103.90
1	AA	687	A	C5-N7-C8	8.33	108.06	103.90
22	BA	514	A	C5-N7-C8	8.33	108.06	103.90
22	BA	1722	A	C4-C5-C6	8.33	121.17	117.00
1	AA	1021	A	C5-N7-C8	8.33	108.06	103.90
1	AA	1480	A	C5-N7-C8	8.33	108.06	103.90
22	BA	492	A	C5-N7-C8	8.33	108.06	103.90
22	BA	2447	G	C6-N1-C2	-8.33	120.10	125.10
22	BA	705	A	C4-C5-C6	8.32	121.16	117.00
22	BA	1780	A	C5-N7-C8	8.32	108.06	103.90
1	AA	321	A	C5-N7-C8	8.32	108.06	103.90
22	BA	1253	A	N3-C4-C5	-8.32	120.98	126.80
22	BA	2170	A	C5-N7-C8	8.32	108.06	103.90
22	BA	2241	A	C5-N7-C8	8.32	108.06	103.90
22	BA	752	A	C5-N7-C8	8.31	108.06	103.90
22	BA	1509	A	C5-N7-C8	8.31	108.06	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	513	A	C5-C6-N6	8.31	130.35	123.70
1	AA	181	A	C5-N7-C8	8.31	108.05	103.90
1	AA	1081	A	C5-N7-C8	8.30	108.05	103.90
22	BA	1528	A	C5-N7-C8	8.31	108.05	103.90
22	BA	1713	A	N3-C4-C5	-8.31	120.99	126.80
22	BA	2566	A	N3-C4-C5	-8.31	120.99	126.80
22	BA	5	A	C5-N7-C8	8.30	108.05	103.90
22	BA	1275	A	C5-N7-C8	8.30	108.05	103.90
22	BA	1385	A	C5-N7-C8	8.29	108.05	103.90
1	AA	583	A	C5-N7-C8	8.29	108.04	103.90
1	AA	1239	A	N3-C4-C5	-8.29	121.00	126.80
22	BA	165	A	C5-N7-C8	8.29	108.04	103.90
22	BA	226	A	C4-C5-C6	8.29	121.14	117.00
1	AA	1257	A	C5-N7-C8	8.28	108.04	103.90
22	BA	1155	A	C5-N7-C8	8.28	108.04	103.90
22	BA	513	A	C4-C5-C6	8.28	121.14	117.00
22	BA	2134	A	C5-N7-C8	8.28	108.04	103.90
1	AA	383	A	N3-C4-N9	8.28	134.02	127.40
22	BA	2366	A	C5-N7-C8	8.28	108.04	103.90
22	BA	342	A	N3-C4-C5	-8.27	121.01	126.80
22	BA	2469	A	C5-C6-N6	8.27	130.32	123.70
1	AA	393	A	C5-N7-C8	8.27	108.03	103.90
22	BA	734	A	C5-N7-C8	8.27	108.03	103.90
22	BA	1535	A	C5-N7-C8	8.27	108.03	103.90
22	BA	2020	A	C5-N7-C8	8.27	108.03	103.90
22	BA	735	A	C4-C5-C6	8.26	121.13	117.00
22	BA	505	A	C5-N7-C8	8.26	108.03	103.90
22	BA	1213	A	C4-C5-C6	8.26	121.13	117.00
1	AA	16	A	N3-C4-C5	-8.26	121.02	126.80
22	BA	101	A	C5-N7-C8	8.26	108.03	103.90
22	BA	900	A	C5-N7-C8	8.25	108.03	103.90
22	BA	1020	A	C5-N7-C8	8.25	108.03	103.90
1	AA	978	A	C5-N7-C8	8.25	108.03	103.90
22	BA	2872	A	N3-C4-C5	-8.25	121.02	126.80
1	AA	1465	A	C5-N7-C8	8.24	108.02	103.90
22	BA	2267	A	C5-N7-C8	8.24	108.02	103.90
1	AA	174	A	C5-N7-C8	8.24	108.02	103.90
1	AA	533	A	C4-C5-C6	8.24	121.12	117.00
22	BA	2309	A	C5-N7-C8	8.24	108.02	103.90
22	BA	643	A	N7-C8-N9	-8.23	109.68	113.80
22	BA	2333	A	N3-C4-C5	-8.23	121.04	126.80
22	BA	2154	A	C5-N7-C8	8.23	108.02	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	71	A	C5-N7-C8	8.23	108.02	103.90
22	BA	2634	A	C5-N7-C8	8.23	108.02	103.90
1	AA	74	A	C5-N7-C8	8.23	108.01	103.90
22	BA	1598	A	C4-C5-C6	8.23	121.11	117.00
1	AA	1170	A	C5-N7-C8	8.23	108.01	103.90
1	AA	1179	A	C5-N7-C8	8.23	108.01	103.90
22	BA	661	A	C5-N7-C8	8.23	108.01	103.90
22	BA	354	A	C5-N7-C8	8.22	108.01	103.90
22	BA	503	A	C5-N7-C8	8.22	108.01	103.90
22	BA	2451	A	N7-C8-N9	-8.22	109.69	113.80
22	BA	2062	A	C5-N7-C8	8.22	108.01	103.90
1	AA	648	A	C5-N7-C8	8.22	108.01	103.90
22	BA	1572	A	C5-C6-N6	8.22	130.28	123.70
1	AA	1499	A	C5-N7-C8	8.22	108.01	103.90
1	AA	729	A	C5-N7-C8	8.21	108.01	103.90
22	BA	346	A	C5-N7-C8	8.21	108.01	103.90
22	BA	1070	A	C5-N7-C8	8.22	108.01	103.90
22	BA	1342	A	C5-N7-C8	8.21	108.01	103.90
22	BA	574	A	C5-N7-C8	8.21	108.01	103.90
22	BA	2077	A	C5-N7-C8	8.21	108.00	103.90
22	BA	602	A	C5-N7-C8	8.21	108.00	103.90
22	BA	504	A	C5-N7-C8	8.20	108.00	103.90
1	AA	918	A	C5-N7-C8	8.20	108.00	103.90
22	BA	750	A	N3-C4-N9	8.20	133.96	127.40
22	BA	1054	A	C5-C6-N6	8.20	130.26	123.70
22	BA	2439	A	C5-N7-C8	8.20	108.00	103.90
1	AA	1151	A	C5-N7-C8	8.19	108.00	103.90
22	BA	1815	A	N3-C4-C5	-8.19	121.06	126.80
1	AA	238	A	C5-N7-C8	8.19	107.99	103.90
22	BA	1640	A	C5-N7-C8	8.19	107.99	103.90
22	BA	2721	A	C4-C5-C6	8.19	121.09	117.00
1	AA	600	A	C5-N7-C8	8.19	107.99	103.90
22	BA	1569	A	N3-C4-C5	-8.19	121.07	126.80
1	AA	466	A	C5-N7-C8	8.18	107.99	103.90
1	AA	498	A	C5-N7-C8	8.18	107.99	103.90
1	AA	845	A	C5-N7-C8	8.18	107.99	103.90
22	BA	167	A	C5-N7-C8	8.18	107.99	103.90
1	AA	1105	A	C8-N9-C4	8.18	109.07	105.80
22	BA	1810	A	C5-C6-N6	8.18	130.25	123.70
22	BA	2587	A	C5-N7-C8	8.18	107.99	103.90
22	BA	2070	A	C5-N7-C8	8.18	107.99	103.90
1	AA	205	A	C5-N7-C8	8.17	107.99	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	937	A	C5-N7-C8	8.17	107.98	103.90
1	AA	1014	A	C5-N7-C8	8.17	107.98	103.90
22	BA	480	A	C4-C5-C6	8.17	121.08	117.00
22	BA	749	A	C5-N7-C8	8.17	107.98	103.90
22	BA	820	A	C4-C5-C6	8.17	121.08	117.00
22	BA	1067	A	C5-N7-C8	8.17	107.98	103.90
1	AA	753	A	C5-N7-C8	8.17	107.98	103.90
22	BA	340	A	C5-N7-C8	8.16	107.98	103.90
23	BB	75	G	C6-N1-C2	-8.16	120.20	125.10
1	AA	802	A	C5-N7-C8	8.16	107.98	103.90
1	AA	1005	A	C5-N7-C8	8.16	107.98	103.90
22	BA	1048	A	C5-N7-C8	8.16	107.98	103.90
22	BA	1522	A	C5-N7-C8	8.16	107.98	103.90
1	AA	306	A	C5-N7-C8	8.16	107.98	103.90
1	AA	865	A	N9-C4-C5	8.16	109.06	105.80
23	BB	104	A	C5-N7-C8	8.16	107.98	103.90
22	BA	14	A	C5-N7-C8	8.15	107.98	103.90
1	AA	382	A	C5-N7-C8	8.15	107.98	103.90
1	AA	814	A	C5-N7-C8	8.15	107.98	103.90
1	AA	819	A	C5-N7-C8	8.15	107.98	103.90
1	AA	649	A	C5-N7-C8	8.15	107.97	103.90
22	BA	1403	A	C5-N7-C8	8.15	107.97	103.90
22	BA	2660	A	C5-N7-C8	8.15	107.97	103.90
1	AA	695	A	C5-N7-C8	8.14	107.97	103.90
1	AA	1016	A	C5-N7-C8	8.14	107.97	103.90
22	BA	507	A	N3-C4-C5	-8.14	121.10	126.80
22	BA	1133	A	C5-N7-C8	8.14	107.97	103.90
1	AA	300	A	C5-C6-N6	8.14	130.21	123.70
1	AA	1171	A	C5-N7-C8	8.14	107.97	103.90
22	BA	216	A	C5-N7-C8	8.14	107.97	103.90
22	BA	310	A	C5-N7-C8	8.14	107.97	103.90
22	BA	466	A	C5-C6-N6	8.14	130.21	123.70
1	AA	130	A	C5-N7-C8	8.13	107.97	103.90
1	AA	364	A	C5-N7-C8	8.13	107.97	103.90
1	AA	397	A	N3-C4-N9	8.13	133.91	127.40
1	AA	635	A	C5-N7-C8	8.13	107.97	103.90
22	BA	783	A	C5-N7-C8	8.13	107.97	103.90
22	BA	1583	A	C5-N7-C8	8.13	107.97	103.90
22	BA	1899	A	C5-N7-C8	8.13	107.97	103.90
1	AA	228	A	C5-N7-C8	8.13	107.96	103.90
22	BA	101	A	N3-C4-N9	8.13	133.90	127.40
22	BA	627	A	C5-N7-C8	8.13	107.96	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	905	A	C5-N7-C8	8.13	107.96	103.90
22	BA	2757	A	C4-C5-C6	8.13	121.06	117.00
22	BA	2077	A	N3-C4-N9	8.12	133.90	127.40
1	AA	274	A	C5-N7-C8	8.12	107.96	103.90
22	BA	1287	A	C5-N7-C8	8.12	107.96	103.90
22	BA	231	A	C5-N7-C8	8.12	107.96	103.90
22	BA	497	A	C5-N7-C8	8.12	107.96	103.90
1	AA	303	A	C5-N7-C8	8.12	107.96	103.90
22	BA	2823	A	C5-N7-C8	8.12	107.96	103.90
22	BA	332	A	C5-N7-C8	8.11	107.96	103.90
22	BA	2327	A	C5-N7-C8	8.11	107.96	103.90
22	BA	789	A	C5-N7-C8	8.11	107.95	103.90
1	AA	1508	A	C4-C5-C6	8.11	121.05	117.00
22	BA	44	A	C5-N7-C8	8.11	107.95	103.90
1	AA	694	A	C5-N7-C8	8.10	107.95	103.90
22	BA	1040	A	C5-N7-C8	8.10	107.95	103.90
22	BA	547	A	C5-N7-C8	8.10	107.95	103.90
1	AA	1012	A	C5-N7-C8	8.10	107.95	103.90
22	BA	2183	A	C5-N7-C8	8.10	107.95	103.90
22	BA	492	A	C4-C5-C6	8.10	121.05	117.00
22	BA	925	A	C5-N7-C8	8.10	107.95	103.90
22	BA	1937	A	N9-C4-C5	8.10	109.04	105.80
22	BA	2163	A	C5-N7-C8	8.10	107.95	103.90
1	AA	199	A	C5-N7-C8	8.09	107.95	103.90
1	AA	246	A	C5-N7-C8	8.09	107.95	103.90
22	BA	449	A	C5-N7-C8	8.09	107.94	103.90
1	AA	190	A	C5-N7-C8	8.09	107.94	103.90
1	AA	1169	A	C5-N7-C8	8.09	107.94	103.90
22	BA	541	A	C5-N7-C8	8.09	107.94	103.90
22	BA	1871	A	C5-N7-C8	8.09	107.94	103.90
22	BA	2251	OMG	P-O3'-C3'	8.09	129.40	119.70
22	BA	84	A	N3-C4-C5	-8.08	121.14	126.80
1	AA	192	A	C5-N7-C8	8.08	107.94	103.90
22	BA	182	A	C5-N7-C8	8.08	107.94	103.90
22	BA	1591	A	C5-N7-C8	8.08	107.94	103.90
22	BA	782	A	C5-N7-C8	8.08	107.94	103.90
23	BB	119	A	C5-N7-C8	8.08	107.94	103.90
22	BA	936	A	C5-N7-C8	8.08	107.94	103.90
22	BA	1089	A	C5-N7-C8	8.08	107.94	103.90
22	BA	1328	A	C5-N7-C8	8.08	107.94	103.90
1	AA	315	A	C5-N7-C8	8.07	107.94	103.90
1	AA	706	A	C5-N7-C8	8.07	107.94	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	877	A	C5-N7-C8	8.07	107.94	103.90
1	AA	253	A	C5-N7-C8	8.06	107.93	103.90
1	AA	1329	A	C5-N7-C8	8.06	107.93	103.90
22	BA	2369	A	C5-N7-C8	8.06	107.93	103.90
1	AA	32	A	C4-C5-C6	8.06	121.03	117.00
1	AA	553	A	C5-N7-C8	8.06	107.93	103.90
1	AA	1333	A	C5-N7-C8	8.06	107.93	103.90
22	BA	1147	A	C5-N7-C8	8.06	107.93	103.90
22	BA	2589	A	C8-N9-C4	8.06	109.02	105.80
22	BA	2317	A	C5-N7-C8	8.05	107.93	103.90
1	AA	816	A	C5-N7-C8	8.05	107.92	103.90
22	BA	1434	A	C5-N7-C8	8.05	107.92	103.90
22	BA	1505	A	C5-N7-C8	8.05	107.92	103.90
22	BA	1508	A	C5-N7-C8	8.05	107.92	103.90
22	BA	2297	A	C5-N7-C8	8.05	107.92	103.90
1	AA	313	A	C5-N7-C8	8.04	107.92	103.90
22	BA	2758	A	C5-N7-C8	8.04	107.92	103.90
1	AA	270	A	C5-N7-C8	8.04	107.92	103.90
1	AA	1502	A	C5-N7-C8	8.04	107.92	103.90
22	BA	83	A	C5-N7-C8	8.04	107.92	103.90
22	BA	1156	A	C5-N7-C8	8.04	107.92	103.90
22	BA	2778	A	C5-N7-C8	8.04	107.92	103.90
22	BA	960	A	C5-N7-C8	8.04	107.92	103.90
1	AA	1408	A	C5-N7-C8	8.04	107.92	103.90
22	BA	1938	A	C5-N7-C8	8.04	107.92	103.90
22	BA	2171	A	C5-N7-C8	8.04	107.92	103.90
1	AA	747	A	C5-N7-C8	8.03	107.92	103.90
1	AA	901	A	C5-C6-N6	8.03	130.13	123.70
22	BA	2750	A	C5-N7-C8	8.03	107.92	103.90
1	AA	1513	A	C5-N7-C8	8.03	107.92	103.90
1	AA	938	A	C5-N7-C8	8.03	107.91	103.90
22	BA	1848	A	C4-C5-C6	8.03	121.01	117.00
22	BA	1590	A	C5-N7-C8	8.02	107.91	103.90
22	BA	1635	A	C5-N7-C8	8.02	107.91	103.90
1	AA	459	A	C5-N7-C8	8.02	107.91	103.90
22	BA	1392	A	C5-N7-C8	8.02	107.91	103.90
1	AA	1256	A	C5-N7-C8	8.02	107.91	103.90
22	BA	804	A	C5-N7-C8	8.02	107.91	103.90
22	BA	2792	A	C5-N7-C8	8.02	107.91	103.90
22	BA	845	A	C5-N7-C8	8.01	107.91	103.90
1	AA	768	A	C5-N7-C8	8.01	107.91	103.90
22	BA	479	A	C5-N7-C8	8.01	107.91	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	336	A	C5-N7-C8	8.01	107.91	103.90
22	BA	920	A	C5-N7-C8	8.01	107.91	103.90
22	BA	983	A	C8-N9-C4	8.01	109.00	105.80
1	AA	143	A	C5-N7-C8	8.01	107.90	103.90
1	AA	182	A	C5-N7-C8	8.01	107.90	103.90
22	BA	644	A	C5-N7-C8	8.01	107.90	103.90
22	BA	1021	A	C5-N7-C8	8.01	107.90	103.90
1	AA	535	A	C5-N7-C8	8.00	107.90	103.90
22	BA	2670	A	C5-N7-C8	8.00	107.90	103.90
1	AA	172	A	C5-N7-C8	8.00	107.90	103.90
22	BA	2450	A	N3-C4-C5	-8.00	121.20	126.80
1	AA	547	A	C5-N7-C8	8.00	107.90	103.90
1	AA	974	A	C5-N7-C8	8.00	107.90	103.90
1	AA	807	A	C5-N7-C8	8.00	107.90	103.90
1	AA	452	A	C5-N7-C8	8.00	107.90	103.90
22	BA	899	A	C5-N7-C8	8.00	107.90	103.90
22	BA	575	A	C5-N7-C8	8.00	107.90	103.90
1	AA	320	A	C5-N7-C8	7.99	107.90	103.90
1	AA	969	A	C5-N7-C8	7.99	107.90	103.90
22	BA	38	A	C5-N7-C8	7.99	107.90	103.90
22	BA	251	A	N3-C4-N9	7.99	133.79	127.40
22	BA	2837	A	C5-N7-C8	7.99	107.89	103.90
1	AA	50	A	C5-N7-C8	7.99	107.89	103.90
1	AA	389	A	C5-N7-C8	7.99	107.89	103.90
23	BB	115	A	C5-N7-C8	7.99	107.89	103.90
22	BA	142	A	C4-C5-C6	7.98	120.99	117.00
22	BA	2721	A	N3-C4-N9	7.98	133.79	127.40
1	AA	865	A	C5-N7-C8	7.98	107.89	103.90
1	AA	712	A	C5-N7-C8	7.98	107.89	103.90
22	BA	1427	A	C5-N7-C8	7.98	107.89	103.90
22	BA	1551	A	C5-N7-C8	7.98	107.89	103.90
22	BA	1246	A	C5-N7-C8	7.97	107.89	103.90
1	AA	572	A	C5-N7-C8	7.97	107.89	103.90
22	BA	222	A	C5-N7-C8	7.97	107.89	103.90
22	BA	1722	A	C5-N7-C8	7.97	107.89	103.90
22	BA	1365	A	C5-N7-C8	7.97	107.89	103.90
1	AA	959	A	C5-N7-C8	7.97	107.88	103.90
22	BA	49	A	C4-C5-C6	7.97	120.98	117.00
1	AA	1146	A	C5-N7-C8	7.97	107.88	103.90
1	AA	915	A	C5-N7-C8	7.96	107.88	103.90
1	AA	1036	A	C5-N7-C8	7.96	107.88	103.90
1	AA	498	A	C4-C5-C6	7.96	120.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1393	A	C5-N7-C8	7.96	107.88	103.90
22	BA	1419	A	C5-N7-C8	7.96	107.88	103.90
22	BA	1490	A	C5-N7-C8	7.96	107.88	103.90
22	BA	10	A	C5-N7-C8	7.96	107.88	103.90
22	BA	627	A	C5-C6-N6	7.96	130.07	123.70
22	BA	849	A	C5-N7-C8	7.96	107.88	103.90
22	BA	2173	A	C5-N7-C8	7.96	107.88	103.90
1	AA	66	A	C5-N7-C8	7.96	107.88	103.90
1	AA	546	A	C5-N7-C8	7.96	107.88	103.90
22	BA	2860	A	C5-N7-C8	7.96	107.88	103.90
22	BA	6	A	C5-N7-C8	7.96	107.88	103.90
22	BA	1096	A	C5-N7-C8	7.95	107.88	103.90
22	BA	1689	A	C5-N7-C8	7.95	107.88	103.90
23	BB	99	A	C5-N7-C8	7.95	107.88	103.90
22	BA	1073	A	C5-N7-C8	7.95	107.88	103.90
1	AA	44	A	C5-N7-C8	7.95	107.88	103.90
1	AA	1437	A	C5-N7-C8	7.95	107.88	103.90
22	BA	2340	A	C8-N9-C4	7.95	108.98	105.80
1	AA	563	A	N3-C4-N9	7.95	133.76	127.40
22	BA	654	A	C5-N7-C8	7.95	107.87	103.90
22	BA	2469	A	C8-N9-C4	7.95	108.98	105.80
1	AA	190	A	N3-C4-N9	7.94	133.75	127.40
1	AA	451	A	C5-N7-C8	7.94	107.87	103.90
22	BA	278	A	N3-C4-N9	7.94	133.75	127.40
22	BA	2879	A	C5-N7-C8	7.94	107.87	103.90
1	AA	746	A	N3-C4-N9	7.94	133.75	127.40
1	AA	1252	A	C5-N7-C8	7.94	107.87	103.90
1	AA	1483	A	C5-N7-C8	7.94	107.87	103.90
22	BA	1046	A	C5-N7-C8	7.94	107.87	103.90
1	AA	975	A	C5-N7-C8	7.94	107.87	103.90
1	AA	1476	A	C5-N7-C8	7.94	107.87	103.90
22	BA	2388	A	C4-C5-C6	7.94	120.97	117.00
1	AA	32	A	N3-C4-N9	7.93	133.75	127.40
1	AA	353	A	C5-N7-C8	7.93	107.87	103.90
1	AA	363	A	C5-N7-C8	7.93	107.87	103.90
22	BA	943	A	C4-C5-C6	7.93	120.97	117.00
22	BA	917	A	C5-N7-C8	7.93	107.87	103.90
22	BA	2314	A	C5-N7-C8	7.93	107.86	103.90
22	BA	2589	A	N3-C4-C5	-7.93	121.25	126.80
1	AA	1000	A	C5-N7-C8	7.93	107.86	103.90
1	AA	1163	A	C5-N7-C8	7.93	107.86	103.90
1	AA	873	A	C4-C5-C6	7.93	120.96	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	439	A	C5-N7-C8	7.93	107.86	103.90
22	BA	1787	A	N3-C4-N9	7.93	133.74	127.40
22	BA	391	A	C5-N7-C8	7.92	107.86	103.90
22	BA	528	A	C5-N7-C8	7.92	107.86	103.90
22	BA	2516	A	C5-N7-C8	7.92	107.86	103.90
1	AA	1117	A	C8-N9-C4	7.92	108.97	105.80
1	AA	1145	A	C5-N7-C8	7.92	107.86	103.90
22	BA	1260	A	C5-N7-C8	7.92	107.86	103.90
1	AA	78	A	C5-N7-C8	7.92	107.86	103.90
22	BA	412	A	C5-N7-C8	7.92	107.86	103.90
22	BA	590	A	C5-N7-C8	7.92	107.86	103.90
22	BA	2142	A	C5-N7-C8	7.92	107.86	103.90
1	AA	1019	A	C5-N7-C8	7.91	107.86	103.90
22	BA	878	A	C5-N7-C8	7.91	107.86	103.90
22	BA	2727	A	C5-C6-N6	7.91	130.03	123.70
1	AA	349	A	C5-N7-C8	7.91	107.86	103.90
22	BA	1553	A	C4-C5-C6	7.91	120.96	117.00
22	BA	1919	A	C5-N7-C8	7.91	107.86	103.90
1	AA	7	A	C5-N7-C8	7.91	107.86	103.90
1	AA	1238	A	C5-N7-C8	7.91	107.86	103.90
22	BA	1413	A	C5-N7-C8	7.91	107.86	103.90
22	BA	1021	A	N3-C4-N9	7.91	133.73	127.40
22	BA	1858	A	C5-N7-C8	7.91	107.85	103.90
1	AA	171	A	C5-N7-C8	7.91	107.85	103.90
22	BA	1090	A	C5-N7-C8	7.91	107.85	103.90
22	BA	2534	A	C5-N7-C8	7.90	107.85	103.90
1	AA	579	A	C5-N7-C8	7.90	107.85	103.90
22	BA	821	A	C5-N7-C8	7.90	107.85	103.90
1	AA	1204	A	C5-N7-C8	7.90	107.85	103.90
1	AA	831	A	C5-N7-C8	7.90	107.85	103.90
1	AA	901	A	C5-N7-C8	7.90	107.85	103.90
22	BA	2335	A	C5-N7-C8	7.89	107.85	103.90
22	BA	278	A	C5-N7-C8	7.89	107.85	103.90
22	BA	272	A	C5-N7-C8	7.89	107.85	103.90
1	AA	109	A	C5-N7-C8	7.89	107.84	103.90
23	BB	108	A	C5-N7-C8	7.89	107.84	103.90
1	AA	712	A	C4-C5-C6	7.89	120.94	117.00
1	AA	1201	A	C5-N7-C8	7.89	107.84	103.90
22	BA	352	A	C5-N7-C8	7.89	107.84	103.90
22	BA	2284	A	N3-C4-N9	7.89	133.71	127.40
1	AA	371	A	C5-N7-C8	7.88	107.84	103.90
22	BA	2273	A	C5-N7-C8	7.88	107.84	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	509	A	C5-N7-C8	7.88	107.84	103.90
1	AA	1398	A	C5-N7-C8	7.88	107.84	103.90
22	BA	152	A	C5-N7-C8	7.88	107.84	103.90
22	BA	2407	A	C4-C5-C6	7.88	120.94	117.00
22	BA	324	A	C5-N7-C8	7.88	107.84	103.90
1	AA	1493	A	C5-N7-C8	7.88	107.84	103.90
22	BA	2003	A	C5-N7-C8	7.87	107.84	103.90
22	BA	2810	A	C5-N7-C8	7.87	107.84	103.90
1	AA	131	A	C5-N7-C8	7.87	107.84	103.90
22	BA	255	A	C4-C5-C6	7.87	120.94	117.00
22	BA	1143	A	C4-C5-C6	7.87	120.94	117.00
22	BA	2158	A	C5-N7-C8	7.87	107.84	103.90
22	BA	2352	A	C5-N7-C8	7.87	107.84	103.90
22	BA	213	A	C8-N9-C4	7.87	108.95	105.80
22	BA	2227	A	C5-N7-C8	7.87	107.83	103.90
22	BA	2541	A	C5-N7-C8	7.87	107.83	103.90
1	AA	1429	A	C5-N7-C8	7.87	107.83	103.90
22	BA	2090	A	C5-N7-C8	7.87	107.83	103.90
1	AA	640	A	C5-N7-C8	7.86	107.83	103.90
1	AA	889	A	C5-N7-C8	7.86	107.83	103.90
1	AA	1431	A	C5-N7-C8	7.86	107.83	103.90
22	BA	676	A	C5-N7-C8	7.86	107.83	103.90
22	BA	1755	A	C5-N7-C8	7.86	107.83	103.90
22	BA	103	A	C5-N7-C8	7.86	107.83	103.90
22	BA	2060	A	C5-N7-C8	7.86	107.83	103.90
22	BA	2749	A	N3-C4-C5	-7.86	121.30	126.80
1	AA	196	A	C5-N7-C8	7.86	107.83	103.90
1	AA	1201	A	C5-C6-N6	7.86	129.98	123.70
22	BA	1794	A	C5-N7-C8	7.85	107.83	103.90
22	BA	960	A	N3-C4-N9	7.85	133.68	127.40
22	BA	2856	A	C5-N7-C8	7.85	107.82	103.90
1	AA	907	A	C5-N7-C8	7.84	107.82	103.90
1	AA	435	A	C5-N7-C8	7.84	107.82	103.90
22	BA	2042	A	C5-N7-C8	7.84	107.82	103.90
22	BA	1029	A	C4-C5-C6	7.84	120.92	117.00
22	BA	1142	A	C5-N7-C8	7.84	107.82	103.90
22	BA	1970	A	C5-N7-C8	7.84	107.82	103.90
22	BA	2094	A	C5-N7-C8	7.84	107.82	103.90
22	BA	2278	A	C5-N7-C8	7.84	107.82	103.90
1	AA	49	U	C5-C4-O4	7.84	130.60	125.90
1	AA	958	A	C5-N7-C8	7.84	107.82	103.90
1	AA	1357	A	C5-N7-C8	7.84	107.82	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1272	A	C5-N7-C8	7.83	107.82	103.90
22	BA	2135	A	C5-N7-C8	7.83	107.82	103.90
1	AA	2	A	C5-N7-C8	7.83	107.81	103.90
1	AA	1346	A	C5-N7-C8	7.83	107.81	103.90
1	AA	595	A	C5-N7-C8	7.83	107.81	103.90
1	AA	780	A	C5-N7-C8	7.83	107.81	103.90
1	AA	1197	A	C4-C5-C6	7.83	120.92	117.00
1	AA	1318	A	C5-N7-C8	7.83	107.81	103.90
22	BA	56	A	C5-N7-C8	7.83	107.81	103.90
22	BA	1749	A	C5-N7-C8	7.83	107.81	103.90
22	BA	1784	A	C5-N7-C8	7.83	107.81	103.90
1	AA	1311	A	C5-N7-C8	7.83	107.81	103.90
22	BA	613	A	C5-N7-C8	7.83	107.81	103.90
22	BA	689	A	C5-N7-C8	7.83	107.81	103.90
22	BA	2052	A	N3-C4-N9	7.83	133.66	127.40
1	AA	1394	A	C5-N7-C8	7.83	107.81	103.90
22	BA	945	A	C5-N7-C8	7.83	107.81	103.90
1	AA	1410	A	C5-N7-C8	7.82	107.81	103.90
22	BA	2101	A	C5-N7-C8	7.82	107.81	103.90
22	BA	2114	A	C5-N7-C8	7.82	107.81	103.90
22	BA	2448	A	C4-C5-C6	7.82	120.91	117.00
23	BB	52	A	C5-N7-C8	7.82	107.81	103.90
1	AA	1046	A	C4-C5-C6	7.82	120.91	117.00
22	BA	1080	A	C5-N7-C8	7.82	107.81	103.90
22	BA	2247	A	C4-C5-C6	7.82	120.91	117.00
1	AA	51	A	C5-N7-C8	7.82	107.81	103.90
1	AA	892	A	C5-N7-C8	7.82	107.81	103.90
22	BA	63	A	C5-N7-C8	7.82	107.81	103.90
22	BA	829	A	C5-N7-C8	7.82	107.81	103.90
22	BA	2478	A	C5-N7-C8	7.82	107.81	103.90
22	BA	608	A	C5-N7-C8	7.81	107.81	103.90
1	AA	1447	A	C5-N7-C8	7.81	107.81	103.90
1	AA	974	A	C8-N9-C4	7.81	108.92	105.80
22	BA	2741	A	C5-N7-C8	7.81	107.80	103.90
1	AA	19	A	N9-C4-C5	7.81	108.92	105.80
22	BA	197	A	C5-N7-C8	7.81	107.80	103.90
22	BA	2425	A	N3-C4-N9	7.81	133.65	127.40
1	AA	1225	A	C5-N7-C8	7.80	107.80	103.90
1	AA	189	A	C5-N7-C8	7.80	107.80	103.90
22	BA	1169	A	C8-N9-C4	7.80	108.92	105.80
22	BA	1634	A	C5-N7-C8	7.80	107.80	103.90
22	BA	781	A	C4-C5-C6	7.80	120.90	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	696	A	C4-C5-C6	7.80	120.90	117.00
1	AA	1507	A	C5-N7-C8	7.80	107.80	103.90
22	BA	2530	A	C5-N7-C8	7.80	107.80	103.90
1	AA	794	A	C5-N7-C8	7.80	107.80	103.90
22	BA	685	A	C5-N7-C8	7.80	107.80	103.90
22	BA	2097	A	C5-N7-C8	7.80	107.80	103.90
22	BA	2328	A	N3-C4-N9	7.80	133.64	127.40
1	AA	65	A	C5-N7-C8	7.79	107.80	103.90
55	B8	73	A	C4-C5-C6	7.79	120.90	117.00
22	BA	742	A	C5-N7-C8	7.79	107.80	103.90
22	BA	1469	A	C4-C5-C6	7.79	120.89	117.00
22	BA	1230	A	C5-N7-C8	7.79	107.80	103.90
23	BB	45	A	C5-N7-C8	7.79	107.80	103.90
1	AA	502	A	C5-N7-C8	7.78	107.79	103.90
1	AA	977	A	C5-N7-C8	7.78	107.79	103.90
22	BA	512	G	O4'-C1'-N9	7.78	114.43	108.20
22	BA	1689	A	C4-C5-C6	7.78	120.89	117.00
22	BA	1787	A	C5-N7-C8	7.78	107.79	103.90
22	BA	2126	A	C5-N7-C8	7.78	107.79	103.90
22	BA	2392	A	C4-C5-C6	7.78	120.89	117.00
22	BA	1872	A	N3-C4-N9	7.78	133.62	127.40
1	AA	749	A	C5-N7-C8	7.78	107.79	103.90
22	BA	2800	A	C5-N7-C8	7.78	107.79	103.90
22	BA	2340	A	C5-N7-C8	7.77	107.79	103.90
22	BA	1127	A	C5-N7-C8	7.77	107.79	103.90
1	AA	906	A	C5-N7-C8	7.77	107.78	103.90
22	BA	311	A	C5-N7-C8	7.77	107.78	103.90
22	BA	2425	A	C4-C5-C6	7.77	120.89	117.00
22	BA	470	A	C4-C5-C6	7.76	120.88	117.00
22	BA	1504	A	C5-N7-C8	7.76	107.78	103.90
22	BA	1773	A	C5-N7-C8	7.76	107.78	103.90
22	BA	2850	A	C4-C5-C6	7.76	120.88	117.00
22	BA	1133	A	N9-C4-C5	7.76	108.91	105.80
22	BA	911	A	C5-N7-C8	7.76	107.78	103.90
1	AA	344	A	C5-N7-C8	7.75	107.78	103.90
1	AA	1441	A	C5-N7-C8	7.75	107.78	103.90
22	BA	676	A	C8-N9-C4	7.75	108.90	105.80
1	AA	728	A	C5-N7-C8	7.75	107.78	103.90
1	AA	1306	A	C5-N7-C8	7.75	107.78	103.90
22	BA	2082	A	C4-C5-C6	7.75	120.88	117.00
1	AA	630	A	C5-N7-C8	7.74	107.77	103.90
1	AA	1428	A	C5-N7-C8	7.74	107.77	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1912	A	C5-N7-C8	7.74	107.77	103.90
1	AA	1350	A	C4-C5-C6	7.74	120.87	117.00
22	BA	1269	A	C4-C5-C6	7.74	120.87	117.00
22	BA	1690	A	C5-N7-C8	7.74	107.77	103.90
1	AA	621	A	C5-N7-C8	7.74	107.77	103.90
1	AA	1413	A	C5-N7-C8	7.74	107.77	103.90
1	AA	59	A	C5-N7-C8	7.73	107.77	103.90
1	AA	1251	A	C5-N7-C8	7.73	107.77	103.90
22	BA	1098	A	C5-N7-C8	7.73	107.76	103.90
22	BA	1810	A	N3-C4-N9	7.73	133.58	127.40
1	AA	197	A	C5-N7-C8	7.73	107.76	103.90
1	AA	1500	A	C5-N7-C8	7.73	107.76	103.90
22	BA	750	A	C5-N7-C8	7.72	107.76	103.90
1	AA	532	A	C5-N7-C8	7.72	107.76	103.90
22	BA	1801	A	C5-N7-C8	7.72	107.76	103.90
1	AA	300	A	N3-C4-N9	7.72	133.58	127.40
22	BA	909	A	C5-N7-C8	7.72	107.76	103.90
22	BA	1453	A	C5-N7-C8	7.72	107.76	103.90
22	BA	2476	A	C5-N7-C8	7.72	107.76	103.90
1	AA	98	A	C5-N7-C8	7.72	107.76	103.90
1	AA	1196	A	C5-N7-C8	7.72	107.76	103.90
1	AA	1248	A	C5-N7-C8	7.71	107.76	103.90
22	BA	1987	A	C5-N7-C8	7.71	107.76	103.90
1	AA	223	A	C5-N7-C8	7.71	107.76	103.90
1	AA	1197	A	C5-N7-C8	7.71	107.75	103.90
23	BB	50	A	C5-N7-C8	7.71	107.76	103.90
22	BA	2322	A	C5-N7-C8	7.71	107.75	103.90
22	BA	71	A	C5-N7-C8	7.71	107.75	103.90
22	BA	2639	A	C5-N7-C8	7.71	107.75	103.90
1	AA	495	A	C5-N7-C8	7.70	107.75	103.90
1	AA	533	A	N3-C4-N9	7.70	133.56	127.40
22	BA	1525	A	C5-N7-C8	7.70	107.75	103.90
22	BA	2727	A	N3-C4-N9	7.70	133.56	127.40
1	AA	718	A	C5-N7-C8	7.70	107.75	103.90
1	AA	766	A	C8-N9-C4	7.70	108.88	105.80
1	AA	1274	A	C5-N7-C8	7.70	107.75	103.90
22	BA	1419	A	C8-N9-C4	7.70	108.88	105.80
22	BA	2019	A	C5-N7-C8	7.70	107.75	103.90
22	BA	1020	A	N3-C4-C5	-7.69	121.42	126.80
22	BA	1321	A	C5-N7-C8	7.69	107.75	103.90
22	BA	1805	A	C5-N7-C8	7.69	107.75	103.90
1	AA	1396	A	C5-N7-C8	7.69	107.75	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	167	A	C4-C5-C6	7.69	120.84	117.00
22	BA	1877	A	C5-N7-C8	7.69	107.75	103.90
1	AA	1191	A	C5-N7-C8	7.69	107.74	103.90
55	B8	76	A	C5-N7-C8	7.69	107.74	103.90
1	AA	706	A	C4-C5-C6	7.68	120.84	117.00
1	AA	1269	A	C5-N7-C8	7.68	107.74	103.90
22	BA	721	A	C5-N7-C8	7.68	107.74	103.90
23	BB	94	A	C5-N7-C8	7.68	107.74	103.90
22	BA	1678	A	C5-N7-C8	7.68	107.74	103.90
22	BA	2169	A	C5-N7-C8	7.68	107.74	103.90
22	BA	2461	A	N3-C4-N9	7.68	133.55	127.40
1	AA	908	A	C4-C5-C6	7.68	120.84	117.00
22	BA	1854	A	N3-C4-N9	7.68	133.54	127.40
1	AA	456	A	C5-N7-C8	7.68	107.74	103.90
1	AA	655	A	C5-N7-C8	7.68	107.74	103.90
22	BA	1701	A	C5-N7-C8	7.68	107.74	103.90
1	AA	1157	A	C5-N7-C8	7.67	107.74	103.90
22	BA	256	A	C5-N7-C8	7.67	107.74	103.90
1	AA	780	A	C4-C5-C6	7.67	120.84	117.00
22	BA	480	A	C5-N7-C8	7.67	107.73	103.90
22	BA	616	A	C5-N7-C8	7.67	107.74	103.90
22	BA	1876	A	C5-N7-C8	7.67	107.74	103.90
22	BA	344	A	C5-N7-C8	7.67	107.73	103.90
1	AA	32	A	C5-N7-C8	7.67	107.73	103.90
1	AA	602	A	C5-N7-C8	7.67	107.73	103.90
22	BA	1336	A	C5-N7-C8	7.67	107.73	103.90
22	BA	1387	A	N3-C4-N9	7.67	133.53	127.40
1	AA	1492	A	C5-N7-C8	7.67	107.73	103.90
1	AA	1468	A	C5-N7-C8	7.66	107.73	103.90
22	BA	735	A	C5-N7-C8	7.66	107.73	103.90
1	AA	77	A	C5-N7-C8	7.66	107.73	103.90
1	AA	139	A	C5-N7-C8	7.66	107.73	103.90
1	AA	996	A	C5-N7-C8	7.66	107.73	103.90
1	AA	1468	A	C4-C5-C6	7.66	120.83	117.00
22	BA	927	A	C5-N7-C8	7.66	107.73	103.90
22	BA	2013	A	C5-N7-C8	7.66	107.73	103.90
1	AA	1216	A	C5-N7-C8	7.66	107.73	103.90
1	AA	1531	A	C5-N7-C8	7.66	107.73	103.90
22	BA	430	A	C5-N7-C8	7.66	107.73	103.90
22	BA	508	A	C5-N7-C8	7.66	107.73	103.90
22	BA	1668	A	C5-C6-N1	7.66	121.53	117.70
22	BA	2298	A	C5-N7-C8	7.66	107.73	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1264	A	N3-C4-C5	-7.65	121.44	126.80
22	BA	675	A	C4-C5-C6	7.65	120.83	117.00
22	BA	947	A	C5-N7-C8	7.65	107.73	103.90
22	BA	1847	A	C4-C5-C6	7.65	120.83	117.00
22	BA	2284	A	C4-C5-C6	7.65	120.83	117.00
22	BA	2887	A	C5-N7-C8	7.65	107.73	103.90
1	AA	129	A	C5-N7-C8	7.65	107.72	103.90
22	BA	2736	A	C5-N7-C8	7.65	107.72	103.90
22	BA	2893	A	C5-N7-C8	7.65	107.72	103.90
22	BA	819	A	C5-N7-C8	7.65	107.72	103.90
22	BA	1569	A	C8-N9-C4	7.65	108.86	105.80
22	BA	1969	A	C4-C5-C6	7.65	120.82	117.00
22	BA	1021	A	C4-C5-C6	7.64	120.82	117.00
22	BA	2411	A	C5-N7-C8	7.64	107.72	103.90
22	BA	2346	A	C5-N7-C8	7.64	107.72	103.90
22	BA	2147	A	C5-N7-C8	7.64	107.72	103.90
22	BA	2734	A	C5-N7-C8	7.64	107.72	103.90
22	BA	2281	A	C5-N7-C8	7.63	107.72	103.90
1	AA	781	A	C5-N7-C8	7.63	107.72	103.90
1	AA	964	A	C5-N7-C8	7.63	107.72	103.90
22	BA	125	A	C5-N7-C8	7.63	107.72	103.90
22	BA	204	A	C5-N7-C8	7.63	107.72	103.90
22	BA	2459	A	C4-C5-C6	7.63	120.81	117.00
1	AA	938	A	N3-C4-N9	7.63	133.50	127.40
1	AA	461	A	C5-N7-C8	7.63	107.71	103.90
22	BA	352	A	C8-N9-C4	7.63	108.85	105.80
22	BA	538	A	C5-N7-C8	7.63	107.71	103.90
22	BA	1969	A	C8-N9-C4	7.63	108.85	105.80
1	AA	994	A	C5-N7-C8	7.62	107.71	103.90
22	BA	2090	A	N3-C4-N9	7.62	133.50	127.40
22	BA	2247	A	C5-N7-C8	7.62	107.71	103.90
22	BA	1156	A	N3-C4-N9	7.62	133.50	127.40
22	BA	1819	A	N3-C4-N9	7.62	133.49	127.40
22	BA	1890	A	C5-N7-C8	7.62	107.71	103.90
22	BA	2873	A	C5-N7-C8	7.62	107.71	103.90
1	AA	1219	A	C5-N7-C8	7.62	107.71	103.90
22	BA	608	A	C4-C5-C6	7.62	120.81	117.00
22	BA	223	A	C5-N7-C8	7.61	107.71	103.90
22	BA	191	A	C4-C5-C6	7.61	120.81	117.00
1	AA	559	A	C5-N7-C8	7.61	107.70	103.90
1	AA	1046	A	C5-N7-C8	7.61	107.71	103.90
22	BA	1403	A	C4-C5-C6	7.61	120.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1275	A	C8-N9-C4	7.61	108.84	105.80
22	BA	1151	A	C5-N7-C8	7.61	107.70	103.90
22	BA	1103	A	C5-N7-C8	7.60	107.70	103.90
22	BA	144	A	C5-N7-C8	7.60	107.70	103.90
22	BA	118	A	C5-N7-C8	7.60	107.70	103.90
22	BA	532	A	C5-N7-C8	7.60	107.70	103.90
22	BA	685	A	N3-C4-N9	7.60	133.48	127.40
22	BA	789	A	N3-C4-N9	7.60	133.48	127.40
22	BA	1373	A	C4-C5-C6	7.60	120.80	117.00
1	AA	120	A	C5-N7-C8	7.60	107.70	103.90
22	BA	1889	A	C5-N7-C8	7.60	107.70	103.90
22	BA	996	A	C5-N7-C8	7.59	107.70	103.90
22	BA	1088	A	N3-C4-N9	7.59	133.47	127.40
22	BA	2054	A	C5-C6-N1	7.59	121.50	117.70
1	AA	759	A	C5-N7-C8	7.59	107.69	103.90
22	BA	603	A	C5-N7-C8	7.59	107.69	103.90
1	AA	1046	A	N3-C4-N9	7.59	133.47	127.40
22	BA	1427	A	C8-N9-C4	7.59	108.83	105.80
22	BA	574	A	N3-C4-N9	7.59	133.47	127.40
22	BA	2468	A	C5-N7-C8	7.59	107.69	103.90
22	BA	2776	A	C5-N7-C8	7.59	107.69	103.90
22	BA	294	A	C5-N7-C8	7.58	107.69	103.90
22	BA	1383	A	C5-N7-C8	7.58	107.69	103.90
1	AA	282	A	C5-N7-C8	7.58	107.69	103.90
1	AA	411	A	C5-N7-C8	7.58	107.69	103.90
22	BA	529	A	C5-N7-C8	7.58	107.69	103.90
22	BA	278	A	C4-C5-C6	7.58	120.79	117.00
1	AA	498	A	C5-C6-N6	7.58	129.76	123.70
1	AA	101	A	C5-N7-C8	7.58	107.69	103.90
1	AA	1201	A	N3-C4-N9	7.58	133.46	127.40
22	BA	127	A	C5-N7-C8	7.57	107.69	103.90
22	BA	2799	A	C5-C6-N6	7.57	129.76	123.70
1	AA	1375	A	C4-C5-C6	7.57	120.78	117.00
22	BA	668	A	C5-N7-C8	7.57	107.69	103.90
22	BA	793	A	C4-C5-C6	7.57	120.79	117.00
22	BA	2497	A	C4-C5-C6	7.57	120.78	117.00
1	AA	28	A	C4-C5-C6	7.57	120.78	117.00
22	BA	309	A	C5-N7-C8	7.57	107.69	103.90
1	AA	356	A	C5-C6-N1	7.57	121.48	117.70
1	AA	415	A	C5-N7-C8	7.57	107.68	103.90
1	AA	1446	A	C5-N7-C8	7.57	107.68	103.90
22	BA	19	A	C5-N7-C8	7.57	107.68	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2095	A	C5-N7-C8	7.57	107.68	103.90
22	BA	2288	A	C5-N7-C8	7.57	107.68	103.90
22	BA	368	A	C4-C5-C6	7.57	120.78	117.00
1	AA	560	A	C5-N7-C8	7.56	107.68	103.90
1	AA	743	A	N3-C4-N9	7.56	133.45	127.40
22	BA	191	A	C5-N7-C8	7.56	107.68	103.90
22	BA	920	A	C8-N9-C4	7.56	108.83	105.80
1	AA	1130	A	C5-N7-C8	7.56	107.68	103.90
1	AA	1246	A	C5-N7-C8	7.56	107.68	103.90
22	BA	368	A	C5-N7-C8	7.56	107.68	103.90
22	BA	1821	A	C5-N7-C8	7.56	107.68	103.90
22	BA	2051	A	N3-C4-N9	7.56	133.45	127.40
22	BA	1937	A	C4-C5-N7	-7.56	106.92	110.70
1	AA	1176	A	C5-N7-C8	7.56	107.68	103.90
22	BA	1960	A	C5-N7-C8	7.55	107.68	103.90
22	BA	2635	A	C5-N7-C8	7.55	107.68	103.90
22	BA	1308	A	N9-C4-C5	7.55	108.82	105.80
22	BA	1998	A	C5-N7-C8	7.55	107.68	103.90
1	AA	397	A	C4-C5-C6	7.55	120.77	117.00
22	BA	1579	A	C5-N7-C8	7.55	107.67	103.90
1	AA	16	A	C5-N7-C8	7.54	107.67	103.90
22	BA	371	A	C4-C5-C6	7.54	120.77	117.00
1	AA	746	A	C4-C5-C6	7.54	120.77	117.00
1	AA	655	A	C4-C5-C6	7.54	120.77	117.00
22	BA	1848	A	N7-C8-N9	-7.54	110.03	113.80
22	BA	2814	A	C5-N7-C8	7.54	107.67	103.90
22	BA	1596	A	C5-N7-C8	7.53	107.67	103.90
22	BA	1773	A	N3-C4-N9	7.53	133.43	127.40
22	BA	2333	A	C8-N9-C4	7.53	108.81	105.80
1	AA	28	A	C5-N7-C8	7.53	107.67	103.90
22	BA	28	A	C5-N7-C8	7.53	107.67	103.90
22	BA	2080	A	C5-N7-C8	7.53	107.67	103.90
1	AA	743	A	C5-C6-N6	7.53	129.72	123.70
22	BA	792	A	C5-N7-C8	7.53	107.67	103.90
1	AA	919	A	C5-N7-C8	7.53	107.66	103.90
22	BA	1204	A	C5-N7-C8	7.53	107.66	103.90
22	BA	1705	A	C5-N7-C8	7.53	107.66	103.90
1	AA	787	A	C5-N7-C8	7.52	107.66	103.90
1	AA	263	A	C5-N7-C8	7.52	107.66	103.90
1	AA	366	A	C5-N7-C8	7.52	107.66	103.90
22	BA	1789	A	C4-C5-C6	7.52	120.76	117.00
22	BA	1000	A	C4-C5-C6	7.52	120.76	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1050	A	C8-N9-C4	7.52	108.81	105.80
22	BA	1650	A	C5-N7-C8	7.52	107.66	103.90
22	BA	503	A	N3-C4-N9	7.52	133.41	127.40
22	BA	1977	A	C5-N7-C8	7.52	107.66	103.90
22	BA	2101	A	C8-N9-C4	7.52	108.81	105.80
22	BA	142	A	C5-N7-C8	7.52	107.66	103.90
22	BA	644	A	C4-C5-C6	7.52	120.76	117.00
22	BA	1789	A	N9-C4-C5	7.52	108.81	105.80
23	BB	58	A	C5-N7-C8	7.52	107.66	103.90
22	BA	892	A	C5-N7-C8	7.51	107.66	103.90
22	BA	173	A	C5-N7-C8	7.51	107.66	103.90
22	BA	447	A	C5-N7-C8	7.51	107.66	103.90
22	BA	2198	A	C5-N7-C8	7.51	107.66	103.90
1	AA	814	A	C4-C5-C6	7.51	120.75	117.00
22	BA	1086	A	C5-N7-C8	7.51	107.66	103.90
55	B8	14	A	C4-C5-C6	7.51	120.75	117.00
1	AA	325	A	C5-N7-C8	7.51	107.65	103.90
22	BA	155	A	C5-N7-C8	7.51	107.65	103.90
22	BA	2738	A	C5-N7-C8	7.51	107.65	103.90
22	BA	2753	A	C5-N7-C8	7.51	107.65	103.90
1	AA	1	A	C5-N7-C8	7.50	107.65	103.90
22	BA	2333	A	C5-N7-C8	7.50	107.65	103.90
22	BA	503	A	C5-C6-N1	7.50	121.45	117.70
1	AA	162	A	C5-N7-C8	7.50	107.65	103.90
1	AA	1289	A	C5-N7-C8	7.50	107.65	103.90
1	AA	1271	A	C5-N7-C8	7.50	107.65	103.90
1	AA	243	A	N9-C4-C5	7.49	108.80	105.80
22	BA	402	A	C5-N7-C8	7.49	107.65	103.90
23	BB	15	A	C5-N7-C8	7.49	107.65	103.90
1	AA	746	A	C5-N7-C8	7.49	107.64	103.90
22	BA	505	A	C4-C5-C6	7.49	120.75	117.00
22	BA	1927	A	C5-N7-C8	7.49	107.64	103.90
22	BA	2740	A	C5-N7-C8	7.49	107.64	103.90
22	BA	161	A	C5-N7-C8	7.49	107.64	103.90
22	BA	478	A	C5-N7-C8	7.49	107.64	103.90
1	AA	383	A	C5-C6-N6	7.49	129.69	123.70
22	BA	990	A	N3-C4-C5	-7.49	121.56	126.80
22	BA	1431	A	N3-C4-N9	7.49	133.39	127.40
1	AA	1324	A	C5-N7-C8	7.48	107.64	103.90
22	BA	401	A	C5-N7-C8	7.48	107.64	103.90
1	AA	767	A	C5-N7-C8	7.48	107.64	103.90
22	BA	2268	A	C4-C5-C6	7.48	120.74	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2513	A	C5-N7-C8	7.48	107.64	103.90
1	AA	441	A	C5-N7-C8	7.47	107.64	103.90
1	AA	1254	A	C5-N7-C8	7.47	107.64	103.90
22	BA	715	A	C5-N7-C8	7.47	107.64	103.90
22	BA	2071	A	C4-C5-C6	7.47	120.74	117.00
1	AA	777	A	C5-N7-C8	7.47	107.63	103.90
22	BA	226	A	N3-C4-N9	7.47	133.38	127.40
22	BA	1237	A	C5-N7-C8	7.47	107.64	103.90
22	BA	1918	A	C5-N7-C8	7.47	107.64	103.90
22	BA	483	A	C5-N7-C8	7.47	107.63	103.90
22	BA	933	A	C5-N7-C8	7.47	107.63	103.90
22	BA	1287	A	C4-C5-C6	7.47	120.73	117.00
22	BA	2199	A	C4-C5-C6	7.47	120.73	117.00
1	AA	487	A	C5-N7-C8	7.46	107.63	103.90
22	BA	1367	A	C4-C5-C6	7.46	120.73	117.00
1	AA	1092	A	C5-N7-C8	7.46	107.63	103.90
22	BA	2082	A	C5-N7-C8	7.46	107.63	103.90
1	AA	539	A	C4-C5-C6	7.46	120.73	117.00
22	BA	89	A	C5-N7-C8	7.46	107.63	103.90
22	BA	430	A	C4-C5-C6	7.46	120.73	117.00
22	BA	2054	A	C5-N7-C8	7.46	107.63	103.90
22	BA	2101	A	C4-C5-C6	7.46	120.73	117.00
22	BA	2191	A	C5-N7-C8	7.46	107.63	103.90
22	BA	199	A	C5-N7-C8	7.46	107.63	103.90
22	BA	2425	A	C5-N7-C8	7.45	107.63	103.90
22	BA	13	A	C4-C5-C6	7.45	120.73	117.00
22	BA	820	A	N3-C4-N9	7.45	133.36	127.40
22	BA	482	A	C5-C6-N6	7.45	129.66	123.70
22	BA	1571	A	C5-N7-C8	7.45	107.62	103.90
22	BA	1494	A	C5-N7-C8	7.45	107.62	103.90
1	AA	3	A	C5-N7-C8	7.45	107.62	103.90
22	BA	730	A	N3-C4-N9	7.45	133.36	127.40
22	BA	1307	A	N3-C4-N9	7.45	133.36	127.40
22	BA	2369	A	C5-C6-N1	7.45	121.42	117.70
22	BA	1544	A	C5-N7-C8	7.44	107.62	103.90
22	BA	2826	A	N3-C4-N9	7.44	133.35	127.40
22	BA	2577	A	C5-N7-C8	7.44	107.62	103.90
22	BA	1810	A	C5-N7-C8	7.44	107.62	103.90
22	BA	2434	A	C5-N7-C8	7.44	107.62	103.90
22	BA	1735	A	N3-C4-N9	7.44	133.35	127.40
1	AA	300	A	C5-N7-C8	7.44	107.62	103.90
22	BA	513	A	N3-C4-N9	7.44	133.35	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1039	A	C5-N7-C8	7.44	107.62	103.90
22	BA	783	A	C4-C5-C6	7.44	120.72	117.00
22	BA	800	A	N3-C4-C5	-7.44	121.59	126.80
1	AA	1081	A	C8-N9-C4	7.43	108.77	105.80
22	BA	91	A	C5-N7-C8	7.43	107.62	103.90
22	BA	404	A	N3-C4-C5	-7.43	121.60	126.80
22	BA	1262	A	C5-N7-C8	7.43	107.62	103.90
1	AA	712	A	N3-C4-N9	7.43	133.35	127.40
22	BA	156	A	C5-N7-C8	7.43	107.62	103.90
22	BA	2009	A	C8-N9-C4	7.43	108.77	105.80
22	BA	1088	A	C4-C5-C6	7.43	120.72	117.00
22	BA	1169	A	C5-N7-C8	7.43	107.61	103.90
22	BA	1819	A	C4-C5-C6	7.43	120.72	117.00
1	AA	72	A	C5-N7-C8	7.43	107.61	103.90
22	BA	1268	A	C5-N7-C8	7.43	107.61	103.90
1	AA	909	A	C5-N7-C8	7.43	107.61	103.90
22	BA	1151	A	C4-C5-C6	7.42	120.71	117.00
22	BA	1580	A	C5-N7-C8	7.42	107.61	103.90
22	BA	2882	A	C5-N7-C8	7.42	107.61	103.90
22	BA	265	A	C5-N7-C8	7.42	107.61	103.90
22	BA	1313	U	C2-N1-C1'	7.42	126.60	117.70
22	BA	2518	A	N3-C4-N9	7.42	133.34	127.40
22	BA	2020	A	C8-N9-C4	7.42	108.77	105.80
22	BA	477	A	C4-C5-C6	7.41	120.71	117.00
22	BA	2727	A	C4-C5-C6	7.41	120.71	117.00
22	BA	256	A	C4-C5-C6	7.41	120.71	117.00
22	BA	1549	A	C5-N7-C8	7.41	107.61	103.90
22	BA	627	A	C8-N9-C4	7.41	108.76	105.80
22	BA	2352	A	C4-C5-C6	7.41	120.71	117.00
22	BA	2590	A	C5-N7-C8	7.41	107.61	103.90
22	BA	514	A	C5-C6-N1	7.41	121.40	117.70
22	BA	756	A	C5-C6-N1	7.41	121.41	117.70
22	BA	1586	A	C5-N7-C8	7.41	107.60	103.90
37	BP	68	GLU	OE1-CD-OE2	-7.41	114.41	123.30
1	AA	1044	A	C5-N7-C8	7.41	107.60	103.90
22	BA	666	A	C5-N7-C8	7.41	107.60	103.90
1	AA	864	A	C5-N7-C8	7.41	107.60	103.90
22	BA	2184	A	C5-N7-C8	7.41	107.60	103.90
22	BA	270	A	C5-N7-C8	7.40	107.60	103.90
1	AA	195	A	C5-N7-C8	7.40	107.60	103.90
1	AA	1465	A	C4-C5-C6	7.40	120.70	117.00
22	BA	279	A	C5-N7-C8	7.40	107.60	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1312	U	C5-C4-O4	7.40	130.34	125.90
22	BA	1354	A	C5-N7-C8	7.40	107.60	103.90
22	BA	454	A	C5-N7-C8	7.40	107.60	103.90
22	BA	1254	A	C5-N7-C8	7.40	107.60	103.90
1	AA	7	A	C8-N9-C4	7.40	108.76	105.80
1	AA	1483	A	N3-C4-N9	7.40	133.32	127.40
22	BA	457	A	C5-N7-C8	7.40	107.60	103.90
22	BA	1495	A	C4-C5-C6	7.40	120.70	117.00
1	AA	373	A	C5-N7-C8	7.39	107.60	103.90
22	BA	1885	A	C5-N7-C8	7.39	107.60	103.90
1	AA	262	A	C5-N7-C8	7.39	107.60	103.90
1	AA	1102	A	C5-N7-C8	7.39	107.59	103.90
1	AA	814	A	N3-C4-N9	7.39	133.31	127.40
22	BA	793	A	C5-N7-C8	7.39	107.59	103.90
22	BA	1027	A	C8-N9-C4	7.39	108.75	105.80
22	BA	2088	A	C5-C6-N1	7.39	121.39	117.70
22	BA	1134	A	C5-N7-C8	7.39	107.59	103.90
1	AA	465	A	C5-N7-C8	7.39	107.59	103.90
1	AA	574	A	C5-N7-C8	7.39	107.59	103.90
1	AA	673	A	C5-N7-C8	7.38	107.59	103.90
22	BA	2328	A	C4-C5-C6	7.38	120.69	117.00
22	BA	2879	A	C4-C5-C6	7.38	120.69	117.00
22	BA	1916	A	C5-N7-C8	7.38	107.59	103.90
22	BA	2461	A	C4-C5-C6	7.38	120.69	117.00
1	AA	155	A	C5-N7-C8	7.38	107.59	103.90
1	AA	642	A	C4-C5-C6	7.38	120.69	117.00
22	BA	221	A	C5-N7-C8	7.38	107.59	103.90
22	BA	1143	A	N3-C4-N9	7.38	133.31	127.40
22	BA	2725	A	C5-N7-C8	7.38	107.59	103.90
22	BA	2835	A	C5-N7-C8	7.38	107.59	103.90
1	AA	1055	A	C5-N7-C8	7.38	107.59	103.90
1	AA	1503	A	C8-N9-C4	7.38	108.75	105.80
22	BA	196	A	C4-C5-C6	7.38	120.69	117.00
22	BA	825	A	N9-C4-C5	7.38	108.75	105.80
22	BA	1609	A	C5-N7-C8	7.38	107.59	103.90
1	AA	33	A	C4-C5-C6	7.38	120.69	117.00
22	BA	176	A	N3-C4-N9	7.37	133.30	127.40
22	BA	819	A	C4-C5-C6	7.37	120.69	117.00
22	BA	1966	A	C5-N7-C8	7.37	107.59	103.90
1	AA	607	A	C5-N7-C8	7.37	107.59	103.90
22	BA	863	A	C5-N7-C8	7.37	107.59	103.90
22	BA	1655	A	C5-N7-C8	7.37	107.58	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1735	A	C4-C5-C6	7.37	120.68	117.00
22	BA	415	A	C5-N7-C8	7.37	107.58	103.90
22	BA	1014	A	C5-N7-C8	7.37	107.58	103.90
22	BA	453	A	C4-C5-C6	7.36	120.68	117.00
22	BA	782	A	N3-C4-N9	7.36	133.29	127.40
22	BA	2205	A	C5-N7-C8	7.36	107.58	103.90
1	AA	977	A	N3-C4-N9	7.36	133.29	127.40
22	BA	172	A	C5-N7-C8	7.36	107.58	103.90
22	BA	943	A	N3-C4-N9	7.36	133.29	127.40
22	BA	1175	A	C5-N7-C8	7.36	107.58	103.90
22	BA	2531	A	C4-C5-C6	7.36	120.68	117.00
22	BA	1791	A	C5-N7-C8	7.36	107.58	103.90
1	AA	1418	A	C5-N7-C8	7.36	107.58	103.90
22	BA	739	A	C5-N7-C8	7.36	107.58	103.90
22	BA	1932	A	C5-N7-C8	7.36	107.58	103.90
22	BA	1439	A	C5-N7-C8	7.35	107.58	103.90
1	AA	448	A	C5-N7-C8	7.35	107.58	103.90
1	AA	1362	A	C5-N7-C8	7.35	107.58	103.90
22	BA	432	A	C5-N7-C8	7.35	107.58	103.90
23	BB	66	A	C4-C5-C6	7.35	120.68	117.00
22	BA	789	A	C8-N9-C4	7.35	108.74	105.80
55	B8	58	A	C5-N7-C8	7.35	107.58	103.90
1	AA	80	A	C4-C5-C6	7.35	120.67	117.00
22	BA	1431	A	C5-N7-C8	7.35	107.58	103.90
22	BA	1260	A	C5-C6-N1	7.35	121.37	117.70
22	BA	1286	A	N3-C4-C5	-7.35	121.66	126.80
22	BA	2826	A	C4-C5-C6	7.35	120.67	117.00
22	BA	670	A	C5-N7-C8	7.35	107.57	103.90
22	BA	119	A	C5-C6-N1	7.34	121.37	117.70
1	AA	33	A	C5-N7-C8	7.34	107.57	103.90
1	AA	983	A	N3-C4-N9	7.34	133.27	127.40
22	BA	226	A	C5-N7-C8	7.34	107.57	103.90
22	BA	945	A	C4-C5-C6	7.34	120.67	117.00
22	BA	1928	A	C5-N7-C8	7.34	107.57	103.90
22	BA	111	A	C5-N7-C8	7.34	107.57	103.90
22	BA	460	A	C5-N7-C8	7.34	107.57	103.90
22	BA	572	A	N3-C4-N9	7.34	133.27	127.40
22	BA	2565	A	C4-C5-C6	7.34	120.67	117.00
1	AA	923	A	C4-C5-C6	7.33	120.67	117.00
1	AA	374	A	C5-N7-C8	7.33	107.57	103.90
22	BA	1829	A	C5-N7-C8	7.33	107.57	103.90
22	BA	1247	A	C8-N9-C4	7.33	108.73	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	599	A	C5-N7-C8	7.33	107.56	103.90
22	BA	2281	A	C8-N9-C4	7.33	108.73	105.80
1	AA	1	A	N3-C4-N9	7.33	133.26	127.40
1	AA	573	A	C5-N7-C8	7.33	107.56	103.90
22	BA	983	A	N3-C4-N9	7.33	133.26	127.40
22	BA	2270	A	C5-N7-C8	7.33	107.56	103.90
1	AA	1349	A	C5-N7-C8	7.32	107.56	103.90
1	AA	460	A	C5-N7-C8	7.32	107.56	103.90
22	BA	391	A	C4-C5-C6	7.32	120.66	117.00
22	BA	2406	A	C5-N7-C8	7.32	107.56	103.90
22	BA	592	A	N3-C4-N9	7.32	133.25	127.40
22	BA	742	A	C5-C6-N1	7.32	121.36	117.70
22	BA	2070	A	N9-C4-C5	7.32	108.73	105.80
1	AA	815	A	C5-N7-C8	7.31	107.56	103.90
1	AA	937	A	C4-C5-C6	7.31	120.66	117.00
22	BA	422	A	C5-N7-C8	7.31	107.56	103.90
22	BA	705	A	C5-N7-C8	7.31	107.56	103.90
55	B8	59	A	C4-C5-C6	7.31	120.66	117.00
1	AA	338	A	C5-N7-C8	7.31	107.56	103.90
22	BA	1009	A	C5-N7-C8	7.31	107.56	103.90
22	BA	910	A	N3-C4-N9	7.31	133.25	127.40
22	BA	1000	A	C5-N7-C8	7.31	107.55	103.90
22	BA	2199	A	C5-N7-C8	7.31	107.55	103.90
1	AA	873	A	N3-C4-N9	7.30	133.24	127.40
22	BA	1241	A	C4-C5-C6	7.30	120.65	117.00
22	BA	1735	A	C8-N9-C4	7.30	108.72	105.80
22	BA	980	A	C5-N7-C8	7.30	107.55	103.90
22	BA	1608	A	C4-C5-C6	7.30	120.65	117.00
1	AA	1155	A	C8-N9-C4	7.30	108.72	105.80
22	BA	2572	A	C5-N7-C8	7.30	107.55	103.90
1	AA	415	A	C4-C5-C6	7.30	120.65	117.00
22	BA	348	A	C5-N7-C8	7.30	107.55	103.90
22	BA	1665	A	C5-N7-C8	7.30	107.55	103.90
22	BA	2273	A	C4-C5-C6	7.30	120.65	117.00
22	BA	2449	U	N3-C2-O2	-7.30	117.09	122.20
1	AA	983	A	C5-N7-C8	7.29	107.55	103.90
22	BA	1969	A	C5-N7-C8	7.29	107.55	103.90
23	BB	58	A	C4-C5-C6	7.29	120.65	117.00
22	BA	251	A	C5-N7-C8	7.29	107.55	103.90
23	BB	53	A	C5-N7-C8	7.29	107.55	103.90
1	AA	1468	A	N3-C4-N9	7.29	133.23	127.40
22	BA	1528	A	N3-C4-N9	7.29	133.23	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	13	A	N9-C4-C5	7.29	108.72	105.80
1	AA	1508	A	C5-N7-C8	7.29	107.54	103.90
22	BA	677	A	C4-C5-C6	7.28	120.64	117.00
22	BA	1359	A	C5-N7-C8	7.28	107.54	103.90
22	BA	347	A	N9-C4-C5	7.28	108.71	105.80
22	BA	2273	A	N3-C4-N9	7.28	133.23	127.40
1	AA	1188	A	C8-N9-C4	7.28	108.71	105.80
1	AA	1261	A	C5-N7-C8	7.28	107.54	103.90
22	BA	574	A	C4-C5-C6	7.28	120.64	117.00
22	BA	1495	A	C5-N7-C8	7.28	107.54	103.90
22	BA	1387	A	C4-C5-C6	7.27	120.64	117.00
55	B8	26	A	C5-N7-C8	7.27	107.54	103.90
1	AA	1225	A	N3-C4-N9	7.27	133.22	127.40
1	AA	1158	C	N1-C2-O2	7.27	123.26	118.90
1	AA	1288	A	C5-N7-C8	7.27	107.53	103.90
55	B8	38	A	C5-N7-C8	7.27	107.53	103.90
1	AA	499	A	C4-C5-C6	7.27	120.63	117.00
22	BA	2826	A	C5-N7-C8	7.26	107.53	103.90
22	BA	1069	A	C8-N9-C4	7.26	108.70	105.80
22	BA	1433	A	C5-N7-C8	7.26	107.53	103.90
22	BA	2287	A	C5-N7-C8	7.26	107.53	103.90
22	BA	2776	A	C8-N9-C4	7.26	108.70	105.80
22	BA	330	A	N3-C4-N9	7.26	133.21	127.40
22	BA	2560	A	C5-N7-C8	7.26	107.53	103.90
22	BA	241	A	C5-N7-C8	7.26	107.53	103.90
22	BA	482	A	N3-C4-N9	7.26	133.21	127.40
22	BA	2518	A	C8-N9-C4	7.26	108.70	105.80
22	BA	1302	A	C5-N7-C8	7.25	107.53	103.90
22	BA	2366	A	N3-C4-N9	7.25	133.20	127.40
1	AA	665	A	C5-N7-C8	7.25	107.53	103.90
1	AA	1188	A	C5-N7-C8	7.25	107.53	103.90
22	BA	1854	A	C5-N7-C8	7.25	107.53	103.90
22	BA	2117	A	C4-C5-C6	7.25	120.63	117.00
1	AA	702	A	C5-N7-C8	7.25	107.53	103.90
22	BA	63	A	C4-C5-C6	7.25	120.62	117.00
22	BA	866	A	C5-N7-C8	7.25	107.53	103.90
22	BA	1077	A	C5-N7-C8	7.25	107.53	103.90
22	BA	1353	A	C5-N7-C8	7.25	107.52	103.90
22	BA	2530	A	C8-N9-C4	7.25	108.70	105.80
22	BA	1213	A	N3-C4-N9	7.25	133.20	127.40
22	BA	1746	A	C5-N7-C8	7.25	107.52	103.90
1	AA	629	A	C5-N7-C8	7.24	107.52	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	470	A	N3-C4-N9	7.24	133.19	127.40
22	BA	2335	A	C4-C5-C6	7.24	120.62	117.00
1	AA	1	A	C4-C5-C6	7.24	120.62	117.00
22	BA	13	A	C5-N7-C8	7.24	107.52	103.90
22	BA	1244	A	C5-N7-C8	7.24	107.52	103.90
22	BA	2426	A	C5-N7-C8	7.24	107.52	103.90
22	BA	2090	A	C5-C6-N1	7.24	121.32	117.70
22	BA	2757	A	N3-C4-N9	7.24	133.19	127.40
1	AA	596	A	N9-C4-C5	7.24	108.69	105.80
22	BA	56	A	N3-C4-N9	7.24	133.19	127.40
22	BA	734	A	N3-C4-N9	7.24	133.19	127.40
22	BA	213	A	C5-N7-C8	7.24	107.52	103.90
1	AA	279	A	C4-C5-C6	7.23	120.62	117.00
22	BA	1698	A	C5-N7-C8	7.23	107.52	103.90
22	BA	2392	A	N3-C4-N9	7.23	133.19	127.40
22	BA	608	A	N3-C4-N9	7.23	133.19	127.40
22	BA	2071	A	C5-N7-C8	7.23	107.52	103.90
1	AA	1082	A	C5-N7-C8	7.23	107.52	103.90
22	BA	197	A	C4-C5-C6	7.23	120.61	117.00
22	BA	582	A	C5-C6-N1	7.23	121.31	117.70
22	BA	1637	A	C5-N7-C8	7.23	107.52	103.90
22	BA	943	A	C5-N7-C8	7.23	107.52	103.90
1	AA	250	A	C5-N7-C8	7.23	107.51	103.90
22	BA	1664	A	N3-C4-N9	7.23	133.18	127.40
22	BA	1735	A	C5-N7-C8	7.23	107.51	103.90
22	BA	52	A	N3-C4-N9	7.22	133.18	127.40
22	BA	181	A	C5-N7-C8	7.22	107.51	103.90
22	BA	2108	A	C5-N7-C8	7.22	107.51	103.90
22	BA	1144	A	C5-N7-C8	7.22	107.51	103.90
22	BA	1786	A	C5-N7-C8	7.21	107.51	103.90
32	BK	102	PRO	CA-N-CD	-7.21	101.40	111.50
22	BA	1502	A	C5-N7-C8	7.21	107.51	103.90
22	BA	1010	A	C4-C5-C6	7.21	120.61	117.00
22	BA	1610	A	C5-N7-C8	7.21	107.51	103.90
1	AA	1111	A	C5-N7-C8	7.21	107.50	103.90
22	BA	1469	A	C5-N7-C8	7.21	107.50	103.90
55	B8	14	A	C5-N7-C8	7.21	107.50	103.90
22	BA	1572	A	C8-N9-C4	7.21	108.68	105.80
22	BA	161	A	N9-C4-C5	7.20	108.68	105.80
22	BA	627	A	N3-C4-N9	7.20	133.16	127.40
22	BA	1794	A	C8-N9-C4	7.20	108.68	105.80
22	BA	1744	A	C4-C5-C6	7.20	120.60	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1093	A	C5-N7-C8	7.20	107.50	103.90
1	AA	1339	A	C4-C5-C6	7.20	120.60	117.00
22	BA	1010	A	C5-N7-C8	7.20	107.50	103.90
22	BA	1287	A	N3-C4-N9	7.20	133.16	127.40
1	AA	1324	A	C4-C5-C6	7.19	120.60	117.00
22	BA	1593	A	C5-N7-C8	7.19	107.50	103.90
22	BA	1899	A	C4-C5-C6	7.19	120.60	117.00
1	AA	1197	A	N3-C4-N9	7.19	133.15	127.40
22	BA	845	A	C5-C6-N1	7.19	121.30	117.70
22	BA	1029	A	C5-N7-C8	7.19	107.50	103.90
22	BA	1009	A	C4-C5-C6	7.19	120.59	117.00
1	AA	784	A	N9-C4-C5	7.19	108.67	105.80
22	BA	693	A	C4-C5-C6	7.19	120.59	117.00
22	BA	1572	A	N3-C4-N9	7.19	133.15	127.40
1	AA	1339	A	C5-N7-C8	7.19	107.49	103.90
22	BA	2358	A	C5-N7-C8	7.19	107.49	103.90
22	BA	2482	A	C5-N7-C8	7.19	107.49	103.90
1	AA	430	A	C8-N9-C4	7.18	108.67	105.80
22	BA	2274	A	C5-N7-C8	7.18	107.49	103.90
1	AA	675	A	C5-N7-C8	7.18	107.49	103.90
22	BA	14	A	C4-C5-C6	7.18	120.59	117.00
22	BA	1274	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1885	A	C4-C5-C6	7.18	120.59	117.00
1	AA	160	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1552	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1803	A	N9-C4-C5	7.18	108.67	105.80
22	BA	2860	A	C4-C5-C6	7.18	120.59	117.00
22	BA	227	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1711	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1532	A	C5-N7-C8	7.18	107.49	103.90
55	B8	38	A	C4-C5-C6	7.18	120.59	117.00
1	AA	509	A	C4-C5-C6	7.17	120.59	117.00
1	AA	938	A	C4-C5-C6	7.17	120.59	117.00
22	BA	362	A	C5-N7-C8	7.17	107.49	103.90
55	B8	26	A	C4-C5-C6	7.17	120.59	117.00
1	AA	327	A	C5-N7-C8	7.17	107.48	103.90
22	BA	1664	A	C5-N7-C8	7.17	107.48	103.90
22	BA	1745	A	C5-N7-C8	7.17	107.48	103.90
22	BA	2719	G	N9-C4-C5	-7.17	102.53	105.40
1	AA	55	A	N3-C4-N9	7.17	133.13	127.40
1	AA	1022	A	C5-N7-C8	7.17	107.48	103.90
22	BA	347	A	C5-N7-C8	7.17	107.48	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	752	A	N9-C4-C5	7.17	108.67	105.80
22	BA	1866	A	C5-N7-C8	7.17	107.48	103.90
1	AA	715	A	C8-N9-C4	7.17	108.67	105.80
22	BA	501	A	C5-N7-C8	7.17	107.48	103.90
22	BA	2726	A	C5-N7-C8	7.17	107.48	103.90
22	BA	1269	A	N3-C4-N9	7.16	133.13	127.40
22	BA	2154	A	C8-N9-C4	7.16	108.67	105.80
22	BA	1373	A	N3-C4-N9	7.16	133.13	127.40
22	BA	2534	A	C8-N9-C4	7.16	108.66	105.80
1	AA	81	A	N3-C4-N9	7.16	133.13	127.40
1	AA	794	A	C4-C5-C6	7.16	120.58	117.00
1	AA	81	A	C4-C5-C6	7.16	120.58	117.00
1	AA	414	A	C8-N9-C4	7.16	108.66	105.80
22	BA	503	A	C4-C5-C6	7.16	120.58	117.00
22	BA	722	A	C5-N7-C8	7.16	107.48	103.90
1	AA	397	A	C5-C6-N1	7.15	121.28	117.70
22	BA	781	A	C5-N7-C8	7.15	107.48	103.90
22	BA	439	A	C5-C6-N1	7.15	121.28	117.70
22	BA	1757	A	C8-N9-C4	7.15	108.66	105.80
22	BA	2886	A	C5-N7-C8	7.15	107.48	103.90
1	AA	1111	A	C4-C5-C6	7.15	120.58	117.00
1	AA	44	A	C4-C5-C6	7.15	120.57	117.00
1	AA	1044	A	C8-N9-C4	7.15	108.66	105.80
23	BB	119	A	C8-N9-C4	7.15	108.66	105.80
1	AA	510	A	C5-N7-C8	7.14	107.47	103.90
22	BA	94	A	C5-N7-C8	7.14	107.47	103.90
22	BA	861	A	C5-N7-C8	7.14	107.47	103.90
1	AA	919	A	N9-C4-C5	7.14	108.66	105.80
22	BA	644	A	N3-C4-N9	7.14	133.12	127.40
22	BA	1085	A	N9-C4-C5	7.14	108.66	105.80
22	BA	2412	A	N3-C4-N9	7.14	133.12	127.40
22	BA	216	A	C4-C5-C6	7.14	120.57	117.00
22	BA	819	A	N3-C4-N9	7.14	133.11	127.40
1	AA	502	A	C4-C5-C6	7.14	120.57	117.00
22	BA	38	A	N9-C4-C5	7.14	108.66	105.80
22	BA	783	A	N3-C4-N9	7.14	133.11	127.40
22	BA	1672	A	N3-C4-N9	7.14	133.11	127.40
22	BA	219	A	C5-N7-C8	7.13	107.47	103.90
22	BA	1655	A	C4-C5-C6	7.13	120.57	117.00
1	AA	26	A	C5-N7-C8	7.13	107.47	103.90
22	BA	538	A	C4-C5-C6	7.13	120.56	117.00
22	BA	2577	A	N3-C4-N9	7.13	133.10	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1408	A	C8-N9-C4	7.13	108.65	105.80
22	BA	1590	A	C8-N9-C4	7.13	108.65	105.80
22	BA	2082	A	N3-C4-N9	7.13	133.10	127.40
22	BA	2899	A	C5-N7-C8	7.13	107.46	103.90
22	BA	845	A	N3-C4-N9	7.13	133.10	127.40
22	BA	1084	A	N9-C4-C5	7.13	108.65	105.80
1	AA	1219	A	C4-C5-C6	7.12	120.56	117.00
22	BA	1111	A	C4-C5-C6	7.12	120.56	117.00
1	AA	676	A	C5-N7-C8	7.12	107.46	103.90
22	BA	1780	A	N9-C4-C5	7.12	108.65	105.80
1	AA	66	A	C4-C5-C6	7.12	120.56	117.00
22	BA	633	A	C5-N7-C8	7.12	107.46	103.90
22	BA	152	A	C4-C5-C6	7.12	120.56	117.00
22	BA	1821	A	N9-C4-C5	7.12	108.65	105.80
22	BA	95	A	C5-N7-C8	7.12	107.46	103.90
23	BB	46	A	C5-N7-C8	7.12	107.46	103.90
22	BA	64	A	C4-C5-C6	7.11	120.56	117.00
22	BA	631	A	C5-N7-C8	7.11	107.46	103.90
22	BA	1494	A	C4-C5-C6	7.11	120.56	117.00
22	BA	2176	A	C5-N7-C8	7.11	107.46	103.90
22	BA	2247	A	N3-C4-N9	7.11	133.09	127.40
22	BA	2813	A	C5-N7-C8	7.11	107.46	103.90
1	AA	162	A	N3-C4-N9	7.11	133.09	127.40
1	AA	1080	A	C5-N7-C8	7.11	107.46	103.90
1	AA	313	A	C4-C5-C6	7.11	120.56	117.00
23	BB	109	A	C5-N7-C8	7.11	107.45	103.90
22	BA	1998	A	C4-C5-C6	7.11	120.55	117.00
22	BA	2062	A	C8-N9-C4	7.11	108.64	105.80
22	BA	2879	A	N3-C4-N9	7.11	133.08	127.40
22	BA	1808	A	C5-N7-C8	7.10	107.45	103.90
22	BA	572	A	N7-C8-N9	-7.10	110.25	113.80
22	BA	1322	A	C5-N7-C8	7.10	107.45	103.90
22	BA	2765	A	N3-C4-N9	7.10	133.08	127.40
22	BA	2657	A	C5-N7-C8	7.10	107.45	103.90
1	AA	366	A	C4-C5-C6	7.10	120.55	117.00
22	BA	2682	A	C5-N7-C8	7.10	107.45	103.90
22	BA	661	A	C4-C5-C6	7.10	120.55	117.00
1	AA	743	A	C5-N7-C8	7.10	107.45	103.90
22	BA	126	A	N9-C4-C5	7.09	108.64	105.80
22	BA	1676	A	C4-C5-C6	7.09	120.55	117.00
1	AA	706	A	N3-C4-N9	7.09	133.07	127.40
1	AA	298	A	C5-N7-C8	7.09	107.45	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	937	A	N3-C4-N9	7.09	133.07	127.40
22	BA	1321	A	N3-C4-N9	7.09	133.07	127.40
1	AA	19	A	C4-C5-N7	-7.09	107.16	110.70
1	AA	1324	A	N3-C4-N9	7.09	133.07	127.40
22	BA	216	A	C8-N9-C4	7.09	108.64	105.80
22	BA	2741	A	C8-N9-C4	7.09	108.64	105.80
1	AA	1280	A	C5-N7-C8	7.09	107.44	103.90
22	BA	1431	A	C8-N9-C4	7.09	108.63	105.80
22	BA	2088	A	C5-N7-C8	7.09	107.44	103.90
55	B8	51	A	C5-N7-C8	7.09	107.44	103.90
1	AA	935	A	C8-N9-C4	7.08	108.63	105.80
22	BA	1637	A	N3-C4-N9	7.08	133.07	127.40
1	AA	630	A	C4-C5-C6	7.08	120.54	117.00
22	BA	802	A	C5-N7-C8	7.08	107.44	103.90
22	BA	2013	A	C5-C6-N1	7.08	121.24	117.70
22	BA	2322	A	C4-C5-C6	7.08	120.54	117.00
22	BA	2412	A	C8-N9-C4	7.08	108.63	105.80
22	BA	233	A	C5-N7-C8	7.08	107.44	103.90
22	BA	730	A	C4-C5-C6	7.08	120.54	117.00
1	AA	195	A	N9-C4-C5	7.07	108.63	105.80
1	AA	563	A	C4-C5-C6	7.07	120.54	117.00
22	BA	207	A	C5-N7-C8	7.07	107.44	103.90
22	BA	2766	A	C5-N7-C8	7.07	107.44	103.90
1	AA	520	A	C4-C5-C6	7.07	120.53	117.00
1	AA	946	A	C5-N7-C8	7.07	107.44	103.90
22	BA	73	A	C5-N7-C8	7.07	107.44	103.90
22	BA	820	A	C5-N7-C8	7.07	107.44	103.90
22	BA	1260	A	N3-C4-N9	7.07	133.06	127.40
22	BA	1301	A	C5-N7-C8	7.07	107.44	103.90
1	AA	28	A	N3-C4-N9	7.07	133.05	127.40
22	BA	401	A	C8-N9-C4	7.07	108.63	105.80
22	BA	382	A	C5-N7-C8	7.07	107.43	103.90
22	BA	53	A	C5-N7-C8	7.06	107.43	103.90
22	BA	1008	A	C5-N7-C8	7.06	107.43	103.90
1	AA	1254	A	C4-C5-C6	7.06	120.53	117.00
22	BA	84	A	N9-C4-C5	7.06	108.62	105.80
1	AA	151	A	C5-N7-C8	7.06	107.43	103.90
1	AA	1130	A	C4-C5-C6	7.06	120.53	117.00
1	AA	1340	A	C8-N9-C4	7.06	108.62	105.80
22	BA	718	A	C4-C5-C6	7.06	120.53	117.00
22	BA	1241	A	N3-C4-N9	7.06	133.05	127.40
22	BA	2598	A	C5-N7-C8	7.06	107.43	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2033	A	C5-N7-C8	7.06	107.43	103.90
22	BA	2850	A	N3-C4-N9	7.06	133.05	127.40
22	BA	2031	A	C4-C5-C6	7.06	120.53	117.00
22	BA	2059	A	C5-N7-C8	7.05	107.43	103.90
22	BA	2449	U	N3-C4-C5	7.05	118.83	114.60
22	BA	2778	A	C4-C5-C6	7.05	120.53	117.00
1	AA	687	A	C4-C5-C6	7.05	120.53	117.00
22	BA	730	A	C5-N7-C8	7.05	107.43	103.90
22	BA	789	A	C5-C6-N1	7.05	121.23	117.70
22	BA	2005	A	C5-N7-C8	7.05	107.43	103.90
22	BA	2108	A	C4-C5-C6	7.05	120.53	117.00
22	BA	429	A	C4-C5-C6	7.05	120.53	117.00
22	BA	471	A	C5-N7-C8	7.05	107.42	103.90
22	BA	2565	A	C5-N7-C8	7.05	107.42	103.90
1	AA	622	A	N9-C4-C5	7.05	108.62	105.80
22	BA	2376	A	C5-N7-C8	7.05	107.42	103.90
1	AA	1019	A	C8-N9-C4	7.05	108.62	105.80
22	BA	28	A	C4-C5-C6	7.05	120.52	117.00
22	BA	2679	A	C5-N7-C8	7.05	107.42	103.90
22	BA	104	A	C5-N7-C8	7.04	107.42	103.90
22	BA	1571	A	C4-C5-C6	7.04	120.52	117.00
1	AA	743	A	C4-C5-C6	7.04	120.52	117.00
22	BA	675	A	C5-N7-C8	7.04	107.42	103.90
22	BA	1705	A	C4-C5-C6	7.04	120.52	117.00
55	B8	76	A	C4-C5-N7	-7.04	107.18	110.70
22	BA	300	A	C5-N7-C8	7.04	107.42	103.90
22	BA	330	A	C5-N7-C8	7.04	107.42	103.90
22	BA	1970	A	N3-C4-N9	7.04	133.03	127.40
22	BA	501	A	C8-N9-C4	7.04	108.62	105.80
22	BA	244	A	C5-N7-C8	7.04	107.42	103.90
1	AA	949	A	C4-C5-C6	7.04	120.52	117.00
22	BA	1286	A	C8-N9-C4	7.04	108.61	105.80
22	BA	2665	A	C4-C5-C6	7.04	120.52	117.00
1	AA	482	A	C5-N7-C8	7.04	107.42	103.90
22	BA	2432	A	N3-C4-N9	7.04	133.03	127.40
55	B8	41	A	C5-N7-C8	7.04	107.42	103.90
22	BA	734	A	C4-C5-C6	7.03	120.52	117.00
22	BA	2381	A	C5-N7-C8	7.03	107.42	103.90
1	AA	790	A	C5-N7-C8	7.03	107.42	103.90
22	BA	1515	A	C5-N7-C8	7.03	107.42	103.90
1	AA	329	A	C5-N7-C8	7.03	107.41	103.90
1	AA	482	A	C4-C5-C6	7.03	120.51	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	655	A	N3-C4-N9	7.03	133.02	127.40
22	BA	675	A	N3-C4-N9	7.03	133.02	127.40
1	AA	143	A	C8-N9-C4	7.02	108.61	105.80
22	BA	753	A	N3-C4-N9	7.02	133.02	127.40
22	BA	2435	A	N9-C4-C5	7.02	108.61	105.80
22	BA	2750	A	C8-N9-C4	7.02	108.61	105.80
1	AA	1332	A	C5-N7-C8	7.02	107.41	103.90
22	BA	2634	A	C4-C5-C6	7.02	120.51	117.00
22	BA	233	A	C4-C5-C6	7.02	120.51	117.00
22	BA	423	A	C5-N7-C8	7.02	107.41	103.90
22	BA	2662	A	C4-C5-C6	7.02	120.51	117.00
22	BA	979	A	C8-N9-C4	7.01	108.61	105.80
22	BA	1572	A	C5-N7-C8	7.01	107.41	103.90
22	BA	6	A	N3-C4-N9	7.01	133.01	127.40
22	BA	119	A	N9-C4-C5	7.01	108.61	105.80
22	BA	528	A	C4-C5-C6	7.01	120.50	117.00
22	BA	2014	A	C5-N7-C8	7.01	107.41	103.90
1	AA	1319	A	C5-N7-C8	7.01	107.41	103.90
22	BA	447	A	C4-C5-C6	7.01	120.50	117.00
22	BA	2386	A	N3-C4-N9	7.01	133.01	127.40
22	BA	2432	A	C5-N7-C8	7.01	107.40	103.90
1	AA	33	A	N3-C4-N9	7.00	133.00	127.40
22	BA	497	A	C4-C5-C6	7.00	120.50	117.00
22	BA	1470	A	C4-C5-C6	7.00	120.50	117.00
22	BA	2114	A	N3-C4-N9	7.00	133.00	127.40
1	AA	1483	A	C8-N9-C4	7.00	108.60	105.80
22	BA	2212	A	C5-N7-C8	7.00	107.40	103.90
1	AA	383	A	C5-N7-C8	7.00	107.40	103.90
1	AA	1171	A	N3-C4-N9	7.00	133.00	127.40
22	BA	332	A	C4-C5-C6	7.00	120.50	117.00
22	BA	1054	A	N3-C4-N9	7.00	133.00	127.40
22	BA	1126	A	C5-N7-C8	7.00	107.40	103.90
22	BA	1253	A	N9-C4-C5	7.00	108.60	105.80
1	AA	19	A	C4-C5-C6	7.00	120.50	117.00
1	AA	675	A	C8-N9-C4	7.00	108.60	105.80
1	AA	393	A	C4-C5-C6	7.00	120.50	117.00
1	AA	946	A	C4-C5-C6	7.00	120.50	117.00
1	AA	10	A	C8-N9-C4	6.99	108.60	105.80
22	BA	173	A	N3-C4-N9	6.99	132.99	127.40
22	BA	742	A	C8-N9-C4	6.99	108.60	105.80
22	BA	320	A	C5-N7-C8	6.99	107.39	103.90
22	BA	2766	A	N3-C4-N9	6.99	132.99	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	349	A	C8-N9-C4	6.99	108.59	105.80
1	AA	414	A	N3-C4-N9	6.99	132.99	127.40
22	BA	603	A	N9-C4-C5	6.99	108.60	105.80
22	BA	975	A	C5-N7-C8	6.99	107.39	103.90
22	BA	1632	A	C5-N7-C8	6.99	107.39	103.90
1	AA	329	A	N3-C4-N9	6.99	132.99	127.40
1	AA	1082	A	N3-C4-N9	6.99	132.99	127.40
1	AA	1375	A	C5-N7-C8	6.98	107.39	103.90
22	BA	575	A	N9-C4-C5	6.98	108.59	105.80
22	BA	996	A	C4-C5-C6	6.98	120.49	117.00
22	BA	1029	A	N3-C4-N9	6.98	132.99	127.40
22	BA	1205	A	C5-N7-C8	6.98	107.39	103.90
1	AA	192	A	C4-C5-C6	6.98	120.49	117.00
1	AA	374	A	C4-C5-C6	6.98	120.49	117.00
1	AA	1507	A	C4-C5-C6	6.98	120.49	117.00
22	BA	502	A	C4-C5-C6	6.98	120.49	117.00
22	BA	1254	A	C8-N9-C4	6.98	108.59	105.80
22	BA	1569	A	C5-N7-C8	6.98	107.39	103.90
1	AA	873	A	C5-N7-C8	6.98	107.39	103.90
1	AA	539	A	N3-C4-N9	6.97	132.98	127.40
22	BA	1966	A	N9-C4-C5	6.97	108.59	105.80
1	AA	430	A	C4-C5-C6	6.97	120.48	117.00
1	AA	461	A	C8-N9-C4	6.97	108.59	105.80
22	BA	149	A	C5-N7-C8	6.97	107.39	103.90
22	BA	384	A	C5-N7-C8	6.97	107.38	103.90
22	BA	804	A	C4-C5-C6	6.97	120.48	117.00
22	BA	1722	A	N3-C4-N9	6.96	132.97	127.40
22	BA	142	A	N3-C4-N9	6.96	132.97	127.40
22	BA	910	A	C8-N9-C4	6.96	108.58	105.80
22	BA	1129	A	C5-N7-C8	6.96	107.38	103.90
23	BB	52	A	C8-N9-C4	6.96	108.58	105.80
1	AA	673	A	C4-C5-C6	6.96	120.48	117.00
1	AA	900	A	C4-C5-C6	6.96	120.48	117.00
1	AA	1152	A	C5-N7-C8	6.96	107.38	103.90
22	BA	739	A	C4-C5-C6	6.96	120.48	117.00
1	AA	1271	A	C8-N9-C4	6.95	108.58	105.80
22	BA	2317	A	N3-C4-N9	6.95	132.96	127.40
22	BA	2705	A	C5-N7-C8	6.95	107.38	103.90
22	BA	497	A	C8-N9-C4	6.95	108.58	105.80
1	AA	179	A	C4-C5-C6	6.95	120.48	117.00
1	AA	815	A	C4-C5-C6	6.95	120.48	117.00
1	AA	1152	A	N3-C4-N9	6.95	132.96	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	73	A	N3-C4-N9	6.95	132.96	127.40
22	BA	1194	A	C5-N7-C8	6.95	107.37	103.90
22	BA	2471	A	C8-N9-C4	6.95	108.58	105.80
22	BA	2328	A	C5-N7-C8	6.95	107.37	103.90
1	AA	560	A	C4-C5-C6	6.95	120.47	117.00
1	AA	1508	A	N3-C4-N9	6.95	132.96	127.40
22	BA	222	A	C8-N9-C4	6.95	108.58	105.80
22	BA	984	A	N3-C4-N9	6.95	132.96	127.40
22	BA	1032	A	C8-N9-C4	6.95	108.58	105.80
23	BB	57	A	C5-N7-C8	6.95	107.37	103.90
22	BA	1746	A	C4-C5-C6	6.94	120.47	117.00
1	AA	139	A	C4-C5-C6	6.94	120.47	117.00
22	BA	2821	A	C5-N7-C8	6.94	107.37	103.90
1	AA	270	A	C4-C5-C6	6.94	120.47	117.00
22	BA	614	A	C8-N9-C4	6.94	108.58	105.80
22	BA	983	A	C4-C5-C6	6.94	120.47	117.00
22	BA	1373	A	C5-N7-C8	6.94	107.37	103.90
22	BA	1690	A	N9-C4-C5	6.94	108.58	105.80
1	AA	554	A	N9-C4-C5	6.94	108.58	105.80
1	AA	1430	A	C5-N7-C8	6.94	107.37	103.90
1	AA	16	A	C8-N9-C4	6.94	108.58	105.80
1	AA	878	A	C5-N7-C8	6.94	107.37	103.90
1	AA	1350	A	N3-C4-N9	6.94	132.95	127.40
22	BA	1551	A	N9-C4-C5	6.94	108.58	105.80
22	BA	2225	A	C8-N9-C4	6.94	108.58	105.80
22	BA	2700	A	C5-N7-C8	6.94	107.37	103.90
22	BA	477	A	C5-N7-C8	6.94	107.37	103.90
1	AA	977	A	C4-C5-C6	6.93	120.47	117.00
22	BA	19	A	N3-C4-N9	6.93	132.95	127.40
22	BA	167	A	N3-C4-N9	6.93	132.95	127.40
22	BA	2873	A	C8-N9-C4	6.93	108.57	105.80
55	B8	21	A	C5-N7-C8	6.93	107.37	103.90
1	AA	119	A	N9-C4-C5	6.93	108.57	105.80
22	BA	541	A	N9-C4-C5	6.93	108.57	105.80
22	BA	2322	A	N3-C4-N9	6.93	132.94	127.40
22	BA	2851	A	C4-C5-C6	6.93	120.47	117.00
22	BA	502	A	N3-C4-N9	6.93	132.94	127.40
22	BA	753	A	C4-C5-C6	6.93	120.46	117.00
22	BA	2386	A	C5-N7-C8	6.93	107.36	103.90
1	AA	746	A	C5-C6-N1	6.92	121.16	117.70
22	BA	160	A	C5-N7-C8	6.92	107.36	103.90
22	BA	1039	A	C8-N9-C4	6.92	108.57	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	B8	6	A	C5-N7-C8	6.92	107.36	103.90
1	AA	716	A	C5-N7-C8	6.92	107.36	103.90
1	AA	1093	A	C4-C5-C6	6.92	120.46	117.00
22	BA	825	A	C4-C5-N7	-6.92	107.24	110.70
22	BA	1614	A	C5-N7-C8	6.92	107.36	103.90
22	BA	1609	A	C8-N9-C4	6.92	108.57	105.80
22	BA	1634	A	C4-C5-C6	6.92	120.46	117.00
55	B8	73	A	N9-C4-C5	6.92	108.57	105.80
22	BA	925	A	C8-N9-C4	6.92	108.57	105.80
22	BA	2407	A	N3-C4-N9	6.92	132.93	127.40
22	BA	2706	A	C5-C6-N1	6.92	121.16	117.70
22	BA	2893	A	C4-C5-C6	6.92	120.46	117.00
22	BA	677	A	C5-N7-C8	6.91	107.36	103.90
22	BA	2497	A	N3-C4-N9	6.91	132.93	127.40
22	BA	2600	A	C8-N9-C4	6.91	108.56	105.80
22	BA	909	A	C5-C6-N1	6.91	121.16	117.70
1	AA	968	A	C5-N7-C8	6.91	107.36	103.90
1	AA	969	A	C4-C5-C6	6.91	120.45	117.00
22	BA	911	A	N3-C4-N9	6.91	132.93	127.40
22	BA	2358	A	C8-N9-C4	6.91	108.56	105.80
23	BB	73	A	C8-N9-C4	6.91	108.56	105.80
1	AA	648	A	C4-C5-C6	6.91	120.45	117.00
22	BA	472	A	C5-N7-C8	6.91	107.35	103.90
22	BA	1431	A	C4-C5-C6	6.91	120.45	117.00
22	BA	1433	A	C4-C5-C6	6.91	120.45	117.00
55	B8	42	A	C5-N7-C8	6.91	107.35	103.90
22	BA	1308	A	C4-C5-N7	-6.91	107.25	110.70
1	AA	1493	A	C8-N9-C4	6.91	108.56	105.80
22	BA	677	A	N3-C4-N9	6.91	132.93	127.40
22	BA	749	A	C8-N9-C4	6.91	108.56	105.80
22	BA	1175	A	N3-C4-N9	6.91	132.93	127.40
22	BA	1395	A	C5-N7-C8	6.90	107.35	103.90
22	BA	2054	A	N3-C4-N9	6.90	132.92	127.40
22	BA	1932	A	C4-C5-C6	6.90	120.45	117.00
22	BA	2809	A	C5-N7-C8	6.90	107.35	103.90
22	BA	1713	A	C8-N9-C4	6.90	108.56	105.80
1	AA	1012	A	C4-C5-C6	6.90	120.45	117.00
1	AA	1447	A	N9-C4-C5	6.90	108.56	105.80
22	BA	1802	A	N3-C4-N9	6.90	132.92	127.40
22	BA	2284	A	C5-N7-C8	6.90	107.35	103.90
1	AA	1081	A	C4-C5-C6	6.89	120.45	117.00
1	AA	1201	A	C4-C5-C6	6.89	120.45	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	592	A	C5-N7-C8	6.89	107.35	103.90
22	BA	1244	A	C4-C5-C6	6.89	120.45	117.00
22	BA	2679	A	C5-C6-N1	6.89	121.15	117.70
55	B8	69	A	C5-N7-C8	6.89	107.35	103.90
1	AA	768	A	C4-C5-C6	6.89	120.45	117.00
22	BA	1713	A	C5-N7-C8	6.89	107.35	103.90
22	BA	466	A	C8-N9-C4	6.89	108.56	105.80
1	AA	10	A	N3-C4-N9	6.89	132.91	127.40
1	AA	790	A	N3-C4-N9	6.89	132.91	127.40
1	AA	8	A	C8-N9-C4	6.89	108.55	105.80
1	AA	1067	A	N9-C4-C5	6.88	108.55	105.80
22	BA	2450	A	C8-N9-C4	6.88	108.55	105.80
1	AA	923	A	C5-N7-C8	6.88	107.34	103.90
1	AA	563	A	C5-C6-N1	6.88	121.14	117.70
22	BA	197	A	N3-C4-N9	6.88	132.91	127.40
22	BA	1637	A	C4-C5-C6	6.88	120.44	117.00
22	BA	1669	A	N3-C4-N9	6.88	132.91	127.40
55	B8	66	A	C5-N7-C8	6.88	107.34	103.90
22	BA	453	A	C5-N7-C8	6.88	107.34	103.90
22	BA	1866	A	C4-C5-C6	6.88	120.44	117.00
1	AA	459	A	C4-C5-C6	6.88	120.44	117.00
22	BA	429	A	C5-N7-C8	6.88	107.34	103.90
22	BA	2433	A	C4-C5-C6	6.88	120.44	117.00
22	BA	2900	A	C5-N7-C8	6.88	107.34	103.90
1	AA	794	A	N3-C4-N9	6.88	132.90	127.40
22	BA	541	A	C4-C5-C6	6.88	120.44	117.00
22	BA	1241	A	C5-N7-C8	6.88	107.34	103.90
22	BA	2820	A	C5-N7-C8	6.88	107.34	103.90
22	BA	1969	A	N3-C4-N9	6.87	132.90	127.40
22	BA	176	A	C5-N7-C8	6.87	107.33	103.90
22	BA	190	A	C4-C5-C6	6.87	120.44	117.00
22	BA	1597	A	C5-C6-N1	6.87	121.14	117.70
1	AA	790	A	C4-C5-C6	6.87	120.43	117.00
22	BA	1610	A	C8-N9-C4	6.87	108.55	105.80
22	BA	1890	A	N3-C4-N9	6.87	132.90	127.40
1	AA	665	A	N9-C4-C5	6.87	108.55	105.80
1	AA	382	A	C4-C5-C6	6.87	120.43	117.00
22	BA	941	A	C5-N7-C8	6.87	107.33	103.90
22	BA	2761	A	C5-N7-C8	6.87	107.33	103.90
1	AA	116	A	C5-N7-C8	6.86	107.33	103.90
22	BA	2169	A	N9-C4-C5	6.86	108.55	105.80
22	BA	2764	A	C5-C6-N1	6.86	121.13	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	449	A	N3-C4-N9	6.86	132.89	127.40
22	BA	1789	A	C4-C5-N7	-6.86	107.27	110.70
22	BA	199	A	C5-C6-N1	6.86	121.13	117.70
22	BA	384	A	C4-C5-C6	6.86	120.43	117.00
22	BA	1336	A	C4-C5-C6	6.86	120.43	117.00
1	AA	907	A	C4-C5-C6	6.86	120.43	117.00
22	BA	2711	A	C5-C6-N1	6.86	121.13	117.70
22	BA	721	A	C8-N9-C4	6.86	108.54	105.80
1	AA	448	A	N3-C4-N9	6.86	132.88	127.40
1	AA	983	A	C4-C5-C6	6.86	120.43	117.00
22	BA	2738	A	C8-N9-C4	6.86	108.54	105.80
1	AA	747	A	C4-C5-C6	6.85	120.43	117.00
22	BA	753	A	C5-N7-C8	6.85	107.33	103.90
22	BA	1393	A	C4-C5-C6	6.85	120.43	117.00
22	BA	1586	A	C4-C5-C6	6.85	120.43	117.00
22	BA	2675	A	C5-N7-C8	6.85	107.33	103.90
22	BA	1470	A	C5-N7-C8	6.85	107.33	103.90
1	AA	151	A	N3-C4-N9	6.85	132.88	127.40
1	AA	364	A	C4-C5-C6	6.85	120.42	117.00
22	BA	2654	A	C5-N7-C8	6.85	107.33	103.90
1	AA	465	A	N3-C4-N9	6.85	132.88	127.40
1	AA	1406	U	C2-N3-C4	-6.85	122.89	127.00
22	BA	219	A	N3-C4-N9	6.85	132.88	127.40
22	BA	2266	A	N3-C4-N9	6.85	132.88	127.40
22	BA	439	A	C4-C5-C6	6.85	120.42	117.00
22	BA	1169	A	N3-C4-N9	6.85	132.88	127.40
22	BA	984	A	C4-C5-C6	6.84	120.42	117.00
22	BA	693	A	C8-N9-C4	6.84	108.54	105.80
1	AA	1299	A	C5-N7-C8	6.84	107.32	103.90
22	BA	471	A	C4-C5-C6	6.84	120.42	117.00
22	BA	522	A	C8-N9-C4	6.84	108.54	105.80
22	BA	1477	A	C5-N7-C8	6.84	107.32	103.90
22	BA	1548	A	C5-N7-C8	6.84	107.32	103.90
22	BA	38	A	C5-C6-N1	6.84	121.12	117.70
22	BA	1230	A	C4-C5-C6	6.84	120.42	117.00
22	BA	2176	A	C4-C5-C6	6.84	120.42	117.00
1	AA	747	A	N9-C4-C5	6.83	108.53	105.80
22	BA	2071	A	N3-C4-N9	6.83	132.87	127.40
1	AA	1257	A	C4-C5-C6	6.83	120.42	117.00
23	BB	73	A	C5-N7-C8	6.83	107.32	103.90
1	AA	149	A	N9-C4-C5	6.83	108.53	105.80
1	AA	279	A	C5-N7-C8	6.83	107.31	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1201	A	C5-C6-N1	6.83	121.11	117.70
1	AA	1418	A	C4-C5-C6	6.83	120.42	117.00
22	BA	73	A	C8-N9-C4	6.83	108.53	105.80
1	AA	715	A	C5-N7-C8	6.83	107.31	103.90
22	BA	1048	A	C4-C5-C6	6.83	120.42	117.00
22	BA	1392	A	N3-C4-N9	6.83	132.86	127.40
1	AA	663	A	C5-N7-C8	6.83	107.31	103.90
1	AA	759	A	C4-C5-C6	6.83	120.41	117.00
22	BA	53	A	C5-C6-N1	6.83	121.11	117.70
22	BA	480	A	N3-C4-N9	6.83	132.86	127.40
1	AA	892	A	C4-C5-C6	6.83	120.41	117.00
22	BA	2101	A	C5-C6-N1	6.83	121.11	117.70
1	AA	408	A	C4-C5-C6	6.82	120.41	117.00
1	AA	452	A	C4-C5-C6	6.82	120.41	117.00
1	AA	596	A	C4-C5-N7	-6.82	107.29	110.70
22	BA	833	A	C5-C6-N1	6.82	121.11	117.70
22	BA	1853	A	C8-N9-C4	6.82	108.53	105.80
22	BA	2471	A	C5-C6-N1	6.82	121.11	117.70
22	BA	2711	A	C5-N7-C8	6.82	107.31	103.90
1	AA	959	A	C4-C5-C6	6.82	120.41	117.00
22	BA	1403	A	N3-C4-N9	6.82	132.85	127.40
22	BA	1650	A	N3-C4-N9	6.82	132.85	127.40
22	BA	2015	A	C5-N7-C8	6.82	107.31	103.90
22	BA	2058	A	C4-C5-C6	6.82	120.41	117.00
1	AA	306	A	C8-N9-C4	6.82	108.53	105.80
1	AA	1360	A	C4-C5-C6	6.82	120.41	117.00
22	BA	272	A	C4-C5-C6	6.81	120.41	117.00
22	BA	1308	A	C4-C5-C6	6.81	120.41	117.00
22	BA	2227	A	N9-C4-C5	6.81	108.53	105.80
22	BA	1328	A	C4-C5-N7	-6.81	107.29	110.70
1	AA	373	A	N3-C4-N9	6.81	132.85	127.40
1	AA	1374	A	N3-C4-N9	6.81	132.85	127.40
22	BA	191	A	N3-C4-N9	6.81	132.85	127.40
22	BA	1469	A	N3-C4-N9	6.81	132.85	127.40
1	AA	415	A	N3-C4-N9	6.81	132.85	127.40
1	AA	502	A	N3-C4-N9	6.81	132.84	127.40
22	BA	609	A	C5-N7-C8	6.81	107.30	103.90
22	BA	793	A	N3-C4-N9	6.81	132.85	127.40
22	BA	1103	A	C4-C5-C6	6.81	120.40	117.00
22	BA	1276	A	C4-C5-C6	6.81	120.40	117.00
22	BA	2590	A	C8-N9-C4	6.81	108.52	105.80
22	BA	2600	A	C5-N7-C8	6.81	107.30	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1213	A	N9-C4-C5	6.81	108.52	105.80
22	BA	19	A	C4-C5-C6	6.80	120.40	117.00
22	BA	1553	A	N3-C4-N9	6.80	132.84	127.40
22	BA	2781	A	C4-C5-C6	6.80	120.40	117.00
1	AA	1081	A	N3-C4-N9	6.80	132.84	127.40
22	BA	2757	A	C5-N7-C8	6.80	107.30	103.90
1	AA	430	A	N3-C4-N9	6.80	132.84	127.40
22	BA	794	A	C4-C5-C6	6.80	120.40	117.00
22	BA	2052	A	C5-C6-N1	6.80	121.10	117.70
22	BA	2635	A	C5-C6-N1	6.80	121.10	117.70
23	BB	29	A	N9-C4-C5	6.80	108.52	105.80
22	BA	1307	A	C5-N7-C8	6.80	107.30	103.90
22	BA	2225	A	N3-C4-N9	6.80	132.84	127.40
22	BA	1009	A	N3-C4-N9	6.80	132.84	127.40
1	AA	1374	A	C8-N9-C4	6.79	108.52	105.80
22	BA	602	A	C4-C5-C6	6.79	120.40	117.00
22	BA	800	A	N9-C4-C5	6.79	108.52	105.80
22	BA	2070	A	C5-C6-N1	6.79	121.10	117.70
22	BA	2564	A	C5-N7-C8	6.79	107.30	103.90
22	BA	1156	A	C4-C5-C6	6.79	120.39	117.00
22	BA	2883	A	C8-N9-C4	6.79	108.52	105.80
1	AA	1219	A	N3-C4-N9	6.79	132.83	127.40
22	BA	443	A	C5-N7-C8	6.79	107.29	103.90
22	BA	990	A	C8-N9-C4	6.79	108.51	105.80
22	BA	83	A	C4-C5-C6	6.78	120.39	117.00
22	BA	752	A	C4-C5-C6	6.78	120.39	117.00
1	AA	77	A	C8-N9-C4	6.78	108.51	105.80
1	AA	98	A	C5-C6-N1	6.78	121.09	117.70
1	AA	371	A	N9-C4-C5	6.78	108.51	105.80
22	BA	626	A	C5-N7-C8	6.78	107.29	103.90
22	BA	1780	A	C4-C5-C6	6.78	120.39	117.00
22	BA	1268	A	C4-C5-C6	6.78	120.39	117.00
22	BA	1744	A	N3-C4-N9	6.78	132.82	127.40
23	BB	99	A	C4-C5-C6	6.78	120.39	117.00
22	BA	2433	A	N3-C4-N9	6.78	132.82	127.40
1	AA	814	A	C8-N9-C4	6.77	108.51	105.80
22	BA	1809	A	C5-N7-C8	6.77	107.29	103.90
1	AA	274	A	C8-N9-C4	6.77	108.51	105.80
1	AA	704	A	C5-N7-C8	6.77	107.29	103.90
22	BA	1785	A	C5-N7-C8	6.77	107.29	103.90
22	BA	2749	A	C8-N9-C4	6.77	108.51	105.80
22	BA	2447	G	C5-C6-N1	6.77	114.89	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1503	A	C8-N9-C4	6.77	108.51	105.80
22	BA	1705	A	N3-C4-N9	6.77	132.81	127.40
22	BA	1998	A	N3-C4-N9	6.77	132.81	127.40
22	BA	2439	A	N3-C4-N9	6.77	132.81	127.40
1	AA	412	A	N9-C4-C5	6.77	108.51	105.80
1	AA	892	A	N3-C4-N9	6.77	132.81	127.40
1	AA	1396	A	C4-C5-C6	6.76	120.38	117.00
22	BA	63	A	N3-C4-N9	6.76	132.81	127.40
22	BA	844	A	C4-C5-C6	6.76	120.38	117.00
22	BA	2225	A	C5-N7-C8	6.76	107.28	103.90
22	BA	2634	A	N3-C4-N9	6.76	132.81	127.40
22	BA	1028	A	C4-C5-C6	6.76	120.38	117.00
55	B8	59	A	C5-N7-C8	6.76	107.28	103.90
1	AA	53	A	C5-N7-C8	6.76	107.28	103.90
1	AA	694	A	C4-C5-C6	6.76	120.38	117.00
22	BA	2741	A	C5-C6-N1	6.76	121.08	117.70
22	BA	190	A	N3-C4-N9	6.76	132.81	127.40
22	BA	592	A	C4-C5-C6	6.76	120.38	117.00
22	BA	716	A	C4-C5-C6	6.76	120.38	117.00
22	BA	1591	A	C4-C5-C6	6.76	120.38	117.00
23	BB	46	A	C4-C5-C6	6.76	120.38	117.00
1	AA	270	A	N3-C4-N9	6.76	132.81	127.40
1	AA	288	A	N9-C4-C5	6.76	108.50	105.80
1	AA	1163	A	N3-C4-N9	6.76	132.81	127.40
1	AA	583	A	C8-N9-C4	6.76	108.50	105.80
22	BA	1057	A	N3-C4-N9	6.76	132.81	127.40
1	AA	609	A	C5-N7-C8	6.75	107.28	103.90
1	AA	49	U	N3-C4-O4	-6.75	114.67	119.40
1	AA	59	A	C4-C5-C6	6.75	120.38	117.00
1	AA	1201	A	C8-N9-C4	6.75	108.50	105.80
22	BA	346	A	C4-C5-C6	6.75	120.38	117.00
22	BA	794	A	C5-N7-C8	6.75	107.28	103.90
22	BA	2114	A	C4-C5-C6	6.75	120.38	117.00
1	AA	309	A	C4-C5-C6	6.75	120.38	117.00
22	BA	1392	A	C4-C5-C6	6.75	120.38	117.00
22	BA	1495	A	N3-C4-N9	6.75	132.80	127.40
22	BA	1596	A	C5-C6-N1	6.75	121.08	117.70
22	BA	1953	A	C5-N7-C8	6.75	107.28	103.90
22	BA	2388	A	N3-C4-N9	6.75	132.80	127.40
22	BA	2287	A	C8-N9-C4	6.75	108.50	105.80
1	AA	860	A	N3-C4-N9	6.75	132.80	127.40
22	BA	2670	A	C8-N9-C4	6.75	108.50	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1456	A	C8-N9-C4	6.75	108.50	105.80
22	BA	1028	A	C5-N7-C8	6.75	107.27	103.90
1	AA	1102	A	C4-C5-C6	6.75	120.37	117.00
22	BA	216	A	N3-C4-N9	6.75	132.80	127.40
22	BA	1470	A	N3-C4-N9	6.75	132.80	127.40
1	AA	60	A	C8-N9-C4	6.74	108.50	105.80
22	BA	586	A	C5-N7-C8	6.74	107.27	103.90
22	BA	1453	A	C8-N9-C4	6.74	108.50	105.80
22	BA	2317	A	C4-C5-C6	6.74	120.37	117.00
22	BA	2792	A	C8-N9-C4	6.74	108.50	105.80
1	AA	781	A	N3-C4-N9	6.74	132.79	127.40
1	AA	412	A	C5-N7-C8	6.74	107.27	103.90
1	AA	523	A	C5-N7-C8	6.74	107.27	103.90
22	BA	1655	A	N3-C4-N9	6.74	132.79	127.40
22	BA	2823	A	N3-C4-N9	6.74	132.79	127.40
1	AA	1179	A	N9-C4-C5	6.74	108.50	105.80
1	AA	1271	A	N3-C4-N9	6.74	132.79	127.40
22	BA	1762	A	N9-C4-C5	6.74	108.50	105.80
22	BA	1847	A	N3-C4-N9	6.74	132.79	127.40
22	BA	1032	A	C5-C6-N1	6.74	121.07	117.70
22	BA	1265	A	C4-C5-C6	6.74	120.37	117.00
1	AA	1163	A	C8-N9-C4	6.73	108.49	105.80
22	BA	2662	A	C5-N7-C8	6.73	107.27	103.90
1	AA	913	A	C8-N9-C4	6.73	108.49	105.80
22	BA	1808	A	C4-C5-C6	6.73	120.37	117.00
22	BA	1900	A	C5-N7-C8	6.73	107.27	103.90
1	AA	116	A	N3-C4-N9	6.73	132.78	127.40
22	BA	173	A	C4-C5-C6	6.73	120.36	117.00
55	B8	51	A	C4-C5-C6	6.73	120.37	117.00
22	BA	632	A	C5-N7-C8	6.73	107.26	103.90
22	BA	515	A	C5-N7-C8	6.73	107.26	103.90
22	BA	1853	A	C5-N7-C8	6.72	107.26	103.90
1	AA	622	A	C5-N7-C8	6.72	107.26	103.90
1	AA	1082	A	C4-C5-C6	6.72	120.36	117.00
22	BA	279	A	C4-C5-C6	6.72	120.36	117.00
1	AA	923	A	N3-C4-N9	6.72	132.78	127.40
22	BA	1205	A	C4-C5-C6	6.72	120.36	117.00
22	BA	661	A	N3-C4-N9	6.72	132.78	127.40
22	BA	2758	A	C8-N9-C4	6.72	108.49	105.80
22	BA	94	A	C4-C5-C6	6.72	120.36	117.00
22	BA	2267	A	C5-C6-N1	6.72	121.06	117.70
22	BA	2281	A	C5-C6-N1	6.72	121.06	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2566	A	C8-N9-C4	6.72	108.49	105.80
22	BA	6	A	C4-C5-C6	6.71	120.36	117.00
22	BA	479	A	C8-N9-C4	6.71	108.48	105.80
22	BA	2227	A	C4-C5-C6	6.71	120.36	117.00
22	BA	1165	A	N9-C4-C5	6.71	108.48	105.80
22	BA	2094	A	C8-N9-C4	6.71	108.48	105.80
22	BA	2407	A	C5-N7-C8	6.71	107.25	103.90
22	BA	621	A	C5-N7-C8	6.71	107.25	103.90
22	BA	1098	A	C4-C5-C6	6.71	120.35	117.00
22	BA	1739	A	C4-C5-C6	6.71	120.35	117.00
22	BA	218	A	N3-C4-N9	6.71	132.76	127.40
22	BA	2453	A	N9-C4-C5	6.71	108.48	105.80
22	BA	2051	A	C5-C6-N1	6.70	121.05	117.70
1	AA	696	A	C5-N7-C8	6.70	107.25	103.90
22	BA	761	A	N9-C4-C5	6.70	108.48	105.80
22	BA	1127	A	C4-C5-C6	6.70	120.35	117.00
22	BA	1772	A	N9-C4-C5	6.70	108.48	105.80
22	BA	905	A	C8-N9-C4	6.70	108.48	105.80
1	AA	321	A	C4-C5-C6	6.70	120.35	117.00
22	BA	412	A	N3-C4-N9	6.70	132.76	127.40
22	BA	633	A	C4-C5-C6	6.70	120.35	117.00
22	BA	1641	A	C5-N7-C8	6.70	107.25	103.90
22	BA	1353	A	C8-N9-C4	6.70	108.48	105.80
22	BA	2598	A	C4-C5-C6	6.70	120.35	117.00
1	AA	414	A	C4-C5-C6	6.69	120.35	117.00
1	AA	1398	A	N3-C4-N9	6.69	132.75	127.40
22	BA	483	A	C4-C5-C6	6.69	120.35	117.00
22	BA	825	A	C4-C5-C6	6.69	120.35	117.00
22	BA	2531	A	C5-N7-C8	6.69	107.25	103.90
23	BB	39	A	C4-C5-C6	6.69	120.35	117.00
1	AA	353	A	C4-C5-C6	6.69	120.34	117.00
1	AA	908	A	N3-C4-N9	6.69	132.75	127.40
1	AA	718	A	C4-C5-C6	6.69	120.34	117.00
1	AA	238	A	C4-C5-C6	6.69	120.34	117.00
1	AA	831	A	C4-C5-C6	6.69	120.34	117.00
22	BA	512	G	C5-N7-C8	-6.69	100.96	104.30
22	BA	783	A	N9-C4-C5	6.69	108.47	105.80
22	BA	1084	A	C4-C5-N7	-6.69	107.36	110.70
22	BA	1496	A	C5-N7-C8	6.69	107.24	103.90
22	BA	1080	A	N9-C4-C5	6.68	108.47	105.80
1	AA	784	A	C4-C5-N7	-6.68	107.36	110.70
1	AA	1437	A	C4-C5-C6	6.68	120.34	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1378	A	N3-C4-N9	6.68	132.75	127.40
1	AA	116	A	C8-N9-C4	6.68	108.47	105.80
1	AA	253	A	C8-N9-C4	6.68	108.47	105.80
1	AA	743	A	C5-C6-N1	6.68	121.04	117.70
22	BA	1028	A	N3-C4-N9	6.68	132.75	127.40
22	BA	1981	A	C8-N9-C4	6.68	108.47	105.80
1	AA	468	A	C8-N9-C4	6.68	108.47	105.80
22	BA	272	A	N3-C4-N9	6.68	132.74	127.40
1	AA	197	A	C8-N9-C4	6.68	108.47	105.80
22	BA	91	A	C8-N9-C4	6.68	108.47	105.80
22	BA	928	A	C5-N7-C8	6.67	107.24	103.90
22	BA	2369	A	N9-C4-C5	6.67	108.47	105.80
1	AA	303	A	C4-C5-C6	6.67	120.34	117.00
22	BA	126	A	C4-C5-C6	6.67	120.34	117.00
1	AA	32	A	C5-C6-N1	6.67	121.03	117.70
1	AA	865	A	C4-C5-N7	-6.67	107.36	110.70
22	BA	1144	A	N3-C4-N9	6.67	132.74	127.40
22	BA	1359	A	N9-C4-C5	6.67	108.47	105.80
22	BA	1788	C	C6-N1-C2	-6.67	117.63	120.30
22	BA	2432	A	C4-C5-C6	6.67	120.34	117.00
22	BA	2665	A	N3-C4-N9	6.67	132.74	127.40
1	AA	161	A	C5-N7-C8	6.67	107.23	103.90
22	BA	1597	A	N3-C4-N9	6.67	132.74	127.40
22	BA	2090	A	C4-C5-C6	6.67	120.33	117.00
1	AA	767	A	C4-C5-C6	6.67	120.33	117.00
1	AA	1170	A	C4-C5-C6	6.67	120.33	117.00
22	BA	255	A	N3-C4-N9	6.67	132.73	127.40
22	BA	582	A	C5-N7-C8	6.67	107.23	103.90
22	BA	1829	A	N3-C4-N9	6.67	132.73	127.40
22	BA	2003	A	C8-N9-C4	6.67	108.47	105.80
22	BA	743	A	C5-N7-C8	6.67	107.23	103.90
22	BA	1054	A	C4-C5-C6	6.66	120.33	117.00
22	BA	2799	A	C5-N7-C8	6.66	107.23	103.90
1	AA	246	A	C8-N9-C4	6.66	108.47	105.80
22	BA	1717	A	C5-N7-C8	6.66	107.23	103.90
1	AA	596	A	C4-C5-C6	6.66	120.33	117.00
1	AA	609	A	C8-N9-C4	6.66	108.46	105.80
1	AA	784	A	C4-C5-C6	6.66	120.33	117.00
22	BA	190	A	C5-N7-C8	6.66	107.23	103.90
22	BA	2003	A	C5-C6-N1	6.66	121.03	117.70
1	AA	329	A	C4-C5-C6	6.66	120.33	117.00
22	BA	1919	A	C8-N9-C4	6.66	108.46	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1952	A	C5-N7-C8	6.66	107.23	103.90
22	BA	1327	A	C8-N9-C4	6.66	108.46	105.80
22	BA	2378	A	C4-C5-C6	6.66	120.33	117.00
1	AA	792	A	C4-C5-C6	6.66	120.33	117.00
1	AA	1101	A	N9-C4-C5	6.66	108.46	105.80
22	BA	1548	A	C4-C5-C6	6.66	120.33	117.00
22	BA	1598	A	C5-N7-C8	6.66	107.23	103.90
22	BA	2270	A	C4-C5-C6	6.66	120.33	117.00
22	BA	2829	A	N9-C4-C5	6.66	108.46	105.80
22	BA	1151	A	N3-C4-N9	6.65	132.72	127.40
1	AA	815	A	N3-C4-N9	6.65	132.72	127.40
22	BA	668	A	C4-C5-C6	6.65	120.33	117.00
22	BA	1717	A	C8-N9-C4	6.65	108.46	105.80
1	AA	787	A	C8-N9-C4	6.65	108.46	105.80
1	AA	1092	A	N9-C4-C5	6.65	108.46	105.80
1	AA	1238	A	N3-C4-N9	6.65	132.72	127.40
22	BA	155	A	C8-N9-C4	6.65	108.46	105.80
22	BA	227	A	N9-C4-C5	6.65	108.46	105.80
1	AA	994	A	C4-C5-C6	6.65	120.33	117.00
1	AA	1346	A	C8-N9-C4	6.65	108.46	105.80
22	BA	1126	A	C4-C5-C6	6.65	120.32	117.00
22	BA	478	A	N3-C4-N9	6.65	132.72	127.40
22	BA	1321	A	C4-C5-C6	6.65	120.32	117.00
1	AA	1191	A	C4-C5-C6	6.65	120.32	117.00
1	AA	1377	A	C4-C5-C6	6.65	120.32	117.00
1	AA	1456	A	C4-C5-C6	6.65	120.32	117.00
22	BA	345	A	N9-C4-C5	6.65	108.46	105.80
22	BA	1672	A	C4-C5-C6	6.64	120.32	117.00
22	BA	1679	A	C4-C5-C6	6.64	120.32	117.00
22	BA	2761	A	C8-N9-C4	6.64	108.46	105.80
1	AA	914	A	C4-C5-C6	6.64	120.32	117.00
22	BA	1603	A	C5-N7-C8	6.64	107.22	103.90
22	BA	2468	A	N3-C4-N9	6.64	132.71	127.40
22	BA	627	A	C5-C6-N1	6.64	121.02	117.70
1	AA	635	A	C4-C5-C6	6.64	120.32	117.00
1	AA	716	A	N3-C4-N9	6.64	132.71	127.40
22	BA	1367	A	C5-N7-C8	6.64	107.22	103.90
22	BA	1772	A	C5-N7-C8	6.64	107.22	103.90
1	AA	499	A	N3-C4-N9	6.64	132.71	127.40
1	AA	573	A	C8-N9-C4	6.64	108.45	105.80
1	AA	600	A	C4-C5-C6	6.64	120.32	117.00
22	BA	477	A	N3-C4-N9	6.64	132.71	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	98	A	C4-C5-C6	6.63	120.32	117.00
1	AA	152	A	N9-C4-C5	6.63	108.45	105.80
1	AA	1465	A	N3-C4-N9	6.63	132.71	127.40
22	BA	152	A	N3-C4-N9	6.63	132.71	127.40
22	BA	917	A	N3-C4-N9	6.63	132.71	127.40
22	BA	182	A	C4-C5-C6	6.63	120.31	117.00
22	BA	1365	A	C4-C5-C6	6.63	120.31	117.00
22	BA	2547	A	C5-N7-C8	6.63	107.21	103.90
1	AA	60	A	C4-C5-C6	6.63	120.31	117.00
1	AA	181	A	C4-C5-C6	6.63	120.31	117.00
22	BA	1490	A	N3-C4-N9	6.62	132.70	127.40
22	BA	1739	A	C5-N7-C8	6.62	107.21	103.90
22	BA	1901	A	C4-C5-C6	6.62	120.31	117.00
22	BA	2577	A	C4-C5-C6	6.62	120.31	117.00
1	AA	907	A	N3-C4-N9	6.62	132.70	127.40
1	AA	914	A	C5-N7-C8	6.62	107.21	103.90
1	AA	1171	A	C4-C5-C6	6.62	120.31	117.00
22	BA	988	A	C8-N9-C4	6.62	108.45	105.80
22	BA	2434	A	C8-N9-C4	6.62	108.45	105.80
22	BA	126	A	C4-C5-N7	-6.62	107.39	110.70
22	BA	332	A	N3-C4-N9	6.62	132.70	127.40
22	BA	2459	A	C5-N7-C8	6.62	107.21	103.90
1	AA	389	A	C5-C6-N1	6.62	121.01	117.70
1	AA	579	A	N3-C4-N9	6.62	132.70	127.40
22	BA	556	A	N3-C4-N9	6.62	132.70	127.40
1	AA	1167	A	C8-N9-C4	6.62	108.45	105.80
22	BA	119	A	C5-N7-C8	6.62	107.21	103.90
22	BA	330	A	C4-C5-C6	6.62	120.31	117.00
22	BA	863	A	C5-C6-N1	6.62	121.01	117.70
22	BA	972	A	C5-C6-N1	6.62	121.01	117.70
22	BA	1189	A	N3-C4-N9	6.62	132.70	127.40
22	BA	1395	A	N9-C4-C5	6.62	108.45	105.80
1	AA	1005	A	C4-C5-C6	6.62	120.31	117.00
22	BA	693	A	N3-C4-N9	6.62	132.69	127.40
22	BA	1260	A	C4-C5-C6	6.62	120.31	117.00
22	BA	1274	A	C4-C5-C6	6.62	120.31	117.00
22	BA	1505	A	N3-C4-N9	6.62	132.69	127.40
22	BA	1757	A	C5-N7-C8	6.62	107.21	103.90
22	BA	1847	A	C5-N7-C8	6.62	107.21	103.90
1	AA	1285	A	C8-N9-C4	6.61	108.45	105.80
23	BB	78	A	C5-N7-C8	6.61	107.21	103.90
55	B8	69	A	C4-C5-C6	6.61	120.31	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	98	A	N3-C4-N9	6.61	132.69	127.40
22	BA	454	A	C4-C5-C6	6.61	120.31	117.00
1	AA	325	A	C4-C5-C6	6.61	120.30	117.00
1	AA	441	A	C4-C5-C6	6.61	120.31	117.00
22	BA	352	A	C4-C5-C6	6.61	120.30	117.00
1	AA	389	A	N3-C4-N9	6.61	132.69	127.40
22	BA	590	A	C4-C5-C6	6.61	120.30	117.00
22	BA	980	A	N3-C4-N9	6.61	132.69	127.40
22	BA	1608	A	C5-N7-C8	6.61	107.20	103.90
22	BA	2198	A	C4-C5-C6	6.61	120.30	117.00
1	AA	509	A	N3-C4-N9	6.61	132.68	127.40
22	BA	1304	A	C4-C5-C6	6.61	120.30	117.00
22	BA	1690	A	C4-C5-C6	6.60	120.30	117.00
22	BA	2298	A	C8-N9-C4	6.60	108.44	105.80
22	BA	1	G	OP1-P-OP2	-6.60	109.70	119.60
22	BA	84	A	C5-N7-C8	6.60	107.20	103.90
22	BA	449	A	C5-C6-N1	6.60	121.00	117.70
1	AA	1000	A	C8-N9-C4	6.60	108.44	105.80
22	BA	1551	A	C4-C5-C6	6.60	120.30	117.00
22	BA	1603	A	C4-C5-C6	6.60	120.30	117.00
22	BA	1652	A	C4-C5-N7	-6.60	107.40	110.70
1	AA	994	A	N3-C4-N9	6.60	132.68	127.40
22	BA	505	A	N3-C4-N9	6.60	132.68	127.40
22	BA	892	A	OP1-P-OP2	-6.60	109.70	119.60
22	BA	1342	A	C8-N9-C4	6.59	108.44	105.80
22	BA	1652	A	N9-C4-C5	6.59	108.44	105.80
1	AA	642	A	N3-C4-N9	6.59	132.67	127.40
1	AA	819	A	C8-N9-C4	6.59	108.44	105.80
1	AA	946	A	N3-C4-N9	6.59	132.67	127.40
22	BA	1669	A	C4-C5-C6	6.59	120.29	117.00
22	BA	466	A	C5-N7-C8	6.59	107.19	103.90
1	AA	1157	A	N3-C4-N9	6.59	132.67	127.40
1	AA	1495	U	N3-C2-O2	-6.59	117.59	122.20
22	BA	788	A	C4-C5-C6	6.59	120.29	117.00
22	BA	988	A	C5-N7-C8	6.59	107.19	103.90
22	BA	1679	A	C5-N7-C8	6.59	107.19	103.90
22	BA	1189	A	C5-N7-C8	6.58	107.19	103.90
22	BA	2577	A	C8-N9-C4	6.58	108.43	105.80
1	AA	554	A	C4-C5-N7	-6.58	107.41	110.70
22	BA	1591	A	N3-C4-N9	6.58	132.67	127.40
22	BA	1641	A	C5-C6-N1	6.58	120.99	117.70
22	BA	2088	A	N3-C4-N9	6.58	132.67	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2170	A	C4-C5-C6	6.58	120.29	117.00
22	BA	2267	A	N3-C4-N9	6.58	132.67	127.40
22	BA	125	A	C8-N9-C4	6.58	108.43	105.80
22	BA	1549	A	N3-C4-N9	6.58	132.66	127.40
22	BA	1677	A	C5-N7-C8	6.58	107.19	103.90
22	BA	1913	A	C8-N9-C4	6.58	108.43	105.80
22	BA	2856	A	C4-C5-C6	6.58	120.29	117.00
1	AA	1176	A	N3-C4-N9	6.58	132.66	127.40
22	BA	602	A	C8-N9-C4	6.58	108.43	105.80
22	BA	2734	A	C8-N9-C4	6.58	108.43	105.80
1	AA	55	A	C4-C5-N7	-6.58	107.41	110.70
22	BA	616	A	C4-C5-C6	6.58	120.29	117.00
22	BA	2461	A	C5-C6-N1	6.58	120.99	117.70
1	AA	131	A	C4-C5-C6	6.58	120.29	117.00
1	AA	174	A	C4-C5-C6	6.58	120.29	117.00
1	AA	482	A	N3-C4-N9	6.58	132.66	127.40
22	BA	320	A	N3-C4-N9	6.58	132.66	127.40
22	BA	2433	A	C5-N7-C8	6.58	107.19	103.90
55	B8	41	A	C4-C5-C6	6.58	120.29	117.00
22	BA	352	A	N3-C4-N9	6.57	132.66	127.40
22	BA	443	A	N3-C4-N9	6.57	132.66	127.40
22	BA	1794	A	C5-C6-N1	6.57	120.99	117.70
22	BA	2176	A	N3-C4-N9	6.57	132.66	127.40
1	AA	595	A	C4-C5-C6	6.57	120.29	117.00
1	AA	1236	A	N3-C4-N9	6.57	132.66	127.40
1	AA	1329	A	C8-N9-C4	6.57	108.43	105.80
22	BA	1387	A	C5-C6-N1	6.57	120.99	117.70
1	AA	766	A	C5-C6-N1	6.57	120.98	117.70
22	BA	391	A	N3-C4-N9	6.57	132.66	127.40
22	BA	1953	A	C8-N9-C4	6.57	108.43	105.80
1	AA	768	A	N3-C4-N9	6.57	132.65	127.40
22	BA	384	A	N3-C4-N9	6.57	132.65	127.40
22	BA	1759	A	C4-C5-C6	6.57	120.28	117.00
22	BA	2711	A	C8-N9-C4	6.57	108.43	105.80
1	AA	1110	A	C4-C5-C6	6.57	120.28	117.00
22	BA	176	A	C4-C5-C6	6.56	120.28	117.00
22	BA	227	A	C4-C5-C6	6.56	120.28	117.00
22	BA	439	A	N3-C4-N9	6.56	132.65	127.40
22	BA	959	A	C4-C5-C6	6.56	120.28	117.00
22	BA	1175	A	C4-C5-C6	6.56	120.28	117.00
22	BA	1754	A	C5-N7-C8	6.56	107.18	103.90
22	BA	563	A	C5-N7-C8	6.56	107.18	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	673	A	N3-C4-N9	6.56	132.65	127.40
1	AA	1429	A	C8-N9-C4	6.56	108.42	105.80
22	BA	83	A	N3-C4-N9	6.56	132.65	127.40
22	BA	309	A	C4-C5-C6	6.56	120.28	117.00
22	BA	345	A	C4-C5-C6	6.56	120.28	117.00
22	BA	2541	A	C8-N9-C4	6.56	108.42	105.80
1	AA	243	A	C4-C5-N7	-6.56	107.42	110.70
1	AA	313	A	N3-C4-N9	6.56	132.65	127.40
22	BA	1080	A	C4-C5-C6	6.56	120.28	117.00
22	BA	1155	A	N9-C4-C5	6.56	108.42	105.80
23	BB	15	A	N9-C4-C5	6.56	108.42	105.80
22	BA	1048	A	N3-C4-N9	6.56	132.65	127.40
22	BA	2191	A	N3-C4-N9	6.56	132.65	127.40
22	BA	342	A	C5-N7-C8	6.55	107.18	103.90
55	B8	26	A	N3-C4-N9	6.55	132.64	127.40
1	AA	181	A	N3-C4-N9	6.55	132.64	127.40
22	BA	716	A	C5-N7-C8	6.55	107.18	103.90
22	BA	1032	A	N9-C4-C5	6.55	108.42	105.80
22	BA	1580	A	C4-C5-C6	6.55	120.28	117.00
1	AA	303	A	N3-C4-N9	6.55	132.64	127.40
1	AA	1332	A	C4-C5-C6	6.55	120.28	117.00
22	BA	739	A	N9-C4-C5	6.55	108.42	105.80
22	BA	2469	A	C5-C6-N1	6.55	120.97	117.70
22	BA	844	A	C5-N7-C8	6.55	107.17	103.90
22	BA	1809	A	N9-C4-C5	6.55	108.42	105.80
1	AA	189	A	C4-C5-C6	6.55	120.27	117.00
1	AA	1055	A	C4-C5-C6	6.55	120.27	117.00
22	BA	788	A	C5-N7-C8	6.55	107.17	103.90
22	BA	1672	A	C8-N9-C4	6.55	108.42	105.80
22	BA	2733	A	C8-N9-C4	6.55	108.42	105.80
1	AA	1254	A	N3-C4-N9	6.54	132.63	127.40
22	BA	71	A	C4-C5-C6	6.54	120.27	117.00
22	BA	1746	A	N3-C4-N9	6.54	132.64	127.40
22	BA	2478	A	C8-N9-C4	6.54	108.42	105.80
1	AA	499	A	C8-N9-C4	6.54	108.42	105.80
1	AA	1229	A	N9-C4-C5	6.54	108.42	105.80
1	AA	1374	A	C4-C5-C6	6.54	120.27	117.00
22	BA	1566	A	C5-N7-C8	6.54	107.17	103.90
22	BA	1593	A	N3-C4-N9	6.54	132.63	127.40
1	AA	26	A	N3-C4-N9	6.54	132.63	127.40
22	BA	222	A	N3-C4-N9	6.54	132.63	127.40
22	BA	492	A	N3-C4-N9	6.54	132.63	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	715	A	C4-C5-C6	6.54	120.27	117.00
22	BA	1669	A	C4-C5-N7	-6.54	107.43	110.70
22	BA	2266	A	C4-C5-C6	6.54	120.27	117.00
22	BA	2531	A	N3-C4-N9	6.54	132.63	127.40
22	BA	2589	A	C5-N7-C8	6.54	107.17	103.90
22	BA	1938	A	C4-C5-C6	6.54	120.27	117.00
22	BA	2183	A	C8-N9-C4	6.54	108.41	105.80
22	BA	368	A	N3-C4-N9	6.53	132.63	127.40
22	BA	1598	A	N3-C4-N9	6.53	132.63	127.40
22	BA	526	A	C8-N9-C4	6.53	108.41	105.80
22	BA	900	A	C4-C5-C6	6.53	120.27	117.00
1	AA	174	A	N9-C4-C5	6.53	108.41	105.80
1	AA	374	A	N3-C4-N9	6.53	132.62	127.40
1	AA	393	A	N3-C4-N9	6.53	132.62	127.40
1	AA	579	A	C8-N9-C4	6.53	108.41	105.80
1	AA	608	A	C5-N7-C8	6.53	107.17	103.90
1	AA	1227	A	C4-C5-C6	6.53	120.27	117.00
1	AA	1238	A	C4-C5-C6	6.53	120.27	117.00
1	AA	1269	A	C8-N9-C4	6.53	108.41	105.80
22	BA	1580	A	C8-N9-C4	6.53	108.41	105.80
23	BB	104	A	C8-N9-C4	6.53	108.41	105.80
22	BA	1912	A	C8-N9-C4	6.53	108.41	105.80
22	BA	532	A	N3-C4-N9	6.53	132.62	127.40
22	BA	1098	A	N3-C4-N9	6.53	132.62	127.40
22	BA	1304	A	N9-C4-C5	6.53	108.41	105.80
22	BA	1932	A	N3-C4-N9	6.53	132.62	127.40
22	BA	2766	A	C5-C6-N1	6.53	120.96	117.70
1	AA	1000	A	N3-C4-N9	6.52	132.62	127.40
22	BA	348	A	C4-C5-C6	6.52	120.26	117.00
22	BA	412	A	C4-C5-C6	6.52	120.26	117.00
22	BA	1420	A	C8-N9-C4	6.52	108.41	105.80
1	AA	487	A	N3-C4-N9	6.52	132.62	127.40
22	BA	2883	A	C5-N7-C8	6.52	107.16	103.90
1	AA	949	A	N3-C4-N9	6.52	132.62	127.40
22	BA	21	A	C5-N7-C8	6.52	107.16	103.90
22	BA	299	A	C5-N7-C8	6.52	107.16	103.90
22	BA	599	A	C8-N9-C4	6.52	108.41	105.80
22	BA	742	A	C4-C5-C6	6.52	120.26	117.00
22	BA	265	A	C4-C5-C6	6.52	120.26	117.00
22	BA	513	A	C5-N7-C8	6.52	107.16	103.90
22	BA	918	A	C5-N7-C8	6.52	107.16	103.90
22	BA	1054	A	C5-N7-C8	6.52	107.16	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2439	A	C4-C5-C6	6.52	120.26	117.00
22	BA	2665	A	C8-N9-C4	6.52	108.41	105.80
22	BA	2080	A	N3-C4-N9	6.52	132.61	127.40
22	BA	1664	A	C4-C5-C6	6.51	120.26	117.00
22	BA	1700	A	C4-C5-C6	6.51	120.26	117.00
22	BA	1916	A	C4-C5-C6	6.51	120.26	117.00
22	BA	1936	A	C5-N7-C8	6.51	107.16	103.90
22	BA	262	A	C4-C5-N7	-6.51	107.44	110.70
22	BA	1549	A	C5-C6-N1	6.51	120.95	117.70
22	BA	1815	A	N9-C4-C5	6.51	108.40	105.80
1	AA	101	A	C4-C5-C6	6.51	120.25	117.00
22	BA	821	A	N9-C4-C5	6.51	108.40	105.80
1	AA	1016	A	C8-N9-C4	6.51	108.40	105.80
1	AA	1213	A	C4-C5-N7	-6.51	107.45	110.70
1	AA	1363	A	C4-C5-C6	6.51	120.25	117.00
22	BA	705	A	N3-C4-N9	6.51	132.60	127.40
22	BA	2117	A	N3-C4-N9	6.51	132.61	127.40
22	BA	1050	A	N3-C4-N9	6.50	132.60	127.40
1	AA	465	A	C4-C5-C6	6.50	120.25	117.00
1	AA	938	A	C5-C6-N1	6.50	120.95	117.70
1	AA	1022	A	C4-C5-C6	6.50	120.25	117.00
1	AA	109	A	C4-C5-C6	6.50	120.25	117.00
1	AA	900	A	C5-N7-C8	6.50	107.15	103.90
1	AA	1216	A	C4-C5-C6	6.50	120.25	117.00
22	BA	1327	A	C5-N7-C8	6.50	107.15	103.90
22	BA	2142	A	N3-C4-N9	6.50	132.60	127.40
22	BA	2814	A	C4-C5-C6	6.50	120.25	117.00
22	BA	1213	A	C8-N9-C4	6.50	108.40	105.80
22	BA	1803	A	C5-N7-C8	6.50	107.15	103.90
22	BA	2090	A	C8-N9-C4	6.50	108.40	105.80
1	AA	313	A	N9-C4-C5	6.50	108.40	105.80
22	BA	127	A	C8-N9-C4	6.50	108.40	105.80
22	BA	706	A	C4-C5-C6	6.50	120.25	117.00
1	AA	560	A	N3-C4-N9	6.50	132.60	127.40
1	AA	1146	A	C4-C5-C6	6.50	120.25	117.00
22	BA	322	A	N9-C4-C5	6.50	108.40	105.80
22	BA	1021	A	C5-C6-N1	6.50	120.95	117.70
22	BA	1050	A	C4-C5-C6	6.50	120.25	117.00
22	BA	1111	A	N3-C4-N9	6.50	132.60	127.40
55	B8	59	A	N3-C4-N9	6.50	132.60	127.40
22	BA	980	A	C4-C5-C6	6.50	120.25	117.00
55	B8	42	A	C4-C5-C6	6.50	120.25	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1394	A	C4-C5-C6	6.49	120.25	117.00
22	BA	401	A	N3-C4-N9	6.49	132.59	127.40
22	BA	1877	A	C4-C5-C6	6.49	120.25	117.00
22	BA	2336	A	N3-C4-N9	6.49	132.59	127.40
22	BA	49	A	N3-C4-N9	6.49	132.59	127.40
1	AA	1067	A	C4-C5-C6	6.49	120.25	117.00
1	AA	1191	A	N3-C4-N9	6.49	132.59	127.40
22	BA	42	A	C5-N7-C8	6.49	107.15	103.90
22	BA	231	A	C5-C6-N1	6.49	120.95	117.70
22	BA	1808	A	N3-C4-N9	6.49	132.59	127.40
22	BA	1901	A	N9-C4-C5	6.49	108.40	105.80
22	BA	2033	A	N9-C4-C5	6.49	108.40	105.80
22	BA	2547	A	C4-C5-C6	6.49	120.25	117.00
22	BA	2900	A	C4-C5-C6	6.49	120.25	117.00
1	AA	432	A	N9-C4-C5	6.49	108.39	105.80
1	AA	574	A	C4-C5-C6	6.49	120.25	117.00
1	AA	1101	A	C4-C5-N7	-6.49	107.45	110.70
1	AA	1196	A	C8-N9-C4	6.49	108.40	105.80
22	BA	752	A	C4-C5-N7	-6.49	107.46	110.70
1	AA	1080	A	C8-N9-C4	6.49	108.39	105.80
22	BA	2327	A	N3-C4-N9	6.49	132.59	127.40
22	BA	2887	A	C4-C5-C6	6.49	120.24	117.00
1	AA	865	A	C4-C5-C6	6.49	120.24	117.00
22	BA	863	A	N3-C4-N9	6.49	132.59	127.40
22	BA	1000	A	N3-C4-N9	6.48	132.59	127.40
1	AA	101	A	N3-C4-N9	6.48	132.59	127.40
22	BA	309	A	N3-C4-N9	6.48	132.59	127.40
22	BA	1918	A	N9-C4-C5	6.48	108.39	105.80
22	BA	2212	A	C4-C5-C6	6.48	120.24	117.00
22	BA	2381	A	C8-N9-C4	6.48	108.39	105.80
22	BA	1366	A	C8-N9-C4	6.48	108.39	105.80
22	BA	1385	A	N9-C4-C5	6.48	108.39	105.80
1	AA	1434	A	C5-C6-N1	6.48	120.94	117.70
22	BA	1144	A	C8-N9-C4	6.48	108.39	105.80
22	BA	1610	A	N3-C4-N9	6.48	132.58	127.40
22	BA	457	A	C8-N9-C4	6.48	108.39	105.80
1	AA	1042	A	C4-C5-C6	6.47	120.24	117.00
1	AA	539	A	C8-N9-C4	6.47	108.39	105.80
22	BA	432	A	C4-C5-C6	6.47	120.24	117.00
22	BA	466	A	C4-C5-C6	6.47	120.24	117.00
22	BA	2241	A	C4-C5-C6	6.47	120.24	117.00
22	BA	2418	A	C8-N9-C4	6.47	108.39	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	363	A	N3-C4-N9	6.47	132.58	127.40
1	AA	906	A	C8-N9-C4	6.47	108.39	105.80
22	BA	764	A	C5-N7-C8	6.47	107.14	103.90
22	BA	1383	A	C4-C5-C6	6.47	120.23	117.00
22	BA	1246	A	C5-C6-N1	6.47	120.93	117.70
22	BA	1877	A	N3-C4-N9	6.47	132.57	127.40
22	BA	165	A	N9-C4-C5	6.47	108.39	105.80
22	BA	599	A	C5-C6-N1	6.47	120.93	117.70
22	BA	936	A	C4-C5-C6	6.46	120.23	117.00
22	BA	1759	A	N3-C4-N9	6.46	132.57	127.40
22	BA	2679	A	N3-C4-N9	6.46	132.57	127.40
22	BA	2727	A	C5-C6-N1	6.46	120.93	117.70
1	AA	262	A	C4-C5-C6	6.46	120.23	117.00
1	AA	802	A	C8-N9-C4	6.46	108.38	105.80
1	AA	1021	A	C8-N9-C4	6.46	108.39	105.80
22	BA	156	A	N3-C4-N9	6.46	132.57	127.40
22	BA	532	A	C4-C5-C6	6.46	120.23	117.00
22	BA	602	A	N3-C4-N9	6.46	132.57	127.40
22	BA	1040	A	C4-C5-C6	6.46	120.23	117.00
22	BA	1085	A	C4-C5-N7	-6.46	107.47	110.70
1	AA	149	A	C4-C5-N7	-6.46	107.47	110.70
1	AA	356	A	N9-C4-C5	6.46	108.38	105.80
1	AA	1170	A	C8-N9-C4	6.46	108.38	105.80
55	B8	14	A	N9-C4-C5	6.46	108.38	105.80
22	BA	756	A	N9-C4-C5	6.46	108.38	105.80
1	AA	77	A	N3-C4-N9	6.45	132.56	127.40
1	AA	845	A	N3-C4-N9	6.45	132.56	127.40
1	AA	1500	A	N3-C4-N9	6.45	132.56	127.40
22	BA	222	A	C4-C5-C6	6.45	120.23	117.00
22	BA	2042	A	C4-C5-C6	6.45	120.23	117.00
55	B8	58	A	C4-C5-C6	6.45	120.23	117.00
1	AA	1227	A	N9-C4-C5	6.45	108.38	105.80
22	BA	472	A	C4-C5-C6	6.45	120.23	117.00
22	BA	1247	A	N3-C4-N9	6.45	132.56	127.40
22	BA	1268	A	N3-C4-N9	6.45	132.56	127.40
22	BA	2052	A	C8-N9-C4	6.45	108.38	105.80
22	BA	2297	A	C4-C5-C6	6.45	120.22	117.00
22	BA	2468	A	C4-C5-C6	6.45	120.22	117.00
22	BA	2700	A	C4-C5-C6	6.45	120.22	117.00
1	AA	263	A	N3-C4-N9	6.45	132.56	127.40
1	AA	448	A	C4-C5-C6	6.45	120.22	117.00
1	AA	1257	A	N3-C4-N9	6.45	132.56	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	56	A	C5-C6-N1	6.45	120.92	117.70
22	BA	1057	A	C4-C5-C6	6.45	120.22	117.00
22	BA	2171	A	C4-C5-C6	6.45	120.22	117.00
22	BA	196	A	N3-C4-N9	6.45	132.56	127.40
22	BA	471	A	N3-C4-N9	6.45	132.56	127.40
22	BA	1378	A	C4-C5-C6	6.45	120.22	117.00
1	AA	1152	A	C4-C5-C6	6.45	120.22	117.00
22	BA	616	A	N3-C4-N9	6.45	132.56	127.40
22	BA	750	A	C8-N9-C4	6.45	108.38	105.80
22	BA	1134	A	C4-C5-C6	6.45	120.22	117.00
22	BA	165	A	C4-C5-C6	6.44	120.22	117.00
22	BA	613	A	C4-C5-C6	6.44	120.22	117.00
1	AA	1287	A	N9-C4-C5	6.44	108.38	105.80
22	BA	347	A	C4-C5-C6	6.44	120.22	117.00
22	BA	670	A	N9-C4-C5	6.44	108.38	105.80
22	BA	2058	A	C5-N7-C8	6.44	107.12	103.90
22	BA	2142	A	C8-N9-C4	6.44	108.38	105.80
22	BA	348	A	N3-C4-N9	6.44	132.55	127.40
22	BA	2726	A	N9-C4-C5	6.44	108.38	105.80
22	BA	2823	A	C4-C5-C6	6.44	120.22	117.00
1	AA	199	A	C8-N9-C4	6.44	108.38	105.80
1	AA	1398	A	C4-C5-C6	6.44	120.22	117.00
1	AA	1410	A	C4-C5-C6	6.44	120.22	117.00
22	BA	1365	A	N3-C4-N9	6.44	132.55	127.40
22	BA	1676	A	N3-C4-N9	6.44	132.55	127.40
22	BA	2171	A	N3-C4-N9	6.44	132.55	127.40
22	BA	2518	A	C4-C5-C6	6.44	120.22	117.00
22	BA	739	A	N3-C4-N9	6.44	132.55	127.40
22	BA	1032	A	C4-C5-N7	-6.44	107.48	110.70
1	AA	572	A	C8-N9-C4	6.43	108.37	105.80
22	BA	722	A	N3-C4-N9	6.43	132.55	127.40
22	BA	1336	A	N3-C4-N9	6.43	132.55	127.40
1	AA	1433	A	N9-C4-C5	6.43	108.37	105.80
22	BA	126	A	N3-C4-N9	6.43	132.55	127.40
22	BA	404	A	C8-N9-C4	6.43	108.37	105.80
22	BA	1762	A	C5-N7-C8	6.43	107.12	103.90
22	BA	2031	A	C8-N9-C4	6.43	108.37	105.80
22	BA	2662	A	N3-C4-N9	6.43	132.55	127.40
1	AA	607	A	C4-C5-C6	6.43	120.22	117.00
22	BA	849	A	C4-C5-C6	6.43	120.22	117.00
22	BA	2448	A	N9-C4-C5	6.43	108.37	105.80
22	BA	2469	A	C5-N7-C8	6.43	107.11	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2753	A	N9-C4-C5	6.43	108.37	105.80
1	AA	1163	A	C4-C5-C6	6.43	120.21	117.00
22	BA	1829	A	C4-C5-C6	6.43	120.21	117.00
22	BA	71	A	N9-C4-C5	6.42	108.37	105.80
22	BA	218	A	C5-N7-C8	6.42	107.11	103.90
22	BA	1342	A	C4-C5-C6	6.42	120.21	117.00
22	BA	1616	A	C5-N7-C8	6.42	107.11	103.90
22	BA	1978	A	C5-N7-C8	6.42	107.11	103.90
22	BA	1987	A	C8-N9-C4	6.42	108.37	105.80
22	BA	2632	A	N9-C4-C5	6.42	108.37	105.80
22	BA	547	A	C4-C5-C6	6.42	120.21	117.00
22	BA	2497	A	C5-N7-C8	6.42	107.11	103.90
23	BB	29	A	C4-C5-N7	-6.42	107.49	110.70
1	AA	1170	A	N3-C4-N9	6.42	132.54	127.40
1	AA	1171	A	C8-N9-C4	6.42	108.37	105.80
22	BA	172	A	C4-C5-C6	6.42	120.21	117.00
22	BA	374	A	N3-C4-N9	6.42	132.54	127.40
1	AA	179	A	N3-C4-N9	6.42	132.54	127.40
22	BA	213	A	N3-C4-N9	6.42	132.54	127.40
22	BA	1665	A	N9-C4-C5	6.42	108.37	105.80
22	BA	1953	A	N3-C4-N9	6.42	132.53	127.40
22	BA	2097	A	C4-C5-C6	6.42	120.21	117.00
22	BA	2288	A	C8-N9-C4	6.42	108.37	105.80
22	BA	2376	A	C8-N9-C4	6.42	108.37	105.80
1	AA	781	A	C4-C5-C6	6.42	120.21	117.00
1	AA	1067	A	C4-C5-N7	-6.42	107.49	110.70
22	BA	196	A	N9-C4-C5	6.42	108.37	105.80
22	BA	299	A	C4-C5-C6	6.42	120.21	117.00
22	BA	1086	A	N9-C4-C5	6.42	108.37	105.80
22	BA	2566	A	C5-N7-C8	6.42	107.11	103.90
1	AA	1180	A	C8-N9-C4	6.41	108.36	105.80
22	BA	1689	A	N9-C4-C5	6.41	108.37	105.80
22	BA	1901	A	C5-N7-C8	6.41	107.11	103.90
22	BA	2037	A	N3-C4-N9	6.41	132.53	127.40
23	BB	99	A	N3-C4-N9	6.41	132.53	127.40
1	AA	673	A	C5-C6-N1	6.41	120.91	117.70
1	AA	1236	A	C4-C5-C6	6.41	120.21	117.00
22	BA	310	A	N3-C4-N9	6.41	132.53	127.40
22	BA	1111	A	N9-C4-C5	6.41	108.36	105.80
22	BA	2749	A	C5-N7-C8	6.41	107.11	103.90
1	AA	696	A	N3-C4-N9	6.41	132.53	127.40
1	AA	872	A	N3-C4-N9	6.41	132.53	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1204	A	N9-C4-C5	6.41	108.36	105.80
55	B8	66	A	C4-C5-C6	6.41	120.20	117.00
1	AA	155	A	N3-C4-N9	6.41	132.53	127.40
22	BA	983	A	C5-N7-C8	6.41	107.11	103.90
22	BA	2142	A	C4-C5-C6	6.41	120.20	117.00
1	AA	964	A	C8-N9-C4	6.41	108.36	105.80
1	AA	1004	A	N3-C4-N9	6.41	132.53	127.40
22	BA	299	A	N3-C4-N9	6.41	132.53	127.40
22	BA	404	A	C5-N7-C8	6.41	107.10	103.90
1	AA	189	A	N3-C4-N9	6.41	132.53	127.40
22	BA	155	A	C5-C6-N1	6.41	120.90	117.70
22	BA	637	A	C8-N9-C4	6.41	108.36	105.80
22	BA	1214	A	C5-N7-C8	6.41	107.10	103.90
22	BA	2101	A	C5-C6-N6	6.41	128.82	123.70
1	AA	1022	A	N3-C4-N9	6.40	132.52	127.40
1	AA	729	A	N9-C4-C5	6.40	108.36	105.80
22	BA	789	A	C4-C5-C6	6.40	120.20	117.00
22	BA	2270	A	N3-C4-N9	6.40	132.52	127.40
1	AA	1418	A	C8-N9-C4	6.40	108.36	105.80
1	AA	1418	A	N3-C4-N9	6.40	132.52	127.40
22	BA	482	A	C8-N9-C4	6.40	108.36	105.80
22	BA	2377	A	C5-N7-C8	6.40	107.10	103.90
23	BB	29	A	C4-C5-C6	6.40	120.20	117.00
1	AA	129	A	C8-N9-C4	6.40	108.36	105.80
22	BA	244	A	N9-C4-C5	6.40	108.36	105.80
22	BA	1008	A	C4-C5-C6	6.40	120.20	117.00
22	BA	1754	A	C4-C5-C6	6.40	120.20	117.00
22	BA	346	A	N3-C4-N9	6.40	132.52	127.40
22	BA	2335	A	N3-C4-N9	6.40	132.52	127.40
1	AA	1499	A	C4-C5-C6	6.40	120.20	117.00
22	BA	751	A	C4-C5-C6	6.40	120.20	117.00
1	AA	78	A	C8-N9-C4	6.39	108.36	105.80
22	BA	927	A	N3-C4-N9	6.39	132.52	127.40
22	BA	2434	A	N9-C4-C5	6.39	108.36	105.80
22	BA	2600	A	C5-C6-N1	6.39	120.90	117.70
1	AA	712	A	C5-C6-N1	6.39	120.90	117.70
22	BA	1347	A	C5-N7-C8	6.39	107.10	103.90
22	BA	1439	A	C4-C5-C6	6.39	120.20	117.00
22	BA	1789	A	N3-C4-N9	6.39	132.51	127.40
22	BA	449	A	C4-C5-C6	6.39	120.19	117.00
22	BA	2478	A	C4-C5-C6	6.39	120.19	117.00
1	AA	78	A	N3-C4-N9	6.39	132.51	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	364	A	N9-C4-C5	6.39	108.36	105.80
22	BA	975	A	N3-C4-N9	6.39	132.51	127.40
1	AA	53	A	C4-C5-C6	6.39	120.19	117.00
22	BA	13	A	N3-C4-N9	6.39	132.51	127.40
22	BA	447	A	N3-C4-N9	6.39	132.51	127.40
1	AA	160	A	N9-C4-C5	6.38	108.35	105.80
22	BA	460	A	C4-C5-C6	6.38	120.19	117.00
22	BA	1505	A	C4-C5-C6	6.38	120.19	117.00
22	BA	800	A	C5-N7-C8	6.38	107.09	103.90
22	BA	1284	A	C5-N7-C8	6.38	107.09	103.90
22	BA	1609	A	N3-C4-N9	6.38	132.51	127.40
22	BA	1652	A	C8-N9-C4	6.38	108.35	105.80
1	AA	389	A	C4-C5-C6	6.38	120.19	117.00
22	BA	927	A	C4-C5-C6	6.38	120.19	117.00
22	BA	1126	A	N3-C4-N9	6.38	132.50	127.40
22	BA	1413	A	C8-N9-C4	6.38	108.35	105.80
22	BA	2062	A	C4-C5-C6	6.38	120.19	117.00
22	BA	2469	A	N3-C4-N9	6.38	132.51	127.40
22	BA	2736	A	C8-N9-C4	6.38	108.35	105.80
22	BA	2761	A	C5-C6-N1	6.38	120.89	117.70
1	AA	250	A	C4-C5-C6	6.38	120.19	117.00
1	AA	630	A	N3-C4-N9	6.38	132.50	127.40
1	AA	909	A	C4-C5-C6	6.38	120.19	117.00
22	BA	1739	A	N3-C4-N9	6.38	132.50	127.40
22	BA	505	A	C8-N9-C4	6.38	108.35	105.80
22	BA	1286	A	C5-N7-C8	6.38	107.09	103.90
22	BA	2764	A	C5-N7-C8	6.38	107.09	103.90
23	BB	109	A	N3-C4-N9	6.38	132.50	127.40
1	AA	199	A	N3-C4-N9	6.38	132.50	127.40
22	BA	131	A	N3-C4-N9	6.38	132.50	127.40
22	BA	439	A	N9-C4-C5	6.38	108.35	105.80
22	BA	613	A	N3-C4-N9	6.38	132.50	127.40
22	BA	900	A	N3-C4-N9	6.38	132.50	127.40
22	BA	1070	A	C4-C5-C6	6.38	120.19	117.00
22	BA	1268	A	C8-N9-C4	6.38	108.35	105.80
22	BA	1698	A	N3-C4-N9	6.38	132.50	127.40
22	BA	218	A	C4-C5-C6	6.38	120.19	117.00
22	BA	1503	A	N3-C4-N9	6.38	132.50	127.40
1	AA	1319	A	N9-C4-C5	6.37	108.35	105.80
22	BA	1275	A	C4-C5-C6	6.37	120.19	117.00
22	BA	1593	A	C4-C5-C6	6.37	120.19	117.00
1	AA	919	A	C4-C5-C6	6.37	120.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	975	A	C4-C5-C6	6.37	120.19	117.00
22	BA	984	A	C5-N7-C8	6.37	107.09	103.90
22	BA	1265	A	N3-C4-N9	6.37	132.50	127.40
22	BA	103	A	C4-C5-C6	6.37	120.18	117.00
22	BA	221	A	C8-N9-C4	6.37	108.35	105.80
22	BA	1378	A	N9-C4-C5	6.37	108.35	105.80
22	BA	1952	A	C4-C5-C6	6.37	120.18	117.00
22	BA	2097	A	N3-C4-N9	6.37	132.50	127.40
22	BA	781	A	N3-C4-N9	6.37	132.49	127.40
23	BB	59	A	C8-N9-C4	6.37	108.35	105.80
22	BA	1900	A	C4-C5-C6	6.37	120.18	117.00
22	BA	2287	A	N3-C4-N9	6.37	132.49	127.40
22	BA	2851	A	N3-C4-N9	6.37	132.49	127.40
1	AA	1130	A	N3-C4-N9	6.36	132.49	127.40
22	BA	1272	A	C4-C5-C6	6.36	120.18	117.00
22	BA	2211	A	C8-N9-C4	6.36	108.34	105.80
1	AA	55	A	C8-N9-C4	6.36	108.34	105.80
1	AA	792	A	N3-C4-N9	6.36	132.49	127.40
22	BA	466	A	N3-C4-N9	6.36	132.49	127.40
22	BA	2297	A	N9-C4-C5	6.36	108.34	105.80
1	AA	306	A	N3-C4-N9	6.36	132.49	127.40
1	AA	532	A	N3-C4-N9	6.36	132.49	127.40
1	AA	236	A	C4-C5-C6	6.36	120.18	117.00
1	AA	431	A	N9-C4-C5	6.36	108.34	105.80
1	AA	958	A	C8-N9-C4	6.36	108.34	105.80
22	BA	91	A	C4-C5-C6	6.36	120.18	117.00
22	BA	1608	A	N3-C4-N9	6.36	132.48	127.40
22	BA	89	A	C5-C6-N1	6.35	120.88	117.70
22	BA	920	A	N3-C4-N9	6.35	132.48	127.40
22	BA	2468	A	C8-N9-C4	6.35	108.34	105.80
1	AA	1158	C	C2-N1-C1'	6.35	125.79	118.80
1	AA	1437	A	N3-C4-N9	6.35	132.48	127.40
22	BA	203	A	C4-C5-C6	6.35	120.18	117.00
22	BA	270	A	C8-N9-C4	6.35	108.34	105.80
22	BA	401	A	C4-C5-C6	6.35	120.18	117.00
22	BA	2336	A	C8-N9-C4	6.35	108.34	105.80
22	BA	715	A	N3-C4-N9	6.35	132.48	127.40
1	AA	432	A	C4-C5-N7	-6.35	107.53	110.70
1	AA	961	U	N1-C2-N3	6.35	118.71	114.90
22	BA	1966	A	C4-C5-C6	6.35	120.17	117.00
22	BA	2346	A	N9-C4-C5	6.35	108.34	105.80
1	AA	1363	A	N3-C4-N9	6.35	132.48	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2352	A	N9-C4-C5	6.35	108.34	105.80
22	BA	173	A	C5-C6-N1	6.35	120.87	117.70
22	BA	743	A	N3-C4-N9	6.35	132.48	127.40
1	AA	767	A	C8-N9-C4	6.34	108.34	105.80
22	BA	340	A	C4-C5-C6	6.34	120.17	117.00
22	BA	428	A	C5-N7-C8	6.34	107.07	103.90
22	BA	1027	A	N3-C4-N9	6.34	132.48	127.40
1	AA	139	A	N3-C4-N9	6.34	132.47	127.40
1	AA	192	A	N9-C4-C5	6.34	108.34	105.80
1	AA	478	A	C8-N9-C4	6.34	108.34	105.80
22	BA	44	A	C5-C6-N1	6.34	120.87	117.70
22	BA	371	A	N3-C4-N9	6.34	132.47	127.40
1	AA	1318	A	C4-C5-C6	6.34	120.17	117.00
1	AA	1375	A	N3-C4-N9	6.34	132.47	127.40
22	BA	19	A	C5-C6-N1	6.34	120.87	117.70
22	BA	64	A	N3-C4-N9	6.34	132.47	127.40
22	BA	2406	A	C8-N9-C4	6.34	108.34	105.80
22	BA	2614	A	N9-C4-C5	6.34	108.34	105.80
1	AA	411	A	C8-N9-C4	6.34	108.34	105.80
1	AA	1012	A	N3-C4-N9	6.34	132.47	127.40
22	BA	1640	A	C4-C5-C6	6.34	120.17	117.00
22	BA	1668	A	C5-N7-C8	6.34	107.07	103.90
22	BA	2459	A	N3-C4-N9	6.34	132.47	127.40
22	BA	2600	A	N3-C4-N9	6.34	132.47	127.40
1	AA	196	A	C8-N9-C4	6.34	108.33	105.80
22	BA	1650	A	C4-C5-C6	6.34	120.17	117.00
23	BB	94	A	C4-C5-C6	6.34	120.17	117.00
22	BA	2835	A	N9-C4-C5	6.33	108.33	105.80
22	BA	1143	A	C5-N7-C8	6.33	107.07	103.90
22	BA	1269	A	C5-C6-N1	6.33	120.87	117.70
22	BA	1307	A	C4-C5-C6	6.33	120.17	117.00
1	AA	327	A	N3-C4-N9	6.33	132.47	127.40
1	AA	595	A	N3-C4-N9	6.33	132.47	127.40
22	BA	56	A	C4-C5-C6	6.33	120.17	117.00
22	BA	945	A	N3-C4-N9	6.33	132.47	127.40
22	BA	2163	A	N3-C4-N9	6.33	132.46	127.40
22	BA	2893	A	C8-N9-C4	6.33	108.33	105.80
22	BA	1678	A	C8-N9-C4	6.33	108.33	105.80
22	BA	1749	A	C8-N9-C4	6.33	108.33	105.80
22	BA	347	A	C5-C6-N1	6.33	120.86	117.70
22	BA	718	A	N3-C4-N9	6.33	132.46	127.40
22	BA	1378	A	C5-C6-N1	6.33	120.86	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2388	A	C4-C5-N7	-6.33	107.54	110.70
22	BA	2829	A	C5-C6-N1	6.33	120.86	117.70
1	AA	1151	A	C4-C5-C6	6.32	120.16	117.00
22	BA	28	A	N9-C4-C5	6.32	108.33	105.80
22	BA	1046	A	C8-N9-C4	6.32	108.33	105.80
22	BA	592	A	C5-C6-N1	6.32	120.86	117.70
22	BA	2340	A	C4-C5-C6	6.32	120.16	117.00
22	BA	2814	A	N9-C4-C5	6.32	108.33	105.80
22	BA	131	A	C8-N9-C4	6.32	108.33	105.80
22	BA	1133	A	C4-C5-N7	-6.32	107.54	110.70
1	AA	777	A	N9-C4-C5	6.32	108.33	105.80
1	AA	1299	A	C8-N9-C4	6.32	108.33	105.80
22	BA	149	A	C4-C5-C6	6.32	120.16	117.00
22	BA	1275	A	C8-N9-C4	6.32	108.33	105.80
22	BA	1698	A	C5-C6-N1	6.32	120.86	117.70
22	BA	1858	A	C5-C6-N1	6.32	120.86	117.70
22	BA	2810	A	C4-C5-C6	6.32	120.16	117.00
37	BP	114	LEU	CA-CB-CG	6.32	129.83	115.30
1	AA	1005	A	N3-C4-N9	6.32	132.45	127.40
22	BA	1285	A	C5-N7-C8	6.32	107.06	103.90
22	BA	2266	A	C5-N7-C8	6.32	107.06	103.90
55	B8	69	A	N3-C4-N9	6.32	132.45	127.40
1	AA	71	A	C8-N9-C4	6.31	108.33	105.80
22	BA	1570	A	C5-N7-C8	6.31	107.06	103.90
22	BA	195	A	N7-C8-N9	-6.31	110.64	113.80
22	BA	279	A	N3-C4-N9	6.31	132.45	127.40
22	BA	802	A	C4-C5-C6	6.31	120.16	117.00
22	BA	1189	A	C4-C5-C6	6.31	120.16	117.00
22	BA	2476	A	N3-C4-N9	6.31	132.45	127.40
22	BA	2781	A	N9-C4-C5	6.31	108.33	105.80
1	AA	753	A	C8-N9-C4	6.31	108.33	105.80
1	AA	1513	A	N3-C4-N9	6.31	132.45	127.40
55	B8	73	A	C4-C5-N7	-6.31	107.55	110.70
22	BA	514	A	N9-C4-C5	6.31	108.32	105.80
1	AA	238	A	N3-C4-N9	6.31	132.45	127.40
1	AA	523	A	N9-C4-C5	6.31	108.32	105.80
22	BA	1001	A	C5-N7-C8	6.31	107.05	103.90
22	BA	1597	A	C8-N9-C4	6.31	108.32	105.80
22	BA	1384	A	C8-N9-C4	6.31	108.32	105.80
1	AA	356	A	N3-C4-N9	6.30	132.44	127.40
1	AA	1287	A	C4-C5-C6	6.30	120.15	117.00
22	BA	344	A	C8-N9-C4	6.30	108.32	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1301	A	N3-C4-N9	6.30	132.44	127.40
1	AA	535	A	C4-C5-C6	6.30	120.15	117.00
1	AA	790	A	C8-N9-C4	6.30	108.32	105.80
1	AA	1368	A	C4-C5-C6	6.30	120.15	117.00
22	BA	5	A	C4-C5-C6	6.30	120.15	117.00
22	BA	94	A	N3-C4-N9	6.30	132.44	127.40
22	BA	219	A	C5-C6-N1	6.30	120.85	117.70
22	BA	1515	A	N9-C4-C5	6.30	108.32	105.80
1	AA	451	A	C4-C5-C6	6.30	120.15	117.00
1	AA	1004	A	C4-C5-C6	6.30	120.15	117.00
22	BA	44	A	N3-C4-N9	6.30	132.44	127.40
22	BA	1302	A	C8-N9-C4	6.30	108.32	105.80
22	BA	1791	A	C4-C5-C6	6.30	120.15	117.00
1	AA	74	A	N9-C4-C5	6.30	108.32	105.80
22	BA	1953	A	C4-C5-C6	6.30	120.15	117.00
1	AA	338	A	N3-C4-N9	6.30	132.44	127.40
1	AA	640	A	C4-C5-C6	6.30	120.15	117.00
1	AA	914	A	N3-C4-N9	6.30	132.44	127.40
22	BA	42	A	C8-N9-C4	6.30	108.32	105.80
22	BA	996	A	N3-C4-N9	6.30	132.44	127.40
22	BA	1669	A	N9-C4-C5	6.30	108.32	105.80
22	BA	1932	A	C5-C6-N1	6.30	120.85	117.70
23	BB	39	A	N3-C4-N9	6.30	132.44	127.40
1	AA	1257	A	C8-N9-C4	6.29	108.32	105.80
22	BA	2037	A	C5-N7-C8	6.29	107.05	103.90
22	BA	2198	A	C8-N9-C4	6.29	108.32	105.80
22	BA	2706	A	C5-N7-C8	6.29	107.05	103.90
1	AA	262	A	N3-C4-N9	6.29	132.44	127.40
1	AA	1306	A	N3-C4-N9	6.29	132.44	127.40
22	BA	131	A	C5-N7-C8	6.29	107.05	103.90
22	BA	925	A	N3-C4-N9	6.29	132.43	127.40
22	BA	1133	A	C4-C5-C6	6.29	120.15	117.00
1	AA	373	A	C8-N9-C4	6.29	108.32	105.80
1	AA	923	A	C5-C6-N1	6.29	120.85	117.70
1	AA	1252	A	C4-C5-C6	6.29	120.14	117.00
22	BA	262	A	C8-N9-C4	6.29	108.32	105.80
22	BA	1634	A	N3-C4-N9	6.29	132.43	127.40
51	B3	32	ILE	CG1-CB-CG2	-6.29	97.56	111.40
55	B8	76	A	C4-C5-C6	6.29	120.14	117.00
1	AA	1044	A	C5-C6-N1	6.29	120.84	117.70
1	AA	1480	A	N9-C4-C5	6.29	108.31	105.80
22	BA	2052	A	C4-C5-C6	6.29	120.14	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2449	U	C5-C4-O4	-6.29	122.13	125.90
23	BB	53	A	N3-C4-N9	6.29	132.43	127.40
1	AA	431	A	C4-C5-N7	-6.29	107.56	110.70
1	AA	969	A	N3-C4-N9	6.29	132.43	127.40
22	BA	1545	A	C5-N7-C8	6.29	107.04	103.90
1	AA	238	A	C8-N9-C4	6.29	108.31	105.80
22	BA	282	A	C4-C5-C6	6.29	120.14	117.00
22	BA	743	A	C4-C5-C6	6.29	120.14	117.00
22	BA	1960	A	C5-C6-N1	6.29	120.84	117.70
22	BA	2778	A	N9-C4-C5	6.29	108.31	105.80
55	B8	21	A	C4-C5-C6	6.29	120.14	117.00
1	AA	802	A	C4-C5-C6	6.28	120.14	117.00
1	AA	1191	A	C8-N9-C4	6.28	108.31	105.80
22	BA	1073	A	N3-C4-N9	6.28	132.43	127.40
1	AA	1333	A	N9-C4-C5	6.28	108.31	105.80
22	BA	44	A	C4-C5-C6	6.28	120.14	117.00
22	BA	1552	A	N3-C4-N9	6.28	132.43	127.40
22	BA	1815	A	C5-C6-N1	6.28	120.84	117.70
1	AA	10	A	C4-C5-C6	6.28	120.14	117.00
1	AA	151	A	C4-C5-C6	6.28	120.14	117.00
22	BA	844	A	N3-C4-N9	6.28	132.42	127.40
22	BA	1936	A	C5-C6-N1	6.28	120.84	117.70
22	BA	877	A	C8-N9-C4	6.28	108.31	105.80
1	AA	600	A	C8-N9-C4	6.28	108.31	105.80
1	AA	1055	A	N3-C4-N9	6.28	132.42	127.40
1	AA	1171	A	C5-C6-N1	6.28	120.84	117.70
22	BA	14	A	N3-C4-N9	6.28	132.42	127.40
22	BA	53	A	N9-C4-C5	6.28	108.31	105.80
22	BA	199	A	N9-C4-C5	6.28	108.31	105.80
22	BA	453	A	N3-C4-N9	6.28	132.42	127.40
22	BA	1027	A	C4-C5-C6	6.28	120.14	117.00
22	BA	1700	A	C8-N9-C4	6.28	108.31	105.80
1	AA	382	A	N3-C4-N9	6.28	132.42	127.40
1	AA	1151	A	N3-C4-N9	6.28	132.42	127.40
22	BA	95	A	C4-C5-C6	6.28	120.14	117.00
22	BA	1378	A	C4-C5-N7	-6.28	107.56	110.70
1	AA	559	A	C4-C5-C6	6.27	120.14	117.00
1	AA	959	A	N3-C4-N9	6.27	132.42	127.40
22	BA	626	A	C4-C5-C6	6.27	120.14	117.00
1	AA	1256	A	C4-C5-C6	6.27	120.14	117.00
22	BA	1504	A	N3-C4-N9	6.27	132.42	127.40
22	BA	947	A	C5-C6-N1	6.27	120.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1545	A	N9-C4-C5	6.27	108.31	105.80
22	BA	2077	A	C5-C6-N1	6.27	120.83	117.70
22	BA	2882	A	N9-C4-C5	6.27	108.31	105.80
22	BA	2900	A	N9-C4-C5	6.27	108.31	105.80
22	BA	311	A	C4-C5-C6	6.27	120.13	117.00
1	AA	1306	A	C4-C5-C6	6.27	120.13	117.00
1	AA	1456	A	N3-C4-N9	6.27	132.41	127.40
1	AA	131	A	N3-C4-N9	6.26	132.41	127.40
1	AA	559	A	N3-C4-N9	6.26	132.41	127.40
1	AA	729	A	N3-C4-N9	6.26	132.41	127.40
22	BA	156	A	C8-N9-C4	6.26	108.31	105.80
22	BA	2080	A	C4-C5-C6	6.26	120.13	117.00
22	BA	2727	A	C5-N7-C8	6.26	107.03	103.90
1	AA	635	A	N3-C4-N9	6.26	132.41	127.40
1	AA	935	A	C4-C5-C6	6.26	120.13	117.00
22	BA	2317	A	C5-C6-N1	6.26	120.83	117.70
22	BA	2705	A	C4-C5-C6	6.26	120.13	117.00
22	BA	1783	A	C8-N9-C4	6.26	108.31	105.80
22	BA	2635	A	N9-C4-C5	6.26	108.31	105.80
1	AA	65	A	C4-C5-C6	6.26	120.13	117.00
1	AA	629	A	C4-C5-C6	6.26	120.13	117.00
22	BA	910	A	C4-C5-C6	6.26	120.13	117.00
22	BA	2868	A	N3-C4-N9	6.26	132.41	127.40
1	AA	1437	A	C8-N9-C4	6.26	108.30	105.80
22	BA	556	A	C5-N7-C8	6.26	107.03	103.90
1	AA	629	A	N3-C4-N9	6.26	132.41	127.40
1	AA	975	A	C8-N9-C4	6.26	108.30	105.80
22	BA	197	A	C5-C6-N1	6.26	120.83	117.70
22	BA	453	A	N9-C4-C5	6.26	108.30	105.80
22	BA	1284	A	C4-C5-C6	6.26	120.13	117.00
22	BA	1745	A	C4-C5-C6	6.26	120.13	117.00
22	BA	2682	A	C8-N9-C4	6.26	108.30	105.80
22	BA	2837	A	N9-C4-C5	6.26	108.30	105.80
22	BA	633	A	C8-N9-C4	6.25	108.30	105.80
22	BA	2733	A	C4-C5-C6	6.25	120.13	117.00
22	BA	2792	A	C4-C5-C6	6.25	120.13	117.00
22	BA	165	A	C4-C5-N7	-6.25	107.57	110.70
22	BA	1156	A	C8-N9-C4	6.25	108.30	105.80
22	BA	643	A	C4-C5-C6	6.25	120.13	117.00
22	BA	1347	A	C4-C5-C6	6.25	120.12	117.00
1	AA	363	A	C4-C5-C6	6.25	120.12	117.00
1	AA	1340	A	C4-C5-C6	6.25	120.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	735	A	N3-C4-N9	6.25	132.40	127.40
22	BA	1711	A	C4-C5-C6	6.25	120.12	117.00
22	BA	2435	A	C4-C5-N7	-6.25	107.58	110.70
1	AA	1036	A	C4-C5-C6	6.25	120.12	117.00
22	BA	5	A	N3-C4-N9	6.25	132.40	127.40
22	BA	126	A	C5-C6-N1	6.25	120.82	117.70
22	BA	2225	A	C4-C5-C6	6.25	120.12	117.00
1	AA	119	A	C4-C5-N7	-6.25	107.58	110.70
1	AA	553	A	C4-C5-C6	6.25	120.12	117.00
1	AA	1357	A	N9-C4-C5	6.25	108.30	105.80
22	BA	262	A	N9-C4-C5	6.25	108.30	105.80
22	BA	2748	A	C5-N7-C8	6.25	107.02	103.90
1	AA	681	A	C4-C5-C6	6.24	120.12	117.00
1	AA	729	A	C4-C5-N7	-6.24	107.58	110.70
1	AA	1248	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1890	A	C5-C6-N1	6.24	120.82	117.70
22	BA	2453	A	C4-C5-N7	-6.24	107.58	110.70
1	AA	728	A	C4-C5-C6	6.24	120.12	117.00
22	BA	231	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1089	A	C4-C5-C6	6.24	120.12	117.00
1	AA	77	A	C4-C5-C6	6.24	120.12	117.00
22	BA	172	A	N3-C4-N9	6.24	132.39	127.40
22	BA	1260	A	C8-N9-C4	6.24	108.30	105.80
22	BA	2051	A	C4-C5-C6	6.24	120.12	117.00
1	AA	1433	A	N3-C4-N9	6.24	132.39	127.40
1	AA	1499	A	N3-C4-N9	6.24	132.39	127.40
22	BA	666	A	C8-N9-C4	6.24	108.30	105.80
22	BA	945	A	N9-C4-C5	6.24	108.30	105.80
22	BA	255	A	C5-N7-C8	6.24	107.02	103.90
22	BA	300	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1809	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1890	A	C8-N9-C4	6.24	108.29	105.80
22	BA	1073	A	C8-N9-C4	6.23	108.29	105.80
22	BA	1265	A	C5-N7-C8	6.23	107.02	103.90
22	BA	2893	A	N3-C4-N9	6.23	132.39	127.40
1	AA	1476	A	C4-C5-C6	6.23	120.12	117.00
22	BA	374	A	C5-C6-N1	6.23	120.82	117.70
22	BA	2080	A	C5-C6-N1	6.23	120.82	117.70
22	BA	2810	A	N9-C4-C5	6.23	108.29	105.80
55	B8	38	A	N3-C4-N9	6.23	132.39	127.40
1	AA	1225	A	C5-C6-N1	6.23	120.81	117.70
22	BA	443	A	C5-C6-N1	6.23	120.82	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	522	A	C5-C6-N1	6.23	120.81	117.70
23	BB	101	A	C4-C5-N7	-6.23	107.58	110.70
55	B8	6	A	C4-C5-C6	6.23	120.11	117.00
1	AA	263	A	C8-N9-C4	6.23	108.29	105.80
1	AA	747	A	C4-C5-N7	-6.23	107.59	110.70
1	AA	1250	A	N9-C4-C5	6.23	108.29	105.80
1	AA	1110	A	N3-C4-N9	6.23	132.38	127.40
1	AA	1431	A	C8-N9-C4	6.23	108.29	105.80
22	BA	167	A	C8-N9-C4	6.23	108.29	105.80
22	BA	1552	A	C8-N9-C4	6.23	108.29	105.80
22	BA	2868	A	C5-N7-C8	6.23	107.01	103.90
22	BA	2899	A	C4-C5-C6	6.23	120.11	117.00
1	AA	781	A	C8-N9-C4	6.23	108.29	105.80
22	BA	933	A	C5-C6-N1	6.23	120.81	117.70
22	BA	1876	A	N3-C4-N9	6.23	132.38	127.40
1	AA	167	A	N9-C4-C5	6.22	108.29	105.80
55	B8	38	A	N9-C4-C5	6.22	108.29	105.80
1	AA	642	A	N9-C4-C5	6.22	108.29	105.80
1	AA	1216	A	N9-C4-C5	6.22	108.29	105.80
22	BA	161	A	C4-C5-N7	-6.22	107.59	110.70
22	BA	1276	A	N9-C4-C5	6.22	108.29	105.80
22	BA	1630	A	N3-C4-N9	6.22	132.38	127.40
22	BA	2126	A	C4-C5-C6	6.22	120.11	117.00
22	BA	2241	A	N3-C4-N9	6.22	132.38	127.40
1	AA	199	A	C4-C5-C6	6.22	120.11	117.00
22	BA	340	A	N3-C4-N9	6.22	132.38	127.40
1	AA	59	A	N3-C4-N9	6.22	132.38	127.40
1	AA	1204	A	C4-C5-C6	6.22	120.11	117.00
22	BA	181	A	N9-C4-C5	6.22	108.29	105.80
22	BA	2327	A	C4-C5-C6	6.22	120.11	117.00
22	BA	526	A	C4-C5-N7	-6.22	107.59	110.70
1	AA	675	A	N3-C4-N9	6.22	132.37	127.40
1	AA	1433	A	C5-C6-N1	6.22	120.81	117.70
22	BA	586	A	C4-C5-C6	6.22	120.11	117.00
22	BA	2281	A	N3-C4-N9	6.22	132.37	127.40
22	BA	2336	A	C4-C5-C6	6.22	120.11	117.00
1	AA	1377	A	N3-C4-N9	6.21	132.37	127.40
1	AA	1447	A	C4-C5-C6	6.21	120.11	117.00
22	BA	320	A	C4-C5-C6	6.21	120.11	117.00
22	BA	582	A	C8-N9-C4	6.21	108.28	105.80
22	BA	2411	A	C8-N9-C4	6.21	108.29	105.80
1	AA	1246	A	C8-N9-C4	6.21	108.28	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	959	A	N3-C4-N9	6.21	132.37	127.40
22	BA	1819	A	C8-N9-C4	6.21	108.28	105.80
1	AA	1169	A	C4-C5-C6	6.21	120.11	117.00
22	BA	144	A	N3-C4-N9	6.21	132.37	127.40
22	BA	262	A	C4-C5-C6	6.21	120.11	117.00
22	BA	532	A	C5-C6-N1	6.21	120.81	117.70
22	BA	722	A	C4-C5-C6	6.21	120.11	117.00
22	BA	1772	A	C5-C6-N1	6.21	120.81	117.70
22	BA	1809	A	N3-C4-N9	6.21	132.37	127.40
22	BA	1848	A	N3-C4-N9	6.21	132.37	127.40
22	BA	528	A	N3-C4-N9	6.21	132.37	127.40
22	BA	1393	A	C8-N9-C4	6.21	108.28	105.80
22	BA	2020	A	C5-C6-N1	6.21	120.80	117.70
22	BA	2587	A	N3-C4-N9	6.21	132.37	127.40
22	BA	2634	A	C5-C6-N1	6.21	120.80	117.70
1	AA	263	A	C4-C5-C6	6.21	120.10	117.00
22	BA	152	A	C5-C6-N1	6.21	120.80	117.70
22	BA	300	A	C8-N9-C4	6.21	108.28	105.80
22	BA	727	A	N3-C4-N9	6.21	132.37	127.40
22	BA	1322	A	N3-C4-N9	6.21	132.37	127.40
22	BA	2198	A	N3-C4-N9	6.21	132.37	127.40
22	BA	920	A	C4-C5-C6	6.21	120.10	117.00
1	AA	918	A	N9-C4-C5	6.20	108.28	105.80
22	BA	538	A	N3-C4-N9	6.20	132.36	127.40
22	BA	1802	A	C5-N7-C8	6.20	107.00	103.90
23	BB	53	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1513	A	C5-C6-N1	6.20	120.80	117.70
22	BA	1853	A	N3-C4-N9	6.20	132.36	127.40
22	BA	2868	A	C4-C5-C6	6.20	120.10	117.00
1	AA	609	A	C4-C5-C6	6.20	120.10	117.00
22	BA	311	A	N9-C4-C5	6.20	108.28	105.80
22	BA	2003	A	N3-C4-N9	6.20	132.36	127.40
22	BA	2706	A	N9-C4-C5	6.20	108.28	105.80
23	BB	109	A	C4-C5-C6	6.20	120.10	117.00
1	AA	223	A	C4-C5-C6	6.20	120.10	117.00
1	AA	845	A	C4-C5-C6	6.20	120.10	117.00
1	AA	1150	A	C4-C5-N7	-6.20	107.60	110.70
22	BA	933	A	C4-C5-C6	6.20	120.10	117.00
22	BA	1668	A	C8-N9-C4	6.20	108.28	105.80
1	AA	949	A	N9-C4-C5	6.19	108.28	105.80
22	BA	1664	A	C5-C6-N1	6.19	120.80	117.70
1	AA	282	A	N3-C4-N9	6.19	132.35	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1176	A	C4-C5-C6	6.19	120.10	117.00
1	AA	1360	A	C8-N9-C4	6.19	108.28	105.80
22	BA	751	A	N3-C4-N9	6.19	132.35	127.40
23	BB	45	A	C4-C5-C6	6.19	120.10	117.00
1	AA	487	A	C4-C5-C6	6.19	120.10	117.00
22	BA	1610	A	C4-C5-C6	6.19	120.09	117.00
22	BA	2311	A	C4-C5-C6	6.19	120.09	117.00
22	BA	2411	A	C4-C5-C6	6.19	120.09	117.00
22	BA	2764	A	N9-C4-C5	6.19	108.28	105.80
55	B8	14	A	N3-C4-N9	6.19	132.35	127.40
1	AA	759	A	N3-C4-N9	6.19	132.35	127.40
22	BA	144	A	C4-C5-C6	6.19	120.09	117.00
22	BA	1583	A	N9-C4-C5	6.19	108.28	105.80
22	BA	1866	A	N3-C4-N9	6.19	132.35	127.40
22	BA	590	A	N3-C4-N9	6.18	132.35	127.40
22	BA	2614	A	C5-N7-C8	6.18	106.99	103.90
22	BA	2781	A	N3-C4-N9	6.18	132.35	127.40
22	BA	654	A	C4-C5-C6	6.18	120.09	117.00
22	BA	792	A	N9-C4-C5	6.18	108.27	105.80
22	BA	1634	A	C8-N9-C4	6.18	108.27	105.80
22	BA	2632	A	C4-C5-C6	6.18	120.09	117.00
1	AA	600	A	N3-C4-N9	6.18	132.34	127.40
1	AA	676	A	C8-N9-C4	6.18	108.27	105.80
1	AA	749	A	N3-C4-N9	6.18	132.34	127.40
22	BA	936	A	N3-C4-N9	6.18	132.34	127.40
22	BA	1586	A	N3-C4-N9	6.18	132.34	127.40
22	BA	2386	A	C4-C5-C6	6.18	120.09	117.00
22	BA	845	A	C4-C5-C6	6.18	120.09	117.00
22	BA	1591	A	C8-N9-C4	6.18	108.27	105.80
1	AA	1513	A	C4-C5-C6	6.18	120.09	117.00
22	BA	199	A	N3-C4-N9	6.18	132.34	127.40
22	BA	526	A	N9-C4-C5	6.18	108.27	105.80
22	BA	781	A	N9-C4-C5	6.18	108.27	105.80
22	BA	1307	A	C5-C6-N1	6.18	120.79	117.70
22	BA	1821	A	C4-C5-C6	6.18	120.09	117.00
22	BA	2042	A	N9-C4-C5	6.18	108.27	105.80
22	BA	2725	A	C4-C5-C6	6.18	120.09	117.00
1	AA	825	A	C8-N9-C4	6.17	108.27	105.80
22	BA	1672	A	C5-N7-C8	6.17	106.99	103.90
1	AA	452	A	N3-C4-N9	6.17	132.34	127.40
1	AA	635	A	C8-N9-C4	6.17	108.27	105.80
22	BA	1165	A	C5-C6-N1	6.17	120.79	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1503	A	C4-C5-C6	6.17	120.09	117.00
22	BA	1609	A	C4-C5-C6	6.17	120.09	117.00
22	BA	2377	A	C4-C5-C6	6.17	120.09	117.00
1	AA	1150	A	C4-C5-C6	6.17	120.09	117.00
22	BA	1103	A	N3-C4-N9	6.17	132.34	127.40
22	BA	1641	A	N9-C4-C5	6.17	108.27	105.80
22	BA	1952	A	N3-C4-N9	6.17	132.34	127.40
22	BA	2829	A	C4-C5-N7	-6.17	107.61	110.70
22	BA	1701	A	N9-C4-C5	6.17	108.27	105.80
1	AA	602	A	C4-C5-C6	6.17	120.08	117.00
1	AA	1016	A	C4-C5-C6	6.17	120.08	117.00
1	AA	1274	A	C4-C5-C6	6.17	120.08	117.00
1	AA	1507	A	N3-C4-N9	6.17	132.34	127.40
22	BA	2516	A	N9-C4-C5	6.17	108.27	105.80
1	AA	101	A	C5-C6-N1	6.17	120.78	117.70
1	AA	554	A	C8-N9-C4	6.17	108.27	105.80
1	AA	1042	A	N3-C4-N9	6.17	132.33	127.40
22	BA	282	A	C8-N9-C4	6.17	108.27	105.80
22	BA	2738	A	C4-C5-C6	6.17	120.08	117.00
22	BA	2766	A	C8-N9-C4	6.17	108.27	105.80
1	AA	767	A	N3-C4-N9	6.17	132.33	127.40
22	BA	721	A	N3-C4-N9	6.17	132.33	127.40
22	BA	1970	A	C8-N9-C4	6.17	108.27	105.80
22	BA	807	U	N1-C2-N3	6.16	118.60	114.90
22	BA	2060	A	C8-N9-C4	6.16	108.27	105.80
55	B8	73	A	N3-C4-N9	6.16	132.33	127.40
1	AA	116	A	C5-C6-N1	6.16	120.78	117.70
1	AA	523	A	C4-C5-C6	6.16	120.08	117.00
1	AA	546	A	C8-N9-C4	6.16	108.26	105.80
22	BA	28	A	C4-C5-N7	-6.16	107.62	110.70
22	BA	1502	A	C8-N9-C4	6.16	108.26	105.80
22	BA	2602	A	C4-C5-N7	-6.16	107.62	110.70
1	AA	171	A	C8-N9-C4	6.16	108.26	105.80
1	AA	288	A	C4-C5-C6	6.16	120.08	117.00
1	AA	1180	A	N3-C4-N9	6.16	132.33	127.40
22	BA	572	A	C5-N7-C8	6.16	106.98	103.90
23	BB	108	A	C5-C6-N1	6.16	120.78	117.70
22	BA	182	A	N3-C4-N9	6.16	132.32	127.40
22	BA	2005	A	C4-C5-C6	6.16	120.08	117.00
22	BA	2311	A	N3-C4-N9	6.16	132.32	127.40
22	BA	2386	A	C5-C6-N1	6.16	120.78	117.70
1	AA	1289	A	C8-N9-C4	6.15	108.26	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	802	A	N3-C4-N9	6.15	132.32	127.40
22	BA	6	A	C5-C6-N1	6.15	120.78	117.70
22	BA	1155	A	C4-C5-C6	6.15	120.08	117.00
22	BA	2705	A	N3-C4-N9	6.15	132.32	127.40
1	AA	583	A	N3-C4-N9	6.15	132.32	127.40
22	BA	1366	A	C5-N7-C8	6.15	106.97	103.90
22	BA	1572	A	C4-C5-C6	6.15	120.08	117.00
22	BA	2590	A	C4-C5-C6	6.15	120.07	117.00
23	BB	78	A	C8-N9-C4	6.15	108.26	105.80
1	AA	1016	A	N3-C4-N9	6.15	132.32	127.40
22	BA	347	A	N3-C4-N9	6.15	132.32	127.40
22	BA	699	A	N9-C4-C5	6.15	108.26	105.80
22	BA	1169	A	C5-C6-N1	6.15	120.77	117.70
22	BA	2108	A	N3-C4-N9	6.15	132.32	127.40
22	BA	1504	A	C4-C5-C6	6.15	120.07	117.00
22	BA	802	A	N3-C4-N9	6.14	132.32	127.40
22	BA	2163	A	C4-C5-C6	6.14	120.07	117.00
1	AA	344	A	C8-N9-C4	6.14	108.26	105.80
22	BA	310	A	C4-C5-C6	6.14	120.07	117.00
22	BA	1077	A	C8-N9-C4	6.14	108.26	105.80
22	BA	2031	A	N3-C4-N9	6.14	132.31	127.40
23	BB	115	A	C4-C5-C6	6.14	120.07	117.00
1	AA	288	A	C4-C5-N7	-6.14	107.63	110.70
22	BA	575	A	C4-C5-N7	-6.14	107.63	110.70
1	AA	366	A	N3-C4-N9	6.14	132.31	127.40
22	BA	522	A	N3-C4-N9	6.14	132.31	127.40
22	BA	981	A	C5-N7-C8	6.14	106.97	103.90
22	BA	1544	A	N3-C4-N9	6.14	132.31	127.40
1	AA	510	A	C8-N9-C4	6.14	108.25	105.80
1	AA	1311	A	N3-C4-N9	6.14	132.31	127.40
22	BA	1365	A	C8-N9-C4	6.14	108.25	105.80
1	AA	50	A	C4-C5-C6	6.14	120.07	117.00
1	AA	1179	A	C4-C5-N7	-6.14	107.63	110.70
22	BA	256	A	N3-C4-N9	6.14	132.31	127.40
22	BA	422	A	C4-C5-C6	6.14	120.07	117.00
22	BA	727	A	C5-N7-C8	6.14	106.97	103.90
22	BA	1144	A	C5-C6-N1	6.14	120.77	117.70
22	BA	1544	A	C5-C6-N1	6.14	120.77	117.70
22	BA	1630	A	C4-C5-C6	6.14	120.07	117.00
22	BA	1805	A	C5-C6-N1	6.14	120.77	117.70
22	BA	2288	A	N3-C4-N9	6.14	132.31	127.40
1	AA	228	A	C4-C5-C6	6.13	120.07	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	478	A	N3-C4-N9	6.13	132.31	127.40
1	AA	878	A	C4-C5-C6	6.13	120.07	117.00
1	AA	1229	A	C4-C5-N7	-6.13	107.63	110.70
22	BA	155	A	N3-C4-N9	6.13	132.31	127.40
22	BA	522	A	C4-C5-C6	6.13	120.07	117.00
22	BA	933	A	N3-C4-N9	6.13	132.31	127.40
22	BA	1494	A	N3-C4-N9	6.13	132.31	127.40
22	BA	1668	A	N9-C4-C5	6.13	108.25	105.80
22	BA	1998	A	N9-C4-C5	6.13	108.25	105.80
1	AA	1219	A	C5-C6-N1	6.13	120.77	117.70
1	AA	1434	A	C8-N9-C4	6.13	108.25	105.80
22	BA	176	A	C8-N9-C4	6.13	108.25	105.80
22	BA	668	A	N9-C4-C5	6.13	108.25	105.80
22	BA	727	A	C8-N9-C4	6.13	108.25	105.80
22	BA	984	A	C5-C6-N1	6.13	120.77	117.70
22	BA	1272	A	C8-N9-C4	6.13	108.25	105.80
22	BA	2126	A	N3-C4-N9	6.13	132.31	127.40
22	BA	2634	A	N9-C4-C5	6.13	108.25	105.80
1	AA	26	A	C5-C6-N1	6.13	120.77	117.70
1	AA	996	A	N9-C4-C5	6.13	108.25	105.80
22	BA	979	A	C5-C6-N1	6.13	120.77	117.70
22	BA	2388	A	N9-C4-C5	6.13	108.25	105.80
22	BA	2809	A	C4-C5-C6	6.13	120.06	117.00
1	AA	325	A	N3-C4-N9	6.13	132.30	127.40
1	AA	1225	A	C4-C5-C6	6.13	120.06	117.00
22	BA	345	A	N3-C4-N9	6.13	132.30	127.40
22	BA	748	G	O4'-C1'-N9	6.13	113.10	108.20
22	BA	863	A	C8-N9-C4	6.13	108.25	105.80
1	AA	74	A	C4-C5-C6	6.13	120.06	117.00
22	BA	1048	A	C8-N9-C4	6.13	108.25	105.80
22	BA	1084	A	C4-C5-C6	6.13	120.06	117.00
22	BA	1246	A	C4-C5-C6	6.12	120.06	117.00
22	BA	176	A	C5-C6-N1	6.12	120.76	117.70
22	BA	1803	A	C5-C6-N1	6.12	120.76	117.70
22	BA	2740	A	C4-C5-C6	6.12	120.06	117.00
1	AA	80	A	N3-C4-N9	6.12	132.30	127.40
22	BA	933	A	N9-C4-C5	6.12	108.25	105.80
22	BA	996	A	C8-N9-C4	6.12	108.25	105.80
22	BA	1977	A	N3-C4-N9	6.12	132.30	127.40
1	AA	1318	A	C8-N9-C4	6.12	108.25	105.80
22	BA	655	A	N9-C4-C5	6.12	108.25	105.80
22	BA	21	A	C5-C6-N1	6.12	120.76	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	415	A	C4-C5-C6	6.12	120.06	117.00
22	BA	2560	A	N9-C4-C5	6.12	108.25	105.80
22	BA	2851	A	N9-C4-C5	6.12	108.25	105.80
1	AA	373	A	C4-C5-C6	6.12	120.06	117.00
22	BA	374	A	C4-C5-C6	6.12	120.06	117.00
22	BA	727	A	C4-C5-C6	6.12	120.06	117.00
22	BA	959	A	C5-N7-C8	6.12	106.96	103.90
1	AA	493	A	C8-N9-C4	6.12	108.25	105.80
22	BA	348	A	C8-N9-C4	6.12	108.25	105.80
22	BA	1700	A	C4-C5-N7	-6.12	107.64	110.70
22	BA	2733	A	N3-C4-N9	6.12	132.29	127.40
22	BA	2799	A	C8-N9-C4	6.12	108.25	105.80
1	AA	718	A	N3-C4-N9	6.11	132.29	127.40
1	AA	1350	A	N9-C4-C5	6.11	108.25	105.80
22	BA	1165	A	C4-C5-N7	-6.11	107.64	110.70
22	BA	1928	A	N9-C4-C5	6.11	108.25	105.80
22	BA	2019	A	C8-N9-C4	6.11	108.25	105.80
22	BA	1086	A	C4-C5-C6	6.11	120.06	117.00
22	BA	2199	A	N3-C4-N9	6.11	132.29	127.40
22	BA	2886	A	C4-C5-C6	6.11	120.06	117.00
1	AA	205	A	C8-N9-C4	6.11	108.25	105.80
1	AA	782	A	C8-N9-C4	6.11	108.25	105.80
1	AA	907	A	C8-N9-C4	6.11	108.25	105.80
22	BA	460	A	N3-C4-N9	6.11	132.29	127.40
22	BA	730	A	C5-C6-N1	6.11	120.75	117.70
22	BA	1918	A	C4-C5-C6	6.11	120.06	117.00
22	BA	677	A	C5-C6-N1	6.11	120.75	117.70
22	BA	1384	A	C4-C5-C6	6.11	120.06	117.00
22	BA	1791	A	N3-C4-N9	6.11	132.29	127.40
22	BA	103	A	N3-C4-N9	6.11	132.29	127.40
22	BA	244	A	C4-C5-C6	6.11	120.05	117.00
22	BA	1785	A	N9-C4-C5	6.11	108.24	105.80
22	BA	2518	A	C5-C6-N1	6.11	120.75	117.70
22	BA	2721	A	C5-C6-N1	6.11	120.75	117.70
22	BA	2809	A	N3-C4-N9	6.11	132.28	127.40
22	BA	2287	A	C4-C5-C6	6.11	120.05	117.00
22	BA	2741	A	N3-C4-N9	6.11	132.28	127.40
1	AA	535	A	N3-C4-N9	6.10	132.28	127.40
1	AA	546	A	N3-C4-N9	6.10	132.28	127.40
22	BA	586	A	N9-C4-C5	6.10	108.24	105.80
22	BA	2602	A	C8-N9-C4	6.10	108.24	105.80
22	BA	2682	A	N3-C4-N9	6.10	132.28	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	64	A	N9-C4-C5	6.10	108.24	105.80
1	AA	456	A	C4-C5-C6	6.10	120.05	117.00
1	AA	496	A	C5-N7-C8	6.10	106.95	103.90
1	AA	1507	A	N9-C4-C5	6.10	108.24	105.80
22	BA	309	A	C5-C6-N1	6.10	120.75	117.70
22	BA	1431	A	C5-C6-N1	6.10	120.75	117.70
22	BA	1590	A	C4-C5-C6	6.10	120.05	117.00
22	BA	1916	A	N3-C4-N9	6.10	132.28	127.40
22	BA	2309	A	C8-N9-C4	6.10	108.24	105.80
22	BA	1027	A	C5-N7-C8	6.10	106.95	103.90
22	BA	1269	A	N9-C4-C5	6.10	108.24	105.80
22	BA	2660	A	N9-C4-C5	6.10	108.24	105.80
1	AA	309	A	N9-C4-C5	6.10	108.24	105.80
1	AA	1000	A	C4-C5-C6	6.10	120.05	117.00
22	BA	2267	A	N9-C4-C5	6.10	108.24	105.80
22	BA	2322	A	C8-N9-C4	6.10	108.24	105.80
22	BA	2821	A	N3-C4-N9	6.10	132.28	127.40
1	AA	60	A	C4-C5-N7	-6.09	107.65	110.70
1	AA	1111	A	N3-C4-N9	6.09	132.28	127.40
1	AA	1157	A	C5-C6-N1	6.09	120.75	117.70
22	BA	172	A	C8-N9-C4	6.09	108.24	105.80
22	BA	621	A	N9-C4-C5	6.09	108.24	105.80
22	BA	1073	A	C4-C5-C6	6.09	120.05	117.00
23	BB	53	A	C8-N9-C4	6.09	108.24	105.80
22	BA	1244	A	N3-C4-N9	6.09	132.28	127.40
1	AA	621	A	C8-N9-C4	6.09	108.24	105.80
1	AA	648	A	N3-C4-N9	6.09	132.27	127.40
22	BA	1237	A	N9-C4-C5	6.09	108.24	105.80
22	BA	2274	A	N9-C4-C5	6.09	108.24	105.80
1	AA	1349	A	N9-C4-C5	6.09	108.24	105.80
22	BA	783	A	C4-C5-N7	-6.09	107.66	110.70
55	B8	51	A	N3-C4-N9	6.09	132.27	127.40
22	BA	1783	A	C4-C5-C6	6.09	120.04	117.00
22	BA	2711	A	N3-C4-N9	6.09	132.27	127.40
22	BA	2860	A	C8-N9-C4	6.09	108.23	105.80
1	AA	1428	A	N9-C4-C5	6.09	108.23	105.80
22	BA	574	A	C5-C6-N1	6.08	120.74	117.70
1	AA	66	A	N3-C4-N9	6.08	132.27	127.40
22	BA	21	A	C4-C5-C6	6.08	120.04	117.00
22	BA	1544	A	N9-C4-C5	6.08	108.23	105.80
22	BA	1801	A	C8-N9-C4	6.08	108.23	105.80
1	AA	2	A	C4-C5-C6	6.08	120.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	729	A	C4-C5-C6	6.08	120.04	117.00
1	AA	1413	A	N9-C4-C5	6.08	108.23	105.80
22	BA	609	A	C4-C5-C6	6.08	120.04	117.00
22	BA	1508	A	C8-N9-C4	6.08	108.23	105.80
22	BA	2212	A	N3-C4-N9	6.08	132.27	127.40
23	BB	45	A	N3-C4-N9	6.08	132.26	127.40
1	AA	336	A	C8-N9-C4	6.08	108.23	105.80
22	BA	382	A	N3-C4-N9	6.08	132.26	127.40
22	BA	1336	A	C5-C6-N1	6.08	120.74	117.70
1	AA	608	A	C8-N9-C4	6.08	108.23	105.80
1	AA	749	A	C4-C5-C6	6.08	120.04	117.00
22	BA	1010	A	C8-N9-C4	6.08	108.23	105.80
22	BA	2602	A	N9-C4-C5	6.08	108.23	105.80
1	AA	72	A	C8-N9-C4	6.08	108.23	105.80
1	AA	900	A	N3-C4-N9	6.08	132.26	127.40
1	AA	1093	A	N3-C4-N9	6.08	132.26	127.40
22	BA	603	A	C4-C5-N7	-6.08	107.66	110.70
22	BA	2632	A	C4-C5-N7	-6.08	107.66	110.70
22	BA	1111	A	C4-C5-N7	-6.08	107.66	110.70
22	BA	2670	A	N3-C4-N9	6.08	132.26	127.40
1	AA	129	A	N3-C4-N9	6.07	132.26	127.40
22	BA	231	A	N3-C4-N9	6.07	132.26	127.40
22	BA	896	A	C4-C5-N7	-6.07	107.66	110.70
22	BA	1095	A	C4-C5-C6	6.07	120.04	117.00
22	BA	1960	A	C4-C5-C6	6.07	120.04	117.00
22	BA	2071	A	N9-C4-C5	6.07	108.23	105.80
22	BA	2411	A	N3-C4-N9	6.07	132.26	127.40
22	BA	2657	A	C4-C5-C6	6.07	120.04	117.00
1	AA	864	A	N3-C4-N9	6.07	132.26	127.40
22	BA	2660	A	C8-N9-C4	6.07	108.23	105.80
1	AA	1346	A	N9-C4-C5	6.07	108.23	105.80
1	AA	1433	A	C4-C5-C6	6.07	120.03	117.00
22	BA	310	A	N9-C4-C5	6.07	108.23	105.80
22	BA	1147	A	C5-C6-N1	6.07	120.73	117.70
22	BA	2781	A	C5-N7-C8	6.07	106.94	103.90
22	BA	71	A	N3-C4-N9	6.07	132.25	127.40
22	BA	2005	A	N3-C4-N9	6.07	132.25	127.40
22	BA	2095	A	C8-N9-C4	6.07	108.23	105.80
22	BA	2639	A	C8-N9-C4	6.07	108.23	105.80
1	AA	26	A	C4-C5-C6	6.07	120.03	117.00
1	AA	1434	A	N3-C4-N9	6.07	132.25	127.40
22	BA	422	A	N3-C4-N9	6.07	132.25	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	563	A	N3-C4-N9	6.07	132.25	127.40
1	AA	435	A	C4-C5-C6	6.07	120.03	117.00
1	AA	579	A	C5-C6-N1	6.07	120.73	117.70
22	BA	204	A	C4-C5-C6	6.07	120.03	117.00
22	BA	1385	A	C4-C5-N7	-6.07	107.67	110.70
22	BA	161	A	C4-C5-C6	6.06	120.03	117.00
22	BA	1439	A	N9-C4-C5	6.06	108.23	105.80
22	BA	1757	A	N3-C4-N9	6.06	132.25	127.40
22	BA	2765	A	C5-C6-N1	6.06	120.73	117.70
22	BA	917	A	C8-N9-C4	6.06	108.22	105.80
23	BB	58	A	N3-C4-N9	6.06	132.25	127.40
1	AA	1431	A	C4-C5-C6	6.06	120.03	117.00
22	BA	1276	A	N3-C4-N9	6.06	132.25	127.40
22	BA	2019	A	N3-C4-N9	6.06	132.25	127.40
22	BA	2614	A	C4-C5-C6	6.06	120.03	117.00
22	BA	2837	A	C5-C6-N1	6.06	120.73	117.70
22	BA	1144	A	C4-C5-C6	6.06	120.03	117.00
22	BA	2378	A	C5-N7-C8	6.06	106.93	103.90
22	BA	2482	A	C4-C5-C6	6.06	120.03	117.00
22	BA	2800	A	C8-N9-C4	6.06	108.22	105.80
23	BB	75	G	N3-C4-C5	-6.06	125.57	128.60
22	BA	2820	A	C8-N9-C4	6.06	108.22	105.80
1	AA	706	A	C5-C6-N1	6.05	120.73	117.70
1	AA	1287	A	C4-C5-N7	-6.05	107.67	110.70
1	AA	1333	A	C4-C5-C6	6.05	120.03	117.00
22	BA	689	A	N3-C4-N9	6.05	132.24	127.40
22	BA	2059	A	C5-C6-N1	6.05	120.73	117.70
1	AA	130	A	C8-N9-C4	6.05	108.22	105.80
1	AA	574	A	N3-C4-N9	6.05	132.24	127.40
22	BA	1866	A	C8-N9-C4	6.05	108.22	105.80
1	AA	520	A	C4-C5-N7	-6.05	107.67	110.70
22	BA	1780	A	C4-C5-N7	-6.05	107.67	110.70
22	BA	1885	A	N3-C4-N9	6.05	132.24	127.40
22	BA	460	A	N9-C4-C5	6.05	108.22	105.80
22	BA	792	A	N3-C4-N9	6.05	132.24	127.40
22	BA	1246	A	N3-C4-N9	6.05	132.24	127.40
22	BA	1889	A	C4-C5-C6	6.05	120.03	117.00
22	BA	1522	A	C8-N9-C4	6.05	108.22	105.80
22	BA	2654	A	N9-C4-C5	6.05	108.22	105.80
23	BB	66	A	C5-N7-C8	6.05	106.92	103.90
1	AA	174	A	C4-C5-N7	-6.05	107.68	110.70
1	AA	270	A	C5-C6-N1	6.05	120.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	573	A	C4-C5-C6	6.05	120.02	117.00
22	BA	362	A	C4-C5-C6	6.05	120.02	117.00
22	BA	415	A	N3-C4-N9	6.05	132.24	127.40
22	BA	1603	A	N3-C4-N9	6.05	132.24	127.40
22	BA	1630	A	C4-C5-N7	-6.05	107.68	110.70
22	BA	2284	A	C5-C6-N1	6.05	120.72	117.70
22	BA	2513	A	N3-C4-N9	6.05	132.24	127.40
22	BA	2725	A	C5-C6-N1	6.05	120.72	117.70
23	BB	34	A	N9-C4-C5	6.05	108.22	105.80
1	AA	663	A	C4-C5-C6	6.04	120.02	117.00
22	BA	2639	A	C4-C5-C6	6.04	120.02	117.00
1	AA	496	A	N3-C4-N9	6.04	132.24	127.40
1	AA	640	A	C8-N9-C4	6.04	108.22	105.80
1	AA	728	A	N3-C4-N9	6.04	132.24	127.40
1	AA	1480	A	C4-C5-C6	6.04	120.02	117.00
22	BA	1549	A	C4-C5-C6	6.04	120.02	117.00
22	BA	1679	A	N3-C4-N9	6.04	132.23	127.40
22	BA	2660	A	C4-C5-N7	-6.04	107.68	110.70
1	AA	1101	A	C4-C5-C6	6.04	120.02	117.00
22	BA	478	A	C4-C5-C6	6.04	120.02	117.00
22	BA	1698	A	C4-C5-C6	6.04	120.02	117.00
22	BA	2851	A	C4-C5-N7	-6.04	107.68	110.70
1	AA	250	A	N3-C4-N9	6.04	132.23	127.40
1	AA	149	A	C4-C5-C6	6.04	120.02	117.00
22	BA	514	A	N3-C4-N9	6.04	132.23	127.40
22	BA	2765	A	C4-C5-C6	6.04	120.02	117.00
1	AA	279	A	N9-C4-C5	6.04	108.22	105.80
1	AA	389	A	N9-C4-C5	6.04	108.22	105.80
1	AA	694	A	N3-C4-N9	6.04	132.23	127.40
1	AA	978	A	C8-N9-C4	6.04	108.22	105.80
22	BA	1040	A	N3-C4-N9	6.04	132.23	127.40
1	AA	621	A	N3-C4-N9	6.04	132.23	127.40
1	AA	655	A	C5-C6-N1	6.04	120.72	117.70
22	BA	2311	A	N9-C4-C5	6.04	108.21	105.80
55	B8	66	A	N9-C4-C5	6.04	108.21	105.80
1	AA	642	A	C4-C5-N7	-6.03	107.68	110.70
1	AA	1534	A	C4-C5-N7	-6.03	107.68	110.70
22	BA	203	A	N3-C4-N9	6.03	132.23	127.40
22	BA	300	A	N3-C4-N9	6.03	132.23	127.40
22	BA	311	A	N3-C4-N9	6.03	132.23	127.40
22	BA	2297	A	C8-N9-C4	6.03	108.21	105.80
22	BA	2733	A	C4-C5-N7	-6.03	107.68	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	310	A	C5-C6-N1	6.03	120.72	117.70
22	BA	1354	A	C4-C5-C6	6.03	120.02	117.00
1	AA	172	A	C8-N9-C4	6.03	108.21	105.80
1	AA	532	A	C8-N9-C4	6.03	108.21	105.80
1	AA	1204	A	N3-C4-N9	6.03	132.22	127.40
22	BA	1635	A	N9-C4-C5	6.03	108.21	105.80
1	AA	1288	A	C5-C6-N1	6.03	120.71	117.70
22	BA	219	A	C4-C5-C6	6.03	120.01	117.00
22	BA	752	A	N3-C4-N9	6.03	132.22	127.40
22	BA	1284	A	C8-N9-C4	6.03	108.21	105.80
22	BA	1998	A	C5-C6-N1	6.03	120.71	117.70
1	AA	223	A	N3-C4-N9	6.03	132.22	127.40
1	AA	253	A	C4-C5-C6	6.03	120.01	117.00
1	AA	439	U	C2-N1-C1'	6.03	124.93	117.70
1	AA	918	A	C4-C5-N7	-6.03	107.69	110.70
1	AA	1151	A	C5-C6-N1	6.03	120.71	117.70
1	AA	1480	A	C4-C5-N7	-6.03	107.69	110.70
22	BA	111	A	C8-N9-C4	6.03	108.21	105.80
22	BA	716	A	N3-C4-N9	6.03	132.22	127.40
22	BA	1803	A	C4-C5-C6	6.03	120.01	117.00
22	BA	2639	A	N3-C4-N9	6.03	132.22	127.40
1	AA	878	A	N3-C4-N9	6.02	132.22	127.40
23	BB	109	A	C8-N9-C4	6.02	108.21	105.80
1	AA	366	A	N9-C4-C5	6.02	108.21	105.80
1	AA	608	A	N3-C4-N9	6.02	132.22	127.40
1	AA	1339	A	N3-C4-N9	6.02	132.22	127.40
1	AA	1340	A	N3-C4-N9	6.02	132.22	127.40
1	AA	1429	A	C4-C5-C6	6.02	120.01	117.00
22	BA	821	A	C4-C5-N7	-6.02	107.69	110.70
22	BA	1095	A	N3-C4-N9	6.02	132.22	127.40
22	BA	1304	A	C5-C6-N1	6.02	120.71	117.70
22	BA	1640	A	N9-C4-C5	6.02	108.21	105.80
22	BA	1901	A	N3-C4-N9	6.02	132.22	127.40
22	BA	721	A	C4-C5-C6	6.02	120.01	117.00
22	BA	928	A	N9-C4-C5	6.02	108.21	105.80
22	BA	1759	A	C5-N7-C8	6.02	106.91	103.90
22	BA	2134	A	C8-N9-C4	6.02	108.21	105.80
55	B8	41	A	N3-C4-N9	6.02	132.22	127.40
1	AA	889	A	C8-N9-C4	6.02	108.21	105.80
1	AA	729	A	C5-C6-N1	6.02	120.71	117.70
1	AA	155	A	C8-N9-C4	6.01	108.21	105.80
1	AA	715	A	C4-C5-C6	6.01	120.01	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	156	A	C5-C6-N1	6.01	120.71	117.70
22	BA	673	C	N1-C2-N3	6.01	123.41	119.20
22	BA	2448	A	C4-C5-N7	-6.01	107.69	110.70
22	BA	2516	A	C4-C5-C6	6.01	120.01	117.00
23	BB	94	A	N9-C4-C5	6.01	108.20	105.80
1	AA	1368	A	N3-C4-N9	6.01	132.21	127.40
1	AA	1531	A	C4-C5-C6	6.01	120.01	117.00
1	AA	607	A	N3-C4-N9	6.01	132.21	127.40
1	AA	1250	A	N3-C4-N9	6.01	132.21	127.40
22	BA	294	A	C8-N9-C4	6.01	108.20	105.80
22	BA	1626	A	C5-N7-C8	6.01	106.91	103.90
22	BA	1970	A	C4-C5-C6	6.01	120.00	117.00
22	BA	1981	A	N9-C4-C5	6.01	108.20	105.80
22	BA	2670	A	C4-C5-C6	6.01	120.00	117.00
1	AA	456	A	N3-C4-N9	6.01	132.21	127.40
22	BA	430	A	N3-C4-N9	6.01	132.21	127.40
22	BA	1308	A	N3-C4-N9	6.01	132.21	127.40
22	BA	1876	A	C4-C5-C6	6.01	120.00	117.00
23	BB	46	A	N3-C4-N9	6.01	132.21	127.40
1	AA	155	A	C4-C5-C6	6.01	120.00	117.00
1	AA	435	A	N3-C4-N9	6.01	132.21	127.40
1	AA	460	A	C4-C5-C6	6.01	120.00	117.00
1	AA	1248	A	N3-C4-N9	6.01	132.21	127.40
1	AA	327	A	C4-C5-C6	6.00	120.00	117.00
22	BA	1545	A	C4-C5-C6	6.00	120.00	117.00
22	BA	1572	A	C5-C6-N1	6.00	120.70	117.70
22	BA	1700	A	N3-C4-N9	6.00	132.20	127.40
1	AA	554	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1274	A	C8-N9-C4	6.00	108.20	105.80
22	BA	2158	A	C8-N9-C4	6.00	108.20	105.80
1	AA	78	A	C4-C5-C6	6.00	120.00	117.00
1	AA	1274	A	N3-C4-N9	6.00	132.20	127.40
22	BA	103	A	C8-N9-C4	6.00	108.20	105.80
22	BA	508	A	N3-C4-N9	6.00	132.20	127.40
22	BA	1508	A	C4-C5-C6	6.00	120.00	117.00
22	BA	2070	A	C4-C5-N7	-6.00	107.70	110.70
22	BA	508	A	C4-C5-C6	6.00	120.00	117.00
22	BA	322	A	C4-C5-N7	-6.00	107.70	110.70
22	BA	2170	A	N3-C4-N9	6.00	132.20	127.40
22	BA	2635	A	C4-C5-C6	6.00	120.00	117.00
22	BA	2706	A	N3-C4-N9	6.00	132.20	127.40
23	BB	34	A	C4-C5-C6	6.00	120.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	889	A	N9-C4-C5	6.00	108.20	105.80
22	BA	332	A	N9-C4-C5	6.00	108.20	105.80
22	BA	354	A	N3-C4-N9	6.00	132.20	127.40
22	BA	460	A	C5-C6-N1	6.00	120.70	117.70
22	BA	1253	A	C5-C6-N1	6.00	120.70	117.70
22	BA	2173	A	N3-C4-N9	6.00	132.20	127.40
22	BA	2448	A	N3-C4-N9	6.00	132.20	127.40
23	BB	34	A	C4-C5-N7	-6.00	107.70	110.70
22	BA	637	A	C5-C6-N1	6.00	120.70	117.70
1	AA	937	A	C8-N9-C4	5.99	108.20	105.80
1	AA	1261	A	N3-C4-N9	5.99	132.19	127.40
22	BA	38	A	C4-C5-C6	5.99	120.00	117.00
22	BA	146	A	C8-N9-C4	5.99	108.20	105.80
22	BA	2135	A	N3-C4-N9	5.99	132.20	127.40
22	BA	2447	G	N3-C4-C5	-5.99	125.60	128.60
1	AA	1394	A	N3-C4-N9	5.99	132.19	127.40
22	BA	1054	A	C8-N9-C4	5.99	108.20	105.80
22	BA	1080	A	C4-C5-N7	-5.99	107.70	110.70
22	BA	1502	A	C4-C5-C6	5.99	120.00	117.00
22	BA	1978	A	N3-C4-N9	5.99	132.19	127.40
1	AA	1157	A	C4-C5-C6	5.99	120.00	117.00
1	AA	1227	A	C5-N7-C8	5.99	106.89	103.90
22	BA	655	A	C8-N9-C4	5.99	108.20	105.80
22	BA	917	A	C4-C5-C6	5.99	120.00	117.00
22	BA	1640	A	N3-C4-N9	5.99	132.19	127.40
22	BA	2530	A	C4-C5-C6	5.99	120.00	117.00
1	AA	441	A	N3-C4-N9	5.99	132.19	127.40
1	AA	864	A	N9-C4-C5	5.99	108.20	105.80
1	AA	1021	A	N3-C4-N9	5.99	132.19	127.40
22	BA	374	A	C8-N9-C4	5.99	108.20	105.80
22	BA	609	A	N9-C4-C5	5.99	108.19	105.80
22	BA	675	A	C8-N9-C4	5.99	108.20	105.80
22	BA	1014	A	C4-C5-C6	5.99	119.99	117.00
22	BA	1858	A	C8-N9-C4	5.99	108.20	105.80
1	AA	192	A	C4-C5-N7	-5.99	107.71	110.70
1	AA	782	A	N3-C4-N9	5.99	132.19	127.40
1	AA	918	A	C4-C5-C6	5.99	119.99	117.00
22	BA	354	A	C8-N9-C4	5.99	108.19	105.80
22	BA	547	A	N3-C4-N9	5.99	132.19	127.40
22	BA	654	A	C8-N9-C4	5.99	108.19	105.80
22	BA	892	A	N9-C4-C5	5.99	108.19	105.80
22	BA	1890	A	C4-C5-C6	5.99	119.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	466	A	C4-C5-C6	5.99	119.99	117.00
1	AA	695	A	N9-C4-C5	5.99	108.19	105.80
1	AA	825	A	N9-C4-C5	5.99	108.19	105.80
1	AA	923	A	N9-C4-C5	5.99	108.19	105.80
22	BA	1067	A	C4-C5-C6	5.99	119.99	117.00
22	BA	1254	A	C4-C5-C6	5.99	119.99	117.00
1	AA	493	A	C4-C5-C6	5.98	119.99	117.00
1	AA	1250	A	C4-C5-C6	5.98	119.99	117.00
22	BA	1525	A	N9-C4-C5	5.98	108.19	105.80
22	BA	1535	A	N3-C4-N9	5.98	132.19	127.40
22	BA	1566	A	N3-C4-N9	5.98	132.19	127.40
22	BA	1978	A	C5-C6-N1	5.98	120.69	117.70
1	AA	495	A	C8-N9-C4	5.98	108.19	105.80
1	AA	573	A	N3-C4-N9	5.98	132.18	127.40
1	AA	915	A	N9-C4-C5	5.98	108.19	105.80
22	BA	1383	A	C8-N9-C4	5.98	108.19	105.80
22	BA	1353	A	C4-C5-C6	5.98	119.99	117.00
1	AA	28	A	C5-C6-N1	5.98	120.69	117.70
1	AA	130	A	N3-C4-N9	5.98	132.18	127.40
1	AA	961	U	C2-N3-C4	-5.98	123.41	127.00
1	AA	1410	A	N3-C4-N9	5.98	132.18	127.40
22	BA	332	A	C5-C6-N1	5.98	120.69	117.70
22	BA	1247	A	C5-C6-N1	5.98	120.69	117.70
22	BA	1276	A	C4-C5-N7	-5.98	107.71	110.70
22	BA	1367	A	N3-C4-N9	5.98	132.18	127.40
22	BA	1596	A	N3-C4-N9	5.98	132.18	127.40
1	AA	694	A	N9-C4-C5	5.98	108.19	105.80
1	AA	702	A	N3-C4-N9	5.98	132.18	127.40
1	AA	1102	A	N3-C4-N9	5.98	132.18	127.40
22	BA	699	A	C4-C5-N7	-5.98	107.71	110.70
1	AA	766	A	N3-C4-N9	5.97	132.18	127.40
1	AA	1180	A	C4-C5-C6	5.97	119.99	117.00
22	BA	975	A	C4-C5-C6	5.97	119.99	117.00
1	AA	274	A	C4-C5-C6	5.97	119.99	117.00
1	AA	1306	A	C8-N9-C4	5.97	108.19	105.80
22	BA	6	A	C8-N9-C4	5.97	108.19	105.80
22	BA	2020	A	N3-C4-N9	5.97	132.18	127.40
1	AA	520	A	N9-C4-C5	5.97	108.19	105.80
22	BA	2297	A	C4-C5-N7	-5.97	107.72	110.70
1	AA	1080	A	C4-C5-C6	5.97	119.98	117.00
22	BA	1070	A	N3-C4-N9	5.97	132.18	127.40
22	BA	1508	A	N3-C4-N9	5.97	132.18	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2778	A	N3-C4-N9	5.97	132.18	127.40
22	BA	2887	A	N3-C4-N9	5.97	132.18	127.40
22	BA	2778	A	C4-C5-N7	-5.97	107.72	110.70
1	AA	702	A	C4-C5-C6	5.97	119.98	117.00
1	AA	1004	A	C8-N9-C4	5.97	108.19	105.80
1	AA	1500	A	C4-C5-C6	5.97	119.98	117.00
22	BA	899	A	N3-C4-N9	5.97	132.17	127.40
1	AA	228	A	C8-N9-C4	5.96	108.19	105.80
1	AA	681	A	N3-C4-N9	5.96	132.17	127.40
1	AA	1150	A	N9-C4-C5	5.96	108.19	105.80
1	AA	1503	A	C4-C5-C6	5.96	119.98	117.00
1	AA	1531	A	N3-C4-N9	5.96	132.17	127.40
22	BA	262	A	C5-C6-N1	5.96	120.68	117.70
22	BA	1637	A	C5-C6-N1	5.96	120.68	117.70
22	BA	2565	A	C8-N9-C4	5.96	108.19	105.80
22	BA	2792	A	N3-C4-N9	5.96	132.17	127.40
22	BA	1819	A	C5-C6-N1	5.96	120.68	117.70
22	BA	2278	A	N9-C4-C5	5.96	108.19	105.80
1	AA	309	A	C8-N9-C4	5.96	108.19	105.80
22	BA	10	A	C8-N9-C4	5.96	108.18	105.80
22	BA	118	A	C4-C5-C6	5.96	119.98	117.00
22	BA	402	A	N3-C4-N9	5.96	132.17	127.40
22	BA	761	A	N3-C4-N9	5.96	132.17	127.40
22	BA	2227	A	C4-C5-N7	-5.96	107.72	110.70
23	BB	34	A	N3-C4-N9	5.96	132.17	127.40
1	AA	1434	A	C4-C5-N7	-5.96	107.72	110.70
22	BA	181	A	C4-C5-C6	5.96	119.98	117.00
22	BA	1981	A	C4-C5-N7	-5.96	107.72	110.70
1	AA	681	A	C8-N9-C4	5.96	108.18	105.80
1	AA	780	A	N9-C4-C5	5.96	108.18	105.80
22	BA	345	A	C4-C5-N7	-5.96	107.72	110.70
22	BA	861	A	N3-C4-N9	5.96	132.17	127.40
22	BA	1899	A	N9-C4-C5	5.96	108.18	105.80
22	BA	1928	A	C4-C5-C6	5.96	119.98	117.00
22	BA	2587	A	C4-C5-C6	5.96	119.98	117.00
1	AA	478	A	C4-C5-N7	-5.96	107.72	110.70
1	AA	978	A	N9-C4-C5	5.96	108.18	105.80
1	AA	1333	A	N3-C4-N9	5.96	132.17	127.40
1	AA	1362	A	C8-N9-C4	5.96	108.18	105.80
9	AI	54	LEU	CB-CG-CD2	-5.96	100.87	111.00
22	BA	483	A	N3-C4-N9	5.96	132.17	127.40
22	BA	984	A	N9-C4-C5	5.96	108.18	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1522	A	N9-C4-C5	5.96	108.18	105.80
22	BA	1889	A	N3-C4-N9	5.96	132.17	127.40
23	BB	104	A	N3-C4-N9	5.96	132.16	127.40
22	BA	2792	A	C5-C6-N1	5.96	120.68	117.70
1	AA	460	A	N3-C4-N9	5.95	132.16	127.40
1	AA	935	A	N3-C4-N9	5.95	132.16	127.40
22	BA	556	A	C5-C6-N1	5.95	120.68	117.70
22	BA	899	A	C4-C5-C6	5.95	119.98	117.00
22	BA	1275	A	N3-C4-N9	5.95	132.16	127.40
1	AA	364	A	N3-C4-N9	5.95	132.16	127.40
1	AA	1251	A	C4-C5-C6	5.95	119.98	117.00
22	BA	614	A	C4-C5-C6	5.95	119.98	117.00
22	BA	1237	A	C5-C6-N1	5.95	120.68	117.70
22	BA	2572	A	C8-N9-C4	5.95	108.18	105.80
55	B8	69	A	N9-C4-C5	5.95	108.18	105.80
1	AA	44	A	N3-C4-N9	5.95	132.16	127.40
1	AA	572	A	C4-C5-C6	5.95	119.97	117.00
1	AA	1287	A	N3-C4-N9	5.95	132.16	127.40
1	AA	1288	A	N3-C4-N9	5.95	132.16	127.40
22	BA	849	A	N3-C4-N9	5.95	132.16	127.40
22	BA	1308	A	C5-C6-N1	5.95	120.67	117.70
55	B8	21	A	N3-C4-N9	5.95	132.16	127.40
1	AA	466	A	N3-C4-N9	5.95	132.16	127.40
1	AA	687	A	C8-N9-C4	5.95	108.18	105.80
1	AA	1441	A	C8-N9-C4	5.95	108.18	105.80
22	BA	925	A	C4-C5-C6	5.95	119.97	117.00
22	BA	1434	A	C4-C5-C6	5.95	119.97	117.00
22	BA	2471	A	N3-C4-N9	5.95	132.16	127.40
22	BA	2482	A	N9-C4-C5	5.95	108.18	105.80
1	AA	996	A	C4-C5-C6	5.95	119.97	117.00
1	AA	1377	A	C8-N9-C4	5.95	108.18	105.80
1	AA	1503	A	N3-C4-N9	5.95	132.16	127.40
22	BA	156	A	C4-C5-C6	5.95	119.97	117.00
22	BA	927	A	C8-N9-C4	5.95	108.18	105.80
22	BA	1385	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1803	A	N3-C4-N9	5.94	132.16	127.40
22	BA	2900	A	C5-C6-N1	5.94	120.67	117.70
22	BA	196	A	C4-C5-N7	-5.94	107.73	110.70
22	BA	1900	A	N3-C4-N9	5.94	132.15	127.40
1	AA	236	A	N9-C4-C5	5.94	108.18	105.80
1	AA	1035	A	C4-C5-C6	5.94	119.97	117.00
1	AA	1280	A	C4-C5-C6	5.94	119.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1311	A	C4-C5-C6	5.94	119.97	117.00
22	BA	632	A	C5-C6-N1	5.94	120.67	117.70
22	BA	706	A	C8-N9-C4	5.94	108.18	105.80
22	BA	751	A	C5-N7-C8	5.94	106.87	103.90
22	BA	833	A	C8-N9-C4	5.94	108.18	105.80
22	BA	2800	A	C4-C5-C6	5.94	119.97	117.00
1	AA	3	A	C4-C5-C6	5.94	119.97	117.00
1	AA	792	A	C4-C5-N7	-5.94	107.73	110.70
22	BA	670	A	C5-C6-N1	5.94	120.67	117.70
22	BA	1020	A	C8-N9-C4	5.94	108.18	105.80
22	BA	1505	A	C5-C6-N1	5.94	120.67	117.70
1	AA	816	A	N3-C4-N9	5.94	132.15	127.40
22	BA	515	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1952	A	C8-N9-C4	5.94	108.17	105.80
1	AA	298	A	N3-C4-N9	5.94	132.15	127.40
1	AA	872	A	C5-C6-N1	5.94	120.67	117.70
22	BA	324	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1353	A	N3-C4-N9	5.94	132.15	127.40
22	BA	1359	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1067	A	N3-C4-N9	5.93	132.15	127.40
22	BA	1548	A	N3-C4-N9	5.93	132.15	127.40
22	BA	1590	A	N3-C4-N9	5.93	132.15	127.40
22	BA	2826	A	C5-C6-N1	5.93	120.67	117.70
1	AA	325	A	C8-N9-C4	5.93	108.17	105.80
1	AA	1042	A	C4-C5-N7	-5.93	107.73	110.70
22	BA	972	A	N9-C4-C5	5.93	108.17	105.80
22	BA	1284	A	N3-C4-N9	5.93	132.15	127.40
22	BA	1809	A	C5-C6-N1	5.93	120.67	117.70
1	AA	749	A	C8-N9-C4	5.93	108.17	105.80
22	BA	217	A	N9-C4-C5	5.93	108.17	105.80
22	BA	1274	A	N3-C4-N9	5.93	132.15	127.40
1	AA	1408	A	N3-C4-N9	5.93	132.14	127.40
22	BA	213	A	C5-C6-N1	5.93	120.67	117.70
22	BA	572	A	N9-C4-C5	5.93	108.17	105.80
22	BA	1583	A	C5-C6-N1	5.93	120.66	117.70
22	BA	1635	A	N3-C4-N9	5.93	132.14	127.40
22	BA	1889	A	N9-C4-C5	5.93	108.17	105.80
22	BA	345	A	C5-C6-N1	5.93	120.66	117.70
1	AA	356	A	C4-C5-N7	-5.93	107.74	110.70
1	AA	579	A	C4-C5-C6	5.93	119.96	117.00
22	BA	118	A	N3-C4-N9	5.93	132.14	127.40
22	BA	146	A	C5-C6-N1	5.93	120.66	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1689	A	N3-C4-N9	5.93	132.14	127.40
55	B8	58	A	N9-C4-C5	5.93	108.17	105.80
1	AA	143	A	C4-C5-C6	5.92	119.96	117.00
1	AA	338	A	C8-N9-C4	5.92	108.17	105.80
1	AA	1349	A	C4-C5-C6	5.92	119.96	117.00
23	BB	50	A	N9-C4-C5	5.92	108.17	105.80
1	AA	152	A	C5-C6-N1	5.92	120.66	117.70
1	AA	533	A	C5-C6-N1	5.92	120.66	117.70
22	BA	402	A	N9-C4-C5	5.92	108.17	105.80
22	BA	2154	A	N3-C4-N9	5.92	132.14	127.40
22	BA	2700	A	N3-C4-N9	5.92	132.14	127.40
1	AA	321	A	N3-C4-N9	5.92	132.14	127.40
1	AA	1105	A	N3-C4-N9	5.92	132.14	127.40
1	AA	1130	A	C8-N9-C4	5.92	108.17	105.80
1	AA	1285	A	C4-C5-N7	-5.92	107.74	110.70
22	BA	1127	A	N3-C4-N9	5.92	132.14	127.40
1	AA	547	A	C4-C5-C6	5.92	119.96	117.00
1	AA	1251	A	N3-C4-N9	5.92	132.14	127.40
1	AA	1429	A	N3-C4-N9	5.92	132.14	127.40
22	BA	73	A	C4-C5-C6	5.92	119.96	117.00
22	BA	1700	A	N9-C4-C5	5.92	108.17	105.80
1	AA	44	A	N9-C4-C5	5.92	108.17	105.80
22	BA	324	A	N3-C4-N9	5.92	132.13	127.40
22	BA	1477	A	C4-C5-C6	5.92	119.96	117.00
22	BA	1665	A	N3-C4-N9	5.92	132.13	127.40
22	BA	1676	A	C5-N7-C8	5.92	106.86	103.90
1	AA	1250	A	C4-C5-N7	-5.92	107.74	110.70
22	BA	2322	A	C5-C6-N1	5.92	120.66	117.70
22	BA	2635	A	N3-C4-N9	5.92	132.13	127.40
22	BA	131	A	C4-C5-C6	5.92	119.96	117.00
22	BA	362	A	N3-C4-N9	5.92	132.13	127.40
1	AA	338	A	C5-C6-N1	5.91	120.66	117.70
22	BA	752	A	C5-C6-N1	5.91	120.66	117.70
22	BA	2734	A	C4-C5-C6	5.91	119.96	117.00
1	AA	466	A	N9-C4-C5	5.91	108.17	105.80
1	AA	919	A	C4-C5-N7	-5.91	107.74	110.70
1	AA	120	A	C4-C5-C6	5.91	119.95	117.00
1	AA	432	A	C8-N9-C4	5.91	108.16	105.80
22	BA	979	A	N9-C4-C5	5.91	108.16	105.80
1	AA	493	A	N3-C4-N9	5.91	132.13	127.40
1	AA	1271	A	C4-C5-C6	5.91	119.95	117.00
1	AA	1394	A	C8-N9-C4	5.91	108.16	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	309	A	N9-C4-C5	5.91	108.16	105.80
22	BA	666	A	C4-C5-C6	5.91	119.95	117.00
22	BA	1502	A	N3-C4-N9	5.91	132.13	127.40
22	BA	2378	A	N3-C4-N9	5.91	132.13	127.40
22	BA	2675	A	C4-C5-C6	5.91	119.95	117.00
22	BA	979	A	C4-C5-N7	-5.91	107.75	110.70
22	BA	1525	A	C4-C5-C6	5.91	119.95	117.00
22	BA	2013	A	N3-C4-N9	5.91	132.13	127.40
22	BA	2191	A	C4-C5-C6	5.91	119.95	117.00
1	AA	1350	A	C4-C5-N7	-5.91	107.75	110.70
22	BA	2725	A	N3-C4-N9	5.91	132.12	127.40
1	AA	794	A	C8-N9-C4	5.90	108.16	105.80
1	AA	825	A	C5-C6-N1	5.90	120.65	117.70
1	AA	909	A	N3-C4-N9	5.90	132.12	127.40
1	AA	1288	A	N9-C4-C5	5.90	108.16	105.80
22	BA	1089	A	N3-C4-N9	5.90	132.12	127.40
22	BA	1490	A	C4-C5-C6	5.90	119.95	117.00
22	BA	265	A	N3-C4-N9	5.90	132.12	127.40
22	BA	905	A	N3-C4-N9	5.90	132.12	127.40
23	BB	52	A	N3-C4-N9	5.90	132.12	127.40
1	AA	19	A	C5-C6-N1	5.90	120.65	117.70
1	AA	704	A	N9-C4-C5	5.90	108.16	105.80
1	AA	1150	A	C8-N9-C4	5.90	108.16	105.80
22	BA	1147	A	N3-C4-N9	5.90	132.12	127.40
22	BA	1794	A	N3-C4-N9	5.90	132.12	127.40
22	BA	706	A	C4-C5-N7	-5.90	107.75	110.70
22	BA	722	A	C8-N9-C4	5.90	108.16	105.80
22	BA	1230	A	N9-C4-C5	5.90	108.16	105.80
22	BA	1755	A	N9-C4-C5	5.90	108.16	105.80
22	BA	2589	A	N3-C4-N9	5.90	132.12	127.40
22	BA	911	A	C5-C6-N1	5.90	120.65	117.70
22	BA	1111	A	C5-C6-N1	5.90	120.65	117.70
22	BA	2062	A	N3-C4-N9	5.90	132.12	127.40
22	BA	2071	A	C5-C6-N1	5.90	120.65	117.70
22	BA	528	A	N9-C4-C5	5.89	108.16	105.80
22	BA	1630	A	N9-C4-C5	5.89	108.16	105.80
22	BA	2117	A	C4-C5-N7	-5.89	107.75	110.70
22	BA	2205	A	C4-C5-C6	5.89	119.95	117.00
22	BA	2675	A	N3-C4-N9	5.89	132.12	127.40
1	AA	179	A	N9-C4-C5	5.89	108.16	105.80
1	AA	468	A	N3-C4-N9	5.89	132.11	127.40
1	AA	495	A	N9-C4-C5	5.89	108.16	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	299	A	N9-C4-C5	5.89	108.16	105.80
22	BA	344	A	C4-C5-C6	5.89	119.95	117.00
22	BA	788	A	N3-C4-N9	5.89	132.11	127.40
22	BA	829	A	C4-C5-C6	5.89	119.95	117.00
55	B8	42	A	N3-C4-N9	5.89	132.11	127.40
1	AA	109	A	N9-C4-C5	5.89	108.16	105.80
1	AA	792	A	N9-C4-C5	5.89	108.16	105.80
1	AA	1468	A	C8-N9-C4	5.89	108.16	105.80
22	BA	668	A	C5-C6-N1	5.89	120.65	117.70
22	BA	821	A	C5-C6-N1	5.89	120.65	117.70
22	BA	975	A	C8-N9-C4	5.89	108.16	105.80
22	BA	2813	A	C8-N9-C4	5.89	108.16	105.80
1	AA	129	A	C4-C5-C6	5.89	119.94	117.00
1	AA	363	A	C8-N9-C4	5.89	108.16	105.80
1	AA	547	A	C8-N9-C4	5.89	108.16	105.80
1	AA	860	A	C4-C5-N7	-5.89	107.75	110.70
1	AA	1188	A	C4-C5-C6	5.89	119.94	117.00
22	BA	160	A	N3-C4-N9	5.89	132.11	127.40
22	BA	262	A	N3-C4-N9	5.89	132.11	127.40
22	BA	423	A	N9-C4-C5	5.89	108.16	105.80
22	BA	1359	A	C4-C5-N7	-5.89	107.75	110.70
22	BA	1535	A	C4-C5-C6	5.89	119.94	117.00
55	B8	26	A	N9-C4-C5	5.89	108.16	105.80
1	AA	572	A	N9-C4-C5	5.89	108.16	105.80
1	AA	831	A	N3-C4-N9	5.89	132.11	127.40
1	AA	1431	A	N3-C4-N9	5.89	132.11	127.40
22	BA	2170	A	C8-N9-C4	5.89	108.16	105.80
22	BA	792	A	C5-C6-N1	5.89	120.64	117.70
22	BA	1635	A	C4-C5-C6	5.89	119.94	117.00
22	BA	1805	A	N3-C4-N9	5.89	132.11	127.40
22	BA	71	A	C4-C5-N7	-5.88	107.76	110.70
22	BA	1938	A	N3-C4-N9	5.88	132.11	127.40
22	BA	2809	A	N9-C4-C5	5.88	108.15	105.80
1	AA	1357	A	C4-C5-C6	5.88	119.94	117.00
22	BA	1755	A	C8-N9-C4	5.88	108.15	105.80
22	BA	2059	A	N3-C4-N9	5.88	132.11	127.40
22	BA	2327	A	C5-C6-N1	5.88	120.64	117.70
1	AA	80	A	C5-N7-C8	5.88	106.84	103.90
1	AA	411	A	N3-C4-N9	5.88	132.10	127.40
22	BA	1090	A	N3-C4-N9	5.88	132.10	127.40
22	BA	1384	A	N9-C4-C5	5.88	108.15	105.80
22	BA	402	A	C4-C5-C6	5.88	119.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	909	A	C8-N9-C4	5.88	108.15	105.80
22	BA	1008	A	N9-C4-C5	5.88	108.15	105.80
22	BA	1155	A	C4-C5-N7	-5.88	107.76	110.70
22	BA	1395	A	C4-C5-C6	5.88	119.94	117.00
22	BA	1571	A	N3-C4-N9	5.88	132.10	127.40
22	BA	219	A	N9-C4-C5	5.88	108.15	105.80
22	BA	1630	A	C8-N9-C4	5.88	108.15	105.80
22	BA	2675	A	C8-N9-C4	5.88	108.15	105.80
22	BA	833	A	N3-C4-N9	5.87	132.10	127.40
22	BA	1151	A	C8-N9-C4	5.87	108.15	105.80
22	BA	2097	A	C5-C6-N1	5.87	120.64	117.70
22	BA	2169	A	C4-C5-C6	5.87	119.94	117.00
22	BA	2587	A	N9-C4-C5	5.87	108.15	105.80
22	BA	804	A	N3-C4-N9	5.87	132.10	127.40
1	AA	309	A	C4-C5-N7	-5.87	107.77	110.70
22	BA	2169	A	N3-C4-N9	5.87	132.10	127.40
1	AA	228	A	N3-C4-N9	5.87	132.09	127.40
1	AA	872	A	C5-N7-C8	5.87	106.83	103.90
22	BA	340	A	C8-N9-C4	5.87	108.15	105.80
22	BA	2748	A	N9-C4-C5	5.87	108.15	105.80
22	BA	2856	A	N9-C4-C5	5.87	108.15	105.80
55	B8	6	A	N9-C4-C5	5.87	108.15	105.80
1	AA	1035	A	C4-C5-N7	-5.87	107.77	110.70
23	BB	108	A	C8-N9-C4	5.87	108.15	105.80
1	AA	949	A	C4-C5-N7	-5.87	107.77	110.70
22	BA	149	A	N3-C4-N9	5.87	132.09	127.40
22	BA	1427	A	C4-C5-C6	5.87	119.93	117.00
22	BA	2184	A	N3-C4-N9	5.87	132.09	127.40
1	AA	1014	A	C8-N9-C4	5.86	108.14	105.80
22	BA	743	A	C5-C6-N1	5.86	120.63	117.70
22	BA	1020	A	C4-C5-C6	5.86	119.93	117.00
22	BA	1226	A	N9-C4-C5	5.86	108.14	105.80
22	BA	1784	A	N3-C4-N9	5.86	132.09	127.40
22	BA	2274	A	C4-C5-C6	5.86	119.93	117.00
22	BA	2453	A	C5-C6-N1	5.86	120.63	117.70
1	AA	382	A	N9-C4-C5	5.86	108.14	105.80
1	AA	1492	A	C4-C5-C6	5.86	119.93	117.00
22	BA	1786	A	N9-C4-C5	5.86	108.14	105.80
22	BA	1960	A	N9-C4-C5	5.86	108.14	105.80
1	AA	553	A	N3-C4-N9	5.86	132.09	127.40
22	BA	233	A	N9-C4-C5	5.86	108.14	105.80
22	BA	927	A	C5-C6-N1	5.86	120.63	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1579	A	N3-C4-N9	5.86	132.09	127.40
1	AA	53	A	N3-C4-N9	5.86	132.09	127.40
1	AA	602	A	N9-C4-C5	5.86	108.14	105.80
22	BA	866	A	C8-N9-C4	5.86	108.14	105.80
1	AA	768	A	C8-N9-C4	5.86	108.14	105.80
1	AA	1476	A	C8-N9-C4	5.86	108.14	105.80
1	AA	1502	A	N3-C4-N9	5.86	132.09	127.40
22	BA	990	A	C4-C5-C6	5.86	119.93	117.00
22	BA	1427	A	N3-C4-N9	5.86	132.09	127.40
22	BA	1665	A	C4-C5-C6	5.86	119.93	117.00
22	BA	2015	A	C8-N9-C4	5.86	108.14	105.80
23	BB	15	A	C4-C5-C6	5.86	119.93	117.00
1	AA	408	A	C4-C5-N7	-5.86	107.77	110.70
1	AA	716	A	C5-C6-N1	5.86	120.63	117.70
22	BA	513	A	C5-C6-N1	5.86	120.63	117.70
22	BA	2037	A	C4-C5-C6	5.86	119.93	117.00
22	BA	693	A	C4-C5-N7	-5.85	107.77	110.70
22	BA	1701	A	C8-N9-C4	5.85	108.14	105.80
22	BA	1913	A	C4-C5-N7	-5.85	107.77	110.70
22	BA	2886	A	N3-C4-N9	5.85	132.08	127.40
1	AA	356	A	C4-C5-C6	5.85	119.93	117.00
1	AA	1251	A	N9-C4-C5	5.85	108.14	105.80
1	AA	1360	A	N3-C4-N9	5.85	132.08	127.40
22	BA	443	A	C8-N9-C4	5.85	108.14	105.80
22	BA	655	A	C4-C5-N7	-5.85	107.77	110.70
22	BA	1126	A	C5-C6-N1	5.85	120.63	117.70
22	BA	1579	A	C4-C5-C6	5.85	119.93	117.00
22	BA	2530	A	N3-C4-N9	5.85	132.08	127.40
1	AA	864	A	C4-C5-C6	5.85	119.92	117.00
22	BA	1553	A	C8-N9-C4	5.85	108.14	105.80
22	BA	2369	A	C4-C5-N7	-5.85	107.77	110.70
1	AA	1145	A	C4-C5-C6	5.85	119.92	117.00
1	AA	1188	A	N3-C4-N9	5.85	132.08	127.40
22	BA	457	A	C5-C6-N1	5.85	120.62	117.70
22	BA	541	A	C4-C5-N7	-5.85	107.78	110.70
22	BA	613	A	N9-C4-C5	5.85	108.14	105.80
1	AA	303	A	C8-N9-C4	5.85	108.14	105.80
1	AA	408	A	N9-C4-C5	5.85	108.14	105.80
22	BA	412	A	C5-C6-N1	5.85	120.62	117.70
22	BA	794	A	N3-C4-N9	5.85	132.08	127.40
22	BA	1262	A	N3-C4-N9	5.85	132.08	127.40
22	BA	2541	A	N9-C4-C5	5.85	108.14	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1196	A	C4-C5-C6	5.85	119.92	117.00
22	BA	661	A	C5-C6-N1	5.85	120.62	117.70
22	BA	241	A	N9-C4-C5	5.84	108.14	105.80
22	BA	1001	A	C8-N9-C4	5.84	108.14	105.80
22	BA	1477	A	N3-C4-N9	5.84	132.07	127.40
22	BA	1630	A	C5-C6-N1	5.84	120.62	117.70
22	BA	2541	A	C4-C5-C6	5.84	119.92	117.00
22	BA	706	A	N9-C4-C5	5.84	108.14	105.80
22	BA	2042	A	C4-C5-N7	-5.84	107.78	110.70
1	AA	411	A	C5-C6-N1	5.84	120.62	117.70
1	AA	1534	A	N9-C4-C5	5.84	108.14	105.80
22	BA	217	A	C5-N7-C8	5.84	106.82	103.90
22	BA	676	A	C5-C6-N1	5.84	120.62	117.70
22	BA	2309	A	N3-C4-N9	5.84	132.07	127.40
1	AA	1340	A	C4-C5-N7	-5.84	107.78	110.70
1	AA	1433	A	C4-C5-N7	-5.84	107.78	110.70
22	BA	1165	A	C4-C5-C6	5.84	119.92	117.00
22	BA	1504	A	C8-N9-C4	5.84	108.14	105.80
22	BA	1760	C	C6-N1-C2	-5.84	117.96	120.30
22	BA	918	A	C5-C6-N1	5.84	120.62	117.70
22	BA	2211	A	C4-C5-C6	5.84	119.92	117.00
23	BB	34	A	C8-N9-C4	5.84	108.14	105.80
1	AA	116	A	C4-C5-C6	5.84	119.92	117.00
1	AA	353	A	N9-C4-C5	5.84	108.13	105.80
22	BA	38	A	N3-C4-N9	5.84	132.07	127.40
22	BA	643	A	N9-C4-C5	5.84	108.14	105.80
22	BA	1086	A	N3-C4-N9	5.84	132.07	127.40
23	BB	57	A	N9-C4-C5	5.84	108.13	105.80
1	AA	553	A	C8-N9-C4	5.83	108.13	105.80
22	BA	538	A	N9-C4-C5	5.83	108.13	105.80
1	AA	172	A	C4-C5-C6	5.83	119.92	117.00
1	AA	510	A	C4-C5-C6	5.83	119.92	117.00
22	BA	718	A	C8-N9-C4	5.83	108.13	105.80
1	AA	1447	A	C4-C5-N7	-5.83	107.78	110.70
22	BA	941	A	C8-N9-C4	5.83	108.13	105.80
22	BA	980	A	C5-C6-N1	5.83	120.62	117.70
22	BA	1690	A	C4-C5-N7	-5.83	107.78	110.70
22	BA	2088	A	C8-N9-C4	5.83	108.13	105.80
1	AA	1434	A	N9-C4-C5	5.83	108.13	105.80
22	BA	231	A	N9-C4-C5	5.83	108.13	105.80
1	AA	1256	A	N9-C4-C5	5.83	108.13	105.80
22	BA	1580	A	N3-C4-N9	5.83	132.06	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	167	A	C4-C5-N7	-5.83	107.79	110.70
22	BA	1913	A	N9-C4-C5	5.83	108.13	105.80
1	AA	130	A	C4-C5-C6	5.83	119.91	117.00
1	AA	338	A	C4-C5-C6	5.83	119.91	117.00
1	AA	574	A	N9-C4-C5	5.83	108.13	105.80
1	AA	743	A	C8-N9-C4	5.83	108.13	105.80
22	BA	644	A	C5-C6-N1	5.83	120.61	117.70
22	BA	1515	A	C8-N9-C4	5.83	108.13	105.80
22	BA	1746	A	C5-C6-N1	5.83	120.61	117.70
22	BA	1871	A	N9-C4-C5	5.83	108.13	105.80
22	BA	2119	A	N9-C4-C5	5.83	108.13	105.80
1	AA	28	A	N9-C4-C5	5.82	108.13	105.80
1	AA	412	A	C5-C6-N1	5.82	120.61	117.70
22	BA	95	A	N3-C4-N9	5.82	132.06	127.40
22	BA	654	A	N3-C4-N9	5.82	132.06	127.40
22	BA	829	A	C8-N9-C4	5.82	108.13	105.80
22	BA	2154	A	C4-C5-C6	5.82	119.91	117.00
22	BA	2564	A	N3-C4-N9	5.82	132.06	127.40
22	BA	2682	A	C5-C6-N1	5.82	120.61	117.70
23	BB	104	A	C4-C5-C6	5.82	119.91	117.00
1	AA	1280	A	N9-C4-C5	5.82	108.13	105.80
22	BA	633	A	N3-C4-N9	5.82	132.06	127.40
22	BA	2809	A	C5-C6-N1	5.82	120.61	117.70
1	AA	353	A	N3-C4-N9	5.82	132.06	127.40
1	AA	787	A	C4-C5-C6	5.82	119.91	117.00
22	BA	529	A	N9-C4-C5	5.82	108.13	105.80
22	BA	2070	A	N3-C4-N9	5.82	132.06	127.40
1	AA	602	A	N3-C4-N9	5.82	132.06	127.40
1	AA	1318	A	N3-C4-N9	5.82	132.06	127.40
22	BA	1347	A	N3-C4-N9	5.82	132.06	127.40
22	BA	2600	A	C4-C5-C6	5.82	119.91	117.00
55	B8	66	A	N3-C4-N9	5.82	132.06	127.40
22	BA	1028	A	C8-N9-C4	5.82	108.13	105.80
22	BA	1987	A	C4-C5-C6	5.82	119.91	117.00
22	BA	2721	A	C5-N7-C8	5.82	106.81	103.90
1	AA	1428	A	C4-C5-C6	5.82	119.91	117.00
22	BA	89	A	C8-N9-C4	5.82	108.13	105.80
22	BA	270	A	N3-C4-N9	5.82	132.05	127.40
22	BA	502	A	C5-N7-C8	5.82	106.81	103.90
22	BA	899	A	C8-N9-C4	5.82	108.13	105.80
22	BA	1509	A	C4-C5-C6	5.82	119.91	117.00
1	AA	1430	A	C8-N9-C4	5.81	108.13	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1020	A	N9-C4-C5	5.81	108.13	105.80
22	BA	2478	A	N3-C4-N9	5.81	132.05	127.40
22	BA	2900	A	N3-C4-N9	5.81	132.05	127.40
1	AA	196	A	C4-C5-C6	5.81	119.91	117.00
1	AA	523	A	N3-C4-N9	5.81	132.05	127.40
1	AA	1046	A	C8-N9-C4	5.81	108.12	105.80
1	AA	1080	A	N3-C4-N9	5.81	132.05	127.40
22	BA	38	A	C4-C5-N7	-5.81	107.79	110.70
22	BA	1090	A	C4-C5-C6	5.81	119.91	117.00
22	BA	1641	A	N3-C4-N9	5.81	132.05	127.40
22	BA	1821	A	C4-C5-N7	-5.81	107.79	110.70
1	AA	949	A	C5-C6-N1	5.81	120.61	117.70
22	BA	1247	A	C4-C5-C6	5.81	119.91	117.00
22	BA	1960	A	N3-C4-N9	5.81	132.05	127.40
1	AA	792	A	C5-C6-N1	5.81	120.61	117.70
1	AA	825	A	C4-C5-N7	-5.81	107.80	110.70
1	AA	1035	A	C8-N9-C4	5.81	108.12	105.80
22	BA	44	A	N9-C4-C5	5.81	108.12	105.80
22	BA	689	A	C8-N9-C4	5.81	108.12	105.80
22	BA	988	A	N3-C4-N9	5.81	132.05	127.40
22	BA	1085	A	C5-C6-N1	5.81	120.61	117.70
22	BA	1503	A	C5-C6-N1	5.81	120.61	117.70
22	BA	1515	A	C5-C6-N1	5.81	120.61	117.70
22	BA	2184	A	N9-C4-C5	5.81	108.12	105.80
1	AA	787	A	N3-C4-N9	5.81	132.05	127.40
1	AA	1333	A	C4-C5-N7	-5.81	107.80	110.70
22	BA	265	A	C8-N9-C4	5.81	108.12	105.80
22	BA	1260	A	C4-C5-N7	-5.81	107.80	110.70
22	BA	1359	A	C8-N9-C4	5.81	108.12	105.80
22	BA	1654	A	N3-C4-N9	5.81	132.05	127.40
22	BA	2070	A	C4-C5-C6	5.81	119.90	117.00
23	BB	34	A	C5-C6-N1	5.81	120.60	117.70
22	BA	223	A	C4-C5-C6	5.81	119.90	117.00
1	AA	197	A	C4-C5-C6	5.80	119.90	117.00
1	AA	807	A	C4-C5-C6	5.80	119.90	117.00
1	AA	1145	A	C8-N9-C4	5.80	108.12	105.80
1	AA	1252	A	N3-C4-N9	5.80	132.04	127.40
22	BA	217	A	N3-C4-N9	5.80	132.04	127.40
22	BA	2453	A	C4-C5-C6	5.80	119.90	117.00
1	AA	243	A	C5-C6-N1	5.80	120.60	117.70
22	BA	1583	A	C4-C5-N7	-5.80	107.80	110.70
22	BA	1583	A	C8-N9-C4	5.80	108.12	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1853	A	C4-C5-C6	5.80	119.90	117.00
22	BA	1981	A	C4-C5-C6	5.80	119.90	117.00
22	BA	2119	A	N3-C4-N9	5.80	132.04	127.40
1	AA	608	A	C5-C6-N1	5.80	120.60	117.70
1	AA	702	A	C8-N9-C4	5.80	108.12	105.80
1	AA	749	A	C5-C6-N1	5.80	120.60	117.70
1	AA	1000	A	C5-C6-N1	5.80	120.60	117.70
22	BA	207	A	C4-C5-C6	5.80	119.90	117.00
22	BA	501	A	N3-C4-N9	5.80	132.04	127.40
22	BA	794	A	N9-C4-C5	5.80	108.12	105.80
22	BA	896	A	N9-C4-C5	5.80	108.12	105.80
1	AA	119	A	C4-C5-C6	5.80	119.90	117.00
22	BA	2169	A	C4-C5-N7	-5.80	107.80	110.70
1	AA	629	A	N9-C4-C5	5.80	108.12	105.80
1	AA	1446	A	N3-C4-N9	5.80	132.04	127.40
22	BA	146	A	N9-C4-C5	5.80	108.12	105.80
22	BA	472	A	N3-C4-N9	5.80	132.04	127.40
22	BA	1829	A	N9-C4-C5	5.80	108.12	105.80
22	BA	1998	A	C4-C5-N7	-5.80	107.80	110.70
1	AA	120	A	C8-N9-C4	5.79	108.12	105.80
1	AA	321	A	C4-C5-N7	-5.79	107.80	110.70
22	BA	2119	A	C4-C5-N7	-5.79	107.80	110.70
1	AA	182	A	C8-N9-C4	5.79	108.12	105.80
1	AA	520	A	N3-C4-N9	5.79	132.03	127.40
22	BA	294	A	C4-C5-C6	5.79	119.90	117.00
22	BA	2268	A	N3-C4-N9	5.79	132.03	127.40
22	BA	2513	A	N9-C4-C5	5.79	108.12	105.80
22	BA	160	A	C4-C5-C6	5.79	119.90	117.00
22	BA	233	A	N3-C4-N9	5.79	132.03	127.40
22	BA	1591	A	C5-C6-N1	5.79	120.60	117.70
22	BA	1596	A	C8-N9-C4	5.79	108.12	105.80
22	BA	2352	A	C4-C5-N7	-5.79	107.80	110.70
1	AA	978	A	C4-C5-N7	-5.79	107.81	110.70
22	BA	515	A	C8-N9-C4	5.79	108.12	105.80
22	BA	1165	A	C8-N9-C4	5.79	108.12	105.80
22	BA	2665	A	C4-C5-N7	-5.79	107.81	110.70
1	AA	2	A	N9-C4-C5	5.79	108.12	105.80
1	AA	174	A	N3-C4-N9	5.79	132.03	127.40
1	AA	298	A	C4-C5-C6	5.79	119.89	117.00
22	BA	49	A	N9-C4-C5	5.79	108.11	105.80
22	BA	2516	A	N3-C4-N9	5.79	132.03	127.40
1	AA	315	A	C4-C5-C6	5.79	119.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1147	A	C4-C5-C6	5.79	119.89	117.00
22	BA	1204	A	C4-C5-N7	-5.79	107.81	110.70
22	BA	2060	A	N3-C4-N9	5.79	132.03	127.40
22	BA	2679	A	C4-C5-C6	5.79	119.89	117.00
1	AA	649	A	N9-C4-C5	5.79	108.11	105.80
22	BA	182	A	C4-C5-N7	-5.79	107.81	110.70
22	BA	632	A	N3-C4-N9	5.79	132.03	127.40
22	BA	1654	A	C5-N7-C8	5.79	106.79	103.90
22	BA	1953	A	C5-C6-N1	5.79	120.59	117.70
22	BA	2471	A	C4-C5-N7	-5.79	107.81	110.70
1	AA	10	A	C5-C6-N1	5.78	120.59	117.70
1	AA	825	A	N3-C4-N9	5.78	132.03	127.40
1	AA	1102	A	N9-C4-C5	5.78	108.11	105.80
1	AA	1110	A	C8-N9-C4	5.78	108.11	105.80
1	AA	1280	A	N3-C4-N9	5.78	132.03	127.40
22	BA	218	A	C5-C6-N1	5.78	120.59	117.70
22	BA	429	A	N9-C4-C5	5.78	108.11	105.80
22	BA	504	A	C8-N9-C4	5.78	108.11	105.80
22	BA	1927	A	N3-C4-N9	5.78	132.03	127.40
1	AA	1513	A	C8-N9-C4	5.78	108.11	105.80
1	AA	72	A	C5-C6-N1	5.78	120.59	117.70
1	AA	546	A	C4-C5-C6	5.78	119.89	117.00
1	AA	1288	A	C4-C5-C6	5.78	119.89	117.00
22	BA	563	A	C5-C6-N1	5.78	120.59	117.70
22	BA	626	A	N3-C4-N9	5.78	132.02	127.40
22	BA	878	A	N9-C4-C5	5.78	108.11	105.80
22	BA	1090	A	C8-N9-C4	5.78	108.11	105.80
22	BA	1304	A	C4-C5-N7	-5.78	107.81	110.70
22	BA	1919	A	N3-C4-N9	5.78	132.02	127.40
22	BA	2058	A	N3-C4-N9	5.78	132.02	127.40
22	BA	2377	A	N3-C4-N9	5.78	132.03	127.40
1	AA	192	A	N3-C4-N9	5.78	132.02	127.40
22	BA	1403	A	N9-C4-C5	5.78	108.11	105.80
22	BA	2821	A	C4-C5-C6	5.78	119.89	117.00
55	B8	58	A	N3-C4-N9	5.78	132.02	127.40
1	AA	831	A	C8-N9-C4	5.78	108.11	105.80
22	BA	1134	A	N9-C4-C5	5.78	108.11	105.80
22	BA	1551	A	N3-C4-N9	5.78	132.02	127.40
22	BA	1785	A	C4-C5-C6	5.78	119.89	117.00
1	AA	371	A	C5-C6-N1	5.77	120.59	117.70
22	BA	223	A	C8-N9-C4	5.77	108.11	105.80
22	BA	422	A	C5-C6-N1	5.77	120.59	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	408	A	N3-C4-N9	5.77	132.02	127.40
1	AA	621	A	C5-C6-N1	5.77	120.59	117.70
1	AA	909	A	N9-C4-C5	5.77	108.11	105.80
1	AA	918	A	N3-C4-N9	5.77	132.02	127.40
9	AI	46	MET	CB-CG-SD	-5.77	95.08	112.40
22	BA	1783	A	N9-C4-C5	5.77	108.11	105.80
22	BA	2015	A	C4-C5-C6	5.77	119.89	117.00
23	BB	108	A	N9-C4-C5	5.77	108.11	105.80
1	AA	451	A	N3-C4-N9	5.77	132.02	127.40
22	BA	2013	A	C8-N9-C4	5.77	108.11	105.80
22	BA	2173	A	C4-C5-C6	5.77	119.89	117.00
1	AA	236	A	C4-C5-N7	-5.77	107.81	110.70
1	AA	583	A	C4-C5-C6	5.77	119.89	117.00
1	AA	753	A	C4-C5-C6	5.77	119.89	117.00
1	AA	845	A	N9-C4-C5	5.77	108.11	105.80
1	AA	1055	A	C8-N9-C4	5.77	108.11	105.80
22	BA	479	A	N9-C4-C5	5.77	108.11	105.80
22	BA	833	A	C5-N7-C8	5.77	106.78	103.90
22	BA	947	A	C8-N9-C4	5.77	108.11	105.80
22	BA	1096	A	C8-N9-C4	5.77	108.11	105.80
22	BA	1504	A	C5-C6-N1	5.77	120.58	117.70
22	BA	1786	A	C5-C6-N1	5.77	120.58	117.70
22	BA	2211	A	C4-C5-N7	-5.77	107.82	110.70
1	AA	1093	A	N9-C4-C5	5.77	108.11	105.80
1	AA	1251	A	C5-C6-N1	5.77	120.58	117.70
22	BA	382	A	C4-C5-C6	5.77	119.88	117.00
22	BA	532	A	N9-C4-C5	5.77	108.11	105.80
22	BA	936	A	C5-C6-N1	5.77	120.58	117.70
22	BA	1169	A	C4-C5-C6	5.77	119.88	117.00
22	BA	1433	A	N3-C4-N9	5.77	132.01	127.40
22	BA	1977	A	C5-C6-N1	5.77	120.58	117.70
1	AA	1044	A	N3-C4-N9	5.77	132.01	127.40
22	BA	160	A	N9-C4-C5	5.77	108.11	105.80
22	BA	541	A	N3-C4-N9	5.77	132.01	127.40
22	BA	2860	A	N3-C4-N9	5.77	132.01	127.40
1	AA	274	A	N3-C4-N9	5.76	132.01	127.40
22	BA	64	A	C4-C5-N7	-5.76	107.82	110.70
22	BA	637	A	N9-C4-C5	5.76	108.11	105.80
22	BA	1579	A	C5-C6-N1	5.76	120.58	117.70
22	BA	1632	A	C4-C5-C6	5.76	119.88	117.00
23	BB	73	A	C4-C5-C6	5.76	119.88	117.00
22	BA	362	A	C8-N9-C4	5.76	108.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2163	A	C4-C5-N7	-5.76	107.82	110.70
1	AA	282	A	C5-C6-N1	5.76	120.58	117.70
22	BA	1342	A	N3-C4-N9	5.76	132.01	127.40
22	BA	1652	A	C4-C5-C6	5.76	119.88	117.00
22	BA	2094	A	C5-C6-N1	5.76	120.58	117.70
1	AA	236	A	N3-C4-N9	5.76	132.01	127.40
1	AA	320	A	N9-C4-C5	5.76	108.10	105.80
22	BA	382	A	C5-C6-N1	5.76	120.58	117.70
22	BA	432	A	C8-N9-C4	5.76	108.10	105.80
22	BA	1805	A	N9-C4-C5	5.76	108.10	105.80
22	BA	320	A	C5-C6-N1	5.76	120.58	117.70
22	BA	1028	A	C5-C6-N1	5.76	120.58	117.70
22	BA	1269	A	C4-C5-N7	-5.76	107.82	110.70
22	BA	1679	A	C8-N9-C4	5.76	108.10	105.80
22	BA	2476	A	C4-C5-C6	5.76	119.88	117.00
1	AA	288	A	C5-C6-N1	5.76	120.58	117.70
1	AA	1256	A	N3-C4-N9	5.76	132.00	127.40
22	BA	632	A	N9-C4-C5	5.76	108.10	105.80
22	BA	1142	A	N9-C4-C5	5.76	108.10	105.80
22	BA	1490	A	C8-N9-C4	5.76	108.10	105.80
22	BA	1785	A	N3-C4-N9	5.76	132.01	127.40
22	BA	1353	A	C5-C6-N1	5.75	120.58	117.70
22	BA	2015	A	N3-C4-N9	5.75	132.00	127.40
1	AA	728	A	N9-C4-C5	5.75	108.10	105.80
1	AA	825	A	C4-C5-C6	5.75	119.88	117.00
22	BA	764	A	N3-C4-N9	5.75	132.00	127.40
22	BA	1096	A	C4-C5-C6	5.75	119.88	117.00
22	BA	1551	A	C5-C6-N1	5.75	120.58	117.70
22	BA	2267	A	C4-C5-C6	5.75	119.88	117.00
22	BA	2418	A	N3-C4-N9	5.75	132.00	127.40
22	BA	990	A	C5-N7-C8	5.75	106.78	103.90
22	BA	1301	A	C5-C6-N1	5.75	120.58	117.70
22	BA	1354	A	N3-C4-N9	5.75	132.00	127.40
22	BA	74	A	N9-C4-C5	5.75	108.10	105.80
22	BA	204	A	N9-C4-C5	5.75	108.10	105.80
22	BA	689	A	C5-C6-N1	5.75	120.57	117.70
22	BA	988	A	C4-C5-C6	5.75	119.87	117.00
22	BA	1142	A	N3-C4-N9	5.75	132.00	127.40
22	BA	1509	A	N3-C4-N9	5.75	132.00	127.40
22	BA	1593	A	C8-N9-C4	5.75	108.10	105.80
22	BA	1745	A	N3-C4-N9	5.75	132.00	127.40
1	AA	131	A	C8-N9-C4	5.75	108.10	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	532	A	C4-C5-C6	5.75	119.87	117.00
22	BA	973	A	C5-N7-C8	5.75	106.77	103.90
22	BA	2837	A	C4-C5-N7	-5.75	107.83	110.70
1	AA	1169	A	N3-C4-N9	5.75	132.00	127.40
22	BA	947	A	N9-C4-C5	5.75	108.10	105.80
22	BA	1040	A	N9-C4-C5	5.75	108.10	105.80
22	BA	2513	A	C4-C5-C6	5.75	119.87	117.00
1	AA	197	A	N3-C4-N9	5.74	132.00	127.40
1	AA	873	A	C8-N9-C4	5.74	108.10	105.80
22	BA	125	A	N3-C4-N9	5.74	132.00	127.40
22	BA	973	A	C5-C6-N1	5.74	120.57	117.70
22	BA	1711	A	N3-C4-N9	5.74	132.00	127.40
22	BA	2547	A	N3-C4-N9	5.74	132.00	127.40
1	AA	1014	A	N9-C4-C5	5.74	108.10	105.80
22	BA	1701	A	C4-C5-N7	-5.74	107.83	110.70
1	AA	195	A	C5-C6-N1	5.74	120.57	117.70
1	AA	364	A	C4-C5-N7	-5.74	107.83	110.70
1	AA	465	A	C5-C6-N1	5.74	120.57	117.70
1	AA	1534	A	C8-N9-C4	5.74	108.10	105.80
22	BA	324	A	C5-C6-N1	5.74	120.57	117.70
22	BA	1387	A	C8-N9-C4	5.74	108.10	105.80
22	BA	1730	C	N1-C2-O2	5.74	122.34	118.90
22	BA	2753	A	C4-C5-N7	-5.74	107.83	110.70
23	BB	115	A	C8-N9-C4	5.74	108.10	105.80
1	AA	782	A	C4-C5-C6	5.74	119.87	117.00
1	AA	1035	A	N3-C4-N9	5.74	131.99	127.40
22	BA	213	A	C4-C5-C6	5.74	119.87	117.00
22	BA	1783	A	N3-C4-N9	5.74	131.99	127.40
22	BA	1785	A	C5-C6-N1	5.74	120.57	117.70
22	BA	2266	A	C5-C6-N1	5.74	120.57	117.70
22	BA	2541	A	N3-C4-N9	5.74	131.99	127.40
22	BA	1393	A	N9-C4-C5	5.74	108.09	105.80
22	BA	2184	A	C4-C5-C6	5.74	119.87	117.00
22	BA	2311	A	C4-C5-N7	-5.74	107.83	110.70
1	AA	71	A	C4-C5-C6	5.74	119.87	117.00
1	AA	181	A	C8-N9-C4	5.74	108.09	105.80
1	AA	777	A	C4-C5-C6	5.74	119.87	117.00
22	BA	10	A	N9-C4-C5	5.74	108.09	105.80
22	BA	1142	A	C5-C6-N1	5.74	120.57	117.70
22	BA	1535	A	C8-N9-C4	5.74	108.09	105.80
22	BA	1614	A	C8-N9-C4	5.74	108.09	105.80
22	BA	2461	A	C8-N9-C4	5.74	108.09	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2534	A	N3-C4-N9	5.74	131.99	127.40
1	AA	665	A	C5-C6-N1	5.73	120.57	117.70
1	AA	673	A	N9-C4-C5	5.73	108.09	105.80
1	AA	1480	A	C8-N9-C4	5.73	108.09	105.80
22	BA	706	A	N3-C4-N9	5.73	131.99	127.40
22	BA	1393	A	C4-C5-N7	-5.73	107.83	110.70
22	BA	2336	A	C4-C5-N7	-5.73	107.83	110.70
1	AA	1261	A	C4-C5-C6	5.73	119.87	117.00
1	AA	1319	A	C4-C5-C6	5.73	119.87	117.00
1	AA	1396	A	N9-C4-C5	5.73	108.09	105.80
22	BA	749	A	N9-C4-C5	5.73	108.09	105.80
22	BA	1635	A	C4-C5-N7	-5.73	107.83	110.70
1	AA	547	A	N3-C4-N9	5.73	131.98	127.40
22	BA	1001	A	C4-C5-C6	5.73	119.86	117.00
22	BA	1640	A	C4-C5-N7	-5.73	107.83	110.70
22	BA	1689	A	C4-C5-N7	-5.73	107.83	110.70
1	AA	459	A	N3-C4-N9	5.73	131.98	127.40
1	AA	2	A	N3-C4-N9	5.73	131.98	127.40
1	AA	1507	A	C5-C6-N1	5.73	120.56	117.70
23	BB	94	A	N3-C4-N9	5.73	131.98	127.40
22	BA	1495	A	N9-C4-C5	5.73	108.09	105.80
1	AA	371	A	C4-C5-N7	-5.72	107.84	110.70
1	AA	1362	A	N3-C4-N9	5.72	131.98	127.40
22	BA	892	A	N3-C4-N9	5.72	131.98	127.40
22	BA	2513	A	C5-C6-N1	5.72	120.56	117.70
1	AA	1229	A	C5-C6-N1	5.72	120.56	117.70
22	BA	1010	A	N3-C4-N9	5.72	131.98	127.40
22	BA	2147	A	C4-C5-C6	5.72	119.86	117.00
1	AA	179	A	C4-C5-N7	-5.72	107.84	110.70
1	AA	1150	A	N3-C4-N9	5.72	131.98	127.40
22	BA	1246	A	N9-C4-C5	5.72	108.09	105.80
1	AA	50	A	N3-C4-N9	5.72	131.98	127.40
22	BA	526	A	C4-C5-C6	5.72	119.86	117.00
22	BA	911	A	C4-C5-C6	5.72	119.86	117.00
22	BA	1147	A	C8-N9-C4	5.72	108.09	105.80
22	BA	1791	A	C5-C6-N1	5.72	120.56	117.70
22	BA	2171	A	C8-N9-C4	5.72	108.09	105.80
22	BA	144	A	C8-N9-C4	5.72	108.09	105.80
1	AA	975	A	N3-C4-N9	5.72	131.97	127.40
1	AA	1036	A	N3-C4-N9	5.72	131.97	127.40
1	AA	1216	A	C4-C5-N7	-5.72	107.84	110.70
22	BA	83	A	C8-N9-C4	5.72	108.09	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	104	A	N3-C4-N9	5.72	131.97	127.40
22	BA	756	A	C8-N9-C4	5.72	108.09	105.80
22	BA	1597	A	C4-C5-C6	5.72	119.86	117.00
22	BA	1784	A	C8-N9-C4	5.72	108.09	105.80
1	AA	649	A	C8-N9-C4	5.71	108.09	105.80
1	AA	1531	A	C8-N9-C4	5.71	108.09	105.80
22	BA	655	A	C4-C5-C6	5.71	119.86	117.00
22	BA	735	A	N9-C4-C5	5.71	108.08	105.80
22	BA	756	A	C4-C5-N7	-5.71	107.84	110.70
22	BA	1885	A	C8-N9-C4	5.71	108.09	105.80
22	BA	2270	A	C5-C6-N1	5.71	120.56	117.70
1	AA	432	A	C4-C5-C6	5.71	119.86	117.00
1	AA	759	A	C8-N9-C4	5.71	108.08	105.80
22	BA	344	A	N3-C4-N9	5.71	131.97	127.40
22	BA	905	A	C4-C5-C6	5.71	119.86	117.00
22	BA	1698	A	N9-C4-C5	5.71	108.08	105.80
22	BA	2516	A	C5-C6-N1	5.71	120.56	117.70
22	BA	2725	A	N9-C4-C5	5.71	108.08	105.80
1	AA	1239	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	1333	A	C5-C6-N1	5.71	120.56	117.70
22	BA	699	A	C8-N9-C4	5.71	108.08	105.80
22	BA	2657	A	N3-C4-N9	5.71	131.97	127.40
22	BA	2810	A	C4-C5-N7	-5.71	107.84	110.70
1	AA	583	A	C5-C6-N1	5.71	120.56	117.70
1	AA	608	A	C4-C5-C6	5.71	119.86	117.00
1	AA	704	A	C8-N9-C4	5.71	108.08	105.80
22	BA	497	A	N3-C4-N9	5.71	131.97	127.40
22	BA	504	A	C4-C5-N7	-5.71	107.84	110.70
22	BA	1046	A	C4-C5-C6	5.71	119.86	117.00
22	BA	1095	A	C4-C5-N7	-5.71	107.84	110.70
22	BA	1383	A	N3-C4-N9	5.71	131.97	127.40
22	BA	1496	A	C4-C5-C6	5.71	119.86	117.00
1	AA	914	A	C8-N9-C4	5.71	108.08	105.80
1	AA	1299	A	N3-C4-N9	5.71	131.97	127.40
1	AA	1368	A	N9-C4-C5	5.71	108.08	105.80
22	BA	616	A	C5-C6-N1	5.71	120.56	117.70
22	BA	1509	A	C8-N9-C4	5.71	108.08	105.80
22	BA	1786	A	N3-C4-N9	5.71	131.97	127.40
22	BA	2740	A	N3-C4-N9	5.71	131.97	127.40
1	AA	243	A	C4-C5-C6	5.71	119.85	117.00
1	AA	365	U	C5-C4-O4	5.71	129.32	125.90
1	AA	1163	A	C5-C6-N1	5.71	120.55	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1332	A	N3-C4-N9	5.71	131.97	127.40
1	AA	1408	A	C5-C6-N1	5.71	120.55	117.70
1	AA	1502	A	C4-C5-C6	5.71	119.85	117.00
22	BA	821	A	C8-N9-C4	5.71	108.08	105.80
22	BA	1327	A	C4-C5-C6	5.71	119.85	117.00
22	BA	1439	A	N3-C4-N9	5.71	131.97	127.40
22	BA	1632	A	N3-C4-N9	5.71	131.97	127.40
22	BA	2227	A	N3-C4-N9	5.71	131.97	127.40
22	BA	2346	A	C4-C5-N7	-5.71	107.85	110.70
22	BA	21	A	N3-C4-N9	5.71	131.96	127.40
22	BA	146	A	C4-C5-N7	-5.71	107.85	110.70
22	BA	804	A	C8-N9-C4	5.71	108.08	105.80
22	BA	1393	A	N3-C4-N9	5.71	131.96	127.40
22	BA	1522	A	C5-C6-N1	5.71	120.55	117.70
22	BA	825	A	N3-C4-N9	5.70	131.96	127.40
1	AA	363	A	C5-C6-N1	5.70	120.55	117.70
1	AA	1196	A	N3-C4-N9	5.70	131.96	127.40
22	BA	1070	A	N9-C4-C5	5.70	108.08	105.80
22	BA	28	A	N3-C4-N9	5.70	131.96	127.40
22	BA	371	A	C8-N9-C4	5.70	108.08	105.80
22	BA	1552	A	C4-C5-C6	5.70	119.85	117.00
22	BA	1932	A	N9-C4-C5	5.70	108.08	105.80
22	BA	2587	A	C5-C6-N1	5.70	120.55	117.70
1	AA	303	A	C5-C6-N1	5.70	120.55	117.70
1	AA	687	A	C4-C5-N7	-5.70	107.85	110.70
1	AA	753	A	N3-C4-N9	5.70	131.96	127.40
1	AA	1500	A	C5-C6-N1	5.70	120.55	117.70
22	BA	514	A	C8-N9-C4	5.70	108.08	105.80
22	BA	668	A	C8-N9-C4	5.70	108.08	105.80
22	BA	1020	A	C4-C5-N7	-5.70	107.85	110.70
22	BA	1088	A	N9-C4-C5	5.70	108.08	105.80
22	BA	1264	A	C5-N7-C8	5.70	106.75	103.90
22	BA	1321	A	C8-N9-C4	5.70	108.08	105.80
22	BA	1470	A	C8-N9-C4	5.70	108.08	105.80
22	BA	1762	A	C5-C6-N1	5.70	120.55	117.70
22	BA	89	A	N9-C4-C5	5.70	108.08	105.80
22	BA	282	A	C4-C5-N7	-5.69	107.85	110.70
22	BA	1801	A	N3-C4-N9	5.69	131.96	127.40
22	BA	2848	G	O4'-C1'-N9	5.69	112.75	108.20
1	AA	792	A	C8-N9-C4	5.69	108.08	105.80
1	AA	983	A	C5-C6-N1	5.69	120.55	117.70
1	AA	1169	A	C8-N9-C4	5.69	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1304	A	N3-C4-N9	5.69	131.95	127.40
1	AA	695	A	C4-C5-N7	-5.69	107.86	110.70
1	AA	1396	A	N3-C4-N9	5.69	131.95	127.40
22	BA	1057	A	C8-N9-C4	5.69	108.08	105.80
22	BA	2042	A	N3-C4-N9	5.69	131.95	127.40
22	BA	2147	A	N9-C4-C5	5.69	108.08	105.80
22	BA	2268	A	C5-N7-C8	5.69	106.75	103.90
22	BA	2328	A	C5-C6-N1	5.69	120.55	117.70
22	BA	2352	A	N3-C4-N9	5.69	131.95	127.40
22	BA	2872	A	C4-C5-C6	5.69	119.84	117.00
55	B8	6	A	C8-N9-C4	5.69	108.08	105.80
22	BA	111	A	N9-C4-C5	5.69	108.08	105.80
22	BA	2014	A	C8-N9-C4	5.69	108.08	105.80
22	BA	2288	A	C4-C5-C6	5.69	119.84	117.00
1	AA	349	A	C4-C5-C6	5.69	119.84	117.00
1	AA	539	A	C5-C6-N1	5.69	120.54	117.70
1	AA	1042	A	N9-C4-C5	5.69	108.08	105.80
22	BA	354	A	C4-C5-C6	5.69	119.84	117.00
22	BA	42	A	C4-C5-C6	5.69	119.84	117.00
22	BA	1395	A	C5-C6-N1	5.69	120.54	117.70
22	BA	1477	A	N9-C4-C5	5.69	108.07	105.80
22	BA	2820	A	N3-C4-N9	5.69	131.95	127.40
1	AA	1413	A	C8-N9-C4	5.68	108.07	105.80
1	AA	60	A	N9-C4-C5	5.68	108.07	105.80
1	AA	509	A	N9-C4-C5	5.68	108.07	105.80
1	AA	1446	A	C8-N9-C4	5.68	108.07	105.80
22	BA	541	A	C5-C6-N1	5.68	120.54	117.70
22	BA	1927	A	C4-C5-C6	5.68	119.84	117.00
22	BA	104	A	C5-C6-N1	5.68	120.54	117.70
22	BA	1420	A	C4-C5-N7	-5.68	107.86	110.70
1	AA	865	A	C5-C6-N1	5.68	120.54	117.70
22	BA	1347	A	N9-C4-C5	5.68	108.07	105.80
22	BA	2879	A	C8-N9-C4	5.68	108.07	105.80
1	AA	50	A	N9-C4-C5	5.68	108.07	105.80
1	AA	1441	A	N3-C4-N9	5.68	131.94	127.40
22	BA	1871	A	C4-C5-C6	5.68	119.84	117.00
1	AA	205	A	N3-C4-N9	5.68	131.94	127.40
1	AA	1117	A	N3-C4-N9	5.68	131.94	127.40
1	AA	1495	U	C2-N1-C1'	5.68	124.51	117.70
22	BA	74	A	C5-N7-C8	5.68	106.74	103.90
22	BA	2560	A	C5-C6-N1	5.68	120.54	117.70
22	BA	2813	A	N3-C4-N9	5.68	131.94	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	39	A	C8-N9-C4	5.68	108.07	105.80
1	AA	74	A	C4-C5-N7	-5.67	107.86	110.70
1	AA	663	A	C8-N9-C4	5.67	108.07	105.80
1	AA	1508	A	C5-C6-N1	5.67	120.54	117.70
22	BA	2411	A	C5-C6-N1	5.67	120.54	117.70
1	AA	306	A	C4-C5-C6	5.67	119.84	117.00
22	BA	614	A	N9-C4-C5	5.67	108.07	105.80
22	BA	1021	A	N9-C4-C5	5.67	108.07	105.80
1	AA	1197	A	C5-C6-N1	5.67	120.54	117.70
22	BA	845	A	C8-N9-C4	5.67	108.07	105.80
22	BA	1126	A	N9-C4-C5	5.67	108.07	105.80
22	BA	2019	A	C4-C5-C6	5.67	119.84	117.00
1	AA	336	A	C4-C5-C6	5.67	119.83	117.00
1	AA	452	A	C8-N9-C4	5.67	108.07	105.80
1	AA	816	A	C4-C5-C6	5.67	119.83	117.00
1	AA	913	A	C4-C5-C6	5.67	119.83	117.00
22	BA	480	A	N9-C4-C5	5.67	108.07	105.80
22	BA	1705	A	C5-C6-N1	5.67	120.53	117.70
22	BA	2886	A	C8-N9-C4	5.67	108.07	105.80
1	AA	1271	A	C5-C6-N1	5.67	120.53	117.70
22	BA	127	A	C4-C5-C6	5.67	119.83	117.00
22	BA	1373	A	C5-C6-N1	5.67	120.53	117.70
1	AA	845	A	C4-C5-N7	-5.67	107.87	110.70
22	BA	529	A	C8-N9-C4	5.67	108.07	105.80
22	BA	1420	A	N3-C4-N9	5.67	131.93	127.40
22	BA	2147	A	N3-C4-N9	5.67	131.93	127.40
22	BA	2654	A	C4-C5-C6	5.67	119.83	117.00
22	BA	2278	A	C4-C5-C6	5.67	119.83	117.00
22	BA	2776	A	N3-C4-N9	5.67	131.93	127.40
1	AA	182	A	N9-C4-C5	5.66	108.06	105.80
22	BA	631	A	N3-C4-N9	5.66	131.93	127.40
22	BA	1085	A	C4-C5-C6	5.66	119.83	117.00
22	BA	1858	A	N9-C4-C5	5.66	108.06	105.80
22	BA	1872	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	2094	A	N3-C4-N9	5.66	131.93	127.40
22	BA	2856	A	N3-C4-N9	5.66	131.93	127.40
1	AA	461	A	N3-C4-N9	5.66	131.93	127.40
1	AA	487	A	C8-N9-C4	5.66	108.06	105.80
22	BA	223	A	N9-C4-C5	5.66	108.06	105.80
22	BA	1069	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	1086	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	1127	A	N9-C4-C5	5.66	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2750	A	C5-C6-N1	5.66	120.53	117.70
1	AA	44	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	614	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	829	A	N3-C4-N9	5.66	131.93	127.40
22	BA	1871	A	C8-N9-C4	5.66	108.06	105.80
1	AA	695	A	C4-C5-C6	5.66	119.83	117.00
1	AA	864	A	C5-C6-N1	5.66	120.53	117.70
1	AA	946	A	C8-N9-C4	5.66	108.06	105.80
22	BA	1384	A	N3-C4-N9	5.66	131.93	127.40
22	BA	2314	A	C8-N9-C4	5.66	108.06	105.80
1	AA	535	A	C8-N9-C4	5.66	108.06	105.80
1	AA	780	A	N3-C4-N9	5.66	131.93	127.40
1	AA	807	A	N3-C4-N9	5.66	131.93	127.40
22	BA	2205	A	N9-C4-C5	5.66	108.06	105.80
1	AA	349	A	N3-C4-N9	5.66	131.92	127.40
1	AA	687	A	N3-C4-N9	5.66	131.92	127.40
22	BA	1070	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	1640	A	C8-N9-C4	5.66	108.06	105.80
22	BA	2134	A	C5-C6-N1	5.66	120.53	117.70
1	AA	389	A	C4-C5-N7	-5.65	107.87	110.70
22	BA	764	A	C5-C6-N1	5.65	120.53	117.70
22	BA	1046	A	N3-C4-N9	5.65	131.92	127.40
22	BA	1496	A	N3-C4-N9	5.65	131.92	127.40
22	BA	1977	A	C8-N9-C4	5.65	108.06	105.80
22	BA	2369	A	N3-C4-N9	5.65	131.92	127.40
1	AA	621	A	C4-C5-C6	5.65	119.83	117.00
22	BA	928	A	C5-C6-N1	5.65	120.53	117.70
22	BA	2577	A	C5-C6-N1	5.65	120.53	117.70
23	BB	57	A	C4-C5-C6	5.65	119.83	117.00
1	AA	475	C	N3-C2-O2	-5.65	117.94	121.90
1	AA	1146	A	N3-C4-N9	5.65	131.92	127.40
22	BA	959	A	N9-C4-C5	5.65	108.06	105.80
22	BA	1307	A	C8-N9-C4	5.65	108.06	105.80
22	BA	1780	A	N3-C4-N9	5.65	131.92	127.40
22	BA	2453	A	N3-C4-N9	5.65	131.92	127.40
1	AA	151	A	C8-N9-C4	5.65	108.06	105.80
1	AA	819	A	N3-C4-N9	5.65	131.92	127.40
1	AA	1377	A	C4-C5-N7	-5.65	107.88	110.70
22	BA	222	A	C5-C6-N1	5.65	120.52	117.70
22	BA	590	A	N9-C4-C5	5.65	108.06	105.80
22	BA	608	A	C8-N9-C4	5.65	108.06	105.80
22	BA	1156	A	C5-C6-N1	5.65	120.52	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	94	A	C4-C5-N7	-5.65	107.88	110.70
55	B8	19	G	O4'-C1'-N9	-5.65	103.68	108.20
22	BA	503	A	N9-C4-C5	5.64	108.06	105.80
1	AA	167	A	C4-C5-C6	5.64	119.82	117.00
1	AA	393	A	N9-C4-C5	5.64	108.06	105.80
1	AA	1110	A	C4-C5-N7	-5.64	107.88	110.70
22	BA	177	G	O4'-C1'-N9	5.64	112.71	108.20
22	BA	753	A	C5-C6-N1	5.64	120.52	117.70
22	BA	1522	A	C4-C5-N7	-5.64	107.88	110.70
22	BA	2430	A	N3-C4-N9	5.64	131.91	127.40
22	BA	800	A	C8-N9-C4	5.64	108.06	105.80
23	BB	15	A	N3-C4-N9	5.64	131.91	127.40
1	AA	1252	A	C8-N9-C4	5.64	108.06	105.80
22	BA	574	A	C8-N9-C4	5.64	108.06	105.80
22	BA	1525	A	C8-N9-C4	5.64	108.06	105.80
22	BA	1711	A	C8-N9-C4	5.64	108.06	105.80
1	AA	315	A	N9-C4-C5	5.64	108.06	105.80
22	BA	849	A	C5-C6-N1	5.64	120.52	117.70
1	AA	753	A	C4-C5-N7	-5.64	107.88	110.70
1	AA	1398	A	C8-N9-C4	5.64	108.06	105.80
1	AA	1476	A	N9-C4-C5	5.64	108.06	105.80
22	BA	10	A	N3-C4-N9	5.64	131.91	127.40
22	BA	324	A	C8-N9-C4	5.64	108.06	105.80
22	BA	556	A	C4-C5-C6	5.64	119.82	117.00
22	BA	1532	A	C4-C5-C6	5.64	119.82	117.00
22	BA	2042	A	C8-N9-C4	5.64	108.05	105.80
22	BA	2135	A	C4-C5-C6	5.64	119.82	117.00
22	BA	2823	A	C8-N9-C4	5.64	108.06	105.80
23	BB	119	A	N3-C4-N9	5.64	131.91	127.40
1	AA	1204	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1332	A	C8-N9-C4	5.63	108.05	105.80
22	BA	896	A	C8-N9-C4	5.63	108.05	105.80
22	BA	909	A	N3-C4-N9	5.63	131.91	127.40
22	BA	182	A	N9-C4-C5	5.63	108.05	105.80
22	BA	1014	A	C8-N9-C4	5.63	108.05	105.80
22	BA	1403	A	C5-C6-N1	5.63	120.52	117.70
22	BA	2031	A	C4-C5-N7	-5.63	107.88	110.70
22	BA	2634	A	C4-C5-N7	-5.63	107.88	110.70
22	BA	2191	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1299	A	C5-C6-N1	5.63	120.52	117.70
22	BA	2199	A	N9-C4-C5	5.63	108.05	105.80
55	B8	41	A	N9-C4-C5	5.63	108.05	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	51	A	C8-N9-C4	5.63	108.05	105.80
1	AA	65	A	N3-C4-N9	5.63	131.90	127.40
1	AA	431	A	C8-N9-C4	5.63	108.05	105.80
1	AA	1155	A	N3-C4-N9	5.63	131.90	127.40
22	BA	391	A	C8-N9-C4	5.63	108.05	105.80
22	BA	415	A	C5-C6-N1	5.63	120.51	117.70
22	BA	1744	A	N9-C4-C5	5.63	108.05	105.80
22	BA	2814	A	C4-C5-N7	-5.63	107.89	110.70
1	AA	288	A	N3-C4-N9	5.63	131.90	127.40
1	AA	1236	A	C5-C6-N1	5.63	120.51	117.70
22	BA	131	A	C5-C6-N1	5.63	120.51	117.70
22	BA	896	A	N3-C4-N9	5.63	131.90	127.40
22	BA	1978	A	N9-C4-C5	5.63	108.05	105.80
1	AA	98	A	C8-N9-C4	5.62	108.05	105.80
1	AA	167	A	N3-C4-N9	5.62	131.90	127.40
1	AA	640	A	N3-C4-N9	5.62	131.90	127.40
1	AA	1176	A	C5-C6-N1	5.62	120.51	117.70
22	BA	118	A	C8-N9-C4	5.62	108.05	105.80
22	BA	430	A	N9-C4-C5	5.62	108.05	105.80
22	BA	900	A	C8-N9-C4	5.62	108.05	105.80
1	AA	600	A	C4-C5-N7	-5.62	107.89	110.70
22	BA	5	A	N9-C4-C5	5.62	108.05	105.80
22	BA	342	A	C8-N9-C4	5.62	108.05	105.80
22	BA	911	A	C8-N9-C4	5.62	108.05	105.80
22	BA	1067	A	N9-C4-C5	5.62	108.05	105.80
49	B1	44	ARG	CG-CD-NE	-5.62	99.99	111.80
1	AA	1005	A	C8-N9-C4	5.62	108.05	105.80
1	AA	1157	A	C8-N9-C4	5.62	108.05	105.80
22	BA	101	A	C8-N9-C4	5.62	108.05	105.80
22	BA	1272	A	N9-C4-C5	5.62	108.05	105.80
22	BA	1616	A	C4-C5-C6	5.62	119.81	117.00
22	BA	1754	A	N3-C4-N9	5.62	131.90	127.40
23	BB	59	A	C5-C6-N6	5.62	128.20	123.70
1	AA	451	A	N9-C4-C5	5.62	108.05	105.80
22	BA	1384	A	C4-C5-N7	-5.62	107.89	110.70
22	BA	1858	A	N3-C4-N9	5.62	131.90	127.40
22	BA	1205	A	N3-C4-N9	5.62	131.90	127.40
22	BA	1509	A	N9-C4-C5	5.62	108.05	105.80
22	BA	2212	A	C8-N9-C4	5.62	108.05	105.80
22	BA	2813	A	C4-C5-C6	5.62	119.81	117.00
1	AA	320	A	C8-N9-C4	5.62	108.05	105.80
1	AA	1396	A	C5-C6-N1	5.62	120.51	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1050	A	C4-C5-N7	-5.62	107.89	110.70
1	AA	236	A	C8-N9-C4	5.62	108.05	105.80
22	BA	340	A	C5-C6-N1	5.62	120.51	117.70
22	BA	1134	A	N3-C4-N9	5.62	131.89	127.40
22	BA	1194	A	N9-C4-C5	5.62	108.05	105.80
22	BA	2097	A	N9-C4-C5	5.62	108.05	105.80
1	AA	33	A	C5-C6-N1	5.61	120.51	117.70
1	AA	478	A	C4-C5-C6	5.61	119.81	117.00
1	AA	1101	A	C8-N9-C4	5.61	108.05	105.80
1	AA	1346	A	C4-C5-N7	-5.61	107.89	110.70
22	BA	592	A	C8-N9-C4	5.61	108.05	105.80
22	BA	1205	A	C8-N9-C4	5.61	108.05	105.80
22	BA	1262	A	N9-C4-C5	5.61	108.05	105.80
22	BA	2134	A	N3-C4-N9	5.61	131.89	127.40
1	AA	246	A	N9-C4-C5	5.61	108.05	105.80
1	AA	8	A	N3-C4-N9	5.61	131.89	127.40
1	AA	172	A	N3-C4-N9	5.61	131.89	127.40
1	AA	609	A	N3-C4-N9	5.61	131.89	127.40
1	AA	1035	A	N9-C4-C5	5.61	108.05	105.80
1	AA	1151	A	C8-N9-C4	5.61	108.04	105.80
22	BA	64	A	C5-C6-N1	5.61	120.50	117.70
22	BA	2899	A	N9-C4-C5	5.61	108.04	105.80
1	AA	648	A	C8-N9-C4	5.61	108.04	105.80
1	AA	918	A	C5-C6-N1	5.61	120.50	117.70
1	AA	1269	A	C4-C5-C6	5.61	119.81	117.00
22	BA	504	A	N3-C4-N9	5.61	131.89	127.40
22	BA	2566	A	C5-C6-N1	5.61	120.50	117.70
1	AA	878	A	C8-N9-C4	5.61	108.04	105.80
22	BA	2009	A	C4-C5-N7	-5.61	107.90	110.70
23	BB	15	A	C4-C5-N7	-5.61	107.90	110.70
1	AA	120	A	N9-C4-C5	5.61	108.04	105.80
22	BA	1677	A	C4-C5-C6	5.61	119.80	117.00
1	AA	1254	A	C5-C6-N1	5.60	120.50	117.70
22	BA	454	A	N9-C4-C5	5.60	108.04	105.80
22	BA	2541	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	74	A	C5-C6-N1	5.60	120.50	117.70
22	BA	1226	A	C5-N7-C8	5.60	106.70	103.90
1	AA	715	A	N3-C4-N9	5.60	131.88	127.40
22	BA	492	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	1096	A	N3-C4-N9	5.60	131.88	127.40
22	BA	1549	A	C8-N9-C4	5.60	108.04	105.80
22	BA	2080	A	N9-C4-C5	5.60	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2376	A	C4-C5-C6	5.60	119.80	117.00
21	AU	2	PRO	CA-N-CD	-5.60	103.66	111.50
22	BA	1040	A	C5-C6-N1	5.60	120.50	117.70
22	BA	1551	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	78	A	C5-C6-N1	5.59	120.50	117.70
1	AA	246	A	C4-C5-N7	-5.59	107.90	110.70
1	AA	1492	A	N3-C4-N9	5.59	131.88	127.40
22	BA	661	A	C4-C5-N7	-5.59	107.90	110.70
22	BA	878	A	C4-C5-C6	5.59	119.80	117.00
22	BA	1784	A	C5-C6-N1	5.59	120.50	117.70
22	BA	2560	A	C4-C5-C6	5.59	119.80	117.00
22	BA	432	A	N3-C4-N9	5.59	131.87	127.40
22	BA	802	A	N9-C4-C5	5.59	108.04	105.80
1	AA	1357	A	C4-C5-N7	-5.59	107.90	110.70
22	BA	616	A	N9-C4-C5	5.59	108.04	105.80
22	BA	1285	A	N9-C4-C5	5.59	108.04	105.80
22	BA	2173	A	N9-C4-C5	5.59	108.04	105.80
1	AA	155	A	C5-C6-N1	5.59	120.49	117.70
1	AA	704	A	C5-C6-N1	5.59	120.50	117.70
1	AA	1246	A	C4-C5-C6	5.59	119.80	117.00
1	AA	1363	A	N9-C4-C5	5.59	108.04	105.80
22	BA	10	A	C4-C5-C6	5.59	119.80	117.00
22	BA	863	A	C4-C5-C6	5.59	119.80	117.00
22	BA	2060	A	C4-C5-C6	5.59	119.79	117.00
22	BA	2734	A	N3-C4-N9	5.59	131.87	127.40
1	AA	675	A	C5-C6-N1	5.59	120.49	117.70
22	BA	1321	A	C5-C6-N1	5.59	120.49	117.70
1	AA	489	C	C2-N1-C1'	5.59	124.94	118.80
1	AA	915	A	C8-N9-C4	5.59	108.03	105.80
22	BA	402	A	C5-C6-N1	5.59	120.49	117.70
22	BA	483	A	C8-N9-C4	5.59	108.03	105.80
22	BA	718	A	C4-C5-N7	-5.59	107.91	110.70
22	BA	1129	A	N9-C4-C5	5.59	108.03	105.80
1	AA	1446	A	C4-C5-C6	5.58	119.79	117.00
22	BA	454	A	N3-C4-N9	5.58	131.87	127.40
22	BA	1057	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	1067	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	1067	A	C8-N9-C4	5.58	108.03	105.80
22	BA	1783	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	3	A	N3-C4-N9	5.58	131.87	127.40
1	AA	313	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	480	A	C4-C5-N7	-5.58	107.91	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2241	A	N9-C4-C5	5.58	108.03	105.80
22	BA	2392	A	C5-N7-C8	5.58	106.69	103.90
22	BA	2856	A	C4-C5-N7	-5.58	107.91	110.70
1	AA	282	A	C4-C5-C6	5.58	119.79	117.00
22	BA	849	A	C8-N9-C4	5.58	108.03	105.80
22	BA	1262	A	C5-C6-N1	5.58	120.49	117.70
22	BA	1640	A	C5-C6-N1	5.58	120.49	117.70
22	BA	1899	A	N3-C4-N9	5.58	131.87	127.40
22	BA	2882	A	C5-C6-N1	5.58	120.49	117.70
1	AA	1021	A	C4-C5-C6	5.58	119.79	117.00
22	BA	84	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	221	A	C4-C5-C6	5.58	119.79	117.00
22	BA	272	A	C5-C6-N1	5.58	120.49	117.70
22	BA	2184	A	C5-C6-N1	5.58	120.49	117.70
22	BA	2572	A	N9-C4-C5	5.58	108.03	105.80
1	AA	143	A	N3-C4-N9	5.58	131.86	127.40
22	BA	547	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	1001	A	N3-C4-N9	5.58	131.86	127.40
1	AA	65	A	N9-C4-C5	5.58	108.03	105.80
22	BA	279	A	C8-N9-C4	5.58	108.03	105.80
22	BA	1744	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	2412	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	2564	A	C4-C5-C6	5.58	119.79	117.00
1	AA	189	A	N9-C4-C5	5.57	108.03	105.80
1	AA	595	A	N9-C4-C5	5.57	108.03	105.80
1	AA	596	A	C5-C6-N1	5.57	120.49	117.70
22	BA	515	A	N3-C4-N9	5.57	131.86	127.40
22	BA	1579	A	C8-N9-C4	5.57	108.03	105.80
22	BA	1652	A	C5-C6-N1	5.57	120.49	117.70
22	BA	2013	A	N9-C4-C5	5.57	108.03	105.80
22	BA	2094	A	C4-C5-C6	5.57	119.79	117.00
22	BA	2183	A	C4-C5-C6	5.57	119.79	117.00
23	BB	94	A	C5-C6-N1	5.57	120.49	117.70
1	AA	1285	A	N9-C4-C5	5.57	108.03	105.80
22	BA	800	A	C4-C5-N7	-5.57	107.91	110.70
22	BA	973	A	N9-C4-C5	5.57	108.03	105.80
22	BA	1847	A	N9-C4-C5	5.57	108.03	105.80
22	BA	2340	A	N3-C4-N9	5.57	131.86	127.40
1	AA	892	A	C5-C6-N1	5.57	120.48	117.70
22	BA	13	A	C4-C5-N7	-5.57	107.92	110.70
22	BA	670	A	N3-C4-N9	5.57	131.86	127.40
22	BA	1690	A	N3-C4-N9	5.57	131.86	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1005	A	C4-C5-N7	-5.57	107.92	110.70
22	BA	632	A	C4-C5-C6	5.57	119.78	117.00
22	BA	936	A	N9-C4-C5	5.57	108.03	105.80
22	BA	1871	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	495	A	C4-C5-N7	-5.57	107.92	110.70
1	AA	716	A	C4-C5-C6	5.57	119.78	117.00
22	BA	1384	A	C5-C6-N1	5.57	120.48	117.70
22	BA	1616	A	N9-C4-C5	5.57	108.03	105.80
1	AA	59	A	N9-C4-C5	5.56	108.03	105.80
1	AA	282	A	N9-C4-C5	5.56	108.03	105.80
22	BA	217	A	C5-C6-N1	5.56	120.48	117.70
1	AA	321	A	N9-C4-C5	5.56	108.03	105.80
22	BA	925	A	C5-C6-N1	5.56	120.48	117.70
22	BA	1570	A	C4-C5-C6	5.56	119.78	117.00
22	BA	1918	A	N3-C4-N9	5.56	131.85	127.40
22	BA	2776	A	C4-C5-C6	5.56	119.78	117.00
1	AA	958	A	N9-C4-C5	5.56	108.02	105.80
22	BA	1244	A	N9-C4-C5	5.56	108.02	105.80
22	BA	1525	A	C5-C6-N1	5.56	120.48	117.70
22	BA	1960	A	C8-N9-C4	5.56	108.02	105.80
1	AA	60	A	N3-C4-N9	5.56	131.85	127.40
1	AA	716	A	C8-N9-C4	5.56	108.02	105.80
1	AA	1236	A	C8-N9-C4	5.56	108.02	105.80
22	BA	866	A	N3-C4-N9	5.56	131.85	127.40
22	BA	1301	A	C4-C5-C6	5.56	119.78	117.00
1	AA	315	A	C8-N9-C4	5.56	108.02	105.80
1	AA	969	A	N9-C4-C5	5.56	108.02	105.80
22	BA	371	A	N9-C4-C5	5.56	108.02	105.80
22	BA	1095	A	C8-N9-C4	5.56	108.02	105.80
22	BA	2019	A	C5-C6-N1	5.56	120.48	117.70
22	BA	2750	A	N3-C4-N9	5.56	131.85	127.40
22	BA	1327	A	N3-C4-N9	5.56	131.84	127.40
1	AA	50	A	C8-N9-C4	5.55	108.02	105.80
1	AA	1236	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	49	A	C8-N9-C4	5.55	108.02	105.80
22	BA	1535	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	1808	A	C8-N9-C4	5.55	108.02	105.80
22	BA	1821	A	N3-C4-N9	5.55	131.84	127.40
22	BA	2679	A	C8-N9-C4	5.55	108.02	105.80
1	AA	665	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	994	A	C8-N9-C4	5.55	108.02	105.80
22	BA	1354	A	N9-C4-C5	5.55	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	747	A	N3-C4-N9	5.55	131.84	127.40
1	AA	784	A	C8-N9-C4	5.55	108.02	105.80
1	AA	1368	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	91	A	N3-C4-N9	5.55	131.84	127.40
22	BA	878	A	C8-N9-C4	5.55	108.02	105.80
22	BA	1336	A	N9-C4-C5	5.55	108.02	105.80
22	BA	1848	A	N9-C4-C5	5.55	108.02	105.80
22	BA	1936	A	C8-N9-C1'	-5.55	117.71	127.70
23	BB	75	G	C5-C6-N1	5.55	114.28	111.50
1	AA	195	A	C4-C5-N7	-5.55	107.92	110.70
1	AA	1256	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	1430	A	C4-C5-C6	5.55	119.78	117.00
22	BA	909	A	N9-C4-C5	5.55	108.02	105.80
22	BA	1165	A	N3-C4-N9	5.55	131.84	127.40
22	BA	2740	A	N9-C4-C5	5.55	108.02	105.80
1	AA	468	A	C5-C6-N1	5.55	120.47	117.70
1	AA	1360	A	C4-C5-N7	-5.55	107.93	110.70
1	AA	26	A	C8-N9-C4	5.55	108.02	105.80
1	AA	313	A	C5-C6-N1	5.55	120.47	117.70
1	AA	1465	A	C5-C6-N1	5.55	120.47	117.70
22	BA	429	A	N3-C4-N9	5.55	131.84	127.40
22	BA	1322	A	C5-C6-N1	5.55	120.47	117.70
22	BA	1354	A	C5-C6-N1	5.55	120.47	117.70
22	BA	2278	A	N3-C4-N9	5.55	131.84	127.40
22	BA	2425	A	C5-C6-N1	5.55	120.47	117.70
1	AA	51	A	N3-C4-N9	5.54	131.84	127.40
1	AA	320	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	968	A	C8-N9-C4	5.54	108.02	105.80
22	BA	1265	A	C5-C6-N1	5.54	120.47	117.70
22	BA	1453	A	N9-C4-C5	5.54	108.02	105.80
22	BA	74	A	N3-C4-N9	5.54	131.84	127.40
22	BA	1525	A	N3-C4-N9	5.54	131.84	127.40
1	AA	8	A	C5-C6-N1	5.54	120.47	117.70
1	AA	66	A	C5-C6-N1	5.54	120.47	117.70
1	AA	149	A	N3-C4-N9	5.54	131.83	127.40
1	AA	754	C	C2-N1-C1'	5.54	124.90	118.80
1	AA	1368	A	C5-C6-N1	5.54	120.47	117.70
22	BA	2009	A	N9-C4-C5	5.54	108.02	105.80
22	BA	2434	A	C5-C6-N1	5.54	120.47	117.70
22	BA	2639	A	C5-C6-N1	5.54	120.47	117.70
1	AA	205	A	N9-C4-C5	5.54	108.02	105.80
22	BA	1978	A	C4-C5-C6	5.54	119.77	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	BL	60	ARG	C-N-CA	5.54	135.55	121.70
1	AA	109	A	N3-C4-N9	5.54	131.83	127.40
22	BA	1876	A	C5-C6-N1	5.54	120.47	117.70
22	BA	2386	A	C8-N9-C4	5.54	108.02	105.80
22	BA	2837	A	C4-C5-C6	5.54	119.77	117.00
23	BB	115	A	N9-C4-C5	5.54	108.02	105.80
22	BA	749	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	456	A	C8-N9-C4	5.54	108.01	105.80
1	AA	459	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	596	A	N3-C4-N9	5.54	131.83	127.40
1	AA	802	A	C5-C6-N1	5.54	120.47	117.70
1	AA	1021	A	C4-C5-N7	-5.54	107.93	110.70
1	AA	1151	A	N9-C4-C5	5.54	108.01	105.80
1	AA	1275	A	N3-C4-N9	5.54	131.83	127.40
1	AA	1289	A	N9-C4-C5	5.54	108.01	105.80
22	BA	84	A	C8-N9-C4	5.54	108.01	105.80
22	BA	322	A	C4-C5-C6	5.54	119.77	117.00
22	BA	1603	A	N9-C4-C5	5.54	108.01	105.80
1	AA	502	A	C5-C6-N1	5.53	120.47	117.70
22	BA	5	A	C4-C5-N7	-5.53	107.93	110.70
22	BA	42	A	N3-C4-N9	5.53	131.83	127.40
22	BA	1378	A	C8-N9-C4	5.53	108.01	105.80
22	BA	2758	A	N9-C4-C5	5.53	108.01	105.80
55	B8	51	A	N9-C4-C5	5.53	108.01	105.80
22	BA	423	A	C5-C6-N1	5.53	120.47	117.70
22	BA	504	A	C4-C5-C6	5.53	119.77	117.00
22	BA	1194	A	C4-C5-C6	5.53	119.77	117.00
1	AA	1110	A	N9-C4-C5	5.53	108.01	105.80
22	BA	1419	A	C5-C6-N1	5.53	120.47	117.70
22	BA	2516	A	C4-C5-N7	-5.53	107.93	110.70
22	BA	207	A	N3-C4-N9	5.53	131.82	127.40
22	BA	508	A	C8-N9-C4	5.53	108.01	105.80
22	BA	1088	A	C4-C5-N7	-5.53	107.94	110.70
22	BA	2163	A	C8-N9-C4	5.53	108.01	105.80
22	BA	2176	A	N9-C4-C5	5.53	108.01	105.80
1	AA	466	A	C4-C5-N7	-5.53	107.94	110.70
1	AA	807	A	N9-C4-C5	5.53	108.01	105.80
1	AA	1014	A	N3-C4-N9	5.53	131.82	127.40
22	BA	1801	A	C4-C5-C6	5.53	119.76	117.00
22	BA	2657	A	N9-C4-C5	5.53	108.01	105.80
22	BA	2820	A	C4-C5-C6	5.53	119.76	117.00
23	BB	66	A	C8-N9-C4	5.53	108.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	236	A	C5-C6-N1	5.53	120.46	117.70
22	BA	1677	A	N3-C4-N9	5.53	131.82	127.40
1	AA	171	A	N9-C4-C5	5.52	108.01	105.80
1	AA	1408	A	C4-C5-C6	5.52	119.76	117.00
22	BA	104	A	C4-C5-C6	5.52	119.76	117.00
22	BA	792	A	C4-C5-C6	5.52	119.76	117.00
22	BA	2058	A	N9-C4-C5	5.52	108.01	105.80
23	BB	104	A	C5-C6-N1	5.52	120.46	117.70
1	AA	1145	A	N9-C4-C5	5.52	108.01	105.80
22	BA	1095	A	N9-C4-C5	5.52	108.01	105.80
22	BA	1700	A	C5-C6-N1	5.52	120.46	117.70
22	BA	354	A	C5-C6-N1	5.52	120.46	117.70
1	AA	59	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	602	A	N9-C4-C5	5.52	108.01	105.80
22	BA	1503	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	2134	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	918	A	N3-C4-N9	5.52	131.81	127.40
22	BA	1237	A	N3-C4-N9	5.52	131.81	127.40
22	BA	1453	A	C5-C6-N1	5.52	120.46	117.70
23	BB	66	A	N3-C4-N9	5.52	131.81	127.40
22	BA	627	A	C4-C5-C6	5.51	119.76	117.00
22	BA	670	A	C4-C5-C6	5.51	119.76	117.00
22	BA	1089	A	N9-C4-C5	5.51	108.01	105.80
22	BA	1505	A	C8-N9-C4	5.51	108.01	105.80
55	B8	42	A	N9-C4-C5	5.51	108.00	105.80
1	AA	253	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	374	A	N9-C4-C5	5.51	108.00	105.80
1	AA	1213	A	C8-N9-C4	5.51	108.00	105.80
22	BA	2587	A	C4-C5-N7	-5.51	107.94	110.70
22	BA	2635	A	C4-C5-N7	-5.51	107.94	110.70
22	BA	2835	A	C4-C5-C6	5.51	119.76	117.00
1	AA	1145	A	N3-C4-N9	5.51	131.81	127.40
1	AA	1169	A	C4-C5-N7	-5.51	107.94	110.70
1	AA	1180	A	C4-C5-N7	-5.51	107.94	110.70
22	BA	2418	A	C4-C5-C6	5.51	119.75	117.00
22	BA	538	A	C4-C5-N7	-5.51	107.95	110.70
22	BA	1237	A	C4-C5-N7	-5.51	107.95	110.70
22	BA	2309	A	C4-C5-C6	5.51	119.75	117.00
22	BA	2829	A	N3-C4-N9	5.51	131.81	127.40
1	AA	753	A	N9-C4-C5	5.51	108.00	105.80
22	BA	1439	A	C4-C5-N7	-5.51	107.95	110.70
22	BA	1938	A	N9-C4-C5	5.51	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2191	A	C5-C6-N1	5.51	120.45	117.70
1	AA	336	A	N9-C4-C5	5.50	108.00	105.80
1	AA	1311	A	C5-C6-N1	5.50	120.45	117.70
22	BA	582	A	N3-C4-N9	5.50	131.80	127.40
22	BA	2119	A	C4-C5-C6	5.50	119.75	117.00
1	AA	238	A	C5-C6-N1	5.50	120.45	117.70
1	AA	1169	A	N9-C4-C5	5.50	108.00	105.80
22	BA	282	A	N3-C4-N9	5.50	131.80	127.40
22	BA	1665	A	C5-C6-N1	5.50	120.45	117.70
22	BA	2800	A	N3-C4-N9	5.50	131.80	127.40
22	BA	104	A	C8-N9-C4	5.50	108.00	105.80
22	BA	1254	A	N3-C4-N9	5.50	131.80	127.40
22	BA	2158	A	C4-C5-C6	5.50	119.75	117.00
22	BA	631	A	C5-C6-N1	5.50	120.45	117.70
23	BB	24	G	C6-N1-C2	-5.50	121.80	125.10
1	AA	448	A	C5-C6-N1	5.50	120.45	117.70
22	BA	371	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	1490	A	C5-C6-N1	5.50	120.45	117.70
22	BA	2241	A	C5-C6-N1	5.50	120.45	117.70
22	BA	195	A	C5-C6-N1	5.50	120.45	117.70
22	BA	2425	A	C8-N9-C4	5.50	108.00	105.80
1	AA	1492	A	C8-N9-C4	5.50	108.00	105.80
22	BA	89	A	N3-C4-N9	5.50	131.80	127.40
22	BA	322	A	N3-C4-N9	5.50	131.80	127.40
22	BA	1142	A	C8-N9-C4	5.50	108.00	105.80
22	BA	1385	A	C8-N9-C4	5.50	108.00	105.80
1	AA	327	A	C5-C6-N1	5.49	120.45	117.70
1	AA	344	A	C4-C5-C6	5.49	119.75	117.00
1	AA	648	A	N9-C4-C5	5.49	108.00	105.80
1	AA	1254	A	N9-C4-C5	5.49	108.00	105.80
22	BA	49	A	C4-C5-N7	-5.49	107.95	110.70
22	BA	981	A	C4-C5-C6	5.49	119.75	117.00
22	BA	1096	A	N9-C4-C5	5.49	108.00	105.80
22	BA	2748	A	C5-C6-N1	5.49	120.45	117.70
1	AA	8	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	493	A	C4-C5-N7	-5.49	107.95	110.70
1	AA	72	A	N3-C4-N9	5.49	131.79	127.40
1	AA	74	A	N3-C4-N9	5.49	131.79	127.40
1	AA	1014	A	C4-C5-C6	5.49	119.75	117.00
22	BA	5	A	C5-C6-N1	5.49	120.45	117.70
22	BA	693	A	C5-C6-N1	5.49	120.44	117.70
22	BA	722	A	C5-C6-N1	5.49	120.44	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1757	A	C4-C5-C6	5.49	119.75	117.00
22	BA	1899	A	C4-C5-N7	-5.49	107.95	110.70
23	BB	99	A	N9-C4-C5	5.49	108.00	105.80
1	AA	465	A	C8-N9-C4	5.49	108.00	105.80
1	AA	572	A	C4-C5-N7	-5.49	107.95	110.70
22	BA	522	A	C4-C5-N7	-5.49	107.96	110.70
22	BA	2211	A	N9-C4-C5	5.49	108.00	105.80
22	BA	2726	A	N3-C4-N9	5.49	131.79	127.40
22	BA	2810	A	N3-C4-N9	5.49	131.79	127.40
1	AA	1145	A	C4-C5-N7	-5.49	107.96	110.70
1	AA	77	A	C5-C6-N1	5.49	120.44	117.70
22	BA	199	A	C4-C5-C6	5.49	119.74	117.00
22	BA	1877	A	C5-C6-N1	5.49	120.44	117.70
23	BB	78	A	C5-C6-N1	5.49	120.44	117.70
1	AA	172	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	321	A	C8-N9-C4	5.48	107.99	105.80
1	AA	533	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	1251	A	C4-C5-N7	-5.48	107.96	110.70
2	AB	193	PRO	CA-N-CD	-5.48	103.82	111.50
22	BA	504	A	N9-C4-C5	5.48	107.99	105.80
22	BA	515	A	C5-C6-N1	5.48	120.44	117.70
22	BA	1654	A	C4-C5-C6	5.48	119.74	117.00
1	AA	1146	A	N9-C4-C5	5.48	107.99	105.80
22	BA	191	A	C5-C6-N1	5.48	120.44	117.70
22	BA	322	A	C5-C6-N1	5.48	120.44	117.70
22	BA	346	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	439	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	1000	A	C8-N9-C4	5.48	107.99	105.80
1	AA	19	A	N3-C4-N9	5.48	131.78	127.40
1	AA	223	A	N9-C4-C5	5.48	107.99	105.80
1	AA	320	A	C4-C5-C6	5.48	119.74	117.00
1	AA	435	A	C8-N9-C4	5.48	107.99	105.80
1	AA	777	A	N3-C4-N9	5.48	131.78	127.40
1	AA	1036	A	N9-C4-C5	5.48	107.99	105.80
22	BA	144	A	C5-C6-N1	5.48	120.44	117.70
22	BA	516	C	C6-N1-C2	-5.48	118.11	120.30
22	BA	945	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	1420	A	N9-C4-C5	5.48	107.99	105.80
22	BA	2534	A	C4-C5-C6	5.48	119.74	117.00
22	BA	2560	A	N3-C4-N9	5.48	131.78	127.40
1	AA	1042	A	C8-N9-C4	5.48	107.99	105.80
22	BA	347	A	C4-C5-N7	-5.48	107.96	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	761	A	C5-N7-C8	5.48	106.64	103.90
22	BA	819	A	C5-C6-N1	5.48	120.44	117.70
22	BA	2513	A	C4-C5-N7	-5.48	107.96	110.70
1	AA	66	A	N9-C4-C5	5.48	107.99	105.80
1	AA	695	A	C8-N9-C4	5.48	107.99	105.80
1	AA	1216	A	C8-N9-C4	5.48	107.99	105.80
1	AA	1350	A	C5-C6-N1	5.48	120.44	117.70
22	BA	272	A	C8-N9-C4	5.48	107.99	105.80
22	BA	346	A	N9-C4-C5	5.48	107.99	105.80
22	BA	1039	A	N3-C4-N9	5.48	131.78	127.40
22	BA	1434	A	N9-C4-C5	5.48	107.99	105.80
22	BA	2273	A	N9-C4-C5	5.48	107.99	105.80
22	BA	2632	A	N3-C4-N9	5.48	131.78	127.40
1	AA	1363	A	C5-C6-N1	5.48	120.44	117.70
22	BA	528	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	547	A	N9-C4-C5	5.48	107.99	105.80
22	BA	2135	A	N9-C4-C5	5.48	107.99	105.80
22	BA	2282	G	O4'-C1'-N9	5.48	112.58	108.20
1	AA	320	A	N3-C4-N9	5.47	131.78	127.40
1	AA	459	A	N9-C4-C5	5.47	107.99	105.80
1	AA	509	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	1152	A	C5-C6-N1	5.47	120.44	117.70
22	BA	197	A	N9-C4-C5	5.47	107.99	105.80
22	BA	529	A	N3-C4-N9	5.47	131.78	127.40
22	BA	2171	A	C4-C5-N7	-5.47	107.96	110.70
22	BA	2211	A	N3-C4-N9	5.47	131.78	127.40
22	BA	2434	A	C4-C5-N7	-5.47	107.96	110.70
1	AA	205	A	C4-C5-N7	-5.47	107.96	110.70
22	BA	449	A	N9-C4-C5	5.47	107.99	105.80
22	BA	501	A	C4-C5-C6	5.47	119.74	117.00
22	BA	2183	A	N3-C4-N9	5.47	131.78	127.40
1	AA	50	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	1167	A	C4-C5-C6	5.47	119.74	117.00
22	BA	529	A	C4-C5-C6	5.47	119.73	117.00
1	AA	172	A	N9-C4-C5	5.47	107.99	105.80
22	BA	10	A	C5-C6-N1	5.47	120.44	117.70
22	BA	979	A	N3-C4-N9	5.47	131.78	127.40
1	AA	162	A	C8-N9-C4	5.47	107.99	105.80
1	AA	1289	A	C4-C5-C6	5.47	119.73	117.00
22	BA	896	A	C4-C5-C6	5.47	119.73	117.00
1	AA	468	A	C4-C5-N7	-5.47	107.97	110.70
1	AA	1036	A	C4-C5-N7	-5.47	107.97	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1398	A	C5-C6-N1	5.47	120.43	117.70
1	AA	1534	A	C4-C5-C6	5.47	119.73	117.00
22	BA	1701	A	C5-C6-N1	5.47	120.43	117.70
22	BA	1889	A	C5-C6-N1	5.47	120.43	117.70
22	BA	2095	A	N9-C4-C5	5.47	107.99	105.80
22	BA	2837	A	N3-C4-N9	5.47	131.77	127.40
22	BA	599	A	C4-C5-C6	5.46	119.73	117.00
22	BA	756	A	N3-C4-N9	5.46	131.77	127.40
22	BA	1096	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	2005	A	C5-C6-N1	5.46	120.43	117.70
1	AA	574	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	294	A	N3-C4-N9	5.46	131.77	127.40
22	BA	844	A	C8-N9-C4	5.46	107.98	105.80
1	AA	889	A	C4-C5-N7	-5.46	107.97	110.70
1	AA	1246	A	N3-C4-N9	5.46	131.77	127.40
22	BA	917	A	C5-C6-N1	5.46	120.43	117.70
22	BA	2014	A	C4-C5-C6	5.46	119.73	117.00
55	B8	21	A	N9-C4-C5	5.46	107.98	105.80
1	AA	1248	A	C8-N9-C4	5.46	107.98	105.80
1	AA	371	A	C8-N9-C4	5.46	107.98	105.80
1	AA	784	A	C5-C6-N1	5.46	120.43	117.70
1	AA	906	A	C5-C6-N1	5.46	120.43	117.70
22	BA	282	A	N9-C4-C5	5.46	107.98	105.80
22	BA	348	A	C5-C6-N1	5.46	120.43	117.70
22	BA	602	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	1302	A	N3-C4-N9	5.46	131.77	127.40
22	BA	1496	A	C8-N9-C4	5.46	107.98	105.80
22	BA	1665	A	C4-C5-N7	-5.46	107.97	110.70
23	BB	15	A	C5-C6-N1	5.46	120.43	117.70
1	AA	1101	A	N3-C4-N9	5.46	131.77	127.40
22	BA	332	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	514	A	C4-C5-C6	5.46	119.73	117.00
22	BA	2632	A	C8-N9-C4	5.46	107.98	105.80
22	BA	2887	A	C8-N9-C4	5.46	107.98	105.80
1	AA	676	A	C4-C5-C6	5.46	119.73	117.00
1	AA	889	A	C5-C6-N1	5.46	120.43	117.70
22	BA	2829	A	C8-N9-C4	5.46	107.98	105.80
1	AA	109	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	1012	A	N9-C4-C5	5.45	107.98	105.80
1	AA	1016	A	C4-C5-N7	-5.45	107.97	110.70
1	AA	1413	A	C4-C5-N7	-5.45	107.97	110.70
22	BA	2119	A	C8-N9-C4	5.45	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2476	A	C8-N9-C4	5.45	107.98	105.80
23	BB	119	A	C5-C6-N1	5.45	120.43	117.70
22	BA	782	A	C5-C6-N1	5.45	120.43	117.70
1	AA	279	A	N3-C4-N9	5.45	131.76	127.40
1	AA	309	A	N3-C4-N9	5.45	131.76	127.40
22	BA	599	A	N3-C4-N9	5.45	131.76	127.40
22	BA	739	A	C5-C6-N1	5.45	120.42	117.70
1	AA	563	A	C8-N9-C4	5.45	107.98	105.80
1	AA	1014	A	C4-C5-N7	-5.45	107.98	110.70
22	BA	972	A	C5-N7-C8	5.45	106.62	103.90
22	BA	2829	A	C4-C5-C6	5.45	119.72	117.00
1	AA	1360	A	N9-C4-C5	5.45	107.98	105.80
1	AA	1480	A	C5-C6-N1	5.45	120.42	117.70
1	AA	51	A	C4-C5-C6	5.45	119.72	117.00
1	AA	171	A	C5-C6-N1	5.45	120.42	117.70
22	BA	1385	A	N3-C4-N9	5.45	131.76	127.40
22	BA	1544	A	C4-C5-C6	5.45	119.72	117.00
1	AA	959	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	1430	A	N3-C4-N9	5.44	131.75	127.40
22	BA	478	A	C5-C6-N1	5.44	120.42	117.70
22	BA	1014	A	N9-C4-C5	5.44	107.98	105.80
22	BA	2542	A	C4-C5-N7	-5.44	107.98	110.70
1	AA	66	A	C8-N9-C4	5.44	107.98	105.80
1	AA	687	A	N9-C4-C5	5.44	107.98	105.80
22	BA	13	A	C5-C6-N1	5.44	120.42	117.70
22	BA	1226	A	C4-C5-C6	5.44	119.72	117.00
22	BA	2314	A	N9-C4-C5	5.44	107.98	105.80
22	BA	590	A	C5-C6-N1	5.44	120.42	117.70
22	BA	1420	A	C4-C5-C6	5.44	119.72	117.00
22	BA	1566	A	C4-C5-C6	5.44	119.72	117.00
1	AA	451	A	C8-N9-C4	5.44	107.97	105.80
1	AA	1311	A	C8-N9-C4	5.44	107.97	105.80
1	AA	1410	A	N9-C4-C5	5.44	107.97	105.80
1	AA	1493	A	N3-C4-N9	5.44	131.75	127.40
22	BA	1129	A	C5-C6-N1	5.44	120.42	117.70
22	BA	1494	A	N9-C4-C5	5.44	107.97	105.80
22	BA	1794	A	C4-C5-C6	5.44	119.72	117.00
1	AA	250	A	C8-N9-C4	5.44	107.97	105.80
22	BA	44	A	C4-C5-N7	-5.44	107.98	110.70
22	BA	2435	A	C4-C5-C6	5.44	119.72	117.00
1	AA	51	A	N9-C4-C5	5.43	107.97	105.80
1	AA	382	A	C4-C5-N7	-5.43	107.98	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	816	A	N9-C4-C5	5.43	107.97	105.80
1	AA	908	A	C4-C5-N7	-5.43	107.98	110.70
22	BA	661	A	C8-N9-C4	5.43	107.97	105.80
1	AA	205	A	C5-C6-N1	5.43	120.42	117.70
22	BA	44	A	C8-N9-C4	5.43	107.97	105.80
22	BA	1744	A	C8-N9-C4	5.43	107.97	105.80
22	BA	1815	A	C5-N7-C8	5.43	106.62	103.90
1	AA	181	A	C5-C6-N1	5.43	120.42	117.70
1	AA	1082	A	C5-C6-N1	5.43	120.42	117.70
22	BA	270	A	C5-C6-N1	5.43	120.42	117.70
22	BA	1342	A	C4-C5-N7	-5.43	107.98	110.70
22	BA	1916	A	N9-C4-C5	5.43	107.97	105.80
23	BB	57	A	N3-C4-N9	5.43	131.75	127.40
1	AA	167	A	C5-C6-N1	5.43	120.42	117.70
1	AA	766	A	C4-C5-N7	-5.43	107.99	110.70
22	BA	1434	A	N3-C4-N9	5.43	131.74	127.40
22	BA	1570	A	N9-C4-C5	5.43	107.97	105.80
22	BA	1586	A	N9-C4-C5	5.43	107.97	105.80
22	BA	1635	A	C8-N9-C4	5.43	107.97	105.80
22	BA	1912	A	C4-C5-C6	5.43	119.72	117.00
22	BA	2117	A	C8-N9-C4	5.43	107.97	105.80
22	BA	2270	A	C8-N9-C4	5.43	107.97	105.80
1	AA	918	A	C8-N9-C4	5.43	107.97	105.80
22	BA	2205	A	N3-C4-N9	5.43	131.74	127.40
1	AA	649	A	C4-C5-C6	5.43	119.71	117.00
1	AA	1155	A	C4-C5-N7	-5.43	107.99	110.70
22	BA	782	A	N9-C4-C5	5.43	107.97	105.80
1	AA	712	A	C8-N9-C4	5.42	107.97	105.80
1	AA	872	A	C4-C5-C6	5.42	119.71	117.00
1	AA	1374	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	1465	A	N9-C4-C5	5.42	107.97	105.80
22	BA	203	A	C5-N7-C8	5.42	106.61	103.90
22	BA	613	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	2736	A	N9-C4-C5	5.42	107.97	105.80
1	AA	344	A	N3-C4-N9	5.42	131.74	127.40
22	BA	721	A	C5-C6-N1	5.42	120.41	117.70
22	BA	2346	A	C8-N9-C4	5.42	107.97	105.80
1	AA	1285	A	C4-C5-C6	5.42	119.71	117.00
22	BA	1987	A	N3-C4-N9	5.42	131.74	127.40
22	BA	2031	A	N9-C4-C5	5.42	107.97	105.80
22	BA	2173	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	3	A	C8-N9-C4	5.42	107.97	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2564	A	C5-C6-N1	5.42	120.41	117.70
1	AA	95	C	C2-N1-C1'	5.42	124.76	118.80
1	AA	228	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	487	A	C5-C6-N1	5.42	120.41	117.70
1	AA	728	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	1151	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	529	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	1301	A	C8-N9-C4	5.42	107.97	105.80
22	BA	1668	A	N3-C4-N9	5.42	131.73	127.40
22	BA	1928	A	C8-N9-C4	5.42	107.97	105.80
22	BA	2014	A	N9-C4-C5	5.42	107.97	105.80
22	BA	2071	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	629	A	C5-C6-N1	5.42	120.41	117.70
1	AA	780	A	C4-C5-N7	-5.42	107.99	110.70
1	AA	1456	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	207	A	N9-C4-C5	5.42	107.97	105.80
22	BA	2117	A	N9-C4-C5	5.42	107.97	105.80
22	BA	2418	A	C5-C6-N1	5.42	120.41	117.70
22	BA	2765	A	C8-N9-C4	5.42	107.97	105.80
1	AA	1158	C	N3-C2-O2	-5.42	118.11	121.90
22	BA	340	A	N9-C4-C5	5.42	107.97	105.80
22	BA	342	A	N9-C4-C5	5.42	107.97	105.80
22	BA	1392	A	C5-C6-N1	5.42	120.41	117.70
1	AA	44	A	C8-N9-C4	5.41	107.97	105.80
1	AA	663	A	N9-C4-C5	5.41	107.97	105.80
22	BA	278	A	C5-C6-N1	5.41	120.41	117.70
22	BA	382	A	C8-N9-C4	5.41	107.97	105.80
22	BA	1583	A	N3-C4-N9	5.41	131.73	127.40
22	BA	2108	A	N9-C4-C5	5.41	107.97	105.80
22	BA	2169	A	C5-C6-N1	5.41	120.41	117.70
22	BA	2433	A	C5-C6-N1	5.41	120.41	117.70
1	AA	1005	A	N9-C4-C5	5.41	107.97	105.80
22	BA	217	A	C4-C5-C6	5.41	119.70	117.00
22	BA	1088	A	C5-C6-N1	5.41	120.41	117.70
22	BA	1515	A	C4-C5-N7	-5.41	108.00	110.70
22	BA	2225	A	C5-C6-N1	5.41	120.41	117.70
22	BA	2274	A	N3-C4-N9	5.41	131.73	127.40
1	AA	892	A	N9-C4-C5	5.41	107.96	105.80
22	BA	1366	A	C5-C6-N1	5.41	120.40	117.70
22	BA	2158	A	N3-C4-N9	5.41	131.73	127.40
22	BA	2314	A	C4-C5-C6	5.41	119.70	117.00
22	BA	2632	A	C5-C6-N1	5.41	120.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	408	A	C8-N9-C4	5.41	107.96	105.80
1	AA	482	A	C5-C6-N1	5.41	120.40	117.70
1	AA	996	A	C4-C5-N7	-5.41	108.00	110.70
22	BA	2314	A	N3-C4-N9	5.41	131.73	127.40
1	AA	441	A	N9-C4-C5	5.41	107.96	105.80
1	AA	1036	A	C8-N9-C4	5.41	107.96	105.80
1	AA	1289	A	N3-C4-N9	5.41	131.72	127.40
22	BA	14	A	N9-C4-C5	5.41	107.96	105.80
22	BA	256	A	N9-C4-C5	5.41	107.96	105.80
22	BA	1214	A	N3-C4-N9	5.41	131.72	127.40
22	BA	1509	A	C4-C5-N7	-5.41	108.00	110.70
23	BB	39	A	C4-C5-N7	-5.41	108.00	110.70
1	AA	101	A	N9-C4-C5	5.40	107.96	105.80
1	AA	860	A	C8-N9-C4	5.40	107.96	105.80
1	AA	906	A	N3-C4-N9	5.40	131.72	127.40
22	BA	1048	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	366	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	681	A	C5-C6-N1	5.40	120.40	117.70
22	BA	1253	A	C5-N7-C8	5.40	106.60	103.90
22	BA	1354	A	C8-N9-C4	5.40	107.96	105.80
22	BA	2381	A	N9-C4-C5	5.40	107.96	105.80
1	AA	81	A	C8-N9-C4	5.40	107.96	105.80
1	AA	649	A	C4-C5-N7	-5.40	108.00	110.70
1	AA	816	A	C8-N9-C4	5.40	107.96	105.80
22	BA	2450	A	N3-C4-N9	5.40	131.72	127.40
22	BA	866	A	C5-C6-N1	5.40	120.40	117.70
22	BA	2753	A	C4-C5-C6	5.40	119.70	117.00
1	AA	819	A	C4-C5-C6	5.40	119.70	117.00
1	AA	900	A	N9-C4-C5	5.40	107.96	105.80
1	AA	1252	A	C5-C6-N1	5.40	120.40	117.70
1	AA	1476	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	146	A	N3-C4-N9	5.40	131.72	127.40
22	BA	503	A	C8-N9-C4	5.40	107.96	105.80
22	BA	849	A	N9-C4-C5	5.40	107.96	105.80
22	BA	1089	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	2873	A	N9-C4-C5	5.40	107.96	105.80
1	AA	676	A	N9-C4-C5	5.40	107.96	105.80
1	AA	1534	A	N3-C4-N9	5.40	131.72	127.40
22	BA	152	A	C8-N9-C4	5.40	107.96	105.80
22	BA	1039	A	C5-C6-N1	5.40	120.40	117.70
1	AA	3	A	N9-C4-C5	5.39	107.96	105.80
22	BA	152	A	N9-C4-C5	5.39	107.96	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1676	A	N9-C4-C5	5.39	107.96	105.80
1	AA	119	A	C5-C6-N1	5.39	120.40	117.70
1	AA	196	A	N3-C4-N9	5.39	131.71	127.40
1	AA	1396	A	C8-N9-C4	5.39	107.96	105.80
1	AA	1480	A	N3-C4-N9	5.39	131.71	127.40
22	BA	1111	A	C8-N9-C4	5.39	107.96	105.80
22	BA	2077	A	N9-C4-C5	5.39	107.96	105.80
1	AA	192	A	C5-C6-N1	5.39	120.40	117.70
1	AA	1275	A	C4-C5-N7	-5.39	108.00	110.70
22	BA	1987	A	N9-C4-C5	5.39	107.96	105.80
1	AA	595	A	C4-C5-N7	-5.39	108.00	110.70
1	AA	1152	A	C8-N9-C4	5.39	107.96	105.80
22	BA	668	A	N3-C4-N9	5.39	131.71	127.40
22	BA	878	A	C4-C5-N7	-5.39	108.01	110.70
22	BA	1230	A	N3-C4-N9	5.39	131.71	127.40
22	BA	2173	A	C8-N9-C4	5.39	107.96	105.80
22	BA	2765	A	C4-C5-N7	-5.39	108.00	110.70
22	BA	2860	A	N9-C4-C5	5.39	107.96	105.80
1	AA	81	A	C4-C5-N7	-5.39	108.01	110.70
22	BA	404	A	C4-C5-C6	5.39	119.69	117.00
22	BA	2091	C	C6-N1-C2	-5.39	118.14	120.30
1	AA	696	A	N9-C4-C5	5.39	107.95	105.80
22	BA	142	A	C5-C6-N1	5.39	120.39	117.70
22	BA	1952	A	C5-C6-N1	5.39	120.39	117.70
1	AA	600	A	N9-C4-C5	5.38	107.95	105.80
1	AA	768	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1357	A	C5-C6-N1	5.38	120.39	117.70
22	BA	892	A	C4-C5-C6	5.38	119.69	117.00
22	BA	2274	A	C5-C6-N1	5.38	120.39	117.70
22	BA	2311	A	C5-C6-N1	5.38	120.39	117.70
22	BA	2314	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	7	A	N3-C4-N9	5.38	131.71	127.40
1	AA	553	A	C5-C6-N1	5.38	120.39	117.70
22	BA	984	A	O4'-C1'-N9	5.38	112.51	108.20
22	BA	2764	A	N3-C4-N9	5.38	131.71	127.40
23	BB	24	G	C5-C6-O6	-5.38	125.37	128.60
1	AA	1394	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	354	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	2062	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	2660	A	C4-C5-C6	5.38	119.69	117.00
22	BA	1287	A	C8-N9-C4	5.38	107.95	105.80
22	BA	1395	A	N3-C4-N9	5.38	131.70	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	52	A	C4-C5-C6	5.38	119.69	117.00
23	BB	109	A	C5-C6-N1	5.38	120.39	117.70
1	AA	393	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	452	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	706	A	C4-C5-N7	-5.38	108.01	110.70
1	AA	1229	A	N3-C4-N9	5.38	131.70	127.40
22	BA	310	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	1469	A	N9-C4-C5	5.38	107.95	105.80
22	BA	1632	A	C8-N9-C4	5.38	107.95	105.80
22	BA	2247	A	C5-C6-N1	5.38	120.39	117.70
22	BA	2883	A	N3-C4-N9	5.38	131.70	127.40
1	AA	1155	A	C4-C5-C6	5.38	119.69	117.00
22	BA	1966	A	C5-C6-N1	5.38	120.39	117.70
1	AA	139	A	C8-N9-C4	5.37	107.95	105.80
1	AA	1105	A	C4-C5-N7	-5.37	108.01	110.70
22	BA	693	A	N9-C4-C5	5.37	107.95	105.80
22	BA	715	A	C5-C6-N1	5.37	120.39	117.70
22	BA	1008	A	N3-C4-N9	5.37	131.70	127.40
22	BA	2432	A	C8-N9-C4	5.37	107.95	105.80
22	BA	2726	A	C4-C5-C6	5.37	119.69	117.00
1	AA	1105	A	C5-C6-N1	5.37	120.39	117.70
22	BA	705	A	N9-C4-C5	5.37	107.95	105.80
22	BA	716	A	N9-C4-C5	5.37	107.95	105.80
22	BA	1147	A	N9-C4-C5	5.37	107.95	105.80
22	BA	1204	A	N3-C4-N9	5.37	131.70	127.40
22	BA	1532	A	N3-C4-N9	5.37	131.70	127.40
22	BA	1532	A	N9-C4-C5	5.37	107.95	105.80
22	BA	2733	A	N9-C4-C5	5.37	107.95	105.80
1	AA	499	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	221	A	N3-C4-N9	5.37	131.70	127.40
22	BA	514	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	735	A	C8-N9-C4	5.37	107.95	105.80
1	AA	1476	A	N3-C4-N9	5.37	131.69	127.40
22	BA	631	A	C4-C5-C6	5.37	119.69	117.00
22	BA	1419	A	N3-C4-N9	5.37	131.69	127.40
22	BA	2346	A	C4-C5-C6	5.37	119.68	117.00
22	BA	2748	A	C4-C5-C6	5.37	119.68	117.00
1	AA	1250	A	C5-C6-N1	5.37	120.38	117.70
22	BA	637	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	2170	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	2450	A	C4-C5-C6	5.37	119.68	117.00
23	BB	50	A	C4-C5-C6	5.37	119.68	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1431	A	C5-C6-N1	5.37	120.38	117.70
22	BA	63	A	C8-N9-C4	5.37	107.95	105.80
1	AA	161	A	N9-C4-C5	5.36	107.95	105.80
1	AA	600	A	C5-C6-N1	5.36	120.38	117.70
1	AA	694	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	706	A	N9-C4-C5	5.36	107.94	105.80
22	BA	340	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	936	A	C8-N9-C4	5.36	107.94	105.80
22	BA	2054	A	C8-N9-C4	5.36	107.95	105.80
22	BA	2126	A	N9-C4-C5	5.36	107.94	105.80
22	BA	2564	A	N9-C4-C5	5.36	107.94	105.80
22	BA	2824	C	C5-C6-N1	5.36	123.68	121.00
1	AA	353	A	C8-N9-C4	5.36	107.94	105.80
1	AA	958	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	1046	A	C5-C6-N1	5.36	120.38	117.70
22	BA	685	A	C5-C6-N1	5.36	120.38	117.70
22	BA	1522	A	N3-C4-N9	5.36	131.69	127.40
22	BA	1548	A	N9-C4-C5	5.36	107.94	105.80
1	AA	262	A	C8-N9-C4	5.36	107.94	105.80
1	AA	263	A	C5-C6-N1	5.36	120.38	117.70
1	AA	482	A	N9-C4-C5	5.36	107.94	105.80
1	AA	502	A	N9-C4-C5	5.36	107.94	105.80
1	AA	1410	A	C8-N9-C4	5.36	107.94	105.80
22	BA	118	A	N9-C4-C5	5.36	107.94	105.80
22	BA	1745	A	C8-N9-C4	5.36	107.94	105.80
22	BA	2738	A	N3-C4-N9	5.36	131.69	127.40
1	AA	495	A	C4-C5-C6	5.36	119.68	117.00
22	BA	1365	A	C5-C6-N1	5.36	120.38	117.70
1	AA	353	A	C4-C5-N7	-5.36	108.02	110.70
1	AA	663	A	N3-C4-N9	5.36	131.69	127.40
1	AA	794	A	C5-C6-N1	5.36	120.38	117.70
22	BA	1801	A	C5-C6-N1	5.36	120.38	117.70
1	AA	1067	A	C8-N9-C4	5.36	107.94	105.80
22	BA	241	A	C5-C6-N1	5.36	120.38	117.70
22	BA	677	A	C8-N9-C4	5.36	107.94	105.80
22	BA	1717	A	C5-C6-N1	5.36	120.38	117.70
22	BA	2335	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	2426	A	N9-C4-C5	5.36	107.94	105.80
22	BA	2682	A	C4-C5-C6	5.36	119.68	117.00
1	AA	649	A	N3-C4-N9	5.35	131.68	127.40
1	AA	1319	A	C4-C5-N7	-5.35	108.02	110.70
22	BA	422	A	N9-C4-C5	5.35	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1912	A	N9-C4-C5	5.35	107.94	105.80
1	AA	71	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	238	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	253	A	N3-C4-N9	5.35	131.68	127.40
1	AA	784	A	N3-C4-N9	5.35	131.68	127.40
1	AA	915	A	C4-C5-N7	-5.35	108.02	110.70
22	BA	104	A	N9-C4-C5	5.35	107.94	105.80
22	BA	556	A	N9-C4-C5	5.35	107.94	105.80
22	BA	1453	A	N3-C4-N9	5.35	131.68	127.40
22	BA	1900	A	N9-C4-C5	5.35	107.94	105.80
22	BA	2267	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	978	A	C4-C5-C6	5.35	119.68	117.00
22	BA	900	A	C4-C5-N7	-5.35	108.03	110.70
22	BA	941	A	N3-C4-N9	5.35	131.68	127.40
22	BA	1650	A	C8-N9-C4	5.35	107.94	105.80
1	AA	451	A	C4-C5-N7	-5.35	108.03	110.70
1	AA	1441	A	C4-C5-N7	-5.35	108.03	110.70
22	BA	111	A	C4-C5-N7	-5.35	108.03	110.70
22	BA	146	A	C4-C5-C6	5.35	119.67	117.00
22	BA	603	A	C4-C5-C6	5.35	119.67	117.00
22	BA	1085	A	N3-C4-N9	5.35	131.68	127.40
22	BA	1434	A	C8-N9-C4	5.35	107.94	105.80
22	BA	1678	A	C4-C5-C6	5.35	119.67	117.00
22	BA	1755	A	C4-C5-N7	-5.35	108.03	110.70
22	BA	1966	A	N3-C4-N9	5.35	131.68	127.40
22	BA	2835	A	C4-C5-N7	-5.35	108.03	110.70
1	AA	1248	A	N9-C4-C5	5.35	107.94	105.80
22	BA	507	A	C8-N9-C4	5.35	107.94	105.80
22	BA	1247	A	C4-C5-N7	-5.35	108.03	110.70
22	BA	1495	A	C5-C6-N1	5.35	120.37	117.70
22	BA	1655	A	N9-C4-C5	5.35	107.94	105.80
22	BA	1900	A	C5-C6-N1	5.35	120.37	117.70
22	BA	2241	A	C4-C5-N7	-5.35	108.03	110.70
22	BA	2298	A	N3-C4-N9	5.35	131.68	127.40
22	BA	2542	A	C5-C6-N1	5.35	120.37	117.70
1	AA	996	A	C8-N9-C4	5.35	107.94	105.80
1	AA	559	A	C8-N9-C4	5.34	107.94	105.80
1	AA	802	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	877	A	N9-C4-C5	5.34	107.94	105.80
1	AA	635	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	181	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	800	A	C4-C5-C6	5.34	119.67	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	99	A	C8-N9-C4	5.34	107.94	105.80
1	AA	152	A	C5-N7-C8	5.34	106.57	103.90
1	AA	205	A	C4-C5-C6	5.34	119.67	117.00
1	AA	430	A	C5-C6-N1	5.34	120.37	117.70
1	AA	1465	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	460	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	793	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1204	A	N9-C4-C5	5.34	107.94	105.80
1	AA	1377	A	N9-C4-C5	5.34	107.94	105.80
22	BA	1913	A	C4-C5-C6	5.34	119.67	117.00
22	BA	2758	A	C4-C5-N7	-5.34	108.03	110.70
23	BB	46	A	C8-N9-C4	5.34	107.94	105.80
1	AA	622	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	964	A	N3-C4-N9	5.34	131.67	127.40
1	AA	1238	A	C8-N9-C4	5.34	107.94	105.80
1	AA	1363	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	478	A	C8-N9-C4	5.34	107.94	105.80
22	BA	482	A	C5-N7-C8	5.34	106.57	103.90
22	BA	599	A	N9-C4-C5	5.34	107.94	105.80
22	BA	861	A	C4-C5-C6	5.34	119.67	117.00
22	BA	947	A	N3-C4-N9	5.34	131.67	127.40
22	BA	2088	A	C4-C5-C6	5.34	119.67	117.00
22	BA	2163	A	N9-C4-C5	5.34	107.93	105.80
22	BA	2327	A	C4-C5-N7	-5.34	108.03	110.70
1	AA	246	A	C4-C5-C6	5.33	119.67	117.00
1	AA	336	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	1508	A	N9-C4-C5	5.33	107.93	105.80
22	BA	635	C	C6-N1-C2	-5.33	118.17	120.30
22	BA	661	A	N9-C4-C5	5.33	107.93	105.80
22	BA	1230	A	C4-C5-N7	-5.33	108.03	110.70
22	BA	1744	A	C5-C6-N1	5.33	120.37	117.70
22	BA	1749	A	N3-C4-N9	5.33	131.67	127.40
22	BA	2327	A	C8-N9-C4	5.33	107.93	105.80
1	AA	1236	A	N9-C4-C5	5.33	107.93	105.80
22	BA	119	A	C8-N9-C4	5.33	107.93	105.80
22	BA	792	A	C4-C5-N7	-5.33	108.03	110.70
22	BA	1142	A	C4-C5-C6	5.33	119.67	117.00
22	BA	1433	A	N9-C4-C5	5.33	107.93	105.80
22	BA	1705	A	N9-C4-C5	5.33	107.93	105.80
22	BA	1877	A	C8-N9-C4	5.33	107.93	105.80
22	BA	2059	A	C4-C5-C6	5.33	119.67	117.00
1	AA	253	A	N9-C4-C5	5.33	107.93	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	165	A	N3-C4-N9	5.33	131.67	127.40
22	BA	1829	A	C5-C6-N1	5.33	120.37	117.70
22	BA	2740	A	C5-C6-N1	5.33	120.36	117.70
1	AA	182	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	1410	A	C5-C6-N1	5.33	120.36	117.70
22	BA	5	A	C8-N9-C4	5.33	107.93	105.80
1	AA	98	A	N9-C4-C5	5.33	107.93	105.80
1	AA	695	A	N3-C4-N9	5.33	131.66	127.40
1	AA	935	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	964	A	C5-C6-N1	5.33	120.36	117.70
1	AA	1357	A	N3-C4-N9	5.33	131.66	127.40
22	BA	749	A	C4-C5-C6	5.33	119.66	117.00
22	BA	1403	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	2	A	C4-C5-N7	-5.33	108.04	110.70
22	BA	182	A	C8-N9-C4	5.33	107.93	105.80
22	BA	1525	A	C4-C5-N7	-5.33	108.04	110.70
1	AA	53	A	C5-C6-N1	5.33	120.36	117.70
1	AA	119	A	N3-C4-N9	5.33	131.66	127.40
1	AA	1368	A	C8-N9-C4	5.33	107.93	105.80
22	BA	1276	A	C5-C6-N1	5.33	120.36	117.70
22	BA	1413	A	C4-C5-C6	5.33	119.66	117.00
22	BA	1655	A	C5-C6-N1	5.33	120.36	117.70
22	BA	1876	A	C8-N9-C4	5.33	107.93	105.80
1	AA	356	A	C8-N9-C4	5.32	107.93	105.80
1	AA	1146	A	C8-N9-C4	5.32	107.93	105.80
1	AA	1319	A	N3-C4-N9	5.32	131.66	127.40
22	BA	172	A	C5-C6-N1	5.32	120.36	117.70
22	BA	764	A	N9-C4-C5	5.32	107.93	105.80
22	BA	2054	A	C4-C5-C6	5.32	119.66	117.00
22	BA	2135	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	2309	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	2814	A	N3-C4-N9	5.32	131.66	127.40
1	AA	160	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	449	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	602	A	C5-C6-N1	5.32	120.36	117.70
1	AA	161	A	C4-C5-C6	5.32	119.66	117.00
1	AA	371	A	C4-C5-C6	5.32	119.66	117.00
1	AA	718	A	C8-N9-C4	5.32	107.93	105.80
1	AA	1082	A	C8-N9-C4	5.32	107.93	105.80
22	BA	10	A	C4-C5-N7	-5.32	108.04	110.70
1	AA	303	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	1241	A	C8-N9-C4	5.32	107.93	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	383	A	C8-N9-C4	5.32	107.93	105.80
1	AA	815	A	C5-C6-N1	5.32	120.36	117.70
1	AA	959	A	N9-C4-C5	5.32	107.93	105.80
22	BA	449	A	C8-N9-C4	5.32	107.93	105.80
55	B8	59	A	N9-C4-C5	5.32	107.93	105.80
1	AA	488	C	C2-N1-C1'	5.32	124.65	118.80
1	AA	1229	A	C8-N9-C4	5.32	107.93	105.80
22	BA	1328	A	C4-C5-C6	5.32	119.66	117.00
22	BA	2268	A	N9-C4-C5	5.32	107.93	105.80
22	BA	2447	G	C5-C6-O6	-5.32	125.41	128.60
22	BA	2757	A	C5-C6-N1	5.32	120.36	117.70
23	BB	101	A	C6-N1-C2	-5.32	115.41	118.60
22	BA	223	A	N3-C4-N9	5.31	131.65	127.40
23	BB	115	A	C4-C5-N7	-5.31	108.04	110.70
22	BA	2665	A	N9-C4-C5	5.31	107.92	105.80
1	AA	1216	A	N3-C4-N9	5.31	131.65	127.40
22	BA	477	A	C8-N9-C4	5.31	107.92	105.80
22	BA	1214	A	C5-C6-N1	5.31	120.36	117.70
22	BA	2449	U	C6-N1-C2	5.31	124.19	121.00
22	BA	2705	A	C8-N9-C4	5.31	107.92	105.80
1	AA	746	A	C8-N9-C4	5.31	107.92	105.80
1	AA	1349	A	N3-C4-N9	5.31	131.65	127.40
1	AA	1500	A	C8-N9-C4	5.31	107.92	105.80
22	BA	793	A	C5-C6-N1	5.31	120.35	117.70
22	BA	1433	A	C8-N9-C4	5.31	107.92	105.80
22	BA	1614	A	C4-C5-C6	5.31	119.65	117.00
22	BA	1749	A	C4-C5-C6	5.31	119.65	117.00
23	BB	29	A	N3-C4-N9	5.31	131.65	127.40
1	AA	412	A	C4-C5-N7	-5.31	108.05	110.70
22	BA	226	A	N9-C4-C5	5.31	107.92	105.80
22	BA	1509	A	C5-C6-N1	5.31	120.35	117.70
1	AA	1441	A	C4-C5-C6	5.30	119.65	117.00
22	BA	582	A	N9-C4-C5	5.30	107.92	105.80
22	BA	2273	A	C5-C6-N1	5.30	120.35	117.70
1	AA	1012	A	C5-C6-N1	5.30	120.35	117.70
22	BA	1805	A	C8-N9-C4	5.30	107.92	105.80
1	AA	1246	A	C5-C6-N1	5.30	120.35	117.70
1	AA	1257	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	1280	A	C8-N9-C4	5.30	107.92	105.80
22	BA	144	A	N9-C4-C5	5.30	107.92	105.80
22	BA	503	A	C4-C5-N7	-5.30	108.05	110.70
22	BA	1927	A	C8-N9-C4	5.30	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2097	A	C8-N9-C4	5.30	107.92	105.80
23	BB	29	A	C5-C6-N1	5.30	120.35	117.70
1	AA	681	A	N9-C4-C5	5.30	107.92	105.80
22	BA	877	A	C4-C5-C6	5.30	119.65	117.00
22	BA	990	A	C6-N1-C2	5.30	121.78	118.60
22	BA	2336	A	C5-C6-N1	5.30	120.35	117.70
1	AA	1167	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	1507	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	535	A	N9-C4-C5	5.30	107.92	105.80
1	AA	583	A	C4-C5-N7	-5.30	108.05	110.70
1	AA	1155	A	C5-C6-N1	5.30	120.35	117.70
22	BA	794	A	C5-C6-N1	5.30	120.35	117.70
22	BA	2572	A	C4-C5-C6	5.30	119.65	117.00
23	BB	115	A	N3-C4-N9	5.30	131.64	127.40
1	AA	8	A	C4-C5-C6	5.29	119.65	117.00
1	AA	309	A	C5-C6-N1	5.29	120.35	117.70
1	AA	452	A	N9-C4-C5	5.29	107.92	105.80
1	AA	523	A	C5-C6-N1	5.29	120.35	117.70
1	AA	648	A	C4-C5-N7	-5.29	108.05	110.70
1	AA	1289	A	C5-C6-N1	5.29	120.35	117.70
1	AA	1299	A	C4-C5-C6	5.29	119.65	117.00
22	BA	346	A	C5-C6-N1	5.29	120.35	117.70
22	BA	1237	A	C4-C5-C6	5.29	119.65	117.00
22	BA	1913	A	N3-C4-N9	5.29	131.63	127.40
22	BA	2369	A	C8-N9-C4	5.29	107.92	105.80
1	AA	51	A	C5-C6-N1	5.29	120.35	117.70
1	AA	1346	A	C5-C6-N1	5.29	120.34	117.70
1	AA	1434	A	C4-C5-C6	5.29	119.65	117.00
22	BA	73	A	N3-C4-N9	5.29	131.63	127.40
22	BA	1098	A	C8-N9-C4	5.29	107.92	105.80
22	BA	1155	A	N3-C4-N9	5.29	131.63	127.40
22	BA	1477	A	C5-C6-N1	5.29	120.35	117.70
22	BA	2761	A	N3-C4-N9	5.29	131.63	127.40
1	AA	65	A	C8-N9-C4	5.29	107.92	105.80
1	AA	270	A	C8-N9-C4	5.29	107.92	105.80
22	BA	125	A	C5-C6-N1	5.29	120.34	117.70
22	BA	479	A	C4-C5-N7	-5.29	108.06	110.70
23	BB	24	G	N3-C4-N9	5.29	129.17	126.00
1	AA	782	A	C4-C5-N7	-5.29	108.06	110.70
1	AA	968	A	N3-C4-N9	5.29	131.63	127.40
1	AA	1375	A	N9-C4-C5	5.29	107.92	105.80
22	BA	497	A	C4-C5-N7	-5.29	108.06	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1275	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	1803	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	1919	A	C4-C5-C6	5.29	119.64	117.00
48	B0	46	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	AA	1428	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	2134	A	N9-C4-C5	5.29	107.92	105.80
1	AA	655	A	N9-C4-C5	5.29	107.91	105.80
1	AA	807	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	1549	A	N9-C4-C5	5.29	107.91	105.80
22	BA	2097	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	2757	A	N9-C4-C5	5.29	107.91	105.80
1	AA	959	A	C8-N9-C4	5.28	107.91	105.80
22	BA	877	A	N3-C4-N9	5.28	131.63	127.40
22	BA	1014	A	N3-C4-N9	5.28	131.63	127.40
22	BA	1272	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	547	A	N9-C4-C5	5.28	107.91	105.80
1	AA	681	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	777	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	958	A	N3-C4-N9	5.28	131.62	127.40
22	BA	861	A	C5-C6-N1	5.28	120.34	117.70
22	BA	2565	A	N3-C4-N9	5.28	131.63	127.40
1	AA	71	A	N3-C4-N9	5.28	131.62	127.40
1	AA	223	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	228	A	N9-C4-C5	5.28	107.91	105.80
22	BA	233	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	415	A	N9-C4-C5	5.28	107.91	105.80
22	BA	1253	A	C8-N9-C4	5.28	107.91	105.80
22	BA	1314	C	C2-N1-C1'	5.28	124.61	118.80
22	BA	1626	A	N9-C4-C5	5.28	107.91	105.80
22	BA	666	A	N3-C4-N9	5.28	131.62	127.40
22	BA	1453	A	C4-C5-C6	5.28	119.64	117.00
23	BB	50	A	C4-C5-N7	-5.28	108.06	110.70
1	AA	298	A	C8-N9-C4	5.28	107.91	105.80
1	AA	729	A	C8-N9-C4	5.28	107.91	105.80
1	AA	1117	A	C4-C5-C6	5.28	119.64	117.00
1	AA	1246	A	N9-C4-C5	5.28	107.91	105.80
22	BA	374	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	1566	A	C8-N9-C4	5.28	107.91	105.80
22	BA	1853	A	C5-C6-N1	5.28	120.34	117.70
1	AA	913	A	N9-C4-C5	5.28	107.91	105.80
22	BA	165	A	C8-N9-C4	5.28	107.91	105.80
22	BA	1413	A	N3-C4-N9	5.28	131.62	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	99	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	204	A	C8-N9-C4	5.27	107.91	105.80
22	BA	483	A	N9-C4-C5	5.27	107.91	105.80
22	BA	1858	A	C4-C5-C6	5.27	119.64	117.00
22	BA	1918	A	C5-C6-N1	5.27	120.34	117.70
1	AA	747	A	C5-C6-N1	5.27	120.34	117.70
1	AA	1111	A	C8-N9-C4	5.27	107.91	105.80
1	AA	1362	A	C4-C5-C6	5.27	119.64	117.00
22	BA	56	A	C8-N9-C4	5.27	107.91	105.80
22	BA	231	A	C8-N9-C4	5.27	107.91	105.80
22	BA	354	A	N9-C4-C5	5.27	107.91	105.80
22	BA	609	A	N3-C4-N9	5.27	131.62	127.40
22	BA	2748	A	N3-C4-N9	5.27	131.62	127.40
22	BA	2887	A	N9-C4-C5	5.27	107.91	105.80
1	AA	130	A	C4-C5-N7	-5.27	108.06	110.70
1	AA	461	A	C5-C6-N1	5.27	120.33	117.70
1	AA	1329	A	C4-C5-C6	5.27	119.63	117.00
22	BA	590	A	C4-C5-N7	-5.27	108.06	110.70
22	BA	668	A	C4-C5-N7	-5.27	108.06	110.70
22	BA	878	A	C5-C6-N1	5.27	120.33	117.70
22	BA	1214	A	C8-N9-C4	5.27	107.91	105.80
22	BA	1626	A	C5-C6-N1	5.27	120.33	117.70
22	BA	1783	A	C5-C6-N1	5.27	120.33	117.70
22	BA	2327	A	N9-C4-C5	5.27	107.91	105.80
22	BA	2835	A	C5-C6-N1	5.27	120.33	117.70
23	BB	39	A	N9-C4-C5	5.27	107.91	105.80
1	AA	28	A	C4-C5-N7	-5.27	108.07	110.70
1	AA	1499	A	N9-C4-C5	5.27	107.91	105.80
1	AA	1092	A	C4-C5-N7	-5.27	108.07	110.70
1	AA	1394	A	N9-C4-C5	5.27	107.91	105.80
22	BA	1616	A	N3-C4-N9	5.27	131.61	127.40
22	BA	2298	A	C5-C6-N1	5.27	120.33	117.70
1	AA	1176	A	C8-N9-C4	5.26	107.91	105.80
1	AA	1431	A	N9-C4-C5	5.26	107.91	105.80
22	BA	412	A	C8-N9-C4	5.26	107.91	105.80
22	BA	423	A	C4-C5-C6	5.26	119.63	117.00
22	BA	1073	A	C5-C6-N1	5.26	120.33	117.70
22	BA	1244	A	C5-C6-N1	5.26	120.33	117.70
22	BA	2020	A	C4-C5-C6	5.26	119.63	117.00
22	BA	2738	A	N9-C4-C5	5.26	107.91	105.80
23	BB	108	A	N3-C4-N9	5.26	131.61	127.40
1	AA	602	A	C5-C6-N1	5.26	120.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	310	A	C8-N9-C4	5.26	107.91	105.80
22	BA	878	A	N3-C4-N9	5.26	131.61	127.40
23	BB	29	A	C8-N9-C4	5.26	107.91	105.80
1	AA	182	A	C4-C5-C6	5.26	119.63	117.00
1	AA	535	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	908	A	N9-C4-C5	5.26	107.91	105.80
22	BA	299	A	C5-C6-N1	5.26	120.33	117.70
22	BA	492	A	C8-N9-C4	5.26	107.91	105.80
22	BA	608	A	C5-C6-N1	5.26	120.33	117.70
22	BA	689	A	C4-C5-C6	5.26	119.63	117.00
22	BA	975	A	C5-C6-N1	5.26	120.33	117.70
22	BA	1552	A	C5-C6-N1	5.26	120.33	117.70
22	BA	2358	A	C4-C5-C6	5.26	119.63	117.00
1	AA	574	A	C8-N9-C4	5.26	107.90	105.80
1	AA	975	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	2154	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	2335	A	C8-N9-C4	5.26	107.90	105.80
1	AA	1146	A	C4-C5-N7	-5.26	108.07	110.70
1	AA	7	A	C4-C5-C6	5.26	119.63	117.00
1	AA	223	A	C8-N9-C4	5.26	107.90	105.80
1	AA	262	A	N9-C4-C5	5.26	107.90	105.80
1	AA	560	A	N9-C4-C5	5.26	107.90	105.80
1	AA	1492	A	N9-C4-C5	5.26	107.90	105.80
22	BA	344	A	C5-C6-N1	5.26	120.33	117.70
22	BA	471	A	C8-N9-C4	5.26	107.90	105.80
22	BA	2449	U	N1-C2-N3	5.26	118.05	114.90
1	AA	171	A	N3-C4-N9	5.25	131.60	127.40
1	AA	1446	A	N9-C4-C5	5.25	107.90	105.80
22	BA	477	A	C5-C6-N1	5.25	120.33	117.70
22	BA	1204	A	C4-C5-C6	5.25	119.63	117.00
1	AA	1318	A	C4-C5-N7	-5.25	108.07	110.70
1	AA	1493	A	C4-C5-C6	5.25	119.63	117.00
22	BA	1021	A	C4-C5-N7	-5.25	108.07	110.70
22	BA	1143	A	C5-C6-N1	5.25	120.33	117.70
22	BA	1194	A	N3-C4-N9	5.25	131.60	127.40
22	BA	2547	A	C8-N9-C4	5.25	107.90	105.80
22	BA	2851	A	C5-C6-N1	5.25	120.33	117.70
1	AA	456	A	N9-C4-C5	5.25	107.90	105.80
1	AA	546	A	C5-C6-N1	5.25	120.33	117.70
1	AA	1012	A	C4-C5-N7	-5.25	108.07	110.70
1	AA	1252	A	N9-C4-C5	5.25	107.90	105.80
1	AA	1289	A	C4-C5-N7	-5.25	108.07	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	142	A	N9-C4-C5	5.25	107.90	105.80
22	BA	173	A	C8-N9-C4	5.25	107.90	105.80
22	BA	453	A	C5-C6-N1	5.25	120.33	117.70
22	BA	899	A	N9-C4-C5	5.25	107.90	105.80
22	BA	1773	A	N9-C4-C5	5.25	107.90	105.80
22	BA	2033	A	C4-C5-C6	5.25	119.62	117.00
49	B1	44	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	AA	456	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	1050	A	C5-C6-N1	5.25	120.33	117.70
22	BA	1787	A	C5-C6-N1	5.25	120.33	117.70
22	BA	1928	A	C4-C5-N7	-5.25	108.08	110.70
1	AA	1362	A	C5-C6-N1	5.25	120.33	117.70
22	BA	819	A	N9-C4-C5	5.25	107.90	105.80
22	BA	1129	A	C8-N9-C4	5.25	107.90	105.80
22	BA	1596	A	C4-C5-C6	5.25	119.62	117.00
1	AA	71	A	N9-C4-C5	5.25	107.90	105.80
1	AA	1329	A	N9-C4-C5	5.25	107.90	105.80
22	BA	1916	A	C8-N9-C4	5.25	107.90	105.80
1	AA	1019	A	N3-C4-N9	5.25	131.60	127.40
22	BA	1784	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	2183	A	C5-C6-N1	5.25	120.32	117.70
22	BA	2298	A	C4-C5-N7	-5.25	108.08	110.70
55	B8	51	A	C8-N9-C4	5.25	107.90	105.80
1	AA	120	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	913	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	160	A	C5-C6-N1	5.24	120.32	117.70
22	BA	191	A	N9-C4-C5	5.24	107.90	105.80
22	BA	1322	A	C8-N9-C4	5.24	107.90	105.80
22	BA	1419	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	1570	A	C5-C6-N1	5.24	120.32	117.70
1	AA	72	A	N9-C4-C5	5.24	107.90	105.80
22	BA	2450	A	C5-N7-C8	5.24	106.52	103.90
22	BA	118	A	C5-C6-N1	5.24	120.32	117.70
22	BA	1054	A	C5-C6-N1	5.24	120.32	117.70
22	BA	2418	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	131	A	N9-C4-C5	5.24	107.89	105.80
1	AA	282	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	306	A	C5-C6-N1	5.24	120.32	117.70
1	AA	547	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	553	A	N9-C4-C5	5.24	107.89	105.80
1	AA	1219	A	N9-C4-C5	5.24	107.89	105.80
22	BA	251	A	N9-C4-C5	5.24	107.89	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	472	A	N9-C4-C5	5.24	107.90	105.80
22	BA	910	A	C5-C6-N1	5.24	120.32	117.70
22	BA	936	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	2406	A	N9-C4-C5	5.24	107.89	105.80
1	AA	1441	A	N9-C4-C5	5.24	107.89	105.80
1	AA	329	A	C5-C6-N1	5.24	120.32	117.70
1	AA	1204	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	2059	A	C8-N9-C4	5.24	107.89	105.80
22	BA	2572	A	C4-C5-N7	-5.24	108.08	110.70
1	AA	223	A	C5-C6-N1	5.23	120.32	117.70
1	AA	1016	A	C5-C6-N1	5.23	120.32	117.70
22	BA	114	U	C2-N1-C1'	5.23	123.98	117.70
22	BA	1237	A	C8-N9-C4	5.23	107.89	105.80
22	BA	1927	A	N9-C4-C5	5.23	107.89	105.80
1	AA	431	A	C4-C5-C6	5.23	119.62	117.00
1	AA	759	A	N9-C4-C5	5.23	107.89	105.80
1	AA	1428	A	C8-N9-C4	5.23	107.89	105.80
22	BA	905	A	C5-C6-N1	5.23	120.32	117.70
22	BA	1274	A	N9-C4-C5	5.23	107.89	105.80
22	BA	1938	A	C8-N9-C4	5.23	107.89	105.80
23	BB	119	A	C4-C5-N7	-5.23	108.08	110.70
22	BA	330	A	C5-C6-N1	5.23	120.32	117.70
22	BA	1274	A	C8-N9-C4	5.23	107.89	105.80
22	BA	1596	A	N9-C4-C5	5.23	107.89	105.80
22	BA	1912	A	N3-C4-N9	5.23	131.58	127.40
22	BA	2095	A	C4-C5-C6	5.23	119.61	117.00
22	BA	2411	A	N9-C4-C5	5.23	107.89	105.80
22	BA	2705	A	N9-C4-C5	5.23	107.89	105.80
22	BA	2706	A	C4-C5-C6	5.23	119.61	117.00
22	BA	2758	A	C4-C5-C6	5.23	119.62	117.00
23	BB	45	A	N9-C4-C5	5.23	107.89	105.80
1	AA	306	A	C4-C5-N7	-5.23	108.08	110.70
1	AA	702	A	C5-C6-N1	5.23	120.31	117.70
22	BA	2476	A	C5-C6-N1	5.23	120.31	117.70
1	AA	781	A	C5-C6-N1	5.23	120.31	117.70
22	BA	155	A	C4-C5-C6	5.23	119.61	117.00
22	BA	632	A	C8-N9-C4	5.23	107.89	105.80
22	BA	654	A	C4-C5-N7	-5.23	108.09	110.70
22	BA	1275	A	N9-C4-C5	5.23	107.89	105.80
22	BA	2378	A	N9-C4-C5	5.23	107.89	105.80
22	BA	2665	A	C5-C6-N1	5.23	120.31	117.70
1	AA	712	A	C4-C5-N7	-5.23	108.09	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2542	A	N3-C4-N9	5.23	131.58	127.40
22	BA	676	A	N3-C4-N9	5.22	131.58	127.40
22	BA	1103	A	C8-N9-C4	5.22	107.89	105.80
22	BA	2873	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	189	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	935	A	C5-C6-N1	5.22	120.31	117.70
22	BA	866	A	N9-C4-C5	5.22	107.89	105.80
22	BA	1654	A	N9-C4-C5	5.22	107.89	105.80
22	BA	1858	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	2335	A	N9-C4-C5	5.22	107.89	105.80
22	BA	2598	A	C8-N9-C4	5.22	107.89	105.80
55	B8	58	A	C8-N9-C4	5.22	107.89	105.80
1	AA	520	A	C8-N9-C4	5.22	107.89	105.80
22	BA	1262	A	C4-C5-C6	5.22	119.61	117.00
22	BA	2119	A	C5-C6-N1	5.22	120.31	117.70
22	BA	2471	A	N9-C4-C5	5.22	107.89	105.80
1	AA	878	A	C5-C6-N1	5.22	120.31	117.70
1	AA	908	A	C8-N9-C4	5.22	107.89	105.80
22	BA	909	A	C4-C5-C6	5.22	119.61	117.00
22	BA	2765	A	N9-C4-C5	5.22	107.89	105.80
22	BA	563	A	C8-N9-C4	5.22	107.89	105.80
22	BA	626	A	N9-C4-C5	5.22	107.89	105.80
55	B8	14	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	448	A	N9-C4-C5	5.22	107.89	105.80
1	AA	663	A	C5-C6-N1	5.22	120.31	117.70
1	AA	958	A	C4-C5-C6	5.22	119.61	117.00
1	AA	1285	A	N3-C4-N9	5.22	131.57	127.40
22	BA	95	A	N9-C4-C5	5.22	107.89	105.80
22	BA	933	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	1029	A	C8-N9-C4	5.22	107.89	105.80
22	BA	2468	A	C5-C6-N1	5.22	120.31	117.70
22	BA	2614	A	N3-C4-N9	5.22	131.57	127.40
22	BA	2776	A	C4-C5-N7	-5.22	108.09	110.70
1	AA	8	A	N9-C4-C5	5.21	107.89	105.80
22	BA	401	A	C5-C6-N1	5.21	120.31	117.70
22	BA	782	A	C4-C5-N7	-5.21	108.09	110.70
22	BA	1598	A	N9-C4-C5	5.21	107.89	105.80
22	BA	2298	A	N9-C4-C5	5.21	107.89	105.80
1	AA	196	A	N9-C4-C5	5.21	107.89	105.80
22	BA	14	A	C8-N9-C4	5.21	107.89	105.80
22	BA	892	A	C5-C6-N1	5.21	120.31	117.70
1	AA	101	A	C8-N9-C4	5.21	107.89	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	816	A	C5-C6-N1	5.21	120.31	117.70
22	BA	1632	A	N9-C4-C5	5.21	107.89	105.80
22	BA	1784	A	C4-C5-C6	5.21	119.61	117.00
1	AA	1349	A	C4-C5-N7	-5.21	108.09	110.70
22	BA	1322	A	C4-C5-C6	5.21	119.61	117.00
1	AA	539	A	C4-C5-N7	-5.21	108.09	110.70
1	AA	1363	A	C8-N9-C4	5.21	107.88	105.80
22	BA	428	A	C8-N9-C4	5.21	107.88	105.80
22	BA	920	A	C5-C6-N1	5.21	120.30	117.70
22	BA	1535	A	N9-C4-C5	5.21	107.88	105.80
22	BA	2060	A	C4-C5-N7	-5.21	108.09	110.70
22	BA	2813	A	C5-C6-N1	5.21	120.31	117.70
1	AA	181	A	N9-C4-C5	5.21	107.88	105.80
1	AA	915	A	C5-C6-N1	5.21	120.30	117.70
1	AA	968	A	C4-C5-C6	5.21	119.60	117.00
1	AA	1256	A	C8-N9-C4	5.21	107.88	105.80
22	BA	447	A	C8-N9-C4	5.21	107.88	105.80
22	BA	1253	A	C4-C5-N7	-5.21	108.10	110.70
22	BA	2009	A	C4-C5-C6	5.21	119.60	117.00
22	BA	2317	A	N9-C4-C5	5.21	107.88	105.80
22	BA	2800	A	N9-C4-C5	5.21	107.88	105.80
55	B8	69	A	C5-C6-N1	5.21	120.30	117.70
1	AA	160	A	C5-C6-N1	5.21	120.30	117.70
22	BA	637	A	N3-C4-N9	5.21	131.56	127.40
22	BA	877	A	C4-C5-N7	-5.21	108.10	110.70
1	AA	640	A	C4-C5-N7	-5.20	108.10	110.70
1	AA	1261	A	C8-N9-C4	5.20	107.88	105.80
22	BA	415	A	C8-N9-C4	5.20	107.88	105.80
22	BA	505	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	793	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	1711	A	C5-C6-N1	5.20	120.30	117.70
22	BA	1913	A	C5-C6-N1	5.20	120.30	117.70
55	B8	38	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	1246	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	1265	A	N9-C4-C5	5.20	107.88	105.80
22	BA	1801	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	2850	A	C4-C5-N7	-5.20	108.10	110.70
1	AA	1105	A	C4-C5-C6	5.20	119.60	117.00
1	AA	1275	A	C4-C5-C6	5.20	119.60	117.00
1	AA	1311	A	N9-C4-C5	5.20	107.88	105.80
1	AA	1324	A	C8-N9-C4	5.20	107.88	105.80
22	BA	1801	A	N9-C4-C5	5.20	107.88	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2813	A	N9-C4-C5	5.20	107.88	105.80
1	AA	315	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	270	A	C4-C5-C6	5.20	119.60	117.00
22	BA	1090	A	N9-C4-C5	5.20	107.88	105.80
22	BA	1713	A	N3-C4-N9	5.20	131.56	127.40
22	BA	1794	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	2589	A	C4-C5-C6	5.20	119.60	117.00
23	BB	119	A	C4-C5-C6	5.20	119.60	117.00
22	BA	1569	A	N3-C4-N9	5.20	131.56	127.40
22	BA	1650	A	C5-C6-N1	5.20	120.30	117.70
1	AA	964	A	C4-C5-C6	5.20	119.60	117.00
1	AA	1092	A	C5-C6-N1	5.20	120.30	117.70
1	AA	1238	A	N9-C4-C5	5.20	107.88	105.80
1	AA	1431	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	706	A	C5-C6-N1	5.20	120.30	117.70
22	BA	735	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	980	A	C8-N9-C4	5.20	107.88	105.80
22	BA	2675	A	C5-C6-N1	5.20	120.30	117.70
1	AA	819	A	C4-C5-N7	-5.19	108.10	110.70
22	BA	945	A	C5-C6-N1	5.19	120.30	117.70
22	BA	1641	A	C4-C5-C6	5.19	119.60	117.00
22	BA	1805	A	C4-C5-N7	-5.19	108.10	110.70
22	BA	2333	A	N3-C4-N9	5.19	131.55	127.40
22	BA	2835	A	N3-C4-N9	5.19	131.56	127.40
1	AA	181	A	C4-C5-N7	-5.19	108.11	110.70
1	AA	441	A	C4-C5-N7	-5.19	108.11	110.70
1	AA	1004	A	C4-C5-N7	-5.19	108.11	110.70
1	AA	1503	A	C4-C5-N7	-5.19	108.10	110.70
22	BA	621	A	C5-C6-N1	5.19	120.30	117.70
22	BA	972	A	N3-C4-N9	5.19	131.55	127.40
22	BA	1366	A	N3-C4-N9	5.19	131.55	127.40
22	BA	1713	A	C5-C6-N1	5.19	120.30	117.70
1	AA	642	A	C5-C6-N1	5.19	120.30	117.70
22	BA	2856	A	C8-N9-C4	5.19	107.88	105.80
23	BB	78	A	N3-C4-N9	5.19	131.55	127.40
1	AA	139	A	C5-C6-N1	5.19	120.29	117.70
22	BA	739	A	C4-C5-N7	-5.19	108.11	110.70
22	BA	1272	A	N3-C4-N9	5.19	131.55	127.40
22	BA	1367	A	N9-C4-C5	5.19	107.88	105.80
22	BA	2037	A	C5-C6-N1	5.19	120.29	117.70
22	BA	2776	A	C5-C6-N1	5.19	120.29	117.70
22	BA	1204	A	C5-C6-N1	5.19	120.29	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1383	A	N9-C4-C5	5.19	107.87	105.80
22	BA	1772	A	N3-C4-N9	5.19	131.55	127.40
1	AA	496	A	C4-C5-C6	5.18	119.59	117.00
1	AA	559	A	N9-C4-C5	5.18	107.87	105.80
22	BA	470	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	2163	A	C5-C6-N1	5.18	120.29	117.70
22	BA	2602	A	N3-C4-N9	5.18	131.55	127.40
22	BA	2726	A	C4-C5-N7	-5.18	108.11	110.70
1	AA	816	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	973	A	N3-C4-N9	5.18	131.55	127.40
22	BA	2590	A	C4-C5-N7	-5.18	108.11	110.70
23	BB	50	A	N3-C4-N9	5.18	131.54	127.40
1	AA	845	A	C5-C6-N1	5.18	120.29	117.70
22	BA	2572	A	N3-C4-N9	5.18	131.54	127.40
22	BA	127	A	N3-C4-N9	5.18	131.54	127.40
22	BA	374	A	N9-C4-C5	5.18	107.87	105.80
22	BA	430	A	C8-N9-C4	5.18	107.87	105.80
22	BA	1810	A	C6-C5-N7	-5.18	128.67	132.30
22	BA	2037	A	C8-N9-C4	5.18	107.87	105.80
22	BA	2274	A	C4-C5-N7	-5.18	108.11	110.70
23	BB	53	A	C5-C6-N1	5.18	120.29	117.70
1	AA	2	A	C8-N9-C4	5.18	107.87	105.80
1	AA	1339	A	N9-C4-C5	5.18	107.87	105.80
1	AA	26	A	N9-C4-C5	5.18	107.87	105.80
22	BA	190	A	C5-C6-N1	5.18	120.29	117.70
22	BA	2430	A	C5-N7-C8	5.18	106.49	103.90
23	BB	101	A	C8-N9-C4	5.18	107.87	105.80
1	AA	553	A	C4-C5-N7	-5.17	108.11	110.70
1	AA	768	A	C5-C6-N1	5.17	120.29	117.70
22	BA	1434	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	1553	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	2183	A	C4-C5-N7	-5.17	108.11	110.70
1	AA	510	A	N3-C4-N9	5.17	131.54	127.40
22	BA	1784	A	N9-C4-C5	5.17	107.87	105.80
22	BA	1987	A	C4-C5-N7	-5.17	108.11	110.70
1	AA	649	A	C5-C6-N1	5.17	120.28	117.70
1	AA	1117	A	C5-C6-N1	5.17	120.28	117.70
1	AA	1269	A	N3-C4-N9	5.17	131.54	127.40
22	BA	1089	A	C8-N9-C4	5.17	107.87	105.80
22	BA	1655	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	1690	A	C5-C6-N1	5.17	120.29	117.70
22	BA	1901	A	C5-C6-N1	5.17	120.29	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	66	A	C4-C5-N7	-5.17	108.11	110.70
1	AA	189	A	C5-C6-N1	5.17	120.28	117.70
22	BA	368	A	N9-C4-C5	5.17	107.87	105.80
22	BA	1678	A	C5-C6-N1	5.17	120.28	117.70
1	AA	59	A	C8-N9-C4	5.17	107.87	105.80
1	AA	451	A	C5-C6-N1	5.17	120.28	117.70
1	AA	478	A	N9-C4-C5	5.17	107.87	105.80
1	AA	1251	A	C8-N9-C4	5.17	107.87	105.80
1	AA	1446	A	C5-C6-N1	5.17	120.28	117.70
1	AA	1499	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	111	A	C4-C5-C6	5.17	119.58	117.00
23	BB	99	A	C5-C6-N1	5.17	120.28	117.70
22	BA	227	A	C4-C5-N7	-5.17	108.12	110.70
22	BA	352	A	C5-C6-N1	5.17	120.28	117.70
22	BA	1098	A	C4-C5-N7	-5.17	108.12	110.70
22	BA	1129	A	N3-C4-N9	5.17	131.53	127.40
22	BA	1503	A	N9-C4-C5	5.17	107.87	105.80
22	BA	1966	A	C4-C5-N7	-5.17	108.12	110.70
22	BA	2733	A	C5-C6-N1	5.17	120.28	117.70
1	AA	109	A	C8-N9-C4	5.17	107.87	105.80
22	BA	1155	A	C5-C6-N1	5.17	120.28	117.70
22	BA	2513	A	C8-N9-C4	5.17	107.87	105.80
55	B8	26	A	C5-C6-N1	5.17	120.28	117.70
22	BA	1324	G	O4'-C1'-N9	5.16	112.33	108.20
22	BA	2284	A	C8-N9-C4	5.16	107.86	105.80
22	BA	2531	A	N9-C4-C5	5.16	107.86	105.80
22	BA	1392	A	N9-C4-C5	5.16	107.86	105.80
22	BA	2336	A	N9-C4-C5	5.16	107.86	105.80
22	BA	2435	A	C5-C6-N1	5.16	120.28	117.70
55	B8	58	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	1329	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	119	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	1502	A	C5-C6-N1	5.16	120.28	117.70
1	AA	961	U	N3-C2-O2	-5.16	118.59	122.20
22	BA	685	A	N9-C4-C5	5.16	107.86	105.80
22	BA	1528	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	1808	A	C5-C6-N1	5.16	120.28	117.70
22	BA	2873	A	C4-C5-C6	5.16	119.58	117.00
1	AA	171	A	C4-C5-N7	-5.16	108.12	110.70
23	BB	45	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	120	A	N3-C4-N9	5.16	131.53	127.40
1	AA	1179	A	C4-C5-C6	5.16	119.58	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	402	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	718	A	N9-C4-C5	5.16	107.86	105.80
22	BA	1275	A	C5-C6-N1	5.16	120.28	117.70
22	BA	1616	A	C5-C6-N1	5.16	120.28	117.70
22	BA	1676	A	C5-C6-N1	5.16	120.28	117.70
22	BA	2700	A	C5-C6-N1	5.16	120.28	117.70
22	BA	1786	A	C4-C5-C6	5.15	119.58	117.00
22	BA	2758	A	N3-C4-N9	5.15	131.52	127.40
1	AA	892	A	C4-C5-N7	-5.15	108.12	110.70
22	BA	1593	A	C5-C6-N1	5.15	120.28	117.70
1	AA	51	A	C4-C5-N7	-5.15	108.12	110.70
1	AA	468	A	N9-C4-C5	5.15	107.86	105.80
1	AA	860	A	N9-C4-C5	5.15	107.86	105.80
1	AA	864	A	C4-C5-N7	-5.15	108.12	110.70
1	AA	913	A	N3-C4-N9	5.15	131.52	127.40
22	BA	422	A	C8-N9-C4	5.15	107.86	105.80
22	BA	715	A	N9-C4-C5	5.15	107.86	105.80
22	BA	821	A	C4-C5-C6	5.15	119.58	117.00
22	BA	1246	A	C8-N9-C4	5.15	107.86	105.80
22	BA	513	A	N9-C4-C5	5.15	107.86	105.80
1	AA	53	A	N9-C4-C5	5.15	107.86	105.80
1	AA	151	A	C5-C6-N1	5.15	120.27	117.70
1	AA	397	A	C4-C5-N7	-5.15	108.13	110.70
1	AA	1324	A	C5-C6-N1	5.15	120.27	117.70
22	BA	515	A	N9-C4-C5	5.15	107.86	105.80
22	BA	676	A	C4-C5-N7	-5.15	108.13	110.70
22	BA	1420	A	C5-C6-N1	5.15	120.27	117.70
22	BA	1672	A	C5-C6-N1	5.15	120.27	117.70
1	AA	10	A	C4-C5-N7	-5.15	108.13	110.70
22	BA	226	A	C4-C5-N7	-5.15	108.13	110.70
22	BA	781	A	C4-C5-N7	-5.15	108.13	110.70
22	BA	900	A	N9-C4-C5	5.15	107.86	105.80
22	BA	1635	A	C5-C6-N1	5.15	120.27	117.70
1	AA	196	A	C4-C5-N7	-5.14	108.13	110.70
1	AA	344	A	N9-C4-C5	5.14	107.86	105.80
1	AA	432	A	N3-C4-N9	5.14	131.51	127.40
1	AA	607	A	N9-C4-C5	5.14	107.86	105.80
1	AA	964	A	N9-C4-C5	5.14	107.86	105.80
1	AA	1111	A	N9-C4-C5	5.14	107.86	105.80
1	AA	1117	A	C4-C5-N7	-5.14	108.13	110.70
1	AA	1167	A	N3-C4-N9	5.14	131.51	127.40
22	BA	111	A	C5-C6-N1	5.14	120.27	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	241	A	C8-N9-C4	5.14	107.86	105.80
22	BA	453	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	2741	A	N9-C4-C5	5.14	107.86	105.80
1	AA	1016	A	N9-C4-C5	5.14	107.86	105.80
22	BA	1314	C	N1-C2-O2	5.14	121.98	118.90
22	BA	1505	A	N9-C4-C5	5.14	107.86	105.80
22	BA	2278	A	C8-N9-C4	5.14	107.86	105.80
22	BA	2433	A	N9-C4-C5	5.14	107.86	105.80
1	AA	1396	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	251	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	1302	A	C4-C5-C6	5.14	119.57	117.00
22	BA	311	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	892	A	C4-C5-N7	-5.14	108.13	110.70
1	AA	975	A	N9-C4-C5	5.14	107.86	105.80
22	BA	2753	A	C8-N9-C4	5.14	107.86	105.80
22	BA	2899	A	N3-C4-N9	5.14	131.51	127.40
1	AA	1238	A	C4-C5-N7	-5.14	108.13	110.70
1	AA	1428	A	N3-C4-N9	5.14	131.51	127.40
22	BA	429	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	1046	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	1143	A	C8-N9-C4	5.14	107.86	105.80
22	BA	1678	A	N3-C4-N9	5.14	131.51	127.40
1	AA	411	A	C4-C5-C6	5.13	119.57	117.00
22	BA	428	A	C4-C5-C6	5.13	119.57	117.00
22	BA	1285	A	C4-C5-C6	5.13	119.57	117.00
22	BA	2158	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	2482	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	2734	A	C5-C6-N1	5.13	120.27	117.70
55	B8	6	A	N3-C4-N9	5.13	131.51	127.40
22	BA	56	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	1090	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	2158	A	N9-C4-C5	5.13	107.85	105.80
1	AA	149	A	C5-C6-N1	5.13	120.27	117.70
1	AA	336	A	N3-C4-N9	5.13	131.50	127.40
1	AA	468	A	C4-C5-C6	5.13	119.56	117.00
1	AA	1150	A	C5-C6-N1	5.13	120.27	117.70
22	BA	1566	A	C5-C6-N1	5.13	120.27	117.70
22	BA	2590	A	N3-C4-N9	5.13	131.50	127.40
22	BA	2860	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	1746	A	N9-C4-C5	5.13	107.85	105.80
22	BA	1805	A	C4-C5-C6	5.13	119.56	117.00
22	BA	2727	A	C8-N9-C4	5.13	107.85	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	161	A	N3-C4-N9	5.13	131.50	127.40
1	AA	718	A	C4-C5-N7	-5.13	108.14	110.70
1	AA	807	A	C8-N9-C4	5.13	107.85	105.80
22	BA	1084	A	N3-C4-N9	5.13	131.50	127.40
22	BA	1544	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	1590	A	C5-C6-N1	5.13	120.26	117.70
22	BA	2188	U	P-O3'-C3'	5.13	125.85	119.70
22	BA	2199	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	2278	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	2381	A	C4-C5-C6	5.13	119.56	117.00
1	AA	228	A	C5-C6-N1	5.13	120.26	117.70
22	BA	918	A	C8-N9-C4	5.13	107.85	105.80
22	BA	1127	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	1395	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	2346	A	C5-C6-N1	5.13	120.26	117.70
22	BA	2602	A	C4-C5-C6	5.13	119.56	117.00
1	AA	640	A	N9-C4-C5	5.12	107.85	105.80
22	BA	507	A	C4-C5-C6	5.12	119.56	117.00
1	AA	831	A	N9-C4-C5	5.12	107.85	105.80
1	AA	1093	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	1261	A	N9-C4-C5	5.12	107.85	105.80
22	BA	309	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	430	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	557	C	C6-N1-C2	-5.12	118.25	120.30
22	BA	1453	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	2719	G	C2-N3-C4	-5.12	109.34	111.90
1	AA	303	A	N9-C4-C5	5.12	107.85	105.80
1	AA	958	A	C5-C6-N1	5.12	120.26	117.70
22	BA	631	A	N9-C4-C5	5.12	107.85	105.80
22	BA	1304	A	C8-N9-C4	5.12	107.85	105.80
22	BA	1579	A	N9-C4-C5	5.12	107.85	105.80
22	BA	1912	A	C5-C6-N1	5.12	120.26	117.70
22	BA	2478	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	2725	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	119	A	C8-N9-C4	5.12	107.85	105.80
22	BA	590	A	C8-N9-C4	5.12	107.85	105.80
22	BA	1103	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	1214	A	N9-C4-C5	5.12	107.85	105.80
22	BA	1829	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	1876	A	N9-C4-C5	5.12	107.85	105.80
22	BA	2273	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	199	A	C5-C6-N1	5.12	120.26	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	629	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	1019	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	1499	A	C8-N9-C4	5.12	107.85	105.80
22	BA	1127	A	C5-C6-N1	5.12	120.26	117.70
22	BA	161	A	C8-N9-C4	5.12	107.85	105.80
22	BA	526	A	C5-C6-N1	5.12	120.26	117.70
22	BA	654	A	N9-C4-C5	5.12	107.85	105.80
22	BA	920	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	1701	A	C4-C5-C6	5.12	119.56	117.00
22	BA	2406	A	N3-C4-N9	5.12	131.49	127.40
1	AA	7	A	C4-C5-N7	-5.11	108.14	110.70
1	AA	430	A	C4-C5-N7	-5.11	108.14	110.70
1	AA	602	A	C4-C5-N7	-5.11	108.14	110.70
1	AA	766	A	N9-C4-C5	5.11	107.85	105.80
1	AA	1274	A	N9-C4-C5	5.11	107.84	105.80
22	BA	1039	A	C4-C5-C6	5.11	119.56	117.00
22	BA	2726	A	C5-C6-N1	5.11	120.25	117.70
22	BA	2810	A	C8-N9-C4	5.11	107.84	105.80
22	BA	1872	A	C8-N9-C4	5.11	107.84	105.80
1	AA	363	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	1238	A	C5-C6-N1	5.11	120.25	117.70
22	BA	167	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	492	A	N9-C4-C5	5.11	107.84	105.80
22	BA	507	A	N3-C4-N9	5.11	131.49	127.40
22	BA	1614	A	N9-C4-C5	5.11	107.84	105.80
22	BA	2147	A	C5-C6-N1	5.11	120.25	117.70
22	BA	2376	A	N9-C4-C5	5.11	107.84	105.80
22	BA	2660	A	N3-C4-N9	5.11	131.49	127.40
1	AA	344	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	1717	A	N3-C4-N9	5.11	131.49	127.40
22	BA	2736	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	2882	A	C4-C5-N7	-5.11	108.15	110.70
1	AA	397	A	N9-C4-C5	5.10	107.84	105.80
1	AA	489	C	N3-C2-O2	-5.10	118.33	121.90
1	AA	768	A	N9-C4-C5	5.10	107.84	105.80
1	AA	977	A	C5-C6-N1	5.10	120.25	117.70
1	AA	1081	A	C5-C6-N1	5.10	120.25	117.70
1	AA	1280	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	197	A	C8-N9-C4	5.10	107.84	105.80
22	BA	2358	A	N3-C4-N9	5.10	131.48	127.40
23	BB	58	A	N9-C4-C5	5.10	107.84	105.80
22	BA	14	A	C5-C6-N1	5.10	120.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	368	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	1413	A	N9-C4-C5	5.10	107.84	105.80
23	BB	46	A	N9-C4-C5	5.10	107.84	105.80
1	AA	728	A	C8-N9-C4	5.10	107.84	105.80
1	AA	937	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	428	A	N9-C4-C5	5.10	107.84	105.80
22	BA	792	A	C8-N9-C4	5.10	107.84	105.80
22	BA	1342	A	N9-C4-C5	5.10	107.84	105.80
22	BA	2478	A	N9-C4-C5	5.10	107.84	105.80
23	BB	108	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	125	A	C4-C5-C6	5.10	119.55	117.00
22	BA	1260	A	N9-C4-C5	5.10	107.84	105.80
22	BA	2882	A	C8-N9-C4	5.10	107.84	105.80
1	AA	974	A	C4-C5-C6	5.10	119.55	117.00
22	BA	1069	A	N9-C4-C5	5.10	107.84	105.80
1	AA	81	A	C5-C6-N1	5.09	120.25	117.70
1	AA	718	A	N9-C4-C5	5.09	107.84	105.80
1	AA	937	A	C5-C6-N1	5.09	120.25	117.70
1	AA	1042	A	C5-C6-N1	5.09	120.25	117.70
22	BA	861	A	N9-C4-C5	5.09	107.84	105.80
22	BA	899	A	C5-C6-N1	5.09	120.25	117.70
22	BA	2482	A	N3-C4-N9	5.09	131.48	127.40
1	AA	1167	A	N9-C4-C5	5.09	107.84	105.80
22	BA	1899	A	C8-N9-C4	5.09	107.84	105.80
22	BA	1970	A	C5-C6-N1	5.09	120.25	117.70
22	BA	2311	A	C8-N9-C4	5.09	107.84	105.80
1	AA	1019	A	C5-C6-N1	5.09	120.25	117.70
22	BA	1678	A	N9-C4-C5	5.09	107.84	105.80
22	BA	1749	A	N9-C4-C5	5.09	107.84	105.80
22	BA	2266	A	N9-C4-C5	5.09	107.84	105.80
22	BA	2366	A	N9-C4-C5	5.09	107.84	105.80
1	AA	349	A	C5-C6-N1	5.09	120.25	117.70
1	AA	872	A	N9-C4-C5	5.09	107.84	105.80
22	BA	83	A	C5-C6-N1	5.09	120.25	117.70
22	BA	575	A	C4-C5-C6	5.09	119.54	117.00
22	BA	2388	A	C5-C6-N1	5.09	120.25	117.70
1	AA	964	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	829	A	N9-C4-C5	5.09	107.83	105.80
22	BA	53	A	N3-C4-N9	5.09	131.47	127.40
22	BA	2598	A	N3-C4-N9	5.09	131.47	127.40
1	AA	274	A	C4-C5-N7	-5.08	108.16	110.70
9	AI	26	GLY	N-CA-C	5.08	125.81	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	905	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	2094	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	144	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	221	A	N9-C4-C5	5.08	107.83	105.80
22	BA	2700	A	N9-C4-C5	5.08	107.83	105.80
1	AA	393	A	C5-C6-N1	5.08	120.24	117.70
22	BA	127	A	N9-C4-C5	5.08	107.83	105.80
22	BA	1046	A	N9-C4-C5	5.08	107.83	105.80
22	BA	1262	A	C8-N9-C4	5.08	107.83	105.80
22	BA	1359	A	C5-C6-N1	5.08	120.24	117.70
22	BA	1571	A	N9-C4-C5	5.08	107.83	105.80
22	BA	1677	A	C8-N9-C4	5.08	107.83	105.80
22	BA	2063	C	C6-N1-C2	-5.08	118.27	120.30
22	BA	2602	A	C5-C6-N1	5.08	120.24	117.70
22	BA	2899	A	C5-C6-N1	5.08	120.24	117.70
1	AA	182	A	N3-C4-N9	5.08	131.46	127.40
1	AA	460	A	C8-N9-C4	5.08	107.83	105.80
1	AA	1274	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	1465	A	C8-N9-C4	5.08	107.83	105.80
22	BA	21	A	C8-N9-C4	5.08	107.83	105.80
22	BA	2407	A	N9-C4-C5	5.08	107.83	105.80
1	AA	131	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	55	A	N9-C4-C5	5.08	107.83	105.80
1	AA	1492	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	332	A	C8-N9-C4	5.08	107.83	105.80
22	BA	1098	A	N9-C4-C5	5.08	107.83	105.80
22	BA	1571	A	C8-N9-C4	5.08	107.83	105.80
22	BA	2135	A	C8-N9-C4	5.08	107.83	105.80
22	BA	2317	A	C4-C5-N7	-5.08	108.16	110.70
1	AA	374	A	C4-C5-N7	-5.07	108.16	110.70
1	AA	459	A	C8-N9-C4	5.07	107.83	105.80
1	AA	621	A	N9-C4-C5	5.07	107.83	105.80
12	AL	102	LEU	CA-CB-CG	5.07	126.97	115.30
22	BA	1226	A	C5-C6-N1	5.07	120.24	117.70
22	BA	1385	A	C5-C6-N1	5.07	120.24	117.70
22	BA	1392	A	C4-C5-N7	-5.07	108.16	110.70
22	BA	1912	A	C4-C5-N7	-5.07	108.16	110.70
22	BA	2761	A	N9-C4-C5	5.07	107.83	105.80
1	AA	675	A	C4-C5-C6	5.07	119.54	117.00
1	AA	1171	A	C4-C5-N7	-5.07	108.16	110.70
22	BA	1590	A	C4-C5-N7	-5.07	108.16	110.70
1	AA	139	A	N9-C4-C5	5.07	107.83	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	111	A	N3-C4-N9	5.07	131.46	127.40
22	BA	1009	A	C5-C6-N1	5.07	120.23	117.70
22	BA	1077	A	N9-C4-C5	5.07	107.83	105.80
22	BA	2461	A	C4-C5-N7	-5.07	108.17	110.70
1	AA	1022	A	N9-C4-C5	5.07	107.83	105.80
22	BA	244	A	N3-C4-N9	5.07	131.46	127.40
22	BA	1515	A	N3-C4-N9	5.07	131.46	127.40
1	AA	270	A	N9-C4-C5	5.07	107.83	105.80
1	AA	363	A	N9-C4-C5	5.07	107.83	105.80
1	AA	635	A	C5-C6-N1	5.07	120.23	117.70
1	AA	1280	A	C5-C6-N1	5.07	120.23	117.70
22	BA	699	A	C4-C5-C6	5.07	119.53	117.00
22	BA	1528	A	N9-C4-C5	5.07	107.83	105.80
22	BA	2005	A	N9-C4-C5	5.07	107.83	105.80
22	BA	2184	A	C4-C5-N7	-5.07	108.17	110.70
1	AA	393	A	C8-N9-C4	5.07	107.83	105.80
1	AA	1021	A	C5-C6-N1	5.07	120.23	117.70
22	BA	1427	A	C5-C6-N1	5.07	120.23	117.70
22	BA	1597	A	C4-C5-N7	-5.07	108.17	110.70
22	BA	1871	A	N3-C4-N9	5.07	131.45	127.40
22	BA	2741	A	C4-C5-C6	5.07	119.53	117.00
22	BA	1807	G	C2-N3-C4	-5.06	109.37	111.90
1	AA	33	A	C8-N9-C4	5.06	107.83	105.80
1	AA	329	A	C8-N9-C4	5.06	107.83	105.80
1	AA	969	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	849	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	1570	A	N3-C4-N9	5.06	131.45	127.40
1	AA	533	A	N9-C4-C5	5.06	107.82	105.80
22	BA	1419	A	N9-C4-C5	5.06	107.83	105.80
22	BA	1918	A	C4-C5-N7	-5.06	108.17	110.70
1	AA	983	A	C8-N9-C4	5.06	107.82	105.80
1	AA	1357	A	C8-N9-C4	5.06	107.82	105.80
22	BA	547	A	C8-N9-C4	5.06	107.82	105.80
22	BA	899	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	1057	A	N9-C4-C5	5.06	107.82	105.80
22	BA	1069	A	N3-C4-N9	5.06	131.45	127.40
22	BA	1634	A	C4-C5-N7	-5.06	108.17	110.70
23	BB	58	A	C8-N9-C4	5.06	107.82	105.80
55	B8	42	A	C8-N9-C4	5.06	107.82	105.80
1	AA	1110	A	C5-C6-N1	5.06	120.23	117.70
1	AA	1329	A	N3-C4-N9	5.06	131.45	127.40
22	BA	844	A	C5-C6-N1	5.06	120.23	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1155	A	C8-N9-C4	5.06	107.82	105.80
22	BA	1313	U	C6-N1-C1'	-5.06	114.12	121.20
22	BA	1591	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	1609	A	C5-C6-N1	5.06	120.23	117.70
22	BA	1705	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	384	A	N9-C4-C5	5.06	107.82	105.80
22	BA	428	A	N3-C4-N9	5.06	131.44	127.40
22	BA	2314	A	C5-C6-N1	5.06	120.23	117.70
1	AA	389	A	C8-N9-C4	5.05	107.82	105.80
1	AA	607	A	C8-N9-C4	5.05	107.82	105.80
1	AA	648	A	C5-C6-N1	5.05	120.23	117.70
1	AA	1014	A	C5-C6-N1	5.05	120.23	117.70
22	BA	181	A	N3-C4-N9	5.05	131.44	127.40
22	BA	861	A	C8-N9-C4	5.05	107.82	105.80
22	BA	1090	A	C5-C6-N1	5.05	120.23	117.70
22	BA	1722	A	C8-N9-C4	5.05	107.82	105.80
22	BA	1916	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	2792	A	C4-C5-N7	-5.05	108.17	110.70
1	AA	974	A	N3-C4-N9	5.05	131.44	127.40
22	BA	563	A	C4-C5-C6	5.05	119.53	117.00
1	AA	7	A	C5-C6-N1	5.05	120.23	117.70
22	BA	1365	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	2317	A	C8-N9-C4	5.05	107.82	105.80
1	AA	44	A	C5-C6-N1	5.05	120.22	117.70
1	AA	50	A	C5-C6-N1	5.05	120.22	117.70
1	AA	130	A	N9-C4-C5	5.05	107.82	105.80
1	AA	819	A	N9-C4-C5	5.05	107.82	105.80
1	AA	1102	A	C4-C5-N7	-5.05	108.17	110.70
1	AA	1288	A	C4-C5-N7	-5.05	108.18	110.70
22	BA	2298	A	C4-C5-C6	5.05	119.53	117.00
55	B8	21	A	C8-N9-C4	5.05	107.82	105.80
1	AA	1531	A	C4-C5-N7	-5.05	108.18	110.70
22	BA	981	A	N3-C4-N9	5.05	131.44	127.40
1	AA	977	A	C8-N9-C4	5.05	107.82	105.80
22	BA	1745	A	N9-C4-C5	5.05	107.82	105.80
1	AA	435	A	C5-C6-N1	5.04	120.22	117.70
22	BA	191	A	C8-N9-C4	5.04	107.82	105.80
22	BA	1285	A	C8-N9-C4	5.04	107.82	105.80
22	BA	2887	A	C5-C6-N1	5.04	120.22	117.70
1	AA	199	A	C4-C5-N7	-5.04	108.18	110.70
1	AA	374	A	C5-C6-N1	5.04	120.22	117.70
22	BA	95	A	C8-N9-C4	5.04	107.82	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2369	A	C4-C5-C6	5.04	119.52	117.00
22	BA	2837	A	C8-N9-C4	5.04	107.82	105.80
1	AA	460	A	N9-C4-C5	5.04	107.82	105.80
1	AA	1102	A	C5-C6-N1	5.04	120.22	117.70
22	BA	1354	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	2322	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	2366	A	C5-C6-N1	5.04	120.22	117.70
1	AA	802	A	N9-C4-C5	5.04	107.82	105.80
22	BA	21	A	N9-C4-C5	5.04	107.82	105.80
22	BA	673	C	N3-C4-C5	5.04	123.92	121.90
22	BA	2183	A	N9-C4-C5	5.04	107.82	105.80
22	BA	1754	A	C8-N9-C4	5.04	107.82	105.80
22	BA	2176	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	2270	A	N9-C4-C5	5.04	107.81	105.80
1	AA	167	A	C8-N9-C4	5.04	107.81	105.80
1	AA	695	A	C5-C6-N1	5.04	120.22	117.70
1	AA	1349	A	C5-C6-N1	5.04	120.22	117.70
22	BA	322	A	C8-N9-C4	5.04	107.81	105.80
22	BA	2288	A	C5-C6-N1	5.04	120.22	117.70
22	BA	2530	A	C5-C6-N1	5.04	120.22	117.70
1	AA	412	A	C8-N9-C4	5.04	107.81	105.80
1	AA	1531	A	N9-C4-C5	5.04	107.81	105.80
22	BA	227	A	N3-C4-N9	5.04	131.43	127.40
22	BA	1040	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	2126	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	2566	A	N9-C4-C5	5.04	107.81	105.80
22	BA	2734	A	N9-C4-C5	5.04	107.81	105.80
1	AA	909	A	C5-C6-N1	5.03	120.22	117.70
1	AA	968	A	N9-C4-C5	5.03	107.81	105.80
1	AA	974	A	C4-C5-N7	-5.03	108.18	110.70
22	BA	94	A	C5-C6-N1	5.03	120.22	117.70
22	BA	918	A	N9-C4-C5	5.03	107.81	105.80
22	BA	1735	A	C5-C6-N1	5.03	120.22	117.70
22	BA	2003	A	C4-C5-N7	-5.03	108.18	110.70
22	BA	2033	A	C4-C5-N7	-5.03	108.18	110.70
22	BA	2205	A	C8-N9-C4	5.03	107.81	105.80
22	BA	2322	A	N9-C4-C5	5.03	107.81	105.80
1	AA	1437	A	C5-C6-N1	5.03	120.22	117.70
22	BA	2516	A	C8-N9-C4	5.03	107.81	105.80
1	AA	195	A	N3-C4-N9	5.03	131.43	127.40
1	AA	546	A	N9-C4-C5	5.03	107.81	105.80
1	AA	1213	A	C4-C5-C6	5.03	119.52	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1225	A	N9-C4-C5	5.03	107.81	105.80
22	BA	182	A	C5-C6-N1	5.03	120.22	117.70
22	BA	1889	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	2005	A	C8-N9-C4	5.03	107.81	105.80
22	BA	2873	A	N3-C4-N9	5.03	131.42	127.40
23	BB	108	A	C4-C5-C6	5.03	119.52	117.00
22	BA	2135	A	C5-C6-N1	5.03	120.21	117.70
1	AA	1180	A	N9-C4-C5	5.03	107.81	105.80
1	AA	1252	A	C4-C5-N7	-5.03	108.19	110.70
1	AA	1428	A	C5-C6-N1	5.03	120.21	117.70
22	BA	644	A	N9-C4-C5	5.03	107.81	105.80
22	BA	2749	A	N9-C4-C5	5.03	107.81	105.80
23	BB	45	A	C8-N9-C4	5.03	107.81	105.80
1	AA	1374	A	C5-C6-N1	5.03	120.21	117.70
22	BA	670	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	981	A	N9-C4-C5	5.03	107.81	105.80
22	BA	2406	A	C4-C5-C6	5.03	119.51	117.00
1	AA	502	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	1214	A	C4-C5-C6	5.02	119.51	117.00
1	AA	1248	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	56	A	N9-C4-C5	5.02	107.81	105.80
22	BA	1347	A	C5-C6-N1	5.02	120.21	117.70
22	BA	1701	A	N3-C4-N9	5.02	131.42	127.40
1	AA	595	A	C8-N9-C4	5.02	107.81	105.80
22	BA	877	A	C5-C6-N1	5.02	120.21	117.70
1	AA	143	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	502	A	C5-C6-N1	5.02	120.21	117.70
22	BA	802	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	1359	A	N3-C4-N9	5.02	131.42	127.40
1	AA	461	A	C4-C5-C6	5.02	119.51	117.00
22	BA	330	A	C8-N9-C4	5.02	107.81	105.80
22	BA	802	A	C5-C6-N1	5.02	120.21	117.70
22	BA	2377	A	N9-C4-C5	5.02	107.81	105.80
22	BA	2406	A	C5-C6-N1	5.02	120.21	117.70
1	AA	1311	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	928	A	C4-C5-C6	5.01	119.51	117.00
23	BB	50	A	C5-C6-N1	5.01	120.21	117.70
22	BA	1328	A	C5-C6-N1	5.01	120.21	117.70
22	BA	1821	A	C5-C6-N1	5.01	120.21	117.70
1	AA	59	A	C5-C6-N1	5.01	120.20	117.70
1	AA	179	A	C5-C6-N1	5.01	120.21	117.70
1	AA	435	A	C4-C5-N7	-5.01	108.19	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1441	A	C5-C6-N1	5.01	120.20	117.70
22	BA	1548	A	C5-C6-N1	5.01	120.21	117.70
22	BA	1597	A	N9-C4-C5	5.01	107.81	105.80
22	BA	2435	A	C8-N9-C4	5.01	107.80	105.80
1	AA	353	A	C5-C6-N1	5.01	120.20	117.70
1	AA	435	A	N9-C4-C5	5.01	107.80	105.80
1	AA	546	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	83	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	103	A	N9-C4-C5	5.01	107.80	105.80
22	BA	457	A	N3-C4-N9	5.01	131.41	127.40
22	BA	470	A	N9-C4-C5	5.01	107.80	105.80
22	BA	1147	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	1713	A	C4-C5-C6	5.01	119.50	117.00
22	BA	1927	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	2171	A	N9-C4-C5	5.01	107.80	105.80
22	BA	2850	A	N9-C4-C5	5.01	107.80	105.80
1	AA	238	A	N9-C4-C5	5.01	107.80	105.80
1	AA	1005	A	C5-C6-N1	5.01	120.20	117.70
1	AA	1246	A	C4-C5-N7	-5.01	108.20	110.70
22	BA	256	A	C4-C5-N7	-5.01	108.20	110.70
22	BA	324	A	N9-C4-C5	5.01	107.80	105.80
22	BA	563	A	N9-C4-C5	5.01	107.80	105.80
22	BA	1057	A	C5-C6-N1	5.01	120.20	117.70
22	BA	1413	A	C4-C5-N7	-5.01	108.20	110.70
22	BA	1987	A	C5-C6-N1	5.01	120.20	117.70
22	BA	2015	A	C5-C6-N1	5.01	120.20	117.70
22	BA	351	C	C2-N1-C1'	5.00	124.31	118.80
22	BA	1755	A	C5-C6-N1	5.00	120.20	117.70
1	AA	478	A	C5-C6-N1	5.00	120.20	117.70
1	AA	509	A	C8-N9-C4	5.00	107.80	105.80
1	AA	694	A	C5-C6-N1	5.00	120.20	117.70
1	AA	815	A	N9-C4-C5	5.00	107.80	105.80
22	BA	2670	A	C5-C6-N1	5.00	120.20	117.70
1	AA	129	A	C4-C5-N7	-5.00	108.20	110.70
1	AA	753	A	C5-C6-N1	5.00	120.20	117.70
1	AA	1429	A	C5-C6-N1	5.00	120.20	117.70
22	BA	344	A	N9-C4-C5	5.00	107.80	105.80
22	BA	1586	A	C4-C5-N7	-5.00	108.20	110.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	AJ	81	GLU	Peptide
51	B3	31	HIS	Peptide
27	BF	142	ASP	Peptide

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	AA	32930	0	16591	430	0
2	AB	1753	0	1780	43	0
3	AC	1624	0	1696	36	0
4	AD	1643	0	1707	41	0
5	AE	1144	0	1185	26	0
6	AF	862	0	864	28	0
7	AG	1181	0	1238	35	0
8	AH	979	0	1031	32	0
9	AI	1022	0	1070	45	0
10	AJ	795	0	836	35	0
11	AK	877	0	887	24	0
12	AL	957	0	1017	14	0
13	AM	883	0	941	50	0
14	AN	799	0	841	26	0
15	AO	714	0	734	13	0
16	AP	649	0	666	16	0
17	AQ	648	0	691	13	0
18	AR	455	0	478	7	0
19	AS	656	0	680	34	0
20	AT	670	0	719	3	0
21	AU	465	0	491	17	0
22	BA	62209	0	31308	391	0
23	BB	2569	0	1301	15	0
24	BC	2082	0	2154	19	0
25	BD	1566	0	1618	15	0
26	BE	1552	0	1619	15	0
27	BF	1410	0	1444	30	0
28	BG	1323	0	1371	18	0
29	BH	1110	0	1148	32	0
30	BI	522	0	520	20	0
31	BJ	1129	0	1162	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BK	946	0	1023	12	0
33	BL	1053	0	1129	18	0
34	BM	1075	0	1155	9	0
35	BN	945	0	989	8	0
36	BO	900	0	935	11	0
37	BP	917	0	962	12	0
38	BQ	947	0	1019	12	0
39	BR	816	0	839	11	0
40	BS	857	0	922	11	0
41	BT	738	0	807	12	0
42	BU	779	0	831	15	0
43	BV	753	0	780	15	0
44	BW	580	0	594	6	0
45	BX	625	0	652	4	0
46	BY	501	0	531	5	0
47	BZ	449	0	488	4	0
48	B0	444	0	458	5	0
49	B1	414	0	442	11	0
50	B2	377	0	418	7	0
51	B3	504	0	572	11	0
52	B4	302	0	340	3	0
53	B5	146	0	143	2	0
54	B7	146	0	77	4	0
55	B8	1646	0	831	19	0
56	AA	35	0	0	0	0
56	B8	1	0	0	0	0
56	BA	132	0	0	1	0
56	BC	1	0	0	0	0
56	BD	1	0	0	0	0
57	AB	1	0	0	0	0
57	B4	1	0	0	0	0
57	BI	1	0	0	0	0
58	BA	15	0	9	0	0
59	AA	168	0	0	3	0
59	AK	1	0	0	0	0
59	AM	1	0	0	0	0
59	AN	2	0	0	0	0
59	B8	1	0	0	1	0
59	BA	608	0	0	4	0
59	BC	7	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	BL	2	0	0	0	0
59	BN	1	0	0	0	0
All	All	145019	0	96734	1531	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 6.

All (1531) 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)
22:BA:962:G:OP1	59:BA:3201:HOH:O	1.58	1.19
22:BA:2107:G:H1	22:BA:2182:U:H3	1.03	1.01
22:BA:2133:G:N2	22:BA:2158:A:N6	2.12	0.98
13:AM:53:ILE:HG22	13:AM:57:ARG:HH21	1.26	0.97
22:BA:2133:G:N2	22:BA:2158:A:C6	2.35	0.94
22:BA:143:C:O2'	41:BT:3:ARG:NH1	2.02	0.93
1:AA:49:U:C5	1:AA:365:U:O4	2.23	0.92
1:AA:445:G:H1	1:AA:489:C:H5	1.11	0.92
1:AA:49:U:C4	1:AA:365:U:O4	2.24	0.91
22:BA:1847:A:HO2'	22:BA:1848:A:H8	0.93	0.90
22:BA:2100:G:O6	22:BA:2189:U:O4	1.93	0.86
1:AA:49:U:O4	1:AA:365:U:O4	1.94	0.85
22:BA:2304:G:H22	22:BA:2312:U:H3	1.21	0.83
22:BA:2100:G:O6	22:BA:2189:U:C4	2.32	0.82
4:AD:184:ARG:NH1	4:AD:187:GLU:OE1	2.12	0.82
19:AS:18:LYS:HB3	19:AS:31:LEU:HD11	1.62	0.82
1:AA:664:G:H22	1:AA:741:G:H1	1.28	0.81
22:BA:882:G:N2	22:BA:883:G:N7	2.28	0.81
22:BA:2133:G:H2'	22:BA:2157:G:H22	1.45	0.81
1:AA:522:C:O2	1:AA:527:G7M:N2	2.13	0.81
22:BA:1250:G:H5''	38:BQ:6:ARG:HD3	1.62	0.81
40:BS:11:ARG:HH22	40:BS:98:LYS:HD3	1.46	0.80
8:AH:12:THR:HG22	8:AH:15:ARG:HH12	1.45	0.80
8:AH:18:GLN:HE21	8:AH:70:ALA:HB1	1.45	0.79
9:AI:25:ASN:OD1	9:AI:59:GLU:HG3	1.81	0.79
1:AA:461:A:H2'	1:AA:462:G:H8	1.48	0.79
9:AI:12:ARG:HG3	9:AI:13:LYS:H	1.47	0.78
3:AC:57:ILE:HG23	3:AC:64:ILE:HD11	1.66	0.78
24:BC:107:PRO:HD2	24:BC:110:LEU:HD22	1.66	0.78
1:AA:1103:C:OP1	2:AB:95:ARG:NH2	2.17	0.77
13:AM:57:ARG:NH1	30:BI:35:ASP:OD1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BP:91:ALA:HB3	37:BP:111:LYS:HG3	1.65	0.77
1:AA:76:G:H1	1:AA:93:U:H3	1.31	0.76
22:BA:1649:G:O2'	35:BN:106:ASP:OD2	2.02	0.76
22:BA:2151:U:H2'	22:BA:2152:G:H8	1.49	0.76
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.19	0.76
11:AK:107:ILE:HD12	21:AU:6:VAL:HG21	1.66	0.76
4:AD:58:LYS:NZ	4:AD:59:GLN:OE1	2.18	0.75
5:AE:115:LEU:HD13	5:AE:123:VAL:HG21	1.68	0.75
16:AP:48:GLU:CD	16:AP:49:GLY:H	1.90	0.75
22:BA:546:U:O2	22:BA:548:G:N2	2.19	0.75
24:BC:5:LYS:NZ	24:BC:14:ARG:O	2.17	0.75
1:AA:1124:G:OP1	10:AJ:37:ARG:NH1	2.20	0.74
22:BA:2133:G:C2	22:BA:2158:A:N6	2.54	0.74
25:BD:12:THR:OG1	37:BP:9:GLU:OE2	2.04	0.74
28:BG:42:GLU:OE2	28:BG:55:ARG:NE	2.20	0.74
4:AD:100:ASN:OD1	4:AD:111:ARG:NH1	2.20	0.74
22:BA:2840:C:H5''	35:BN:53:THR:HG21	1.70	0.73
35:BN:32:GLU:OE1	35:BN:86:ARG:NH2	2.20	0.73
55:B8:18:G:O2'	55:B8:57:G:N2	2.21	0.73
4:AD:188:ARG:NH1	4:AD:191:LEU:O	2.21	0.73
42:BU:34:VAL:HG13	42:BU:67:VAL:HG12	1.71	0.73
1:AA:1516:2MG:N2	1:AA:1519:MA6:OP2	2.21	0.72
22:BA:1847:A:O2'	22:BA:1848:A:H8	1.71	0.72
1:AA:673:A:H2'	1:AA:674:G:C8	2.24	0.72
22:BA:2720:U:OP1	37:BP:53:ARG:NH2	2.23	0.72
22:BA:636:G:OP2	33:BL:109:LYS:NZ	2.23	0.72
22:BA:2107:G:N2	22:BA:2182:U:O2	2.18	0.72
51:B3:28:ASN:O	51:B3:36:LYS:NZ	2.22	0.72
22:BA:1102:C:H2'	22:BA:1103:A:H8	1.55	0.72
13:AM:79:ARG:NH1	19:AS:65:GLU:OE2	2.21	0.72
1:AA:208:U:C2	1:AA:211:G:O6	2.43	0.72
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.72	0.72
26:BE:111:GLU:OE2	26:BE:114:ARG:NH1	2.23	0.71
30:BI:18:CYS:SG	30:BI:20:ASN:ND2	2.62	0.71
7:AG:16:PRO:HB3	9:AI:46:MET:HE1	1.72	0.71
28:BG:25:THR:OG1	28:BG:32:GLU:OE2	2.08	0.71
44:BW:66:LYS:NZ	44:BW:85:GLU:OE2	2.23	0.71
47:BZ:3:LYS:NZ	47:BZ:59:GLU:OXT	2.23	0.71
25:BD:77:ARG:NH2	25:BD:200:ASP:OD1	2.24	0.71
27:BF:16:LEU:HD23	27:BF:28:VAL:HG13	1.73	0.71
1:AA:458:U:H2'	1:AA:459:A:C8	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:382:A:H2'	1:AA:383:A:C8	2.26	0.71
6:AF:86:ARG:NH1	18:AR:64:TYR:O	2.24	0.71
9:AI:46:MET:N	9:AI:46:MET:SD	2.64	0.71
26:BE:97:ASN:HB2	26:BE:100:MET:HG3	1.73	0.70
22:BA:2105:U:H2'	22:BA:2106:U:C6	2.27	0.70
1:AA:544:G:OP1	4:AD:56:ARG:NH2	2.23	0.70
7:AG:69:VAL:HG13	7:AG:100:ALA:HB1	1.73	0.70
29:BH:57:LYS:HA	29:BH:60:GLU:HG2	1.74	0.70
44:BW:19:LYS:HG3	44:BW:41:ARG:HH22	1.57	0.70
10:AJ:37:ARG:HA	10:AJ:37:ARG:HH11	1.56	0.69
26:BE:7:ASP:OD2	26:BE:122:GLU:N	2.19	0.69
7:AG:140:ASP:OD1	7:AG:143:ARG:NH1	2.26	0.69
1:AA:1086:U:H3	1:AA:1099:G:H22	1.40	0.69
1:AA:1147:C:O2	9:AI:18:ARG:NH2	2.24	0.69
1:AA:1254:A:OP2	10:AJ:45:ARG:NH2	2.21	0.69
22:BA:962:G:P	59:BA:3201:HOH:O	2.39	0.69
42:BU:26:LYS:NZ	42:BU:37:GLU:OE2	2.20	0.69
1:AA:537:G:OP1	12:AL:110:ARG:NH2	2.23	0.69
22:BA:1366:A:OP1	45:BX:2:SER:OG	2.11	0.69
9:AI:106:ARG:NH1	9:AI:107:ASP:O	2.26	0.69
1:AA:1119:C:OP1	9:AI:85:ARG:NH1	2.22	0.68
1:AA:1380:U:O2'	7:AG:3:ARG:NH1	2.26	0.68
1:AA:208:U:O2	1:AA:211:G:O6	2.10	0.68
22:BA:2278:A:OP1	34:BM:10:ARG:NH2	2.26	0.68
40:BS:48:LYS:O	40:BS:52:GLU:HG3	1.92	0.68
2:AB:164:ILE:HD13	2:AB:186:ILE:HD13	1.76	0.68
22:BA:2299:U:OP2	27:BF:71:ARG:NH1	2.23	0.68
9:AI:24:GLY:O	9:AI:25:ASN:HB2	1.93	0.68
22:BA:1667:G:O2'	22:BA:1991:U:O4	2.10	0.68
22:BA:2106:U:H2'	22:BA:2107:G:H8	1.58	0.68
1:AA:1266:G:N2	1:AA:1269:A:OP2	2.21	0.67
22:BA:183:C:H42	22:BA:213:A:H61	1.42	0.67
22:BA:2305:U:H5''	27:BF:131:GLY:HA3	1.76	0.67
21:AU:31:GLU:OE1	21:AU:34:ARG:NH2	2.25	0.67
40:BS:72:THR:OG1	40:BS:108:SER:OG	2.13	0.67
22:BA:286:U:H2'	22:BA:287:G:H8	1.60	0.67
22:BA:1799:G:N7	24:BC:178:SER:OG	2.26	0.67
22:BA:2469:A:N6	22:BA:2481:G:O2'	2.26	0.67
27:BF:102:ARG:HG2	30:BI:24:ILE:HD11	1.76	0.67
27:BF:105:THR:HA	30:BI:38:SER:HB3	1.75	0.67
12:AL:114:ARG:HB2	12:AL:119:VAL:HB	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:83:LEU:HD11	19:AS:66:MET:CG	2.25	0.67
22:BA:1069:A:H5''	22:BA:1070:A:C8	2.30	0.67
28:BG:86:LYS:HG2	28:BG:165:ALA:HB2	1.74	0.67
11:AK:64:GLN:NE2	11:AK:68:GLU:OE1	2.27	0.67
19:AS:67:VAL:O	30:BI:56:ARG:NH1	2.28	0.67
21:AU:4:ILE:HD12	21:AU:19:PHE:HA	1.76	0.67
1:AA:78:A:H2'	1:AA:79:G:C8	2.30	0.67
22:BA:1417:C:HO2'	22:BA:1587:G:HO2'	1.36	0.66
2:AB:7:ARG:O	2:AB:11:LYS:NZ	2.28	0.66
2:AB:59:LYS:O	2:AB:63:ARG:NE	2.29	0.66
1:AA:49:U:H5	1:AA:365:U:O4	1.76	0.66
22:BA:881:G:H21	22:BA:896:A:H62	1.42	0.66
1:AA:616:G:O2'	16:AP:47:GLU:OE2	2.07	0.66
1:AA:951:G:OP2	13:AM:101:ARG:NH2	2.28	0.66
1:AA:1071:C:H2'	1:AA:1072:G:H8	1.61	0.66
22:BA:1607:C:N4	22:BA:1622:G:OP2	2.28	0.66
23:BB:1:U:H2'	23:BB:2:G:H8	1.61	0.66
29:BH:21:VAL:HG21	29:BH:25:TYR:HD2	1.61	0.66
1:AA:652:U:O4	1:AA:752:G:O2'	2.14	0.65
22:BA:639:U:H2'	22:BA:640:C:C6	2.31	0.65
29:BH:113:SER:O	29:BH:116:ARG:NH2	2.25	0.65
1:AA:216:U:H2'	1:AA:217:C:C6	2.31	0.65
22:BA:2134:A:N6	22:BA:2157:G:O2'	2.30	0.65
48:B0:46:ASP:OD2	48:B0:46:ASP:N	2.29	0.65
1:AA:79:G:H2'	1:AA:80:A:C8	2.31	0.65
29:BH:111:ALA:HB3	29:BH:114:GLU:HG3	1.79	0.65
11:AK:107:ILE:CD1	21:AU:6:VAL:HG21	2.27	0.65
4:AD:65:TYR:OH	4:AD:95:GLU:OE2	2.15	0.65
1:AA:946:A:H2'	1:AA:947:G:C8	2.32	0.65
3:AC:73:PRO:HB3	3:AC:105:GLU:HG3	1.78	0.64
36:BO:84:GLU:HG2	36:BO:85:LYS:HD2	1.79	0.64
1:AA:1363:A:O2'	1:AA:1365:G:N7	2.28	0.64
1:AA:458:U:H2'	1:AA:459:A:H8	1.61	0.64
22:BA:548:G:O2'	22:BA:549:G:O4'	2.15	0.64
1:AA:1305:G:H21	1:AA:1332:A:H2	1.44	0.64
22:BA:1174:U:O2	22:BA:1177:G:N1	2.30	0.64
22:BA:2068:U:H3	22:BA:2430:A:H2	1.43	0.64
22:BA:2030:6MZ:H2	22:BA:2499:C:H5''	1.80	0.63
8:AH:106:THR:HG23	8:AH:108:LYS:H	1.63	0.63
1:AA:1178:G:N7	9:AI:99:ARG:NH2	2.46	0.63
50:B2:24:THR:HG23	50:B2:27:GLY:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1317:C:H42	14:AN:53:ARG:HH11	1.47	0.63
36:BO:76:LYS:O	36:BO:80:GLU:HG3	1.98	0.63
1:AA:974:A:OP1	14:AN:69:ARG:NH2	2.30	0.63
1:AA:1288:A:H2'	1:AA:1289:A:C8	2.34	0.62
5:AE:153:VAL:HG23	5:AE:156:LYS:HE2	1.81	0.62
1:AA:1038:C:H2'	1:AA:1039:G:H8	1.63	0.62
1:AA:1287:A:H2'	1:AA:1288:A:C8	2.34	0.62
6:AF:38:ARG:NH1	6:AF:98:GLU:O	2.32	0.62
8:AH:92:LEU:O	8:AH:117:ARG:NH2	2.32	0.62
1:AA:31:G:O2'	1:AA:48:C:N4	2.32	0.62
34:BM:77:PRO:HG2	34:BM:80:VAL:HG21	1.79	0.62
1:AA:1026:G:N1	1:AA:1035:A:C5	2.67	0.62
24:BC:251:GLN:NE2	24:BC:252:THR:O	2.32	0.62
1:AA:254:G:OP1	17:AQ:70:THR:OG1	2.15	0.62
22:BA:2102:G:H1	22:BA:2187:U:H3	1.46	0.62
27:BF:56:ASP:OD2	27:BF:57:LEU:N	2.33	0.62
8:AH:18:GLN:NE2	8:AH:70:ALA:HB1	2.14	0.62
14:AN:90:ARG:HB3	14:AN:92:GLU:OE1	2.00	0.62
1:AA:456:A:H2'	1:AA:457:G:C8	2.35	0.62
1:AA:1321:U:O2'	19:AS:78:ARG:NH2	2.33	0.62
22:BA:1724:G:H1	22:BA:1736:U:H3	1.48	0.62
22:BA:2184:A:H2'	22:BA:2185:U:C6	2.34	0.61
1:AA:1273:C:H2'	1:AA:1274:A:O4'	2.01	0.61
22:BA:183:C:N4	22:BA:213:A:H61	1.99	0.61
27:BF:115:ARG:HG3	30:BI:47:LYS:HE3	1.81	0.61
11:AK:23:ILE:HG21	11:AK:96:THR:HG21	1.81	0.61
1:AA:1229:A:OP2	13:AM:113:ARG:NH2	2.28	0.61
1:AA:1530:G:O6	21:AU:46:LYS:NZ	2.27	0.61
1:AA:337:G:H2'	1:AA:338:A:C8	2.35	0.61
1:AA:1118:U:OP1	9:AI:11:ARG:NH1	2.28	0.61
22:BA:2106:U:H2'	22:BA:2107:G:C8	2.36	0.61
1:AA:1250:A:H2'	1:AA:1251:A:C8	2.35	0.61
13:AM:66:GLU:HG3	13:AM:67:GLY:H	1.65	0.61
38:BQ:112:LYS:HE3	39:BR:49:ILE:HB	1.83	0.61
22:BA:636:G:N1	33:BL:76:GLU:OE1	2.29	0.61
26:BE:2:GLU:HG2	26:BE:13:THR:HA	1.82	0.61
1:AA:746:A:H2'	1:AA:747:A:C8	2.36	0.61
6:AF:3:HIS:HB2	6:AF:92:THR:O	2.01	0.61
1:AA:1101:A:N7	2:AB:171:ILE:HD11	2.16	0.60
22:BA:1720:U:H2'	22:BA:1721:G:O4'	2.01	0.60
22:BA:1869:G:N2	22:BA:1871:A:O2'	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BR:38:VAL:HG23	39:BR:54:VAL:HG22	1.83	0.60
1:AA:1239:A:H62	1:AA:1299:A:H62	1.47	0.60
27:BF:110:ARG:HH22	27:BF:139:PRO:HB3	1.65	0.60
1:AA:335:C:H2'	1:AA:336:A:C8	2.36	0.60
7:AG:113:ASP:OD1	7:AG:114:LYS:N	2.34	0.60
22:BA:2845:U:H5''	37:BP:52:ASN:O	2.01	0.60
32:BK:40:LYS:HD3	32:BK:58:LEU:O	2.02	0.60
1:AA:405:U:O4	4:AD:2:ALA:N	2.34	0.60
6:AF:3:HIS:HB3	6:AF:92:THR:HG23	1.83	0.60
4:AD:78:GLU:OE2	4:AD:81:ARG:NH2	2.30	0.60
10:AJ:16:ARG:O	10:AJ:20:GLN:NE2	2.34	0.60
1:AA:1175:G:H2'	1:AA:1176:A:H8	1.66	0.60
22:BA:2188:U:HO2'	22:BA:2189:U:H6	1.48	0.60
1:AA:891:U:H2'	1:AA:892:A:H8	1.66	0.60
3:AC:138:VAL:HG21	3:AC:168:TYR:HD2	1.65	0.60
19:AS:67:VAL:HG13	30:BI:56:ARG:NH2	2.17	0.60
22:BA:534:U:O2'	38:BQ:49:ASP:OD2	2.16	0.60
22:BA:962:G:OP1	56:BA:3083:MG:MG	1.43	0.60
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.37	0.60
13:AM:83:LEU:HD11	19:AS:66:MET:HG2	1.84	0.60
47:BZ:3:LYS:HD2	47:BZ:4:THR:O	2.01	0.60
55:B8:23:C:H2'	55:B8:24:G:H8	1.67	0.60
1:AA:427:U:OP1	4:AD:13:ARG:NH1	2.34	0.60
22:BA:1814:G:OP2	22:BA:1815:A:O2'	2.12	0.60
39:BR:43:ASN:O	39:BR:46:GLU:HG2	2.01	0.60
1:AA:932:C:OP1	7:AG:4:ARG:NE	2.25	0.60
22:BA:285:G:H1	22:BA:355:U:H3	1.47	0.60
22:BA:1173:U:O2'	22:BA:1174:U:O4'	2.19	0.60
37:BP:68:GLU:OE1	37:BP:68:GLU:N	2.34	0.60
9:AI:55:VAL:HG12	9:AI:57:MET:HG2	1.83	0.59
49:B1:43:VAL:O	49:B1:44:ARG:HB2	2.02	0.59
1:AA:999:C:N3	1:AA:1042:A:N6	2.49	0.59
3:AC:28:GLU:OE1	3:AC:28:GLU:N	2.35	0.59
39:BR:41:ILE:HD12	39:BR:103:ALA:HB2	1.84	0.59
9:AI:97:GLU:HA	9:AI:100:LYS:HE2	1.85	0.59
22:BA:1245:G:OP1	33:BL:13:LYS:NZ	2.31	0.59
22:BA:2100:G:C2	22:BA:2101:A:H1'	2.37	0.59
22:BA:2159:G:H2'	22:BA:2160:C:C6	2.38	0.59
54:B7:5:C:H2'	54:B7:6:G:C8	2.36	0.59
22:BA:277:G:OP2	22:BA:277:G:N2	2.27	0.59
22:BA:2115:G:OP1	22:BA:2166:U:O2'	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BB:13:G:O2'	23:BB:15:A:OP2	2.21	0.59
3:AC:175:LEU:HD23	3:AC:182:ILE:HD13	1.85	0.59
4:AD:58:LYS:NZ	4:AD:69:GLU:OE2	2.25	0.59
12:AL:4:VAL:HG23	17:AQ:34:TYR:HB3	1.84	0.59
11:AK:107:ILE:HD13	21:AU:12:PHE:CE2	2.38	0.59
22:BA:195:A:H8	59:BA:3403:HOH:O	1.81	0.59
42:BU:51:ALA:O	42:BU:52:LEU:HG	2.02	0.59
1:AA:86:G:H1'	1:AA:87:C:C5	2.38	0.59
22:BA:1096:A:H2'	22:BA:1097:U:O4'	2.03	0.59
22:BA:2124:G:H1	22:BA:2174:C:H42	1.51	0.59
24:BC:154:LEU:HD13	24:BC:176:LEU:HD21	1.83	0.59
1:AA:1038:C:H2'	1:AA:1039:G:C8	2.38	0.59
2:AB:165:ASP:OD2	2:AB:168:HIS:HB2	2.03	0.59
10:AJ:63:ASP:OD1	14:AN:98:LYS:NZ	2.36	0.59
16:AP:52:LEU:HD12	16:AP:57:ILE:HD11	1.85	0.59
18:AR:48:ARG:HB2	18:AR:51:TYR:CD2	2.38	0.59
23:BB:51:G:OP1	36:BO:63:LYS:NZ	2.22	0.59
22:BA:585:G:N7	38:BQ:6:ARG:NH1	2.51	0.58
46:BY:49:ASP:OD1	46:BY:52:ARG:NH2	2.35	0.58
2:AB:23:TRP:CZ3	2:AB:25:PRO:HA	2.38	0.58
1:AA:49:U:O4	1:AA:365:U:C4	2.56	0.58
22:BA:2162:G:OP2	22:BA:2164:C:N4	2.36	0.58
1:AA:399:G:H2'	1:AA:400:C:C6	2.39	0.58
1:AA:677:U:H3	1:AA:713:G:H22	1.51	0.58
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.50	0.58
22:BA:24:G:N2	40:BS:78:GLU:OE2	2.36	0.58
22:BA:285:G:N2	22:BA:355:U:O2	2.29	0.58
22:BA:1438:U:H2'	22:BA:1439:A:H8	1.68	0.58
22:BA:1704:C:H2'	22:BA:1705:A:H8	1.68	0.58
39:BR:6:GLN:HG2	39:BR:11:GLN:HG2	1.85	0.58
1:AA:1244:G:H2'	1:AA:1245:C:C6	2.38	0.58
9:AI:84:THR:HG23	9:AI:98:LEU:HD13	1.85	0.58
28:BG:2:SER:OG	28:BG:6:LYS:NZ	2.37	0.58
29:BH:21:VAL:HG21	29:BH:25:TYR:CD2	2.38	0.58
19:AS:41:PHE:H	19:AS:44:MET:CE	2.16	0.58
1:AA:600:A:O3'	8:AH:89:LYS:NZ	2.35	0.58
7:AG:18:PHE:CZ	7:AG:58:GLU:HG2	2.39	0.58
22:BA:856:G:H2'	22:BA:857:G:C8	2.38	0.58
55:B8:71:C:H2'	55:B8:72:G:C8	2.39	0.58
1:AA:324:G:N1	1:AA:327:A:OP2	2.32	0.58
1:AA:1315:U:O2'	1:AA:1360:A:O2'	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:47:LEU:HD11	7:AG:62:PHE:HB2	1.86	0.58
8:AH:24:ALA:HB1	8:AH:60:GLU:OE2	2.04	0.58
22:BA:1175:A:H8	22:BA:1176:U:C4	2.22	0.58
1:AA:1317:C:N3	14:AN:53:ARG:HD2	2.19	0.57
9:AI:26:GLY:N	9:AI:59:GLU:O	2.37	0.57
22:BA:2107:G:H2'	22:BA:2108:A:C8	2.39	0.57
22:BA:2636:C:O2'	25:BD:45:TYR:OH	2.18	0.57
1:AA:84:U:O2'	1:AA:87:C:N3	2.36	0.57
1:AA:841:C:C2	1:AA:843:U:H5''	2.39	0.57
3:AC:100:GLN:NE2	3:AC:102:ASN:OD1	2.37	0.57
22:BA:2030:6MZ:C2	22:BA:2499:C:H5''	2.34	0.57
1:AA:1055:A:O2'	3:AC:161:GLU:O	2.21	0.57
1:AA:1347:G:O6	9:AI:12:ARG:NH2	2.36	0.57
1:AA:1386:G:H2'	1:AA:1387:G:H8	1.68	0.57
49:B1:37:LYS:HG2	49:B1:48:ILE:HD13	1.86	0.57
22:BA:2185:U:H2'	22:BA:2186:G:C8	2.39	0.57
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.40	0.57
22:BA:994:C:O2	39:BR:10:LYS:NZ	2.37	0.57
55:B8:3:G:H4'	55:B8:4:U:OP1	2.05	0.57
1:AA:189:A:H2'	1:AA:190:A:C8	2.39	0.57
1:AA:1092:A:H2'	1:AA:1093:A:C8	2.40	0.57
1:AA:1280:A:OP1	10:AJ:9:ARG:NH1	2.37	0.57
22:BA:2102:G:N2	22:BA:2187:U:O2	2.30	0.57
7:AG:16:PRO:HB3	9:AI:46:MET:CE	2.34	0.57
8:AH:96:MET:HB3	8:AH:100:GLY:H	1.70	0.57
22:BA:545:U:O2'	22:BA:546:U:O4'	2.19	0.57
22:BA:2134:A:H8	22:BA:2157:G:H21	1.51	0.57
1:AA:1218:C:H2'	1:AA:1219:A:H8	1.70	0.57
4:AD:85:ASN:OD1	4:AD:88:GLU:N	2.30	0.57
28:BG:24:ILE:HD13	28:BG:72:LEU:HD21	1.87	0.57
1:AA:823:C:HO2'	8:AH:2:SER:N	2.03	0.57
31:BJ:36:LEU:O	31:BJ:121:LYS:NZ	2.35	0.57
22:BA:2151:U:H2'	22:BA:2152:G:C8	2.34	0.56
1:AA:958:A:H5'	19:AS:55:ARG:HH12	1.70	0.56
27:BF:80:ARG:HH22	55:B8:56:C:N4	2.03	0.56
1:AA:78:A:H2'	1:AA:79:G:H8	1.69	0.56
1:AA:1244:G:H2'	1:AA:1245:C:H6	1.71	0.56
16:AP:36:VAL:HG13	16:AP:53:ASP:HB2	1.87	0.56
21:AU:12:PHE:CE1	21:AU:16:LEU:HD23	2.41	0.56
22:BA:356:G:H2'	22:BA:357:C:C6	2.41	0.56
22:BA:356:G:H2'	22:BA:357:C:H6	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1266:G:O2'	22:BA:2012:G:O6	2.16	0.56
22:BA:2131:U:H5'	22:BA:2132:U:H5''	1.86	0.56
22:BA:2314:A:H2'	22:BA:2315:G:H8	1.69	0.56
1:AA:436:C:H2'	1:AA:437:U:C6	2.40	0.56
19:AS:12:ASP:OD2	19:AS:35:SER:OG	2.16	0.56
22:BA:2273:A:H2'	22:BA:2274:A:C8	2.41	0.56
28:BG:149:ARG:HA	28:BG:162:VAL:HG13	1.87	0.56
22:BA:1738:G:O2'	22:BA:1739:A:O5'	2.24	0.56
1:AA:335:C:H2'	1:AA:336:A:H8	1.70	0.56
1:AA:461:A:H2'	1:AA:462:G:C8	2.37	0.56
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.41	0.56
2:AB:135:LEU:O	2:AB:139:ARG:HB2	2.04	0.56
5:AE:83:HIS:CE1	5:AE:147:MET:HG3	2.41	0.56
11:AK:64:GLN:HG2	11:AK:99:ALA:HB2	1.88	0.56
1:AA:672:U:H2'	1:AA:673:A:C8	2.40	0.56
1:AA:714:G:H2'	1:AA:715:A:C8	2.41	0.56
4:AD:164:GLN:OE1	4:AD:164:GLN:N	2.35	0.56
13:AM:3:ARG:HG2	13:AM:9:ILE:HG13	1.88	0.56
8:AH:25:VAL:HG13	8:AH:63:LEU:HD11	1.86	0.56
13:AM:81:MET:O	13:AM:92:ARG:NH2	2.39	0.56
24:BC:29:PRO:HG2	24:BC:34:LEU:HD11	1.87	0.56
1:AA:1123:U:O2'	10:AJ:39:PRO:O	2.23	0.56
9:AI:123:ARG:NH1	9:AI:124:ARG:O	2.39	0.56
22:BA:1069:A:H5''	22:BA:1070:A:H8	1.70	0.56
45:BX:72:ARG:NH1	45:BX:78:TYR:OH	2.37	0.56
1:AA:1229:A:P	13:AM:113:ARG:HH22	2.29	0.55
3:AC:16:LYS:NZ	3:AC:181:ASP:OD2	2.38	0.55
8:AH:96:MET:HG3	8:AH:99:LEU:HB2	1.88	0.55
24:BC:3:VAL:HG12	24:BC:19:VAL:HG22	1.87	0.55
29:BH:12:LEU:HD11	29:BH:25:TYR:HE2	1.71	0.55
22:BA:2484:G:OP1	34:BM:44:ARG:NH2	2.39	0.55
2:AB:48:PRO:O	2:AB:51:ASN:N	2.39	0.55
1:AA:279:A:H5'	1:AA:279:A:H8	1.71	0.55
1:AA:490:C:H2'	1:AA:491:G:H8	1.71	0.55
1:AA:1033:G:H2'	1:AA:1034:G:C8	2.42	0.55
1:AA:1166:G:N1	1:AA:1169:A:OP2	2.39	0.55
3:AC:191:THR:HG23	3:AC:193:TYR:H	1.72	0.55
6:AF:40:GLU:OE1	6:AF:100:SER:OG	2.19	0.55
13:AM:3:ARG:NH1	27:BF:110:ARG:HH11	2.04	0.55
1:AA:90:C:H2'	1:AA:91:U:C6	2.42	0.55
5:AE:104:GLY:H	5:AE:122:ASN:HD22	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:59:THR:HG22	11:AK:61:PHE:H	1.71	0.55
28:BG:170:ARG:NH1	52:B4:29:ALA:O	2.37	0.55
22:BA:880:G:H2'	22:BA:881:G:H8	1.71	0.55
26:BE:194:LYS:O	26:BE:197:GLU:HG2	2.07	0.55
31:BJ:110:PRO:O	31:BJ:115:GLY:HA3	2.06	0.55
36:BO:43:ASN:ND2	36:BO:45:SER:OG	2.40	0.55
51:B3:31:HIS:C	51:B3:33:LEU:H	2.10	0.55
51:B3:32:ILE:H	51:B3:32:ILE:HD12	1.72	0.55
55:B8:69:A:H2'	55:B8:70:C:C6	2.42	0.55
4:AD:152:GLN:HG3	4:AD:154:ARG:H	1.72	0.55
7:AG:116:MET:HA	7:AG:119:ARG:HB3	1.88	0.55
22:BA:277:G:H4'	22:BA:278:A:C5	2.42	0.55
22:BA:1068:G:N2	22:BA:1095:A:O3'	2.33	0.55
22:BA:1816:C:N4	24:BC:35:GLU:OE1	2.38	0.55
1:AA:1040:U:H2'	1:AA:1041:G:C8	2.42	0.55
13:AM:17:ILE:O	13:AM:20:THR:OG1	2.24	0.55
22:BA:1084:A:H2'	22:BA:1085:A:C8	2.42	0.55
1:AA:377:G:H2'	1:AA:378:G:H8	1.72	0.55
37:BP:112:GLU:OE1	37:BP:114:LEU:HD23	2.07	0.55
1:AA:384:G:H2'	1:AA:385:C:C6	2.42	0.54
1:AA:1314:C:H2'	1:AA:1315:U:H6	1.72	0.54
22:BA:2788:C:H2'	22:BA:2789:C:C6	2.42	0.54
1:AA:279:A:H5'	1:AA:279:A:C8	2.42	0.54
1:AA:674:G:H2'	1:AA:675:A:C8	2.42	0.54
4:AD:12:SER:OG	4:AD:17:THR:O	2.17	0.54
22:BA:1182:G:H2'	22:BA:1183:U:O4'	2.06	0.54
22:BA:2394:C:H5''	33:BL:63:LYS:HE2	1.89	0.54
34:BM:31:PHE:CZ	34:BM:110:GLU:HB2	2.42	0.54
1:AA:512:U:H2'	1:AA:513:C:C6	2.42	0.54
6:AF:101:PRO:HG2	18:AR:25:ASP:OD1	2.07	0.54
22:BA:636:G:N2	33:BL:76:GLU:OE1	2.40	0.54
22:BA:286:U:H2'	22:BA:287:G:C8	2.40	0.54
26:BE:154:ASP:OD2	26:BE:155:GLU:N	2.40	0.54
1:AA:1157:A:H1'	1:AA:1181:G:N2	2.22	0.54
7:AG:18:PHE:HZ	7:AG:58:GLU:HG2	1.72	0.54
1:AA:946:A:H2'	1:AA:947:G:H8	1.73	0.54
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.40	0.54
1:AA:1261:A:N6	1:AA:1274:A:O2'	2.39	0.54
2:AB:68:LEU:HD13	2:AB:158:PRO:HB3	1.90	0.54
2:AB:151:ILE:HB	2:AB:154:MET:HE2	1.90	0.54
9:AI:55:VAL:HG21	9:AI:94:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1225:G:OP1	39:BR:71:LYS:NZ	2.37	0.54
38:BQ:87:SER:HB2	39:BR:51:VAL:HG13	1.89	0.54
1:AA:1310:G:OP2	13:AM:87:ARG:NH2	2.41	0.54
1:AA:1036:A:H2'	1:AA:1037:C:C6	2.43	0.54
8:AH:76:GLN:NE2	8:AH:77:ARG:O	2.41	0.54
10:AJ:21:ALA:O	10:AJ:24:GLU:HG3	2.07	0.54
22:BA:2182:U:O4	22:BA:2183:A:N6	2.41	0.54
26:BE:21:ARG:O	26:BE:114:ARG:NH2	2.40	0.54
1:AA:539:A:H2'	1:AA:540:G:H8	1.73	0.54
1:AA:859:G:H2'	1:AA:860:A:H8	1.72	0.54
22:BA:2100:G:H1	22:BA:2189:U:H3	1.54	0.54
10:AJ:52:LEU:HD21	10:AJ:59:LYS:HD2	1.89	0.54
6:AF:22:ILE:O	6:AF:26:THR:HG23	2.09	0.53
7:AG:56:LYS:HD2	7:AG:57:SER:HB2	1.90	0.53
8:AH:77:ARG:NH1	8:AH:126:ILE:O	2.40	0.53
12:AL:55:VAL:HG11	12:AL:80:ILE:HD11	1.91	0.53
13:AM:4:ILE:HG22	13:AM:5:ALA:N	2.23	0.53
19:AS:41:PHE:H	19:AS:44:MET:HE2	1.72	0.53
22:BA:849:A:H2'	22:BA:850:U:C6	2.43	0.53
22:BA:2451:A:C2	53:B5:23:ARG:HG2	2.43	0.53
42:BU:7:ARG:NH2	42:BU:8:ASP:OD2	2.40	0.53
1:AA:76:G:O6	1:AA:93:U:O4	2.26	0.53
1:AA:745:G:H2'	1:AA:746:A:H8	1.74	0.53
6:AF:44:ARG:HA	6:AF:58:HIS:HA	1.90	0.53
6:AF:44:ARG:CB	6:AF:56:LYS:HE2	2.39	0.53
22:BA:1704:C:H2'	22:BA:1705:A:C8	2.43	0.53
23:BB:1:U:H2'	23:BB:2:G:C8	2.41	0.53
24:BC:71:LYS:HG2	24:BC:74:ILE:HD12	1.90	0.53
1:AA:459:A:H2'	1:AA:460:A:H8	1.73	0.53
2:AB:187:VAL:HG21	2:AB:199:VAL:HG13	1.90	0.53
22:BA:1071:G:H2'	22:BA:1072:C:C6	2.44	0.53
1:AA:398:U:H2'	1:AA:399:G:H8	1.73	0.53
2:AB:80:VAL:HA	2:AB:214:LEU:HD21	1.91	0.53
22:BA:534:U:H2'	22:BA:535:G:H8	1.73	0.53
22:BA:955:PSU:OP1	34:BM:86:LYS:NZ	2.36	0.53
43:BV:56:PHE:CE1	43:BV:61:LEU:HD21	2.44	0.53
51:B3:32:ILE:HG22	51:B3:32:ILE:O	2.08	0.53
1:AA:492:C:H2'	1:AA:493:A:C8	2.44	0.53
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.35	0.53
1:AA:1526:G:H2'	1:AA:1527:U:C6	2.44	0.53
22:BA:323:C:H2'	26:BE:163:ASN:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:810:U:C4	33:BL:29:LYS:O	2.62	0.53
23:BB:42:C:C5	27:BF:66:LEU:HD22	2.43	0.53
2:AB:57:LEU:HD23	2:AB:60:ILE:HD11	1.89	0.53
2:AB:128:LYS:HD2	2:AB:128:LYS:O	2.08	0.53
13:AM:3:ARG:HH12	27:BF:110:ARG:HE	1.55	0.53
15:AO:76:ALA:O	15:AO:79:THR:OG1	2.23	0.53
43:BV:45:ASP:OD1	43:BV:46:LYS:N	2.42	0.53
55:B8:23:C:H2'	55:B8:24:G:C8	2.43	0.53
22:BA:1179:G:H2'	22:BA:1180:U:C6	2.43	0.53
22:BA:2562:U:OP1	32:BK:40:LYS:NZ	2.39	0.53
14:AN:39:GLU:HA	14:AN:42:TRP:HB3	1.91	0.53
32:BK:104:THR:HG22	32:BK:105:ARG:H	1.73	0.53
33:BL:109:LYS:HG2	33:BL:126:ARG:HB2	1.91	0.53
1:AA:695:A:H2'	1:AA:696:A:C8	2.44	0.53
4:AD:129:VAL:HG21	4:AD:146:ARG:NH2	2.24	0.53
11:AK:126:LYS:HD2	21:AU:37:PHE:CB	2.38	0.53
29:BH:7:ASP:OD1	29:BH:8:LYS:N	2.36	0.53
1:AA:460:A:H2'	1:AA:461:A:C8	2.44	0.53
1:AA:1060:U:H4'	10:AJ:53:ILE:HG13	1.91	0.53
10:AJ:21:ALA:O	10:AJ:25:ILE:HD12	2.09	0.53
1:AA:1316:G:N2	1:AA:1318:A:H3'	2.24	0.52
3:AC:138:VAL:HG21	3:AC:168:TYR:CD2	2.44	0.52
22:BA:2728:U:HO2'	22:BA:2729:G:H8	1.55	0.52
29:BH:68:ARG:NH2	29:BH:134:VAL:HB	2.24	0.52
40:BS:109:ASP:OD1	40:BS:110:ARG:HG3	2.09	0.52
1:AA:859:G:H2'	1:AA:860:A:C8	2.45	0.52
7:AG:46:ALA:HB2	7:AG:117:ALA:HA	1.91	0.52
8:AH:79:SER:HB2	8:AH:85:ILE:H	1.74	0.52
22:BA:549:G:HO2'	22:BA:550:C:H6	1.57	0.52
22:BA:871:U:H2'	22:BA:872:U:C6	2.45	0.52
22:BA:948:C:H1'	22:BA:984:A:C8	2.44	0.52
22:BA:1069:A:C4	22:BA:1096:A:H5''	2.45	0.52
41:BT:11:LEU:O	46:BY:29:ARG:NH2	2.43	0.52
42:BU:26:LYS:HD3	42:BU:37:GLU:HG2	1.89	0.52
1:AA:459:A:H2'	1:AA:460:A:C8	2.44	0.52
22:BA:2058:A:O2'	53:B5:14:ASN:ND2	2.41	0.52
33:BL:59:ARG:HG2	33:BL:59:ARG:HH11	1.74	0.52
36:BO:84:GLU:OE2	36:BO:85:LYS:NZ	2.38	0.52
1:AA:232:G:H1'	1:AA:262:A:N1	2.24	0.52
1:AA:427:U:OP2	1:AA:428:G:O2'	2.23	0.52
1:AA:674:G:H2'	1:AA:675:A:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:19:VAL:HG23	9:AI:65:ILE:HG12	1.90	0.52
22:BA:720:U:H2'	22:BA:721:A:H8	1.74	0.52
22:BA:1469:A:H2'	22:BA:1470:A:C8	2.45	0.52
1:AA:618:C:O2'	16:AP:14:ARG:NH1	2.42	0.52
6:AF:9:MET:HG2	6:AF:59:TYR:CD1	2.45	0.52
11:AK:107:ILE:HG21	21:AU:12:PHE:CE2	2.45	0.52
13:AM:3:ARG:NH1	27:BF:110:ARG:HE	2.08	0.52
28:BG:94:TYR:HA	28:BG:106:SER:O	2.10	0.52
1:AA:1080:A:OP1	5:AE:52:LYS:HD2	2.09	0.52
14:AN:28:ALA:HB3	14:AN:29:ILE:HD12	1.92	0.52
22:BA:1328:A:H2'	22:BA:1330:C:C5	2.45	0.52
52:B4:16:ILE:HG12	52:B4:25:VAL:HG22	1.90	0.52
1:AA:713:G:H2'	1:AA:714:G:C8	2.44	0.52
9:AI:54:LEU:HD23	9:AI:54:LEU:H	1.74	0.52
22:BA:355:U:H2'	22:BA:356:G:H8	1.73	0.52
22:BA:1636:U:H2'	22:BA:1637:A:C8	2.45	0.52
43:BV:62:THR:HG22	43:BV:71:LYS:HD3	1.90	0.52
48:B0:38:HIS:ND1	48:B0:39:LEU:O	2.41	0.52
1:AA:3:A:H5''	1:AA:4:U:H5'	1.92	0.52
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.45	0.52
22:BA:1494:A:H2'	22:BA:1495:A:C8	2.44	0.52
33:BL:79:LEU:HD11	33:BL:112:LEU:HD12	1.92	0.52
49:B1:6:ARG:HG3	49:B1:24:THR:HB	1.91	0.52
1:AA:22:G:H2'	1:AA:23:C:C6	2.44	0.52
14:AN:32:ASP:OD2	14:AN:33:VAL:N	2.42	0.52
18:AR:48:ARG:HD3	18:AR:51:TYR:HE2	1.75	0.52
22:BA:207:A:H2'	22:BA:208:C:O4'	2.10	0.52
22:BA:848:C:H2'	22:BA:849:A:C8	2.45	0.52
22:BA:1059:G:H3'	22:BA:1060:U:H2'	1.91	0.52
47:BZ:37:GLU:O	47:BZ:38:ARG:NH1	2.42	0.52
1:AA:945:G:C2	1:AA:946:A:C8	2.98	0.52
19:AS:48:THR:HG22	19:AS:61:PHE:CD1	2.45	0.52
1:AA:539:A:H2'	1:AA:540:G:C8	2.45	0.51
1:AA:1372:U:OP1	9:AI:74:GLY:N	2.41	0.51
22:BA:1889:A:H2'	22:BA:1890:A:C8	2.45	0.51
41:BT:89:GLU:OE1	41:BT:89:GLU:N	2.39	0.51
43:BV:35:GLU:OE1	43:BV:35:GLU:N	2.35	0.51
22:BA:581:C:H2'	22:BA:582:A:C8	2.45	0.51
1:AA:1040:U:H2'	1:AA:1041:G:H8	1.76	0.51
1:AA:1135:U:H2'	1:AA:1137:C:C5	2.45	0.51
2:AB:129:LEU:HD11	2:AB:134:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:455:G:H2'	1:AA:456:A:C8	2.45	0.51
1:AA:728:A:H2'	1:AA:729:A:C8	2.46	0.51
1:AA:1014:A:H2'	1:AA:1015:G:C8	2.45	0.51
22:BA:1683:U:H2'	22:BA:1684:G:H8	1.75	0.51
1:AA:323:U:OP1	20:AT:25:ARG:NH2	2.37	0.51
1:AA:440:C:C2	1:AA:441:A:C8	2.98	0.51
1:AA:672:U:H2'	1:AA:673:A:H8	1.76	0.51
1:AA:1308:U:OP2	13:AM:100:GLN:NE2	2.41	0.51
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.25	0.51
19:AS:42:PRO:O	19:AS:45:ILE:HG12	2.11	0.51
22:BA:1199:U:H1'	38:BQ:4:VAL:HG22	1.92	0.51
22:BA:1594:U:H2'	22:BA:1595:C:C6	2.46	0.51
1:AA:1005:A:N6	1:AA:1024:G:O2'	2.38	0.51
22:BA:2191:A:H2'	22:BA:2192:U:C6	2.46	0.51
49:B1:5:ILE:HB	49:B1:28:ARG:NH2	2.25	0.51
6:AF:2:ARG:HD3	6:AF:91:ARG:NE	2.26	0.51
22:BA:715:A:H2'	22:BA:716:A:C8	2.44	0.51
22:BA:1636:U:H2'	22:BA:1637:A:H8	1.76	0.51
22:BA:2662:A:O5'	22:BA:2662:A:H8	1.94	0.51
33:BL:22:GLY:O	33:BL:28:GLY:HA3	2.11	0.51
43:BV:24:ASN:OD1	43:BV:44:HIS:HB3	2.10	0.51
1:AA:951:G:O2'	1:AA:970:C:O2'	2.28	0.51
7:AG:16:PRO:HG2	7:AG:44:TYR:OH	2.11	0.51
22:BA:687:C:H1'	50:B2:4:THR:HG22	1.92	0.51
22:BA:884:U:H1'	22:BA:893:C:C2	2.46	0.51
29:BH:70:GLU:C	29:BH:72:ILE:H	2.14	0.51
29:BH:82:SER:HB2	29:BH:90:LEU:HD11	1.91	0.51
2:AB:145:GLU:O	2:AB:149:GLY:N	2.43	0.51
3:AC:118:ASP:HA	3:AC:121:THR:HG22	1.93	0.51
15:AO:79:THR:O	15:AO:82:ILE:HG12	2.11	0.51
17:AQ:53:CYS:HA	17:AQ:81:LYS:NZ	2.25	0.51
22:BA:645:C:H2'	22:BA:647:G:C8	2.46	0.51
1:AA:410:G:OP1	4:AD:26:ARG:NH2	2.37	0.51
1:AA:617:G:H5'	16:AP:47:GLU:OE2	2.11	0.51
3:AC:156:ARG:H	3:AC:163:ALA:HA	1.76	0.51
6:AF:44:ARG:HB2	6:AF:56:LYS:HE2	1.93	0.51
11:AK:107:ILE:HG21	21:AU:12:PHE:HE2	1.74	0.51
1:AA:462:G:C5	1:AA:463:U:C4	2.99	0.50
1:AA:1137:C:H4'	1:AA:1138:G:O5'	2.11	0.50
13:AM:4:ILE:HG22	13:AM:5:ALA:H	1.75	0.50
15:AO:64:ARG:NH2	15:AO:68:ASP:OD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1438:U:H2'	22:BA:1439:A:C8	2.46	0.50
22:BA:2150:C:H2'	22:BA:2151:U:C6	2.47	0.50
1:AA:1036:A:H2'	1:AA:1037:C:H6	1.75	0.50
13:AM:3:ARG:HH11	27:BF:110:ARG:HH11	1.58	0.50
19:AS:44:MET:HA	19:AS:47:LEU:HD13	1.92	0.50
22:BA:5:A:H2'	22:BA:6:A:C8	2.45	0.50
22:BA:849:A:H2'	22:BA:850:U:H6	1.76	0.50
6:AF:16:GLU:OE2	6:AF:17:GLN:HG3	2.11	0.50
22:BA:284:U:H3	22:BA:356:G:H1	1.58	0.50
41:BT:54:GLU:HG3	41:BT:88:LYS:HB2	1.93	0.50
2:AB:94:HIS:HB2	2:AB:146:ASN:O	2.11	0.50
6:AF:3:HIS:CD2	6:AF:95:ALA:N	2.80	0.50
22:BA:2680:U:O2'	22:BA:2681:C:H5'	2.11	0.50
1:AA:147:G:H2'	1:AA:148:G:C8	2.47	0.50
1:AA:456:A:H61	1:AA:475:C:H42	1.59	0.50
1:AA:1026:G:C6	1:AA:1035:A:N6	2.80	0.50
1:AA:244:U:O4	1:AA:906:A:H1'	2.12	0.50
3:AC:152:GLU:OE2	3:AC:199:LYS:HD2	2.12	0.50
5:AE:15:LEU:HA	5:AE:37:THR:HG22	1.92	0.50
14:AN:47:LYS:O	14:AN:50:THR:HG22	2.11	0.50
22:BA:643:A:C8	49:B1:44:ARG:NH1	2.80	0.50
22:BA:2188:U:O2'	22:BA:2189:U:H6	1.94	0.50
48:B0:31:ASP:OD1	48:B0:32:LYS:N	2.44	0.50
1:AA:411:A:P	4:AD:26:ARG:HH22	2.33	0.50
1:AA:1241:G:H2'	1:AA:1242:G:H8	1.75	0.50
1:AA:1328:C:H5''	13:AM:28:THR:HG21	1.93	0.50
5:AE:62:LYS:O	5:AE:66:LYS:HG3	2.10	0.50
7:AG:26:PHE:CA	7:AG:101:MET:HE1	2.42	0.50
22:BA:1062:G:C6	22:BA:1077:A:N1	2.80	0.50
22:BA:1104:C:H2'	22:BA:1105:U:C6	2.46	0.50
25:BD:46:ARG:NH2	25:BD:88:GLU:O	2.44	0.50
1:AA:514:C:H2'	1:AA:515:G:H8	1.77	0.50
1:AA:1022:A:H2'	1:AA:1023:U:O4'	2.12	0.50
1:AA:1464:U:H2'	1:AA:1465:A:H8	1.77	0.50
4:AD:85:ASN:HD22	5:AE:101:GLU:CD	2.15	0.50
5:AE:34:THR:HG22	5:AE:52:LYS:HG2	1.94	0.50
13:AM:53:ILE:CG2	13:AM:57:ARG:HH21	2.11	0.50
13:AM:71:ARG:HH21	27:BF:115:ARG:HH22	1.60	0.50
17:AQ:17:MET:SD	17:AQ:20:SER:HB2	2.51	0.50
20:AT:2:ALA:HB3	20:AT:8:LYS:HG2	1.93	0.50
42:BU:51:ALA:C	42:BU:53:ASN:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:96:U:H2'	1:AA:97:G:C8	2.46	0.50
1:AA:204:G:N2	1:AA:465:A:OP1	2.44	0.50
1:AA:390:U:H2'	1:AA:391:G:H8	1.77	0.50
9:AI:45:ARG:HD3	9:AI:49:ARG:NH2	2.27	0.50
22:BA:2314:A:H2'	22:BA:2315:G:C8	2.47	0.50
1:AA:413:G:N2	1:AA:428:G:H1'	2.26	0.49
22:BA:568:U:H1'	22:BA:2030:6MZ:H9C1	1.94	0.49
22:BA:1614:A:C6	40:BS:87:PRO:HB3	2.47	0.49
22:BA:1923:U:H2'	22:BA:1924:C:C6	2.47	0.49
22:BA:2470:G:OP1	34:BM:55:ARG:NH1	2.44	0.49
29:BH:16:GLY:HA2	29:BH:47:PHE:CE2	2.47	0.49
1:AA:1071:C:H2'	1:AA:1072:G:C8	2.43	0.49
13:AM:68:ASP:OD1	13:AM:69:LEU:N	2.44	0.49
22:BA:285:G:H2'	22:BA:286:U:C6	2.47	0.49
22:BA:1079:C:H2'	22:BA:1080:A:C8	2.47	0.49
29:BH:125:THR:HA	29:BH:146:VAL:HG21	1.94	0.49
1:AA:1238:A:H2	1:AA:1241:G:N3	2.10	0.49
1:AA:1526:G:H2'	1:AA:1527:U:H6	1.77	0.49
22:BA:548:G:N3	22:BA:548:G:H2'	2.26	0.49
22:BA:1548:A:H2'	22:BA:1549:A:C8	2.47	0.49
22:BA:2291:U:OP1	22:BA:2380:C:O2'	2.24	0.49
1:AA:195:A:H2'	1:AA:196:A:C8	2.46	0.49
1:AA:235:C:H2'	1:AA:236:A:C8	2.48	0.49
1:AA:1518:MA6:O5'	1:AA:1518:MA6:H8	2.12	0.49
39:BR:44:GLY:O	39:BR:45:GLU:HG2	2.13	0.49
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.94	0.49
2:AB:14:VAL:HA	2:AB:203:ASN:HB2	1.94	0.49
5:AE:161:VAL:HG12	5:AE:162:GLU:H	1.77	0.49
22:BA:2420:C:OP1	51:B3:34:THR:OG1	2.21	0.49
44:BW:19:LYS:HG3	44:BW:41:ARG:NH2	2.24	0.49
1:AA:995:C:N3	1:AA:1046:A:O2'	2.38	0.49
1:AA:1119:C:H2'	1:AA:1120:C:C6	2.47	0.49
1:AA:1297:G:O2'	7:AG:114:LYS:NZ	2.25	0.49
6:AF:18:VAL:HG11	6:AF:58:HIS:NE2	2.28	0.49
13:AM:54:ASP:OD2	30:BI:17:SER:HB2	2.12	0.49
14:AN:49:GLN:HE22	19:AS:12:ASP:HA	1.76	0.49
22:BA:1156:A:C8	38:BQ:51:ARG:HG2	2.47	0.49
22:BA:2557:G:H2'	22:BA:2558:C:C6	2.47	0.49
28:BG:133:LEU:HB3	28:BG:141:ILE:HD11	1.95	0.49
29:BH:114:GLU:OE2	29:BH:134:VAL:HA	2.12	0.49
36:BO:16:ARG:O	36:BO:20:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BQ:97:ASP:OD2	39:BR:13:ARG:NE	2.46	0.49
1:AA:1124:G:H3'	10:AJ:37:ARG:NH2	2.27	0.49
8:AH:112:THR:HG23	8:AH:115:ALA:H	1.77	0.49
22:BA:2103:C:O2'	22:BA:2104:C:H5'	2.12	0.49
30:BI:48:GLN:N	30:BI:48:GLN:OE1	2.45	0.49
32:BK:43:ILE:HD12	32:BK:56:ASP:HB2	1.94	0.49
40:BS:59:GLU:OE2	40:BS:66:ILE:HD11	2.12	0.49
1:AA:1006:G:O6	1:AA:1024:G:H1'	2.12	0.49
2:AB:20:THR:O	2:AB:23:TRP:HD1	1.95	0.49
12:AL:39:THR:HG21	12:AL:49:LEU:HB3	1.95	0.49
22:BA:2531:A:H62	28:BG:177:LYS:NZ	2.10	0.49
32:BK:70:ARG:HD2	32:BK:76:VAL:HG22	1.94	0.49
33:BL:29:LYS:O	33:BL:29:LYS:HG2	2.13	0.49
37:BP:31:TRP:CE3	37:BP:38:LYS:HG2	2.48	0.49
1:AA:88:U:O2'	1:AA:89:U:H6	1.95	0.49
1:AA:696:A:H2'	1:AA:697:U:H6	1.78	0.49
3:AC:24:ALA:HB1	3:AC:28:GLU:HG2	1.95	0.49
22:BA:545:U:H1'	22:BA:548:G:H1	1.77	0.49
22:BA:1099:G:H2'	22:BA:1100:C:C6	2.48	0.49
22:BA:1277:G:O2'	35:BN:24:MET:HG2	2.13	0.49
26:BE:122:GLU:OE1	26:BE:190:ALA:HB3	2.12	0.49
1:AA:89:U:H2'	1:AA:90:C:C6	2.48	0.49
1:AA:390:U:H2'	1:AA:391:G:C8	2.47	0.49
1:AA:1126:U:OP1	10:AJ:7:ARG:NH1	2.44	0.49
2:AB:133:GLU:N	2:AB:133:GLU:OE1	2.46	0.49
2:AB:134:ALA:O	2:AB:138:THR:HB	2.13	0.49
3:AC:82:GLU:OE1	3:AC:82:GLU:N	2.44	0.49
7:AG:116:MET:O	7:AG:120:LEU:N	2.23	0.49
46:BY:56:LEU:HA	46:BY:59:GLU:HG2	1.94	0.49
55:B8:46:G:H2'	55:B8:47:U:H5'	1.94	0.49
3:AC:25:ASN:OD1	3:AC:26:THR:N	2.41	0.48
5:AE:90:THR:OG1	5:AE:135:ASN:ND2	2.46	0.48
7:AG:37:SER:OG	9:AI:41:ARG:NE	2.46	0.48
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.78	0.48
22:BA:2162:G:O3'	22:BA:2163:A:H8	1.96	0.48
1:AA:1026:G:N1	1:AA:1035:A:C6	2.81	0.48
1:AA:1151:A:O2'	1:AA:1152:A:H5''	2.13	0.48
1:AA:1360:A:H2'	1:AA:1361:G:C8	2.48	0.48
4:AD:197:GLU:N	4:AD:197:GLU:OE1	2.47	0.48
14:AN:30:ILE:HG12	14:AN:44:ALA:CB	2.43	0.48
14:AN:32:ASP:HB3	14:AN:34:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:B3:31:HIS:O	51:B3:33:LEU:N	2.46	0.48
1:AA:216:U:H2'	1:AA:217:C:H6	1.75	0.48
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.47	0.48
16:AP:48:GLU:OE2	16:AP:49:GLY:N	2.45	0.48
22:BA:250:G:H2'	22:BA:251:A:C8	2.47	0.48
32:BK:102:PRO:HB3	32:BK:121:GLU:HG3	1.94	0.48
37:BP:34:GLU:OE2	37:BP:39:ARG:NH1	2.37	0.48
1:AA:868:C:H2'	1:AA:869:G:O4'	2.13	0.48
5:AE:108:GLY:O	5:AE:112:ARG:HG3	2.13	0.48
10:AJ:28:THR:O	10:AJ:32:THR:HG23	2.13	0.48
22:BA:848:C:H2'	22:BA:849:A:H8	1.79	0.48
22:BA:876:C:H2'	22:BA:877:A:O4'	2.12	0.48
22:BA:2300:C:H2'	22:BA:2301:C:H6	1.78	0.48
27:BF:73:SER:OG	27:BF:81:GLN:N	2.45	0.48
38:BQ:48:ARG:HH11	38:BQ:49:ASP:CG	2.17	0.48
43:BV:7:GLU:OE2	43:BV:7:GLU:N	2.46	0.48
1:AA:834:U:H2'	1:AA:835:U:C6	2.48	0.48
1:AA:993:G:H2'	1:AA:995:C:H41	1.78	0.48
1:AA:1035:A:H2'	1:AA:1036:A:C8	2.48	0.48
13:AM:3:ARG:HH21	13:AM:7:ILE:CG2	2.26	0.48
14:AN:42:TRP:CZ2	14:AN:46:LEU:HD21	2.49	0.48
22:BA:358:U:H2'	22:BA:359:G:H8	1.77	0.48
22:BA:2327:A:H2'	22:BA:2328:A:C8	2.48	0.48
41:BT:18:GLU:O	41:BT:22:THR:HG23	2.14	0.48
55:B8:2:G:O2'	55:B8:3:G:H2'	2.14	0.48
1:AA:203:G:H1'	1:AA:465:A:H62	1.78	0.48
6:AF:42:TRP:HE3	6:AF:59:TYR:HD2	1.62	0.48
7:AG:113:ASP:OD2	7:AG:122:ASN:ND2	2.46	0.48
13:AM:53:ILE:HG22	13:AM:57:ARG:NH2	2.10	0.48
15:AO:77:ARG:HA	15:AO:80:GLN:HE22	1.78	0.48
22:BA:1100:C:H2'	22:BA:1101:U:O4'	2.14	0.48
22:BA:2100:G:C6	22:BA:2101:A:C4	3.01	0.48
22:BA:2189:U:C4	22:BA:2190:G:N7	2.81	0.48
22:BA:2285:C:P	49:B1:6:ARG:HH21	2.36	0.48
22:BA:2311:A:N3	27:BF:85:ILE:HD11	2.29	0.48
29:BH:99:ILE:HD13	29:BH:130:VAL:HG11	1.96	0.48
31:BJ:21:THR:HG22	31:BJ:61:LYS:HD2	1.94	0.48
1:AA:944:G:N1	1:AA:1338:G:OP2	2.42	0.48
7:AG:26:PHE:HA	7:AG:101:MET:HE1	1.96	0.48
22:BA:477:A:H2'	22:BA:478:A:C8	2.49	0.48
22:BA:720:U:H2'	22:BA:721:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:896:A:H2'	22:BA:897:C:H5'	1.95	0.48
22:BA:1007:C:OP1	31:BJ:37:ARG:NH2	2.47	0.48
22:BA:2377:A:H2'	22:BA:2378:A:C8	2.49	0.48
28:BG:38:ASN:ND2	28:BG:64:GLN:OE1	2.47	0.48
29:BH:42:LYS:O	29:BH:45:GLU:HG3	2.14	0.48
1:AA:1230:C:H5'	55:B8:30:C:H5''	1.96	0.48
3:AC:10:ILE:HD13	14:AN:98:LYS:HD3	1.96	0.48
7:AG:71:PRO:O	7:AG:96:ARG:HG2	2.14	0.48
9:AI:20:PHE:HB3	9:AI:22:LYS:HZ2	1.79	0.48
22:BA:2542:A:H5''	22:BA:2766:A:O2'	2.13	0.48
1:AA:137:U:H3	1:AA:226:G:H1	1.61	0.48
1:AA:858:G:O6	1:AA:869:G:H3'	2.13	0.48
1:AA:1326:U:H2'	1:AA:1327:C:H6	1.79	0.48
2:AB:106:THR:HA	2:AB:109:GLN:NE2	2.29	0.48
3:AC:40:ARG:NH1	3:AC:55:ILE:O	2.35	0.48
11:AK:107:ILE:O	11:AK:107:ILE:HG13	2.13	0.48
22:BA:1794:A:H2'	22:BA:1795:C:C6	2.49	0.48
22:BA:2285:C:OP2	49:B1:6:ARG:NH2	2.35	0.48
33:BL:78:ARG:HG2	33:BL:113:ALA:HB3	1.94	0.48
1:AA:180:U:O2'	1:AA:181:A:H5'	2.14	0.48
1:AA:464:U:H2'	1:AA:466:A:OP2	2.13	0.48
1:AA:736:C:H2'	1:AA:737:C:C6	2.49	0.48
1:AA:1294:G:H2'	1:AA:1295:U:C6	2.48	0.48
6:AF:18:VAL:O	6:AF:22:ILE:HG13	2.14	0.48
9:AI:43:THR:HA	9:AI:46:MET:CE	2.44	0.48
19:AS:27:ASP:C	19:AS:28:LYS:HD2	2.35	0.48
19:AS:67:VAL:O	30:BI:56:ARG:CZ	2.61	0.48
22:BA:1434:A:H2'	22:BA:1435:G:C8	2.49	0.48
1:AA:1129:C:H4'	9:AI:18:ARG:HH12	1.79	0.47
4:AD:35:GLU:CD	4:AD:35:GLU:H	2.17	0.47
22:BA:1538:G:H2'	22:BA:1539:U:C6	2.49	0.47
23:BB:79:G:O6	43:BV:14:LYS:NZ	2.42	0.47
26:BE:121:VAL:O	26:BE:190:ALA:N	2.46	0.47
1:AA:269:C:H2'	1:AA:270:A:C8	2.48	0.47
1:AA:346:G:OP1	37:BP:39:ARG:NH2	2.30	0.47
1:AA:524:G:H2'	1:AA:525:C:C6	2.49	0.47
1:AA:996:A:H2'	1:AA:997:U:C6	2.49	0.47
1:AA:1288:A:H2'	1:AA:1289:A:H8	1.77	0.47
22:BA:2106:U:C2	22:BA:2107:G:C8	3.02	0.47
22:BA:2160:C:H2'	22:BA:2161:C:C6	2.49	0.47
22:BA:2291:U:H2'	22:BA:2292:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BK:38:ILE:HD11	32:BK:112:PHE:HZ	1.78	0.47
55:B8:19:G:H4'	55:B8:20:U:OP2	2.14	0.47
1:AA:1403:C:N4	54:B7:6:G:OP2	2.46	0.47
3:AC:93:ASP:OD1	3:AC:94:ILE:N	2.47	0.47
11:AK:126:LYS:HD2	21:AU:37:PHE:HB2	1.96	0.47
19:AS:68:GLY:HA3	30:BI:56:ARG:HH12	1.79	0.47
22:BA:2818:U:H2'	22:BA:2819:G:H8	1.79	0.47
50:B2:44:VAL:HG23	50:B2:44:VAL:O	2.13	0.47
1:AA:417:G:H2'	1:AA:418:C:C6	2.49	0.47
3:AC:69:HIS:HA	3:AC:104:ALA:O	2.14	0.47
10:AJ:50:THR:OG1	10:AJ:64:GLN:NE2	2.26	0.47
22:BA:602:A:O2'	22:BA:604:G:O2'	2.15	0.47
22:BA:1019:U:OP1	22:BA:1035:U:O2'	2.22	0.47
22:BA:1798:U:OP2	24:BC:271:ARG:NH2	2.42	0.47
31:BJ:23:LYS:NZ	31:BJ:142:ILE:OXT	2.38	0.47
1:AA:675:A:H1'	11:AK:118:HIS:CD2	2.49	0.47
22:BA:1106:G:H2'	22:BA:1107:G:H8	1.79	0.47
22:BA:1809:A:H2'	22:BA:1810:A:C8	2.50	0.47
22:BA:2116:G:N7	22:BA:2165:C:N4	2.62	0.47
24:BC:133:ARG:HD3	29:BH:123:ARG:NH2	2.29	0.47
27:BF:108:VAL:HA	27:BF:111:ILE:HG13	1.97	0.47
2:AB:6:MET:O	2:AB:9:MET:HG2	2.14	0.47
8:AH:29:SER:HB2	8:AH:59:LEU:HB2	1.96	0.47
9:AI:37:GLN:OE1	9:AI:37:GLN:N	2.47	0.47
10:AJ:10:LEU:O	10:AJ:71:LEU:HD12	2.15	0.47
12:AL:89:D2T:OD1	12:AL:89:D2T:N	2.46	0.47
22:BA:302:C:O2'	22:BA:303:G:H8	1.98	0.47
22:BA:358:U:H2'	22:BA:359:G:C8	2.50	0.47
22:BA:1428:C:C5	22:BA:1569:A:H5''	2.49	0.47
55:B8:71:C:H2'	55:B8:72:G:H8	1.75	0.47
1:AA:22:G:H2'	1:AA:23:C:H6	1.78	0.47
1:AA:162:A:O5'	1:AA:162:A:H8	1.96	0.47
1:AA:362:G:H8	59:AA:1739:HOH:O	1.92	0.47
1:AA:458:U:C2	1:AA:459:A:N7	2.82	0.47
5:AE:83:HIS:CE1	8:AH:96:MET:HE1	2.50	0.47
5:AE:150:PRO:HB2	5:AE:164:ILE:HG23	1.97	0.47
22:BA:645:C:O2'	22:BA:646:U:H5'	2.15	0.47
22:BA:1509:A:H2'	22:BA:1510:G:C8	2.50	0.47
22:BA:1724:G:H2'	22:BA:1725:U:C6	2.49	0.47
24:BC:155:ALA:HB2	24:BC:162:VAL:HG23	1.96	0.47
26:BE:152:GLU:N	26:BE:152:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BJ:69:ARG:O	31:BJ:90:GLU:HG3	2.14	0.47
38:BQ:107:THR:O	38:BQ:111:GLU:HG2	2.14	0.47
40:BS:88:ARG:NH2	40:BS:94:ASP:OD2	2.47	0.47
42:BU:85:PHE:CE1	42:BU:94:ARG:HG2	2.50	0.47
1:AA:2:A:H1'	1:AA:613:C:O2'	2.14	0.47
1:AA:496:A:H5'	1:AA:497:G:OP2	2.15	0.47
1:AA:522:C:H41	12:AL:50:ARG:NH2	2.13	0.47
3:AC:22:TRP:HB3	3:AC:59:ARG:HB2	1.95	0.47
3:AC:81:GLY:O	3:AC:84:VAL:HG22	2.15	0.47
5:AE:13:GLU:HB2	5:AE:64:MET:CE	2.45	0.47
7:AG:111:ARG:HD3	7:AG:119:ARG:HG3	1.96	0.47
9:AI:26:GLY:HA2	9:AI:61:LEU:O	2.14	0.47
10:AJ:36:VAL:HG12	10:AJ:76:ILE:HG22	1.97	0.47
10:AJ:83:THR:HA	10:AJ:86:ALA:HB3	1.97	0.47
22:BA:959:A:H2'	22:BA:960:A:C8	2.50	0.47
34:BM:20:LEU:HD13	43:BV:81:PRO:HG2	1.97	0.47
1:AA:441:A:H1'	1:AA:497:G:N2	2.29	0.47
1:AA:1320:C:O2	19:AS:72:GLY:HA3	2.15	0.47
13:AM:67:GLY:O	13:AM:71:ARG:HG2	2.15	0.47
15:AO:89:ARG:NH2	22:BA:713:G:O6	2.30	0.47
31:BJ:19:ASP:OD1	31:BJ:21:THR:HG23	2.15	0.47
42:BU:28:VAL:HG22	42:BU:34:VAL:HG12	1.97	0.47
1:AA:384:G:H2'	1:AA:385:C:H6	1.80	0.47
1:AA:1367:C:OP2	9:AI:114:LYS:NZ	2.41	0.47
7:AG:67:GLU:HG2	7:AG:70:ARG:NH2	2.30	0.47
8:AH:10:MET:HG3	8:AH:27:MET:SD	2.54	0.47
22:BA:141:G:C6	41:BT:1:MET:HE1	2.50	0.47
22:BA:1104:C:H2'	22:BA:1105:U:H6	1.80	0.47
1:AA:56:U:H2'	1:AA:57:G:C8	2.50	0.46
1:AA:1106:G:H2'	1:AA:1107:C:C6	2.50	0.46
2:AB:89:GLN:NE2	2:AB:225:ARG:HH11	2.12	0.46
18:AR:26:ILE:O	18:AR:30:LYS:HG2	2.14	0.46
1:AA:17:U:H2'	1:AA:18:C:C6	2.51	0.46
1:AA:131:A:H2'	1:AA:132:C:C6	2.49	0.46
1:AA:737:C:H2'	1:AA:738:C:H6	1.80	0.46
22:BA:684:G:OP1	50:B2:16:HIS:ND1	2.46	0.46
22:BA:2467:C:H2'	22:BA:2468:A:O4'	2.15	0.46
35:BN:21:PHE:CE1	35:BN:24:MET:HE3	2.50	0.46
1:AA:1026:G:C2	1:AA:1027:C:C2	3.04	0.46
22:BA:811:U:H2'	33:BL:21:ARG:HA	1.96	0.46
22:BA:881:G:N2	22:BA:896:A:H62	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:208:U:H3	1:AA:211:G:H1	1.60	0.46
1:AA:869:G:H8	59:AA:1750:HOH:O	1.94	0.46
16:AP:55:ASP:OD1	16:AP:56:ARG:N	2.47	0.46
22:BA:639:U:H2'	22:BA:640:C:H6	1.79	0.46
29:BH:132:PHE:HB2	29:BH:140:ALA:HB3	1.98	0.46
54:B7:1:C:H2'	54:B7:2:G:H8	1.80	0.46
1:AA:494:G:H2'	1:AA:496:A:H8	1.79	0.46
1:AA:976:G:OP2	1:AA:1358:U:O2'	2.32	0.46
4:AD:125:VAL:HG22	4:AD:143:VAL:HG22	1.97	0.46
6:AF:45:ARG:HD3	6:AF:59:TYR:CE2	2.50	0.46
9:AI:51:PRO:HA	9:AI:54:LEU:HD21	1.98	0.46
22:BA:285:G:C6	22:BA:356:G:C6	3.04	0.46
1:AA:109:A:H5'	1:AA:110:C:H5	1.81	0.46
1:AA:191:G:H2'	1:AA:192:A:C8	2.51	0.46
1:AA:439:U:O4'	4:AD:120:HIS:HD2	1.99	0.46
5:AE:104:GLY:O	5:AE:122:ASN:HA	2.15	0.46
51:B3:31:HIS:O	51:B3:33:LEU:HG	2.16	0.46
1:AA:300:A:O5'	1:AA:300:A:H8	1.98	0.46
1:AA:398:U:H2'	1:AA:399:G:C8	2.50	0.46
1:AA:674:G:H21	11:AK:118:HIS:HB2	1.81	0.46
1:AA:918:A:H2'	1:AA:919:A:C8	2.51	0.46
18:AR:48:ARG:HD3	18:AR:51:TYR:CE2	2.51	0.46
22:BA:3:U:H2'	22:BA:4:U:C6	2.51	0.46
22:BA:1430:G:H2'	22:BA:1431:A:O4'	2.16	0.46
22:BA:2094:A:H5'	29:BH:25:TYR:CD1	2.51	0.46
1:AA:875:U:O2'	8:AH:15:ARG:NH1	2.47	0.46
1:AA:1507:A:H2'	1:AA:1508:A:C8	2.51	0.46
3:AC:156:ARG:HH21	3:AC:193:TYR:HD1	1.64	0.46
5:AE:150:PRO:HB3	5:AE:164:ILE:HA	1.97	0.46
9:AI:34:SER:HB3	9:AI:37:GLN:OE1	2.16	0.46
22:BA:172:A:H2'	22:BA:173:A:C8	2.51	0.46
22:BA:721:A:H2'	22:BA:722:A:C8	2.51	0.46
22:BA:2236:U:H2'	22:BA:2237:G:O4'	2.15	0.46
23:BB:51:G:H5''	36:BO:64:TYR:CD2	2.51	0.46
24:BC:5:LYS:HD3	24:BC:17:VAL:HG22	1.98	0.46
40:BS:2:GLU:HG2	40:BS:108:SER:HB3	1.98	0.46
1:AA:1366:C:O2'	10:AJ:62:ARG:NH2	2.49	0.46
2:AB:6:MET:HA	2:AB:9:MET:HE3	1.97	0.46
10:AJ:59:LYS:HE2	10:AJ:62:ARG:NH2	2.31	0.46
22:BA:281:C:H2'	22:BA:282:A:C8	2.51	0.46
22:BA:1080:A:H2'	22:BA:1081:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BI:30:HIS:CG	30:BI:31:ASP:N	2.84	0.46
1:AA:477:C:H2'	1:AA:479:U:O4'	2.16	0.46
1:AA:958:A:H5'	19:AS:55:ARG:NH1	2.31	0.46
1:AA:1147:C:H2'	1:AA:1148:U:C6	2.50	0.46
2:AB:108:ARG:HA	2:AB:111:ILE:HG12	1.97	0.46
7:AG:61:ALA:HA	7:AG:64:VAL:HG12	1.97	0.46
10:AJ:37:ARG:NH1	10:AJ:37:ARG:HA	2.30	0.46
22:BA:2830:C:OP2	25:BD:59:ARG:HD2	2.15	0.46
1:AA:1119:C:H2'	1:AA:1120:C:H6	1.80	0.45
22:BA:64:A:H2'	22:BA:65:U:C6	2.52	0.45
22:BA:645:C:H2'	22:BA:647:G:N7	2.31	0.45
22:BA:1069:A:N3	22:BA:1096:A:H5''	2.30	0.45
22:BA:1102:C:C2	22:BA:1103:A:C8	3.04	0.45
22:BA:1614:A:C2	40:BS:93:ALA:HB2	2.51	0.45
22:BA:2128:G:H2'	22:BA:2129:C:H6	1.80	0.45
22:BA:2687:U:H2'	22:BA:2688:G:O4'	2.16	0.45
54:B7:2:G:N2	54:B7:3:C:O4'	2.49	0.45
1:AA:408:A:O3'	4:AD:23:SER:OG	2.33	0.45
1:AA:844:G:N2	1:AA:845:A:O2'	2.50	0.45
1:AA:1226:C:OP2	13:AM:102:THR:HG21	2.16	0.45
6:AF:3:HIS:CD2	6:AF:65:GLU:OE2	2.69	0.45
10:AJ:7:ARG:HB3	10:AJ:101:SER:OG	2.16	0.45
22:BA:469:G:O6	50:B2:37:LYS:HE2	2.16	0.45
22:BA:2125:G:H22	22:BA:2171:A:P	2.39	0.45
27:BF:23:ASN:OD1	27:BF:24:SER:N	2.49	0.45
28:BG:160:LYS:HB3	28:BG:160:LYS:HE2	1.77	0.45
1:AA:86:G:H1'	1:AA:87:C:H5	1.77	0.45
1:AA:545:C:H5'	4:AD:69:GLU:HG3	1.98	0.45
2:AB:126:PHE:HD1	2:AB:128:LYS:HG3	1.82	0.45
9:AI:20:PHE:HB3	9:AI:22:LYS:NZ	2.31	0.45
9:AI:46:MET:O	9:AI:50:GLN:N	2.50	0.45
22:BA:1870:C:H2'	22:BA:1871:A:C8	2.52	0.45
29:BH:95:GLY:H	29:BH:98:ASP:HB2	1.81	0.45
46:BY:3:ALA:O	46:BY:7:ARG:NH2	2.49	0.45
1:AA:149:A:H2'	1:AA:150:U:C6	2.51	0.45
1:AA:1317:C:H42	14:AN:53:ARG:NH1	2.14	0.45
8:AH:78:VAL:HG12	8:AH:85:ILE:HD12	1.99	0.45
16:AP:48:GLU:CD	16:AP:49:GLY:N	2.66	0.45
22:BA:240:C:OP2	22:BA:241:A:O2'	2.24	0.45
22:BA:1859:U:H2'	22:BA:1860:G:C8	2.51	0.45
22:BA:2068:U:N3	22:BA:2430:A:H2	2.12	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BB:42:C:C6	27:BF:66:LEU:HB2	2.51	0.45
1:AA:461:A:C4	1:AA:462:G:N7	2.85	0.45
1:AA:600:A:H2'	1:AA:601:G:C8	2.51	0.45
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.51	0.45
3:AC:62:LYS:HD2	3:AC:63:SER:HB3	1.98	0.45
10:AJ:12:ALA:HB3	10:AJ:18:ILE:HB	1.99	0.45
22:BA:880:G:H2'	22:BA:881:G:C8	2.51	0.45
22:BA:2031:A:C6	22:BA:2498:OMC:H1'	2.52	0.45
22:BA:2170:A:H1'	22:BA:2171:A:C8	2.51	0.45
22:BA:2183:A:H2'	22:BA:2184:A:C8	2.52	0.45
24:BC:247:PRO:HG2	24:BC:248:TRP:CZ3	2.51	0.45
1:AA:91:U:H2'	1:AA:92:U:H6	1.81	0.45
1:AA:718:A:C8	11:AK:118:HIS:HB3	2.51	0.45
1:AA:1333:A:H2'	1:AA:1334:G:O4'	2.16	0.45
10:AJ:83:THR:O	10:AJ:87:LEU:HG	2.16	0.45
22:BA:1065:U:H2'	22:BA:1066:U:O4'	2.16	0.45
24:BC:41:GLY:O	24:BC:43:ARG:NH1	2.38	0.45
29:BH:90:LEU:HB3	29:BH:123:ARG:O	2.17	0.45
33:BL:81:ASP:HB3	33:BL:100:ILE:HD13	1.98	0.45
1:AA:79:G:C6	1:AA:80:A:C6	3.04	0.45
1:AA:96:U:H2'	1:AA:97:G:H8	1.81	0.45
1:AA:954:G:H2'	1:AA:955:U:C6	2.51	0.45
1:AA:1250:A:OP1	9:AI:68:LYS:HD2	2.15	0.45
1:AA:1404:C:H2'	1:AA:1405:G:C8	2.51	0.45
2:AB:121:SER:OG	2:AB:122:GLN:N	2.49	0.45
7:AG:143:ARG:O	7:AG:146:GLU:HG3	2.16	0.45
13:AM:69:LEU:O	13:AM:73:ILE:HG13	2.17	0.45
15:AO:4:SER:O	15:AO:8:THR:HG23	2.16	0.45
15:AO:67:LEU:HD11	15:AO:87:LEU:HD13	1.98	0.45
24:BC:76:ALA:HB2	24:BC:96:TYR:CD1	2.52	0.45
24:BC:133:ARG:HD3	29:BH:123:ARG:CZ	2.47	0.45
25:BD:46:ARG:NH2	25:BD:89:GLU:OE2	2.50	0.45
3:AC:73:PRO:HB3	3:AC:105:GLU:CG	2.45	0.45
5:AE:113:ALA:O	5:AE:117:VAL:HG22	2.17	0.45
11:AK:113:VAL:HG12	11:AK:113:VAL:O	2.17	0.45
22:BA:1545:A:H2'	22:BA:1546:G:O4'	2.16	0.45
22:BA:2251:OMG:HM23	22:BA:2251:OMG:H1'	1.57	0.45
1:AA:1055:A:O2'	3:AC:156:ARG:NH1	2.49	0.45
2:AB:128:LYS:NZ	2:AB:137:ARG:HH21	2.15	0.45
4:AD:146:ARG:HD3	4:AD:148:LYS:HG2	1.98	0.45
9:AI:43:THR:HA	9:AI:46:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:37:ARG:N	10:AJ:75:ASP:O	2.48	0.45
13:AM:64:VAL:O	13:AM:69:LEU:HB2	2.16	0.45
22:BA:356:G:C6	22:BA:357:C:C4	3.05	0.45
22:BA:2109:U:OP1	22:BA:2149:U:O2'	2.34	0.45
22:BA:2554:U:H2'	22:BA:2555:U:C6	2.51	0.45
43:BV:72:VAL:HB	43:BV:91:PHE:HB3	1.98	0.45
1:AA:409:U:P	4:AD:23:SER:HG	2.40	0.45
1:AA:1229:A:H2'	1:AA:1230:C:C6	2.52	0.45
2:AB:94:HIS:ND1	2:AB:146:ASN:HB3	2.32	0.45
8:AH:36:ILE:HD11	8:AH:126:ILE:HD13	1.99	0.45
19:AS:48:THR:HG22	19:AS:61:PHE:HD1	1.80	0.45
21:AU:39:GLU:O	21:AU:39:GLU:HG2	2.17	0.45
22:BA:534:U:H2'	22:BA:535:G:C8	2.52	0.45
22:BA:1071:G:N2	22:BA:1089:A:HO2'	2.15	0.45
22:BA:1223:G:N2	22:BA:1226:A:OP2	2.42	0.45
32:BK:102:PRO:HD3	37:BP:68:GLU:OE2	2.17	0.45
55:B8:75:C:OP1	59:B8:201:HOH:O	2.21	0.45
1:AA:438:U:H4'	1:AA:439:U:H5'	1.99	0.44
1:AA:979:C:N4	59:AA:1722:HOH:O	2.50	0.44
1:AA:1243:C:H2'	1:AA:1244:G:H8	1.82	0.44
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.52	0.44
1:AA:1477:U:H2'	1:AA:1478:U:C6	2.52	0.44
4:AD:13:ARG:HB3	4:AD:36:GLN:O	2.16	0.44
4:AD:196:ASN:OD1	4:AD:199:LEU:HG	2.17	0.44
22:BA:882:G:N2	22:BA:895:U:H1'	2.32	0.44
22:BA:2102:G:H2'	22:BA:2103:C:O4'	2.17	0.44
22:BA:2271:G:OP1	44:BW:18:ALA:HB1	2.17	0.44
23:BB:48:U:H2'	23:BB:49:C:C6	2.52	0.44
27:BF:80:ARG:HH12	55:B8:56:C:N4	2.15	0.44
42:BU:71:ALA:HB3	42:BU:80:ALA:HB1	1.99	0.44
1:AA:1060:U:H2'	1:AA:1061:G:H8	1.82	0.44
1:AA:1175:G:H2'	1:AA:1176:A:C8	2.50	0.44
6:AF:66:ALA:HB3	6:AF:71:ILE:HD11	1.99	0.44
7:AG:108:ALA:HA	7:AG:123:GLU:HG3	1.98	0.44
7:AG:111:ARG:HD3	7:AG:119:ARG:CG	2.48	0.44
22:BA:1738:G:HO2'	22:BA:1739:A:P	2.40	0.44
22:BA:1872:A:H2'	22:BA:1873:G:O4'	2.17	0.44
27:BF:134:GLU:HG3	27:BF:136:ILE:H	1.82	0.44
50:B2:16:HIS:HB2	50:B2:44:VAL:CG2	2.48	0.44
55:B8:69:A:H2'	55:B8:70:C:H6	1.81	0.44
1:AA:91:U:H2'	1:AA:92:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1220:G:H1'	19:AS:52:HIS:CE1	2.52	0.44
1:AA:1314:C:OP2	19:AS:5:LEU:HD13	2.18	0.44
4:AD:101:VAL:HG11	4:AD:137:VAL:HG21	1.99	0.44
9:AI:26:GLY:HA3	9:AI:59:GLU:O	2.17	0.44
9:AI:46:MET:HE2	9:AI:46:MET:HB2	1.93	0.44
11:AK:52:PHE:O	11:AK:53:ARG:HD2	2.18	0.44
14:AN:29:ILE:O	14:AN:32:ASP:HB2	2.17	0.44
15:AO:47:LYS:O	15:AO:53:ARG:NH2	2.50	0.44
22:BA:784:G:H5'	22:BA:785:G:OP1	2.16	0.44
22:BA:1062:G:C4	22:BA:1063:G:C8	3.05	0.44
22:BA:1085:A:H2'	22:BA:1086:A:C4	2.52	0.44
22:BA:1526:C:H2'	22:BA:1527:G:O4'	2.17	0.44
22:BA:2185:U:H2'	22:BA:2186:G:H8	1.80	0.44
22:BA:2532:G:O6	28:BG:177:LYS:HE3	2.18	0.44
23:BB:41:G:HO2'	23:BB:42:C:P	2.40	0.44
41:BT:2:ILE:HD13	41:BT:42:GLU:HG2	1.98	0.44
1:AA:312:C:H2'	1:AA:313:A:C8	2.53	0.44
1:AA:414:A:C4	1:AA:415:A:C8	3.06	0.44
1:AA:456:A:H2'	1:AA:457:G:H8	1.82	0.44
1:AA:463:U:H2'	1:AA:464:U:C2	2.52	0.44
1:AA:555:U:H2'	1:AA:556:C:C6	2.53	0.44
1:AA:996:A:H2'	1:AA:997:U:H6	1.82	0.44
4:AD:184:ARG:NH1	4:AD:186:PRO:HA	2.32	0.44
13:AM:56:LEU:O	13:AM:60:VAL:HG23	2.18	0.44
22:BA:82:U:H2'	22:BA:83:A:C8	2.52	0.44
22:BA:857:G:H2'	22:BA:858:G:O4'	2.17	0.44
22:BA:2567:G:H2'	22:BA:2568:U:C6	2.53	0.44
22:BA:2698:U:H2'	22:BA:2699:C:C6	2.52	0.44
29:BH:87:GLU:HG3	29:BH:89:LYS:HB3	1.99	0.44
30:BI:34:LEU:H	30:BI:34:LEU:HD23	1.81	0.44
45:BX:43:GLU:CD	45:BX:45:ARG:HE	2.21	0.44
1:AA:178:C:H2'	1:AA:179:A:H8	1.83	0.44
2:AB:47:VAL:HG23	2:AB:48:PRO:HD3	1.99	0.44
22:BA:284:U:H2'	22:BA:285:G:H8	1.82	0.44
23:BB:54:G:H21	27:BF:26:MET:CE	2.30	0.44
32:BK:102:PRO:HB3	32:BK:121:GLU:CG	2.48	0.44
35:BN:21:PHE:CD1	35:BN:24:MET:HE3	2.53	0.44
41:BT:3:ARG:HB3	41:BT:5:GLU:HG3	1.99	0.44
1:AA:236:A:H2'	1:AA:237:G:C8	2.53	0.44
1:AA:1011:C:H2'	1:AA:1012:A:H8	1.83	0.44
2:AB:99:GLY:O	2:AB:103:ASN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:120:LYS:HB3	9:AI:120:LYS:HE2	1.72	0.44
13:AM:56:LEU:O	13:AM:59:GLU:HG2	2.18	0.44
13:AM:58:ASP:OD1	13:AM:58:ASP:N	2.51	0.44
14:AN:73:PHE:CZ	14:AN:78:GLY:HA2	2.52	0.44
22:BA:1075:C:H2'	22:BA:1076:C:C6	2.53	0.44
22:BA:1810:A:O5'	22:BA:1810:A:H8	2.01	0.44
22:BA:2419:U:H4'	49:B1:22:THR:HG21	2.00	0.44
1:AA:111:G:O6	1:AA:330:C:N4	2.47	0.44
1:AA:950:U:H2'	1:AA:951:G:H8	1.82	0.44
1:AA:1309:G:N7	13:AM:98:ARG:NH2	2.66	0.44
7:AG:46:ALA:HB1	7:AG:120:LEU:HB3	2.00	0.44
9:AI:54:LEU:HD11	9:AI:98:LEU:HD23	1.99	0.44
12:AL:110:ARG:HD2	12:AL:110:ARG:HA	1.77	0.44
32:BK:101:GLY:HA2	37:BP:68:GLU:OE2	2.18	0.44
41:BT:56:GLU:HG2	41:BT:57:VAL:HG23	1.99	0.44
1:AA:90:C:H2'	1:AA:91:U:H6	1.83	0.44
1:AA:298:A:H2'	1:AA:299:G:C8	2.52	0.44
1:AA:1220:G:P	14:AN:53:ARG:HH22	2.41	0.44
9:AI:12:ARG:HG3	9:AI:13:LYS:N	2.25	0.44
22:BA:1746:A:H2'	22:BA:1747:U:C6	2.53	0.44
24:BC:145:GLU:HB2	24:BC:188:CYS:HB3	1.99	0.44
36:BO:39:VAL:HG12	36:BO:48:LEU:HD12	2.00	0.44
40:BS:73:LYS:HB2	40:BS:106:VAL:HB	2.00	0.44
1:AA:269:C:H2'	1:AA:270:A:H8	1.82	0.44
1:AA:601:G:OP1	8:AH:89:LYS:NZ	2.51	0.44
22:BA:2125:G:N2	22:BA:2171:A:O5'	2.50	0.44
22:BA:2305:U:H2'	22:BA:2306:C:C6	2.53	0.44
22:BA:2898:U:H2'	22:BA:2899:A:C8	2.52	0.44
23:BB:54:G:H21	27:BF:26:MET:HE3	1.83	0.44
31:BJ:60:ASP:OD1	31:BJ:60:ASP:N	2.40	0.44
22:BA:703:U:H2'	22:BA:704:G:O4'	2.17	0.43
22:BA:948:C:P	59:BA:3202:HOH:O	2.59	0.43
22:BA:1791:A:C8	22:BA:1792:G:C8	3.06	0.43
22:BA:2148:G:H2'	22:BA:2149:U:C6	2.53	0.43
22:BA:2176:A:H2'	22:BA:2177:C:C6	2.52	0.43
2:AB:145:GLU:OE1	2:AB:145:GLU:N	2.43	0.43
4:AD:95:GLU:HA	4:AD:100:ASN:HD22	1.83	0.43
7:AG:37:SER:O	7:AG:40:GLU:HG2	2.17	0.43
19:AS:5:LEU:HG	19:AS:7:LYS:H	1.84	0.43
22:BA:1054:A:H2'	22:BA:1055:G:O4'	2.18	0.43
22:BA:1079:C:H2'	22:BA:1080:A:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2328:A:H2'	22:BA:2329:U:C6	2.53	0.43
37:BP:68:GLU:O	37:BP:68:GLU:HG2	2.18	0.43
1:AA:737:C:H2'	1:AA:738:C:C6	2.54	0.43
1:AA:745:G:H2'	1:AA:746:A:C8	2.52	0.43
3:AC:51:SER:O	3:AC:70:THR:OG1	2.36	0.43
3:AC:105:GLU:OE1	3:AC:105:GLU:HA	2.17	0.43
5:AE:104:GLY:H	5:AE:122:ASN:ND2	2.16	0.43
22:BA:548:G:O2'	22:BA:549:G:O5'	2.35	0.43
22:BA:593:U:H2'	22:BA:594:U:C6	2.52	0.43
33:BL:82:LEU:HD22	33:BL:90:VAL:HG21	2.00	0.43
1:AA:377:G:H2'	1:AA:378:G:C8	2.51	0.43
1:AA:1072:G:H2'	1:AA:1073:U:C6	2.54	0.43
1:AA:1236:A:H4'	1:AA:1304:G:H4'	2.00	0.43
10:AJ:29:ALA:O	10:AJ:32:THR:OG1	2.25	0.43
22:BA:2:G:H2'	22:BA:3:U:C6	2.53	0.43
22:BA:360:U:C4	22:BA:361:G:C6	3.07	0.43
22:BA:832:U:H2'	22:BA:833:A:C8	2.53	0.43
22:BA:2156:G:H2'	22:BA:2157:G:O4'	2.18	0.43
33:BL:19:LEU:HD22	33:BL:27:LEU:HD22	2.00	0.43
1:AA:160:A:H2'	1:AA:161:A:O4'	2.17	0.43
1:AA:193:C:H2'	1:AA:194:C:C6	2.53	0.43
1:AA:1317:C:N4	14:AN:53:ARG:HH11	2.12	0.43
9:AI:21:ILE:CG2	9:AI:61:LEU:HD23	2.48	0.43
13:AM:60:VAL:HG12	13:AM:65:VAL:HG21	2.01	0.43
13:AM:71:ARG:NH2	27:BF:115:ARG:HH22	2.15	0.43
24:BC:71:LYS:NZ	24:BC:100:GLU:OE1	2.31	0.43
25:BD:136:ASN:OD1	25:BD:139:SER:OG	2.36	0.43
27:BF:126:GLY:O	27:BF:158:THR:OG1	2.28	0.43
1:AA:212:G:C4	1:AA:213:G:C8	3.07	0.43
1:AA:954:G:H21	1:AA:1227:A:H62	1.67	0.43
1:AA:1120:C:H2'	1:AA:1121:U:H6	1.84	0.43
1:AA:1314:C:C2	1:AA:1315:U:C5	3.07	0.43
2:AB:56:GLU:O	2:AB:59:LYS:HG2	2.19	0.43
10:AJ:56:HIS:CG	10:AJ:57:VAL:H	2.36	0.43
13:AM:25:VAL:HA	13:AM:29:ARG:HD2	2.00	0.43
21:AU:41:PRO:HA	21:AU:44:GLU:HG3	2.01	0.43
22:BA:1263:U:O2'	48:B0:8:PRO:HD2	2.18	0.43
22:BA:2250:G:O2'	22:BA:2496:C:OP1	2.26	0.43
27:BF:8:TYR:HA	27:BF:12:VAL:HB	2.01	0.43
44:BW:71:VAL:HG22	44:BW:78:LYS:HD2	2.00	0.43
1:AA:627:G:H2'	1:AA:628:G:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:999:C:H2'	1:AA:1000:A:C8	2.54	0.43
1:AA:1023:U:H2'	1:AA:1024:G:C4	2.54	0.43
1:AA:1026:G:N2	1:AA:1035:A:C4	2.86	0.43
1:AA:1088:G:H21	1:AA:1167:A:H61	1.65	0.43
1:AA:1412:C:H2'	1:AA:1413:A:C8	2.54	0.43
3:AC:112:ASP:O	3:AC:116:VAL:HG23	2.18	0.43
4:AD:104:ARG:HA	4:AD:104:ARG:HD3	1.77	0.43
20:AT:24:ARG:HA	20:AT:24:ARG:HD3	1.79	0.43
22:BA:535:G:C6	22:BA:559:G:C6	3.07	0.43
22:BA:1251:C:OP2	38:BQ:6:ARG:HD2	2.18	0.43
22:BA:1733:G:H2'	22:BA:1734:G:H8	1.82	0.43
25:BD:56:LYS:HD2	25:BD:59:ARG:HG3	2.00	0.43
33:BL:62:PRO:HG2	51:B3:25:LYS:HD3	2.01	0.43
6:AF:7:VAL:HG22	6:AF:61:LEU:HD13	2.01	0.43
11:AK:14:LYS:HA	11:AK:14:LYS:HD2	1.72	0.43
16:AP:70:ARG:O	16:AP:74:LEU:HD13	2.19	0.43
22:BA:1433:A:H2'	22:BA:1434:A:O4'	2.19	0.43
22:BA:1506:U:H2'	22:BA:1507:C:C6	2.54	0.43
35:BN:20:MET:HG2	35:BN:24:MET:HE1	1.99	0.43
41:BT:1:MET:HB3	41:BT:2:ILE:H	1.60	0.43
1:AA:1124:G:P	10:AJ:37:ARG:HH12	2.39	0.43
4:AD:28:ILE:HD12	4:AD:34:ILE:HG21	2.00	0.43
5:AE:132:ASN:O	5:AE:136:VAL:HG23	2.18	0.43
8:AH:96:MET:CG	8:AH:99:LEU:HB2	2.49	0.43
15:AO:21:ASP:OD1	15:AO:24:SER:HB3	2.18	0.43
22:BA:612:G:H2'	22:BA:614:A:C8	2.53	0.43
22:BA:1202:G:O6	22:BA:1244:A:N6	2.52	0.43
22:BA:2281:A:C2'	22:BA:2282:G:H5'	2.49	0.43
22:BA:2530:A:N6	28:BG:156:PRO:HG3	2.33	0.43
30:BI:16:CYS:SG	30:BI:17:SER:N	2.92	0.43
46:BY:5:GLU:OE1	46:BY:5:GLU:N	2.41	0.43
1:AA:757:U:H2'	1:AA:758:C:O4'	2.19	0.43
1:AA:826:C:O2	8:AH:16:ASN:ND2	2.52	0.43
10:AJ:80:THR:O	10:AJ:82:LYS:N	2.51	0.43
22:BA:141:G:H3'	22:BA:141:G:N3	2.33	0.43
22:BA:355:U:H2'	22:BA:356:G:C8	2.52	0.43
22:BA:2489:U:H2'	22:BA:2490:G:O4'	2.19	0.43
1:AA:304:U:O2'	1:AA:305:G:H5'	2.19	0.42
1:AA:320:A:H2'	1:AA:321:A:O4'	2.18	0.42
1:AA:1213:A:O2'	1:AA:1215:G:N7	2.41	0.42
1:AA:1315:U:O2	1:AA:1360:A:H2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:150:PRO:HA	5:AE:153:VAL:HG12	2.01	0.42
11:AK:23:ILE:HD13	11:AK:84:VAL:HG13	2.00	0.42
22:BA:248:G:H5'	22:BA:250:G:N7	2.34	0.42
22:BA:2143:C:H2'	22:BA:2144:G:C8	2.54	0.42
1:AA:264:C:O2'	17:AQ:66:PRO:O	2.33	0.42
1:AA:680:C:H2'	1:AA:681:A:H8	1.84	0.42
1:AA:876:C:H1'	8:AH:12:THR:HG21	2.01	0.42
1:AA:947:G:H2'	1:AA:948:C:H6	1.84	0.42
1:AA:1163:A:H2'	1:AA:1164:G:C8	2.54	0.42
1:AA:1198:G:H2'	1:AA:1199:U:C6	2.55	0.42
6:AF:4:TYR:CE2	6:AF:71:ILE:HG13	2.54	0.42
22:BA:1068:G:N3	22:BA:1095:A:O2'	2.50	0.42
30:BI:30:HIS:CG	30:BI:31:ASP:H	2.38	0.42
34:BM:36:VAL:HG21	34:BM:129:THR:HG23	2.01	0.42
43:BV:68:LYS:NZ	43:BV:69:GLU:O	2.34	0.42
1:AA:179:A:C5	1:AA:180:U:C4	3.07	0.42
1:AA:413:G:H21	1:AA:428:G:H1'	1.84	0.42
1:AA:565:U:H3'	1:AA:566:G:H2'	2.01	0.42
1:AA:864:A:H5''	5:AE:90:THR:HB	2.02	0.42
1:AA:910:C:OP2	12:AL:18:LYS:NZ	2.52	0.42
1:AA:1174:G:H2'	1:AA:1175:G:H8	1.83	0.42
4:AD:58:LYS:HB3	4:AD:58:LYS:HE3	1.73	0.42
9:AI:50:GLN:O	9:AI:53:GLU:HG2	2.20	0.42
10:AJ:15:HIS:NE2	10:AJ:16:ARG:HG3	2.35	0.42
13:AM:16:VAL:HG13	13:AM:17:ILE:HD12	2.01	0.42
17:AQ:28:PHE:CZ	17:AQ:37:PHE:HB3	2.54	0.42
22:BA:1506:U:H2'	22:BA:1507:C:H6	1.85	0.42
22:BA:1590:A:H2'	22:BA:1591:A:C8	2.55	0.42
30:BI:11:GLU:HB2	30:BI:25:ARG:HE	1.84	0.42
31:BJ:111:LYS:HD2	31:BJ:111:LYS:N	2.34	0.42
42:BU:18:ASP:OD2	42:BU:40:ASN:N	2.47	0.42
51:B3:26:HIS:CE1	51:B3:48:ALA:HB2	2.54	0.42
1:AA:559:A:H4'	1:AA:560:A:H3'	2.01	0.42
1:AA:908:A:H2'	1:AA:909:A:C8	2.54	0.42
1:AA:1125:U:O2'	1:AA:1126:U:H2'	2.18	0.42
2:AB:139:ARG:O	2:AB:143:LYS:N	2.51	0.42
16:AP:8:ARG:NH2	16:AP:15:PRO:HB3	2.35	0.42
19:AS:71:LEU:HD23	19:AS:71:LEU:HA	1.84	0.42
22:BA:280:U:H2'	22:BA:281:C:C6	2.53	0.42
22:BA:281:C:H2'	22:BA:282:A:H8	1.84	0.42
22:BA:287:G:H2'	22:BA:288:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2014:A:H2'	22:BA:2015:A:C8	2.53	0.42
1:AA:106:C:H2'	1:AA:107:G:O4'	2.20	0.42
1:AA:628:G:H2'	1:AA:629:A:C8	2.54	0.42
2:AB:9:MET:HE3	2:AB:47:VAL:HG12	1.99	0.42
7:AG:47:LEU:HG	7:AG:58:GLU:OE2	2.19	0.42
15:AO:77:ARG:HA	15:AO:80:GLN:NE2	2.34	0.42
21:AU:7:ARG:O	21:AU:10:GLU:HG2	2.19	0.42
22:BA:1230:A:H2'	22:BA:1231:U:O4'	2.19	0.42
22:BA:1282:U:H2'	22:BA:1283:G:O4'	2.20	0.42
22:BA:1300:G:H4'	22:BA:1301:A:H5''	2.00	0.42
22:BA:2116:G:O6	22:BA:2171:A:N6	2.52	0.42
22:BA:2246:G:H2'	22:BA:2247:A:C8	2.54	0.42
38:BQ:35:ALA:O	38:BQ:39:VAL:HG23	2.20	0.42
1:AA:80:A:N3	1:AA:81:A:H1'	2.34	0.42
1:AA:302:G:H2'	1:AA:303:A:H8	1.85	0.42
1:AA:590:U:H2'	1:AA:591:U:C6	2.54	0.42
1:AA:1144:G:N2	1:AA:1146:A:H62	2.17	0.42
7:AG:25:LYS:O	7:AG:29:ILE:HG13	2.20	0.42
8:AH:113:ASP:N	8:AH:113:ASP:OD1	2.53	0.42
9:AI:26:GLY:CA	9:AI:59:GLU:O	2.68	0.42
13:AM:49:SER:HB3	13:AM:52:GLN:HG3	2.02	0.42
18:AR:68:LEU:HD23	18:AR:68:LEU:HA	1.74	0.42
22:BA:882:G:N1	22:BA:895:U:O2	2.52	0.42
29:BH:129:GLU:HG2	29:BH:141:LYS:HE2	2.01	0.42
1:AA:517:G:H8	1:AA:517:G:OP2	2.02	0.42
1:AA:922:G:H2'	1:AA:923:A:C8	2.55	0.42
1:AA:1238:A:OP1	1:AA:1335:U:O2'	2.23	0.42
7:AG:149:LYS:HB2	7:AG:149:LYS:HE2	1.75	0.42
13:AM:39:ILE:HD12	13:AM:56:LEU:HD21	2.02	0.42
13:AM:83:LEU:HD22	19:AS:65:GLU:OE1	2.19	0.42
19:AS:53:ASN:OD1	19:AS:56:GLN:N	2.36	0.42
19:AS:64:ASP:O	19:AS:67:VAL:HG12	2.20	0.42
22:BA:249:C:O2	51:B3:12:LYS:NZ	2.52	0.42
22:BA:347:A:H2'	22:BA:348:A:C8	2.55	0.42
22:BA:1538:G:H2'	22:BA:1539:U:H6	1.85	0.42
22:BA:2159:G:H2'	22:BA:2160:C:H6	1.82	0.42
27:BF:102:ARG:CG	30:BI:24:ILE:HD11	2.47	0.42
29:BH:129:GLU:OE1	29:BH:143:ILE:HG22	2.20	0.42
32:BK:63:VAL:HG23	32:BK:64:ARG:HG3	2.01	0.42
49:B1:25:LYS:HE2	49:B1:51:GLU:OE1	2.20	0.42
1:AA:161:A:H2'	1:AA:162:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:323:U:H2'	1:AA:324:G:O4'	2.20	0.42
1:AA:405:U:OP2	4:AD:3:ARG:NH1	2.53	0.42
1:AA:590:U:H2'	1:AA:591:U:H6	1.84	0.42
1:AA:642:A:N7	8:AH:107:SER:HA	2.35	0.42
1:AA:736:C:H2'	1:AA:737:C:H6	1.84	0.42
1:AA:1025:U:H4'	1:AA:1026:G:C8	2.54	0.42
1:AA:1187:G:H2'	1:AA:1188:A:C8	2.55	0.42
1:AA:1216:A:H2'	1:AA:1217:C:H6	1.85	0.42
10:AJ:27:GLU:OE1	10:AJ:27:GLU:N	2.45	0.42
22:BA:746:PSU:H6	22:BA:746:PSU:H2'	1.66	0.42
22:BA:1509:A:H2'	22:BA:1510:G:H8	1.83	0.42
22:BA:2579:C:O2'	25:BD:136:ASN:OD1	2.38	0.42
26:BE:87:ALA:O	26:BE:88:ARG:NH2	2.53	0.42
29:BH:87:GLU:CG	29:BH:89:LYS:HB3	2.50	0.42
30:BI:45:THR:HA	30:BI:48:GLN:HE22	1.84	0.42
31:BJ:121:LYS:HB2	31:BJ:121:LYS:HE3	1.79	0.42
42:BU:86:ARG:HG2	42:BU:95:PHE:CD1	2.55	0.42
1:AA:309:A:H2'	1:AA:310:G:H8	1.85	0.42
1:AA:412:A:C2	1:AA:414:A:H1'	2.55	0.42
1:AA:501:C:H2'	1:AA:502:A:C8	2.55	0.42
1:AA:780:A:OP1	11:AK:125:LYS:HG2	2.19	0.42
13:AM:29:ARG:HH11	13:AM:29:ARG:HB2	1.84	0.42
14:AN:20:PHE:C	14:AN:22:LYS:H	2.23	0.42
17:AQ:30:LYS:HB2	17:AQ:37:PHE:CE2	2.55	0.42
22:BA:464:U:H2'	22:BA:465:G:O4'	2.19	0.42
22:BA:875:G:H2'	22:BA:876:C:C6	2.55	0.42
22:BA:884:U:H1'	22:BA:893:C:N3	2.34	0.42
22:BA:1141:U:H4'	22:BA:1142:A:O4'	2.20	0.42
22:BA:2183:A:O2'	22:BA:2184:A:H5'	2.20	0.42
1:AA:219:U:H2'	1:AA:220:G:H8	1.85	0.42
1:AA:511:C:HO2'	1:AA:512:U:H6	1.68	0.42
1:AA:634:C:H2'	1:AA:635:A:C8	2.55	0.42
1:AA:948:C:OP1	13:AM:108:THR:HG22	2.20	0.42
1:AA:981:U:H5	1:AA:982:U:HO2'	1.67	0.42
1:AA:1329:A:H5'	13:AM:29:ARG:NH1	2.35	0.42
11:AK:81:ASN:HB3	11:AK:106:ARG:HB3	2.02	0.42
12:AL:114:ARG:HH21	12:AL:121:ARG:HB2	1.84	0.42
22:BA:742:A:H2'	22:BA:743:A:C8	2.54	0.42
22:BA:1105:U:H2'	22:BA:1106:G:H8	1.84	0.42
22:BA:1327:A:H2'	22:BA:1328:A:O4'	2.20	0.42
22:BA:1853:A:H2'	22:BA:1854:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2119:A:O2'	22:BA:2120:G:H5'	2.20	0.42
36:BO:56:LYS:HA	36:BO:56:LYS:HD2	1.66	0.42
49:B1:9:ILE:HD12	49:B1:51:GLU:HG3	2.02	0.42
1:AA:696:A:H2'	1:AA:697:U:C6	2.55	0.41
1:AA:947:G:H2'	1:AA:948:C:C6	2.55	0.41
1:AA:1512:U:H2'	1:AA:1513:A:C8	2.55	0.41
16:AP:44:SER:C	16:AP:46:LYS:H	2.24	0.41
30:BI:58:ASP:OD1	30:BI:58:ASP:N	2.53	0.41
33:BL:9:ALA:O	33:BL:12:SER:OG	2.23	0.41
1:AA:722:G:N3	1:AA:722:G:H2'	2.35	0.41
3:AC:47:LEU:HD22	3:AC:76:VAL:HG12	2.02	0.41
4:AD:73:ARG:O	4:AD:77:LYS:HG3	2.21	0.41
8:AH:87:LYS:HG3	8:AH:125:ILE:HD11	2.02	0.41
22:BA:1062:G:C6	22:BA:1063:G:C5	3.08	0.41
22:BA:1357:C:H2'	22:BA:1358:G:O4'	2.20	0.41
22:BA:1654:A:O2'	25:BD:118:PHE:O	2.33	0.41
22:BA:2148:G:H2'	22:BA:2149:U:H6	1.85	0.41
29:BH:88:GLY:O	29:BH:125:THR:HG22	2.20	0.41
43:BV:77:VAL:HG23	43:BV:89:ILE:HG12	2.01	0.41
1:AA:82:G:N1	1:AA:88:U:O2	2.54	0.41
1:AA:134:G:H1'	1:AA:325:A:N7	2.36	0.41
1:AA:900:A:O5'	1:AA:900:A:H8	2.02	0.41
1:AA:1035:A:H2'	1:AA:1036:A:H8	1.85	0.41
1:AA:1308:U:H2'	1:AA:1309:G:C8	2.56	0.41
3:AC:121:THR:O	3:AC:125:GLU:HG3	2.20	0.41
7:AG:126:ASP:HB2	7:AG:131:LYS:HB2	2.01	0.41
11:AK:107:ILE:HD13	21:AU:12:PHE:HE2	1.81	0.41
19:AS:55:ARG:HG3	19:AS:56:GLN:HG2	2.01	0.41
22:BA:475:C:O2	22:BA:479:A:N6	2.48	0.41
22:BA:493:G:H2'	22:BA:494:G:O4'	2.21	0.41
22:BA:1260:A:H2'	22:BA:1261:C:O4'	2.20	0.41
22:BA:1610:A:H5'	22:BA:1610:A:H8	1.85	0.41
22:BA:1858:A:H2'	22:BA:1859:U:O4'	2.21	0.41
22:BA:2241:A:H2'	22:BA:2242:G:C8	2.55	0.41
22:BA:2574:G:O2'	25:BD:148:GLN:HB3	2.20	0.41
55:B8:66:A:H2'	55:B8:67:U:C6	2.55	0.41
1:AA:618:C:O2	1:AA:622:A:N6	2.53	0.41
1:AA:1021:A:H2'	1:AA:1022:A:C8	2.55	0.41
1:AA:1130:A:H2'	1:AA:1131:G:H8	1.86	0.41
1:AA:1151:A:O2'	1:AA:1152:A:H8	2.03	0.41
1:AA:1180:A:H8	1:AA:1180:A:O5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1229:A:H2'	1:AA:1230:C:H6	1.85	0.41
2:AB:187:VAL:HG13	2:AB:191:SER:HB3	2.03	0.41
3:AC:42:TYR:OH	3:AC:90:VAL:HG11	2.20	0.41
5:AE:154:ALA:HB1	5:AE:159:LYS:O	2.20	0.41
6:AF:9:MET:SD	6:AF:59:TYR:CE1	3.14	0.41
22:BA:638:G:H2'	22:BA:639:U:C6	2.55	0.41
22:BA:2070:A:H2'	22:BA:2071:A:O4'	2.21	0.41
22:BA:2122:U:H2'	22:BA:2123:G:O4'	2.20	0.41
26:BE:127:GLU:OE1	26:BE:127:GLU:N	2.34	0.41
29:BH:16:GLY:HA2	29:BH:47:PHE:CZ	2.55	0.41
1:AA:310:G:H5''	16:AP:31:ARG:HB2	2.01	0.41
1:AA:779:C:H2'	1:AA:780:A:O4'	2.21	0.41
1:AA:1402:4OC:HM23	1:AA:1402:4OC:H1'	1.88	0.41
2:AB:100:MET:HA	2:AB:107:VAL:HG21	2.02	0.41
6:AF:34:GLY:C	6:AF:35:LYS:HD3	2.41	0.41
6:AF:44:ARG:HB3	6:AF:56:LYS:HE2	2.02	0.41
6:AF:103:VAL:HG12	6:AF:106:LYS:HZ3	1.86	0.41
17:AQ:4:LYS:HG3	17:AQ:4:LYS:O	2.21	0.41
17:AQ:7:THR:HG21	17:AQ:60:GLU:OE2	2.20	0.41
22:BA:482:A:H4'	42:BU:45:HIS:ND1	2.36	0.41
22:BA:760:G:H2'	22:BA:761:A:O4'	2.20	0.41
22:BA:828:U:H2'	22:BA:829:A:C8	2.55	0.41
42:BU:26:LYS:HA	42:BU:26:LYS:HD2	1.85	0.41
55:B8:21:A:N6	55:B8:46:G:H2'	2.36	0.41
1:AA:545:C:H2'	1:AA:546:A:O4'	2.21	0.41
1:AA:1372:U:H2'	1:AA:1373:G:O4'	2.20	0.41
12:AL:73:ASN:C	12:AL:74:LEU:HD12	2.41	0.41
13:AM:19:LEU:HD23	13:AM:19:LEU:HA	1.91	0.41
19:AS:17:LYS:HD3	19:AS:17:LYS:HA	1.75	0.41
19:AS:51:VAL:O	19:AS:57:HIS:HA	2.20	0.41
22:BA:141:G:C6	41:BT:1:MET:CE	3.04	0.41
22:BA:1473:G:C6	22:BA:1474:U:C4	3.09	0.41
22:BA:2032:G:C5	25:BD:150:MEQ:HE3	2.55	0.41
22:BA:2038:G:H2'	22:BA:2039:U:O4'	2.20	0.41
22:BA:2316:G:H2'	22:BA:2317:A:C8	2.56	0.41
28:BG:52:PHE:CE1	28:BG:72:LEU:HD22	2.55	0.41
42:BU:26:LYS:HE2	42:BU:26:LYS:HB3	1.89	0.41
43:BV:10:LYS:HE2	43:BV:10:LYS:HA	2.03	0.41
44:BW:26:PHE:O	44:BW:29:GLU:HG3	2.21	0.41
55:B8:46:G:C2'	55:B8:47:U:H5'	2.50	0.41
1:AA:860:A:H2'	1:AA:861:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:974:A:H4'	1:AA:975:A:H3'	2.03	0.41
2:AB:133:GLU:O	2:AB:137:ARG:HB2	2.21	0.41
3:AC:50:ALA:O	3:AC:70:THR:OG1	2.35	0.41
3:AC:58:GLU:O	3:AC:64:ILE:HD12	2.21	0.41
8:AH:30:SER:O	8:AH:34:VAL:HG23	2.21	0.41
13:AM:86:TYR:H	19:AS:73:GLU:HB3	1.86	0.41
14:AN:49:GLN:HG3	19:AS:13:LEU:HD23	2.03	0.41
22:BA:274:C:H2'	22:BA:275:C:O4'	2.21	0.41
22:BA:1870:C:O2'	22:BA:1871:A:O5'	2.39	0.41
35:BN:35:LYS:HB2	35:BN:112:TYR:CE2	2.55	0.41
41:BT:37:ASP:OD1	41:BT:37:ASP:N	2.52	0.41
1:AA:680:C:H2'	1:AA:681:A:C8	2.56	0.41
1:AA:986:U:H2'	1:AA:987:G:O4'	2.21	0.41
2:AB:78:GLU:HG2	2:AB:79:ALA:N	2.35	0.41
4:AD:202:GLU:OE1	5:AE:112:ARG:NH2	2.52	0.41
8:AH:52:GLU:O	8:AH:57:PRO:HA	2.20	0.41
15:AO:21:ASP:O	15:AO:27:VAL:HG21	2.21	0.41
22:BA:1094:U:H1'	22:BA:1097:U:H5	1.85	0.41
22:BA:1098:A:C6	22:BA:1099:G:C5	3.09	0.41
22:BA:1386:C:H2'	22:BA:1387:A:C8	2.55	0.41
25:BD:1:MET:CE	25:BD:205:PRO:HG3	2.50	0.41
27:BF:64:LYS:HD3	30:BI:5:ILE:HD12	2.02	0.41
28:BG:29:LYS:HE2	28:BG:29:LYS:HB3	1.73	0.41
29:BH:89:LYS:HB2	29:BH:89:LYS:HE3	1.94	0.41
48:B0:38:HIS:HB3	48:B0:44:THR:HG22	2.03	0.41
1:AA:219:U:C2	1:AA:220:G:C8	3.08	0.41
1:AA:1020:G:H2'	1:AA:1021:A:C8	2.56	0.41
1:AA:1026:G:C6	1:AA:1035:A:C6	3.09	0.41
1:AA:1026:G:C2	1:AA:1035:A:C5	3.09	0.41
1:AA:1032:G:H3'	1:AA:1032:G:N3	2.36	0.41
1:AA:1343:G:H2'	1:AA:1344:C:C6	2.55	0.41
2:AB:154:MET:SD	2:AB:156:GLY:O	2.78	0.41
3:AC:56:VAL:HG22	3:AC:67:THR:HB	2.03	0.41
4:AD:57:GLU:HG3	4:AD:200:ILE:HD11	2.03	0.41
4:AD:62:ARG:CZ	4:AD:69:GLU:HG2	2.51	0.41
7:AG:57:SER:O	7:AG:60:GLU:N	2.54	0.41
21:AU:4:ILE:CD1	21:AU:19:PHE:HA	2.47	0.41
22:BA:251:A:O5'	22:BA:251:A:H8	2.04	0.41
22:BA:568:U:H4'	22:BA:945:A:N6	2.36	0.41
22:BA:657:U:H2'	22:BA:658:U:C6	2.56	0.41
22:BA:880:G:N3	22:BA:881:G:C8	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1365:A:OP2	45:BX:2:SER:HB3	2.21	0.41
22:BA:2188:U:O2'	22:BA:2189:U:O5'	2.39	0.41
22:BA:2818:U:H2'	22:BA:2819:G:C8	2.56	0.41
23:BB:49:C:H2'	23:BB:50:A:C8	2.56	0.41
27:BF:117:LEU:O	27:BF:178:ARG:N	2.51	0.41
28:BG:76:VAL:O	28:BG:80:THR:OG1	2.39	0.41
32:BK:105:ARG:HG2	32:BK:122:VAL:HG12	2.03	0.41
43:BV:21:ARG:HA	43:BV:25:LYS:O	2.21	0.41
1:AA:190:A:O5'	1:AA:190:A:H8	2.03	0.41
1:AA:208:U:N3	1:AA:211:G:N1	2.66	0.41
1:AA:815:A:OP2	1:AA:816:A:H5''	2.21	0.41
1:AA:1326:U:H2'	1:AA:1327:C:C6	2.55	0.41
2:AB:126:PHE:CD1	2:AB:128:LYS:HG3	2.55	0.41
10:AJ:87:LEU:O	10:AJ:90:LEU:HD22	2.20	0.41
22:BA:357:C:H2'	22:BA:358:U:H6	1.86	0.41
22:BA:1654:A:H2'	22:BA:1655:A:H8	1.85	0.41
22:BA:1808:A:H3'	22:BA:1809:A:C8	2.55	0.41
22:BA:1874:C:H2'	22:BA:1875:G:O4'	2.21	0.41
23:BB:24:G:N7	23:BB:56:G:H2'	2.36	0.41
23:BB:79:G:N7	43:BV:14:LYS:NZ	2.69	0.41
25:BD:55:LYS:HD3	25:BD:60:VAL:HG12	2.03	0.41
26:BE:158:PHE:O	26:BE:162:ARG:HG3	2.21	0.41
29:BH:65:ALA:O	29:BH:69:ALA:N	2.54	0.41
29:BH:99:ILE:O	29:BH:103:VAL:HG23	2.21	0.41
1:AA:108:G:H5'	1:AA:109:A:H5''	2.03	0.40
1:AA:202:G:H21	1:AA:465:A:H61	1.69	0.40
1:AA:467:U:H3'	1:AA:468:A:C5'	2.52	0.40
1:AA:950:U:H2'	1:AA:951:G:C8	2.55	0.40
4:AD:124:MET:HG3	4:AD:128:ARG:C	2.41	0.40
10:AJ:20:GLN:OE1	10:AJ:20:GLN:N	2.54	0.40
16:AP:50:THR:HG23	16:AP:50:THR:O	2.22	0.40
22:BA:1558:C:O4'	22:BA:1560:G:C8	2.74	0.40
22:BA:2064:C:H2'	22:BA:2065:C:C6	2.56	0.40
22:BA:2255:G:O2'	55:B8:3:G:OP2	2.34	0.40
22:BA:2588:G:O6	22:BA:2607:G:C6	2.74	0.40
29:BH:46:PHE:CD1	29:BH:50:ARG:HD2	2.56	0.40
36:BO:88:LYS:NZ	36:BO:89:ASP:OD2	2.48	0.40
39:BR:22:LEU:HD12	39:BR:23:GLU:O	2.20	0.40
1:AA:415:A:C4	1:AA:416:G:C8	3.08	0.40
1:AA:455:G:H2'	1:AA:456:A:H8	1.84	0.40
1:AA:600:A:H2'	1:AA:601:G:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:600:A:H5''	8:AH:89:LYS:HE2	2.02	0.40
1:AA:981:U:O2'	14:AN:61:ARG:NE	2.54	0.40
1:AA:1427:C:H2'	1:AA:1428:A:C8	2.56	0.40
3:AC:119:SER:O	3:AC:123:GLN:HG3	2.21	0.40
4:AD:60:LYS:NZ	4:AD:194:ASP:O	2.50	0.40
13:AM:63:PHE:HB2	13:AM:65:VAL:HG13	2.04	0.40
13:AM:66:GLU:CG	13:AM:67:GLY:H	2.33	0.40
14:AN:42:TRP:O	14:AN:46:LEU:HD23	2.21	0.40
17:AQ:60:GLU:O	17:AQ:76:VAL:HG22	2.21	0.40
22:BA:2:G:H2'	22:BA:3:U:H6	1.86	0.40
22:BA:84:A:OP1	42:BU:6:ARG:NH1	2.54	0.40
22:BA:711:G:C6	22:BA:721:A:C6	3.08	0.40
22:BA:1405:U:H2'	22:BA:1406:U:C6	2.56	0.40
22:BA:1774:C:O2	22:BA:1774:C:H2'	2.20	0.40
22:BA:2478:A:H5'	52:B4:32:LYS:HE2	2.04	0.40
29:BH:44:ILE:HD12	29:BH:44:ILE:H	1.87	0.40
36:BO:27:VAL:HG21	36:BO:40:ILE:HD12	2.02	0.40
49:B1:13:SER:HB3	49:B1:49:TYR:CZ	2.56	0.40
1:AA:383:A:H8	1:AA:383:A:O5'	2.04	0.40
1:AA:1027:C:H2'	1:AA:1028:C:C6	2.56	0.40
1:AA:1152:A:H2'	1:AA:1153:G:O4'	2.21	0.40
1:AA:1317:C:C4	14:AN:53:ARG:HD2	2.57	0.40
1:AA:1345:U:OP1	9:AI:122:ARG:NH1	2.54	0.40
5:AE:14:LYS:HD2	5:AE:113:ALA:HB1	2.03	0.40
7:AG:111:ARG:HD2	7:AG:123:GLU:HG2	2.03	0.40
11:AK:126:LYS:HD2	21:AU:37:PHE:HB3	2.01	0.40
13:AM:7:ILE:O	13:AM:7:ILE:HG22	2.21	0.40
16:AP:22:ALA:HA	16:AP:33:ILE:HG13	2.02	0.40
17:AQ:65:ARG:O	17:AQ:67:LEU:HD12	2.21	0.40
22:BA:2364:C:H2'	22:BA:2365:G:O4'	2.21	0.40
25:BD:12:THR:OG1	25:BD:13:ARG:N	2.53	0.40
28:BG:67:THR:O	28:BG:71:LEU:HG	2.22	0.40
34:BM:53:MET:O	34:BM:57:VAL:HG22	2.22	0.40
51:B3:31:HIS:C	51:B3:33:LEU:N	2.74	0.40
1:AA:110:C:O2'	16:AP:25:ARG:O	2.39	0.40
1:AA:181:A:H4'	1:AA:182:A:H5'	2.02	0.40
1:AA:407:U:H2'	1:AA:408:A:C8	2.56	0.40
1:AA:470:C:H2'	1:AA:471:U:H6	1.86	0.40
1:AA:613:C:H2'	1:AA:614:C:C6	2.56	0.40
1:AA:668:G:H21	15:AO:46:HIS:HE1	1.69	0.40
1:AA:1158:C:N3	1:AA:1160:G:C8	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	2.04	0.40
12:AL:107:VAL:HG21	12:AL:110:ARG:HD3	2.04	0.40
14:AN:54:ASP:HA	14:AN:59:ARG:HD3	2.04	0.40
17:AQ:9:GLN:OE1	17:AQ:79:VAL:HG21	2.21	0.40
22:BA:879:G:C2	22:BA:880:G:C8	3.10	0.40
22:BA:2176:A:H2'	22:BA:2177:C:C5	2.56	0.40
22:BA:2847:U:H2'	22:BA:2848:G:O4'	2.22	0.40
31:BJ:118:MET:HA	31:BJ:121:LYS:HE2	2.02	0.40
50:B2:16:HIS:HB2	50:B2:44:VAL:HG21	2.03	0.40
1:AA:302:G:H2'	1:AA:303:A:C8	2.56	0.40
1:AA:526:C:OP2	12:AL:88:LYS:HE3	2.22	0.40
1:AA:900:A:H2'	1:AA:901:A:C8	2.56	0.40
1:AA:1220:G:H1'	19:AS:52:HIS:ND1	2.36	0.40
1:AA:1236:A:H2'	1:AA:1237:C:C6	2.57	0.40
6:AF:3:HIS:HD2	6:AF:95:ALA:N	2.19	0.40
6:AF:4:TYR:HA	6:AF:90:MET:O	2.22	0.40
10:AJ:12:ALA:HB2	10:AJ:96:VAL:HG12	2.02	0.40
15:AO:75:VAL:O	15:AO:79:THR:HG23	2.21	0.40
17:AQ:19:LYS:HG3	17:AQ:47:HIS:CE1	2.57	0.40
22:BA:1115:G:O2'	22:BA:1116:G:H5''	2.21	0.40
22:BA:1704:C:N4	22:BA:1705:A:H62	2.20	0.40
26:BE:157:LEU:HD12	26:BE:157:LEU:HA	1.89	0.40
43:BV:2:PHE:HB3	43:BV:50:MET:CE	2.51	0.40
47:BZ:48:ILE:HG21	47:BZ:57:VAL:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	222/241 (92%)	209 (94%)	13 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
4	AD	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
5	AE	153/167 (92%)	148 (97%)	5 (3%)	0	100	100
6	AF	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	AG	149/179 (83%)	143 (96%)	6 (4%)	0	100	100
8	AH	127/130 (98%)	127 (100%)	0	0	100	100
9	AI	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
10	AJ	97/103 (94%)	89 (92%)	6 (6%)	2 (2%)	5	22
11	AK	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
12	AL	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
13	AM	112/118 (95%)	104 (93%)	8 (7%)	0	100	100
14	AN	99/102 (97%)	88 (89%)	11 (11%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	AP	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
17	AQ	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
18	AR	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
19	AS	80/92 (87%)	74 (92%)	6 (8%)	0	100	100
20	AT	84/87 (97%)	84 (100%)	0	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
25	BD	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	25	56
26	BE	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
27	BF	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
28	BG	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
29	BH	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
30	BI	64/70 (91%)	58 (91%)	6 (9%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	BL	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
34	BM	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
35	BN	116/127 (91%)	109 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BO	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
37	BP	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	BS	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	BT	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
42	BU	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
43	BV	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
44	BW	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	BX	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
46	BY	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	BZ	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	B0	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
49	B1	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
50	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
51	B3	62/65 (95%)	57 (92%)	3 (5%)	2 (3%)	3	13
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	B5	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
All	All	5590/5931 (94%)	5378 (96%)	207 (4%)	5 (0%)	50	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	BD	149	ASN
51	B3	32	ILE
51	B3	33	LEU
10	AJ	57	VAL
10	AJ	58	ASN

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	
2	AB	186/199 (94%)	183 (98%)	3 (2%)	58	84
3	AC	170/190 (90%)	168 (99%)	2 (1%)	67	89
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	118/126 (94%)	118 (100%)	0	100	100
6	AF	92/116 (79%)	92 (100%)	0	100	100
7	AG	124/147 (84%)	123 (99%)	1 (1%)	79	93
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	104 (99%)	1 (1%)	73	91
10	AJ	87/90 (97%)	87 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	102/103 (99%)	102 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	78 (99%)	1 (1%)	65	88
15	AO	76/77 (99%)	76 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	71/79 (90%)	70 (99%)	1 (1%)	62	86
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	48/61 (79%)	48 (100%)	0	100	100
24	BC	216/218 (99%)	216 (100%)	0	100	100
25	BD	163/163 (100%)	162 (99%)	1 (1%)	84	95
26	BE	165/165 (100%)	165 (100%)	0	100	100
27	BF	148/150 (99%)	147 (99%)	1 (1%)	81	94
28	BG	137/138 (99%)	136 (99%)	1 (1%)	81	94
29	BH	114/114 (100%)	114 (100%)	0	100	100
30	BI	59/62 (95%)	58 (98%)	1 (2%)	56	83
31	BJ	116/116 (100%)	116 (100%)	0	100	100
32	BK	104/104 (100%)	103 (99%)	1 (1%)	73	91
33	BL	103/103 (100%)	103 (100%)	0	100	100
34	BM	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	BN	98/103 (95%)	98 (100%)	0	100	100
36	BO	87/87 (100%)	86 (99%)	1 (1%)	70	90
37	BP	99/100 (99%)	99 (100%)	0	100	100
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	84 (100%)	0	100	100
40	BS	93/93 (100%)	93 (100%)	0	100	100
41	BT	80/84 (95%)	80 (100%)	0	100	100
42	BU	83/85 (98%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	78 (100%)	0	100	100
44	BW	57/63 (90%)	57 (100%)	0	100	100
45	BX	67/68 (98%)	67 (100%)	0	100	100
46	BY	54/55 (98%)	54 (100%)	0	100	100
47	BZ	48/49 (98%)	48 (100%)	0	100	100
48	B0	47/48 (98%)	46 (98%)	1 (2%)	48	78
49	B1	45/49 (92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	38 (100%)	0	100	100
51	B3	51/52 (98%)	51 (100%)	0	100	100
52	B4	34/34 (100%)	34 (100%)	0	100	100
53	B5	17/17 (100%)	16 (94%)	1 (6%)	16	45
All	All	4650/4844 (96%)	4633 (100%)	17 (0%)	88	97

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	63	ARG
2	AB	128	LYS
2	AB	193	PRO
3	AC	62	LYS
3	AC	79	LYS
7	AG	56	LYS
9	AI	106	ARG
14	AN	27	LYS
19	AS	29	LYS
25	BD	33	ARG
27	BF	14	LYS

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Mol	Chain	Res	Type
28	BG	153	ARG
30	BI	62	LYS
32	BK	94	PRO
36	BO	63	LYS
48	B0	40	ARG
53	B5	24	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
5	AE	122	ASN
5	AE	135	ASN
6	AF	3	HIS
8	AH	18	GLN
28	BG	38	ASN
36	BO	43	ASN
53	B5	14	ASN
53	B5	17	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	238 (15%)	7 (0%)
22	BA	2890/2897 (99%)	417 (14%)	23 (0%)
23	BB	119/120 (99%)	13 (10%)	1 (0%)
54	B7	6/7 (85%)	3 (50%)	1 (16%)
55	B8	76/77 (98%)	12 (15%)	2 (2%)
All	All	4621/4635 (99%)	683 (14%)	34 (0%)

All (683) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G
1	AA	44	A
1	AA	47	C

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Mol	Chain	Res	Type
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	76	G
1	AA	78	A
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	87	C
1	AA	88	U
1	AA	89	U
1	AA	98	A
1	AA	101	A
1	AA	116	A
1	AA	119	A
1	AA	120	A
1	AA	122	G
1	AA	130	A
1	AA	131	A
1	AA	141	G
1	AA	151	A
1	AA	163	C
1	AA	164	G
1	AA	166	U
1	AA	181	A
1	AA	182	A
1	AA	197	A
1	AA	205	A
1	AA	210	C
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	270	A
1	AA	289	G
1	AA	299	G

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Mol	Chain	Res	Type
1	AA	306	A
1	AA	321	A
1	AA	328	C
1	AA	352	C
1	AA	354	G
1	AA	356	A
1	AA	367	U
1	AA	372	C
1	AA	382	A
1	AA	384	G
1	AA	392	C
1	AA	393	A
1	AA	397	A
1	AA	406	G
1	AA	409	U
1	AA	412	A
1	AA	413	G
1	AA	429	U
1	AA	435	A
1	AA	437	U
1	AA	439	U
1	AA	440	C
1	AA	448	A
1	AA	456	A
1	AA	459	A
1	AA	465	A
1	AA	467	U
1	AA	468	A
1	AA	478	A
1	AA	479	U
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	488	C
1	AA	495	A
1	AA	496	A
1	AA	499	A
1	AA	509	A
1	AA	511	C
1	AA	513	C
1	AA	515	G
1	AA	516	PSU

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Mol	Chain	Res	Type
1	AA	518	C
1	AA	527	G7M
1	AA	529	G
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	560	A
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	579	A
1	AA	588	G
1	AA	596	A
1	AA	633	G
1	AA	653	U
1	AA	665	A
1	AA	702	A
1	AA	703	G
1	AA	718	A
1	AA	721	G
1	AA	722	G
1	AA	723	U
1	AA	724	G
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	760	G
1	AA	777	A
1	AA	781	A
1	AA	790	A
1	AA	792	A
1	AA	793	U
1	AA	794	A
1	AA	802	A
1	AA	815	A
1	AA	817	C
1	AA	819	A
1	AA	828	U
1	AA	836	G
1	AA	841	C

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Mol	Chain	Res	Type
1	AA	842	U
1	AA	843	U
1	AA	849	G
1	AA	872	A
1	AA	914	A
1	AA	926	G
1	AA	934	C
1	AA	935	A
1	AA	958	A
1	AA	959	A
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	974	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	992	U
1	AA	993	G
1	AA	1004	A
1	AA	1005	A
1	AA	1009	U
1	AA	1012	A
1	AA	1014	A
1	AA	1020	G
1	AA	1021	A
1	AA	1026	G
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U
1	AA	1036	A
1	AA	1044	A
1	AA	1045	C
1	AA	1046	A
1	AA	1065	U
1	AA	1067	A
1	AA	1092	A
1	AA	1093	A
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A

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Mol	Chain	Res	Type
1	AA	1108	G
1	AA	1132	C
1	AA	1133	G
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1157	A
1	AA	1159	U
1	AA	1169	A
1	AA	1172	C
1	AA	1173	U
1	AA	1184	G
1	AA	1191	A
1	AA	1196	A
1	AA	1197	A
1	AA	1201	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1229	A
1	AA	1238	A
1	AA	1256	A
1	AA	1258	G
1	AA	1260	G
1	AA	1280	A
1	AA	1285	A
1	AA	1289	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
1	AA	1320	C
1	AA	1332	A
1	AA	1340	A
1	AA	1346	A

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Mol	Chain	Res	Type
1	AA	1348	U
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1419	G
1	AA	1432	G
1	AA	1441	A
1	AA	1446	A
1	AA	1454	G
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1502	A
1	AA	1503	A
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
22	BA	10	A
22	BA	12	U
22	BA	14	A
22	BA	34	U
22	BA	35	G
22	BA	42	A
22	BA	51	G
22	BA	61	C
22	BA	71	A
22	BA	74	A
22	BA	75	G
22	BA	101	A
22	BA	103	A
22	BA	118	A
22	BA	119	A
22	BA	120	U
22	BA	125	A
22	BA	142	A
22	BA	143	C
22	BA	163	C
22	BA	165	A
22	BA	181	A

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Mol	Chain	Res	Type
22	BA	196	A
22	BA	197	A
22	BA	201	C
22	BA	204	A
22	BA	215	G
22	BA	216	A
22	BA	221	A
22	BA	222	A
22	BA	233	A
22	BA	248	G
22	BA	264	C
22	BA	265	A
22	BA	272	A
22	BA	276	U
22	BA	278	A
22	BA	302	C
22	BA	303	G
22	BA	311	A
22	BA	330	A
22	BA	383	C
22	BA	385	C
22	BA	386	G
22	BA	396	G
22	BA	402	A
22	BA	406	G
22	BA	411	G
22	BA	412	A
22	BA	477	A
22	BA	480	A
22	BA	481	G
22	BA	489	G
22	BA	491	G
22	BA	505	A
22	BA	509	C
22	BA	510	C
22	BA	532	A
22	BA	544	C
22	BA	546	U
22	BA	547	A
22	BA	548	G
22	BA	549	G
22	BA	550	C

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Mol	Chain	Res	Type
22	BA	563	A
22	BA	573	U
22	BA	575	A
22	BA	586	A
22	BA	588	U
22	BA	603	A
22	BA	614	A
22	BA	616	A
22	BA	637	A
22	BA	644	A
22	BA	645	C
22	BA	646	U
22	BA	647	G
22	BA	652	U
22	BA	653	U
22	BA	654	A
22	BA	655	A
22	BA	668	A
22	BA	676	A
22	BA	685	A
22	BA	686	U
22	BA	696	G
22	BA	730	A
22	BA	735	A
22	BA	738	G
22	BA	747	5MU
22	BA	764	A
22	BA	765	C
22	BA	775	G
22	BA	776	G
22	BA	782	A
22	BA	784	G
22	BA	785	G
22	BA	787	C
22	BA	789	A
22	BA	792	A
22	BA	794	A
22	BA	805	G
22	BA	806	C
22	BA	812	C
22	BA	827	U
22	BA	828	U

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Mol	Chain	Res	Type
22	BA	829	A
22	BA	846	U
22	BA	859	G
22	BA	869	G
22	BA	884	U
22	BA	896	A
22	BA	897	C
22	BA	905	A
22	BA	907	G
22	BA	910	A
22	BA	911	A
22	BA	914	G
22	BA	931	U
22	BA	932	U
22	BA	945	A
22	BA	946	C
22	BA	958	U
22	BA	961	C
22	BA	974	G
22	BA	983	A
22	BA	984	A
22	BA	985	C
22	BA	988	A
22	BA	996	A
22	BA	1009	A
22	BA	1012	U
22	BA	1013	C
22	BA	1022	G
22	BA	1026	G
22	BA	1033	U
22	BA	1040	A
22	BA	1046	A
22	BA	1047	G
22	BA	1054	A
22	BA	1069	A
22	BA	1070	A
22	BA	1071	G
22	BA	1083	U
22	BA	1084	A
22	BA	1085	A
22	BA	1088	A
22	BA	1102	C

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Mol	Chain	Res	Type
22	BA	1106	G
22	BA	1112	G
22	BA	1126	A
22	BA	1130	U
22	BA	1132	U
22	BA	1133	A
22	BA	1134	A
22	BA	1135	C
22	BA	1136	G
22	BA	1142	A
22	BA	1173	U
22	BA	1174	U
22	BA	1175	A
22	BA	1176	U
22	BA	1206	G
22	BA	1212	G
22	BA	1247	A
22	BA	1248	G
22	BA	1250	G
22	BA	1253	A
22	BA	1256	G
22	BA	1268	A
22	BA	1271	G
22	BA	1272	A
22	BA	1274	A
22	BA	1275	A
22	BA	1287	A
22	BA	1293	C
22	BA	1300	G
22	BA	1301	A
22	BA	1303	G
22	BA	1321	A
22	BA	1329	U
22	BA	1352	U
22	BA	1365	A
22	BA	1379	U
22	BA	1383	A
22	BA	1392	A
22	BA	1395	A
22	BA	1403	A
22	BA	1416	G
22	BA	1419	A

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Mol	Chain	Res	Type
22	BA	1428	C
22	BA	1434	A
22	BA	1452	G
22	BA	1453	A
22	BA	1458	U
22	BA	1460	U
22	BA	1478	G
22	BA	1482	G
22	BA	1493	C
22	BA	1494	A
22	BA	1508	A
22	BA	1509	A
22	BA	1515	A
22	BA	1566	A
22	BA	1569	A
22	BA	1576	U
22	BA	1578	U
22	BA	1585	C
22	BA	1606	C
22	BA	1608	A
22	BA	1609	A
22	BA	1610	A
22	BA	1626	A
22	BA	1630	A
22	BA	1647	U
22	BA	1648	U
22	BA	1649	G
22	BA	1674	G
22	BA	1675	C
22	BA	1677	A
22	BA	1698	A
22	BA	1730	C
22	BA	1739	A
22	BA	1757	A
22	BA	1758	U
22	BA	1764	C
22	BA	1773	A
22	BA	1782	U
22	BA	1786	A
22	BA	1787	A
22	BA	1800	C
22	BA	1801	A

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Mol	Chain	Res	Type
22	BA	1802	A
22	BA	1808	A
22	BA	1811	G
22	BA	1816	C
22	BA	1829	A
22	BA	1830	C
22	BA	1839	G
22	BA	1848	A
22	BA	1871	A
22	BA	1872	A
22	BA	1873	G
22	BA	1900	A
22	BA	1905	C
22	BA	1906	G
22	BA	1913	A
22	BA	1914	C
22	BA	1929	G
22	BA	1930	G
22	BA	1936	A
22	BA	1937	A
22	BA	1938	A
22	BA	1939	5MU
22	BA	1955	U
22	BA	1960	A
22	BA	1965	C
22	BA	1966	A
22	BA	1967	C
22	BA	1970	A
22	BA	1971	U
22	BA	1972	G
22	BA	1982	U
22	BA	1991	U
22	BA	1993	U
22	BA	2006	C
22	BA	2021	C
22	BA	2023	C
22	BA	2027	G
22	BA	2031	A
22	BA	2033	A
22	BA	2035	G
22	BA	2036	C
22	BA	2043	C

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Mol	Chain	Res	Type
22	BA	2054	A
22	BA	2055	C
22	BA	2056	G
22	BA	2060	A
22	BA	2061	G
22	BA	2062	A
22	BA	2069	G7M
22	BA	2077	A
22	BA	2080	A
22	BA	2093	G
22	BA	2101	A
22	BA	2110	G
22	BA	2111	U
22	BA	2112	G
22	BA	2113	U
22	BA	2115	G
22	BA	2116	G
22	BA	2117	A
22	BA	2118	U
22	BA	2119	A
22	BA	2121	G
22	BA	2123	G
22	BA	2124	G
22	BA	2125	G
22	BA	2126	A
22	BA	2128	G
22	BA	2131	U
22	BA	2132	U
22	BA	2133	G
22	BA	2134	A
22	BA	2145	C
22	BA	2146	C
22	BA	2147	A
22	BA	2158	A
22	BA	2159	G
22	BA	2161	C
22	BA	2162	G
22	BA	2163	A
22	BA	2164	C
22	BA	2165	C
22	BA	2169	A
22	BA	2170	A

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Mol	Chain	Res	Type
22	BA	2171	A
22	BA	2172	U
22	BA	2173	A
22	BA	2188	U
22	BA	2189	U
22	BA	2190	G
22	BA	2198	A
22	BA	2204	G
22	BA	2211	A
22	BA	2225	A
22	BA	2238	G
22	BA	2239	G
22	BA	2240	U
22	BA	2251	OMG
22	BA	2252	G
22	BA	2261	C
22	BA	2268	A
22	BA	2278	A
22	BA	2283	C
22	BA	2286	G
22	BA	2287	A
22	BA	2288	A
22	BA	2294	G
22	BA	2302	U
22	BA	2303	G
22	BA	2305	U
22	BA	2308	G
22	BA	2322	A
22	BA	2325	G
22	BA	2327	A
22	BA	2333	A
22	BA	2334	U
22	BA	2336	A
22	BA	2347	C
22	BA	2368	C
22	BA	2369	A
22	BA	2383	G
22	BA	2385	C
22	BA	2396	G
22	BA	2406	A
22	BA	2419	U
22	BA	2425	A

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Mol	Chain	Res	Type
22	BA	2426	A
22	BA	2427	C
22	BA	2429	G
22	BA	2435	A
22	BA	2440	C
22	BA	2441	U
22	BA	2445	2MG
22	BA	2448	A
22	BA	2469	A
22	BA	2476	A
22	BA	2491	U
22	BA	2498	OMC
22	BA	2502	G
22	BA	2504	PSU
22	BA	2505	G
22	BA	2507	C
22	BA	2518	A
22	BA	2529	G
22	BA	2535	G
22	BA	2547	A
22	BA	2556	C
22	BA	2566	A
22	BA	2567	G
22	BA	2573	C
22	BA	2582	G
22	BA	2602	A
22	BA	2609	U
22	BA	2613	U
22	BA	2615	U
22	BA	2629	U
22	BA	2630	G
22	BA	2661	G
22	BA	2689	U
22	BA	2690	U
22	BA	2705	A
22	BA	2713	U
22	BA	2714	G
22	BA	2716	C
22	BA	2726	A
22	BA	2727	A
22	BA	2733	A
22	BA	2744	G

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Mol	Chain	Res	Type
22	BA	2748	A
22	BA	2778	A
22	BA	2799	A
22	BA	2800	A
22	BA	2820	A
22	BA	2821	A
22	BA	2835	A
22	BA	2843	G
22	BA	2849	U
22	BA	2850	A
22	BA	2861	U
22	BA	2873	A
22	BA	2874	C
22	BA	2880	C
22	BA	2883	A
22	BA	2884	U
22	BA	2885	G
23	BB	13	G
23	BB	15	A
23	BB	24	G
23	BB	26	C
23	BB	35	C
23	BB	44	G
23	BB	45	A
23	BB	53	A
23	BB	56	G
23	BB	66	A
23	BB	89	U
23	BB	90	C
23	BB	109	A
54	B7	4	C
54	B7	6	G
54	B7	7	U
55	B8	3	G
55	B8	4	U
55	B8	5	G
55	B8	6	A
55	B8	14	A
55	B8	17	C
55	B8	19	G
55	B8	21	A
55	B8	47	U

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Mol	Chain	Res	Type
55	B8	59	A
55	B8	74	C
55	B8	76	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	119	A
1	AA	428	G
1	AA	958	A
1	AA	1092	A
1	AA	1225	A
1	AA	1299	A
1	AA	1493	A
22	BA	125	A
22	BA	196	A
22	BA	479	A
22	BA	764	A
22	BA	784	G
22	BA	984	A
22	BA	1142	A
22	BA	1253	A
22	BA	1286	A
22	BA	1427	A
22	BA	1608	A
22	BA	1609	A
22	BA	1738	G
22	BA	1757	A
22	BA	1847	A
22	BA	2146	C
22	BA	2162	G
22	BA	2188	U
22	BA	2251	OMG
22	BA	2311	A
22	BA	2468	A
22	BA	2518	A
22	BA	2873	A
23	BB	66	A
54	B7	5	C
55	B8	2	G
55	B8	3	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	PSU	BA	1917	22	18,21,22	4.07	7 (38%)	22,30,33	1.88	5 (22%)
1	PSU	AA	516	1,56	18,21,22	4.19	6 (33%)	22,30,33	1.95	6 (27%)
1	2MG	AA	1516	1	18,26,27	2.32	7 (38%)	16,38,41	1.48	4 (25%)
22	5MU	BA	1939	22	19,22,23	0.76	0	28,32,35	1.17	3 (10%)
1	G7M	AA	527	1	20,26,27	2.43	6 (30%)	17,39,42	1.09	1 (5%)
22	PSU	BA	2504	22	18,21,22	3.88	6 (33%)	22,30,33	1.72	4 (18%)
22	PSU	BA	2580	22	18,21,22	3.77	7 (38%)	22,30,33	2.14	6 (27%)
22	PSU	BA	746	22,56	18,21,22	1.47	3 (16%)	22,30,33	2.42	5 (22%)
22	2MA	BA	2503	22,56	19,25,26	3.11	6 (31%)	21,37,40	1.83	3 (14%)
1	2MG	AA	966	1	18,26,27	2.46	7 (38%)	16,38,41	1.46	3 (18%)
1	5MC	AA	967	1	18,22,23	3.43	7 (38%)	26,32,35	1.06	2 (7%)
22	5MC	BA	1962	22	18,22,23	3.07	7 (38%)	26,32,35	1.26	5 (19%)
22	1MG	BA	745	22	18,26,27	2.36	5 (27%)	19,39,42	1.44	2 (10%)
22	3TD	BA	1915	22	18,22,23	4.06	8 (44%)	22,32,35	1.97	4 (18%)
34	4D4	BM	81	34	9,11,12	2.44	3 (33%)	8,13,15	1.06	0
22	G7M	BA	2069	22	20,26,27	2.14	6 (30%)	17,39,42	1.25	2 (11%)
22	6MZ	BA	2030	22	18,25,26	2.95	5 (27%)	16,36,39	2.58	4 (25%)
1	4OC	AA	1402	1	20,23,24	2.90	8 (40%)	26,32,35	0.97	2 (7%)
22	OMC	BA	2498	22,56	19,22,23	2.64	7 (36%)	26,31,34	1.05	1 (3%)
22	PSU	BA	2457	22	18,21,22	3.66	7 (38%)	22,30,33	2.28	5 (22%)
22	OMG	BA	2251	22,55	18,26,27	2.30	8 (44%)	19,38,41	1.86	4 (21%)
22	5MU	BA	747	22	19,22,23	0.82	1 (5%)	28,32,35	1.26	3 (10%)
22	OMU	BA	2552	22	19,22,23	2.64	7 (36%)	26,31,34	1.92	5 (19%)
22	2MG	BA	1835	22	18,26,27	2.19	7 (38%)	16,38,41	1.70	4 (25%)
1	5MC	AA	1407	1	18,22,23	3.26	7 (38%)	26,32,35	1.00	1 (3%)
22	PSU	BA	955	22	18,21,22	3.80	6 (33%)	22,30,33	2.17	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	AA	1518	1	18,26,27	1.34	2 (11%)	19,38,41	3.38	2 (10%)
22	PSU	BA	2605	22	18,21,22	3.73	7 (38%)	22,30,33	1.88	4 (18%)
25	MEQ	BD	150	25	8,9,10	1.37	2 (25%)	5,10,12	1.46	1 (20%)
1	2MG	AA	1207	1	18,26,27	2.45	7 (38%)	16,38,41	1.42	4 (25%)
22	PSU	BA	2604	22	18,21,22	3.82	6 (33%)	22,30,33	2.05	5 (22%)
1	UR3	AA	1498	1	19,22,23	3.03	8 (42%)	26,32,35	1.40	3 (11%)
22	PSU	BA	1911	22	18,21,22	4.12	6 (33%)	22,30,33	2.00	5 (22%)
1	MA6	AA	1519	1	18,26,27	1.32	1 (5%)	19,38,41	3.57	2 (10%)
12	D2T	AL	89	12	7,9,10	1.07	0	6,11,13	2.56	2 (33%)
22	6MZ	BA	1618	22	18,25,26	2.93	5 (27%)	16,36,39	2.21	4 (25%)
22	2MG	BA	2445	22	18,26,27	2.28	6 (33%)	16,38,41	1.80	4 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	BA	1917	22	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
22	5MU	BA	1939	22	-	2/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
22	PSU	BA	2504	22	-	2/7/25/26	0/2/2/2
22	PSU	BA	2580	22	-	1/7/25/26	0/2/2/2
22	PSU	BA	746	22,56	-	2/7/25/26	0/2/2/2
22	2MA	BA	2503	22,56	-	1/3/25/26	0/3/3/3
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
22	5MC	BA	1962	22	-	0/7/25/26	0/2/2/2
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
22	3TD	BA	1915	22	-	2/7/25/26	0/2/2/2
34	4D4	BM	81	34	-	2/11/12/14	-
22	G7M	BA	2069	22	-	1/3/25/26	0/3/3/3
22	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	1/9/29/30	0/2/2/2
22	OMC	BA	2498	22,56	-	2/9/27/28	0/2/2/2
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMG	BA	2251	22,55	-	3/5/27/28	0/3/3/3
22	5MU	BA	747	22	-	0/7/25/26	0/2/2/2
22	OMU	BA	2552	22	-	0/9/27/28	0/2/2/2
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
25	MEQ	BD	150	25	-	2/8/9/11	-
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
22	PSU	BA	1911	22	-	2/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
22	6MZ	BA	1618	22	-	0/5/27/28	0/3/3/3
22	2MG	BA	2445	22	-	2/5/27/28	0/3/3/3

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C6-C5	11.67	1.48	1.35
1	AA	516	PSU	C6-C5	11.19	1.48	1.35
22	BA	1911	PSU	C6-C5	10.95	1.48	1.35
22	BA	1618	6MZ	C6-N6	10.93	1.52	1.35
22	BA	2030	6MZ	C6-N6	10.86	1.52	1.35
22	BA	1917	PSU	C6-C5	10.81	1.47	1.35
22	BA	2604	PSU	C6-C5	10.42	1.47	1.35
22	BA	955	PSU	C6-C5	10.17	1.47	1.35
22	BA	2580	PSU	C6-C5	10.15	1.47	1.35
22	BA	2504	PSU	C6-C5	10.13	1.47	1.35
22	BA	2605	PSU	C6-C5	9.83	1.46	1.35
22	BA	2457	PSU	C6-C5	9.77	1.46	1.35
22	BA	1911	PSU	C2-N1	9.45	1.49	1.36
1	AA	516	PSU	C2-N1	9.32	1.49	1.36
22	BA	1917	PSU	C2-N1	9.17	1.49	1.36
22	BA	2504	PSU	C2-N1	8.97	1.48	1.36
1	AA	967	5MC	C6-C5	8.80	1.49	1.34
22	BA	955	PSU	C2-N1	8.75	1.48	1.36
1	AA	1407	5MC	C6-C5	8.70	1.48	1.34
22	BA	2605	PSU	C2-N1	8.60	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1498	UR3	C2-N1	8.55	1.50	1.38
22	BA	1915	3TD	C2-N1	8.36	1.48	1.37
22	BA	2604	PSU	C2-N1	8.25	1.47	1.36
22	BA	2457	PSU	C2-N1	8.22	1.47	1.36
22	BA	2580	PSU	C2-N1	8.08	1.47	1.36
22	BA	2503	2MA	C4-N3	7.63	1.47	1.35
22	BA	1962	5MC	C6-C5	7.48	1.46	1.34
1	AA	516	PSU	C2-N3	7.04	1.49	1.37
22	BA	1911	PSU	C2-N3	6.69	1.49	1.37
22	BA	1917	PSU	C2-N3	6.69	1.49	1.37
22	BA	2503	2MA	C2-N3	6.61	1.45	1.34
22	BA	2504	PSU	C2-N3	6.44	1.48	1.37
22	BA	2604	PSU	C2-N3	6.38	1.48	1.37
22	BA	2580	PSU	C2-N3	6.24	1.48	1.37
1	AA	967	5MC	C4-N3	6.22	1.44	1.34
1	AA	1402	4OC	C4-N3	6.14	1.43	1.32
1	AA	1402	4OC	C6-C5	6.04	1.49	1.35
22	BA	2457	PSU	C2-N3	6.01	1.47	1.37
22	BA	955	PSU	C2-N3	5.89	1.47	1.37
1	AA	967	5MC	C2-N3	5.86	1.48	1.36
22	BA	2605	PSU	C2-N3	5.82	1.47	1.37
22	BA	745	1MG	C2-N3	5.77	1.45	1.34
22	BA	2503	2MA	C2-N1	5.74	1.44	1.34
22	BA	1962	5MC	C4-N3	5.74	1.43	1.34
22	BA	2552	OMU	C2-N3	5.70	1.48	1.38
1	AA	1498	UR3	C6-C5	5.70	1.48	1.35
1	AA	1402	4OC	C2-N3	5.69	1.47	1.36
22	BA	2552	OMU	C2-N1	5.68	1.47	1.38
1	AA	527	G7M	C2-N3	5.64	1.46	1.33
34	BM	81	4D4	CZ-NE	5.56	1.44	1.33
1	AA	1407	5MC	C4-N3	5.50	1.43	1.34
1	AA	1407	5MC	C2-N3	5.40	1.47	1.36
22	BA	1962	5MC	C2-N3	5.40	1.47	1.36
22	BA	2498	OMC	C2-N3	5.30	1.47	1.36
22	BA	2498	OMC	C6-C5	5.28	1.47	1.35
1	AA	966	2MG	C2-N2	5.28	1.45	1.33
1	AA	1207	2MG	C2-N2	5.21	1.45	1.33
22	BA	2552	OMU	C6-C5	5.09	1.46	1.35
22	BA	1915	3TD	C1'-C5	-5.02	1.38	1.50
22	BA	1915	3TD	C6-N1	4.99	1.44	1.36
1	AA	527	G7M	C4-N3	4.95	1.49	1.37
22	BA	2503	2MA	C6-N1	4.86	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1516	2MG	C2-N2	4.86	1.44	1.33
1	AA	1207	2MG	C2-N1	4.84	1.44	1.36
1	AA	966	2MG	C4-N3	4.83	1.49	1.37
1	AA	516	PSU	C6-N1	4.81	1.44	1.36
22	BA	1917	PSU	C6-N1	4.79	1.44	1.36
1	AA	966	2MG	C2-N1	4.74	1.44	1.36
22	BA	1911	PSU	C6-N1	4.72	1.44	1.36
1	AA	1207	2MG	C4-N3	4.62	1.48	1.37
1	AA	1498	UR3	C2-N3	4.61	1.47	1.39
1	AA	527	G7M	C6-N1	4.55	1.44	1.37
22	BA	2069	G7M	C2-N3	4.48	1.44	1.33
1	AA	1516	2MG	C4-N3	4.47	1.48	1.37
22	BA	745	1MG	C4-N3	4.46	1.48	1.37
22	BA	2251	OMG	C2-N3	4.44	1.44	1.33
22	BA	2251	OMG	C4-N3	4.43	1.48	1.37
22	BA	2069	G7M	C4-N3	4.38	1.48	1.37
22	BA	2504	PSU	C6-N1	4.38	1.43	1.36
22	BA	2445	2MG	C2-N2	4.38	1.43	1.33
22	BA	2498	OMC	C4-N3	4.37	1.43	1.34
22	BA	1835	2MG	C2-N2	4.33	1.43	1.33
22	BA	2498	OMC	C4-N4	4.28	1.44	1.33
1	AA	1498	UR3	O4-C4	-4.27	1.14	1.23
1	AA	967	5MC	C4-N4	4.26	1.45	1.34
1	AA	1402	4OC	C4-N4	4.26	1.44	1.35
22	BA	1915	3TD	C2-N3	4.20	1.47	1.38
22	BA	2605	PSU	C6-N1	4.19	1.43	1.36
22	BA	745	1MG	C2-N2	4.19	1.41	1.34
22	BA	955	PSU	C6-N1	4.17	1.43	1.36
1	AA	1407	5MC	C4-N4	4.15	1.44	1.34
22	BA	1835	2MG	C4-N3	4.13	1.47	1.37
22	BA	2604	PSU	C6-N1	4.13	1.43	1.36
22	BA	2445	2MG	C4-N3	4.12	1.47	1.37
1	AA	1516	2MG	C2-N1	4.12	1.43	1.36
22	BA	2251	OMG	C2-N2	4.09	1.43	1.34
1	AA	967	5MC	C6-N1	4.08	1.45	1.38
1	AA	527	G7M	C2-N2	4.04	1.43	1.34
22	BA	1962	5MC	C4-N4	4.03	1.44	1.34
22	BA	2445	2MG	C2-N1	3.99	1.43	1.36
22	BA	2069	G7M	C6-N1	3.93	1.43	1.37
1	AA	516	PSU	C4-N3	3.91	1.46	1.38
22	BA	2445	2MG	C5-C4	-3.89	1.33	1.43
1	AA	967	5MC	C2-N1	3.87	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2580	PSU	C6-N1	3.85	1.42	1.36
22	BA	2498	OMC	C2-N1	3.85	1.48	1.40
22	BA	1835	2MG	C2-N1	3.83	1.42	1.36
1	AA	1407	5MC	C6-N1	3.76	1.44	1.38
22	BA	2457	PSU	C6-N1	3.74	1.42	1.36
1	AA	1207	2MG	C6-N1	3.66	1.43	1.37
22	BA	2069	G7M	C2-N2	3.66	1.42	1.34
22	BA	1962	5MC	C2-N1	3.60	1.47	1.40
1	AA	1402	4OC	C5-C4	3.57	1.48	1.40
22	BA	1911	PSU	C4-N3	3.54	1.45	1.38
22	BA	1835	2MG	C5-C4	-3.52	1.34	1.43
22	BA	745	1MG	C5-C4	-3.52	1.34	1.43
22	BA	1917	PSU	C4-N3	3.50	1.45	1.38
22	BA	2498	OMC	O2-C2	-3.48	1.17	1.23
1	AA	1407	5MC	C2-N1	3.39	1.47	1.40
1	AA	1402	4OC	C2-N1	3.37	1.47	1.40
1	AA	966	2MG	C6-N1	3.37	1.42	1.37
1	AA	1519	MA6	C5-C4	-3.26	1.32	1.40
22	BA	2445	2MG	O6-C6	-3.25	1.16	1.23
22	BA	2251	OMG	C5-C4	-3.25	1.34	1.43
22	BA	2552	OMU	O2-C2	-3.24	1.17	1.23
22	BA	2552	OMU	O4-C4	-3.23	1.18	1.24
1	AA	527	G7M	C5-C6	3.22	1.53	1.45
1	AA	1407	5MC	O2-C2	-3.21	1.17	1.23
22	BA	2504	PSU	C4-N3	3.21	1.44	1.38
22	BA	1962	5MC	C6-N1	3.19	1.43	1.38
22	BA	1962	5MC	O2-C2	-3.18	1.17	1.23
22	BA	2552	OMU	C4-N3	3.15	1.44	1.38
1	AA	1518	MA6	C5-C4	-3.14	1.32	1.40
1	AA	1516	2MG	C5-C4	-3.12	1.35	1.43
22	BA	2030	6MZ	C5-C4	-3.12	1.32	1.40
34	BM	81	4D4	CZ-NH2	3.10	1.44	1.32
22	BA	2604	PSU	C4-N3	3.07	1.44	1.38
22	BA	746	PSU	C4-N3	-3.06	1.33	1.38
1	AA	1516	2MG	C6-N1	3.03	1.42	1.37
1	AA	1402	4OC	O2-C2	-3.02	1.18	1.23
22	BA	1835	2MG	O6-C6	-3.00	1.17	1.23
22	BA	1618	6MZ	C2-N3	2.98	1.36	1.32
22	BA	2580	PSU	C4-N3	2.97	1.44	1.38
22	BA	2580	PSU	O4'-C1'	-2.93	1.39	1.43
22	BA	2457	PSU	O4-C4	-2.91	1.18	1.23
1	AA	1516	2MG	C5-C6	2.88	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	967	5MC	O2-C2	-2.87	1.18	1.23
1	AA	1402	4OC	C6-N1	2.87	1.44	1.38
1	AA	1207	2MG	C5-C6	2.85	1.53	1.47
22	BA	1618	6MZ	C5-C4	-2.83	1.33	1.40
1	AA	966	2MG	C5-C4	-2.82	1.35	1.43
1	AA	1498	UR3	C5-C4	2.79	1.51	1.43
22	BA	2605	PSU	O4-C4	-2.79	1.18	1.23
1	AA	966	2MG	C5-C6	2.78	1.53	1.47
22	BA	1835	2MG	C6-N1	2.77	1.42	1.37
1	AA	1207	2MG	C5-C4	-2.75	1.36	1.43
1	AA	1498	UR3	O2-C2	-2.72	1.17	1.22
22	BA	745	1MG	O6-C6	-2.72	1.17	1.22
22	BA	955	PSU	C4-N3	2.71	1.43	1.38
22	BA	2251	OMG	O6-C6	-2.70	1.17	1.23
22	BA	2251	OMG	C6-N1	2.70	1.41	1.37
22	BA	1915	3TD	O2-C2	-2.68	1.18	1.23
22	BA	2604	PSU	O4-C4	-2.68	1.18	1.23
22	BA	2605	PSU	C4-N3	2.64	1.43	1.38
1	AA	527	G7M	C2-N1	2.62	1.44	1.37
22	BA	746	PSU	C6-C5	2.62	1.38	1.35
22	BA	2503	2MA	C6-C5	2.60	1.52	1.43
22	BA	955	PSU	O4-C4	-2.58	1.18	1.23
22	BA	2251	OMG	C5-C6	2.58	1.52	1.47
1	AA	1516	2MG	O6-C6	-2.51	1.18	1.23
22	BA	2580	PSU	O4-C4	-2.47	1.18	1.23
22	BA	2030	6MZ	C4-N3	-2.47	1.32	1.35
22	BA	2457	PSU	C4-N3	2.46	1.43	1.38
22	BA	2503	2MA	C6-N6	-2.45	1.24	1.34
22	BA	2445	2MG	C6-N1	2.45	1.41	1.37
22	BA	2069	G7M	C5-C6	2.43	1.51	1.45
22	BA	1917	PSU	O4-C4	-2.43	1.19	1.23
22	BA	1911	PSU	O4-C4	-2.42	1.19	1.23
25	BD	150	MEQ	OE1-CD	-2.42	1.18	1.23
1	AA	966	2MG	O6-C6	-2.42	1.18	1.23
1	AA	1498	UR3	C6-N1	2.38	1.43	1.38
22	BA	2069	G7M	C2-N1	2.38	1.43	1.37
22	BA	1618	6MZ	C9-N6	2.38	1.49	1.45
34	BM	81	4D4	CZ-NH1	-2.35	1.25	1.34
22	BA	2030	6MZ	C2-N3	2.34	1.35	1.32
1	AA	516	PSU	O4'-C1'	-2.32	1.40	1.43
22	BA	2030	6MZ	C9-N6	2.31	1.49	1.45
22	BA	2498	OMC	C6-N1	2.31	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2504	PSU	O4-C4	-2.31	1.19	1.23
25	BD	150	MEQ	CD-NE2	2.29	1.45	1.34
1	AA	1498	UR3	C3U-N3	-2.20	1.43	1.47
1	AA	1207	2MG	O6-C6	-2.19	1.18	1.23
22	BA	1618	6MZ	C4-N3	-2.18	1.32	1.35
22	BA	1917	PSU	C1'-C5	2.18	1.55	1.50
22	BA	2251	OMG	C2-N1	2.16	1.43	1.37
22	BA	1915	3TD	C4-N3	2.12	1.45	1.40
22	BA	1835	2MG	C5-C6	2.12	1.51	1.47
22	BA	746	PSU	C2-N1	-2.08	1.33	1.36
22	BA	2457	PSU	O4'-C1'	-2.08	1.41	1.43
22	BA	1915	3TD	O4-C4	-2.05	1.18	1.23
22	BA	747	5MU	C5M-C5	-2.05	1.45	1.50
22	BA	2552	OMU	C6-N1	2.02	1.42	1.38
1	AA	1518	MA6	C10-N6	-2.01	1.41	1.45
22	BA	2605	PSU	C1'-C5	2.01	1.54	1.50

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N1-C6-N6	-13.95	102.37	117.06
1	AA	1518	MA6	N1-C6-N6	-13.36	103.00	117.06
22	BA	746	PSU	N1-C2-N3	7.79	123.96	115.13
22	BA	2503	2MA	C2-N3-C4	6.69	120.95	115.52
22	BA	1915	3TD	N1-C2-N3	6.40	121.19	116.14
1	AA	1519	MA6	N3-C2-N1	-6.28	118.86	128.68
22	BA	2552	OMU	C4-N3-C2	-6.05	118.60	126.58
1	AA	1518	MA6	N3-C2-N1	-5.75	119.69	128.68
22	BA	2457	PSU	C4-N3-C2	-5.64	118.21	126.34
22	BA	2457	PSU	N1-C2-N3	5.63	121.51	115.13
22	BA	2030	6MZ	N3-C2-N1	-5.62	119.89	128.68
22	BA	1618	6MZ	N3-C2-N1	-5.53	120.04	128.68
22	BA	2030	6MZ	C9-N6-C6	-5.45	118.17	122.87
22	BA	1618	6MZ	C9-N6-C6	-5.20	118.39	122.87
22	BA	955	PSU	N1-C2-N3	5.16	120.98	115.13
22	BA	2580	PSU	N1-C2-N3	5.15	120.96	115.13
22	BA	955	PSU	C4-N3-C2	-5.07	119.03	126.34
22	BA	1911	PSU	C4-N3-C2	-4.97	119.19	126.34
22	BA	2605	PSU	C4-N3-C2	-4.94	119.22	126.34
22	BA	746	PSU	O2-C2-N1	-4.89	117.41	122.79
22	BA	1917	PSU	C4-N3-C2	-4.88	119.30	126.34
1	AA	1498	UR3	C4-N3-C2	-4.84	120.01	124.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2604	PSU	N1-C2-N3	4.74	120.51	115.13
22	BA	2552	OMU	N3-C2-N1	4.72	121.16	114.89
22	BA	2580	PSU	C4-N3-C2	-4.70	119.57	126.34
22	BA	746	PSU	C4-N3-C2	-4.66	119.63	126.34
22	BA	2604	PSU	C4-N3-C2	-4.60	119.72	126.34
22	BA	2504	PSU	C4-N3-C2	-4.60	119.72	126.34
22	BA	2030	6MZ	C2-N1-C6	4.59	120.52	116.59
22	BA	1911	PSU	N1-C2-N3	4.50	120.23	115.13
22	BA	2030	6MZ	C1'-N9-C4	-4.39	118.93	126.64
1	AA	516	PSU	C4-N3-C2	-4.37	120.05	126.34
12	AL	89	D2T	CB1-SB-CB	4.34	110.29	102.44
1	AA	516	PSU	N1-C2-N3	4.31	120.01	115.13
22	BA	2605	PSU	N1-C2-N3	4.28	119.98	115.13
22	BA	1915	3TD	C4-N3-C2	-4.28	119.97	124.61
22	BA	1917	PSU	N1-C2-N3	4.22	119.92	115.13
22	BA	745	1MG	C5-C6-N1	4.17	120.17	113.90
22	BA	2445	2MG	CM2-N2-C2	-4.13	114.73	123.86
22	BA	2580	PSU	C6-N1-C2	-4.12	118.47	122.68
22	BA	2445	2MG	C5-C6-N1	4.00	121.01	113.95
22	BA	1835	2MG	C5-C6-N1	3.98	120.98	113.95
22	BA	2251	OMG	O3'-C3'-C2'	3.90	122.25	111.17
22	BA	955	PSU	C6-N1-C2	-3.85	118.74	122.68
22	BA	1835	2MG	CM2-N2-C2	-3.85	115.36	123.86
22	BA	2504	PSU	N1-C2-N3	3.79	119.43	115.13
22	BA	2251	OMG	C5-C6-N1	3.63	120.35	113.95
22	BA	2457	PSU	C6-N1-C2	-3.62	118.98	122.68
22	BA	2604	PSU	C6-N1-C2	-3.60	119.00	122.68
1	AA	966	2MG	C5-C6-N1	3.58	120.27	113.95
1	AA	516	PSU	C6-C5-C4	3.57	120.70	118.20
1	AA	1516	2MG	C5-C6-N1	3.53	120.19	113.95
22	BA	955	PSU	C6-C5-C4	3.53	120.66	118.20
12	AL	89	D2T	OD2-CG-CB	3.50	120.71	113.15
22	BA	2580	PSU	C6-C5-C4	3.49	120.64	118.20
22	BA	2552	OMU	C5-C4-N3	3.44	119.99	114.84
22	BA	2457	PSU	C6-C5-C4	3.40	120.58	118.20
22	BA	2503	2MA	N3-C2-N1	-3.37	119.58	125.73
1	AA	516	PSU	C6-N1-C2	-3.35	119.25	122.68
22	BA	747	5MU	C4-N3-C2	-3.35	123.01	127.35
1	AA	1207	2MG	C5-C6-N1	3.32	119.82	113.95
22	BA	2604	PSU	O2-C2-N1	-3.31	119.15	122.79
22	BA	1618	6MZ	C2-N1-C6	3.30	119.42	116.59
22	BA	2251	OMG	C2-N1-C6	-3.20	119.21	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1911	PSU	C6-C5-C4	3.19	120.43	118.20
1	AA	1407	5MC	C5-C6-N1	-3.14	120.10	123.34
1	AA	967	5MC	C5-C6-N1	-3.11	120.14	123.34
22	BA	747	5MU	C6-C5-C4	3.06	120.59	118.03
22	BA	1911	PSU	C6-N1-C2	-3.04	119.57	122.68
22	BA	2604	PSU	C6-C5-C4	3.04	120.32	118.20
22	BA	2605	PSU	C6-N1-C2	-2.96	119.66	122.68
22	BA	1915	3TD	C6-C5-C4	2.92	120.24	118.22
22	BA	2445	2MG	O6-C6-C5	-2.90	118.71	124.37
22	BA	2457	PSU	O2-C2-N1	-2.90	119.60	122.79
1	AA	527	G7M	C2-N1-C6	-2.90	119.76	125.10
22	BA	745	1MG	C8-N7-C5	2.87	108.46	102.99
22	BA	1917	PSU	C6-N1-C2	-2.87	119.75	122.68
22	BA	1939	5MU	C4-N3-C2	-2.84	123.67	127.35
22	BA	1962	5MC	C5-C6-N1	-2.80	120.46	123.34
22	BA	1939	5MU	C6-C5-C4	2.76	120.34	118.03
22	BA	2251	OMG	C8-N7-C5	2.76	108.24	102.99
1	AA	1498	UR3	C6-N1-C2	-2.65	119.42	121.79
22	BA	2504	PSU	C6-N1-C2	-2.64	119.98	122.68
22	BA	2445	2MG	C8-N7-C5	2.58	107.91	102.99
22	BA	1835	2MG	O6-C6-C5	-2.58	119.33	124.37
1	AA	1516	2MG	C8-N7-C5	2.58	107.91	102.99
22	BA	1911	PSU	O2-C2-N1	-2.57	119.96	122.79
22	BA	746	PSU	C5-C6-N1	-2.57	118.25	122.11
1	AA	966	2MG	C8-N7-C5	2.56	107.87	102.99
22	BA	2498	OMC	O2-C2-N3	-2.53	118.22	122.33
22	BA	1962	5MC	CM5-C5-C6	-2.53	119.47	122.85
22	BA	1917	PSU	C6-C5-C4	2.50	119.95	118.20
22	BA	2552	OMU	O4-C4-C5	-2.50	120.76	125.16
1	AA	1207	2MG	C8-N7-C5	2.50	107.75	102.99
22	BA	2069	G7M	N2-C2-N1	2.49	122.02	116.71
22	BA	1917	PSU	O2-C2-N1	-2.49	120.05	122.79
1	AA	1498	UR3	C1'-N1-C2	2.47	121.16	116.99
1	AA	1207	2MG	CM2-N2-C2	-2.47	118.41	123.86
22	BA	2069	G7M	C2-N1-C6	-2.45	120.59	125.10
1	AA	516	PSU	O2-C2-N1	-2.45	120.10	122.79
1	AA	1516	2MG	CM2-N2-C2	-2.43	118.50	123.86
22	BA	2580	PSU	O2-C2-N1	-2.41	120.14	122.79
1	AA	1402	4OC	C6-C5-C4	2.40	119.89	116.96
22	BA	1962	5MC	C1'-N1-C6	-2.36	117.20	121.12
1	AA	966	2MG	O6-C6-C5	-2.35	119.78	124.37
22	BA	2503	2MA	CM2-C2-N1	2.35	120.81	117.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1835	2MG	C8-N7-C5	2.32	107.40	102.99
22	BA	2580	PSU	O4'-C1'-C2'	2.30	108.39	105.14
1	AA	1207	2MG	O6-C6-C5	-2.30	119.88	124.37
22	BA	747	5MU	C5-C4-N3	2.28	117.26	115.31
22	BA	2605	PSU	C6-C5-C4	2.26	119.78	118.20
22	BA	1962	5MC	O2-C2-N3	-2.25	118.67	122.33
22	BA	1618	6MZ	C1'-N9-C4	-2.24	122.70	126.64
1	AA	516	PSU	O4'-C1'-C2'	2.24	108.30	105.14
22	BA	1962	5MC	C1'-N1-C2	2.24	123.41	118.42
22	BA	2552	OMU	O2-C2-N1	-2.23	119.82	122.79
22	BA	2504	PSU	C6-C5-C4	2.20	119.73	118.20
22	BA	955	PSU	O2-C2-N1	-2.15	120.43	122.79
22	BA	746	PSU	C6-C5-C4	2.11	119.67	118.20
22	BA	1939	5MU	C5-C6-N1	-2.10	121.18	123.34
1	AA	1402	4OC	CM4-N4-C4	-2.09	118.38	122.45
1	AA	967	5MC	CM5-C5-C6	-2.08	120.07	122.85
1	AA	1516	2MG	O6-C6-C5	-2.07	120.33	124.37
25	BD	150	MEQ	CG-CD-NE2	2.06	119.15	116.29
22	BA	1915	3TD	O4'-C1'-C2'	2.02	107.99	105.14

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	AA	966	2MG	O4'-C4'-C5'-O5'
34	BM	81	4D4	NE-CD-CG-CB
22	BA	746	PSU	C2'-C1'-C5-C4
22	BA	1915	3TD	C3'-C4'-C5'-O5'
22	BA	1915	3TD	O4'-C4'-C5'-O5'
22	BA	2030	6MZ	O4'-C4'-C5'-O5'
22	BA	2251	OMG	C1'-C2'-O2'-CM2
22	BA	2504	PSU	O4'-C4'-C5'-O5'
1	AA	527	G7M	O4'-C4'-C5'-O5'
22	BA	2504	PSU	C3'-C4'-C5'-O5'
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
22	BA	2030	6MZ	C3'-C4'-C5'-O5'
22	BA	2251	OMG	C3'-C4'-C5'-O5'
22	BA	2445	2MG	C3'-C4'-C5'-O5'
22	BA	1911	PSU	O4'-C4'-C5'-O5'
25	BD	150	MEQ	NE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
25	BD	150	MEQ	OE1-CD-CG-CB
1	AA	1519	MA6	C3'-C4'-C5'-O5'
22	BA	2251	OMG	O4'-C4'-C5'-O5'
22	BA	2445	2MG	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
1	AA	1402	4OC	O4'-C4'-C5'-O5'
22	BA	1939	5MU	O4'-C4'-C5'-O5'
22	BA	1911	PSU	C3'-C4'-C5'-O5'
34	BM	81	4D4	CG-CD-NE-CZ
22	BA	2580	PSU	O4'-C4'-C5'-O5'
22	BA	1939	5MU	C3'-C4'-C5'-O5'
22	BA	2498	OMC	O4'-C4'-C5'-O5'
22	BA	746	PSU	O4'-C1'-C5-C6
22	BA	2069	G7M	O4'-C4'-C5'-O5'
22	BA	2498	OMC	C2'-C1'-N1-C2
22	BA	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1516	2MG	1	0
1	AA	527	G7M	1	0
22	BA	746	PSU	1	0
22	BA	2030	6MZ	3	0
1	AA	1402	4OC	1	0
22	BA	2498	OMC	1	0
22	BA	2251	OMG	1	0
22	BA	955	PSU	1	0
1	AA	1518	MA6	1	0
25	BD	150	MEQ	1	0
1	AA	1519	MA6	1	0
12	AL	89	D2T	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 173 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	TRP	BA	3001	-	14,16,16	0.86	1 (7%)	16,22,22	1.13	2 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	TRP	BA	3001	-	-	0/7/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	3001	TRP	OXT-C	-2.20	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	TRP	OXT-C-O	-2.59	118.21	124.09
58	BA	3001	TRP	OXT-C-CA	2.15	120.71	113.38

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.83
1	BA	2099:U	O3'	2100:G	P	3.52