Full wwPDB EM Validation Report (i)

Mar 19, 2022 – 08:28 am GMT

PDB ID	:	7QGU
EMDB ID	:	EMD-13959
Title	:	Structure of the B. subtilis disome - stalled 70S ribosome
Authors	:	Kratzat, H.; Buschauer, R.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2021-12-10
Resolution	:	4.75 Å(reported)

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

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

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

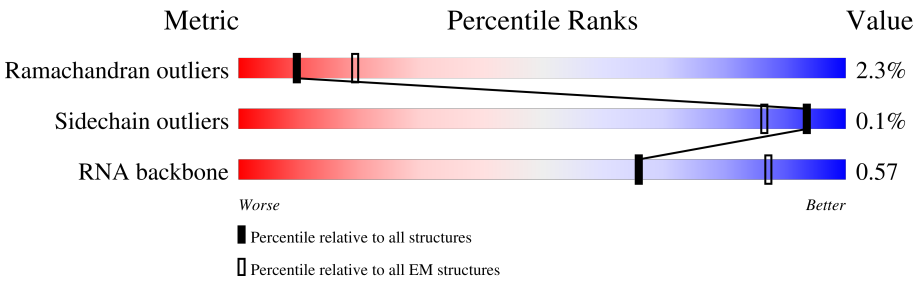
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.75 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	2928	55% 32% 12% •
2	B	119	53% 32% 8% • 6%
3	C	277	40% 99% •
4	D	208	6% 97% •
5	E	207	16% 97% • •
6	F	179	14% 97% • •
7	G	179	• 97% • •
8	H	166	11% 68% 6% 26%

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Mol	Chain	Length	Quality of chain
9	I	141	60% 93% 6%
10	J	145	7% 97%
11	K	122	29% 98%
12	L	146	17% 99%
13	M	144	17% 96%
14	N	120	98%
15	O	120	95% 5%
16	P	115	10% 99%
17	Q	119	98%
18	R	102	7% 97%
19	S	113	15% 91% 5%
20	T	95	6% 98%
21	U	103	6% 94%
22	V	94	12% 87% 13%
23	X	149	78% 83% 16%
24	Y	62	48% 90% 6%
25	Z	66	9% 98%
26	a	59	7% 97%
27	b	59	12% 90% 8%
28	c	49	27% 98%
29	d	44	23% 100%
30	e	66	20% 95%
31	f	37	97%
32	W	1555	65% 26% 8%
33	g	246	13% 89% 9%

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Mol	Chain	Length	Quality of chain
34	h	218	6% 96%
35	i	200	98%
36	j	166	6% 97%
37	k	95	32% 98%
38	l	156	8% 97%
39	m	132	98%
40	n	130	5% 96%
41	o	102	5% 96%
42	p	131	30% 89% 10%
43	q	138	14% 94% 5%
44	r	121	7% 90% 8%
45	s	61	8% 93% 5%
46	t	89	97%
47	u	90	97%
48	v	87	11% 99%
49	w	79	32% 86% 10%
50	x	92	89% 9%
51	y	88	5% 97%
52	z	77	5% 71% 22% 5%
53	2	95	25% 20% 5% 75%
54	3	66	9% 65% 32%

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 135606 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2923	62767	28002	11589	20253	2923	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1558	C	G	conflict	GB 1864548803

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	112	2395	1068	435	780	112	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	275	2111	1312	416	377	6	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	207	1575	988	290	292	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	205	1561	980	289	290	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	178	1404	893	245	259	7	0	0

- Molecule 7 is a protein called Ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	175	1342	835	248	257	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	123	955	602	163	189	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	154	THR	ALA	variant	UNP A0A063X7V1

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	133	981	617	173	185	6	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	142	1123	710	206	202	5	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	122	920	571	173	172	4	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	146	1081	671	207	201	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	138	1097	703	208	181	5	0	0

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	119	953	583	186	180	4	0	0

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	120	912	564	176	171	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	P	114	936	595	184	157	0	0

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	117	940	591	189	156	4	0	0

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	R	101	786	501	139	146	0	0

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	109	842	525	164	150	3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	93	752	472	137	139	4	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	100	754	473	141	137	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	V	82	630	390	123	117	0	0

- Molecule 23 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	X	149	733	435	149	149	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	58	444	275	92	75	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	65	530	328	102	98	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	58	455	281	89	84	1	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	54	426	262	86	71	7	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	48	401	244	80	73	4	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	44	367	222	89	54	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	64	512	321	107	82	2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	36	288	181	59	44	4	0	0

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
32	W	1544	33115	14768	6067	10736	1544	0	0

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	g	224	896	448	224	224	0	0

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	h	210	840	420	210	210	0	0

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	i	199	797	398	199	200	0	0

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	j	165	661	330	165	166	0	0

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	k	95	381	190	95	96	0	0

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	l	153	613	306	153	154	0	0

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	m	131	525	262	131	132	0	0

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	n	130	521	260	130	131	0	0

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	o	102	409	204	102	103	0	0

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	p	118	472	236	118	118	0	0

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	q	137	549	274	137	138	0	0

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	r	119	476	238	119	119	0	0

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	s	60	241	120	60	61	0	0

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	t	88	353	176	88	89	0	0

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	u	89	357	178	89	90	0	0

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	v	86	345	172	86	87	0	0

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	w	71	285	142	71	72	0	0

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
50	x	84	336	168	84	84	0	0

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	y	86	345	172	86	87	0	0

- Molecule 52 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	z	77	1643	731	290	545	77	0	0

- Molecule 53 is a protein called YqzJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	2	24	107	64	28	14	1	0	0

- Molecule 54 is a protein called 50S ribosomal protein L31.

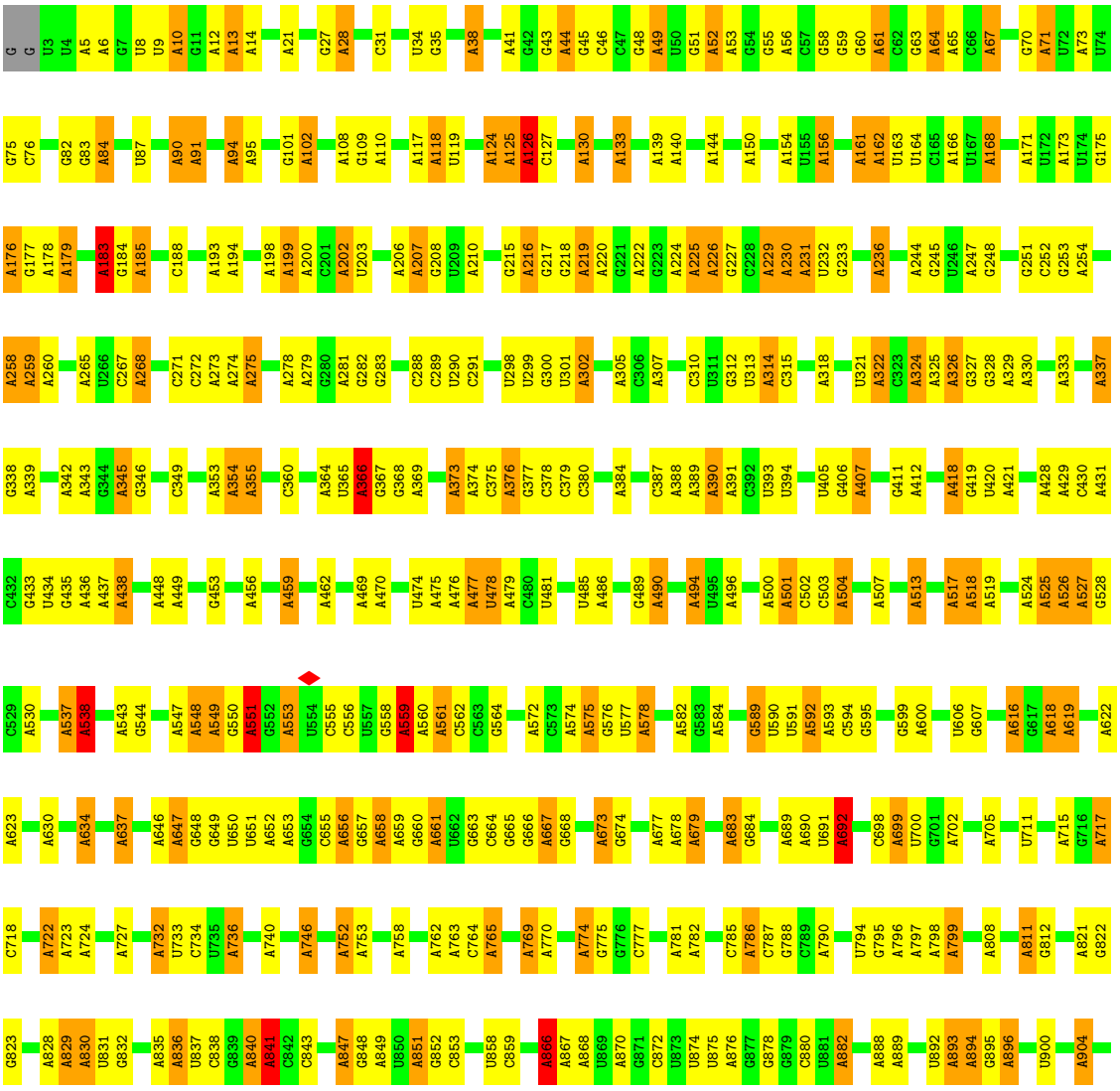
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	3	45	366	227	66	71	2	0	0

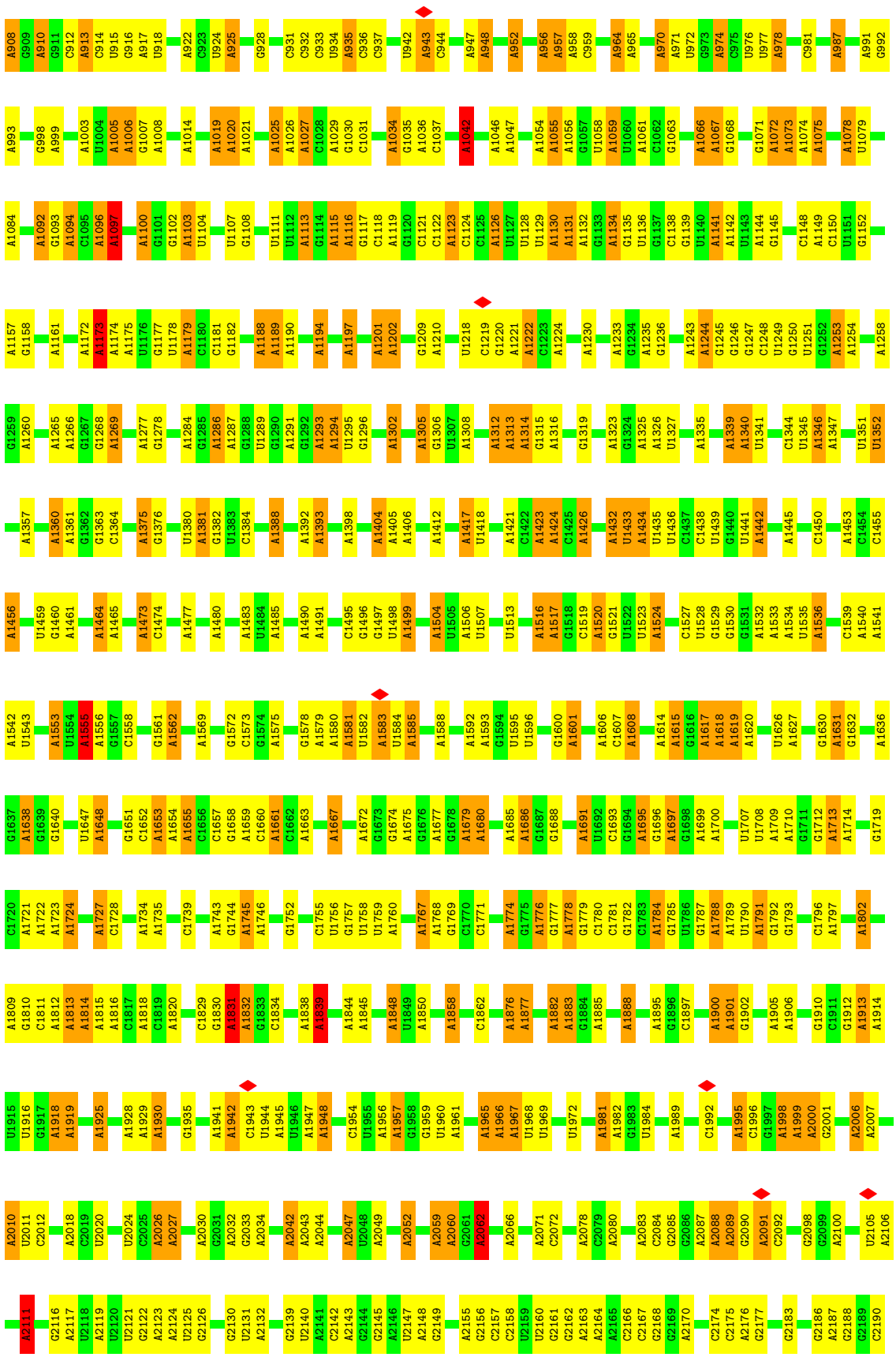
3 Residue-property plots (i)

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

- Molecule 1: 23S rRNA

Chain A: 55% 32% 12%

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A993 G998 A999 A1003 U1004 A1005 A1006 G1007 A1008 A1014 A1019 A1020 A1021 A1025 A1026 A1027 C1028 A1029 G1030 C1031 A1034 G1035 A1036 C1037 A1042 A1046 A1047 A1054 A1055 A1056 G1057 U1058 A1059 U1060 A1061 C1062 G1063 A1066 A1067 G1068 G1071 A1072 A1073 A1074 A1075 A1078 U1079
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C1720 A1721 A1722 A1723 A1724 A1727 C1728 A1734 A1735 C1739 A1743 G1744 A1745 A1746 G1752 C1755 U1756 G1757 U1758 U1759 A1760 A1767 A1768 G1769 C1770 C1771 A1774 G1775 A1776 G1777 A1778 G1779 C1780 C1781 G1782 C1783 A1784 G1785 U1786 G1787 A1788 A1789 U1790 A1791 G1792 G1793 C1796 A1797 A1802
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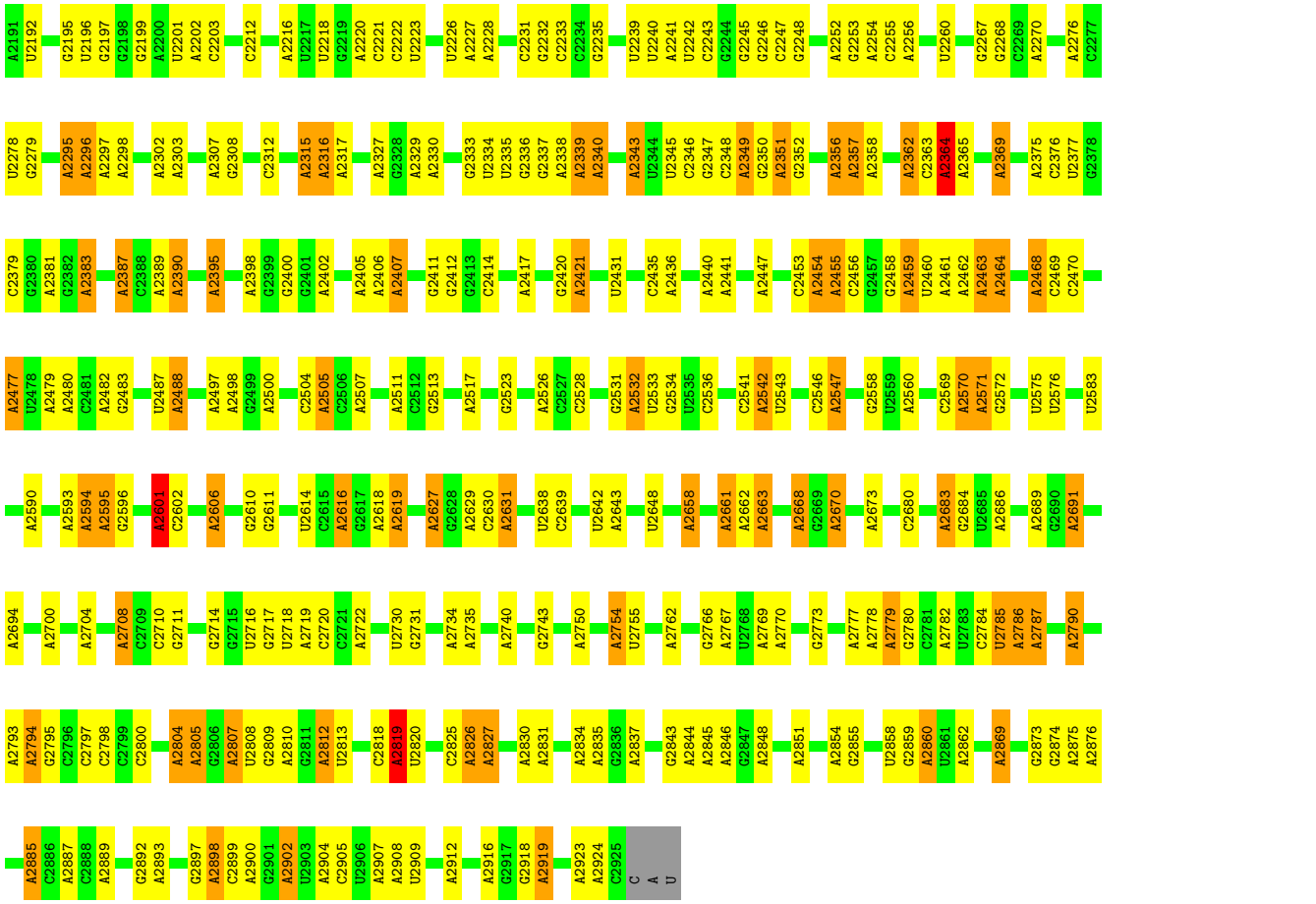
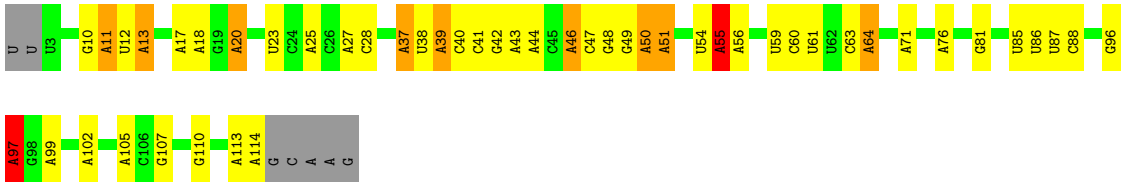


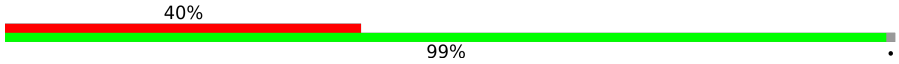
- Molecule 2: 5S rRNA

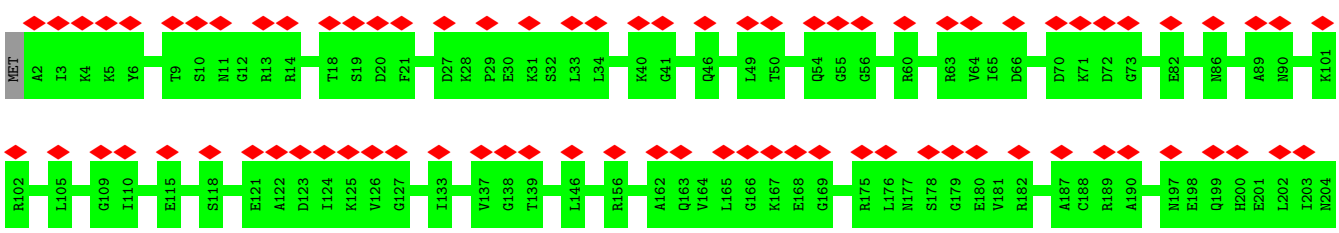
Chain B:

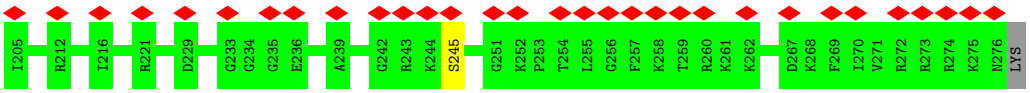


- Molecule 3: 50S ribosomal protein L2

Chain C:

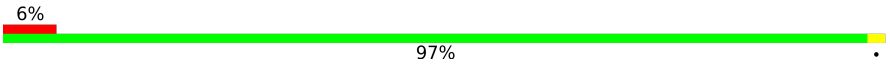


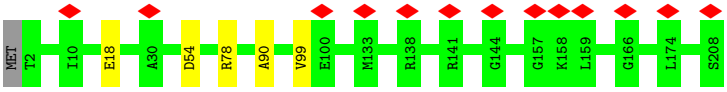




• Molecule 4: 50S ribosomal protein L3

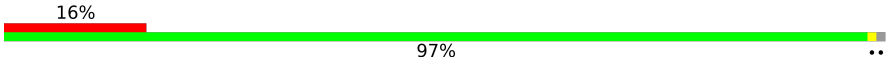
Chain D:

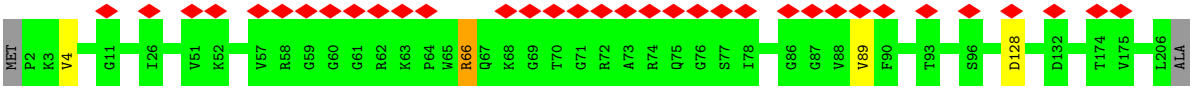




• Molecule 5: 50S ribosomal protein L4

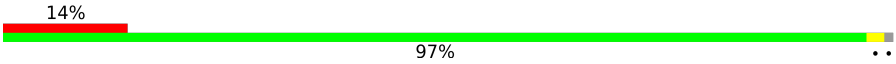
Chain E:

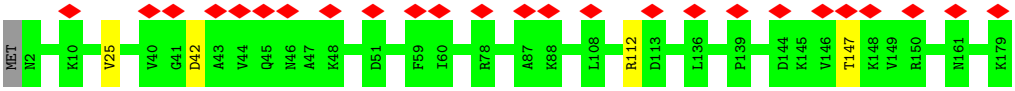




• Molecule 6: 50S ribosomal protein L5

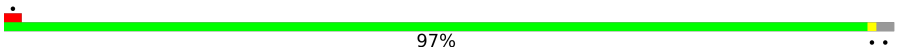
Chain F:

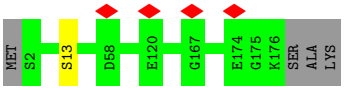




• Molecule 7: Ribosomal protein L6

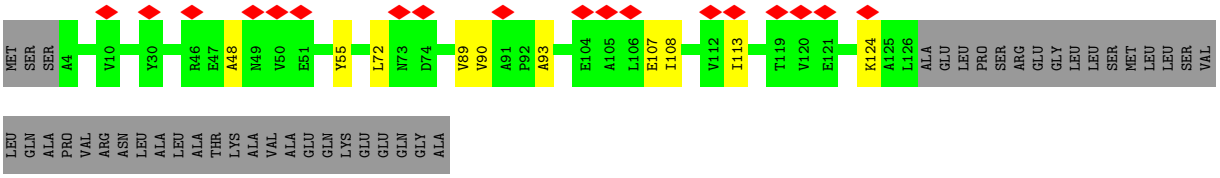
Chain G:





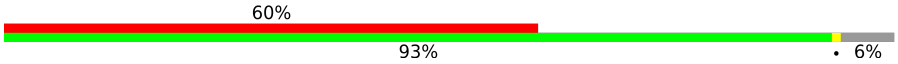
• Molecule 8: 50S ribosomal protein L10

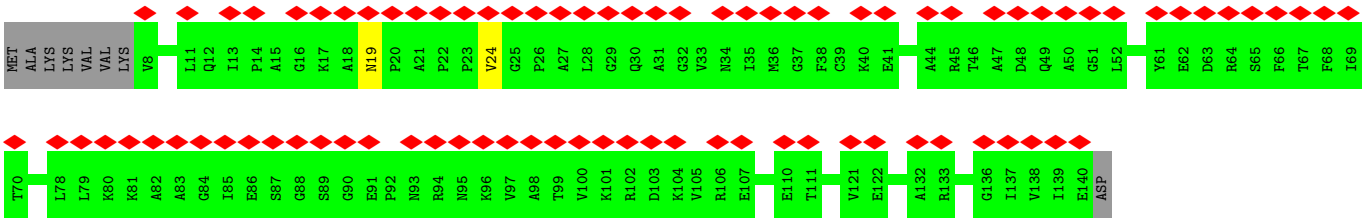
Chain H:



• Molecule 9: 50S ribosomal protein L11

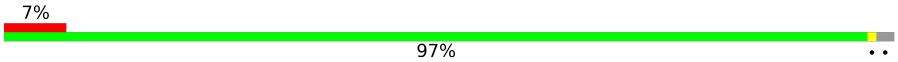
Chain I:

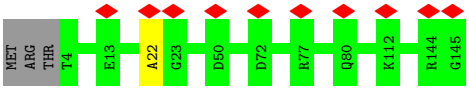




- Molecule 10: 50S ribosomal protein L13

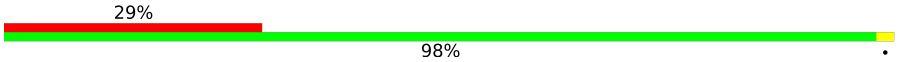
Chain J:

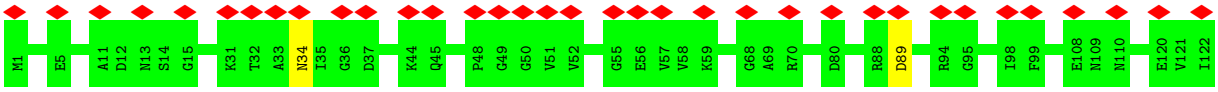




- Molecule 11: 50S ribosomal protein L14

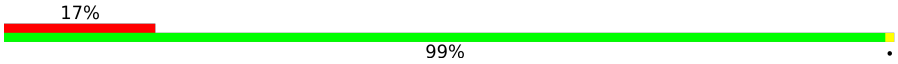
Chain K:

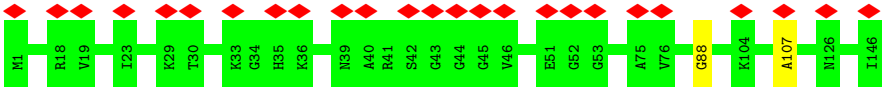




- Molecule 12: 50S ribosomal protein L15

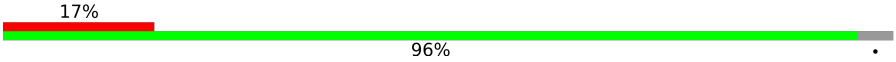
Chain L:

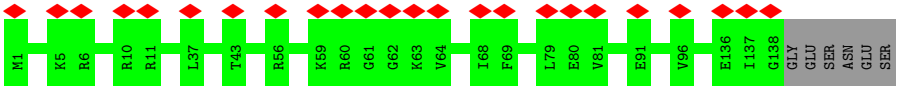




- Molecule 13: 50S ribosomal protein L16

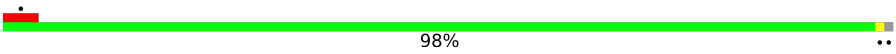
Chain M:

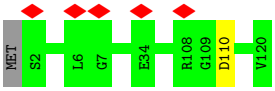




- Molecule 14: 50S ribosomal protein L17

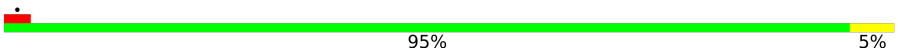
Chain N:

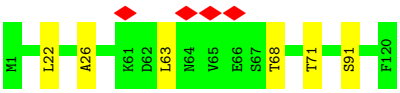




- Molecule 15: 50S ribosomal protein L18

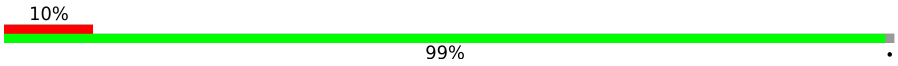
Chain O:

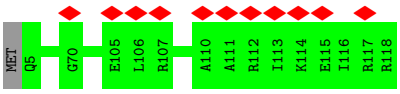




• Molecule 16: 50S ribosomal protein L19

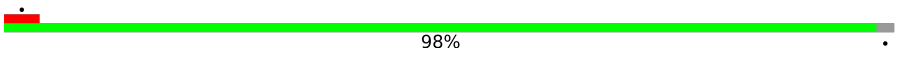
Chain P:

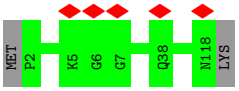




• Molecule 17: 50S ribosomal protein L20

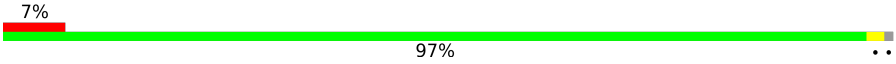
Chain Q:

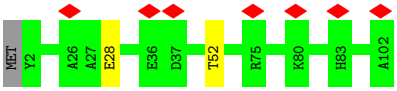




• Molecule 18: 50S ribosomal protein L21

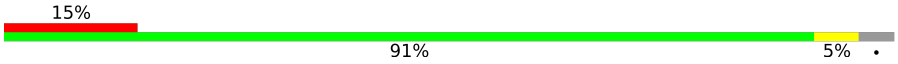
Chain R:

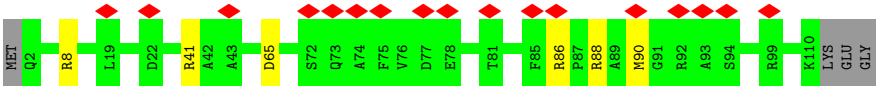




• Molecule 19: 50S ribosomal protein L22

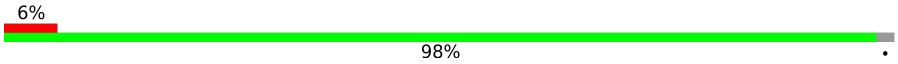
Chain S:

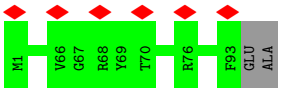




• Molecule 20: 50S ribosomal protein L23

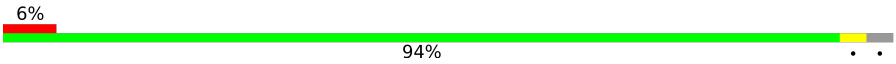
Chain T:

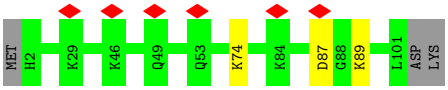




• Molecule 21: 50S ribosomal protein L24

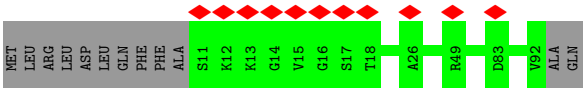
Chain U:





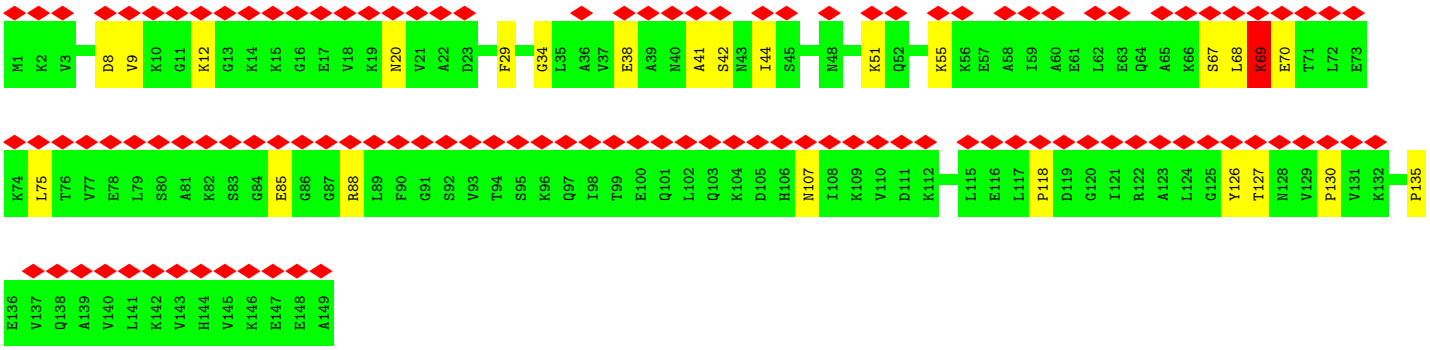
• Molecule 22: 50S ribosomal protein L27

Chain V: 12% 87% 13%



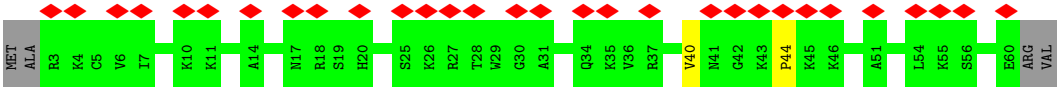
• Molecule 23: 50S ribosomal protein L9

Chain X: 78% 83% 16%



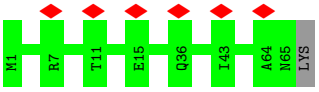
• Molecule 24: 50S ribosomal protein L28

Chain Y: 48% 90% 6%



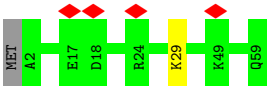
• Molecule 25: 50S ribosomal protein L29

Chain Z: 9% 98%



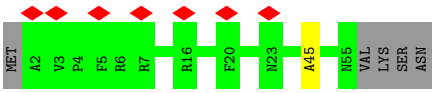
• Molecule 26: 50S ribosomal protein L30

Chain a: 7% 97%



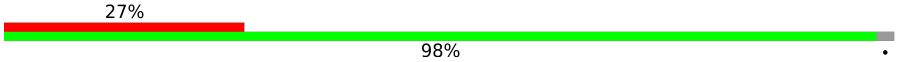
• Molecule 27: 50S ribosomal protein L32

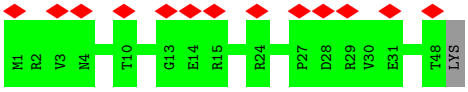
Chain b: 12% 90% 8%



- Molecule 28: 50S ribosomal protein L33

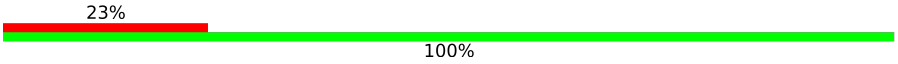
Chain c:

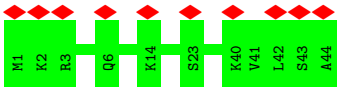




- Molecule 29: 50S ribosomal protein L34

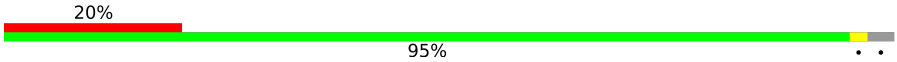
Chain d:

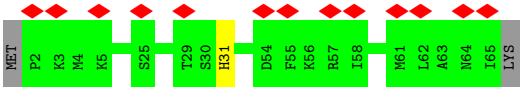




- Molecule 30: 50S ribosomal protein L35

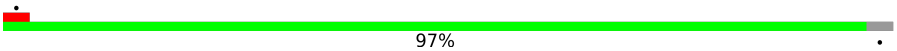
Chain e:

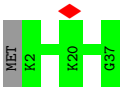




- Molecule 31: 50S ribosomal protein L36

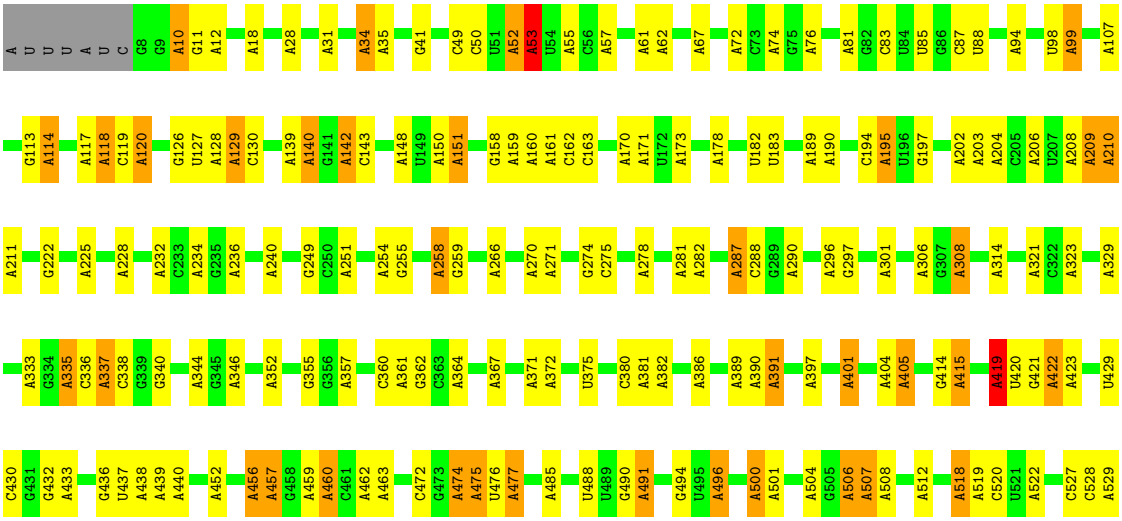
Chain f:

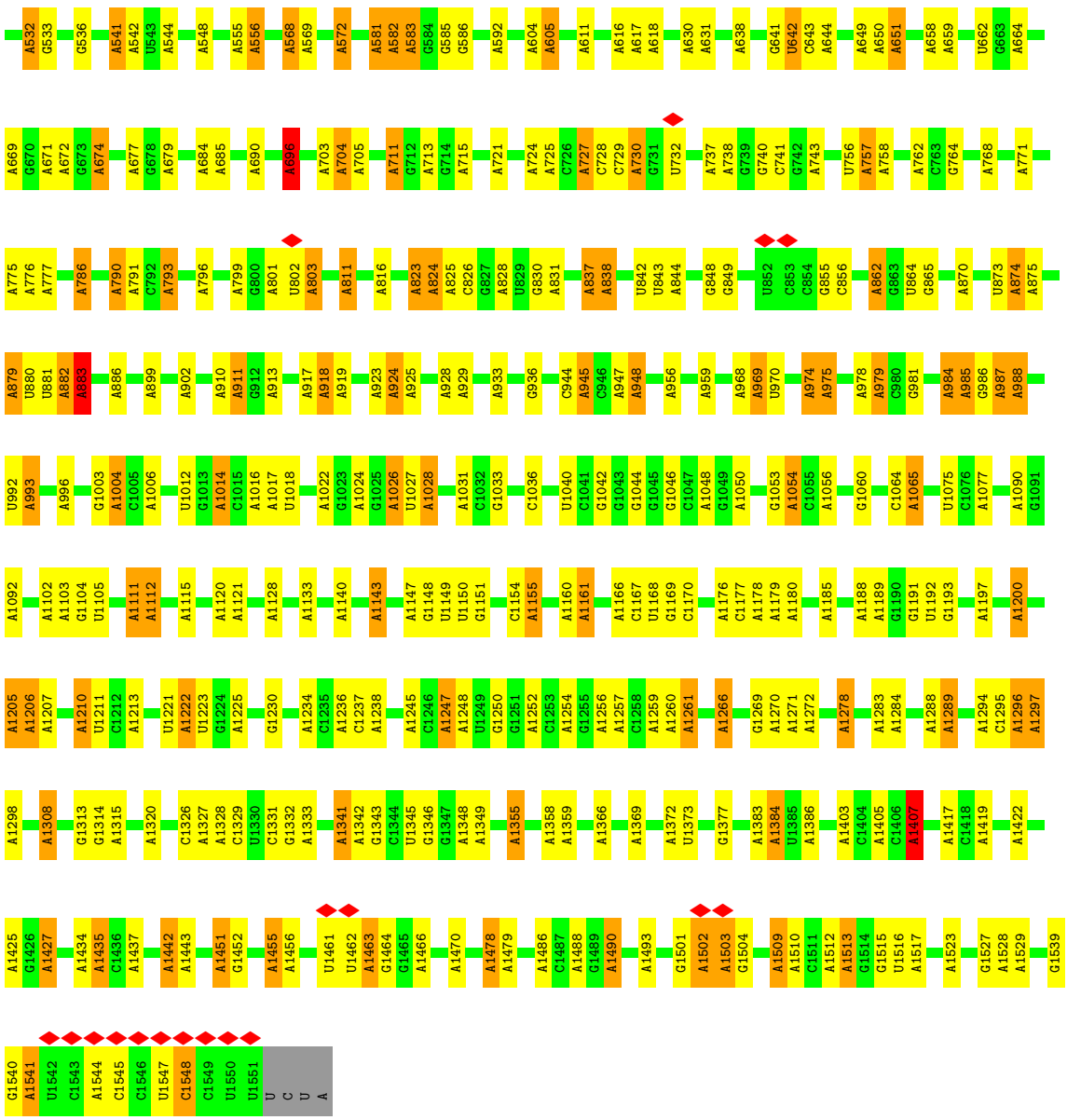




- Molecule 32: 16S rRNA

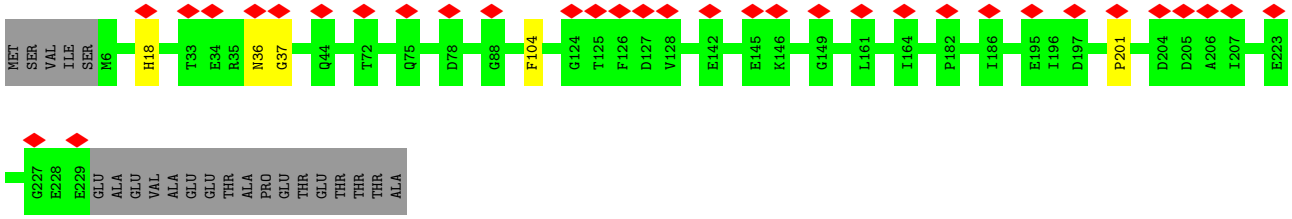
Chain W:





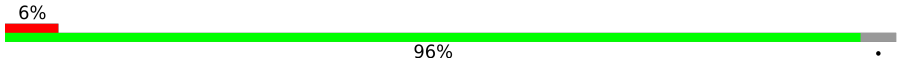
- Molecule 33: 30S ribosomal protein S2

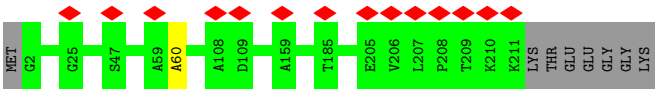
Chain g:



- Molecule 34: 30S ribosomal protein S3

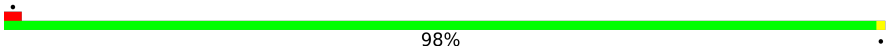
Chain h:

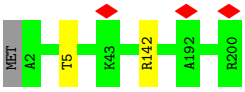




• Molecule 35: 30S ribosomal protein S4

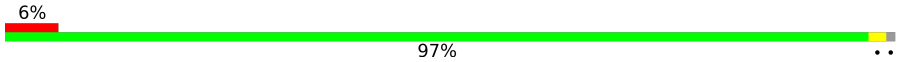
Chain i:

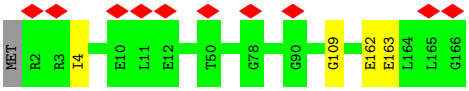




• Molecule 36: 30S ribosomal protein S5

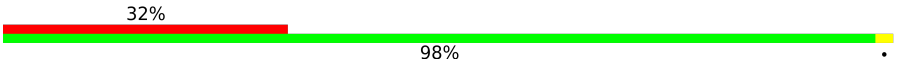
Chain j:

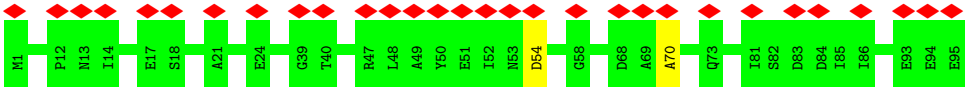




• Molecule 37: 30S ribosomal protein S6

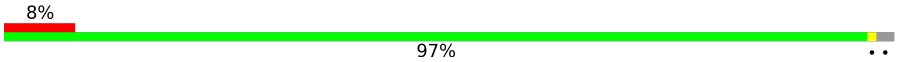
Chain k:

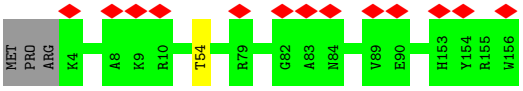




• Molecule 38: 30S ribosomal protein S7

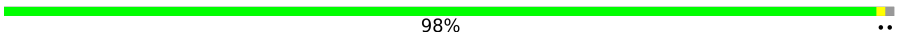
Chain l:





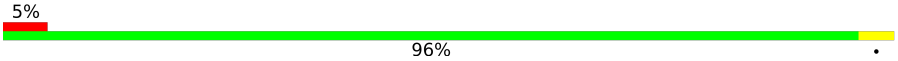
• Molecule 39: 30S ribosomal protein S8

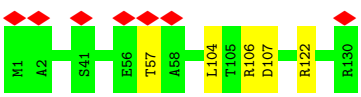
Chain m:



• Molecule 40: 30S ribosomal protein S9

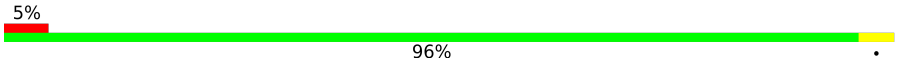
Chain n:

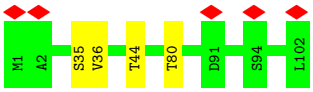




• Molecule 41: 30S ribosomal protein S10

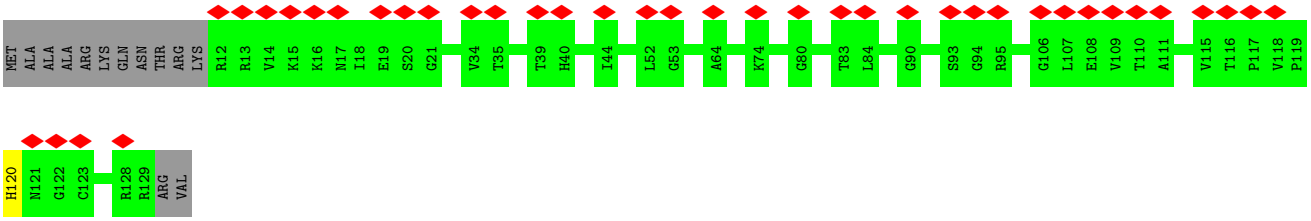
Chain o:





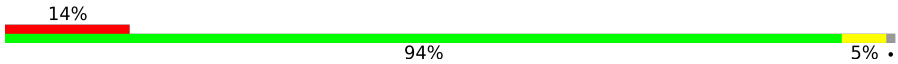
• Molecule 42: 30S ribosomal protein S11

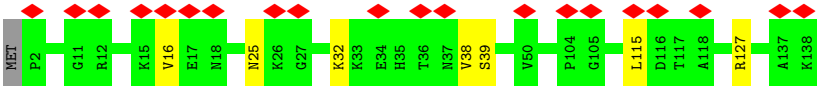
Chain p:



• Molecule 43: 30S ribosomal protein S12

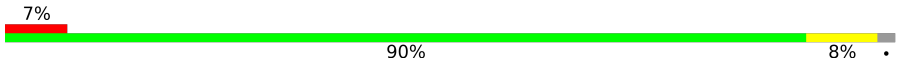
Chain q:

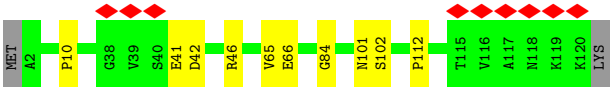




• Molecule 44: 30S ribosomal protein S13

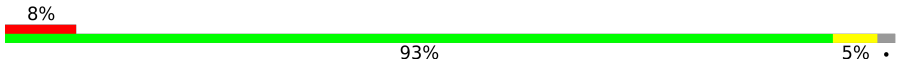
Chain r:

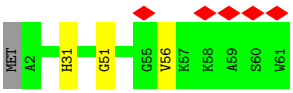




• Molecule 45: 30S ribosomal protein S14 type Z

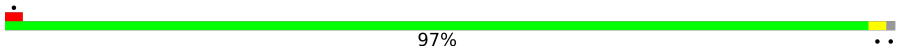
Chain s:

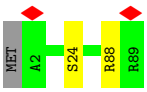




• Molecule 46: 30S ribosomal protein S15

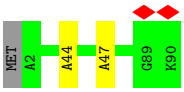
Chain t:





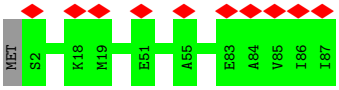
• Molecule 47: 30S ribosomal protein S16

Chain u: 97%



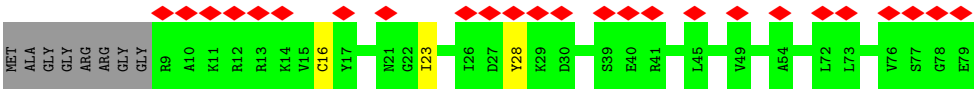
• Molecule 48: 30S ribosomal protein S17

Chain v: 11% 99%



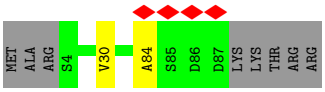
• Molecule 49: 30S ribosomal protein S18

Chain w: 32% 86% 10%



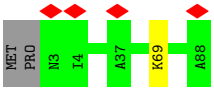
• Molecule 50: 30S ribosomal protein S19

Chain x: 89% 9%



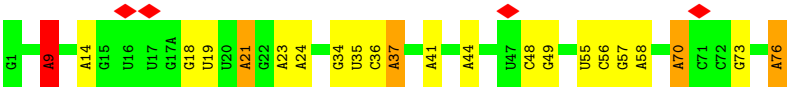
• Molecule 51: 30S ribosomal protein S20

Chain y: 5% 97%



• Molecule 52: P-site tRNA

Chain z: 5% 71% 22% 5%

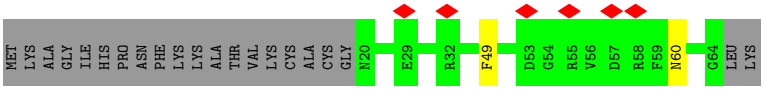


• Molecule 53: YqzJ

Chain 2: 25% 20% 5% 75%

- Molecule 54: 50S ribosomal protein L31

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12739	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.709	Depositor
Minimum map value	-0.823	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	650.4, 650.4, 650.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	A	1.37	1874/70307 (2.7%)	2.92	7344/109687 (6.7%)
2	B	1.30	64/2678 (2.4%)	2.78	247/4174 (5.9%)
3	C	0.27	0/2148	0.48	0/2881
4	D	0.28	0/1597	0.47	0/2140
5	E	0.27	0/1580	0.50	0/2132
6	F	0.29	0/1423	0.50	0/1910
7	G	0.24	0/1360	0.43	0/1832
8	H	0.26	0/963	0.49	0/1298
9	I	0.26	0/995	0.48	0/1346
10	J	0.26	0/1146	0.49	0/1542
11	K	0.28	0/927	0.47	0/1245
12	L	0.23	0/1093	0.44	0/1457
13	M	0.21	0/1120	0.38	0/1496
14	N	0.26	0/960	0.50	0/1284
15	O	0.30	0/921	0.54	1/1236 (0.1%)
16	P	0.24	0/949	0.44	0/1269
17	Q	0.27	0/952	0.45	0/1266
18	R	0.28	0/797	0.53	0/1070
19	S	0.34	0/851	0.59	0/1146
20	T	0.30	0/759	0.47	0/1011
21	U	0.27	0/764	0.52	0/1022
22	V	0.30	0/638	0.50	0/847
23	X	0.64	1/732 (0.1%)	1.01	5/1016 (0.5%)
24	Y	0.30	0/448	0.58	0/596
25	Z	0.24	0/531	0.48	0/707
26	a	0.24	0/457	0.44	0/613
27	b	0.23	0/433	0.48	0/574
28	c	0.26	0/406	0.44	0/540
29	d	0.21	0/370	0.44	0/483
30	e	0.23	0/519	0.48	0/680
31	f	0.20	0/291	0.37	0/383
32	W	1.36	968/37074 (2.6%)	2.90	3819/57834 (6.6%)
33	g	0.32	0/895	0.40	0/1117
34	h	0.29	0/839	0.38	0/1047

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	i	0.26	0/796	0.41	0/992
36	j	0.26	0/660	0.46	0/822
37	k	0.31	0/380	0.41	0/472
38	l	0.27	0/612	0.39	0/762
39	m	0.24	0/524	0.43	0/652
40	n	0.26	0/520	0.51	0/647
41	o	0.28	0/408	0.39	0/507
42	p	0.22	0/471	0.42	0/587
43	q	0.24	0/548	0.50	0/682
44	r	0.31	0/475	0.52	0/592
45	s	0.21	0/240	0.49	0/297
46	t	0.27	0/352	0.42	0/437
47	u	0.27	0/356	0.41	0/442
48	v	0.27	0/344	0.43	0/427
49	w	0.31	0/284	0.43	0/352
50	x	0.33	0/335	0.46	0/417
51	y	0.26	0/344	0.40	0/427
52	z	1.04	30/1834 (1.6%)	2.18	104/2858 (3.6%)
53	2	0.50	0/106	1.02	0/122
54	3	0.29	0/373	0.45	0/497
All	All	1.19	2937/147885 (2.0%)	2.58	11520/221872 (5.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	79
2	B	0	2
5	E	0	1
19	S	0	2
23	X	0	2
32	W	0	33
52	z	0	2
All	All	0	121

All (2937) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	508	A	C8-N7	8.39	1.37	1.31
1	A	1188	A	C8-N7	8.37	1.37	1.31

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	526	A	C8-N7	8.21	1.37	1.31
1	A	2916	A	C8-N7	8.17	1.37	1.31
1	A	504	A	C8-N7	8.14	1.37	1.31
1	A	374	A	C8-N7	8.14	1.37	1.31
32	W	439	A	C8-N7	8.13	1.37	1.31
1	A	1417	A	C8-N7	8.10	1.37	1.31
32	W	150	A	C8-N7	8.10	1.37	1.31
1	A	2898	A	C8-N7	8.09	1.37	1.31
32	W	631	A	C8-N7	8.08	1.37	1.31
32	W	1372	A	C8-N7	8.06	1.37	1.31
1	A	2793	A	C8-N7	8.05	1.37	1.31
1	A	1814	A	C8-N7	8.02	1.37	1.31
32	W	457	A	C8-N7	8.01	1.37	1.31
32	W	151	A	C8-N7	7.97	1.37	1.31
32	W	1056	A	C8-N7	7.97	1.37	1.31
1	A	224	A	C8-N7	7.97	1.37	1.31
1	A	732	A	C8-N7	7.97	1.37	1.31
1	A	207	A	C8-N7	7.96	1.37	1.31
32	W	1355	A	C8-N7	7.96	1.37	1.31
1	A	1078	A	C8-N7	7.96	1.37	1.31
32	W	862	A	C8-N7	7.95	1.37	1.31
1	A	2807	A	C8-N7	7.95	1.37	1.31
1	A	118	A	C8-N7	7.95	1.37	1.31
1	A	2295	A	C8-N7	7.95	1.37	1.31
1	A	1347	A	C8-N7	7.95	1.37	1.31
32	W	254	A	C8-N7	7.93	1.37	1.31
1	A	501	A	C8-N7	7.93	1.37	1.31
32	W	1247	A	C8-N7	7.92	1.37	1.31
1	A	2089	A	C8-N7	7.92	1.37	1.31
32	W	1358	A	C8-N7	7.92	1.37	1.31
32	W	266	A	C8-N7	7.92	1.37	1.31
1	A	389	A	C8-N7	7.91	1.37	1.31
32	W	899	A	C8-N7	7.91	1.37	1.31
1	A	1919	A	C8-N7	7.91	1.37	1.31
1	A	1905	A	C8-N7	7.91	1.37	1.31
32	W	506	A	C8-N7	7.91	1.37	1.31
2	B	17	A	C8-N7	7.90	1.37	1.31
32	W	757	A	C8-N7	7.90	1.37	1.31
1	A	1179	A	C8-N7	7.90	1.37	1.31
1	A	1434	A	C8-N7	7.90	1.37	1.31
32	W	1022	A	C8-N7	7.89	1.37	1.31
1	A	1339	A	C8-N7	7.89	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	1443	A	C8-N7	7.89	1.37	1.31
1	A	702	A	C8-N7	7.89	1.37	1.31
1	A	811	A	C8-N7	7.89	1.37	1.31
1	A	494	A	C8-N7	7.88	1.37	1.31
1	A	1473	A	C8-N7	7.88	1.37	1.31
1	A	1201	A	C8-N7	7.88	1.37	1.31
32	W	674	A	C8-N7	7.88	1.37	1.31
32	W	775	A	C8-N7	7.88	1.37	1.31
1	A	219	A	C8-N7	7.88	1.37	1.31
2	B	50	A	C8-N7	7.88	1.37	1.31
1	A	448	A	C8-N7	7.88	1.37	1.31
32	W	1257	A	C8-N7	7.87	1.37	1.31
32	W	28	A	C8-N7	7.87	1.37	1.31
1	A	126	A	C8-N7	7.87	1.37	1.31
32	W	139	A	C8-N7	7.86	1.37	1.31
32	W	1133	A	C8-N7	7.86	1.37	1.31
1	A	216	A	C8-N7	7.86	1.37	1.31
1	A	470	A	C8-N7	7.86	1.37	1.31
1	A	723	A	C8-N7	7.85	1.37	1.31
1	A	1161	A	C8-N7	7.85	1.37	1.31
1	A	2083	A	C8-N7	7.85	1.37	1.31
1	A	1579	A	C8-N7	7.84	1.37	1.31
32	W	367	A	C8-N7	7.84	1.37	1.31
1	A	183	A	C8-N7	7.84	1.37	1.31
1	A	314	A	C8-N7	7.84	1.37	1.31
32	W	419	A	C8-N7	7.84	1.37	1.31
1	A	1340	A	C8-N7	7.83	1.37	1.31
1	A	782	A	C8-N7	7.83	1.37	1.31
32	W	296	A	C8-N7	7.83	1.37	1.31
32	W	452	A	C8-N7	7.83	1.37	1.31
32	W	786	A	C8-N7	7.83	1.37	1.31
1	A	1789	A	C8-N7	7.82	1.37	1.31
1	A	1982	A	C8-N7	7.82	1.37	1.31
32	W	541	A	C8-N7	7.82	1.37	1.31
1	A	1157	A	C8-N7	7.82	1.37	1.31
32	W	1422	A	C8-N7	7.81	1.37	1.31
32	W	721	A	C8-N7	7.81	1.37	1.31
32	W	1451	A	C8-N7	7.81	1.37	1.31
32	W	690	A	C8-N7	7.81	1.37	1.31
1	A	1066	A	C8-N7	7.81	1.37	1.31
32	W	1213	A	C8-N7	7.81	1.37	1.31
1	A	965	A	C8-N7	7.80	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	A	C8-N7	7.80	1.37	1.31
1	A	999	A	C8-N7	7.80	1.37	1.31
1	A	2526	A	C8-N7	7.80	1.37	1.31
32	W	925	A	C8-N7	7.80	1.37	1.31
1	A	2834	A	C8-N7	7.80	1.37	1.31
32	W	1298	A	C8-N7	7.80	1.37	1.31
1	A	179	A	C8-N7	7.79	1.37	1.31
1	A	2908	A	C8-N7	7.79	1.37	1.31
1	A	547	A	C8-N7	7.79	1.37	1.31
1	A	553	A	C8-N7	7.79	1.37	1.31
1	A	1504	A	C8-N7	7.79	1.37	1.31
1	A	2062	A	C8-N7	7.79	1.36	1.31
1	A	2668	A	C8-N7	7.79	1.36	1.31
1	A	345	A	C8-N7	7.78	1.36	1.31
1	A	1995	A	C8-N7	7.78	1.36	1.31
32	W	777	A	C8-N7	7.78	1.36	1.31
1	A	6	A	C8-N7	7.78	1.36	1.31
1	A	1555	A	C8-N7	7.78	1.36	1.31
1	A	1925	A	C8-N7	7.78	1.36	1.31
1	A	2447	A	C8-N7	7.78	1.36	1.31
32	W	148	A	C8-N7	7.78	1.36	1.31
32	W	1207	A	C8-N7	7.78	1.36	1.31
1	A	1123	A	C8-N7	7.78	1.36	1.31
1	A	1941	A	C8-N7	7.78	1.36	1.31
1	A	2893	A	C8-N7	7.78	1.36	1.31
32	W	1050	A	C8-N7	7.77	1.36	1.31
1	A	428	A	C8-N7	7.77	1.36	1.31
1	A	1020	A	C8-N7	7.77	1.36	1.31
1	A	1067	A	C8-N7	7.77	1.36	1.31
1	A	176	A	C8-N7	7.76	1.36	1.31
1	A	652	A	C8-N7	7.76	1.36	1.31
1	A	1906	A	C8-N7	7.76	1.36	1.31
1	A	646	A	C8-N7	7.76	1.36	1.31
1	A	2398	A	C8-N7	7.76	1.36	1.31
1	A	952	A	C8-N7	7.76	1.36	1.31
1	A	1119	A	C8-N7	7.76	1.36	1.31
1	A	2047	A	C8-N7	7.76	1.36	1.31
1	A	2364	A	C8-N7	7.76	1.36	1.31
32	W	438	A	C8-N7	7.76	1.36	1.31
32	W	1333	A	C8-N7	7.76	1.36	1.31
1	A	1269	A	C8-N7	7.76	1.36	1.31
32	W	1327	A	C8-N7	7.76	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1308	A	C8-N7	7.76	1.36	1.31
1	A	1005	A	C8-N7	7.75	1.36	1.31
1	A	1788	A	C8-N7	7.75	1.36	1.31
2	B	18	A	C8-N7	7.75	1.36	1.31
32	W	1470	A	C8-N7	7.75	1.36	1.31
1	A	1026	A	C8-N7	7.75	1.36	1.31
1	A	1966	A	C8-N7	7.74	1.36	1.31
32	W	824	A	C8-N7	7.74	1.36	1.31
32	W	1425	A	C8-N7	7.74	1.36	1.31
1	A	173	A	C8-N7	7.74	1.36	1.31
1	A	273	A	C8-N7	7.74	1.36	1.31
32	W	401	A	C8-N7	7.74	1.36	1.31
32	W	910	A	C8-N7	7.74	1.36	1.31
32	W	968	A	C8-N7	7.74	1.36	1.31
1	A	2356	A	C8-N7	7.74	1.36	1.31
32	W	190	A	C8-N7	7.74	1.36	1.31
1	A	477	A	C8-N7	7.74	1.36	1.31
1	A	647	A	C8-N7	7.74	1.36	1.31
32	W	1261	A	C8-N7	7.74	1.36	1.31
32	W	1510	A	C8-N7	7.74	1.36	1.31
1	A	867	A	C8-N7	7.73	1.36	1.31
1	A	575	A	C8-N7	7.73	1.36	1.31
1	A	659	A	C8-N7	7.73	1.36	1.31
1	A	2349	A	C8-N7	7.73	1.36	1.31
32	W	159	A	C8-N7	7.73	1.36	1.31
32	W	1386	A	C8-N7	7.73	1.36	1.31
32	W	208	A	C8-N7	7.73	1.36	1.31
32	W	475	A	C8-N7	7.73	1.36	1.31
1	A	2078	A	C8-N7	7.73	1.36	1.31
32	W	240	A	C8-N7	7.73	1.36	1.31
32	W	1128	A	C8-N7	7.73	1.36	1.31
1	A	384	A	C8-N7	7.72	1.36	1.31
1	A	1432	A	C8-N7	7.72	1.36	1.31
1	A	1844	A	C8-N7	7.72	1.36	1.31
32	W	1342	A	C8-N7	7.72	1.36	1.31
1	A	1592	A	C8-N7	7.72	1.36	1.31
32	W	713	A	C8-N7	7.72	1.36	1.31
32	W	1434	A	C8-N7	7.72	1.36	1.31
1	A	44	A	C8-N7	7.72	1.36	1.31
1	A	161	A	C8-N7	7.72	1.36	1.31
1	A	429	A	C8-N7	7.72	1.36	1.31
1	A	2769	A	C8-N7	7.72	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	105	A	C8-N7	7.72	1.36	1.31
32	W	500	A	C8-N7	7.72	1.36	1.31
32	W	1435	A	C8-N7	7.72	1.36	1.31
1	A	896	A	C8-N7	7.72	1.36	1.31
32	W	975	A	C8-N7	7.72	1.36	1.31
1	A	333	A	C8-N7	7.71	1.36	1.31
1	A	2343	A	C8-N7	7.71	1.36	1.31
32	W	929	A	C8-N7	7.71	1.36	1.31
32	W	485	A	C8-N7	7.71	1.36	1.31
1	A	717	A	C8-N7	7.71	1.36	1.31
1	A	1115	A	C8-N7	7.71	1.36	1.31
1	A	1224	A	C8-N7	7.71	1.36	1.31
32	W	1120	A	C8-N7	7.71	1.36	1.31
32	W	52	A	C8-N7	7.71	1.36	1.31
1	A	329	A	C8-N7	7.71	1.36	1.31
1	A	388	A	C8-N7	7.71	1.36	1.31
1	A	1406	A	C8-N7	7.71	1.36	1.31
1	A	2329	A	C8-N7	7.71	1.36	1.31
32	W	189	A	C8-N7	7.71	1.36	1.31
1	A	199	A	C8-N7	7.71	1.36	1.31
1	A	507	A	C8-N7	7.71	1.36	1.31
1	A	1142	A	C8-N7	7.70	1.36	1.31
32	W	1254	A	C8-N7	7.70	1.36	1.31
1	A	1412	A	C8-N7	7.70	1.36	1.31
32	W	1437	A	C8-N7	7.70	1.36	1.31
1	A	618	A	C8-N7	7.70	1.36	1.31
1	A	2375	A	C8-N7	7.70	1.36	1.31
32	W	917	A	C8-N7	7.70	1.36	1.31
32	W	1256	A	C8-N7	7.70	1.36	1.31
32	W	1419	A	C8-N7	7.70	1.36	1.31
1	A	166	A	C8-N7	7.70	1.36	1.31
1	A	2315	A	C8-N7	7.70	1.36	1.31
1	A	2498	A	C8-N7	7.70	1.36	1.31
1	A	2902	A	C8-N7	7.70	1.36	1.31
32	W	1486	A	C8-N7	7.70	1.36	1.31
1	A	888	A	C8-N7	7.70	1.36	1.31
1	A	2779	A	C8-N7	7.70	1.36	1.31
32	W	117	A	C8-N7	7.70	1.36	1.31
32	W	1466	A	C8-N7	7.70	1.36	1.31
1	A	2686	A	C8-N7	7.69	1.36	1.31
1	A	490	A	C8-N7	7.69	1.36	1.31
1	A	2919	A	C8-N7	7.69	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	507	A	C8-N7	7.69	1.36	1.31
32	W	664	A	C8-N7	7.69	1.36	1.31
32	W	1503	A	C8-N7	7.69	1.36	1.31
1	A	524	A	C8-N7	7.69	1.36	1.31
1	A	592	A	C8-N7	7.69	1.36	1.31
1	A	1055	A	C8-N7	7.69	1.36	1.31
1	A	1784	A	C8-N7	7.69	1.36	1.31
1	A	2601	A	C8-N7	7.69	1.36	1.31
52	z	44	A	C8-N7	7.69	1.36	1.31
1	A	322	A	C8-N7	7.69	1.36	1.31
32	W	1512	A	C8-N7	7.69	1.36	1.31
1	A	476	A	C8-N7	7.68	1.36	1.31
1	A	1914	A	C8-N7	7.68	1.36	1.31
1	A	1948	A	C8-N7	7.68	1.36	1.31
1	A	2071	A	C8-N7	7.68	1.36	1.31
2	B	55	A	C8-N7	7.68	1.36	1.31
32	W	1140	A	C8-N7	7.68	1.36	1.31
1	A	479	A	C8-N7	7.68	1.36	1.31
1	A	1302	A	C8-N7	7.68	1.36	1.31
1	A	1774	A	C8-N7	7.68	1.36	1.31
1	A	2339	A	C8-N7	7.68	1.36	1.31
1	A	2479	A	C8-N7	7.68	1.36	1.31
32	W	232	A	C8-N7	7.68	1.36	1.31
32	W	886	A	C8-N7	7.68	1.36	1.31
1	A	64	A	C8-N7	7.68	1.36	1.31
32	W	816	A	C8-N7	7.68	1.36	1.31
1	A	1113	A	C8-N7	7.68	1.36	1.31
1	A	364	A	C8-N7	7.68	1.36	1.31
1	A	1540	A	C8-N7	7.67	1.36	1.31
2	B	114	A	C8-N7	7.67	1.36	1.31
1	A	2080	A	C8-N7	7.67	1.36	1.31
1	A	185	A	C8-N7	7.67	1.36	1.31
1	A	2673	A	C8-N7	7.67	1.36	1.31
1	A	2683	A	C8-N7	7.67	1.36	1.31
1	A	2722	A	C8-N7	7.67	1.36	1.31
32	W	928	A	C8-N7	7.67	1.36	1.31
1	A	1697	A	C8-N7	7.67	1.36	1.31
1	A	1588	A	C8-N7	7.67	1.36	1.31
1	A	1722	A	C8-N7	7.67	1.36	1.31
1	A	2500	A	C8-N7	7.67	1.36	1.31
1	A	2593	A	C8-N7	7.67	1.36	1.31
1	A	2618	A	C8-N7	7.67	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	170	A	C8-N7	7.67	1.36	1.31
32	W	801	A	C8-N7	7.67	1.36	1.31
32	W	1289	A	C8-N7	7.67	1.36	1.31
1	A	1876	A	C8-N7	7.67	1.36	1.31
32	W	658	A	C8-N7	7.67	1.36	1.31
1	A	786	A	C8-N7	7.66	1.36	1.31
32	W	529	A	C8-N7	7.66	1.36	1.31
32	W	1359	A	C8-N7	7.66	1.36	1.31
1	A	1305	A	C8-N7	7.66	1.36	1.31
1	A	2000	A	C8-N7	7.66	1.36	1.31
32	W	923	A	C8-N7	7.66	1.36	1.31
1	A	1003	A	C8-N7	7.66	1.36	1.31
1	A	1008	A	C8-N7	7.66	1.36	1.31
32	W	1320	A	C8-N7	7.66	1.36	1.31
1	A	436	A	C8-N7	7.66	1.36	1.31
1	A	144	A	C8-N7	7.66	1.36	1.31
1	A	1532	A	C8-N7	7.66	1.36	1.31
1	A	2317	A	C8-N7	7.66	1.36	1.31
1	A	2547	A	C8-N7	7.66	1.36	1.31
32	W	1210	A	C8-N7	7.66	1.36	1.31
1	A	200	A	C8-N7	7.65	1.36	1.31
1	A	922	A	C8-N7	7.65	1.36	1.31
1	A	1061	A	C8-N7	7.65	1.36	1.31
32	W	67	A	C8-N7	7.65	1.36	1.31
32	W	1248	A	C8-N7	7.65	1.36	1.31
1	A	1580	A	C8-N7	7.65	1.36	1.31
1	A	1677	A	C8-N7	7.65	1.36	1.31
32	W	290	A	C8-N7	7.65	1.36	1.31
32	W	924	A	C8-N7	7.65	1.36	1.31
1	A	421	A	C8-N7	7.65	1.36	1.31
1	A	762	A	C8-N7	7.65	1.36	1.31
1	A	2330	A	C8-N7	7.65	1.36	1.31
1	A	2754	A	C8-N7	7.65	1.36	1.31
2	B	76	A	C8-N7	7.65	1.36	1.31
32	W	278	A	C8-N7	7.65	1.36	1.31
1	A	1074	A	C8-N7	7.65	1.36	1.31
1	A	1895	A	C8-N7	7.65	1.36	1.31
1	A	281	A	C8-N7	7.65	1.36	1.31
1	A	560	A	C8-N7	7.65	1.36	1.31
1	A	692	A	C8-N7	7.65	1.36	1.31
1	A	991	A	C8-N7	7.65	1.36	1.31
1	A	1710	A	C8-N7	7.65	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2875	A	C8-N7	7.65	1.36	1.31
1	A	957	A	C8-N7	7.65	1.36	1.31
1	A	847	A	C8-N7	7.64	1.36	1.31
1	A	1084	A	C8-N7	7.64	1.36	1.31
2	B	37	A	C8-N7	7.64	1.36	1.31
32	W	1252	A	C8-N7	7.64	1.36	1.31
1	A	496	A	C8-N7	7.64	1.36	1.31
32	W	18	A	C8-N7	7.64	1.36	1.31
32	W	605	A	C8-N7	7.64	1.36	1.31
32	W	959	A	C8-N7	7.64	1.36	1.31
32	W	1541	A	C8-N7	7.64	1.36	1.31
32	W	228	A	C8-N7	7.64	1.36	1.31
32	W	357	A	C8-N7	7.64	1.36	1.31
1	A	354	A	C8-N7	7.64	1.36	1.31
32	W	352	A	C8-N7	7.64	1.36	1.31
32	W	978	A	C8-N7	7.64	1.36	1.31
1	A	1746	A	C8-N7	7.64	1.36	1.31
1	A	342	A	C8-N7	7.63	1.36	1.31
1	A	2440	A	C8-N7	7.63	1.36	1.31
1	A	2830	A	C8-N7	7.63	1.36	1.31
1	A	2860	A	C8-N7	7.63	1.36	1.31
32	W	386	A	C8-N7	7.63	1.36	1.31
1	A	202	A	C8-N7	7.63	1.36	1.31
1	A	102	A	C8-N7	7.63	1.36	1.31
1	A	244	A	C8-N7	7.63	1.36	1.31
1	A	1516	A	C8-N7	7.63	1.36	1.31
32	W	1017	A	C8-N7	7.63	1.36	1.31
1	A	1815	A	C8-N7	7.63	1.36	1.31
1	A	2670	A	C8-N7	7.63	1.36	1.31
32	W	1456	A	C8-N7	7.63	1.36	1.31
1	A	582	A	C8-N7	7.62	1.36	1.31
1	A	1346	A	C8-N7	7.62	1.36	1.31
1	A	1615	A	C8-N7	7.62	1.36	1.31
32	W	730	A	C8-N7	7.62	1.36	1.31
32	W	947	A	C8-N7	7.62	1.36	1.31
32	W	62	A	C8-N7	7.62	1.36	1.31
32	W	831	A	C8-N7	7.62	1.36	1.31
1	A	917	A	C8-N7	7.62	1.36	1.31
1	A	2900	A	C8-N7	7.62	1.36	1.31
1	A	1313	A	C8-N7	7.62	1.36	1.31
1	A	893	A	C8-N7	7.62	1.36	1.31
1	A	2767	A	C8-N7	7.62	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	A	C8-N7	7.62	1.36	1.31
1	A	1490	A	C8-N7	7.62	1.36	1.31
1	A	1601	A	C8-N7	7.62	1.36	1.31
32	W	160	A	C8-N7	7.62	1.36	1.31
32	W	556	A	C8-N7	7.62	1.36	1.31
32	W	1238	A	C8-N7	7.62	1.36	1.31
1	A	456	A	C8-N7	7.61	1.36	1.31
1	A	2777	A	C8-N7	7.61	1.36	1.31
32	W	1417	A	C8-N7	7.61	1.36	1.31
1	A	5	A	C8-N7	7.61	1.36	1.31
1	A	1465	A	C8-N7	7.61	1.36	1.31
1	A	1614	A	C8-N7	7.61	1.36	1.31
1	A	2034	A	C8-N7	7.61	1.36	1.31
1	A	2826	A	C8-N7	7.61	1.36	1.31
2	B	39	A	C8-N7	7.61	1.36	1.31
32	W	738	A	C8-N7	7.61	1.36	1.31
1	A	1541	A	C8-N7	7.61	1.36	1.31
1	A	2740	A	C8-N7	7.61	1.36	1.31
32	W	142	A	C8-N7	7.61	1.36	1.31
1	A	21	A	C8-N7	7.61	1.36	1.31
1	A	851	A	C8-N7	7.61	1.36	1.31
1	A	2030	A	C8-N7	7.61	1.36	1.31
1	A	2778	A	C8-N7	7.61	1.36	1.31
1	A	2812	A	C8-N7	7.61	1.36	1.31
1	A	2819	A	C8-N7	7.61	1.36	1.31
32	W	129	A	C8-N7	7.61	1.36	1.31
32	W	1236	A	C8-N7	7.61	1.36	1.31
1	A	10	A	C8-N7	7.61	1.36	1.31
1	A	139	A	C8-N7	7.61	1.36	1.31
1	A	774	A	C8-N7	7.61	1.36	1.31
1	A	1361	A	C8-N7	7.61	1.36	1.31
1	A	1553	A	C8-N7	7.61	1.36	1.31
32	W	173	A	C8-N7	7.61	1.36	1.31
32	W	333	A	C8-N7	7.61	1.36	1.31
32	W	404	A	C8-N7	7.61	1.36	1.31
32	W	512	A	C8-N7	7.61	1.36	1.31
32	W	611	A	C8-N7	7.61	1.36	1.31
32	W	870	A	C8-N7	7.61	1.36	1.31
32	W	974	A	C8-N7	7.61	1.36	1.31
1	A	1019	A	C8-N7	7.60	1.36	1.31
1	A	1034	A	C8-N7	7.60	1.36	1.31
1	A	1291	A	C8-N7	7.60	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	371	A	C8-N7	7.60	1.36	1.31
32	W	659	A	C8-N7	7.60	1.36	1.31
52	z	23	A	C8-N7	7.60	1.36	1.31
1	A	2643	A	C8-N7	7.60	1.36	1.31
32	W	210	A	C8-N7	7.60	1.36	1.31
1	A	530	A	C8-N7	7.60	1.36	1.31
1	A	781	A	C8-N7	7.60	1.36	1.31
1	A	1405	A	C8-N7	7.60	1.36	1.31
1	A	2006	A	C8-N7	7.60	1.36	1.31
1	A	49	A	C8-N7	7.60	1.36	1.31
1	A	925	A	C8-N7	7.60	1.36	1.31
1	A	1426	A	C8-N7	7.60	1.36	1.31
1	A	2042	A	C8-N7	7.60	1.36	1.31
32	W	209	A	C8-N7	7.60	1.36	1.31
32	W	459	A	C8-N7	7.60	1.36	1.31
32	W	638	A	C8-N7	7.60	1.36	1.31
1	A	1636	A	C8-N7	7.60	1.36	1.31
1	A	1700	A	C8-N7	7.60	1.36	1.31
32	W	372	A	C8-N7	7.60	1.36	1.31
32	W	569	A	C8-N7	7.60	1.36	1.31
1	A	2338	A	C8-N7	7.59	1.36	1.31
32	W	282	A	C8-N7	7.59	1.36	1.31
2	B	102	A	C8-N7	7.59	1.36	1.31
32	W	118	A	C8-N7	7.59	1.36	1.31
32	W	684	A	C8-N7	7.59	1.36	1.31
32	W	1054	A	C8-N7	7.59	1.36	1.31
1	A	1797	A	C8-N7	7.59	1.36	1.31
1	A	1942	A	C8-N7	7.59	1.36	1.31
1	A	2462	A	C8-N7	7.59	1.36	1.31
1	A	2297	A	C8-N7	7.59	1.36	1.31
32	W	771	A	C8-N7	7.59	1.36	1.31
1	A	1536	A	C8-N7	7.59	1.36	1.31
1	A	2619	A	C8-N7	7.59	1.36	1.31
2	B	113	A	C8-N7	7.59	1.36	1.31
32	W	301	A	C8-N7	7.59	1.36	1.31
1	A	821	A	C8-N7	7.59	1.36	1.31
1	A	1583	A	C8-N7	7.59	1.36	1.31
1	A	2087	A	C8-N7	7.59	1.36	1.31
1	A	2406	A	C8-N7	7.59	1.36	1.31
1	A	2923	A	C8-N7	7.59	1.36	1.31
32	W	415	A	C8-N7	7.59	1.36	1.31
1	A	537	A	C8-N7	7.58	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	27	A	C8-N7	7.58	1.36	1.31
32	W	423	A	C8-N7	7.58	1.36	1.31
1	A	71	A	C8-N7	7.58	1.36	1.31
1	A	2477	A	C8-N7	7.58	1.36	1.31
1	A	2750	A	C8-N7	7.58	1.36	1.31
32	W	53	A	C8-N7	7.58	1.36	1.31
1	A	765	A	C8-N7	7.58	1.36	1.31
1	A	849	A	C8-N7	7.58	1.36	1.31
1	A	1585	A	C8-N7	7.58	1.36	1.31
32	W	791	A	C8-N7	7.58	1.36	1.31
32	W	1407	A	C8-N7	7.58	1.36	1.31
1	A	14	A	C8-N7	7.58	1.36	1.31
1	A	462	A	C8-N7	7.58	1.36	1.31
1	A	1036	A	C8-N7	7.58	1.36	1.31
1	A	2835	A	C8-N7	7.58	1.36	1.31
32	W	679	A	C8-N7	7.58	1.36	1.31
1	A	67	A	C8-N7	7.58	1.36	1.31
1	A	150	A	C8-N7	7.58	1.36	1.31
1	A	418	A	C8-N7	7.58	1.36	1.31
32	W	583	A	C8-N7	7.58	1.36	1.31
32	W	618	A	C8-N7	7.58	1.36	1.31
32	W	956	A	C8-N7	7.58	1.36	1.31
1	A	1189	A	C8-N7	7.58	1.36	1.31
32	W	251	A	C8-N7	7.58	1.36	1.31
1	A	130	A	C8-N7	7.58	1.36	1.31
1	A	259	A	C8-N7	7.58	1.36	1.31
1	A	1092	A	C8-N7	7.58	1.36	1.31
1	A	1357	A	C8-N7	7.58	1.36	1.31
1	A	1655	A	C8-N7	7.58	1.36	1.31
32	W	382	A	C8-N7	7.58	1.36	1.31
32	W	1090	A	C8-N7	7.58	1.36	1.31
32	W	1271	A	C8-N7	7.58	1.36	1.31
32	W	1509	A	C8-N7	7.58	1.36	1.31
32	W	203	A	C8-N7	7.57	1.36	1.31
32	W	271	A	C8-N7	7.57	1.36	1.31
32	W	1348	A	C8-N7	7.57	1.36	1.31
1	A	500	A	C8-N7	7.57	1.36	1.31
1	A	2052	A	C8-N7	7.57	1.36	1.31
32	W	1014	A	C8-N7	7.57	1.36	1.31
1	A	61	A	C8-N7	7.57	1.36	1.31
1	A	1130	A	C8-N7	7.57	1.36	1.31
1	A	1506	A	C8-N7	7.57	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1663	A	C8-N7	7.57	1.36	1.31
1	A	1735	A	C8-N7	7.57	1.36	1.31
32	W	258	A	C8-N7	7.57	1.36	1.31
32	W	762	A	C8-N7	7.57	1.36	1.31
32	W	1006	A	C8-N7	7.57	1.36	1.31
32	W	1102	A	C8-N7	7.57	1.36	1.31
1	A	1900	A	C8-N7	7.57	1.36	1.31
32	W	1488	A	C8-N7	7.57	1.36	1.31
1	A	125	A	C8-N7	7.57	1.36	1.31
1	A	330	A	C8-N7	7.57	1.36	1.31
1	A	373	A	C8-N7	7.57	1.36	1.31
1	A	2594	A	C8-N7	7.57	1.36	1.31
2	B	44	A	C8-N7	7.57	1.36	1.31
1	A	543	A	C8-N7	7.57	1.36	1.31
1	A	2455	A	C8-N7	7.57	1.36	1.31
32	W	55	A	C8-N7	7.57	1.36	1.31
32	W	671	A	C8-N7	7.57	1.36	1.31
32	W	389	A	C8-N7	7.56	1.36	1.31
32	W	1176	A	C8-N7	7.56	1.36	1.31
1	A	247	A	C8-N7	7.56	1.36	1.31
1	A	1326	A	C8-N7	7.56	1.36	1.31
1	A	1818	A	C8-N7	7.56	1.36	1.31
32	W	211	A	C8-N7	7.56	1.36	1.31
32	W	902	A	C8-N7	7.56	1.36	1.31
32	W	1121	A	C8-N7	7.56	1.36	1.31
1	A	210	A	C8-N7	7.56	1.36	1.31
1	A	572	A	C8-N7	7.56	1.36	1.31
1	A	656	A	C8-N7	7.56	1.36	1.31
1	A	658	A	C8-N7	7.56	1.36	1.31
1	A	2362	A	C8-N7	7.56	1.36	1.31
1	A	2845	A	C8-N7	7.56	1.36	1.31
1	A	391	A	C8-N7	7.56	1.36	1.31
32	W	390	A	C8-N7	7.56	1.36	1.31
32	W	1222	A	C8-N7	7.56	1.36	1.31
1	A	978	A	C8-N7	7.56	1.36	1.31
1	A	1144	A	C8-N7	7.56	1.36	1.31
1	A	1499	A	C8-N7	7.56	1.36	1.31
1	A	2606	A	C8-N7	7.56	1.36	1.31
32	W	874	A	C8-N7	7.56	1.36	1.31
1	A	2889	A	C8-N7	7.56	1.36	1.31
1	A	265	A	C8-N7	7.55	1.36	1.31
1	A	437	A	C8-N7	7.55	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	829	A	C8-N7	7.55	1.36	1.31
1	A	1266	A	C8-N7	7.55	1.36	1.31
1	A	1456	A	C8-N7	7.55	1.36	1.31
1	A	2351	A	C8-N7	7.55	1.36	1.31
32	W	10	A	C8-N7	7.55	1.36	1.31
32	W	140	A	C8-N7	7.55	1.36	1.31
32	W	696	A	C8-N7	7.55	1.36	1.31
32	W	1328	A	C8-N7	7.55	1.36	1.31
32	W	474	A	C8-N7	7.55	1.36	1.31
32	W	993	A	C8-N7	7.55	1.36	1.31
1	A	231	A	C8-N7	7.55	1.36	1.31
1	A	908	A	C8-N7	7.55	1.36	1.31
1	A	1360	A	C8-N7	7.55	1.36	1.31
32	W	724	A	C8-N7	7.55	1.36	1.31
1	A	124	A	C8-N7	7.55	1.36	1.31
1	A	722	A	C8-N7	7.55	1.36	1.31
1	A	1230	A	C8-N7	7.55	1.36	1.31
1	A	1957	A	C8-N7	7.55	1.36	1.31
1	A	2595	A	C8-N7	7.55	1.36	1.31
1	A	2662	A	C8-N7	7.55	1.36	1.31
32	W	120	A	C8-N7	7.55	1.36	1.31
32	W	715	A	C8-N7	7.55	1.36	1.31
2	B	25	A	C8-N7	7.55	1.36	1.31
32	W	669	A	C8-N7	7.55	1.36	1.31
1	A	222	A	C8-N7	7.55	1.36	1.31
1	A	1882	A	C8-N7	7.55	1.36	1.31
1	A	1961	A	C8-N7	7.55	1.36	1.31
1	A	2661	A	C8-N7	7.55	1.36	1.31
32	W	456	A	C8-N7	7.55	1.36	1.31
32	W	651	A	C8-N7	7.55	1.36	1.31
32	W	737	A	C8-N7	7.55	1.36	1.31
1	A	1210	A	C8-N7	7.54	1.36	1.31
1	A	407	A	C8-N7	7.54	1.36	1.31
1	A	904	A	C8-N7	7.54	1.36	1.31
1	A	2532	A	C8-N7	7.54	1.36	1.31
32	W	171	A	C8-N7	7.54	1.36	1.31
32	W	703	A	C8-N7	7.54	1.36	1.31
32	W	1077	A	C8-N7	7.54	1.36	1.31
1	A	987	A	C8-N7	7.54	1.36	1.31
1	A	2505	A	C8-N7	7.54	1.36	1.31
1	A	2912	A	C8-N7	7.54	1.36	1.31
1	A	1533	A	C8-N7	7.54	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1314	A	C8-N7	7.54	1.36	1.31
1	A	2060	A	C8-N7	7.54	1.36	1.31
1	A	808	A	C8-N7	7.54	1.36	1.31
1	A	1244	A	C8-N7	7.54	1.36	1.31
1	A	1445	A	C8-N7	7.54	1.36	1.31
1	A	1695	A	C8-N7	7.54	1.36	1.31
1	A	2007	A	C8-N7	7.54	1.36	1.31
1	A	2804	A	C8-N7	7.54	1.36	1.31
32	W	1180	A	C8-N7	7.54	1.36	1.31
1	A	2629	A	C8-N7	7.53	1.36	1.31
1	A	302	A	C8-N7	7.53	1.36	1.31
1	A	947	A	C8-N7	7.53	1.36	1.31
1	A	970	A	C8-N7	7.53	1.36	1.31
1	A	1277	A	C8-N7	7.53	1.36	1.31
1	A	1617	A	C8-N7	7.53	1.36	1.31
1	A	1699	A	C8-N7	7.53	1.36	1.31
1	A	1850	A	C8-N7	7.53	1.36	1.31
1	A	2869	A	C8-N7	7.53	1.36	1.31
32	W	987	A	C8-N7	7.53	1.36	1.31
32	W	913	A	C8-N7	7.53	1.36	1.31
32	W	1225	A	C8-N7	7.53	1.36	1.31
1	A	1126	A	C8-N7	7.53	1.36	1.31
1	A	1778	A	C8-N7	7.53	1.36	1.31
1	A	1913	A	C8-N7	7.53	1.36	1.31
52	z	41	A	C8-N7	7.53	1.36	1.31
1	A	337	A	C8-N7	7.53	1.36	1.31
1	A	584	A	C8-N7	7.53	1.36	1.31
1	A	1096	A	C8-N7	7.53	1.36	1.31
1	A	1258	A	C8-N7	7.53	1.36	1.31
1	A	2461	A	C8-N7	7.53	1.36	1.31
32	W	202	A	C8-N7	7.53	1.36	1.31
32	W	81	A	C8-N7	7.52	1.36	1.31
32	W	568	A	C8-N7	7.52	1.36	1.31
1	A	1312	A	C8-N7	7.52	1.36	1.31
1	A	2316	A	C8-N7	7.52	1.36	1.31
1	A	2542	A	C8-N7	7.52	1.36	1.31
32	W	522	A	C8-N7	7.52	1.36	1.31
32	W	882	A	C8-N7	7.52	1.36	1.31
1	A	339	A	C8-N7	7.52	1.36	1.31
1	A	948	A	C8-N7	7.52	1.36	1.31
1	A	2307	A	C8-N7	7.52	1.36	1.31
1	A	2480	A	C8-N7	7.52	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	504	A	C8-N7	7.52	1.36	1.31
32	W	630	A	C8-N7	7.52	1.36	1.31
32	W	1178	A	C8-N7	7.52	1.36	1.31
32	W	1384	A	C8-N7	7.52	1.36	1.31
1	A	2298	A	C8-N7	7.52	1.36	1.31
32	W	837	A	C8-N7	7.52	1.36	1.31
32	W	1197	A	C8-N7	7.52	1.36	1.31
32	W	1405	A	C8-N7	7.52	1.36	1.31
1	A	1929	A	C8-N7	7.52	1.36	1.31
32	W	793	A	C8-N7	7.52	1.36	1.31
32	W	844	A	C8-N7	7.52	1.36	1.31
1	A	1197	A	C8-N7	7.51	1.36	1.31
1	A	1202	A	C8-N7	7.51	1.36	1.31
1	A	2088	A	C8-N7	7.51	1.36	1.31
32	W	281	A	C8-N7	7.51	1.36	1.31
32	W	650	A	C8-N7	7.51	1.36	1.31
32	W	704	A	C8-N7	7.51	1.36	1.31
32	W	945	A	C8-N7	7.51	1.36	1.31
1	A	133	A	C8-N7	7.51	1.36	1.31
1	A	1375	A	C8-N7	7.51	1.36	1.31
1	A	1534	A	C8-N7	7.51	1.36	1.31
1	A	2381	A	C8-N7	7.51	1.36	1.31
1	A	2389	A	C8-N7	7.51	1.36	1.31
32	W	796	A	C8-N7	7.51	1.36	1.31
1	A	1381	A	C8-N7	7.51	1.36	1.31
1	A	1812	A	C8-N7	7.51	1.36	1.31
32	W	321	A	C8-N7	7.51	1.36	1.31
32	W	617	A	C8-N7	7.51	1.36	1.31
32	W	985	A	C8-N7	7.51	1.36	1.31
32	W	1529	A	C8-N7	7.51	1.36	1.31
1	A	549	A	C8-N7	7.51	1.36	1.31
1	A	1014	A	C8-N7	7.51	1.36	1.31
1	A	1141	A	C8-N7	7.51	1.36	1.31
1	A	1194	A	C8-N7	7.51	1.36	1.31
1	A	1392	A	C8-N7	7.51	1.36	1.31
1	A	1845	A	C8-N7	7.51	1.36	1.31
1	A	2507	A	C8-N7	7.51	1.36	1.31
1	A	325	A	C8-N7	7.51	1.36	1.31
1	A	828	A	C8-N7	7.51	1.36	1.31
1	A	178	A	C8-N7	7.51	1.36	1.31
1	A	376	A	C8-N7	7.51	1.36	1.31
1	A	705	A	C8-N7	7.51	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1679	A	C8-N7	7.51	1.36	1.31
1	A	1734	A	C8-N7	7.51	1.36	1.31
32	W	31	A	C8-N7	7.51	1.36	1.31
32	W	491	A	C8-N7	7.51	1.36	1.31
1	A	162	A	C8-N7	7.50	1.36	1.31
1	A	230	A	C8-N7	7.50	1.36	1.31
1	A	2387	A	C8-N7	7.50	1.36	1.31
32	W	236	A	C8-N7	7.50	1.36	1.31
1	A	469	A	C8-N7	7.50	1.36	1.31
1	A	763	A	C8-N7	7.50	1.36	1.31
1	A	1556	A	C8-N7	7.50	1.36	1.31
1	A	1885	A	C8-N7	7.50	1.36	1.31
1	A	1989	A	C8-N7	7.50	1.36	1.31
32	W	604	A	C8-N7	7.50	1.36	1.31
32	W	1143	A	C8-N7	7.50	1.36	1.31
32	W	1160	A	C8-N7	7.50	1.36	1.31
32	W	329	A	C8-N7	7.50	1.36	1.31
1	A	2846	A	C8-N7	7.50	1.36	1.31
32	W	677	A	C8-N7	7.50	1.36	1.31
1	A	653	A	C8-N7	7.50	1.36	1.31
1	A	1097	A	C8-N7	7.50	1.36	1.31
1	A	1175	A	C8-N7	7.50	1.36	1.31
1	A	2049	A	C8-N7	7.50	1.36	1.31
1	A	2810	A	C8-N7	7.50	1.36	1.31
32	W	803	A	C8-N7	7.50	1.36	1.31
1	A	1388	A	C8-N7	7.49	1.36	1.31
1	A	2907	A	C8-N7	7.49	1.36	1.31
2	B	46	A	C8-N7	7.49	1.36	1.31
32	W	1523	A	C8-N7	7.49	1.36	1.31
1	A	91	A	C8-N7	7.49	1.36	1.31
1	A	964	A	C8-N7	7.49	1.36	1.31
1	A	1956	A	C8-N7	7.49	1.36	1.31
1	A	958	A	C8-N7	7.49	1.36	1.31
1	A	1222	A	C8-N7	7.49	1.36	1.31
1	A	2837	A	C8-N7	7.49	1.36	1.31
32	W	1206	A	C8-N7	7.49	1.36	1.31
32	W	1490	A	C8-N7	7.49	1.36	1.31
1	A	279	A	C8-N7	7.49	1.36	1.31
1	A	1235	A	C8-N7	7.49	1.36	1.31
1	A	1947	A	C8-N7	7.49	1.36	1.31
32	W	581	A	C8-N7	7.49	1.36	1.31
32	W	725	A	C8-N7	7.49	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2027	A	C8-N7	7.49	1.36	1.31
32	W	711	A	C8-N7	7.49	1.36	1.31
32	W	1185	A	C8-N7	7.49	1.36	1.31
1	A	324	A	C8-N7	7.49	1.36	1.31
1	A	699	A	C8-N7	7.49	1.36	1.31
1	A	1930	A	C8-N7	7.49	1.36	1.31
1	A	2876	A	C8-N7	7.49	1.36	1.31
32	W	463	A	C8-N7	7.49	1.36	1.31
1	A	12	A	C8-N7	7.48	1.36	1.31
1	A	236	A	C8-N7	7.48	1.36	1.31
1	A	1485	A	C8-N7	7.48	1.36	1.31
1	A	2734	A	C8-N7	7.48	1.36	1.31
32	W	969	A	C8-N7	7.48	1.36	1.31
1	A	1424	A	C8-N7	7.48	1.36	1.31
1	A	65	A	C8-N7	7.48	1.36	1.31
1	A	229	A	C8-N7	7.48	1.36	1.31
1	A	486	A	C8-N7	7.48	1.36	1.31
32	W	270	A	C8-N7	7.48	1.36	1.31
1	A	1685	A	C8-N7	7.48	1.36	1.31
1	A	870	A	C8-N7	7.48	1.36	1.31
1	A	1116	A	C8-N7	7.48	1.36	1.31
1	A	1233	A	C8-N7	7.48	1.36	1.31
1	A	1287	A	C8-N7	7.48	1.36	1.31
1	A	1672	A	C8-N7	7.48	1.36	1.31
1	A	2904	A	C8-N7	7.48	1.36	1.31
32	W	823	A	C8-N7	7.48	1.36	1.31
32	W	825	A	C8-N7	7.48	1.36	1.31
32	W	979	A	C8-N7	7.48	1.36	1.31
1	A	41	A	C8-N7	7.48	1.36	1.31
32	W	381	A	C8-N7	7.48	1.36	1.31
1	A	1802	A	C8-N7	7.47	1.36	1.31
32	W	685	A	C8-N7	7.47	1.36	1.31
32	W	1259	A	C8-N7	7.47	1.36	1.31
1	A	548	A	C8-N7	7.47	1.36	1.31
1	A	736	A	C8-N7	7.47	1.36	1.31
1	A	876	A	C8-N7	7.47	1.36	1.31
1	A	1480	A	C8-N7	7.47	1.36	1.31
1	A	1981	A	C8-N7	7.47	1.36	1.31
32	W	532	A	C8-N7	7.47	1.36	1.31
32	W	582	A	C8-N7	7.47	1.36	1.31
32	W	616	A	C8-N7	7.47	1.36	1.31
1	A	616	A	C8-N7	7.47	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1029	A	C8-N7	7.47	1.36	1.31
52	z	14	A	C8-N7	7.47	1.36	1.31
1	A	678	A	C8-N7	7.47	1.36	1.31
1	A	1286	A	C8-N7	7.47	1.36	1.31
1	A	1132	A	C8-N7	7.46	1.36	1.31
1	A	1421	A	C8-N7	7.46	1.36	1.31
1	A	2421	A	C8-N7	7.46	1.36	1.31
32	W	206	A	C8-N7	7.46	1.36	1.31
32	W	799	A	C8-N7	7.46	1.36	1.31
1	A	1945	A	C8-N7	7.46	1.36	1.31
1	A	2383	A	C8-N7	7.46	1.36	1.31
32	W	1383	A	C8-N7	7.46	1.36	1.31
1	A	260	A	C8-N7	7.46	1.36	1.31
1	A	275	A	C8-N7	7.46	1.36	1.31
1	A	343	A	C8-N7	7.46	1.36	1.31
1	A	637	A	C8-N7	7.46	1.36	1.31
32	W	35	A	C8-N7	7.46	1.36	1.31
1	A	525	A	C8-N7	7.46	1.36	1.31
1	A	889	A	C8-N7	7.46	1.36	1.31
1	A	2719	A	C8-N7	7.46	1.36	1.31
2	B	64	A	C8-N7	7.46	1.36	1.31
32	W	422	A	C8-N7	7.46	1.36	1.31
32	W	649	A	C8-N7	7.46	1.36	1.31
32	W	1260	A	C8-N7	7.46	1.36	1.31
1	A	412	A	C8-N7	7.46	1.36	1.31
1	A	1724	A	C8-N7	7.46	1.36	1.31
1	A	2694	A	C8-N7	7.46	1.36	1.31
1	A	2831	A	C8-N7	7.46	1.36	1.31
32	W	879	A	C8-N7	7.46	1.36	1.31
32	W	1297	A	C8-N7	7.46	1.36	1.31
32	W	1513	A	C8-N7	7.46	1.36	1.31
1	A	593	A	C8-N7	7.46	1.36	1.31
1	A	2100	A	C8-N7	7.46	1.36	1.31
1	A	2390	A	C8-N7	7.46	1.36	1.31
32	W	544	A	C8-N7	7.46	1.36	1.31
1	A	769	A	C8-N7	7.45	1.36	1.31
1	A	1745	A	C8-N7	7.45	1.36	1.31
1	A	438	A	C8-N7	7.45	1.36	1.31
1	A	1524	A	C8-N7	7.45	1.36	1.31
1	A	1675	A	C8-N7	7.45	1.36	1.31
32	W	195	A	C8-N7	7.45	1.36	1.31
32	W	323	A	C8-N7	7.45	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	743	A	C8-N7	7.45	1.36	1.31
32	W	988	A	C8-N7	7.45	1.36	1.31
1	A	220	A	C8-N7	7.45	1.36	1.31
1	A	449	A	C8-N7	7.45	1.36	1.31
1	A	519	A	C8-N7	7.45	1.36	1.31
1	A	740	A	C8-N7	7.45	1.36	1.31
1	A	1743	A	C8-N7	7.45	1.36	1.31
32	W	107	A	C8-N7	7.45	1.36	1.31
32	W	1103	A	C8-N7	7.45	1.36	1.31
32	W	1155	A	C8-N7	7.45	1.36	1.31
32	W	1528	A	C8-N7	7.45	1.36	1.31
1	A	830	A	C8-N7	7.45	1.36	1.31
1	A	1174	A	C8-N7	7.45	1.36	1.31
1	A	1631	A	C8-N7	7.45	1.36	1.31
1	A	274	A	C8-N7	7.45	1.36	1.31
1	A	758	A	C8-N7	7.45	1.36	1.31
1	A	1542	A	C8-N7	7.45	1.36	1.31
1	A	1606	A	C8-N7	7.45	1.36	1.31
1	A	1627	A	C8-N7	7.45	1.36	1.31
1	A	2302	A	C8-N7	7.45	1.36	1.31
32	W	919	A	C8-N7	7.45	1.36	1.31
32	W	572	A	C8-N7	7.44	1.36	1.31
1	A	198	A	C8-N7	7.44	1.36	1.31
1	A	1131	A	C8-N7	7.44	1.36	1.31
1	A	1325	A	C8-N7	7.44	1.36	1.31
1	A	1791	A	C8-N7	7.44	1.36	1.31
1	A	2018	A	C8-N7	7.44	1.36	1.31
2	B	71	A	C8-N7	7.44	1.36	1.31
32	W	1111	A	C8-N7	7.44	1.36	1.31
52	z	24	A	C8-N7	7.44	1.36	1.31
1	A	1809	A	C8-N7	7.44	1.36	1.31
32	W	592	A	C8-N7	7.44	1.36	1.31
1	A	1054	A	C8-N7	7.44	1.36	1.31
32	W	1294	A	C8-N7	7.44	1.36	1.31
1	A	318	A	C8-N7	7.44	1.36	1.31
1	A	1483	A	C8-N7	7.44	1.36	1.31
1	A	2059	A	C8-N7	7.44	1.36	1.31
1	A	2417	A	C8-N7	7.44	1.36	1.31
1	A	2517	A	C8-N7	7.44	1.36	1.31
32	W	1179	A	C8-N7	7.44	1.36	1.31
1	A	683	A	C8-N7	7.43	1.36	1.31
1	A	1723	A	C8-N7	7.43	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2066	A	C8-N7	7.43	1.36	1.31
32	W	1092	A	C8-N7	7.43	1.36	1.31
32	W	1455	A	C8-N7	7.43	1.36	1.31
1	A	2091	A	C8-N7	7.43	1.36	1.31
1	A	2296	A	C8-N7	7.43	1.36	1.31
1	A	2590	A	C8-N7	7.43	1.36	1.31
1	A	2924	A	C8-N7	7.43	1.36	1.31
32	W	776	A	C8-N7	7.43	1.36	1.31
1	A	882	A	C8-N7	7.43	1.36	1.31
1	A	974	A	C8-N7	7.43	1.36	1.31
1	A	770	A	C8-N7	7.43	1.36	1.31
1	A	1284	A	C8-N7	7.43	1.36	1.31
1	A	1721	A	C8-N7	7.43	1.36	1.31
1	A	1816	A	C8-N7	7.43	1.36	1.31
1	A	1848	A	C8-N7	7.43	1.36	1.31
1	A	2663	A	C8-N7	7.43	1.36	1.31
1	A	790	A	C8-N7	7.43	1.36	1.31
1	A	2560	A	C8-N7	7.43	1.36	1.31
1	A	715	A	C8-N7	7.43	1.36	1.31
1	A	2762	A	C8-N7	7.43	1.36	1.31
32	W	178	A	C8-N7	7.43	1.36	1.31
32	W	314	A	C8-N7	7.43	1.36	1.31
32	W	496	A	C8-N7	7.43	1.36	1.31
32	W	542	A	C8-N7	7.43	1.36	1.31
52	z	58	A	C8-N7	7.43	1.36	1.31
1	A	84	A	C8-N7	7.42	1.36	1.31
1	A	326	A	C8-N7	7.42	1.36	1.31
1	A	894	A	C8-N7	7.42	1.36	1.31
1	A	1569	A	C8-N7	7.42	1.36	1.31
1	A	1608	A	C8-N7	7.42	1.36	1.31
1	A	2851	A	C8-N7	7.42	1.36	1.31
1	A	2887	A	C8-N7	7.42	1.36	1.31
32	W	204	A	C8-N7	7.42	1.36	1.31
32	W	344	A	C8-N7	7.42	1.36	1.31
32	W	883	A	C8-N7	7.42	1.36	1.31
32	W	984	A	C8-N7	7.42	1.36	1.31
1	A	2365	A	C8-N7	7.42	1.36	1.31
1	A	38	A	C8-N7	7.42	1.36	1.31
1	A	193	A	C8-N7	7.42	1.36	1.31
1	A	1877	A	C8-N7	7.42	1.36	1.31
1	A	2276	A	C8-N7	7.42	1.36	1.31
1	A	2327	A	C8-N7	7.42	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	477	A	C8-N7	7.42	1.36	1.31
32	W	1366	A	C8-N7	7.42	1.36	1.31
1	A	475	A	C8-N7	7.42	1.36	1.31
1	A	1638	A	C8-N7	7.42	1.36	1.31
1	A	2787	A	C8-N7	7.42	1.36	1.31
32	W	768	A	C8-N7	7.42	1.36	1.31
32	W	1245	A	C8-N7	7.42	1.36	1.31
52	z	70	A	C8-N7	7.42	1.36	1.31
32	W	501	A	C8-N7	7.42	1.36	1.31
32	W	1115	A	C8-N7	7.42	1.36	1.31
1	A	561	A	C8-N7	7.42	1.36	1.31
1	A	2770	A	C8-N7	7.42	1.36	1.31
32	W	225	A	C8-N7	7.42	1.36	1.31
1	A	1654	A	C8-N7	7.41	1.36	1.31
32	W	306	A	C8-N7	7.41	1.36	1.31
1	A	13	A	C8-N7	7.41	1.36	1.31
1	A	156	A	C8-N7	7.41	1.36	1.31
1	A	1253	A	C8-N7	7.41	1.36	1.31
1	A	73	A	C8-N7	7.41	1.36	1.31
1	A	971	A	C8-N7	7.41	1.36	1.31
1	A	1593	A	C8-N7	7.41	1.36	1.31
1	A	2357	A	C8-N7	7.41	1.36	1.31
23	X	69	LYS	C-O	-7.41	1.09	1.23
32	W	1463	A	C8-N7	7.41	1.36	1.31
32	W	758	A	C8-N7	7.41	1.36	1.31
32	W	1028	A	C8-N7	7.41	1.36	1.31
1	A	431	A	C8-N7	7.41	1.36	1.31
1	A	2570	A	C8-N7	7.41	1.36	1.31
32	W	1205	A	C8-N7	7.41	1.36	1.31
1	A	1027	A	C8-N7	7.41	1.36	1.31
1	A	1686	A	C8-N7	7.41	1.36	1.31
32	W	1517	A	C8-N7	7.41	1.36	1.31
52	z	21	A	C8-N7	7.41	1.36	1.31
1	A	667	A	C8-N7	7.40	1.36	1.31
1	A	1323	A	C8-N7	7.40	1.36	1.31
1	A	2735	A	C8-N7	7.40	1.36	1.31
32	W	1403	A	C8-N7	7.40	1.36	1.31
1	A	1265	A	C8-N7	7.40	1.36	1.31
1	A	1998	A	C8-N7	7.40	1.36	1.31
2	B	51	A	C8-N7	7.40	1.36	1.31
32	W	72	A	C8-N7	7.40	1.36	1.31
1	A	28	A	C8-N7	7.40	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	A	C8-N7	7.40	1.36	1.31
1	A	1491	A	C8-N7	7.40	1.36	1.31
32	W	1283	A	C8-N7	7.40	1.36	1.31
1	A	943	A	C8-N7	7.40	1.36	1.31
1	A	1667	A	C8-N7	7.40	1.36	1.31
1	A	369	A	C8-N7	7.40	1.36	1.31
32	W	61	A	C8-N7	7.40	1.36	1.31
1	A	2511	A	C8-N7	7.39	1.36	1.31
32	W	644	A	C8-N7	7.39	1.36	1.31
1	A	2794	A	C8-N7	7.39	1.36	1.31
32	W	364	A	C8-N7	7.39	1.36	1.31
32	W	1200	A	C8-N7	7.39	1.36	1.31
1	A	171	A	C8-N7	7.39	1.36	1.31
1	A	278	A	C8-N7	7.39	1.36	1.31
2	B	43	A	C8-N7	7.39	1.36	1.31
32	W	1266	A	C8-N7	7.39	1.36	1.31
1	A	1059	A	C8-N7	7.39	1.36	1.31
1	A	1767	A	C8-N7	7.39	1.36	1.31
1	A	2854	A	C8-N7	7.39	1.36	1.31
32	W	440	A	C8-N7	7.39	1.36	1.31
32	W	1189	A	C8-N7	7.39	1.36	1.31
1	A	353	A	C8-N7	7.38	1.36	1.31
32	W	1270	A	C8-N7	7.38	1.36	1.31
1	A	1335	A	C8-N7	7.38	1.36	1.31
1	A	1398	A	C8-N7	7.38	1.36	1.31
1	A	2303	A	C8-N7	7.38	1.36	1.31
1	A	623	A	C8-N7	7.38	1.36	1.31
1	A	753	A	C8-N7	7.38	1.36	1.31
32	W	1161	A	C8-N7	7.38	1.36	1.31
1	A	268	A	C8-N7	7.38	1.36	1.31
32	W	335	A	C8-N7	7.38	1.36	1.31
32	W	1048	A	C8-N7	7.38	1.36	1.31
1	A	1918	A	C8-N7	7.38	1.36	1.31
1	A	2032	A	C8-N7	7.37	1.36	1.31
1	A	2708	A	C8-N7	7.37	1.36	1.31
32	W	555	A	C8-N7	7.37	1.36	1.31
32	W	1024	A	C8-N7	7.37	1.36	1.31
1	A	619	A	C8-N7	7.37	1.36	1.31
1	A	727	A	C8-N7	7.37	1.36	1.31
1	A	1149	A	C8-N7	7.37	1.36	1.31
32	W	519	A	C8-N7	7.37	1.36	1.31
32	W	828	A	C8-N7	7.37	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	1188	A	C8-N7	7.37	1.36	1.31
32	W	1349	A	C8-N7	7.37	1.36	1.31
1	A	355	A	C8-N7	7.37	1.36	1.31
1	A	2571	A	C8-N7	7.37	1.36	1.31
1	A	2848	A	C8-N7	7.37	1.36	1.31
1	A	2463	A	C8-N7	7.37	1.36	1.31
1	A	2497	A	C8-N7	7.37	1.36	1.31
1	A	1254	A	C8-N7	7.37	1.36	1.31
1	A	1423	A	C8-N7	7.37	1.36	1.31
1	A	2044	A	C8-N7	7.37	1.36	1.31
32	W	838	A	C8-N7	7.37	1.36	1.31
1	A	1316	A	C8-N7	7.36	1.36	1.31
1	A	2454	A	C8-N7	7.36	1.36	1.31
1	A	2700	A	C8-N7	7.36	1.36	1.31
32	W	337	A	C8-N7	7.36	1.36	1.31
1	A	1464	A	C8-N7	7.36	1.36	1.31
32	W	1493	A	C8-N7	7.36	1.36	1.31
32	W	1502	A	C8-N7	7.36	1.36	1.31
1	A	677	A	C8-N7	7.36	1.36	1.31
32	W	460	A	C8-N7	7.36	1.36	1.31
32	W	34	A	C8-N7	7.36	1.36	1.31
1	A	835	A	C8-N7	7.36	1.36	1.31
1	A	2616	A	C8-N7	7.36	1.36	1.31
1	A	2844	A	C8-N7	7.36	1.36	1.31
52	z	9	A	C8-N7	7.36	1.36	1.31
1	A	1100	A	C8-N7	7.35	1.36	1.31
1	A	1831	A	C8-N7	7.35	1.36	1.31
1	A	117	A	C8-N7	7.35	1.36	1.31
1	A	1072	A	C8-N7	7.35	1.36	1.31
32	W	74	A	C8-N7	7.35	1.36	1.31
1	A	459	A	C8-N7	7.35	1.36	1.31
1	A	1713	A	C8-N7	7.35	1.36	1.31
1	A	1581	A	C8-N7	7.35	1.36	1.31
2	B	97	A	C8-N7	7.35	1.36	1.31
32	W	433	A	C8-N7	7.35	1.36	1.31
1	A	2369	A	C8-N7	7.34	1.36	1.31
1	A	2658	A	C8-N7	7.34	1.36	1.31
32	W	1147	A	C8-N7	7.34	1.36	1.31
32	W	1479	A	C8-N7	7.34	1.36	1.31
32	W	12	A	C8-N7	7.34	1.36	1.31
1	A	746	A	C8-N7	7.34	1.36	1.31
1	A	1838	A	C8-N7	7.34	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1888	A	C8-N7	7.34	1.36	1.31
1	A	2340	A	C8-N7	7.34	1.36	1.31
1	A	2026	A	C8-N7	7.34	1.36	1.31
1	A	2464	A	C8-N7	7.34	1.36	1.31
1	A	206	A	C8-N7	7.34	1.36	1.31
1	A	2790	A	C8-N7	7.34	1.36	1.31
2	B	20	A	C8-N7	7.34	1.36	1.31
32	W	346	A	C8-N7	7.34	1.36	1.31
32	W	1442	A	C8-N7	7.34	1.36	1.31
1	A	868	A	C8-N7	7.33	1.36	1.31
32	W	1284	A	C8-N7	7.33	1.36	1.31
1	A	622	A	C8-N7	7.33	1.36	1.31
1	A	1075	A	C8-N7	7.33	1.36	1.31
32	W	672	A	C8-N7	7.33	1.36	1.31
1	A	1461	A	C8-N7	7.33	1.36	1.31
1	A	2786	A	C8-N7	7.33	1.36	1.31
1	A	2270	A	C8-N7	7.33	1.36	1.31
2	B	56	A	C8-N7	7.33	1.36	1.31
32	W	1004	A	C8-N7	7.33	1.36	1.31
1	A	1477	A	C8-N7	7.33	1.36	1.31
32	W	128	A	C8-N7	7.33	1.36	1.31
1	A	194	A	C8-N7	7.32	1.36	1.31
1	A	1260	A	C8-N7	7.32	1.36	1.31
1	A	2482	A	C8-N7	7.32	1.36	1.31
32	W	1166	A	C8-N7	7.32	1.36	1.31
1	A	90	A	C8-N7	7.32	1.36	1.31
1	A	1243	A	C8-N7	7.32	1.36	1.31
1	A	1965	A	C8-N7	7.32	1.36	1.31
1	A	2704	A	C8-N7	7.32	1.36	1.31
1	A	305	A	C8-N7	7.32	1.36	1.31
1	A	307	A	C8-N7	7.32	1.36	1.31
1	A	1046	A	C8-N7	7.32	1.36	1.31
1	A	1727	A	C8-N7	7.32	1.36	1.31
32	W	234	A	C8-N7	7.32	1.36	1.31
1	A	95	A	C8-N7	7.31	1.36	1.31
1	A	2405	A	C8-N7	7.31	1.36	1.31
32	W	1031	A	C8-N7	7.31	1.36	1.31
32	W	1296	A	C8-N7	7.31	1.36	1.31
1	A	140	A	C8-N7	7.31	1.36	1.31
1	A	1056	A	C8-N7	7.31	1.36	1.31
1	A	1221	A	C8-N7	7.30	1.36	1.31
1	A	1517	A	C8-N7	7.30	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1999	A	C8-N7	7.30	1.36	1.31
1	A	56	A	C8-N7	7.30	1.36	1.31
1	A	1047	A	C8-N7	7.29	1.36	1.31
32	W	911	A	C8-N7	7.29	1.36	1.31
1	A	2862	A	C8-N7	7.29	1.36	1.31
32	W	705	A	C8-N7	7.29	1.36	1.31
32	W	1369	A	C8-N7	7.29	1.36	1.31
1	A	517	A	C8-N7	7.29	1.36	1.31
1	A	634	A	C8-N7	7.29	1.36	1.31
1	A	1653	A	C8-N7	7.29	1.36	1.31
32	W	811	A	C8-N7	7.29	1.36	1.31
1	A	225	A	C8-N7	7.29	1.36	1.31
1	A	2106	A	C8-N7	7.29	1.36	1.31
1	A	1562	A	C8-N7	7.29	1.36	1.31
1	A	108	A	C8-N7	7.28	1.36	1.31
1	A	2782	A	C8-N7	7.28	1.36	1.31
32	W	518	A	C8-N7	7.28	1.36	1.31
1	A	1901	A	C8-N7	7.28	1.36	1.31
1	A	518	A	C8-N7	7.28	1.36	1.31
32	W	875	A	C8-N7	7.28	1.36	1.31
1	A	390	A	C8-N7	7.28	1.36	1.31
1	A	2689	A	C8-N7	7.28	1.36	1.31
32	W	727	A	C8-N7	7.28	1.36	1.31
1	A	2805	A	C8-N7	7.27	1.36	1.31
1	A	1404	A	C8-N7	7.27	1.36	1.31
32	W	1272	A	C8-N7	7.27	1.36	1.31
52	z	76	A	C8-N7	7.27	1.36	1.31
32	W	948	A	C8-N7	7.27	1.36	1.31
1	A	1042	A	C8-N7	7.26	1.36	1.31
1	A	1025	A	C8-N7	7.26	1.36	1.31
32	W	1112	A	C8-N7	7.26	1.36	1.31
1	A	690	A	C8-N7	7.26	1.36	1.31
1	A	913	A	C8-N7	7.26	1.36	1.31
1	A	1768	A	C8-N7	7.25	1.36	1.31
32	W	790	A	C8-N7	7.25	1.36	1.31
1	A	993	A	C8-N7	7.25	1.36	1.31
2	B	13	A	C8-N7	7.25	1.36	1.31
32	W	933	A	C8-N7	7.25	1.36	1.31
32	W	1341	A	C8-N7	7.25	1.36	1.31
1	A	724	A	C8-N7	7.25	1.36	1.31
1	A	1832	A	C8-N7	7.25	1.36	1.31
32	W	548	A	C8-N7	7.25	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	996	A	C8-N7	7.25	1.36	1.31
32	W	361	A	C8-N7	7.24	1.36	1.31
1	A	1575	A	C8-N7	7.24	1.36	1.31
32	W	94	A	C8-N7	7.24	1.36	1.31
32	W	287	A	C8-N7	7.24	1.36	1.31
32	W	918	A	C8-N7	7.24	1.36	1.31
32	W	1065	A	C8-N7	7.24	1.36	1.31
1	A	1813	A	C8-N7	7.24	1.36	1.31
1	A	2358	A	C8-N7	7.24	1.36	1.31
1	A	1620	A	C8-N7	7.23	1.36	1.31
1	A	254	A	C8-N7	7.23	1.36	1.31
1	A	2043	A	C8-N7	7.23	1.36	1.31
1	A	1073	A	C8-N7	7.22	1.36	1.31
1	A	2441	A	C8-N7	7.22	1.36	1.31
1	A	1021	A	C8-N7	7.22	1.36	1.31
1	A	110	A	C8-N7	7.22	1.36	1.31
32	W	462	A	C8-N7	7.22	1.36	1.31
1	A	1776	A	C8-N7	7.22	1.36	1.31
1	A	1453	A	C8-N7	7.21	1.36	1.31
1	A	1858	A	C8-N7	7.21	1.36	1.31
1	A	630	A	C8-N7	7.21	1.36	1.31
1	A	1760	A	C8-N7	7.21	1.36	1.31
1	A	2827	A	C8-N7	7.21	1.36	1.31
2	B	11	A	C8-N7	7.21	1.36	1.31
1	A	1619	A	C8-N7	7.21	1.36	1.31
32	W	114	A	C8-N7	7.21	1.36	1.31
1	A	600	A	C8-N7	7.20	1.36	1.31
1	A	1103	A	C8-N7	7.20	1.36	1.31
1	A	2436	A	C8-N7	7.20	1.36	1.31
1	A	752	A	C8-N7	7.20	1.36	1.31
1	A	1520	A	C8-N7	7.19	1.36	1.31
1	A	1967	A	C8-N7	7.19	1.36	1.31
1	A	2395	A	C8-N7	7.19	1.36	1.31
1	A	258	A	C8-N7	7.18	1.36	1.31
1	A	2402	A	C8-N7	7.18	1.36	1.31
1	A	866	A	C8-N7	7.18	1.36	1.31
1	A	661	A	C8-N7	7.18	1.36	1.31
1	A	578	A	C8-N7	7.17	1.36	1.31
32	W	1016	A	C8-N7	7.17	1.36	1.31
32	W	1315	A	C8-N7	7.17	1.36	1.31
32	W	1288	A	C8-N7	7.16	1.36	1.31
1	A	1680	A	C8-N7	7.16	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1691	A	C8-N7	7.16	1.36	1.31
32	W	57	A	C8-N7	7.16	1.36	1.31
1	A	689	A	C8-N7	7.16	1.36	1.31
1	A	956	A	C8-N7	7.16	1.36	1.31
1	A	1648	A	C8-N7	7.15	1.36	1.31
32	W	397	A	C8-N7	7.14	1.36	1.31
1	A	574	A	C8-N7	7.13	1.36	1.31
1	A	910	A	C8-N7	7.12	1.36	1.31
1	A	1839	A	C8-N7	7.12	1.36	1.31
1	A	1714	A	C8-N7	7.12	1.36	1.31
1	A	1820	A	C8-N7	7.12	1.36	1.31
1	A	2111	A	C8-N7	7.12	1.36	1.31
32	W	1234	A	C8-N7	7.11	1.36	1.31
1	A	1709	A	C8-N7	7.11	1.36	1.31
1	A	226	A	C8-N7	7.10	1.36	1.31
1	A	559	A	C8-N7	7.10	1.36	1.31
1	A	1094	A	C8-N7	7.10	1.36	1.31
32	W	161	A	C8-N7	7.09	1.36	1.31
32	W	76	A	C8-N7	7.09	1.36	1.31
1	A	1442	A	C8-N7	7.09	1.36	1.31
1	A	1618	A	C8-N7	7.09	1.36	1.31
1	A	538	A	C8-N7	7.07	1.36	1.31
1	A	1393	A	C8-N7	7.07	1.36	1.31
1	A	551	A	C8-N7	7.07	1.36	1.31
32	W	1478	A	C8-N7	7.05	1.36	1.31
1	A	1006	A	C8-N7	7.04	1.36	1.31
1	A	1691	A	N3-C4	7.04	1.39	1.34
32	W	993	A	N3-C4	7.04	1.39	1.34
1	A	935	A	C8-N7	7.03	1.36	1.31
1	A	1190	A	C8-N7	7.02	1.36	1.31
1	A	2468	A	C8-N7	6.99	1.36	1.31
32	W	391	A	C8-N7	6.99	1.36	1.31
1	A	44	A	N3-C4	6.98	1.39	1.34
32	W	405	A	C8-N7	6.98	1.36	1.31
32	W	308	A	C8-N7	6.98	1.36	1.31
1	A	1885	A	N3-C4	6.97	1.39	1.34
1	A	52	A	C8-N7	6.97	1.36	1.31
1	A	2459	A	C8-N7	6.97	1.36	1.31
32	W	572	A	N3-C4	6.97	1.39	1.34
1	A	168	A	C8-N7	6.94	1.36	1.31
1	A	1928	A	C8-N7	6.94	1.36	1.31
1	A	1094	A	N3-C4	6.93	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	404	A	N3-C4	6.93	1.39	1.34
32	W	405	A	N3-C4	6.92	1.39	1.34
1	A	922	A	N3-C4	6.92	1.39	1.34
1	A	1714	A	N3-C4	6.92	1.39	1.34
1	A	527	A	C8-N7	6.91	1.36	1.31
32	W	55	A	N3-C4	6.91	1.39	1.34
2	B	99	A	C8-N7	6.91	1.36	1.31
32	W	99	A	C8-N7	6.91	1.36	1.31
32	W	996	A	N3-C4	6.90	1.39	1.34
1	A	732	A	N3-C4	6.90	1.39	1.34
1	A	1900	A	N3-C4	6.90	1.39	1.34
1	A	1134	A	N3-C4	6.90	1.39	1.34
32	W	114	A	N3-C4	6.90	1.39	1.34
1	A	2407	A	C8-N7	6.89	1.36	1.31
32	W	541	A	N3-C4	6.88	1.39	1.34
32	W	1427	A	C8-N7	6.88	1.36	1.31
1	A	2786	A	N3-C4	6.87	1.39	1.34
1	A	2027	A	N3-C4	6.87	1.39	1.34
32	W	1298	A	N3-C4	6.87	1.39	1.34
1	A	278	A	N3-C4	6.87	1.39	1.34
32	W	902	A	N3-C4	6.86	1.39	1.34
1	A	1942	A	N3-C4	6.86	1.39	1.34
32	W	1178	A	N3-C4	6.85	1.39	1.34
32	W	1271	A	N3-C4	6.85	1.39	1.34
1	A	1302	A	N3-C4	6.84	1.39	1.34
32	W	202	A	N3-C4	6.84	1.39	1.34
1	A	530	A	N3-C4	6.84	1.39	1.34
1	A	1562	A	N3-C4	6.84	1.39	1.34
1	A	281	A	N3-C4	6.83	1.39	1.34
32	W	423	A	N3-C4	6.83	1.39	1.34
1	A	2358	A	N3-C4	6.82	1.39	1.34
1	A	2812	A	N3-C4	6.82	1.39	1.34
32	W	346	A	N3-C4	6.82	1.39	1.34
1	A	2349	A	N3-C4	6.82	1.39	1.34
1	A	2560	A	N3-C4	6.81	1.39	1.34
1	A	634	A	N3-C4	6.81	1.39	1.34
1	A	774	A	N3-C4	6.81	1.39	1.34
32	W	281	A	N3-C4	6.81	1.39	1.34
1	A	1130	A	N3-C4	6.81	1.39	1.34
1	A	2691	A	C8-N7	6.81	1.36	1.31
32	W	160	A	N3-C4	6.81	1.39	1.34
1	A	2831	A	N3-C4	6.80	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	1024	A	N3-C4	6.80	1.39	1.34
32	W	1234	A	N3-C4	6.80	1.39	1.34
1	A	2505	A	N3-C4	6.79	1.39	1.34
1	A	90	A	N3-C4	6.79	1.39	1.34
1	A	326	A	N3-C4	6.79	1.39	1.34
32	W	727	A	N3-C4	6.79	1.39	1.34
1	A	324	A	N3-C4	6.79	1.39	1.34
32	W	978	A	N3-C4	6.79	1.39	1.34
1	A	345	A	N3-C4	6.79	1.39	1.34
1	A	2924	A	N3-C4	6.79	1.39	1.34
32	W	1245	A	N3-C4	6.78	1.39	1.34
1	A	2405	A	N3-C4	6.78	1.39	1.34
1	A	226	A	N3-C4	6.78	1.39	1.34
32	W	321	A	N3-C4	6.78	1.39	1.34
1	A	1883	A	C8-N7	6.78	1.36	1.31
1	A	1134	A	C8-N7	6.77	1.36	1.31
32	W	1143	A	N3-C4	6.77	1.39	1.34
1	A	353	A	N3-C4	6.77	1.39	1.34
1	A	1025	A	N3-C4	6.77	1.39	1.34
2	B	20	A	N3-C4	6.77	1.39	1.34
32	W	1103	A	N3-C4	6.76	1.39	1.34
32	W	1308	A	C8-N7	6.76	1.36	1.31
1	A	1222	A	N3-C4	6.76	1.39	1.34
1	A	2338	A	N3-C4	6.76	1.39	1.34
1	A	526	A	N3-C4	6.76	1.39	1.34
1	A	2898	A	N3-C4	6.76	1.39	1.34
32	W	1256	A	N3-C4	6.76	1.39	1.34
1	A	2066	A	N3-C4	6.76	1.39	1.34
1	A	2030	A	N3-C4	6.75	1.39	1.34
1	A	1316	A	N3-C4	6.75	1.39	1.34
1	A	2893	A	N3-C4	6.75	1.39	1.34
1	A	2402	A	N3-C4	6.75	1.38	1.34
1	A	307	A	N3-C4	6.75	1.38	1.34
1	A	2339	A	N3-C4	6.75	1.38	1.34
32	W	74	A	N3-C4	6.75	1.38	1.34
1	A	553	A	N3-C4	6.75	1.38	1.34
1	A	673	A	C8-N7	6.75	1.36	1.31
1	A	1760	A	N3-C4	6.74	1.38	1.34
1	A	2844	A	N3-C4	6.74	1.38	1.34
1	A	2916	A	N3-C4	6.74	1.38	1.34
1	A	1524	A	N3-C4	6.74	1.38	1.34
1	A	2059	A	N3-C4	6.74	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	705	A	N3-C4	6.74	1.38	1.34
32	W	979	A	N3-C4	6.74	1.38	1.34
32	W	793	A	N3-C4	6.74	1.38	1.34
32	W	1308	A	N3-C4	6.74	1.38	1.34
2	B	71	A	N3-C4	6.74	1.38	1.34
1	A	500	A	N3-C4	6.73	1.38	1.34
1	A	2830	A	N3-C4	6.73	1.38	1.34
2	B	11	A	N3-C4	6.73	1.38	1.34
2	B	64	A	N3-C4	6.73	1.38	1.34
32	W	1289	A	N3-C4	6.73	1.38	1.34
1	A	2827	A	N3-C4	6.73	1.38	1.34
32	W	1155	A	N3-C4	6.73	1.38	1.34
32	W	1225	A	N3-C4	6.73	1.38	1.34
1	A	1326	A	N3-C4	6.73	1.38	1.34
1	A	1877	A	N3-C4	6.73	1.38	1.34
32	W	389	A	N3-C4	6.73	1.38	1.34
1	A	373	A	N3-C4	6.73	1.38	1.34
1	A	407	A	N3-C4	6.73	1.38	1.34
1	A	2047	A	N3-C4	6.73	1.38	1.34
1	A	948	A	N3-C4	6.73	1.38	1.34
32	W	507	A	N3-C4	6.72	1.38	1.34
1	A	1360	A	N3-C4	6.72	1.38	1.34
32	W	799	A	N3-C4	6.72	1.38	1.34
1	A	339	A	N3-C4	6.72	1.38	1.34
1	A	1556	A	N3-C4	6.72	1.38	1.34
32	W	270	A	N3-C4	6.72	1.38	1.34
1	A	679	A	C8-N7	6.72	1.36	1.31
1	A	970	A	N3-C4	6.72	1.38	1.34
1	A	1677	A	N3-C4	6.72	1.38	1.34
1	A	2862	A	N3-C4	6.71	1.38	1.34
2	B	18	A	N3-C4	6.71	1.38	1.34
32	W	1026	A	C8-N7	6.71	1.36	1.31
32	W	1147	A	N3-C4	6.71	1.38	1.34
1	A	1710	A	N3-C4	6.71	1.38	1.34
32	W	649	A	N3-C4	6.71	1.38	1.34
52	z	37	A	C8-N7	6.71	1.36	1.31
1	A	449	A	N3-C4	6.71	1.38	1.34
1	A	559	A	N3-C4	6.71	1.38	1.34
32	W	1502	A	N3-C4	6.71	1.38	1.34
32	W	1528	A	N3-C4	6.71	1.38	1.34
1	A	2497	A	N3-C4	6.70	1.38	1.34
1	A	2700	A	N3-C4	6.70	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	1358	A	N3-C4	6.70	1.38	1.34
1	A	1483	A	N3-C4	6.70	1.38	1.34
1	A	2480	A	N3-C4	6.70	1.38	1.34
1	A	185	A	N3-C4	6.70	1.38	1.34
1	A	1654	A	N3-C4	6.70	1.38	1.34
1	A	1197	A	N3-C4	6.69	1.38	1.34
1	A	1709	A	N3-C4	6.69	1.38	1.34
1	A	2381	A	N3-C4	6.69	1.38	1.34
32	W	933	A	N3-C4	6.69	1.38	1.34
1	A	1672	A	N3-C4	6.69	1.38	1.34
1	A	2845	A	N3-C4	6.69	1.38	1.34
32	W	519	A	N3-C4	6.69	1.38	1.34
32	W	1278	A	C8-N7	6.69	1.36	1.31
1	A	95	A	N3-C4	6.69	1.38	1.34
32	W	128	A	N3-C4	6.69	1.38	1.34
32	W	721	A	N3-C4	6.69	1.38	1.34
1	A	575	A	N3-C4	6.69	1.38	1.34
1	A	2869	A	N3-C4	6.69	1.38	1.34
32	W	987	A	N3-C4	6.69	1.38	1.34
32	W	1327	A	N3-C4	6.69	1.38	1.34
1	A	1375	A	N3-C4	6.68	1.38	1.34
2	B	13	A	N3-C4	6.68	1.38	1.34
1	A	1381	A	N3-C4	6.68	1.38	1.34
1	A	1858	A	N3-C4	6.68	1.38	1.34
1	A	913	A	N3-C4	6.68	1.38	1.34
32	W	638	A	N3-C4	6.68	1.38	1.34
32	W	801	A	N3-C4	6.68	1.38	1.34
1	A	593	A	N3-C4	6.68	1.38	1.34
1	A	952	A	N3-C4	6.68	1.38	1.34
32	W	611	A	N3-C4	6.68	1.38	1.34
1	A	1814	A	N3-C4	6.68	1.38	1.34
32	W	1512	A	N3-C4	6.68	1.38	1.34
1	A	2461	A	N3-C4	6.67	1.38	1.34
32	W	658	A	N3-C4	6.67	1.38	1.34
32	W	1348	A	N3-C4	6.67	1.38	1.34
32	W	1297	A	N3-C4	6.67	1.38	1.34
1	A	1103	A	N3-C4	6.67	1.38	1.34
1	A	2885	A	C8-N7	6.67	1.36	1.31
1	A	524	A	N3-C4	6.67	1.38	1.34
1	A	2500	A	N3-C4	6.67	1.38	1.34
1	A	6	A	N3-C4	6.67	1.38	1.34
1	A	2511	A	N3-C4	6.67	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2694	A	N3-C4	6.67	1.38	1.34
52	z	9	A	N3-C4	6.67	1.38	1.34
1	A	459	A	N3-C4	6.67	1.38	1.34
1	A	1392	A	N3-C4	6.67	1.38	1.34
1	A	2447	A	N3-C4	6.67	1.38	1.34
1	A	618	A	N3-C4	6.66	1.38	1.34
32	W	99	A	N3-C4	6.66	1.38	1.34
1	A	1906	A	N3-C4	6.66	1.38	1.34
1	A	1945	A	N3-C4	6.66	1.38	1.34
1	A	600	A	N3-C4	6.66	1.38	1.34
1	A	910	A	N3-C4	6.66	1.38	1.34
1	A	2383	A	N3-C4	6.66	1.38	1.34
32	W	1435	A	N3-C4	6.66	1.38	1.34
1	A	2854	A	N3-C4	6.66	1.38	1.34
1	A	130	A	N3-C4	6.66	1.38	1.34
1	A	867	A	N3-C4	6.66	1.38	1.34
1	A	1005	A	N3-C4	6.66	1.38	1.34
1	A	2317	A	N3-C4	6.66	1.38	1.34
2	B	46	A	N3-C4	6.66	1.38	1.34
32	W	94	A	N3-C4	6.66	1.38	1.34
32	W	659	A	N3-C4	6.65	1.38	1.34
32	W	1470	A	N3-C4	6.65	1.38	1.34
1	A	753	A	N3-C4	6.65	1.38	1.34
1	A	1113	A	N3-C4	6.65	1.38	1.34
1	A	168	A	N3-C4	6.65	1.38	1.34
1	A	538	A	N3-C4	6.65	1.38	1.34
1	A	1144	A	N3-C4	6.65	1.38	1.34
32	W	234	A	N3-C4	6.65	1.38	1.34
32	W	1017	A	N3-C4	6.65	1.38	1.34
32	W	151	A	N3-C4	6.64	1.38	1.34
32	W	677	A	N3-C4	6.64	1.38	1.34
32	W	928	A	N3-C4	6.64	1.38	1.34
1	A	1092	A	N3-C4	6.64	1.38	1.34
1	A	1340	A	N3-C4	6.64	1.38	1.34
1	A	1844	A	N3-C4	6.64	1.38	1.34
1	A	2571	A	N3-C4	6.64	1.38	1.34
1	A	2662	A	N3-C4	6.64	1.38	1.34
32	W	62	A	N3-C4	6.64	1.38	1.34
32	W	711	A	N3-C4	6.64	1.38	1.34
1	A	14	A	N3-C4	6.64	1.38	1.34
1	A	52	A	N3-C4	6.64	1.38	1.34
1	A	1700	A	N3-C4	6.64	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	672	A	N3-C4	6.64	1.38	1.34
1	A	231	A	N3-C4	6.64	1.38	1.34
32	W	831	A	N3-C4	6.64	1.38	1.34
32	W	1488	A	N3-C4	6.64	1.38	1.34
1	A	1312	A	N3-C4	6.64	1.38	1.34
1	A	551	A	N3-C4	6.64	1.38	1.34
1	A	1536	A	N3-C4	6.64	1.38	1.34
32	W	500	A	N3-C4	6.64	1.38	1.34
1	A	229	A	N3-C4	6.63	1.38	1.34
1	A	646	A	N3-C4	6.63	1.38	1.34
1	A	1588	A	N3-C4	6.63	1.38	1.34
1	A	219	A	N3-C4	6.63	1.38	1.34
1	A	1084	A	N3-C4	6.63	1.38	1.34
1	A	935	A	N3-C4	6.63	1.38	1.34
1	A	236	A	N3-C4	6.63	1.38	1.34
1	A	1258	A	N3-C4	6.63	1.38	1.34
1	A	2479	A	N3-C4	6.63	1.38	1.34
32	W	364	A	N3-C4	6.63	1.38	1.34
32	W	886	A	N3-C4	6.63	1.38	1.34
1	A	202	A	N3-C4	6.63	1.38	1.34
1	A	1638	A	N3-C4	6.63	1.38	1.34
1	A	1685	A	N3-C4	6.63	1.38	1.34
1	A	1838	A	N3-C4	6.63	1.38	1.34
1	A	1456	A	N3-C4	6.62	1.38	1.34
1	A	1925	A	N3-C4	6.62	1.38	1.34
1	A	762	A	N3-C4	6.62	1.38	1.34
32	W	1294	A	N3-C4	6.62	1.38	1.34
1	A	254	A	N3-C4	6.62	1.38	1.34
1	A	781	A	N3-C4	6.62	1.38	1.34
1	A	1506	A	N3-C4	6.62	1.38	1.34
1	A	1614	A	N3-C4	6.62	1.38	1.34
32	W	1284	A	N3-C4	6.62	1.38	1.34
1	A	1464	A	N3-C4	6.62	1.38	1.34
32	W	12	A	N3-C4	6.62	1.38	1.34
1	A	330	A	N3-C4	6.62	1.38	1.34
1	A	1876	A	N3-C4	6.62	1.38	1.34
32	W	771	A	N3-C4	6.62	1.38	1.34
32	W	1205	A	N3-C4	6.62	1.38	1.34
32	W	899	A	N3-C4	6.62	1.38	1.34
1	A	124	A	N3-C4	6.62	1.38	1.34
1	A	894	A	N3-C4	6.62	1.38	1.34
1	A	1404	A	N3-C4	6.62	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	A	N3-C4	6.61	1.38	1.34
1	A	513	A	N3-C4	6.61	1.38	1.34
1	A	1585	A	N3-C4	6.61	1.38	1.34
32	W	1490	A	N3-C4	6.61	1.38	1.34
32	W	1509	A	N3-C4	6.61	1.38	1.34
1	A	999	A	N3-C4	6.61	1.38	1.34
1	A	2846	A	N3-C4	6.61	1.38	1.34
1	A	302	A	N3-C4	6.61	1.38	1.34
1	A	418	A	N3-C4	6.61	1.38	1.34
1	A	486	A	N3-C4	6.61	1.38	1.34
1	A	504	A	N3-C4	6.61	1.38	1.34
1	A	513	A	C8-N7	6.61	1.36	1.31
1	A	2044	A	N3-C4	6.61	1.38	1.34
32	W	335	A	N3-C4	6.61	1.38	1.34
1	A	678	A	N3-C4	6.61	1.38	1.34
1	A	2407	A	N3-C4	6.61	1.38	1.34
32	W	225	A	N3-C4	6.61	1.38	1.34
52	z	23	A	N3-C4	6.61	1.38	1.34
1	A	2362	A	N3-C4	6.61	1.38	1.34
32	W	730	A	N3-C4	6.61	1.38	1.34
1	A	21	A	N3-C4	6.60	1.38	1.34
1	A	548	A	N3-C4	6.60	1.38	1.34
1	A	1989	A	N3-C4	6.60	1.38	1.34
1	A	247	A	N3-C4	6.60	1.38	1.34
1	A	438	A	N3-C4	6.60	1.38	1.34
1	A	1188	A	N3-C4	6.60	1.38	1.34
1	A	2463	A	N3-C4	6.60	1.38	1.34
32	W	139	A	N3-C4	6.60	1.38	1.34
1	A	61	A	N3-C4	6.60	1.38	1.34
1	A	171	A	N3-C4	6.60	1.38	1.34
1	A	462	A	N3-C4	6.60	1.38	1.34
1	A	616	A	N3-C4	6.60	1.38	1.34
1	A	782	A	N3-C4	6.60	1.38	1.34
1	A	1357	A	N3-C4	6.60	1.38	1.34
32	W	344	A	N3-C4	6.60	1.38	1.34
32	W	947	A	N3-C4	6.60	1.38	1.34
1	A	38	A	N3-C4	6.60	1.38	1.34
1	A	1284	A	N3-C4	6.60	1.38	1.34
32	W	1004	A	N3-C4	6.60	1.38	1.34
1	A	1661	A	C8-N7	6.59	1.36	1.31
1	A	1713	A	N3-C4	6.59	1.38	1.34
1	A	1746	A	N3-C4	6.59	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1947	A	N3-C4	6.59	1.38	1.34
1	A	2619	A	N3-C4	6.59	1.38	1.34
32	W	475	A	N3-C4	6.59	1.38	1.34
32	W	618	A	N3-C4	6.59	1.38	1.34
32	W	823	A	N3-C4	6.59	1.38	1.34
1	A	456	A	N3-C4	6.59	1.38	1.34
1	A	673	A	N3-C4	6.59	1.38	1.34
1	A	198	A	N3-C4	6.59	1.38	1.34
1	A	947	A	N3-C4	6.59	1.38	1.34
1	A	1615	A	N3-C4	6.59	1.38	1.34
32	W	282	A	N3-C4	6.59	1.38	1.34
32	W	440	A	N3-C4	6.59	1.38	1.34
32	W	504	A	N3-C4	6.59	1.38	1.34
52	z	24	A	N3-C4	6.59	1.38	1.34
1	A	1029	A	N3-C4	6.59	1.38	1.34
1	A	1230	A	N3-C4	6.59	1.38	1.34
32	W	1443	A	N3-C4	6.59	1.38	1.34
1	A	2060	A	N3-C4	6.59	1.38	1.34
1	A	2091	A	N3-C4	6.59	1.38	1.34
32	W	452	A	N3-C4	6.59	1.38	1.34
1	A	1957	A	N3-C4	6.59	1.38	1.34
1	A	2629	A	N3-C4	6.59	1.38	1.34
1	A	2778	A	N3-C4	6.59	1.38	1.34
1	A	2834	A	N3-C4	6.59	1.38	1.34
32	W	704	A	N3-C4	6.59	1.38	1.34
1	A	1655	A	N3-C4	6.58	1.38	1.34
32	W	757	A	N3-C4	6.58	1.38	1.34
1	A	1631	A	N3-C4	6.58	1.38	1.34
32	W	61	A	N3-C4	6.58	1.38	1.34
32	W	838	A	N3-C4	6.58	1.38	1.34
32	W	1320	A	N3-C4	6.58	1.38	1.34
1	A	1406	A	N3-C4	6.58	1.38	1.34
1	A	1581	A	N3-C4	6.58	1.38	1.34
1	A	1695	A	N3-C4	6.58	1.38	1.34
1	A	1815	A	N3-C4	6.58	1.38	1.34
1	A	2740	A	N3-C4	6.58	1.38	1.34
32	W	208	A	N3-C4	6.58	1.38	1.34
32	W	419	A	N3-C4	6.58	1.38	1.34
32	W	1341	A	N3-C4	6.58	1.38	1.34
1	A	964	A	N3-C4	6.58	1.38	1.34
1	A	1398	A	N3-C4	6.58	1.38	1.34
32	W	491	A	N3-C4	6.58	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	893	A	N3-C4	6.58	1.38	1.34
1	A	1116	A	N3-C4	6.58	1.38	1.34
1	A	2782	A	N3-C4	6.58	1.38	1.34
32	W	1222	A	N3-C4	6.58	1.38	1.34
1	A	2532	A	N3-C4	6.58	1.38	1.34
32	W	1451	A	N3-C4	6.58	1.38	1.34
1	A	494	A	N3-C4	6.58	1.38	1.34
1	A	2590	A	N3-C4	6.58	1.38	1.34
1	A	578	A	N3-C4	6.57	1.38	1.34
1	A	630	A	N3-C4	6.57	1.38	1.34
1	A	1308	A	N3-C4	6.57	1.38	1.34
1	A	1619	A	N3-C4	6.57	1.38	1.34
1	A	2627	A	N3-C4	6.57	1.38	1.34
2	B	50	A	N3-C4	6.57	1.38	1.34
1	A	314	A	N3-C4	6.57	1.38	1.34
1	A	2670	A	N3-C4	6.57	1.38	1.34
1	A	428	A	N3-C4	6.57	1.38	1.34
1	A	763	A	N3-C4	6.57	1.38	1.34
1	A	1006	A	N3-C4	6.57	1.38	1.34
1	A	1194	A	N3-C4	6.57	1.38	1.34
1	A	1235	A	N3-C4	6.57	1.38	1.34
1	A	1724	A	N3-C4	6.57	1.38	1.34
32	W	34	A	N3-C4	6.57	1.38	1.34
32	W	397	A	N3-C4	6.57	1.38	1.34
32	W	1236	A	N3-C4	6.57	1.38	1.34
1	A	765	A	N3-C4	6.57	1.38	1.34
1	A	835	A	N3-C4	6.57	1.38	1.34
1	A	1533	A	N3-C4	6.57	1.38	1.34
1	A	2083	A	N3-C4	6.57	1.38	1.34
1	A	2330	A	N3-C4	6.57	1.38	1.34
2	B	99	A	N3-C4	6.57	1.38	1.34
32	W	52	A	N3-C4	6.57	1.38	1.34
32	W	401	A	N3-C4	6.57	1.38	1.34
1	A	244	A	N3-C4	6.57	1.38	1.34
1	A	525	A	N3-C4	6.57	1.38	1.34
1	A	1540	A	N3-C4	6.57	1.38	1.34
32	W	948	A	N3-C4	6.57	1.38	1.34
1	A	543	A	N3-C4	6.56	1.38	1.34
1	A	1426	A	N3-C4	6.56	1.38	1.34
1	A	2708	A	N3-C4	6.56	1.38	1.34
1	A	2722	A	N3-C4	6.56	1.38	1.34
1	A	2754	A	N3-C4	6.56	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	1065	A	N3-C4	6.56	1.38	1.34
1	A	133	A	N3-C4	6.56	1.38	1.34
1	A	1253	A	N3-C4	6.56	1.38	1.34
1	A	518	A	N3-C4	6.56	1.38	1.34
1	A	1813	A	N3-C4	6.56	1.38	1.34
1	A	2887	A	N3-C4	6.56	1.38	1.34
32	W	975	A	N3-C4	6.56	1.38	1.34
32	W	1266	A	N3-C4	6.56	1.38	1.34
32	W	1355	A	N3-C4	6.56	1.38	1.34
1	A	1305	A	N3-C4	6.56	1.38	1.34
1	A	1490	A	N3-C4	6.56	1.38	1.34
32	W	875	A	N3-C4	6.56	1.38	1.34
32	W	1014	A	N3-C4	6.56	1.38	1.34
32	W	1056	A	N3-C4	6.56	1.38	1.34
32	W	1213	A	N3-C4	6.56	1.38	1.34
52	z	70	A	N3-C4	6.56	1.38	1.34
1	A	1042	A	N3-C4	6.56	1.38	1.34
1	A	94	A	N3-C4	6.55	1.38	1.34
1	A	527	A	N3-C4	6.55	1.38	1.34
1	A	1339	A	N3-C4	6.55	1.38	1.34
1	A	2351	A	N3-C4	6.55	1.38	1.34
1	A	2627	A	C8-N7	6.55	1.36	1.31
32	W	290	A	N3-C4	6.55	1.38	1.34
32	W	522	A	N3-C4	6.55	1.38	1.34
32	W	959	A	N3-C4	6.55	1.38	1.34
32	W	1128	A	N3-C4	6.55	1.38	1.34
1	A	1073	A	N3-C4	6.55	1.38	1.34
32	W	439	A	N3-C4	6.55	1.38	1.34
32	W	1206	A	N3-C4	6.55	1.38	1.34
1	A	475	A	N3-C4	6.55	1.38	1.34
1	A	1075	A	N3-C4	6.55	1.38	1.34
1	A	1347	A	N3-C4	6.55	1.38	1.34
32	W	762	A	N3-C4	6.55	1.38	1.34
32	W	1403	A	N3-C4	6.55	1.38	1.34
1	A	537	A	N3-C4	6.55	1.38	1.34
1	A	592	A	N3-C4	6.55	1.38	1.34
1	A	1453	A	N3-C4	6.55	1.38	1.34
32	W	415	A	N3-C4	6.55	1.38	1.34
32	W	433	A	N3-C4	6.55	1.38	1.34
1	A	770	A	N3-C4	6.55	1.38	1.34
1	A	1434	A	N3-C4	6.55	1.38	1.34
32	W	178	A	N3-C4	6.55	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	422	A	N3-C4	6.55	1.38	1.34
32	W	532	A	N3-C4	6.55	1.38	1.34
32	W	31	A	N3-C4	6.55	1.38	1.34
1	A	469	A	N3-C4	6.54	1.38	1.34
1	A	2904	A	N3-C4	6.54	1.38	1.34
32	W	758	A	N3-C4	6.54	1.38	1.34
1	A	1047	A	N3-C4	6.54	1.38	1.34
1	A	1243	A	N3-C4	6.54	1.38	1.34
1	A	1653	A	N3-C4	6.54	1.38	1.34
1	A	1743	A	N3-C4	6.54	1.38	1.34
1	A	2900	A	N3-C4	6.54	1.38	1.34
32	W	501	A	N3-C4	6.54	1.38	1.34
1	A	429	A	N3-C4	6.54	1.38	1.34
1	A	1995	A	N3-C4	6.54	1.38	1.34
32	W	361	A	N3-C4	6.54	1.38	1.34
32	W	616	A	N3-C4	6.54	1.38	1.34
32	W	913	A	N3-C4	6.54	1.38	1.34
1	A	126	A	N3-C4	6.54	1.38	1.34
2	B	44	A	N3-C4	6.54	1.38	1.34
32	W	1200	A	N3-C4	6.54	1.38	1.34
1	A	866	A	N3-C4	6.54	1.38	1.34
1	A	1361	A	N3-C4	6.54	1.38	1.34
1	A	2042	A	N3-C4	6.54	1.38	1.34
1	A	2668	A	N3-C4	6.54	1.38	1.34
32	W	323	A	N3-C4	6.54	1.38	1.34
32	W	690	A	N3-C4	6.54	1.38	1.34
52	z	41	A	N3-C4	6.54	1.38	1.34
1	A	987	A	N3-C4	6.54	1.38	1.34
32	W	150	A	N3-C4	6.54	1.38	1.34
1	A	2923	A	N3-C4	6.54	1.38	1.34
32	W	1383	A	N3-C4	6.54	1.38	1.34
1	A	974	A	N3-C4	6.53	1.38	1.34
1	A	1405	A	N3-C4	6.53	1.38	1.34
1	A	1941	A	N3-C4	6.53	1.38	1.34
1	A	2343	A	N3-C4	6.53	1.38	1.34
1	A	2356	A	N3-C4	6.53	1.38	1.34
32	W	1121	A	N3-C4	6.53	1.38	1.34
32	W	776	A	N3-C4	6.53	1.38	1.34
1	A	210	A	N3-C4	6.53	1.38	1.34
1	A	652	A	N3-C4	6.53	1.38	1.34
1	A	661	A	N3-C4	6.53	1.38	1.34
1	A	1224	A	N3-C4	6.53	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2794	A	N3-C4	6.53	1.38	1.34
32	W	173	A	N3-C4	6.53	1.38	1.34
32	W	266	A	N3-C4	6.53	1.38	1.34
1	A	1812	A	N3-C4	6.53	1.38	1.34
32	W	306	A	N3-C4	6.53	1.38	1.34
32	W	1111	A	N3-C4	6.53	1.38	1.34
1	A	724	A	N3-C4	6.53	1.38	1.34
1	A	1845	A	N3-C4	6.53	1.38	1.34
32	W	506	A	N3-C4	6.53	1.38	1.34
32	W	1407	A	N3-C4	6.53	1.38	1.34
1	A	1569	A	N3-C4	6.53	1.38	1.34
1	A	2315	A	N3-C4	6.53	1.38	1.34
32	W	518	A	N3-C4	6.53	1.38	1.34
32	W	240	A	N3-C4	6.52	1.38	1.34
32	W	1328	A	N3-C4	6.52	1.38	1.34
52	z	58	A	N3-C4	6.52	1.38	1.34
1	A	715	A	N3-C4	6.52	1.38	1.34
1	A	1323	A	N3-C4	6.52	1.38	1.34
2	B	51	A	N3-C4	6.52	1.38	1.34
1	A	2365	A	N3-C4	6.52	1.38	1.34
32	W	457	A	N3-C4	6.52	1.38	1.34
32	W	1541	A	N3-C4	6.52	1.38	1.34
1	A	49	A	N3-C4	6.52	1.38	1.34
1	A	479	A	N3-C4	6.52	1.38	1.34
1	A	868	A	N3-C4	6.52	1.38	1.34
1	A	888	A	N3-C4	6.52	1.38	1.34
1	A	1930	A	N3-C4	6.52	1.38	1.34
1	A	2270	A	N3-C4	6.52	1.38	1.34
1	A	322	A	N3-C4	6.52	1.38	1.34
1	A	476	A	N3-C4	6.52	1.38	1.34
1	A	623	A	N3-C4	6.52	1.38	1.34
1	A	2316	A	N3-C4	6.52	1.38	1.34
1	A	2441	A	N3-C4	6.52	1.38	1.34
32	W	195	A	N3-C4	6.52	1.38	1.34
32	W	685	A	N3-C4	6.52	1.38	1.34
1	A	139	A	N3-C4	6.52	1.38	1.34
1	A	2006	A	N3-C4	6.52	1.38	1.34
32	W	542	A	N3-C4	6.52	1.38	1.34
32	W	544	A	N3-C4	6.52	1.38	1.34
1	A	41	A	N3-C4	6.51	1.38	1.34
1	A	1680	A	N3-C4	6.51	1.38	1.34
1	A	2542	A	N3-C4	6.51	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	189	A	N3-C4	6.51	1.38	1.34
32	W	1180	A	N3-C4	6.51	1.38	1.34
1	A	752	A	N3-C4	6.51	1.38	1.34
32	W	1022	A	N3-C4	6.51	1.38	1.34
1	A	390	A	N3-C4	6.51	1.38	1.34
1	A	1066	A	N3-C4	6.51	1.38	1.34
1	A	1174	A	N3-C4	6.51	1.38	1.34
1	A	1516	A	N3-C4	6.51	1.38	1.34
1	A	1580	A	N3-C4	6.51	1.38	1.34
1	A	1617	A	N3-C4	6.51	1.38	1.34
1	A	1850	A	N3-C4	6.51	1.38	1.34
1	A	2307	A	N3-C4	6.51	1.38	1.34
32	W	308	A	N3-C4	6.51	1.38	1.34
32	W	1259	A	N3-C4	6.51	1.38	1.34
1	A	1480	A	N3-C4	6.51	1.38	1.34
1	A	2735	A	N3-C4	6.51	1.38	1.34
32	W	67	A	N3-C4	6.51	1.38	1.34
32	W	548	A	N3-C4	6.51	1.38	1.34
32	W	1102	A	N3-C4	6.51	1.38	1.34
1	A	991	A	N3-C4	6.51	1.38	1.34
1	A	1036	A	N3-C4	6.51	1.38	1.34
32	W	911	A	N3-C4	6.51	1.38	1.34
32	W	1315	A	N3-C4	6.51	1.38	1.34
1	A	384	A	N3-C4	6.51	1.38	1.34
1	A	470	A	N3-C4	6.51	1.38	1.34
1	A	870	A	N3-C4	6.51	1.38	1.34
1	A	1809	A	N3-C4	6.51	1.38	1.34
1	A	1914	A	N3-C4	6.50	1.38	1.34
32	W	206	A	N3-C4	6.50	1.38	1.34
32	W	1366	A	N3-C4	6.50	1.38	1.34
32	W	1386	A	N3-C4	6.50	1.38	1.34
1	A	904	A	N3-C4	6.50	1.38	1.34
32	W	53	A	N3-C4	6.50	1.38	1.34
32	W	203	A	N3-C4	6.50	1.38	1.34
32	W	496	A	N3-C4	6.50	1.38	1.34
1	A	1667	A	N3-C4	6.50	1.38	1.34
1	A	2049	A	N3-C4	6.50	1.38	1.34
1	A	2375	A	N3-C4	6.50	1.38	1.34
32	W	72	A	N3-C4	6.50	1.38	1.34
32	W	140	A	N3-C4	6.50	1.38	1.34
32	W	713	A	N3-C4	6.50	1.38	1.34
32	W	1478	A	N3-C4	6.50	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1027	A	N3-C4	6.50	1.38	1.34
1	A	1593	A	N3-C4	6.50	1.38	1.34
32	W	679	A	N3-C4	6.50	1.38	1.34
32	W	1133	A	N3-C4	6.50	1.38	1.34
1	A	736	A	N3-C4	6.50	1.38	1.34
1	A	1491	A	N3-C4	6.50	1.38	1.34
1	A	1517	A	N3-C4	6.50	1.38	1.34
1	A	1620	A	N3-C4	6.50	1.38	1.34
1	A	2673	A	N3-C4	6.50	1.38	1.34
32	W	883	A	N3-C4	6.50	1.38	1.34
32	W	1405	A	N3-C4	6.50	1.38	1.34
1	A	2071	A	N3-C4	6.50	1.38	1.34
1	A	2464	A	N3-C4	6.50	1.38	1.34
32	W	357	A	N3-C4	6.50	1.38	1.34
32	W	367	A	N3-C4	6.50	1.38	1.34
32	W	825	A	N3-C4	6.50	1.38	1.34
1	A	1541	A	N3-C4	6.49	1.38	1.34
1	A	2468	A	N3-C4	6.49	1.38	1.34
1	A	2805	A	N3-C4	6.49	1.38	1.34
1	A	2826	A	N3-C4	6.49	1.38	1.34
32	W	204	A	N3-C4	6.49	1.38	1.34
32	W	390	A	N3-C4	6.49	1.38	1.34
32	W	790	A	N3-C4	6.49	1.38	1.34
32	W	1417	A	N3-C4	6.49	1.38	1.34
1	A	1774	A	N3-C4	6.49	1.38	1.34
32	W	828	A	N3-C4	6.49	1.38	1.34
1	A	1014	A	N3-C4	6.49	1.38	1.34
1	A	2052	A	N3-C4	6.49	1.38	1.34
1	A	1663	A	N3-C4	6.49	1.38	1.34
1	A	2032	A	N3-C4	6.49	1.38	1.34
32	W	314	A	N3-C4	6.49	1.38	1.34
32	W	391	A	N3-C4	6.49	1.38	1.34
32	W	1278	A	N3-C4	6.49	1.38	1.34
1	A	258	A	N3-C4	6.49	1.38	1.34
32	W	1503	A	N3-C4	6.49	1.38	1.34
1	A	376	A	N3-C4	6.49	1.38	1.34
1	A	1287	A	N3-C4	6.49	1.38	1.34
32	W	381	A	N3-C4	6.49	1.38	1.34
32	W	617	A	N3-C4	6.49	1.38	1.34
32	W	1384	A	N3-C4	6.49	1.38	1.34
32	W	1517	A	N3-C4	6.48	1.38	1.34
1	A	355	A	N3-C4	6.48	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	896	A	N3-C4	6.48	1.38	1.34
1	A	993	A	N3-C4	6.48	1.38	1.34
1	A	1190	A	N3-C4	6.48	1.38	1.34
1	A	1056	A	N3-C4	6.48	1.38	1.34
32	W	1427	A	N3-C4	6.48	1.38	1.34
1	A	154	A	N3-C4	6.48	1.38	1.34
1	A	622	A	N3-C4	6.48	1.38	1.34
1	A	1579	A	N3-C4	6.48	1.38	1.34
1	A	1735	A	N3-C4	6.48	1.38	1.34
1	A	1768	A	N3-C4	6.48	1.38	1.34
32	W	474	A	N3-C4	6.48	1.38	1.34
1	A	1485	A	N3-C4	6.48	1.38	1.34
32	W	462	A	N3-C4	6.48	1.38	1.34
32	W	1434	A	N3-C4	6.48	1.38	1.34
1	A	437	A	N3-C4	6.47	1.38	1.34
1	A	549	A	N3-C4	6.47	1.38	1.34
1	A	790	A	N3-C4	6.47	1.38	1.34
32	W	1257	A	N3-C4	6.47	1.38	1.34
1	A	1918	A	N3-C4	6.47	1.38	1.34
32	W	171	A	N3-C4	6.47	1.38	1.34
32	W	968	A	N3-C4	6.47	1.38	1.34
1	A	207	A	N3-C4	6.47	1.38	1.34
1	A	2837	A	N3-C4	6.47	1.38	1.34
1	A	1269	A	N3-C4	6.47	1.38	1.34
1	A	1532	A	N3-C4	6.47	1.38	1.34
1	A	2421	A	N3-C4	6.47	1.38	1.34
1	A	2851	A	N3-C4	6.47	1.38	1.34
32	W	372	A	N3-C4	6.47	1.38	1.34
32	W	485	A	N3-C4	6.47	1.38	1.34
32	W	1455	A	N3-C4	6.47	1.38	1.34
32	W	18	A	N3-C4	6.47	1.38	1.34
1	A	13	A	N3-C4	6.47	1.38	1.34
1	A	692	A	N3-C4	6.47	1.38	1.34
1	A	958	A	N3-C4	6.47	1.38	1.34
1	A	1277	A	N3-C4	6.47	1.38	1.34
32	W	460	A	N3-C4	6.47	1.38	1.34
32	W	1028	A	N3-C4	6.47	1.38	1.34
1	A	1233	A	N3-C4	6.46	1.38	1.34
1	A	1966	A	N3-C4	6.46	1.38	1.34
32	W	333	A	N3-C4	6.46	1.38	1.34
32	W	508	A	N3-C4	6.46	1.38	1.34
32	W	1486	A	N3-C4	6.46	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	A	N3-C4	6.46	1.38	1.34
32	W	120	A	N3-C4	6.46	1.38	1.34
32	W	1179	A	N3-C4	6.46	1.38	1.34
1	A	162	A	N3-C4	6.46	1.38	1.34
1	A	1115	A	N3-C4	6.46	1.38	1.34
1	A	1202	A	N3-C4	6.46	1.38	1.34
1	A	1998	A	N3-C4	6.46	1.38	1.34
1	A	2912	A	N3-C4	6.46	1.38	1.34
1	A	431	A	N3-C4	6.46	1.38	1.34
1	A	584	A	N3-C4	6.46	1.38	1.34
1	A	2686	A	N3-C4	6.46	1.38	1.34
32	W	604	A	N3-C4	6.46	1.38	1.34
1	A	225	A	N3-C4	6.46	1.38	1.34
1	A	1313	A	N3-C4	6.46	1.38	1.34
1	A	2807	A	N3-C4	6.46	1.38	1.34
2	B	113	A	N3-C4	6.46	1.38	1.34
32	W	28	A	N3-C4	6.46	1.38	1.34
32	W	945	A	N3-C4	6.46	1.38	1.34
1	A	166	A	N3-C4	6.46	1.38	1.34
1	A	889	A	N3-C4	6.46	1.38	1.34
1	A	2689	A	N3-C4	6.46	1.38	1.34
32	W	236	A	N3-C4	6.46	1.38	1.34
32	W	529	A	N3-C4	6.46	1.38	1.34
32	W	1048	A	N3-C4	6.46	1.38	1.34
32	W	1160	A	N3-C4	6.46	1.38	1.34
32	W	1333	A	N3-C4	6.46	1.38	1.34
1	A	1008	A	N3-C4	6.46	1.38	1.34
1	A	2440	A	N3-C4	6.46	1.38	1.34
32	W	1272	A	N3-C4	6.46	1.38	1.34
1	A	156	A	N3-C4	6.45	1.38	1.34
1	A	1465	A	N3-C4	6.45	1.38	1.34
1	A	1895	A	N3-C4	6.45	1.38	1.34
32	W	1140	A	N3-C4	6.45	1.38	1.34
1	A	161	A	N3-C4	6.45	1.38	1.34
1	A	421	A	N3-C4	6.45	1.38	1.34
1	A	519	A	N3-C4	6.45	1.38	1.34
1	A	1189	A	N3-C4	6.45	1.38	1.34
32	W	159	A	N3-C4	6.45	1.38	1.34
32	W	1197	A	N3-C4	6.45	1.38	1.34
52	z	14	A	N3-C4	6.45	1.38	1.34
1	A	200	A	N3-C4	6.45	1.38	1.34
1	A	769	A	N3-C4	6.45	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	882	A	N3-C4	6.45	1.38	1.34
1	A	1265	A	N3-C4	6.45	1.38	1.34
1	A	2908	A	N3-C4	6.45	1.38	1.34
1	A	2340	A	N3-C4	6.45	1.38	1.34
32	W	1437	A	N3-C4	6.45	1.38	1.34
1	A	199	A	N3-C4	6.45	1.38	1.34
1	A	1126	A	N3-C4	6.45	1.38	1.34
1	A	1393	A	N3-C4	6.45	1.38	1.34
32	W	882	A	N3-C4	6.45	1.38	1.34
2	B	56	A	N3-C4	6.44	1.38	1.34
1	A	56	A	N3-C4	6.44	1.38	1.34
1	A	73	A	N3-C4	6.44	1.38	1.34
1	A	2389	A	N3-C4	6.44	1.38	1.34
1	A	677	A	N3-C4	6.44	1.38	1.34
1	A	1314	A	N3-C4	6.44	1.38	1.34
1	A	1555	A	N3-C4	6.44	1.38	1.34
1	A	2088	A	N3-C4	6.44	1.38	1.34
32	W	278	A	N3-C4	6.44	1.38	1.34
32	W	438	A	N3-C4	6.44	1.38	1.34
2	B	114	A	N3-C4	6.44	1.38	1.34
1	A	619	A	N3-C4	6.44	1.38	1.34
1	A	705	A	N3-C4	6.44	1.38	1.34
1	A	1335	A	N3-C4	6.44	1.38	1.34
1	A	1461	A	N3-C4	6.44	1.38	1.34
1	A	1697	A	N3-C4	6.44	1.38	1.34
1	A	2329	A	N3-C4	6.44	1.38	1.34
1	A	1175	A	N3-C4	6.44	1.38	1.34
1	A	1473	A	N3-C4	6.44	1.38	1.34
1	A	1802	A	N3-C4	6.44	1.38	1.34
32	W	1349	A	N3-C4	6.44	1.38	1.34
1	A	1699	A	N3-C4	6.43	1.38	1.34
1	A	2885	A	N3-C4	6.43	1.38	1.34
32	W	791	A	N3-C4	6.43	1.38	1.34
52	z	44	A	N3-C4	6.43	1.38	1.34
1	A	849	A	N3-C4	6.43	1.38	1.34
1	A	1100	A	N3-C4	6.43	1.38	1.34
1	A	2482	A	N3-C4	6.43	1.38	1.34
32	W	35	A	N3-C4	6.43	1.38	1.34
32	W	569	A	N3-C4	6.43	1.38	1.34
32	W	918	A	N3-C4	6.43	1.38	1.34
1	A	117	A	N3-C4	6.43	1.38	1.34
1	A	1542	A	N3-C4	6.43	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1797	A	N3-C4	6.43	1.38	1.34
1	A	1839	A	N3-C4	6.43	1.38	1.34
32	W	879	A	N3-C4	6.43	1.38	1.34
1	A	268	A	N3-C4	6.43	1.38	1.34
1	A	273	A	N3-C4	6.43	1.38	1.34
1	A	978	A	N3-C4	6.43	1.38	1.34
1	A	1961	A	N3-C4	6.43	1.38	1.34
1	A	2298	A	N3-C4	6.43	1.38	1.34
1	A	2661	A	N3-C4	6.43	1.38	1.34
1	A	305	A	N3-C4	6.42	1.38	1.34
1	A	1776	A	N3-C4	6.42	1.38	1.34
1	A	1789	A	N3-C4	6.42	1.38	1.34
1	A	2100	A	N3-C4	6.42	1.38	1.34
1	A	2106	A	N3-C4	6.42	1.38	1.34
32	W	296	A	N3-C4	6.42	1.38	1.34
32	W	1466	A	N3-C4	6.42	1.38	1.34
1	A	2302	A	N3-C4	6.42	1.38	1.34
32	W	1248	A	N3-C4	6.42	1.38	1.34
32	W	1529	A	N3-C4	6.42	1.38	1.34
1	A	1421	A	N3-C4	6.42	1.38	1.34
1	A	2570	A	N3-C4	6.42	1.38	1.34
1	A	2902	A	N3-C4	6.42	1.38	1.34
32	W	725	A	N3-C4	6.42	1.38	1.34
32	W	1176	A	N3-C4	6.42	1.38	1.34
32	W	1442	A	N3-C4	6.42	1.38	1.34
32	W	738	A	N3-C4	6.42	1.38	1.34
1	A	354	A	N3-C4	6.42	1.38	1.34
1	A	2704	A	N3-C4	6.42	1.38	1.34
32	W	170	A	N3-C4	6.42	1.38	1.34
32	W	1493	A	N3-C4	6.42	1.38	1.34
1	A	265	A	N3-C4	6.42	1.38	1.34
1	A	325	A	N3-C4	6.42	1.38	1.34
1	A	1097	A	N3-C4	6.42	1.38	1.34
1	A	1504	A	N3-C4	6.42	1.38	1.34
1	A	2517	A	N3-C4	6.42	1.38	1.34
32	W	228	A	N3-C4	6.42	1.38	1.34
32	W	974	A	N3-C4	6.42	1.38	1.34
32	W	1510	A	N3-C4	6.42	1.38	1.34
1	A	28	A	N3-C4	6.42	1.38	1.34
1	A	84	A	N3-C4	6.42	1.38	1.34
1	A	477	A	N3-C4	6.42	1.38	1.34
32	W	1120	A	N3-C4	6.42	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	A	N3-C4	6.41	1.38	1.34
32	W	1006	A	N3-C4	6.41	1.38	1.34
32	W	1523	A	N3-C4	6.41	1.38	1.34
1	A	1132	A	N3-C4	6.41	1.38	1.34
1	A	2876	A	N3-C4	6.41	1.38	1.34
2	B	37	A	N3-C4	6.41	1.38	1.34
2	B	76	A	N3-C4	6.41	1.38	1.34
32	W	1092	A	N3-C4	6.41	1.38	1.34
1	A	12	A	N3-C4	6.41	1.38	1.34
1	A	333	A	N3-C4	6.41	1.38	1.34
1	A	851	A	N3-C4	6.41	1.38	1.34
1	A	1179	A	N3-C4	6.41	1.38	1.34
1	A	2276	A	N3-C4	6.41	1.38	1.34
2	B	55	A	N3-C4	6.41	1.38	1.34
32	W	1288	A	N3-C4	6.41	1.38	1.34
1	A	279	A	N3-C4	6.41	1.38	1.34
1	A	1142	A	N3-C4	6.41	1.38	1.34
1	A	1816	A	N3-C4	6.41	1.38	1.34
1	A	2364	A	N3-C4	6.41	1.38	1.34
1	A	2395	A	N3-C4	6.41	1.38	1.34
32	W	715	A	N3-C4	6.41	1.38	1.34
32	W	1185	A	N3-C4	6.41	1.38	1.34
1	A	1020	A	N3-C4	6.41	1.38	1.34
32	W	669	A	N3-C4	6.41	1.38	1.34
1	A	727	A	N3-C4	6.41	1.38	1.34
1	A	1123	A	N3-C4	6.41	1.38	1.34
2	B	17	A	N3-C4	6.41	1.38	1.34
32	W	1252	A	N3-C4	6.41	1.38	1.34
32	W	1456	A	N3-C4	6.41	1.38	1.34
1	A	125	A	N3-C4	6.40	1.38	1.34
1	A	2526	A	N3-C4	6.40	1.38	1.34
32	W	816	A	N3-C4	6.40	1.38	1.34
1	A	108	A	N3-C4	6.40	1.38	1.34
1	A	917	A	N3-C4	6.40	1.38	1.34
1	A	1424	A	N3-C4	6.40	1.38	1.34
1	A	1686	A	N3-C4	6.40	1.38	1.34
1	A	2369	A	N3-C4	6.40	1.38	1.34
32	W	81	A	N3-C4	6.40	1.38	1.34
32	W	352	A	N3-C4	6.40	1.38	1.34
32	W	775	A	N3-C4	6.40	1.38	1.34
1	A	412	A	N3-C4	6.40	1.38	1.34
1	A	1131	A	N3-C4	6.40	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1965	A	N3-C4	6.40	1.38	1.34
1	A	1982	A	N3-C4	6.40	1.38	1.34
1	A	2907	A	N3-C4	6.40	1.38	1.34
32	W	1463	A	N3-C4	6.40	1.38	1.34
1	A	2683	A	N3-C4	6.40	1.38	1.34
32	W	630	A	N3-C4	6.40	1.38	1.34
1	A	683	A	N3-C4	6.40	1.38	1.34
1	A	1055	A	N3-C4	6.40	1.38	1.34
1	A	1679	A	N3-C4	6.40	1.38	1.34
1	A	2303	A	N3-C4	6.40	1.38	1.34
32	W	917	A	N3-C4	6.40	1.38	1.34
1	A	517	A	N3-C4	6.40	1.38	1.34
1	A	786	A	N3-C4	6.40	1.38	1.34
1	A	1848	A	N3-C4	6.40	1.38	1.34
1	A	329	A	N3-C4	6.39	1.38	1.34
1	A	2295	A	N3-C4	6.39	1.38	1.34
1	A	2919	A	N3-C4	6.39	1.38	1.34
32	W	650	A	N3-C4	6.39	1.38	1.34
32	W	925	A	N3-C4	6.39	1.38	1.34
1	A	173	A	N3-C4	6.39	1.38	1.34
1	A	561	A	N3-C4	6.39	1.38	1.34
1	A	1161	A	N3-C4	6.39	1.38	1.34
1	A	1592	A	N3-C4	6.39	1.38	1.34
1	A	647	A	N3-C4	6.39	1.38	1.34
1	A	1072	A	N3-C4	6.39	1.38	1.34
1	A	1210	A	N3-C4	6.39	1.38	1.34
2	B	27	A	N3-C4	6.39	1.38	1.34
32	W	329	A	N3-C4	6.39	1.38	1.34
32	W	463	A	N3-C4	6.39	1.38	1.34
32	W	923	A	N3-C4	6.39	1.38	1.34
1	A	828	A	N3-C4	6.38	1.38	1.34
1	A	1723	A	N3-C4	6.38	1.38	1.34
1	A	2454	A	N3-C4	6.38	1.38	1.34
32	W	271	A	N3-C4	6.38	1.38	1.34
32	W	1369	A	N3-C4	6.38	1.38	1.34
1	A	2593	A	N3-C4	6.38	1.38	1.34
1	A	2769	A	N3-C4	6.38	1.38	1.34
32	W	512	A	N3-C4	6.38	1.38	1.34
1	A	723	A	N3-C4	6.38	1.38	1.34
1	A	758	A	N3-C4	6.38	1.38	1.34
1	A	1221	A	N3-C4	6.38	1.38	1.34
32	W	382	A	N3-C4	6.38	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	651	A	N3-C4	6.38	1.38	1.34
1	A	1260	A	N3-C4	6.38	1.38	1.34
1	A	1534	A	N3-C4	6.38	1.38	1.34
32	W	76	A	N3-C4	6.38	1.38	1.34
1	A	956	A	N3-C4	6.38	1.38	1.34
1	A	2417	A	N3-C4	6.38	1.38	1.34
1	A	2848	A	N3-C4	6.38	1.38	1.34
32	W	210	A	N3-C4	6.38	1.38	1.34
32	W	985	A	N3-C4	6.38	1.38	1.34
1	A	259	A	N3-C4	6.38	1.38	1.34
1	A	2750	A	N3-C4	6.38	1.38	1.34
32	W	57	A	N3-C4	6.38	1.38	1.34
1	A	1575	A	N3-C4	6.37	1.38	1.34
1	A	2296	A	N3-C4	6.37	1.38	1.34
1	A	2719	A	N3-C4	6.37	1.38	1.34
32	W	811	A	N3-C4	6.37	1.38	1.34
1	A	1606	A	N3-C4	6.37	1.38	1.34
1	A	2357	A	N3-C4	6.37	1.38	1.34
1	A	2595	A	N3-C4	6.37	1.38	1.34
1	A	821	A	N3-C4	6.37	1.38	1.34
1	A	957	A	N3-C4	6.37	1.38	1.34
1	A	1788	A	N3-C4	6.37	1.38	1.34
1	A	2498	A	N3-C4	6.37	1.38	1.34
1	A	2762	A	N3-C4	6.37	1.38	1.34
32	W	592	A	N3-C4	6.37	1.38	1.34
32	W	862	A	N3-C4	6.37	1.38	1.34
1	A	102	A	N3-C4	6.37	1.38	1.34
1	A	637	A	N3-C4	6.37	1.38	1.34
1	A	1054	A	N3-C4	6.37	1.38	1.34
1	A	65	A	N3-C4	6.37	1.38	1.34
1	A	699	A	N3-C4	6.37	1.38	1.34
1	A	1948	A	N3-C4	6.37	1.38	1.34
32	W	148	A	N3-C4	6.37	1.38	1.34
32	W	824	A	N3-C4	6.37	1.38	1.34
32	W	984	A	N3-C4	6.37	1.38	1.34
1	A	388	A	N3-C4	6.36	1.38	1.34
1	A	658	A	N3-C4	6.36	1.38	1.34
1	A	1721	A	N3-C4	6.36	1.38	1.34
1	A	337	A	N3-C4	6.36	1.38	1.34
1	A	722	A	N3-C4	6.36	1.38	1.34
32	W	1031	A	N3-C4	6.36	1.38	1.34
1	A	1675	A	N3-C4	6.36	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	870	A	N3-C4	6.36	1.38	1.34
1	A	222	A	N3-C4	6.36	1.38	1.34
1	A	1286	A	N3-C4	6.36	1.38	1.34
1	A	1767	A	N3-C4	6.36	1.38	1.34
32	W	796	A	N3-C4	6.36	1.38	1.34
32	W	803	A	N3-C4	6.36	1.38	1.34
1	A	1967	A	N3-C4	6.36	1.38	1.34
32	W	456	A	N3-C4	6.36	1.38	1.34
1	A	1882	A	N3-C4	6.35	1.38	1.34
1	A	1157	A	N3-C4	6.35	1.38	1.34
32	W	337	A	N3-C4	6.35	1.38	1.34
32	W	459	A	N3-C4	6.35	1.38	1.34
1	A	829	A	N3-C4	6.35	1.38	1.34
1	A	572	A	N3-C4	6.35	1.38	1.34
1	A	1149	A	N3-C4	6.35	1.38	1.34
1	A	1445	A	N3-C4	6.35	1.38	1.34
1	A	1913	A	N3-C4	6.35	1.38	1.34
32	W	251	A	N3-C4	6.35	1.38	1.34
32	W	777	A	N3-C4	6.35	1.38	1.34
32	W	910	A	N3-C4	6.35	1.38	1.34
32	W	956	A	N3-C4	6.35	1.38	1.34
32	W	1115	A	N3-C4	6.35	1.38	1.34
1	A	448	A	N3-C4	6.35	1.38	1.34
1	A	1784	A	N3-C4	6.35	1.38	1.34
1	A	943	A	N3-C4	6.35	1.38	1.34
1	A	1956	A	N3-C4	6.35	1.38	1.34
1	A	2663	A	N3-C4	6.35	1.38	1.34
32	W	1270	A	N3-C4	6.35	1.38	1.34
1	A	1059	A	N3-C4	6.34	1.38	1.34
1	A	2000	A	N3-C4	6.34	1.38	1.34
32	W	129	A	N3-C4	6.34	1.38	1.34
32	W	1238	A	N3-C4	6.34	1.38	1.34
1	A	260	A	N3-C4	6.34	1.38	1.34
1	A	391	A	N3-C4	6.34	1.38	1.34
1	A	1627	A	N3-C4	6.34	1.38	1.34
1	A	2860	A	N3-C4	6.34	1.38	1.34
32	W	190	A	N3-C4	6.34	1.38	1.34
1	A	71	A	N3-C4	6.34	1.38	1.34
1	A	118	A	N3-C4	6.34	1.38	1.34
1	A	1412	A	N3-C4	6.34	1.38	1.34
1	A	1553	A	N3-C4	6.34	1.38	1.34
1	A	2691	A	N3-C4	6.34	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	477	A	N3-C4	6.34	1.38	1.34
32	W	724	A	N3-C4	6.34	1.38	1.34
1	A	179	A	N3-C4	6.34	1.38	1.34
1	A	1346	A	N3-C4	6.34	1.38	1.34
1	A	1608	A	N3-C4	6.34	1.38	1.34
1	A	908	A	N3-C4	6.33	1.38	1.34
32	W	10	A	N3-C4	6.33	1.38	1.34
32	W	1372	A	N3-C4	6.33	1.38	1.34
1	A	1325	A	N3-C4	6.33	1.38	1.34
1	A	2777	A	N3-C4	6.33	1.38	1.34
1	A	2889	A	N3-C4	6.33	1.38	1.34
32	W	1054	A	N3-C4	6.33	1.38	1.34
1	A	1254	A	N3-C4	6.33	1.38	1.34
1	A	1883	A	N3-C4	6.33	1.38	1.34
1	A	2111	A	N3-C4	6.33	1.38	1.34
1	A	2793	A	N3-C4	6.33	1.38	1.34
1	A	1818	A	N3-C4	6.33	1.38	1.34
1	A	110	A	N3-C4	6.33	1.38	1.34
1	A	1734	A	N3-C4	6.33	1.38	1.34
1	A	1888	A	N3-C4	6.33	1.38	1.34
32	W	1261	A	N3-C4	6.33	1.38	1.34
1	A	274	A	N3-C4	6.33	1.38	1.34
32	W	161	A	N3-C4	6.33	1.38	1.34
32	W	1050	A	N3-C4	6.33	1.38	1.34
1	A	389	A	N3-C4	6.33	1.38	1.34
1	A	1034	A	N3-C4	6.33	1.38	1.34
1	A	1919	A	N3-C4	6.33	1.38	1.34
1	A	2387	A	N3-C4	6.33	1.38	1.34
1	A	2770	A	N3-C4	6.33	1.38	1.34
1	A	193	A	N3-C4	6.32	1.38	1.34
1	A	653	A	N3-C4	6.32	1.38	1.34
1	A	1442	A	N3-C4	6.32	1.38	1.34
1	A	2810	A	N3-C4	6.32	1.38	1.34
32	W	1166	A	N3-C4	6.32	1.38	1.34
1	A	53	A	N3-C4	6.32	1.38	1.34
32	W	1026	A	N3-C4	6.32	1.38	1.34
1	A	5	A	N3-C4	6.32	1.38	1.34
1	A	2658	A	N3-C4	6.32	1.38	1.34
1	A	2819	A	N3-C4	6.32	1.38	1.34
1	A	67	A	N3-C4	6.32	1.38	1.34
1	A	318	A	N3-C4	6.32	1.38	1.34
1	A	2477	A	N3-C4	6.32	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2043	A	N3-C4	6.32	1.38	1.34
1	A	144	A	N3-C4	6.31	1.38	1.34
1	A	1477	A	N3-C4	6.31	1.38	1.34
1	A	2078	A	N3-C4	6.31	1.38	1.34
32	W	1422	A	N3-C4	6.31	1.38	1.34
1	A	176	A	N3-C4	6.31	1.38	1.34
1	A	1791	A	N3-C4	6.31	1.38	1.34
1	A	2080	A	N3-C4	6.31	1.38	1.34
1	A	2767	A	N3-C4	6.31	1.38	1.34
32	W	1479	A	N3-C4	6.31	1.38	1.34
1	A	689	A	N3-C4	6.31	1.38	1.34
1	A	1244	A	N3-C4	6.31	1.38	1.34
1	A	2779	A	N3-C4	6.31	1.38	1.34
2	B	43	A	N3-C4	6.31	1.38	1.34
1	A	150	A	N3-C4	6.31	1.38	1.34
1	A	2459	A	N3-C4	6.31	1.38	1.34
1	A	656	A	N3-C4	6.31	1.38	1.34
1	A	702	A	N3-C4	6.31	1.38	1.34
1	A	1423	A	N3-C4	6.30	1.38	1.34
1	A	1618	A	N3-C4	6.30	1.38	1.34
1	A	224	A	N3-C4	6.30	1.38	1.34
1	A	1831	A	N3-C4	6.30	1.38	1.34
32	W	924	A	N3-C4	6.30	1.38	1.34
32	W	1254	A	N3-C4	6.30	1.38	1.34
1	A	808	A	N3-C4	6.30	1.38	1.34
1	A	1928	A	N3-C4	6.30	1.38	1.34
1	A	2297	A	N3-C4	6.30	1.38	1.34
1	A	2643	A	N3-C4	6.30	1.38	1.34
1	A	2790	A	N3-C4	6.30	1.38	1.34
32	W	556	A	N3-C4	6.30	1.38	1.34
32	W	1296	A	N3-C4	6.30	1.38	1.34
1	A	1583	A	N3-C4	6.30	1.38	1.34
1	A	847	A	N3-C4	6.30	1.38	1.34
1	A	2007	A	N3-C4	6.30	1.38	1.34
2	B	97	A	N3-C4	6.29	1.38	1.34
32	W	568	A	N3-C4	6.29	1.38	1.34
32	W	671	A	N3-C4	6.29	1.38	1.34
1	A	343	A	N3-C4	6.29	1.38	1.34
32	W	1016	A	N3-C4	6.29	1.38	1.34
32	W	1189	A	N3-C4	6.29	1.38	1.34
1	A	1141	A	N3-C4	6.29	1.38	1.34
32	W	1359	A	N3-C4	6.29	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	1210	A	N3-C4	6.29	1.38	1.34
1	A	717	A	N3-C4	6.29	1.38	1.34
1	A	746	A	N3-C4	6.29	1.38	1.34
1	A	1905	A	N3-C4	6.29	1.38	1.34
1	A	830	A	N3-C4	6.29	1.38	1.34
1	A	2327	A	N3-C4	6.29	1.38	1.34
1	A	2406	A	N3-C4	6.29	1.38	1.34
1	A	2507	A	N3-C4	6.29	1.38	1.34
32	W	118	A	N3-C4	6.29	1.38	1.34
32	W	844	A	N3-C4	6.29	1.38	1.34
1	A	496	A	N3-C4	6.28	1.38	1.34
1	A	2398	A	N3-C4	6.28	1.38	1.34
32	W	737	A	N3-C4	6.28	1.38	1.34
1	A	1096	A	N3-C4	6.28	1.38	1.34
1	A	364	A	N3-C4	6.28	1.38	1.34
1	A	582	A	N3-C4	6.28	1.38	1.34
32	W	581	A	N3-C4	6.28	1.38	1.34
52	z	76	A	N3-C4	6.28	1.38	1.34
1	A	194	A	N3-C4	6.28	1.38	1.34
1	A	1019	A	N3-C4	6.28	1.38	1.34
1	A	2390	A	N3-C4	6.28	1.38	1.34
2	B	39	A	N3-C4	6.28	1.38	1.34
32	W	874	A	N3-C4	6.27	1.38	1.34
1	A	1291	A	N3-C4	6.27	1.38	1.34
1	A	2034	A	N3-C4	6.27	1.38	1.34
1	A	2547	A	N3-C4	6.27	1.38	1.34
32	W	1419	A	N3-C4	6.27	1.38	1.34
1	A	436	A	N3-C4	6.27	1.38	1.34
1	A	1003	A	N3-C4	6.27	1.38	1.34
1	A	1119	A	N3-C4	6.27	1.38	1.34
32	W	684	A	N3-C4	6.27	1.38	1.34
32	W	142	A	N3-C4	6.27	1.38	1.34
32	W	605	A	N3-C4	6.27	1.38	1.34
1	A	2087	A	N3-C4	6.27	1.38	1.34
32	W	703	A	N3-C4	6.27	1.38	1.34
1	A	1820	A	N3-C4	6.27	1.38	1.34
32	W	582	A	N3-C4	6.27	1.38	1.34
1	A	230	A	N3-C4	6.26	1.38	1.34
32	W	644	A	N3-C4	6.26	1.38	1.34
1	A	690	A	N3-C4	6.26	1.38	1.34
1	A	1417	A	N3-C4	6.26	1.38	1.34
1	A	1722	A	N3-C4	6.26	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	A	N3-C4	6.26	1.38	1.34
32	W	1513	A	N3-C4	6.26	1.38	1.34
1	A	275	A	N3-C4	6.26	1.38	1.34
1	A	547	A	N3-C4	6.26	1.38	1.34
1	A	1601	A	N3-C4	6.26	1.38	1.34
1	A	1067	A	N3-C4	6.26	1.38	1.34
32	W	555	A	N3-C4	6.26	1.38	1.34
32	W	929	A	N3-C4	6.26	1.38	1.34
1	A	507	A	N3-C4	6.25	1.38	1.34
1	A	971	A	N3-C4	6.25	1.38	1.34
32	W	254	A	N3-C4	6.25	1.38	1.34
32	W	1112	A	N3-C4	6.25	1.38	1.34
1	A	369	A	N3-C4	6.25	1.38	1.34
32	W	1090	A	N3-C4	6.25	1.38	1.34
1	A	876	A	N3-C4	6.25	1.38	1.34
1	A	1727	A	N3-C4	6.25	1.38	1.34
1	A	2616	A	N3-C4	6.25	1.38	1.34
32	W	107	A	N3-C4	6.25	1.38	1.34
32	W	969	A	N3-C4	6.25	1.38	1.34
1	A	2787	A	N3-C4	6.25	1.38	1.34
32	W	919	A	N3-C4	6.25	1.38	1.34
1	A	64	A	N3-C4	6.25	1.38	1.34
32	W	258	A	N3-C4	6.24	1.38	1.34
1	A	2062	A	N3-C4	6.24	1.38	1.34
1	A	1520	A	N3-C4	6.24	1.38	1.34
1	A	1388	A	N3-C4	6.24	1.38	1.34
1	A	1778	A	N3-C4	6.24	1.38	1.34
32	W	786	A	N3-C4	6.24	1.38	1.34
32	W	988	A	N3-C4	6.24	1.38	1.34
2	B	105	A	N3-C4	6.23	1.38	1.34
32	W	664	A	N3-C4	6.23	1.38	1.34
1	A	1021	A	N3-C4	6.23	1.38	1.34
1	A	2835	A	N3-C4	6.23	1.38	1.34
1	A	1432	A	N3-C4	6.23	1.38	1.34
1	A	2436	A	N3-C4	6.23	1.38	1.34
1	A	2875	A	N3-C4	6.23	1.38	1.34
1	A	2804	A	N3-C4	6.23	1.38	1.34
32	W	117	A	N3-C4	6.23	1.38	1.34
1	A	2734	A	N3-C4	6.22	1.38	1.34
1	A	1981	A	N3-C4	6.22	1.38	1.34
32	W	674	A	N3-C4	6.22	1.38	1.34
1	A	490	A	N3-C4	6.22	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	287	A	N3-C4	6.22	1.38	1.34
32	W	386	A	N3-C4	6.22	1.38	1.34
1	A	1499	A	N3-C4	6.21	1.38	1.34
32	W	211	A	N3-C4	6.21	1.38	1.34
1	A	1061	A	N3-C4	6.21	1.38	1.34
1	A	2594	A	N3-C4	6.21	1.38	1.34
1	A	1648	A	N3-C4	6.21	1.38	1.34
1	A	574	A	N3-C4	6.20	1.38	1.34
1	A	1636	A	N3-C4	6.20	1.38	1.34
1	A	2455	A	N3-C4	6.20	1.38	1.34
1	A	374	A	N3-C4	6.20	1.38	1.34
32	W	301	A	N3-C4	6.20	1.38	1.34
32	W	1247	A	N3-C4	6.20	1.38	1.34
32	W	1342	A	N3-C4	6.20	1.38	1.34
1	A	2618	A	N3-C4	6.20	1.38	1.34
32	W	631	A	N3-C4	6.20	1.38	1.34
1	A	1901	A	N3-C4	6.20	1.38	1.34
32	W	1188	A	N3-C4	6.19	1.38	1.34
32	W	1425	A	N3-C4	6.19	1.38	1.34
1	A	1745	A	N3-C4	6.19	1.38	1.34
32	W	1077	A	N3-C4	6.19	1.38	1.34
52	z	21	A	N3-C4	6.19	1.38	1.34
32	W	837	A	N3-C4	6.18	1.38	1.34
32	W	371	A	N3-C4	6.18	1.38	1.34
1	A	2018	A	N3-C4	6.18	1.38	1.34
32	W	768	A	N3-C4	6.18	1.38	1.34
1	A	965	A	N3-C4	6.17	1.38	1.34
1	A	1266	A	N3-C4	6.17	1.38	1.34
1	A	216	A	N3-C4	6.17	1.38	1.34
1	A	659	A	N3-C4	6.17	1.38	1.34
1	A	811	A	N3-C4	6.17	1.38	1.34
2	B	25	A	N3-C4	6.16	1.38	1.34
1	A	178	A	N3-C4	6.16	1.38	1.34
1	A	679	A	N3-C4	6.16	1.38	1.34
1	A	2089	A	N3-C4	6.15	1.38	1.34
1	A	2606	A	N3-C4	6.15	1.38	1.34
1	A	10	A	N3-C4	6.15	1.38	1.34
1	A	560	A	N3-C4	6.15	1.38	1.34
1	A	1201	A	N3-C4	6.15	1.38	1.34
32	W	1260	A	N3-C4	6.14	1.38	1.34
32	W	232	A	N3-C4	6.14	1.38	1.34
1	A	140	A	N3-C4	6.13	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1999	A	N3-C4	6.13	1.38	1.34
1	A	2026	A	N3-C4	6.13	1.38	1.34
1	A	1078	A	N3-C4	6.13	1.38	1.34
32	W	1161	A	N3-C4	6.13	1.38	1.34
1	A	925	A	N3-C4	6.12	1.38	1.34
32	W	743	A	N3-C4	6.12	1.38	1.34
1	A	1046	A	N3-C4	6.12	1.38	1.34
1	A	740	A	N3-C4	6.11	1.38	1.34
32	W	583	A	N3-C4	6.11	1.38	1.34
1	A	2462	A	N3-C4	6.11	1.38	1.34
1	A	1832	A	N3-C4	6.10	1.38	1.34
32	W	209	A	N3-C4	6.10	1.38	1.34
1	A	183	A	N3-C4	6.09	1.38	1.34
1	A	1929	A	N3-C4	6.09	1.38	1.34
32	W	1283	A	N3-C4	6.08	1.38	1.34
1	A	2601	A	N3-C4	6.07	1.38	1.34
1	A	220	A	N3-C4	6.04	1.38	1.34
1	A	667	A	N3-C4	6.03	1.38	1.34
1	A	1661	A	N7-C5	6.03	1.42	1.39
52	z	37	A	N7-C5	6.03	1.42	1.39
32	W	1207	A	N3-C4	6.02	1.38	1.34
1	A	1026	A	N3-C4	6.01	1.38	1.34
1	A	1074	A	N3-C4	5.99	1.38	1.34
1	A	501	A	N3-C4	5.90	1.38	1.34
32	W	696	A	N3-C4	5.87	1.38	1.34
32	W	1548	C	C2-N3	5.68	1.40	1.35
1	A	1103	A	C2-N3	5.49	1.38	1.33
32	W	933	A	C2-N3	5.42	1.38	1.33
32	W	1278	A	C2-N3	5.38	1.38	1.33
32	W	1425	A	C2-N3	5.38	1.38	1.33
1	A	527	A	C2-N3	5.37	1.38	1.33
1	A	2329	A	C2-N3	5.36	1.38	1.33
32	W	1166	A	C2-N3	5.36	1.38	1.33
1	A	1638	A	C2-N3	5.36	1.38	1.33
32	W	99	A	C2-N3	5.36	1.38	1.33
1	A	956	A	C2-N3	5.35	1.38	1.33
1	A	1999	A	C2-N3	5.35	1.38	1.33
32	W	1026	A	C2-N3	5.34	1.38	1.33
1	A	1667	A	C2-N3	5.34	1.38	1.33
1	A	513	A	C2-N3	5.32	1.38	1.33
1	A	2844	A	C2-N3	5.32	1.38	1.33
1	A	173	A	C2-N3	5.31	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	z	70	A	C2-N3	5.31	1.38	1.33
1	A	2436	A	C2-N3	5.30	1.38	1.33
52	z	76	A	C2-N3	5.30	1.38	1.33
1	A	2570	A	C2-N3	5.29	1.38	1.33
32	W	1435	A	C2-N3	5.29	1.38	1.33
1	A	41	A	C2-N3	5.29	1.38	1.33
32	W	507	A	C2-N3	5.29	1.38	1.33
32	W	604	A	C2-N3	5.29	1.38	1.33
32	W	1270	A	C2-N3	5.29	1.38	1.33
1	A	1768	A	C2-N3	5.28	1.38	1.33
1	A	2683	A	C2-N3	5.28	1.38	1.33
32	W	605	A	C2-N3	5.28	1.38	1.33
1	A	1710	A	C2-N3	5.28	1.38	1.33
1	A	2629	A	C2-N3	5.28	1.38	1.33
1	A	2351	A	C2-N3	5.27	1.38	1.33
1	A	1636	A	C2-N3	5.27	1.38	1.33
1	A	518	A	C2-N3	5.26	1.38	1.33
1	A	1442	A	C2-N3	5.26	1.38	1.33
32	W	76	A	C2-N3	5.26	1.38	1.33
32	W	405	A	C2-N3	5.26	1.38	1.33
1	A	56	A	C2-N3	5.26	1.38	1.33
1	A	2735	A	C2-N3	5.25	1.38	1.33
32	W	1272	A	C2-N3	5.25	1.38	1.33
1	A	391	A	C2-N3	5.25	1.38	1.33
1	A	2885	A	C2-N3	5.25	1.38	1.33
32	W	282	A	C2-N3	5.25	1.38	1.33
1	A	1989	A	C2-N3	5.25	1.38	1.33
1	A	108	A	C2-N3	5.24	1.38	1.33
2	B	25	A	C2-N3	5.24	1.38	1.33
1	A	462	A	C2-N3	5.24	1.38	1.33
1	A	1831	A	C2-N3	5.24	1.38	1.33
2	B	99	A	C2-N3	5.24	1.38	1.33
1	A	634	A	C2-N3	5.24	1.38	1.33
32	W	1296	A	C2-N3	5.24	1.38	1.33
1	A	1008	A	C2-N3	5.24	1.38	1.33
1	A	1945	A	C2-N3	5.24	1.38	1.33
1	A	260	A	C2-N3	5.23	1.38	1.33
1	A	679	A	C2-N3	5.23	1.38	1.33
1	A	156	A	C2-N3	5.23	1.38	1.33
32	W	1384	A	C2-N3	5.23	1.38	1.33
1	A	2498	A	C2-N3	5.23	1.38	1.33
1	A	2500	A	C2-N3	5.23	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2827	A	C2-N3	5.23	1.38	1.33
1	A	1820	A	C2-N3	5.23	1.38	1.33
1	A	2662	A	C2-N3	5.23	1.38	1.33
32	W	685	A	C2-N3	5.23	1.38	1.33
1	A	656	A	C2-N3	5.23	1.38	1.33
1	A	1714	A	C2-N3	5.22	1.38	1.33
32	W	161	A	C2-N3	5.22	1.38	1.33
1	A	851	A	C2-N3	5.22	1.38	1.33
32	W	1529	A	C2-N3	5.22	1.38	1.33
1	A	1675	A	C2-N3	5.22	1.38	1.33
32	W	758	A	C2-N3	5.22	1.38	1.33
32	W	1349	A	C2-N3	5.22	1.38	1.33
32	W	1517	A	C2-N3	5.22	1.38	1.33
32	W	364	A	C2-N3	5.21	1.38	1.33
32	W	724	A	C2-N3	5.21	1.38	1.33
32	W	1160	A	C2-N3	5.21	1.38	1.33
1	A	2049	A	C2-N3	5.21	1.38	1.33
1	A	2407	A	C2-N3	5.21	1.38	1.33
1	A	935	A	C2-N3	5.21	1.38	1.33
1	A	1006	A	C2-N3	5.21	1.38	1.33
32	W	838	A	C2-N3	5.21	1.38	1.33
1	A	1357	A	C2-N3	5.21	1.38	1.33
1	A	2691	A	C2-N3	5.21	1.38	1.33
32	W	1256	A	C2-N3	5.21	1.38	1.33
1	A	549	A	C2-N3	5.21	1.38	1.33
1	A	1778	A	C2-N3	5.21	1.38	1.33
1	A	2627	A	C2-N3	5.21	1.38	1.33
32	W	94	A	C2-N3	5.21	1.38	1.33
1	A	2663	A	C2-N3	5.20	1.38	1.33
1	A	2831	A	C2-N3	5.20	1.38	1.33
1	A	268	A	C2-N3	5.20	1.38	1.33
2	B	27	A	C2-N3	5.20	1.38	1.33
1	A	1100	A	C2-N3	5.20	1.38	1.33
1	A	2805	A	C2-N3	5.20	1.38	1.33
32	W	790	A	C2-N3	5.20	1.38	1.33
32	W	1112	A	C2-N3	5.20	1.38	1.33
1	A	1901	A	C2-N3	5.20	1.38	1.33
1	A	699	A	C2-N3	5.20	1.38	1.33
1	A	964	A	C2-N3	5.20	1.38	1.33
32	W	671	A	C2-N3	5.20	1.38	1.33
2	B	13	A	C2-N3	5.19	1.38	1.33
1	A	1126	A	C2-N3	5.19	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	46	A	C2-N3	5.19	1.38	1.33
32	W	721	A	C2-N3	5.19	1.38	1.33
32	W	947	A	C2-N3	5.19	1.38	1.33
1	A	429	A	C2-N3	5.19	1.38	1.33
1	A	1392	A	C2-N3	5.19	1.38	1.33
32	W	57	A	C2-N3	5.19	1.38	1.33
32	W	664	A	C2-N3	5.19	1.38	1.33
1	A	44	A	C2-N3	5.19	1.38	1.33
32	W	617	A	C2-N3	5.19	1.38	1.33
32	W	1528	A	C2-N3	5.19	1.38	1.33
1	A	2594	A	C2-N3	5.19	1.38	1.33
1	A	2754	A	C2-N3	5.19	1.38	1.33
32	W	452	A	C2-N3	5.19	1.38	1.33
1	A	1096	A	C2-N3	5.19	1.38	1.33
1	A	1480	A	C2-N3	5.19	1.38	1.33
1	A	124	A	C2-N3	5.18	1.38	1.33
1	A	1483	A	C2-N3	5.18	1.38	1.33
1	A	1490	A	C2-N3	5.18	1.38	1.33
1	A	2106	A	C2-N3	5.18	1.38	1.33
32	W	1188	A	C2-N3	5.18	1.38	1.33
1	A	144	A	C2-N3	5.18	1.38	1.33
1	A	917	A	C2-N3	5.18	1.38	1.33
32	W	870	A	C2-N3	5.18	1.38	1.33
1	A	559	A	C2-N3	5.18	1.38	1.33
1	A	1534	A	C2-N3	5.18	1.38	1.33
32	W	140	A	C2-N3	5.18	1.38	1.33
32	W	308	A	C2-N3	5.18	1.38	1.33
32	W	1328	A	C2-N3	5.18	1.38	1.33
1	A	1141	A	C2-N3	5.18	1.38	1.33
32	W	287	A	C2-N3	5.18	1.38	1.33
1	A	517	A	C2-N3	5.18	1.38	1.33
32	W	715	A	C2-N3	5.18	1.38	1.33
1	A	2307	A	C2-N3	5.17	1.38	1.33
32	W	504	A	C2-N3	5.17	1.38	1.33
32	W	796	A	C2-N3	5.17	1.38	1.33
32	W	1143	A	C2-N3	5.17	1.38	1.33
1	A	1477	A	C2-N3	5.17	1.38	1.33
32	W	1427	A	C2-N3	5.17	1.38	1.33
1	A	95	A	C2-N3	5.17	1.38	1.33
52	z	24	A	C2-N3	5.17	1.38	1.33
1	A	162	A	C2-N3	5.17	1.38	1.33
32	W	301	A	C2-N3	5.17	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	844	A	C2-N3	5.17	1.38	1.33
1	A	2900	A	C2-N3	5.17	1.38	1.33
2	B	39	A	C2-N3	5.17	1.38	1.33
32	W	793	A	C2-N3	5.17	1.38	1.33
1	A	1277	A	C2-N3	5.16	1.38	1.33
32	W	948	A	C2-N3	5.16	1.38	1.33
32	W	1022	A	C2-N3	5.16	1.38	1.33
1	A	722	A	C2-N3	5.16	1.38	1.33
1	A	2395	A	C2-N3	5.16	1.38	1.33
1	A	2862	A	C2-N3	5.16	1.38	1.33
32	W	882	A	C2-N3	5.16	1.38	1.33
32	W	918	A	C2-N3	5.16	1.38	1.33
1	A	943	A	C2-N3	5.16	1.38	1.33
1	A	1686	A	C2-N3	5.16	1.38	1.33
1	A	1695	A	C2-N3	5.16	1.38	1.33
1	A	2111	A	C2-N3	5.16	1.38	1.33
1	A	2837	A	C2-N3	5.16	1.38	1.33
32	W	34	A	C2-N3	5.16	1.38	1.33
32	W	485	A	C2-N3	5.16	1.38	1.33
32	W	1245	A	C2-N3	5.16	1.38	1.33
1	A	254	A	C2-N3	5.16	1.38	1.33
1	A	1709	A	C2-N3	5.16	1.38	1.33
1	A	2924	A	C2-N3	5.16	1.38	1.33
32	W	786	A	C2-N3	5.16	1.38	1.33
1	A	1776	A	C2-N3	5.16	1.38	1.33
32	W	512	A	C2-N3	5.16	1.38	1.33
32	W	542	A	C2-N3	5.16	1.38	1.33
1	A	337	A	C2-N3	5.16	1.38	1.33
1	A	763	A	C2-N3	5.16	1.38	1.33
1	A	2661	A	C2-N3	5.16	1.38	1.33
1	A	2907	A	C2-N3	5.16	1.38	1.33
32	W	18	A	C2-N3	5.16	1.38	1.33
1	A	185	A	C2-N3	5.15	1.38	1.33
1	A	117	A	C2-N3	5.15	1.38	1.33
1	A	507	A	C2-N3	5.15	1.38	1.33
1	A	560	A	C2-N3	5.15	1.38	1.33
1	A	908	A	C2-N3	5.15	1.38	1.33
1	A	2455	A	C2-N3	5.15	1.38	1.33
1	A	2511	A	C2-N3	5.15	1.38	1.33
1	A	2812	A	C2-N3	5.15	1.38	1.33
32	W	278	A	C2-N3	5.15	1.38	1.33
32	W	1442	A	C2-N3	5.15	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	A	C2-N3	5.15	1.38	1.33
1	A	830	A	C2-N3	5.15	1.38	1.33
1	A	2875	A	C2-N3	5.15	1.38	1.33
32	W	1161	A	C2-N3	5.15	1.38	1.33
1	A	870	A	C2-N3	5.15	1.38	1.33
1	A	1816	A	C2-N3	5.15	1.38	1.33
1	A	1393	A	C2-N3	5.15	1.38	1.33
1	A	1789	A	C2-N3	5.14	1.38	1.33
32	W	371	A	C2-N3	5.14	1.38	1.33
32	W	1315	A	C2-N3	5.14	1.38	1.33
1	A	1802	A	C2-N3	5.14	1.38	1.33
1	A	2270	A	C2-N3	5.14	1.38	1.33
32	W	1050	A	C2-N3	5.14	1.38	1.33
32	W	1513	A	C2-N3	5.14	1.38	1.33
1	A	6	A	C2-N3	5.14	1.38	1.33
1	A	71	A	C2-N3	5.14	1.38	1.33
1	A	828	A	C2-N3	5.14	1.38	1.33
1	A	889	A	C2-N3	5.14	1.38	1.33
1	A	1286	A	C2-N3	5.14	1.38	1.33
1	A	2532	A	C2-N3	5.14	1.38	1.33
32	W	548	A	C2-N3	5.14	1.38	1.33
32	W	837	A	C2-N3	5.14	1.38	1.33
32	W	1288	A	C2-N3	5.14	1.38	1.33
1	A	616	A	C2-N3	5.13	1.38	1.33
1	A	1424	A	C2-N3	5.13	1.38	1.33
1	A	2026	A	C2-N3	5.13	1.38	1.33
2	B	50	A	C2-N3	5.13	1.38	1.33
32	W	281	A	C2-N3	5.13	1.38	1.33
32	W	1004	A	C2-N3	5.13	1.38	1.33
1	A	715	A	C2-N3	5.13	1.38	1.33
1	A	978	A	C2-N3	5.13	1.38	1.33
1	A	1075	A	C2-N3	5.13	1.38	1.33
1	A	1617	A	C2-N3	5.13	1.38	1.33
1	A	1791	A	C2-N3	5.13	1.38	1.33
32	W	433	A	C2-N3	5.13	1.38	1.33
1	A	140	A	C2-N3	5.13	1.38	1.33
1	A	194	A	C2-N3	5.13	1.38	1.33
1	A	910	A	C2-N3	5.13	1.38	1.33
1	A	1858	A	C2-N3	5.13	1.38	1.33
32	W	31	A	C2-N3	5.13	1.38	1.33
1	A	829	A	C2-N3	5.13	1.38	1.33
1	A	1025	A	C2-N3	5.13	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1339	A	C2-N3	5.13	1.38	1.33
1	A	1653	A	C2-N3	5.13	1.38	1.33
1	A	2734	A	C2-N3	5.13	1.38	1.33
2	B	18	A	C2-N3	5.13	1.38	1.33
2	B	97	A	C2-N3	5.13	1.38	1.33
32	W	460	A	C2-N3	5.13	1.38	1.33
32	W	1463	A	C2-N3	5.13	1.38	1.33
1	A	2402	A	C2-N3	5.12	1.38	1.33
32	W	1486	A	C2-N3	5.12	1.38	1.33
1	A	2030	A	C2-N3	5.12	1.38	1.33
1	A	2790	A	C2-N3	5.12	1.38	1.33
1	A	970	A	C2-N3	5.12	1.38	1.33
1	A	1222	A	C2-N3	5.12	1.38	1.33
1	A	1784	A	C2-N3	5.12	1.38	1.33
1	A	2616	A	C2-N3	5.12	1.38	1.33
32	W	1283	A	C2-N3	5.12	1.38	1.33
1	A	5	A	C2-N3	5.12	1.38	1.33
1	A	1423	A	C2-N3	5.12	1.38	1.33
1	A	1426	A	C2-N3	5.12	1.38	1.33
1	A	1541	A	C2-N3	5.12	1.38	1.33
1	A	1888	A	C2-N3	5.12	1.38	1.33
1	A	736	A	C2-N3	5.12	1.38	1.33
1	A	1019	A	C2-N3	5.12	1.38	1.33
32	W	1327	A	C2-N3	5.12	1.38	1.33
1	A	436	A	C2-N3	5.12	1.38	1.33
1	A	551	A	C2-N3	5.12	1.38	1.33
1	A	1672	A	C2-N3	5.12	1.38	1.33
1	A	1942	A	C2-N3	5.12	1.38	1.33
2	B	105	A	C2-N3	5.12	1.38	1.33
32	W	228	A	C2-N3	5.12	1.38	1.33
1	A	305	A	C2-N3	5.11	1.38	1.33
1	A	1161	A	C2-N3	5.11	1.38	1.33
32	W	361	A	C2-N3	5.11	1.38	1.33
32	W	508	A	C5-C4	-5.11	1.35	1.38
32	W	690	A	C2-N3	5.11	1.38	1.33
32	W	816	A	C2-N3	5.11	1.38	1.33
32	W	1342	A	C2-N3	5.11	1.38	1.33
1	A	244	A	C2-N3	5.11	1.38	1.33
1	A	486	A	C2-N3	5.11	1.38	1.33
1	A	1654	A	C2-N3	5.11	1.38	1.33
1	A	2052	A	C2-N3	5.11	1.38	1.33
1	A	1190	A	C2-N3	5.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1258	A	C2-N3	5.11	1.38	1.33
32	W	684	A	C2-N3	5.11	1.38	1.33
32	W	917	A	C2-N3	5.11	1.38	1.33
32	W	1456	A	C2-N3	5.11	1.38	1.33
1	A	1361	A	C2-N3	5.11	1.38	1.33
1	A	2406	A	C2-N3	5.11	1.38	1.33
1	A	2846	A	C2-N3	5.11	1.38	1.33
1	A	91	A	C2-N3	5.11	1.38	1.33
1	A	150	A	C2-N3	5.11	1.38	1.33
1	A	330	A	C2-N3	5.11	1.38	1.33
1	A	1131	A	C2-N3	5.11	1.38	1.33
1	A	1142	A	C2-N3	5.11	1.38	1.33
1	A	1839	A	C2-N3	5.11	1.38	1.33
1	A	1981	A	C2-N3	5.11	1.38	1.33
1	A	2302	A	C2-N3	5.11	1.38	1.33
1	A	2459	A	C2-N3	5.11	1.38	1.33
1	A	2668	A	C2-N3	5.11	1.38	1.33
1	A	2750	A	C2-N3	5.11	1.38	1.33
32	W	142	A	C2-N3	5.11	1.38	1.33
1	A	2387	A	C2-N3	5.11	1.38	1.33
1	A	2769	A	C2-N3	5.11	1.38	1.33
32	W	1247	A	C2-N3	5.11	1.38	1.33
1	A	219	A	C2-N3	5.10	1.38	1.33
1	A	389	A	C2-N3	5.10	1.38	1.33
1	A	496	A	C2-N3	5.10	1.38	1.33
1	A	2043	A	C2-N3	5.10	1.38	1.33
32	W	968	A	C2-N3	5.10	1.38	1.33
1	A	1618	A	C2-N3	5.10	1.38	1.33
32	W	582	A	C2-N3	5.10	1.38	1.33
32	W	1308	A	C2-N3	5.10	1.38	1.33
1	A	2904	A	C2-N3	5.10	1.38	1.33
1	A	110	A	C2-N3	5.10	1.38	1.33
1	A	974	A	C2-N3	5.10	1.38	1.33
1	A	1956	A	C2-N3	5.10	1.38	1.33
1	A	2047	A	C2-N3	5.10	1.38	1.33
32	W	271	A	C2-N3	5.10	1.38	1.33
32	W	669	A	C2-N3	5.10	1.38	1.33
1	A	13	A	C2-N3	5.10	1.38	1.33
1	A	224	A	C2-N3	5.10	1.38	1.33
1	A	543	A	C2-N3	5.10	1.38	1.33
1	A	774	A	C5-C4	-5.10	1.35	1.38
1	A	1119	A	C2-N3	5.10	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1722	A	C2-N3	5.10	1.38	1.33
1	A	2673	A	C2-N3	5.10	1.38	1.33
32	W	53	A	C2-N3	5.10	1.38	1.33
32	W	81	A	C2-N3	5.10	1.38	1.33
32	W	1016	A	C2-N3	5.10	1.38	1.33
1	A	2722	A	C2-N3	5.10	1.38	1.33
32	W	335	A	C2-N3	5.10	1.38	1.33
32	W	1493	A	C2-N3	5.10	1.38	1.33
1	A	130	A	C2-N3	5.09	1.38	1.33
1	A	216	A	C2-N3	5.09	1.38	1.33
1	A	866	A	C2-N3	5.09	1.38	1.33
1	A	882	A	C2-N3	5.09	1.38	1.33
1	A	1499	A	C2-N3	5.09	1.38	1.33
1	A	2526	A	C2-N3	5.09	1.38	1.33
32	W	314	A	C2-N3	5.09	1.38	1.33
32	W	1261	A	C2-N3	5.09	1.38	1.33
1	A	1235	A	C2-N3	5.09	1.38	1.33
32	W	35	A	C2-N3	5.09	1.38	1.33
32	W	1028	A	C2-N3	5.09	1.38	1.33
1	A	275	A	C2-N3	5.09	1.38	1.33
1	A	519	A	C2-N3	5.09	1.38	1.33
1	A	547	A	C2-N3	5.09	1.38	1.33
1	A	1614	A	C2-N3	5.09	1.38	1.33
1	A	1727	A	C2-N3	5.09	1.38	1.33
1	A	2517	A	C2-N3	5.09	1.38	1.33
1	A	692	A	C2-N3	5.09	1.38	1.33
1	A	1221	A	C2-N3	5.09	1.38	1.33
1	A	2835	A	C2-N3	5.09	1.38	1.33
1	A	2889	A	C2-N3	5.09	1.38	1.33
32	W	491	A	C2-N3	5.09	1.38	1.33
32	W	824	A	C2-N3	5.09	1.38	1.33
1	A	572	A	C2-N3	5.09	1.38	1.33
1	A	1606	A	C2-N3	5.09	1.38	1.33
32	W	1014	A	C2-N3	5.09	1.38	1.33
1	A	1832	A	C2-N3	5.09	1.38	1.33
1	A	2670	A	C2-N3	5.09	1.38	1.33
32	W	1140	A	C2-N3	5.09	1.38	1.33
32	W	1434	A	C2-N3	5.09	1.38	1.33
32	W	1490	A	C2-N3	5.09	1.38	1.33
1	A	199	A	C2-N3	5.08	1.38	1.33
1	A	1516	A	C2-N3	5.08	1.38	1.33
1	A	1540	A	C2-N3	5.08	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1928	A	C2-N3	5.08	1.38	1.33
1	A	2810	A	C2-N3	5.08	1.38	1.33
32	W	956	A	C2-N3	5.08	1.38	1.33
1	A	1174	A	C2-N3	5.08	1.38	1.33
1	A	2080	A	C2-N3	5.08	1.38	1.33
1	A	220	A	C2-N3	5.08	1.38	1.33
1	A	1059	A	C2-N3	5.08	1.38	1.33
32	W	651	A	C2-N3	5.08	1.38	1.33
32	W	1271	A	C2-N3	5.08	1.38	1.33
32	W	1437	A	C2-N3	5.08	1.38	1.33
1	A	1506	A	C2-N3	5.08	1.38	1.33
1	A	1583	A	C2-N3	5.08	1.38	1.33
1	A	1723	A	C2-N3	5.08	1.38	1.33
1	A	1767	A	C2-N3	5.08	1.38	1.33
32	W	1405	A	C2-N3	5.08	1.38	1.33
1	A	318	A	C2-N3	5.08	1.38	1.33
1	A	2018	A	C2-N3	5.08	1.38	1.33
2	B	55	A	C2-N3	5.08	1.38	1.33
1	A	1335	A	C2-N3	5.08	1.38	1.33
1	A	1850	A	C2-N3	5.08	1.38	1.33
1	A	2088	A	C2-N3	5.08	1.38	1.33
32	W	390	A	C2-N3	5.08	1.38	1.33
1	A	61	A	C2-N3	5.08	1.38	1.33
1	A	226	A	C2-N3	5.08	1.38	1.33
1	A	265	A	C2-N3	5.08	1.38	1.33
1	A	678	A	C2-N3	5.08	1.38	1.33
1	A	690	A	C2-N3	5.08	1.38	1.33
1	A	896	A	C2-N3	5.08	1.38	1.33
1	A	1026	A	C2-N3	5.08	1.38	1.33
1	A	1877	A	C2-N3	5.08	1.38	1.33
2	B	51	A	C2-N3	5.08	1.38	1.33
1	A	118	A	C2-N3	5.07	1.38	1.33
1	A	705	A	C2-N3	5.07	1.38	1.33
1	A	2316	A	C2-N3	5.07	1.38	1.33
32	W	74	A	C2-N3	5.07	1.38	1.33
32	W	266	A	C5-C4	-5.07	1.35	1.38
32	W	1115	A	C2-N3	5.07	1.38	1.33
1	A	325	A	C2-N3	5.07	1.38	1.33
1	A	2000	A	C2-N3	5.07	1.38	1.33
1	A	2421	A	C2-N3	5.07	1.38	1.33
1	A	259	A	C2-N3	5.07	1.38	1.33
1	A	592	A	C2-N3	5.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1224	A	C2-N3	5.07	1.38	1.33
1	A	1517	A	C2-N3	5.07	1.38	1.33
1	A	1580	A	C2-N3	5.07	1.38	1.33
32	W	266	A	C2-N3	5.07	1.38	1.33
32	W	439	A	C2-N3	5.07	1.38	1.33
32	W	1236	A	C2-N3	5.07	1.38	1.33
1	A	1627	A	C2-N3	5.07	1.38	1.33
1	A	2027	A	C2-N3	5.07	1.38	1.33
1	A	2658	A	C2-N3	5.07	1.38	1.33
32	W	650	A	C2-N3	5.07	1.38	1.33
1	A	428	A	C2-N3	5.07	1.38	1.33
1	A	475	A	C2-N3	5.07	1.38	1.33
1	A	1398	A	C2-N3	5.07	1.38	1.33
1	A	1445	A	C2-N3	5.07	1.38	1.33
1	A	1520	A	C2-N3	5.07	1.38	1.33
1	A	1697	A	C2-N3	5.07	1.38	1.33
1	A	2357	A	C2-N3	5.07	1.38	1.33
32	W	1065	A	C2-N3	5.07	1.38	1.33
32	W	1120	A	C2-N3	5.07	1.38	1.33
1	A	630	A	C2-N3	5.07	1.38	1.33
1	A	2686	A	C2-N3	5.07	1.38	1.33
1	A	2704	A	C2-N3	5.07	1.38	1.33
32	W	649	A	C2-N3	5.07	1.38	1.33
32	W	743	A	C2-N3	5.07	1.38	1.33
1	A	724	A	C2-N3	5.06	1.38	1.33
1	A	1036	A	C2-N3	5.06	1.38	1.33
1	A	1788	A	C2-N3	5.06	1.38	1.33
1	A	10	A	C2-N3	5.06	1.38	1.33
1	A	281	A	C2-N3	5.06	1.38	1.33
1	A	847	A	C2-N3	5.06	1.38	1.33
1	A	1027	A	C2-N3	5.06	1.38	1.33
32	W	423	A	C2-N3	5.06	1.38	1.33
32	W	440	A	C2-N3	5.06	1.38	1.33
32	W	737	A	C2-N3	5.06	1.38	1.33
32	W	910	A	C2-N3	5.06	1.38	1.33
32	W	1417	A	C2-N3	5.06	1.38	1.33
32	W	1455	A	C2-N3	5.06	1.38	1.33
1	A	1914	A	C2-N3	5.06	1.38	1.33
32	W	1048	A	C2-N3	5.06	1.38	1.33
1	A	1029	A	C2-N3	5.06	1.38	1.33
1	A	1746	A	C2-N3	5.06	1.38	1.33
1	A	1967	A	C2-N3	5.06	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	206	A	C2-N3	5.06	1.38	1.33
32	W	1017	A	C2-N3	5.06	1.38	1.33
32	W	1179	A	C2-N3	5.06	1.38	1.33
1	A	421	A	C2-N3	5.06	1.38	1.33
1	A	661	A	C2-N3	5.06	1.38	1.33
1	A	2078	A	C2-N3	5.06	1.38	1.33
32	W	296	A	C2-N3	5.06	1.38	1.33
32	W	1031	A	C2-N3	5.06	1.38	1.33
1	A	329	A	C2-N3	5.05	1.38	1.33
1	A	376	A	C2-N3	5.05	1.38	1.33
1	A	537	A	C2-N3	5.05	1.38	1.33
1	A	683	A	C2-N3	5.05	1.38	1.33
1	A	1895	A	C2-N3	5.05	1.38	1.33
1	A	2441	A	C2-N3	5.05	1.38	1.33
32	W	61	A	C2-N3	5.05	1.38	1.33
32	W	337	A	C2-N3	5.05	1.38	1.33
32	W	638	A	C2-N3	5.05	1.38	1.33
1	A	193	A	C2-N3	5.05	1.38	1.33
32	W	679	A	C2-N3	5.05	1.38	1.33
1	A	90	A	C2-N3	5.05	1.38	1.33
1	A	1906	A	C2-N3	5.05	1.38	1.33
1	A	2571	A	C5-C4	-5.05	1.35	1.38
32	W	386	A	C2-N3	5.05	1.38	1.33
32	W	875	A	C2-N3	5.05	1.38	1.33
1	A	1524	A	C2-N3	5.05	1.38	1.33
1	A	2454	A	C2-N3	5.05	1.38	1.33
32	W	984	A	C2-N3	5.05	1.38	1.33
52	z	23	A	C2-N3	5.05	1.38	1.33
1	A	53	A	C2-N3	5.05	1.38	1.33
1	A	1608	A	C2-N3	5.05	1.38	1.33
1	A	1244	A	C2-N3	5.05	1.38	1.33
1	A	1677	A	C2-N3	5.05	1.38	1.33
1	A	2779	A	C2-N3	5.05	1.38	1.33
32	W	1222	A	C2-N3	5.05	1.38	1.33
32	W	696	A	C2-N3	5.04	1.38	1.33
32	W	1238	A	C2-N3	5.04	1.38	1.33
1	A	958	A	C2-N3	5.04	1.38	1.33
1	A	1504	A	C2-N3	5.04	1.38	1.33
1	A	2860	A	C2-N3	5.04	1.38	1.33
32	W	1155	A	C2-N3	5.04	1.38	1.33
1	A	230	A	C2-N3	5.04	1.38	1.33
1	A	538	A	C2-N3	5.04	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	584	A	C2-N3	5.04	1.38	1.33
1	A	893	A	C2-N3	5.04	1.38	1.33
1	A	1072	A	C2-N3	5.04	1.38	1.33
1	A	1132	A	C2-N3	5.04	1.38	1.33
1	A	1144	A	C2-N3	5.04	1.38	1.33
1	A	1197	A	C2-N3	5.04	1.38	1.33
1	A	1760	A	C2-N3	5.04	1.38	1.33
32	W	160	A	C2-N3	5.04	1.38	1.33
32	W	306	A	C2-N3	5.04	1.38	1.33
32	W	592	A	C2-N3	5.04	1.38	1.33
52	z	14	A	C2-N3	5.04	1.38	1.33
1	A	278	A	C2-N3	5.04	1.38	1.33
1	A	646	A	C2-N3	5.04	1.38	1.33
1	A	1809	A	C2-N3	5.04	1.38	1.33
32	W	1451	A	C2-N3	5.04	1.38	1.33
1	A	1055	A	C2-N3	5.04	1.38	1.33
1	A	1179	A	C2-N3	5.04	1.38	1.33
1	A	1210	A	C2-N3	5.04	1.38	1.33
1	A	1882	A	C2-N3	5.04	1.38	1.33
2	B	44	A	C2-N3	5.04	1.38	1.33
32	W	883	A	C2-N3	5.04	1.38	1.33
32	W	1541	A	C2-N3	5.04	1.38	1.33
1	A	73	A	C2-N3	5.04	1.38	1.33
1	A	171	A	C2-N3	5.04	1.38	1.33
1	A	2044	A	C2-N3	5.04	1.38	1.33
32	W	1479	A	C2-N3	5.04	1.38	1.33
32	W	1502	A	C2-N3	5.04	1.38	1.33
1	A	582	A	C2-N3	5.04	1.38	1.33
1	A	673	A	C5-C4	-5.04	1.35	1.38
1	A	1005	A	C2-N3	5.04	1.38	1.33
1	A	1034	A	C2-N3	5.04	1.38	1.33
1	A	1084	A	C2-N3	5.04	1.38	1.33
1	A	1134	A	C2-N3	5.04	1.38	1.33
1	A	1265	A	C2-N3	5.04	1.38	1.33
1	A	2389	A	C2-N3	5.04	1.38	1.33
1	A	2793	A	C2-N3	5.04	1.38	1.33
32	W	389	A	C2-N3	5.04	1.38	1.33
32	W	422	A	C2-N3	5.04	1.38	1.33
32	W	630	A	C2-N3	5.04	1.38	1.33
32	W	1369	A	C2-N3	5.04	1.38	1.33
52	z	58	A	C2-N3	5.04	1.38	1.33
1	A	12	A	C2-N3	5.03	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	A	C2-N3	5.03	1.38	1.33
1	A	578	A	C2-N3	5.03	1.38	1.33
1	A	637	A	C2-N3	5.03	1.38	1.33
1	A	971	A	C2-N3	5.03	1.38	1.33
1	A	1113	A	C2-N3	5.03	1.38	1.33
1	A	1700	A	C2-N3	5.03	1.38	1.33
2	B	71	A	C2-N3	5.03	1.38	1.33
32	W	404	A	C2-N3	5.03	1.38	1.33
1	A	1432	A	C2-N3	5.03	1.38	1.33
32	W	1207	A	C2-N3	5.03	1.38	1.33
1	A	133	A	C2-N3	5.03	1.38	1.33
1	A	689	A	C2-N3	5.03	1.38	1.33
1	A	740	A	C2-N3	5.03	1.38	1.33
1	A	894	A	C2-N3	5.03	1.38	1.33
1	A	1054	A	C2-N3	5.03	1.38	1.33
1	A	1900	A	C2-N3	5.03	1.38	1.33
1	A	2295	A	C2-N3	5.03	1.38	1.33
32	W	232	A	C2-N3	5.03	1.38	1.33
32	W	1248	A	C2-N3	5.03	1.38	1.33
1	A	1966	A	C2-N3	5.03	1.38	1.33
1	A	2340	A	C2-N3	5.03	1.38	1.33
1	A	2369	A	C2-N3	5.03	1.38	1.33
32	W	67	A	C2-N3	5.03	1.38	1.33
32	W	352	A	C2-N3	5.03	1.38	1.33
32	W	1210	A	C2-N3	5.03	1.38	1.33
1	A	1056	A	C2-N3	5.03	1.38	1.33
1	A	1061	A	C2-N3	5.03	1.38	1.33
1	A	1149	A	C2-N3	5.03	1.38	1.33
1	A	1845	A	C2-N3	5.03	1.38	1.33
32	W	803	A	C2-N3	5.03	1.38	1.33
32	W	911	A	C2-N3	5.03	1.38	1.33
32	W	1056	A	C2-N3	5.03	1.38	1.33
32	W	1205	A	C2-N3	5.03	1.38	1.33
32	W	1478	A	C2-N3	5.03	1.38	1.33
1	A	456	A	C2-N3	5.03	1.38	1.33
1	A	769	A	C2-N3	5.03	1.38	1.33
1	A	1453	A	C2-N3	5.03	1.38	1.33
32	W	611	A	C2-N3	5.03	1.38	1.33
1	A	913	A	C2-N3	5.02	1.38	1.33
1	A	2417	A	C2-N3	5.02	1.38	1.33
1	A	2777	A	C5-C4	-5.02	1.35	1.38
1	A	2845	A	C2-N3	5.02	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	W	507	A	C5-C4	-5.02	1.35	1.38
32	W	1466	A	C2-N3	5.02	1.38	1.33
1	A	758	A	C2-N3	5.02	1.38	1.33
1	A	1347	A	C2-N3	5.02	1.38	1.33
1	A	2087	A	C2-N3	5.02	1.38	1.33
1	A	2507	A	C2-N3	5.02	1.38	1.33
1	A	2770	A	C2-N3	5.02	1.38	1.33
1	A	2787	A	C2-N3	5.02	1.38	1.33
32	W	52	A	C2-N3	5.02	1.38	1.33
32	W	72	A	C2-N3	5.02	1.38	1.33
32	W	107	A	C2-N3	5.02	1.38	1.33
32	W	203	A	C2-N3	5.02	1.38	1.33
32	W	928	A	C2-N3	5.02	1.38	1.33
32	W	1090	A	C2-N3	5.02	1.38	1.33
1	A	876	A	C2-N3	5.02	1.38	1.33
1	A	2343	A	C2-N3	5.02	1.38	1.33
32	W	725	A	C2-N3	5.02	1.38	1.33
1	A	343	A	C2-N3	5.02	1.38	1.33
1	A	653	A	C2-N3	5.02	1.38	1.33
1	A	1115	A	C2-N3	5.02	1.38	1.33
1	A	1619	A	C2-N3	5.02	1.38	1.33
1	A	2590	A	C2-N3	5.02	1.38	1.33
32	W	382	A	C2-N3	5.02	1.38	1.33
52	z	21	A	C2-N3	5.02	1.38	1.33
1	A	154	A	C2-N3	5.02	1.38	1.33
1	A	222	A	C2-N3	5.02	1.38	1.33
1	A	1194	A	C2-N3	5.02	1.38	1.33
1	A	1323	A	C2-N3	5.02	1.38	1.33
32	W	254	A	C2-N3	5.02	1.38	1.33
32	W	1103	A	C2-N3	5.02	1.38	1.33
32	W	1176	A	C2-N3	5.02	1.38	1.33
52	z	44	A	C2-N3	5.02	1.38	1.33
32	W	713	A	C2-N3	5.02	1.38	1.33
32	W	831	A	C2-N3	5.02	1.38	1.33
1	A	717	A	C2-N3	5.01	1.38	1.33
1	A	948	A	C2-N3	5.01	1.38	1.33
32	W	475	A	C2-N3	5.01	1.38	1.33
32	W	1257	A	C2-N3	5.01	1.38	1.33
1	A	727	A	C2-N3	5.01	1.38	1.33
1	A	1421	A	C2-N3	5.01	1.38	1.33
1	A	1585	A	C2-N3	5.01	1.38	1.33
1	A	1685	A	C2-N3	5.01	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	A	C2-N3	5.01	1.38	1.33
1	A	166	A	C2-N3	5.01	1.38	1.33
1	A	991	A	C5-C4	-5.01	1.35	1.38
1	A	1562	A	C2-N3	5.01	1.38	1.33
1	A	1710	A	C5-C4	-5.01	1.35	1.38
1	A	1774	A	C2-N3	5.01	1.38	1.33
32	W	923	A	C2-N3	5.01	1.38	1.33
32	W	1092	A	C2-N3	5.01	1.38	1.33
32	W	1419	A	C2-N3	5.01	1.38	1.33
1	A	65	A	C2-N3	5.01	1.38	1.33
1	A	673	A	C2-N3	5.01	1.38	1.33
1	A	746	A	C2-N3	5.01	1.38	1.33
1	A	2071	A	C2-N3	5.01	1.38	1.33
32	W	705	A	C2-N3	5.01	1.38	1.33
32	W	1383	A	C2-N3	5.01	1.38	1.33
1	A	265	A	C5-C4	-5.01	1.35	1.38
1	A	1266	A	C2-N3	5.01	1.38	1.33
1	A	786	A	C2-N3	5.01	1.38	1.33
1	A	1734	A	C2-N3	5.01	1.38	1.33
32	W	321	A	C2-N3	5.01	1.38	1.33
32	W	367	A	C2-N3	5.01	1.38	1.33
1	A	38	A	C2-N3	5.00	1.38	1.33
1	A	52	A	C2-N3	5.00	1.38	1.33
1	A	469	A	C2-N3	5.00	1.38	1.33
1	A	2919	A	C2-N3	5.00	1.38	1.33
32	W	55	A	C2-N3	5.00	1.38	1.33
32	W	618	A	C2-N3	5.00	1.38	1.33
1	A	225	A	C2-N3	5.00	1.38	1.33
1	A	868	A	C2-N3	5.00	1.38	1.33
1	A	1254	A	C2-N3	5.00	1.38	1.33
1	A	1405	A	C2-N3	5.00	1.38	1.33
32	W	532	A	C2-N3	5.00	1.38	1.33
32	W	768	A	C2-N3	5.00	1.38	1.33
1	A	677	A	C2-N3	5.00	1.38	1.33
1	A	753	A	C2-N3	5.00	1.38	1.33
1	A	888	A	C2-N3	5.00	1.38	1.33
1	A	2834	A	C2-N3	5.00	1.38	1.33

All (11520) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1691	A	C2-N3-C4	20.51	120.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1134	A	C2-N3-C4	20.48	120.84	110.60
32	W	1308	A	C2-N3-C4	20.41	120.80	110.60
1	A	226	A	C2-N3-C4	20.26	120.73	110.60
1	A	732	A	C2-N3-C4	20.18	120.69	110.60
32	W	993	A	C2-N3-C4	20.13	120.66	110.60
32	W	195	A	C2-N3-C4	20.12	120.66	110.60
1	A	593	A	C2-N3-C4	20.02	120.61	110.60
1	A	1714	A	C2-N3-C4	19.97	120.58	110.60
1	A	1581	A	C2-N3-C4	19.95	120.58	110.60
32	W	1234	A	C2-N3-C4	19.93	120.56	110.60
32	W	405	A	C2-N3-C4	19.87	120.54	110.60
32	W	1288	A	C2-N3-C4	19.84	120.52	110.60
32	W	572	A	C2-N3-C4	19.76	120.48	110.60
1	A	2786	A	C2-N3-C4	19.73	120.46	110.60
1	A	1046	A	C2-N3-C4	19.66	120.43	110.60
1	A	1132	A	C2-N3-C4	19.58	120.39	110.60
1	A	437	A	C2-N3-C4	19.57	120.39	110.60
1	A	1491	A	C2-N3-C4	19.57	120.39	110.60
32	W	674	A	C2-N3-C4	19.55	120.38	110.60
1	A	1480	A	C2-N3-C4	19.50	120.35	110.60
32	W	1341	A	C2-N3-C4	19.50	120.35	110.60
1	A	560	A	C2-N3-C4	19.49	120.35	110.60
32	W	987	A	C2-N3-C4	19.49	120.35	110.60
1	A	948	A	C2-N3-C4	19.47	120.33	110.60
1	A	913	A	C2-N3-C4	19.47	120.33	110.60
1	A	732	A	N1-C2-N3	-19.44	119.58	129.30
1	A	1506	A	C2-N3-C4	19.43	120.32	110.60
32	W	727	A	C2-N3-C4	19.43	120.31	110.60
32	W	128	A	C2-N3-C4	19.42	120.31	110.60
1	A	438	A	C2-N3-C4	19.41	120.30	110.60
1	A	1360	A	C2-N3-C4	19.40	120.30	110.60
2	B	11	A	C2-N3-C4	19.39	120.30	110.60
1	A	925	A	C2-N3-C4	19.36	120.28	110.60
1	A	2339	A	C2-N3-C4	19.34	120.27	110.60
1	A	2794	A	C2-N3-C4	19.33	120.27	110.60
2	B	71	A	C2-N3-C4	19.32	120.26	110.60
32	W	151	A	C2-N3-C4	19.31	120.26	110.60
1	A	390	A	C2-N3-C4	19.30	120.25	110.60
32	W	1358	A	N1-C2-N3	-19.30	119.65	129.30
1	A	736	A	C2-N3-C4	19.28	120.24	110.60
1	A	957	A	C2-N3-C4	19.28	120.24	110.60
1	A	1073	A	C2-N3-C4	19.27	120.24	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1358	A	C2-N3-C4	19.27	120.24	110.60
1	A	1905	A	C2-N3-C4	19.27	120.23	110.60
1	A	2532	A	C2-N3-C4	19.26	120.23	110.60
32	W	507	A	C2-N3-C4	19.25	120.23	110.60
1	A	935	A	C2-N3-C4	19.24	120.22	110.60
1	A	1778	A	C2-N3-C4	19.23	120.21	110.60
1	A	1930	A	C2-N3-C4	19.22	120.21	110.60
32	W	674	A	N1-C2-N3	-19.22	119.69	129.30
1	A	183	A	N1-C2-N3	-19.22	119.69	129.30
1	A	765	A	C2-N3-C4	19.22	120.21	110.60
1	A	161	A	C2-N3-C4	19.21	120.21	110.60
1	A	1286	A	C2-N3-C4	19.21	120.21	110.60
1	A	1667	A	C2-N3-C4	19.21	120.21	110.60
32	W	956	A	C2-N3-C4	19.21	120.20	110.60
1	A	867	A	C2-N3-C4	19.20	120.20	110.60
32	W	862	A	N1-C2-N3	-19.20	119.70	129.30
1	A	2459	A	C2-N3-C4	19.20	120.20	110.60
1	A	1074	A	C2-N3-C4	19.20	120.20	110.60
1	A	1305	A	N1-C2-N3	-19.20	119.70	129.30
1	A	2807	A	N1-C2-N3	-19.19	119.70	129.30
1	A	527	A	C2-N3-C4	19.19	120.19	110.60
1	A	2062	A	N1-C2-N3	-19.19	119.71	129.30
1	A	1555	A	N1-C2-N3	-19.18	119.71	129.30
32	W	1160	A	C2-N3-C4	19.18	120.19	110.60
32	W	844	A	C2-N3-C4	19.18	120.19	110.60
1	A	690	A	C2-N3-C4	19.18	120.19	110.60
1	A	1905	A	N1-C2-N3	-19.18	119.71	129.30
32	W	737	A	C2-N3-C4	19.18	120.19	110.60
1	A	133	A	C2-N3-C4	19.18	120.19	110.60
1	A	1005	A	C2-N3-C4	19.18	120.19	110.60
1	A	1442	A	C2-N3-C4	19.17	120.19	110.60
1	A	1398	A	C2-N3-C4	19.17	120.18	110.60
32	W	899	A	N1-C2-N3	-19.17	119.72	129.30
52	z	23	A	C2-N3-C4	19.16	120.18	110.60
1	A	2083	A	C2-N3-C4	19.16	120.18	110.60
32	W	254	A	N1-C2-N3	-19.16	119.72	129.30
1	A	318	A	C2-N3-C4	19.15	120.18	110.60
1	A	1655	A	C2-N3-C4	19.15	120.18	110.60
1	A	1097	A	N1-C2-N3	-19.15	119.72	129.30
1	A	1123	A	N1-C2-N3	-19.15	119.72	129.30
1	A	574	A	C2-N3-C4	19.15	120.17	110.60
1	A	2089	A	N1-C2-N3	-19.15	119.73	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1485	A	C2-N3-C4	19.14	120.17	110.60
1	A	1919	A	N1-C2-N3	-19.14	119.73	129.30
1	A	2689	A	C2-N3-C4	19.14	120.17	110.60
1	A	108	A	C2-N3-C4	19.14	120.17	110.60
1	A	652	A	C2-N3-C4	19.14	120.17	110.60
1	A	689	A	C2-N3-C4	19.14	120.17	110.60
1	A	847	A	N1-C2-N3	-19.14	119.73	129.30
2	B	102	A	C2-N3-C4	19.14	120.17	110.60
32	W	631	A	N1-C2-N3	-19.14	119.73	129.30
32	W	945	A	C2-N3-C4	19.13	120.17	110.60
1	A	1019	A	C2-N3-C4	19.13	120.17	110.60
1	A	1388	A	C2-N3-C4	19.13	120.17	110.60
1	A	849	A	C2-N3-C4	19.13	120.16	110.60
32	W	1155	A	C2-N3-C4	19.13	120.16	110.60
1	A	1096	A	C2-N3-C4	19.12	120.16	110.60
32	W	381	A	C2-N3-C4	19.12	120.16	110.60
32	W	151	A	N1-C2-N3	-19.12	119.74	129.30
1	A	2807	A	C2-N3-C4	19.12	120.16	110.60
1	A	130	A	C2-N3-C4	19.12	120.16	110.60
32	W	114	A	C2-N3-C4	19.12	120.16	110.60
1	A	1536	A	C2-N3-C4	19.12	120.16	110.60
32	W	1178	A	C2-N3-C4	19.11	120.16	110.60
1	A	2735	A	C2-N3-C4	19.11	120.16	110.60
32	W	506	A	C2-N3-C4	19.11	120.16	110.60
32	W	811	A	C2-N3-C4	19.11	120.16	110.60
1	A	2790	A	C2-N3-C4	19.11	120.15	110.60
1	A	1914	A	N1-C2-N3	-19.11	119.75	129.30
32	W	713	A	N1-C2-N3	-19.11	119.75	129.30
1	A	1417	A	N1-C2-N3	-19.10	119.75	129.30
32	W	649	A	C2-N3-C4	19.10	120.15	110.60
32	W	899	A	C2-N3-C4	19.10	120.15	110.60
32	W	1372	A	N1-C2-N3	-19.10	119.75	129.30
1	A	1877	A	C2-N3-C4	19.10	120.15	110.60
1	A	118	A	N1-C2-N3	-19.09	119.75	129.30
32	W	630	A	C2-N3-C4	19.09	120.15	110.60
1	A	2889	A	C2-N3-C4	19.09	120.14	110.60
52	z	14	A	C2-N3-C4	19.08	120.14	110.60
1	A	364	A	C2-N3-C4	19.08	120.14	110.60
1	A	526	A	N1-C2-N3	-19.08	119.76	129.30
1	A	882	A	C2-N3-C4	19.08	120.14	110.60
32	W	170	A	C2-N3-C4	19.08	120.14	110.60
1	A	526	A	C2-N3-C4	19.08	120.14	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1375	A	C2-N3-C4	19.08	120.14	110.60
1	A	1562	A	C2-N3-C4	19.08	120.14	110.60
32	W	74	A	C2-N3-C4	19.08	120.14	110.60
1	A	910	A	C2-N3-C4	19.08	120.14	110.60
1	A	965	A	C2-N3-C4	19.08	120.14	110.60
32	W	462	A	C2-N3-C4	19.08	120.14	110.60
32	W	555	A	C2-N3-C4	19.08	120.14	110.60
1	A	1097	A	C2-N3-C4	19.07	120.14	110.60
1	A	1919	A	C2-N3-C4	19.07	120.14	110.60
32	W	1115	A	C2-N3-C4	19.07	120.13	110.60
1	A	1174	A	C2-N3-C4	19.07	120.13	110.60
1	A	1914	A	C2-N3-C4	19.07	120.13	110.60
1	A	2719	A	C2-N3-C4	19.07	120.13	110.60
32	W	439	A	C2-N3-C4	19.07	120.13	110.60
32	W	1455	A	C2-N3-C4	19.07	120.13	110.60
1	A	1266	A	C2-N3-C4	19.06	120.13	110.60
1	A	500	A	C2-N3-C4	19.06	120.13	110.60
2	B	71	A	N1-C2-N3	-19.06	119.77	129.30
1	A	2826	A	C2-N3-C4	19.06	120.13	110.60
32	W	129	A	C2-N3-C4	19.06	120.13	110.60
32	W	477	A	C2-N3-C4	19.06	120.13	110.60
1	A	353	A	C2-N3-C4	19.06	120.13	110.60
1	A	342	A	C2-N3-C4	19.05	120.13	110.60
1	A	634	A	C2-N3-C4	19.05	120.13	110.60
1	A	943	A	C2-N3-C4	19.05	120.13	110.60
2	B	114	A	C2-N3-C4	19.05	120.13	110.60
1	A	265	A	C2-N3-C4	19.05	120.12	110.60
32	W	775	A	C2-N3-C4	19.05	120.12	110.60
1	A	1532	A	C2-N3-C4	19.05	120.12	110.60
1	A	2329	A	C2-N3-C4	19.05	120.12	110.60
32	W	258	A	C2-N3-C4	19.05	120.12	110.60
1	A	154	A	C2-N3-C4	19.05	120.12	110.60
32	W	508	A	N1-C2-N3	-19.05	119.78	129.30
32	W	301	A	C2-N3-C4	19.04	120.12	110.60
32	W	671	A	C2-N3-C4	19.04	120.12	110.60
1	A	64	A	N1-C2-N3	-19.04	119.78	129.30
1	A	1222	A	C2-N3-C4	19.04	120.12	110.60
32	W	150	A	N1-C2-N3	-19.04	119.78	129.30
32	W	1523	A	C2-N3-C4	19.04	120.12	110.60
32	W	1359	A	C2-N3-C4	19.04	120.12	110.60
1	A	1392	A	C2-N3-C4	19.04	120.12	110.60
1	A	1490	A	C2-N3-C4	19.03	120.12	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2369	A	C2-N3-C4	19.03	120.11	110.60
2	B	13	A	C2-N3-C4	19.03	120.12	110.60
32	W	415	A	N1-C2-N3	-19.03	119.78	129.30
32	W	438	A	C2-N3-C4	19.03	120.11	110.60
32	W	978	A	C2-N3-C4	19.03	120.11	110.60
1	A	1325	A	C2-N3-C4	19.03	120.11	110.60
32	W	631	A	C2-N3-C4	19.03	120.11	110.60
32	W	1372	A	C2-N3-C4	19.03	120.11	110.60
1	A	1269	A	C2-N3-C4	19.03	120.11	110.60
1	A	171	A	C2-N3-C4	19.02	120.11	110.60
1	A	758	A	C2-N3-C4	19.02	120.11	110.60
32	W	1236	A	C2-N3-C4	19.02	120.11	110.60
1	A	1520	A	C2-N3-C4	19.02	120.11	110.60
1	A	2091	A	C2-N3-C4	19.02	120.11	110.60
1	A	2547	A	C2-N3-C4	19.02	120.11	110.60
2	B	46	A	C2-N3-C4	19.02	120.11	110.60
32	W	457	A	N1-C2-N3	-19.02	119.79	129.30
32	W	1260	A	C2-N3-C4	19.02	120.11	110.60
1	A	765	A	N1-C2-N3	-19.02	119.79	129.30
1	A	2479	A	C2-N3-C4	19.02	120.11	110.60
1	A	176	A	C2-N3-C4	19.01	120.11	110.60
1	A	1473	A	N1-C2-N3	-19.01	119.79	129.30
1	A	1524	A	C2-N3-C4	19.01	120.11	110.60
32	W	1206	A	C2-N3-C4	19.01	120.11	110.60
1	A	572	A	N1-C2-N3	-19.01	119.80	129.30
32	W	985	A	N1-C2-N3	-19.01	119.80	129.30
52	z	41	A	C2-N3-C4	19.01	120.10	110.60
1	A	2848	A	C2-N3-C4	19.01	120.10	110.60
1	A	1480	A	N1-C2-N3	-19.00	119.80	129.30
1	A	1784	A	N1-C2-N3	-19.00	119.80	129.30
32	W	57	A	C2-N3-C4	19.00	120.10	110.60
32	W	886	A	C2-N3-C4	19.00	120.10	110.60
1	A	49	A	C2-N3-C4	19.00	120.10	110.60
1	A	1601	A	C2-N3-C4	19.00	120.10	110.60
1	A	1254	A	C2-N3-C4	19.00	120.10	110.60
1	A	1405	A	C2-N3-C4	19.00	120.10	110.60
1	A	1876	A	C2-N3-C4	19.00	120.10	110.60
32	W	438	A	N1-C2-N3	-19.00	119.80	129.30
32	W	658	A	C2-N3-C4	19.00	120.10	110.60
32	W	333	A	C2-N3-C4	19.00	120.10	110.60
32	W	713	A	C2-N3-C4	19.00	120.10	110.60
32	W	777	A	C2-N3-C4	19.00	120.10	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1243	A	C2-N3-C4	19.00	120.10	110.60
1	A	1636	A	C2-N3-C4	19.00	120.10	110.60
1	A	28	A	C2-N3-C4	18.99	120.10	110.60
1	A	275	A	C2-N3-C4	18.99	120.10	110.60
1	A	715	A	C2-N3-C4	18.99	120.10	110.60
1	A	1456	A	C2-N3-C4	18.99	120.10	110.60
1	A	2007	A	C2-N3-C4	18.99	120.10	110.60
1	A	2343	A	C2-N3-C4	18.99	120.10	110.60
32	W	768	A	C2-N3-C4	18.99	120.10	110.60
32	W	1004	A	C2-N3-C4	18.99	120.09	110.60
52	z	24	A	C2-N3-C4	18.99	120.09	110.60
1	A	1029	A	C2-N3-C4	18.99	120.09	110.60
1	A	2722	A	C2-N3-C4	18.99	120.09	110.60
32	W	251	A	C2-N3-C4	18.99	120.09	110.60
32	W	913	A	C2-N3-C4	18.99	120.09	110.60
32	W	1050	A	N1-C2-N3	-18.99	119.81	129.30
32	W	1189	A	C2-N3-C4	18.99	120.09	110.60
1	A	305	A	C2-N3-C4	18.98	120.09	110.60
1	A	1260	A	C2-N3-C4	18.98	120.09	110.60
1	A	1313	A	C2-N3-C4	18.98	120.09	110.60
32	W	150	A	C2-N3-C4	18.98	120.09	110.60
32	W	988	A	N1-C2-N3	-18.98	119.81	129.30
52	z	14	A	N1-C2-N3	-18.98	119.81	129.30
32	W	1369	A	C2-N3-C4	18.98	120.09	110.60
1	A	369	A	C2-N3-C4	18.98	120.09	110.60
2	B	25	A	N1-C2-N3	-18.98	119.81	129.30
1	A	2662	A	C2-N3-C4	18.98	120.09	110.60
32	W	796	A	C2-N3-C4	18.98	120.09	110.60
32	W	1419	A	C2-N3-C4	18.98	120.09	110.60
1	A	1046	A	N1-C2-N3	-18.98	119.81	129.30
1	A	1157	A	C2-N3-C4	18.98	120.09	110.60
2	B	102	A	N1-C2-N3	-18.98	119.81	129.30
32	W	72	A	C2-N3-C4	18.98	120.09	110.60
32	W	190	A	C2-N3-C4	18.98	120.09	110.60
1	A	94	A	C2-N3-C4	18.97	120.09	110.60
32	W	282	A	C2-N3-C4	18.97	120.09	110.60
32	W	1143	A	C2-N3-C4	18.97	120.09	110.60
1	A	504	A	C2-N3-C4	18.97	120.09	110.60
1	A	2026	A	C2-N3-C4	18.97	120.09	110.60
1	A	2317	A	C2-N3-C4	18.97	120.09	110.60
32	W	397	A	C2-N3-C4	18.97	120.09	110.60
1	A	1421	A	C2-N3-C4	18.97	120.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	391	A	C2-N3-C4	18.97	120.08	110.60
1	A	418	A	C2-N3-C4	18.97	120.08	110.60
1	A	2032	A	C2-N3-C4	18.97	120.08	110.60
32	W	361	A	C2-N3-C4	18.97	120.08	110.60
32	W	382	A	C2-N3-C4	18.97	120.08	110.60
1	A	781	A	C2-N3-C4	18.97	120.08	110.60
1	A	952	A	C2-N3-C4	18.97	120.08	110.60
1	A	2663	A	C2-N3-C4	18.97	120.08	110.60
1	A	2779	A	C2-N3-C4	18.97	120.08	110.60
1	A	231	A	C2-N3-C4	18.97	120.08	110.60
1	A	342	A	N1-C2-N3	-18.97	119.82	129.30
1	A	547	A	C2-N3-C4	18.97	120.08	110.60
1	A	1026	A	C2-N3-C4	18.97	120.08	110.60
32	W	456	A	C2-N3-C4	18.97	120.08	110.60
1	A	2668	A	C2-N3-C4	18.96	120.08	110.60
1	A	1233	A	C2-N3-C4	18.96	120.08	110.60
1	A	2447	A	C2-N3-C4	18.96	120.08	110.60
32	W	361	A	N1-C2-N3	-18.96	119.82	129.30
1	A	374	A	N1-C2-N3	-18.96	119.82	129.30
32	W	581	A	C2-N3-C4	18.96	120.08	110.60
32	W	919	A	C2-N3-C4	18.96	120.08	110.60
1	A	185	A	C2-N3-C4	18.96	120.08	110.60
1	A	1426	A	C2-N3-C4	18.96	120.08	110.60
1	A	1483	A	C2-N3-C4	18.96	120.08	110.60
1	A	1691	A	N1-C2-N3	-18.96	119.82	129.30
32	W	542	A	N1-C2-N3	-18.96	119.82	129.30
1	A	2402	A	C2-N3-C4	18.96	120.08	110.60
32	W	837	A	N1-C2-N3	-18.96	119.82	129.30
1	A	1266	A	N1-C2-N3	-18.96	119.82	129.30
1	A	2375	A	N1-C2-N3	-18.96	119.82	129.30
1	A	1813	A	C2-N3-C4	18.95	120.08	110.60
1	A	281	A	C2-N3-C4	18.95	120.08	110.60
1	A	1617	A	C2-N3-C4	18.95	120.08	110.60
32	W	10	A	N1-C2-N3	-18.95	119.82	129.30
32	W	457	A	C2-N3-C4	18.95	120.08	110.60
1	A	1061	A	N1-C2-N3	-18.95	119.83	129.30
1	A	1325	A	N1-C2-N3	-18.95	119.82	129.30
1	A	656	A	C2-N3-C4	18.95	120.08	110.60
1	A	2845	A	C2-N3-C4	18.95	120.08	110.60
32	W	925	A	C2-N3-C4	18.95	120.07	110.60
1	A	1123	A	C2-N3-C4	18.95	120.07	110.60
1	A	1555	A	C2-N3-C4	18.95	120.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	A	C2-N3-C4	18.95	120.07	110.60
1	A	91	A	C2-N3-C4	18.95	120.07	110.60
1	A	1126	A	C2-N3-C4	18.95	120.07	110.60
1	A	1141	A	C2-N3-C4	18.95	120.07	110.60
1	A	2643	A	C2-N3-C4	18.95	120.07	110.60
1	A	2902	A	C2-N3-C4	18.95	120.07	110.60
32	W	10	A	C2-N3-C4	18.95	120.07	110.60
32	W	1488	A	C2-N3-C4	18.95	120.07	110.60
52	z	21	A	C2-N3-C4	18.95	120.07	110.60
1	A	677	A	C2-N3-C4	18.94	120.07	110.60
1	A	683	A	C2-N3-C4	18.94	120.07	110.60
1	A	1119	A	C2-N3-C4	18.94	120.07	110.60
1	A	1579	A	C2-N3-C4	18.94	120.07	110.60
1	A	1767	A	C2-N3-C4	18.94	120.07	110.60
1	A	2777	A	N1-C2-N3	-18.94	119.83	129.30
32	W	870	A	C2-N3-C4	18.94	120.07	110.60
1	A	56	A	C2-N3-C4	18.94	120.07	110.60
32	W	1213	A	C2-N3-C4	18.94	120.07	110.60
1	A	1417	A	C2-N3-C4	18.94	120.07	110.60
1	A	2769	A	C2-N3-C4	18.94	120.07	110.60
32	W	208	A	C2-N3-C4	18.94	120.07	110.60
32	W	1355	A	C2-N3-C4	18.94	120.07	110.60
1	A	925	A	N1-C2-N3	-18.94	119.83	129.30
1	A	1844	A	N1-C2-N3	-18.94	119.83	129.30
1	A	2507	A	N1-C2-N3	-18.94	119.83	129.30
1	A	2686	A	N1-C2-N3	-18.94	119.83	129.30
32	W	1179	A	C2-N3-C4	18.94	120.07	110.60
1	A	851	A	C2-N3-C4	18.93	120.07	110.60
1	A	1844	A	C2-N3-C4	18.93	120.07	110.60
1	A	2421	A	C2-N3-C4	18.93	120.07	110.60
1	A	2462	A	C2-N3-C4	18.93	120.07	110.60
1	A	2893	A	C2-N3-C4	18.93	120.07	110.60
32	W	61	A	C2-N3-C4	18.93	120.07	110.60
1	A	210	A	C2-N3-C4	18.93	120.07	110.60
1	A	1026	A	N1-C2-N3	-18.93	119.83	129.30
32	W	968	A	C2-N3-C4	18.93	120.07	110.60
32	W	1517	A	C2-N3-C4	18.93	120.06	110.60
1	A	21	A	C2-N3-C4	18.93	120.06	110.60
1	A	1608	A	C2-N3-C4	18.93	120.06	110.60
1	A	2349	A	C2-N3-C4	18.93	120.06	110.60
1	A	222	A	C2-N3-C4	18.93	120.06	110.60
1	A	808	A	C2-N3-C4	18.93	120.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2049	A	C2-N3-C4	18.93	120.06	110.60
2	B	18	A	C2-N3-C4	18.93	120.06	110.60
32	W	1342	A	C2-N3-C4	18.93	120.06	110.60
32	W	1451	A	C2-N3-C4	18.93	120.06	110.60
1	A	389	A	C2-N3-C4	18.93	120.06	110.60
1	A	723	A	N1-C2-N3	-18.93	119.84	129.30
32	W	211	A	C2-N3-C4	18.93	120.06	110.60
32	W	390	A	C2-N3-C4	18.93	120.06	110.60
32	W	824	A	C2-N3-C4	18.93	120.06	110.60
32	W	1308	A	N1-C2-N3	-18.93	119.84	129.30
32	W	1510	A	C2-N3-C4	18.93	120.06	110.60
1	A	139	A	N1-C2-N3	-18.92	119.84	129.30
1	A	618	A	C2-N3-C4	18.92	120.06	110.60
1	A	658	A	C2-N3-C4	18.92	120.06	110.60
1	A	1131	A	C2-N3-C4	18.92	120.06	110.60
1	A	1941	A	N1-C2-N3	-18.92	119.84	129.30
32	W	1502	A	C2-N3-C4	18.92	120.06	110.60
1	A	1631	A	C2-N3-C4	18.92	120.06	110.60
32	W	1128	A	C2-N3-C4	18.92	120.06	110.60
1	A	216	A	C2-N3-C4	18.92	120.06	110.60
1	A	1638	A	C2-N3-C4	18.92	120.06	110.60
32	W	452	A	C2-N3-C4	18.92	120.06	110.60
1	A	161	A	N1-C2-N3	-18.92	119.84	129.30
1	A	496	A	C2-N3-C4	18.92	120.06	110.60
1	A	1553	A	C2-N3-C4	18.92	120.06	110.60
1	A	530	A	C2-N3-C4	18.92	120.06	110.60
1	A	1072	A	C2-N3-C4	18.92	120.06	110.60
1	A	1677	A	C2-N3-C4	18.92	120.06	110.60
1	A	1308	A	C2-N3-C4	18.92	120.06	110.60
1	A	412	A	C2-N3-C4	18.91	120.06	110.60
1	A	600	A	C2-N3-C4	18.91	120.06	110.60
1	A	908	A	C2-N3-C4	18.91	120.06	110.60
1	A	1743	A	C2-N3-C4	18.91	120.06	110.60
1	A	1918	A	C2-N3-C4	18.91	120.06	110.60
1	A	2762	A	C2-N3-C4	18.91	120.06	110.60
32	W	1355	A	N1-C2-N3	-18.91	119.84	129.30
1	A	118	A	C2-N3-C4	18.91	120.06	110.60
1	A	790	A	C2-N3-C4	18.91	120.06	110.60
1	A	1305	A	C2-N3-C4	18.91	120.06	110.60
1	A	2351	A	C2-N3-C4	18.91	120.06	110.60
32	W	118	A	C2-N3-C4	18.91	120.06	110.60
32	W	1403	A	C2-N3-C4	18.91	120.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1055	A	C2-N3-C4	18.91	120.06	110.60
1	A	2375	A	C2-N3-C4	18.91	120.06	110.60
1	A	702	A	C2-N3-C4	18.91	120.06	110.60
1	A	1663	A	C2-N3-C4	18.91	120.06	110.60
1	A	1685	A	C2-N3-C4	18.91	120.06	110.60
1	A	1700	A	C2-N3-C4	18.91	120.06	110.60
32	W	139	A	C2-N3-C4	18.91	120.06	110.60
1	A	593	A	N1-C2-N3	-18.91	119.85	129.30
1	A	1464	A	C2-N3-C4	18.91	120.05	110.60
1	A	2694	A	C2-N3-C4	18.91	120.05	110.60
1	A	2837	A	C2-N3-C4	18.91	120.05	110.60
1	A	2862	A	C2-N3-C4	18.91	120.05	110.60
32	W	522	A	C2-N3-C4	18.91	120.05	110.60
1	A	470	A	C2-N3-C4	18.91	120.05	110.60
32	W	171	A	C2-N3-C4	18.91	120.05	110.60
1	A	1820	A	C2-N3-C4	18.91	120.05	110.60
32	W	148	A	C2-N3-C4	18.91	120.05	110.60
32	W	254	A	C2-N3-C4	18.91	120.05	110.60
32	W	721	A	C2-N3-C4	18.91	120.05	110.60
32	W	776	A	N1-C2-N3	-18.91	119.85	129.30
1	A	1858	A	C2-N3-C4	18.90	120.05	110.60
1	A	2111	A	C2-N3-C4	18.90	120.05	110.60
1	A	1713	A	N1-C2-N3	-18.90	119.85	129.30
1	A	2461	A	C2-N3-C4	18.90	120.05	110.60
32	W	1298	A	C2-N3-C4	18.90	120.05	110.60
32	W	1425	A	C2-N3-C4	18.90	120.05	110.60
1	A	2898	A	C2-N3-C4	18.90	120.05	110.60
1	A	384	A	C2-N3-C4	18.90	120.05	110.60
1	A	389	A	N1-C2-N3	-18.90	119.85	129.30
1	A	1760	A	C2-N3-C4	18.90	120.05	110.60
1	A	1913	A	C2-N3-C4	18.90	120.05	110.60
1	A	2088	A	N1-C2-N3	-18.90	119.85	129.30
2	B	25	A	C2-N3-C4	18.90	120.05	110.60
32	W	28	A	C2-N3-C4	18.90	120.05	110.60
32	W	592	A	C2-N3-C4	18.90	120.05	110.60
32	W	996	A	C2-N3-C4	18.90	120.05	110.60
1	A	2338	A	C2-N3-C4	18.90	120.05	110.60
32	W	306	A	C2-N3-C4	18.90	120.05	110.60
1	A	1308	A	N1-C2-N3	-18.90	119.85	129.30
1	A	1814	A	N1-C2-N3	-18.90	119.85	129.30
32	W	173	A	C2-N3-C4	18.90	120.05	110.60
32	W	228	A	C2-N3-C4	18.90	120.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	364	A	C2-N3-C4	18.90	120.05	110.60
32	W	791	A	C2-N3-C4	18.90	120.05	110.60
1	A	677	A	N1-C2-N3	-18.89	119.85	129.30
1	A	724	A	C2-N3-C4	18.89	120.05	110.60
1	A	1210	A	C2-N3-C4	18.89	120.05	110.60
1	A	1784	A	C2-N3-C4	18.89	120.05	110.60
1	A	1848	A	C2-N3-C4	18.89	120.05	110.60
1	A	2078	A	C2-N3-C4	18.89	120.05	110.60
32	W	159	A	C2-N3-C4	18.89	120.05	110.60
32	W	659	A	C2-N3-C4	18.89	120.05	110.60
1	A	1473	A	C2-N3-C4	18.89	120.05	110.60
1	A	2754	A	C2-N3-C4	18.89	120.05	110.60
32	W	12	A	C2-N3-C4	18.89	120.05	110.60
32	W	617	A	C2-N3-C4	18.89	120.05	110.60
1	A	477	A	N1-C2-N3	-18.89	119.86	129.30
1	A	1132	A	N1-C2-N3	-18.89	119.86	129.30
1	A	1713	A	C2-N3-C4	18.89	120.05	110.60
1	A	2042	A	C2-N3-C4	18.89	120.05	110.60
1	A	2812	A	C2-N3-C4	18.89	120.05	110.60
32	W	1111	A	C2-N3-C4	18.89	120.05	110.60
1	A	322	A	C2-N3-C4	18.89	120.04	110.60
1	A	1347	A	N1-C2-N3	-18.89	119.86	129.30
1	A	2087	A	C2-N3-C4	18.89	120.05	110.60
1	A	2295	A	C2-N3-C4	18.89	120.04	110.60
32	W	776	A	C2-N3-C4	18.89	120.05	110.60
1	A	139	A	C2-N3-C4	18.89	120.04	110.60
1	A	476	A	C2-N3-C4	18.89	120.04	110.60
1	A	821	A	C2-N3-C4	18.89	120.04	110.60
1	A	156	A	C2-N3-C4	18.89	120.04	110.60
1	A	1556	A	C2-N3-C4	18.89	120.04	110.60
1	A	1965	A	C2-N3-C4	18.89	120.04	110.60
1	A	2032	A	N1-C2-N3	-18.89	119.86	129.30
1	A	2686	A	C2-N3-C4	18.89	120.04	110.60
1	A	2876	A	N1-C2-N3	-18.89	119.86	129.30
32	W	1259	A	C2-N3-C4	18.89	120.04	110.60
32	W	1261	A	N1-C2-N3	-18.89	119.86	129.30
32	W	1486	A	C2-N3-C4	18.89	120.04	110.60
1	A	44	A	C2-N3-C4	18.88	120.04	110.60
1	A	314	A	C2-N3-C4	18.88	120.04	110.60
1	A	1131	A	N1-C2-N3	-18.88	119.86	129.30
1	A	1258	A	C2-N3-C4	18.88	120.04	110.60
32	W	485	A	C2-N3-C4	18.88	120.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1541	A	C2-N3-C4	18.88	120.04	110.60
1	A	659	A	C2-N3-C4	18.88	120.04	110.60
32	W	541	A	C2-N3-C4	18.88	120.04	110.60
32	W	979	A	C2-N3-C4	18.88	120.04	110.60
1	A	1141	A	N1-C2-N3	-18.88	119.86	129.30
1	A	1432	A	N1-C2-N3	-18.88	119.86	129.30
1	A	2018	A	N1-C2-N3	-18.88	119.86	129.30
1	A	2898	A	N1-C2-N3	-18.88	119.86	129.30
1	A	41	A	C2-N3-C4	18.88	120.04	110.60
1	A	479	A	C2-N3-C4	18.88	120.04	110.60
1	A	1189	A	N1-C2-N3	-18.88	119.86	129.30
1	A	1542	A	C2-N3-C4	18.88	120.04	110.60
1	A	1709	A	C2-N3-C4	18.88	120.04	110.60
1	A	2480	A	C2-N3-C4	18.88	120.04	110.60
1	A	947	A	C2-N3-C4	18.88	120.04	110.60
1	A	1157	A	N1-C2-N3	-18.88	119.86	129.30
1	A	1406	A	C2-N3-C4	18.88	120.04	110.60
1	A	1900	A	C2-N3-C4	18.88	120.04	110.60
1	A	2365	A	C2-N3-C4	18.88	120.04	110.60
2	B	50	A	C2-N3-C4	18.88	120.04	110.60
2	B	51	A	C2-N3-C4	18.88	120.04	110.60
1	A	324	A	C2-N3-C4	18.88	120.04	110.60
1	A	1036	A	N1-C2-N3	-18.88	119.86	129.30
1	A	1244	A	C2-N3-C4	18.88	120.04	110.60
1	A	2916	A	N1-C2-N3	-18.88	119.86	129.30
32	W	1386	A	C2-N3-C4	18.88	120.04	110.60
1	A	1774	A	C2-N3-C4	18.87	120.04	110.60
1	A	1995	A	C2-N3-C4	18.87	120.04	110.60
1	A	2594	A	C2-N3-C4	18.87	120.04	110.60
1	A	2767	A	C2-N3-C4	18.87	120.04	110.60
32	W	140	A	C2-N3-C4	18.87	120.04	110.60
32	W	225	A	C2-N3-C4	18.87	120.04	110.60
32	W	703	A	N1-C2-N3	-18.87	119.86	129.30
32	W	1147	A	C2-N3-C4	18.87	120.04	110.60
1	A	549	A	C2-N3-C4	18.87	120.04	110.60
1	A	876	A	C2-N3-C4	18.87	120.04	110.60
1	A	2670	A	N1-C2-N3	-18.87	119.86	129.30
32	W	1407	A	N1-C2-N3	-18.87	119.86	129.30
1	A	456	A	C2-N3-C4	18.87	120.03	110.60
1	A	1189	A	C2-N3-C4	18.87	120.03	110.60
1	A	1895	A	C2-N3-C4	18.87	120.03	110.60
1	A	1928	A	C2-N3-C4	18.87	120.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1999	A	C2-N3-C4	18.87	120.04	110.60
1	A	2356	A	C2-N3-C4	18.87	120.04	110.60
1	A	2362	A	C2-N3-C4	18.87	120.03	110.60
32	W	1493	A	C2-N3-C4	18.87	120.03	110.60
1	A	547	A	N1-C2-N3	-18.87	119.86	129.30
1	A	1347	A	C2-N3-C4	18.87	120.03	110.60
1	A	2295	A	N1-C2-N3	-18.87	119.87	129.30
1	A	2389	A	C2-N3-C4	18.87	120.03	110.60
1	A	2500	A	C2-N3-C4	18.87	120.03	110.60
1	A	2593	A	C2-N3-C4	18.87	120.03	110.60
1	A	683	A	N1-C2-N3	-18.87	119.87	129.30
32	W	793	A	C2-N3-C4	18.87	120.03	110.60
32	W	1252	A	C2-N3-C4	18.87	120.03	110.60
1	A	889	A	C2-N3-C4	18.87	120.03	110.60
1	A	2358	A	C2-N3-C4	18.87	120.03	110.60
32	W	801	A	C2-N3-C4	18.87	120.03	110.60
32	W	1050	A	C2-N3-C4	18.87	120.03	110.60
32	W	1320	A	C2-N3-C4	18.87	120.03	110.60
1	A	10	A	C2-N3-C4	18.86	120.03	110.60
1	A	1930	A	N1-C2-N3	-18.86	119.87	129.30
1	A	2089	A	C2-N3-C4	18.86	120.03	110.60
32	W	234	A	C2-N3-C4	18.86	120.03	110.60
32	W	240	A	C2-N3-C4	18.86	120.03	110.60
32	W	496	A	C2-N3-C4	18.86	120.03	110.60
32	W	984	A	C2-N3-C4	18.86	120.03	110.60
32	W	1422	A	N1-C2-N3	-18.86	119.87	129.30
1	A	1302	A	N1-C2-N3	-18.86	119.87	129.30
1	A	1423	A	C2-N3-C4	18.86	120.03	110.60
1	A	1918	A	N1-C2-N3	-18.86	119.87	129.30
1	A	49	A	N1-C2-N3	-18.86	119.87	129.30
1	A	1287	A	C2-N3-C4	18.86	120.03	110.60
1	A	1424	A	C2-N3-C4	18.86	120.03	110.60
1	A	2018	A	C2-N3-C4	18.86	120.03	110.60
1	A	2778	A	C2-N3-C4	18.86	120.03	110.60
1	A	2831	A	C2-N3-C4	18.86	120.03	110.60
1	A	2854	A	C2-N3-C4	18.86	120.03	110.60
1	A	2912	A	C2-N3-C4	18.86	120.03	110.60
32	W	1065	A	C2-N3-C4	18.86	120.03	110.60
52	z	70	A	C2-N3-C4	18.86	120.03	110.60
1	A	64	A	C2-N3-C4	18.86	120.03	110.60
1	A	867	A	N1-C2-N3	-18.86	119.87	129.30
1	A	1036	A	C2-N3-C4	18.86	120.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1735	A	C2-N3-C4	18.86	120.03	110.60
1	A	2704	A	C2-N3-C4	18.86	120.03	110.60
32	W	775	A	N1-C2-N3	-18.86	119.87	129.30
32	W	1092	A	C2-N3-C4	18.86	120.03	110.60
32	W	1185	A	C2-N3-C4	18.86	120.03	110.60
1	A	144	A	C2-N3-C4	18.86	120.03	110.60
1	A	1981	A	C2-N3-C4	18.86	120.03	110.60
1	A	2455	A	N1-C2-N3	-18.86	119.87	129.30
32	W	1288	A	N1-C2-N3	-18.86	119.87	129.30
1	A	572	A	C2-N3-C4	18.86	120.03	110.60
1	A	830	A	C2-N3-C4	18.86	120.03	110.60
1	A	971	A	C2-N3-C4	18.86	120.03	110.60
1	A	1142	A	C2-N3-C4	18.86	120.03	110.60
1	A	1760	A	N1-C2-N3	-18.86	119.87	129.30
32	W	206	A	C2-N3-C4	18.86	120.03	110.60
32	W	737	A	N1-C2-N3	-18.86	119.87	129.30
32	W	1054	A	C2-N3-C4	18.86	120.03	110.60
1	A	477	A	C2-N3-C4	18.85	120.03	110.60
1	A	1579	A	N1-C2-N3	-18.85	119.87	129.30
1	A	1675	A	C2-N3-C4	18.85	120.03	110.60
1	A	2315	A	C2-N3-C4	18.85	120.03	110.60
1	A	2876	A	C2-N3-C4	18.85	120.03	110.60
32	W	711	A	C2-N3-C4	18.85	120.03	110.60
32	W	902	A	C2-N3-C4	18.85	120.03	110.60
32	W	1272	A	C2-N3-C4	18.85	120.03	110.60
1	A	659	A	N1-C2-N3	-18.85	119.87	129.30
1	A	970	A	C2-N3-C4	18.85	120.03	110.60
1	A	2398	A	C2-N3-C4	18.85	120.03	110.60
32	W	440	A	C2-N3-C4	18.85	120.03	110.60
1	A	73	A	C2-N3-C4	18.85	120.03	110.60
1	A	273	A	C2-N3-C4	18.85	120.03	110.60
1	A	2570	A	C2-N3-C4	18.85	120.03	110.60
1	A	2916	A	C2-N3-C4	18.85	120.03	110.60
2	B	99	A	C2-N3-C4	18.85	120.03	110.60
32	W	99	A	C2-N3-C4	18.85	120.03	110.60
32	W	344	A	C2-N3-C4	18.85	120.03	110.60
32	W	512	A	C2-N3-C4	18.85	120.03	110.60
1	A	206	A	C2-N3-C4	18.85	120.02	110.60
1	A	978	A	C2-N3-C4	18.85	120.02	110.60
1	A	2869	A	C2-N3-C4	18.85	120.03	110.60
32	W	372	A	C2-N3-C4	18.85	120.03	110.60
32	W	1161	A	C2-N3-C4	18.85	120.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	407	A	C2-N3-C4	18.85	120.02	110.60
1	A	476	A	N1-C2-N3	-18.85	119.88	129.30
1	A	560	A	N1-C2-N3	-18.85	119.88	129.30
1	A	1672	A	C2-N3-C4	18.85	120.02	110.60
1	A	2767	A	N1-C2-N3	-18.85	119.88	129.30
32	W	271	A	C2-N3-C4	18.85	120.02	110.60
1	A	95	A	C2-N3-C4	18.85	120.02	110.60
1	A	1116	A	C2-N3-C4	18.85	120.02	110.60
1	A	849	A	N1-C2-N3	-18.84	119.88	129.30
1	A	1404	A	C2-N3-C4	18.84	120.02	110.60
1	A	1998	A	C2-N3-C4	18.84	120.02	110.60
1	A	2606	A	N1-C2-N3	-18.84	119.88	129.30
1	A	2782	A	C2-N3-C4	18.84	120.02	110.60
32	W	542	A	C2-N3-C4	18.84	120.02	110.60
1	A	762	A	C2-N3-C4	18.84	120.02	110.60
1	A	2908	A	C2-N3-C4	18.84	120.02	110.60
32	W	1048	A	N1-C2-N3	-18.84	119.88	129.30
32	W	1056	A	C2-N3-C4	18.84	120.02	110.60
1	A	226	A	N1-C2-N3	-18.84	119.88	129.30
1	A	376	A	C2-N3-C4	18.84	120.02	110.60
1	A	616	A	C2-N3-C4	18.84	120.02	110.60
1	A	637	A	C2-N3-C4	18.84	120.02	110.60
1	A	922	A	C2-N3-C4	18.84	120.02	110.60
1	A	1059	A	C2-N3-C4	18.84	120.02	110.60
1	A	1284	A	C2-N3-C4	18.84	120.02	110.60
1	A	2571	A	C2-N3-C4	18.84	120.02	110.60
32	W	202	A	C2-N3-C4	18.84	120.02	110.60
1	A	364	A	N1-C2-N3	-18.84	119.88	129.30
1	A	2844	A	C2-N3-C4	18.84	120.02	110.60
32	W	837	A	C2-N3-C4	18.84	120.02	110.60
32	W	1048	A	C2-N3-C4	18.84	120.02	110.60
32	W	1419	A	N1-C2-N3	-18.84	119.88	129.30
1	A	260	A	C2-N3-C4	18.84	120.02	110.60
1	A	548	A	C2-N3-C4	18.84	120.02	110.60
1	A	647	A	N1-C2-N3	-18.84	119.88	129.30
1	A	1144	A	C2-N3-C4	18.84	120.02	110.60
32	W	76	A	N1-C2-N3	-18.84	119.88	129.30
1	A	894	A	C2-N3-C4	18.84	120.02	110.60
1	A	965	A	N1-C2-N3	-18.84	119.88	129.30
1	A	1816	A	C2-N3-C4	18.84	120.02	110.60
1	A	2700	A	C2-N3-C4	18.84	120.02	110.60
1	A	2740	A	C2-N3-C4	18.84	120.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	64	A	C2-N3-C4	18.84	120.02	110.60
32	W	460	A	N1-C2-N3	-18.84	119.88	129.30
1	A	699	A	C2-N3-C4	18.84	120.02	110.60
1	A	1357	A	C2-N3-C4	18.84	120.02	110.60
1	A	1533	A	C2-N3-C4	18.84	120.02	110.60
1	A	2908	A	N1-C2-N3	-18.84	119.88	129.30
2	B	76	A	C2-N3-C4	18.84	120.02	110.60
32	W	386	A	N1-C2-N3	-18.84	119.88	129.30
32	W	556	A	C2-N3-C4	18.84	120.02	110.60
32	W	1222	A	C2-N3-C4	18.84	120.02	110.60
32	W	1510	A	N1-C2-N3	-18.84	119.88	129.30
1	A	2819	A	N1-C2-N3	-18.83	119.88	129.30
32	W	76	A	C2-N3-C4	18.83	120.02	110.60
32	W	1261	A	C2-N3-C4	18.83	120.02	110.60
32	W	1386	A	N1-C2-N3	-18.83	119.88	129.30
1	A	91	A	N1-C2-N3	-18.83	119.88	129.30
1	A	225	A	C2-N3-C4	18.83	120.02	110.60
1	A	723	A	C2-N3-C4	18.83	120.02	110.60
1	A	2923	A	C2-N3-C4	18.83	120.02	110.60
32	W	459	A	C2-N3-C4	18.83	120.02	110.60
32	W	1028	A	C2-N3-C4	18.83	120.02	110.60
32	W	1207	A	C2-N3-C4	18.83	120.02	110.60
1	A	821	A	N1-C2-N3	-18.83	119.88	129.30
1	A	1188	A	N1-C2-N3	-18.83	119.88	129.30
1	A	1617	A	N1-C2-N3	-18.83	119.88	129.30
1	A	1699	A	C2-N3-C4	18.83	120.02	110.60
32	W	18	A	N1-C2-N3	-18.83	119.88	129.30
32	W	357	A	C2-N3-C4	18.83	120.02	110.60
32	W	650	A	C2-N3-C4	18.83	120.02	110.60
1	A	1906	A	C2-N3-C4	18.83	120.02	110.60
1	A	1906	A	N1-C2-N3	-18.83	119.89	129.30
32	W	456	A	N1-C2-N3	-18.83	119.89	129.30
32	W	506	A	N1-C2-N3	-18.83	119.89	129.30
32	W	605	A	C2-N3-C4	18.83	120.01	110.60
32	W	1161	A	N1-C2-N3	-18.83	119.89	129.30
32	W	1210	A	C2-N3-C4	18.83	120.01	110.60
32	W	1437	A	C2-N3-C4	18.83	120.02	110.60
32	W	1488	A	N1-C2-N3	-18.83	119.89	129.30
1	A	1461	A	C2-N3-C4	18.83	120.01	110.60
1	A	1680	A	C2-N3-C4	18.83	120.01	110.60
1	A	2834	A	C2-N3-C4	18.83	120.01	110.60
2	B	44	A	C2-N3-C4	18.83	120.01	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	677	A	C2-N3-C4	18.83	120.01	110.60
32	W	1490	A	C2-N3-C4	18.83	120.01	110.60
1	A	166	A	N1-C2-N3	-18.82	119.89	129.30
1	A	326	A	C2-N3-C4	18.82	120.01	110.60
1	A	702	A	N1-C2-N3	-18.82	119.89	129.30
1	A	870	A	C2-N3-C4	18.82	120.01	110.60
1	A	1119	A	N1-C2-N3	-18.82	119.89	129.30
1	A	1845	A	C2-N3-C4	18.82	120.01	110.60
32	W	664	A	C2-N3-C4	18.82	120.01	110.60
32	W	777	A	N1-C2-N3	-18.82	119.89	129.30
32	W	1257	A	C2-N3-C4	18.82	120.01	110.60
1	A	1885	A	C2-N3-C4	18.82	120.01	110.60
1	A	2034	A	C2-N3-C4	18.82	120.01	110.60
1	A	2071	A	C2-N3-C4	18.82	120.01	110.60
1	A	2356	A	N1-C2-N3	-18.82	119.89	129.30
32	W	757	A	C2-N3-C4	18.82	120.01	110.60
1	A	957	A	N1-C2-N3	-18.82	119.89	129.30
1	A	1202	A	C2-N3-C4	18.82	120.01	110.60
1	A	1588	A	C2-N3-C4	18.82	120.01	110.60
32	W	669	A	C2-N3-C4	18.82	120.01	110.60
32	W	924	A	C2-N3-C4	18.82	120.01	110.60
32	W	1016	A	C2-N3-C4	18.82	120.01	110.60
1	A	125	A	C2-N3-C4	18.82	120.01	110.60
1	A	1654	A	C2-N3-C4	18.82	120.01	110.60
1	A	524	A	C2-N3-C4	18.82	120.01	110.60
1	A	551	A	C2-N3-C4	18.82	120.01	110.60
1	A	1710	A	C2-N3-C4	18.82	120.01	110.60
1	A	2830	A	C2-N3-C4	18.82	120.01	110.60
32	W	287	A	C2-N3-C4	18.82	120.01	110.60
1	A	71	A	C2-N3-C4	18.82	120.01	110.60
1	A	504	A	N1-C2-N3	-18.82	119.89	129.30
1	A	999	A	C2-N3-C4	18.82	120.01	110.60
32	W	266	A	C2-N3-C4	18.82	120.01	110.60
1	A	345	A	C2-N3-C4	18.82	120.01	110.60
1	A	1269	A	N1-C2-N3	-18.82	119.89	129.30
1	A	2088	A	C2-N3-C4	18.82	120.01	110.60
1	A	2507	A	C2-N3-C4	18.82	120.01	110.60
32	W	1503	A	C2-N3-C4	18.82	120.01	110.60
1	A	1941	A	C2-N3-C4	18.81	120.01	110.60
2	B	39	A	C2-N3-C4	18.81	120.01	110.60
1	A	418	A	N1-C2-N3	-18.81	119.89	129.30
1	A	1506	A	N1-C2-N3	-18.81	119.89	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1838	A	C2-N3-C4	18.81	120.01	110.60
1	A	1948	A	C2-N3-C4	18.81	120.01	110.60
1	A	2479	A	N1-C2-N3	-18.81	119.89	129.30
1	A	2875	A	C2-N3-C4	18.81	120.01	110.60
2	B	113	A	C2-N3-C4	18.81	120.01	110.60
32	W	569	A	C2-N3-C4	18.81	120.01	110.60
32	W	638	A	C2-N3-C4	18.81	120.01	110.60
32	W	762	A	C2-N3-C4	18.81	120.01	110.60
1	A	102	A	C2-N3-C4	18.81	120.00	110.60
1	A	388	A	C2-N3-C4	18.81	120.01	110.60
32	W	1200	A	C2-N3-C4	18.81	120.01	110.60
1	A	53	A	C2-N3-C4	18.81	120.00	110.60
1	A	224	A	N1-C2-N3	-18.81	119.89	129.30
1	A	1103	A	C2-N3-C4	18.81	120.00	110.60
1	A	1465	A	C2-N3-C4	18.81	120.00	110.60
32	W	159	A	N1-C2-N3	-18.81	119.90	129.30
32	W	1256	A	C2-N3-C4	18.81	120.00	110.60
1	A	207	A	N1-C2-N3	-18.81	119.90	129.30
1	A	1746	A	C2-N3-C4	18.81	120.00	110.60
1	A	2907	A	C2-N3-C4	18.81	120.00	110.60
32	W	1247	A	N1-C2-N3	-18.81	119.90	129.30
1	A	808	A	N1-C2-N3	-18.81	119.90	129.30
1	A	1614	A	C2-N3-C4	18.81	120.00	110.60
1	A	2875	A	N1-C2-N3	-18.81	119.90	129.30
32	W	582	A	C2-N3-C4	18.81	120.00	110.60
32	W	1266	A	C2-N3-C4	18.81	120.00	110.60
1	A	431	A	C2-N3-C4	18.80	120.00	110.60
1	A	2463	A	C2-N3-C4	18.80	120.00	110.60
1	A	2683	A	N1-C2-N3	-18.80	119.90	129.30
32	W	55	A	C2-N3-C4	18.80	120.00	110.60
32	W	323	A	C2-N3-C4	18.80	120.00	110.60
32	W	1248	A	C2-N3-C4	18.80	120.00	110.60
1	A	828	A	N1-C2-N3	-18.80	119.90	129.30
1	A	888	A	C2-N3-C4	18.80	120.00	110.60
1	A	2893	A	N1-C2-N3	-18.80	119.90	129.30
32	W	314	A	C2-N3-C4	18.80	120.00	110.60
1	A	179	A	C2-N3-C4	18.80	120.00	110.60
1	A	592	A	C2-N3-C4	18.80	120.00	110.60
1	A	1144	A	N1-C2-N3	-18.80	119.90	129.30
1	A	1575	A	C2-N3-C4	18.80	120.00	110.60
1	A	2100	A	C2-N3-C4	18.80	120.00	110.60
1	A	2560	A	C2-N3-C4	18.80	120.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	35	A	C2-N3-C4	18.80	120.00	110.60
32	W	529	A	C2-N3-C4	18.80	120.00	110.60
1	A	222	A	N1-C2-N3	-18.80	119.90	129.30
1	A	653	A	C2-N3-C4	18.80	120.00	110.60
1	A	699	A	N1-C2-N3	-18.80	119.90	129.30
32	W	518	A	C2-N3-C4	18.80	120.00	110.60
1	A	126	A	N1-C2-N3	-18.80	119.90	129.30
1	A	494	A	N1-C2-N3	-18.80	119.90	129.30
1	A	1346	A	C2-N3-C4	18.80	120.00	110.60
1	A	2052	A	C2-N3-C4	18.80	120.00	110.60
1	A	2303	A	C2-N3-C4	18.80	120.00	110.60
32	W	460	A	C2-N3-C4	18.80	120.00	110.60
1	A	12	A	C2-N3-C4	18.80	120.00	110.60
1	A	274	A	C2-N3-C4	18.80	120.00	110.60
1	A	1100	A	C2-N3-C4	18.80	120.00	110.60
1	A	1592	A	C2-N3-C4	18.80	120.00	110.60
1	A	2303	A	N1-C2-N3	-18.80	119.90	129.30
1	A	2900	A	C2-N3-C4	18.80	120.00	110.60
32	W	1417	A	C2-N3-C4	18.80	120.00	110.60
1	A	268	A	C2-N3-C4	18.79	120.00	110.60
1	A	279	A	C2-N3-C4	18.79	120.00	110.60
1	A	1453	A	C2-N3-C4	18.79	120.00	110.60
1	A	2027	A	C2-N3-C4	18.79	120.00	110.60
32	W	433	A	C2-N3-C4	18.79	120.00	110.60
32	W	730	A	N1-C2-N3	-18.79	119.90	129.30
32	W	1188	A	C2-N3-C4	18.79	120.00	110.60
1	A	1499	A	C2-N3-C4	18.79	120.00	110.60
1	A	1776	A	C2-N3-C4	18.79	120.00	110.60
32	W	1451	A	N1-C2-N3	-18.79	119.91	129.30
1	A	619	A	C2-N3-C4	18.79	120.00	110.60
1	A	705	A	C2-N3-C4	18.79	119.99	110.60
1	A	1149	A	N1-C2-N3	-18.79	119.91	129.30
32	W	62	A	C2-N3-C4	18.79	120.00	110.60
32	W	386	A	C2-N3-C4	18.79	120.00	110.60
2	B	55	A	N1-C2-N3	-18.79	119.91	129.30
32	W	948	A	C2-N3-C4	18.79	119.99	110.60
1	A	154	A	N1-C2-N3	-18.79	119.91	129.30
1	A	210	A	N1-C2-N3	-18.79	119.91	129.30
1	A	956	A	C2-N3-C4	18.79	119.99	110.60
32	W	381	A	N1-C2-N3	-18.79	119.91	129.30
32	W	803	A	C2-N3-C4	18.79	119.99	110.60
32	W	838	A	C2-N3-C4	18.79	119.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1349	A	C2-N3-C4	18.79	119.99	110.60
1	A	2477	A	C2-N3-C4	18.79	119.99	110.60
1	A	2673	A	C2-N3-C4	18.79	119.99	110.60
32	W	67	A	C2-N3-C4	18.79	119.99	110.60
32	W	462	A	N1-C2-N3	-18.79	119.91	129.30
32	W	1509	A	C2-N3-C4	18.79	119.99	110.60
1	A	1061	A	C2-N3-C4	18.78	119.99	110.60
1	A	1929	A	C2-N3-C4	18.78	119.99	110.60
32	W	52	A	C2-N3-C4	18.78	119.99	110.60
32	W	367	A	C2-N3-C4	18.78	119.99	110.60
32	W	1112	A	C2-N3-C4	18.78	119.99	110.60
1	A	200	A	C2-N3-C4	18.78	119.99	110.60
1	A	1593	A	C2-N3-C4	18.78	119.99	110.60
1	A	2066	A	C2-N3-C4	18.78	119.99	110.60
1	A	2455	A	C2-N3-C4	18.78	119.99	110.60
1	A	314	A	N1-C2-N3	-18.78	119.91	129.30
1	A	1585	A	C2-N3-C4	18.78	119.99	110.60
1	A	1677	A	N1-C2-N3	-18.78	119.91	129.30
1	A	2043	A	C2-N3-C4	18.78	119.99	110.60
1	A	2860	A	C2-N3-C4	18.78	119.99	110.60
2	B	97	A	C2-N3-C4	18.78	119.99	110.60
32	W	422	A	N1-C2-N3	-18.78	119.91	129.30
32	W	879	A	N1-C2-N3	-18.78	119.91	129.30
1	A	224	A	C2-N3-C4	18.78	119.99	110.60
1	A	575	A	C2-N3-C4	18.78	119.99	110.60
1	A	1434	A	C2-N3-C4	18.78	119.99	110.60
1	A	1453	A	N1-C2-N3	-18.78	119.91	129.30
1	A	2532	A	N1-C2-N3	-18.78	119.91	129.30
32	W	1284	A	C2-N3-C4	18.78	119.99	110.60
32	W	1512	A	N1-C2-N3	-18.78	119.91	129.30
1	A	84	A	C2-N3-C4	18.78	119.99	110.60
1	A	307	A	C2-N3-C4	18.78	119.99	110.60
1	A	1456	A	N1-C2-N3	-18.78	119.91	129.30
1	A	1679	A	C2-N3-C4	18.78	119.99	110.60
1	A	2436	A	C2-N3-C4	18.78	119.99	110.60
32	W	371	A	C2-N3-C4	18.78	119.99	110.60
32	W	1120	A	C2-N3-C4	18.78	119.99	110.60
32	W	1422	A	C2-N3-C4	18.78	119.99	110.60
1	A	258	A	C2-N3-C4	18.78	119.99	110.60
1	A	448	A	C2-N3-C4	18.78	119.99	110.60
1	A	1882	A	C2-N3-C4	18.78	119.99	110.60
32	W	532	A	C2-N3-C4	18.78	119.99	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	823	A	C2-N3-C4	18.78	119.99	110.60
1	A	438	A	N1-C2-N3	-18.77	119.91	129.30
1	A	486	A	C2-N3-C4	18.77	119.99	110.60
1	A	770	A	C2-N3-C4	18.77	119.99	110.60
1	A	958	A	C2-N3-C4	18.77	119.99	110.60
1	A	1020	A	C2-N3-C4	18.77	119.99	110.60
1	A	2668	A	N1-C2-N3	-18.77	119.91	129.30
1	A	2787	A	C2-N3-C4	18.77	119.99	110.60
1	A	2889	A	N1-C2-N3	-18.77	119.91	129.30
1	A	330	A	C2-N3-C4	18.77	119.99	110.60
1	A	1115	A	C2-N3-C4	18.77	119.99	110.60
1	A	2887	A	C2-N3-C4	18.77	119.99	110.60
32	W	1056	A	N1-C2-N3	-18.77	119.91	129.30
1	A	162	A	N1-C2-N3	-18.77	119.92	129.30
1	A	173	A	C2-N3-C4	18.77	119.99	110.60
1	A	652	A	N1-C2-N3	-18.77	119.92	129.30
1	A	868	A	C2-N3-C4	18.77	119.98	110.60
32	W	208	A	N1-C2-N3	-18.77	119.91	129.30
32	W	228	A	N1-C2-N3	-18.77	119.92	129.30
32	W	1435	A	C2-N3-C4	18.77	119.98	110.60
32	W	1442	A	C2-N3-C4	18.77	119.99	110.60
32	W	1470	A	C2-N3-C4	18.77	119.99	110.60
1	A	782	A	C2-N3-C4	18.77	119.98	110.60
1	A	1404	A	N1-C2-N3	-18.77	119.92	129.30
1	A	2417	A	C2-N3-C4	18.77	119.98	110.60
1	A	1116	A	N1-C2-N3	-18.77	119.92	129.30
1	A	1361	A	C2-N3-C4	18.77	119.98	110.60
1	A	1627	A	C2-N3-C4	18.77	119.98	110.60
1	A	1809	A	C2-N3-C4	18.77	119.98	110.60
32	W	12	A	N1-C2-N3	-18.77	119.92	129.30
32	W	206	A	N1-C2-N3	-18.77	119.92	129.30
32	W	210	A	C2-N3-C4	18.77	119.98	110.60
32	W	544	A	C2-N3-C4	18.77	119.98	110.60
32	W	1479	A	C2-N3-C4	18.77	119.98	110.60
1	A	622	A	C2-N3-C4	18.77	119.98	110.60
1	A	658	A	N1-C2-N3	-18.77	119.92	129.30
1	A	763	A	N1-C2-N3	-18.77	119.92	129.30
1	A	896	A	C2-N3-C4	18.77	119.98	110.60
1	A	1174	A	N1-C2-N3	-18.77	119.92	129.30
1	A	2406	A	C2-N3-C4	18.77	119.98	110.60
1	A	2421	A	N1-C2-N3	-18.77	119.92	129.30
1	A	1534	A	C2-N3-C4	18.77	119.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2618	A	N1-C2-N3	-18.77	119.92	129.30
32	W	485	A	N1-C2-N3	-18.77	119.92	129.30
32	W	1102	A	N1-C2-N3	-18.77	119.92	129.30
32	W	1207	A	N1-C2-N3	-18.77	119.92	129.30
1	A	769	A	C2-N3-C4	18.76	119.98	110.60
1	A	1029	A	N1-C2-N3	-18.76	119.92	129.30
1	A	1388	A	N1-C2-N3	-18.76	119.92	129.30
1	A	1569	A	C2-N3-C4	18.76	119.98	110.60
1	A	1767	A	N1-C2-N3	-18.76	119.92	129.30
1	A	2270	A	C2-N3-C4	18.76	119.98	110.60
1	A	2919	A	C2-N3-C4	18.76	119.98	110.60
32	W	287	A	N1-C2-N3	-18.76	119.92	129.30
32	W	874	A	C2-N3-C4	18.76	119.98	110.60
32	W	1247	A	C2-N3-C4	18.76	119.98	110.60
52	z	44	A	C2-N3-C4	18.76	119.98	110.60
1	A	763	A	C2-N3-C4	18.76	119.98	110.60
1	A	1695	A	C2-N3-C4	18.76	119.98	110.60
1	A	2750	A	C2-N3-C4	18.76	119.98	110.60
32	W	423	A	C2-N3-C4	18.76	119.98	110.60
1	A	273	A	N1-C2-N3	-18.76	119.92	129.30
1	A	475	A	N1-C2-N3	-18.76	119.92	129.30
1	A	893	A	C2-N3-C4	18.76	119.98	110.60
2	B	55	A	C2-N3-C4	18.76	119.98	110.60
2	B	56	A	C2-N3-C4	18.76	119.98	110.60
32	W	474	A	C2-N3-C4	18.76	119.98	110.60
32	W	532	A	N1-C2-N3	-18.76	119.92	129.30
32	W	592	A	N1-C2-N3	-18.76	119.92	129.30
32	W	816	A	N1-C2-N3	-18.76	119.92	129.30
32	W	875	A	C2-N3-C4	18.76	119.98	110.60
32	W	1077	A	C2-N3-C4	18.76	119.98	110.60
1	A	978	A	N1-C2-N3	-18.76	119.92	129.30
1	A	1078	A	C2-N3-C4	18.76	119.98	110.60
1	A	1313	A	N1-C2-N3	-18.76	119.92	129.30
1	A	1314	A	C2-N3-C4	18.76	119.98	110.60
1	A	1516	A	C2-N3-C4	18.76	119.98	110.60
1	A	1606	A	C2-N3-C4	18.76	119.98	110.60
1	A	2315	A	N1-C2-N3	-18.76	119.92	129.30
1	A	2734	A	C2-N3-C4	18.76	119.98	110.60
1	A	2810	A	N1-C2-N3	-18.76	119.92	129.30
1	A	324	A	N1-C2-N3	-18.76	119.92	129.30
1	A	507	A	C2-N3-C4	18.76	119.98	110.60
1	A	717	A	N1-C2-N3	-18.76	119.92	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1224	A	C2-N3-C4	18.76	119.98	110.60
1	A	1277	A	C2-N3-C4	18.76	119.98	110.60
1	A	1312	A	C2-N3-C4	18.76	119.98	110.60
1	A	1517	A	N1-C2-N3	-18.76	119.92	129.30
1	A	2316	A	C2-N3-C4	18.76	119.98	110.60
1	A	2464	A	C2-N3-C4	18.76	119.98	110.60
1	A	2511	A	C2-N3-C4	18.76	119.98	110.60
1	A	2673	A	N1-C2-N3	-18.76	119.92	129.30
32	W	34	A	C2-N3-C4	18.76	119.98	110.60
32	W	1254	A	C2-N3-C4	18.76	119.98	110.60
32	W	1270	A	N1-C2-N3	-18.76	119.92	129.30
32	W	1479	A	N1-C2-N3	-18.76	119.92	129.30
1	A	333	A	C2-N3-C4	18.76	119.98	110.60
1	A	1056	A	C2-N3-C4	18.76	119.98	110.60
1	A	73	A	N1-C2-N3	-18.75	119.92	129.30
1	A	1686	A	C2-N3-C4	18.75	119.98	110.60
1	A	1788	A	C2-N3-C4	18.75	119.98	110.60
1	A	2047	A	C2-N3-C4	18.75	119.98	110.60
1	A	2060	A	C2-N3-C4	18.75	119.98	110.60
32	W	306	A	N1-C2-N3	-18.75	119.92	129.30
32	W	824	A	N1-C2-N3	-18.75	119.92	129.30
32	W	974	A	C2-N3-C4	18.75	119.98	110.60
32	W	1166	A	C2-N3-C4	18.75	119.98	110.60
1	A	692	A	C2-N3-C4	18.75	119.98	110.60
1	A	1541	A	C2-N3-C4	18.75	119.98	110.60
1	A	1685	A	N1-C2-N3	-18.75	119.92	129.30
32	W	644	A	C2-N3-C4	18.75	119.98	110.60
1	A	337	A	C2-N3-C4	18.75	119.98	110.60
1	A	908	A	N1-C2-N3	-18.75	119.92	129.30
1	A	1005	A	N1-C2-N3	-18.75	119.92	129.30
1	A	1340	A	C2-N3-C4	18.75	119.97	110.60
1	A	1517	A	C2-N3-C4	18.75	119.97	110.60
1	A	2594	A	N1-C2-N3	-18.75	119.92	129.30
32	W	142	A	C2-N3-C4	18.75	119.98	110.60
32	W	170	A	N1-C2-N3	-18.75	119.92	129.30
32	W	500	A	C2-N3-C4	18.75	119.98	110.60
32	W	548	A	C2-N3-C4	18.75	119.97	110.60
32	W	715	A	C2-N3-C4	18.75	119.98	110.60
1	A	124	A	C2-N3-C4	18.75	119.97	110.60
2	B	51	A	N1-C2-N3	-18.75	119.92	129.30
32	W	321	A	N1-C2-N3	-18.75	119.92	129.30
32	W	685	A	C2-N3-C4	18.75	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	374	A	C2-N3-C4	18.75	119.97	110.60
1	A	1201	A	N1-C2-N3	-18.75	119.92	129.30
1	A	1326	A	N1-C2-N3	-18.75	119.93	129.30
1	A	1818	A	C2-N3-C4	18.75	119.97	110.60
1	A	437	A	N1-C2-N3	-18.75	119.93	129.30
1	A	449	A	C2-N3-C4	18.75	119.97	110.60
1	A	1072	A	N1-C2-N3	-18.75	119.93	129.30
1	A	1202	A	N1-C2-N3	-18.75	119.93	129.30
32	W	886	A	N1-C2-N3	-18.75	119.93	129.30
1	A	373	A	C2-N3-C4	18.75	119.97	110.60
1	A	519	A	N1-C2-N3	-18.75	119.93	129.30
1	A	851	A	N1-C2-N3	-18.75	119.93	129.30
1	A	1034	A	C2-N3-C4	18.75	119.97	110.60
1	A	1042	A	N1-C2-N3	-18.75	119.93	129.30
1	A	1789	A	C2-N3-C4	18.75	119.97	110.60
1	A	1789	A	N1-C2-N3	-18.75	119.93	129.30
1	A	2658	A	C2-N3-C4	18.75	119.97	110.60
32	W	389	A	C2-N3-C4	18.75	119.97	110.60
32	W	786	A	C2-N3-C4	18.75	119.97	110.60
32	W	882	A	C2-N3-C4	18.75	119.97	110.60
32	W	1541	A	N1-C2-N3	-18.75	119.93	129.30
1	A	110	A	C2-N3-C4	18.74	119.97	110.60
1	A	1727	A	C2-N3-C4	18.74	119.97	110.60
32	W	993	A	N1-C2-N3	-18.74	119.93	129.30
32	W	1115	A	N1-C2-N3	-18.74	119.93	129.30
32	W	1463	A	C2-N3-C4	18.74	119.97	110.60
1	A	1412	A	C2-N3-C4	18.74	119.97	110.60
1	A	1948	A	N1-C2-N3	-18.74	119.93	129.30
1	A	2106	A	C2-N3-C4	18.74	119.97	110.60
1	A	2390	A	C2-N3-C4	18.74	119.97	110.60
32	W	204	A	C2-N3-C4	18.74	119.97	110.60
32	W	419	A	N1-C2-N3	-18.74	119.93	129.30
32	W	459	A	N1-C2-N3	-18.74	119.93	129.30
32	W	968	A	N1-C2-N3	-18.74	119.93	129.30
1	A	1947	A	C2-N3-C4	18.74	119.97	110.60
1	A	2316	A	N1-C2-N3	-18.74	119.93	129.30
1	A	2793	A	N1-C2-N3	-18.74	119.93	129.30
32	W	190	A	N1-C2-N3	-18.74	119.93	129.30
32	W	730	A	C2-N3-C4	18.74	119.97	110.60
1	A	429	A	C2-N3-C4	18.74	119.97	110.60
1	A	847	A	C2-N3-C4	18.74	119.97	110.60
1	A	1084	A	C2-N3-C4	18.74	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	53	A	C2-N3-C4	18.74	119.97	110.60
32	W	94	A	C2-N3-C4	18.74	119.97	110.60
32	W	440	A	N1-C2-N3	-18.74	119.93	129.30
32	W	491	A	C2-N3-C4	18.74	119.97	110.60
1	A	339	A	C2-N3-C4	18.74	119.97	110.60
1	A	582	A	C2-N3-C4	18.74	119.97	110.60
1	A	1608	A	N1-C2-N3	-18.74	119.93	129.30
1	A	2517	A	C2-N3-C4	18.74	119.97	110.60
1	A	1084	A	N1-C2-N3	-18.74	119.93	129.30
2	B	43	A	C2-N3-C4	18.74	119.97	110.60
32	W	31	A	N1-C2-N3	-18.74	119.93	129.30
32	W	211	A	N1-C2-N3	-18.74	119.93	129.30
32	W	335	A	C2-N3-C4	18.74	119.97	110.60
32	W	463	A	C2-N3-C4	18.74	119.97	110.60
32	W	910	A	C2-N3-C4	18.74	119.97	110.60
32	W	947	A	N1-C2-N3	-18.74	119.93	129.30
32	W	1140	A	C2-N3-C4	18.74	119.97	110.60
32	W	1234	A	N1-C2-N3	-18.74	119.93	129.30
32	W	1342	A	N1-C2-N3	-18.74	119.93	129.30
32	W	1427	A	C2-N3-C4	18.74	119.97	110.60
1	A	673	A	C2-N3-C4	18.73	119.97	110.60
1	A	740	A	C2-N3-C4	18.73	119.97	110.60
1	A	1340	A	N1-C2-N3	-18.73	119.93	129.30
1	A	2302	A	C2-N3-C4	18.73	119.97	110.60
1	A	2708	A	C2-N3-C4	18.73	119.97	110.60
1	A	2845	A	N1-C2-N3	-18.73	119.93	129.30
32	W	67	A	N1-C2-N3	-18.73	119.93	129.30
32	W	1006	A	C2-N3-C4	18.73	119.97	110.60
32	W	1077	A	N1-C2-N3	-18.73	119.93	129.30
32	W	1205	A	C2-N3-C4	18.73	119.97	110.60
32	W	1296	A	N1-C2-N3	-18.73	119.93	129.30
1	A	1620	A	C2-N3-C4	18.73	119.97	110.60
1	A	1814	A	C2-N3-C4	18.73	119.97	110.60
32	W	925	A	N1-C2-N3	-18.73	119.93	129.30
32	W	1225	A	C2-N3-C4	18.73	119.97	110.60
32	W	1271	A	C2-N3-C4	18.73	119.97	110.60
1	A	38	A	C2-N3-C4	18.73	119.97	110.60
1	A	462	A	C2-N3-C4	18.73	119.97	110.60
1	A	1194	A	C2-N3-C4	18.73	119.97	110.60
32	W	743	A	C2-N3-C4	18.73	119.97	110.60
32	W	910	A	N1-C2-N3	-18.73	119.93	129.30
1	A	124	A	N1-C2-N3	-18.73	119.94	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	268	A	N1-C2-N3	-18.73	119.94	129.30
1	A	1054	A	C2-N3-C4	18.73	119.97	110.60
32	W	236	A	C2-N3-C4	18.73	119.97	110.60
1	A	193	A	C2-N3-C4	18.73	119.96	110.60
1	A	575	A	N1-C2-N3	-18.73	119.94	129.30
1	A	829	A	C2-N3-C4	18.73	119.96	110.60
1	A	1316	A	C2-N3-C4	18.73	119.96	110.60
1	A	1393	A	C2-N3-C4	18.73	119.96	110.60
2	B	11	A	N1-C2-N3	-18.73	119.94	129.30
32	W	270	A	C2-N3-C4	18.73	119.96	110.60
32	W	679	A	C2-N3-C4	18.73	119.96	110.60
32	W	796	A	N1-C2-N3	-18.73	119.94	129.30
1	A	1230	A	C2-N3-C4	18.73	119.96	110.60
1	A	2708	A	N1-C2-N3	-18.73	119.94	129.30
32	W	61	A	N1-C2-N3	-18.73	119.94	129.30
32	W	917	A	C2-N3-C4	18.73	119.96	110.60
1	A	278	A	C2-N3-C4	18.73	119.96	110.60
1	A	578	A	C2-N3-C4	18.73	119.96	110.60
1	A	1014	A	C2-N3-C4	18.73	119.96	110.60
1	A	1700	A	N1-C2-N3	-18.73	119.94	129.30
1	A	1925	A	C2-N3-C4	18.73	119.96	110.60
2	B	17	A	N1-C2-N3	-18.73	119.94	129.30
32	W	382	A	N1-C2-N3	-18.73	119.94	129.30
32	W	582	A	N1-C2-N3	-18.73	119.94	129.30
32	W	1111	A	N1-C2-N3	-18.73	119.94	129.30
32	W	1178	A	N1-C2-N3	-18.73	119.94	129.30
32	W	1266	A	N1-C2-N3	-18.73	119.94	129.30
1	A	1113	A	C2-N3-C4	18.72	119.96	110.60
1	A	1326	A	C2-N3-C4	18.72	119.96	110.60
1	A	1421	A	N1-C2-N3	-18.72	119.94	129.30
32	W	178	A	C2-N3-C4	18.72	119.96	110.60
32	W	422	A	C2-N3-C4	18.72	119.96	110.60
32	W	724	A	N1-C2-N3	-18.72	119.94	129.30
1	A	260	A	N1-C2-N3	-18.72	119.94	129.30
1	A	1540	A	C2-N3-C4	18.72	119.96	110.60
1	A	2777	A	C2-N3-C4	18.72	119.96	110.60
32	W	391	A	C2-N3-C4	18.72	119.96	110.60
32	W	404	A	C2-N3-C4	18.72	119.96	110.60
1	A	5	A	C2-N3-C4	18.72	119.96	110.60
32	W	771	A	C2-N3-C4	18.72	119.96	110.60
1	A	71	A	N1-C2-N3	-18.72	119.94	129.30
1	A	219	A	C2-N3-C4	18.72	119.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	421	A	C2-N3-C4	18.72	119.96	110.60
1	A	519	A	C2-N3-C4	18.72	119.96	110.60
1	A	781	A	N1-C2-N3	-18.72	119.94	129.30
1	A	469	A	C2-N3-C4	18.72	119.96	110.60
1	A	1601	A	N1-C2-N3	-18.72	119.94	129.30
32	W	556	A	N1-C2-N3	-18.72	119.94	129.30
1	A	1797	A	C2-N3-C4	18.72	119.96	110.60
1	A	1956	A	C2-N3-C4	18.72	119.96	110.60
1	A	2327	A	C2-N3-C4	18.72	119.96	110.60
1	A	2618	A	C2-N3-C4	18.72	119.96	110.60
32	W	541	A	N1-C2-N3	-18.72	119.94	129.30
32	W	703	A	C2-N3-C4	18.72	119.96	110.60
32	W	1028	A	N1-C2-N3	-18.72	119.94	129.30
32	W	1090	A	N1-C2-N3	-18.72	119.94	129.30
32	W	1417	A	N1-C2-N3	-18.72	119.94	129.30
32	W	1502	A	N1-C2-N3	-18.72	119.94	129.30
1	A	6	A	C2-N3-C4	18.71	119.96	110.60
1	A	1961	A	C2-N3-C4	18.71	119.96	110.60
32	W	768	A	N1-C2-N3	-18.71	119.94	129.30
32	W	1205	A	N1-C2-N3	-18.71	119.94	129.30
32	W	1528	A	C2-N3-C4	18.71	119.96	110.60
1	A	2091	A	N1-C2-N3	-18.71	119.94	129.30
2	B	27	A	C2-N3-C4	18.71	119.96	110.60
32	W	195	A	N1-C2-N3	-18.71	119.94	129.30
32	W	696	A	C2-N3-C4	18.71	119.96	110.60
32	W	929	A	C2-N3-C4	18.71	119.96	110.60
1	A	259	A	C2-N3-C4	18.71	119.96	110.60
1	A	1405	A	N1-C2-N3	-18.71	119.94	129.30
1	A	1615	A	C2-N3-C4	18.71	119.96	110.60
1	A	1945	A	N1-C2-N3	-18.71	119.94	129.30
1	A	2338	A	N1-C2-N3	-18.71	119.94	129.30
1	A	2661	A	N1-C2-N3	-18.71	119.94	129.30
52	z	21	A	N1-C2-N3	-18.71	119.94	129.30
1	A	436	A	C2-N3-C4	18.71	119.95	110.60
1	A	538	A	C2-N3-C4	18.71	119.95	110.60
1	A	1580	A	C2-N3-C4	18.71	119.95	110.60
1	A	1581	A	N1-C2-N3	-18.71	119.94	129.30
1	A	1942	A	N1-C2-N3	-18.71	119.94	129.30
1	A	2851	A	C2-N3-C4	18.71	119.95	110.60
32	W	31	A	C2-N3-C4	18.71	119.95	110.60
32	W	337	A	C2-N3-C4	18.71	119.95	110.60
32	W	519	A	C2-N3-C4	18.71	119.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	704	A	C2-N3-C4	18.71	119.96	110.60
32	W	825	A	C2-N3-C4	18.71	119.96	110.60
1	A	61	A	C2-N3-C4	18.71	119.95	110.60
1	A	230	A	C2-N3-C4	18.71	119.95	110.60
1	A	811	A	C2-N3-C4	18.71	119.95	110.60
1	A	2083	A	N1-C2-N3	-18.71	119.95	129.30
1	A	2570	A	N1-C2-N3	-18.71	119.95	129.30
32	W	120	A	C2-N3-C4	18.71	119.95	110.60
32	W	128	A	N1-C2-N3	-18.71	119.95	129.30
32	W	985	A	C2-N3-C4	18.71	119.95	110.60
32	W	1004	A	N1-C2-N3	-18.71	119.95	129.30
32	W	1017	A	N1-C2-N3	-18.71	119.95	129.30
32	W	1022	A	C2-N3-C4	18.71	119.95	110.60
32	W	1185	A	N1-C2-N3	-18.71	119.95	129.30
32	W	1210	A	N1-C2-N3	-18.71	119.95	129.30
32	W	1327	A	C2-N3-C4	18.71	119.95	110.60
1	A	2719	A	N1-C2-N3	-18.71	119.95	129.30
1	A	166	A	C2-N3-C4	18.70	119.95	110.60
1	A	618	A	N1-C2-N3	-18.70	119.95	129.30
1	A	717	A	C2-N3-C4	18.70	119.95	110.60
1	A	2062	A	C2-N3-C4	18.70	119.95	110.60
32	W	117	A	C2-N3-C4	18.70	119.95	110.60
32	W	323	A	N1-C2-N3	-18.70	119.95	129.30
32	W	1102	A	C2-N3-C4	18.70	119.95	110.60
1	A	150	A	C2-N3-C4	18.70	119.95	110.60
1	A	231	A	N1-C2-N3	-18.70	119.95	129.30
1	A	943	A	N1-C2-N3	-18.70	119.95	129.30
1	A	1047	A	C2-N3-C4	18.70	119.95	110.60
1	A	1323	A	C2-N3-C4	18.70	119.95	110.60
1	A	1723	A	C2-N3-C4	18.70	119.95	110.60
1	A	1929	A	N1-C2-N3	-18.70	119.95	129.30
32	W	333	A	N1-C2-N3	-18.70	119.95	129.30
32	W	690	A	C2-N3-C4	18.70	119.95	110.60
32	W	816	A	C2-N3-C4	18.70	119.95	110.60
32	W	870	A	N1-C2-N3	-18.70	119.95	129.30
1	A	623	A	C2-N3-C4	18.70	119.95	110.60
1	A	727	A	C2-N3-C4	18.70	119.95	110.60
1	A	1277	A	N1-C2-N3	-18.70	119.95	129.30
32	W	933	A	C2-N3-C4	18.70	119.95	110.60
1	A	14	A	C2-N3-C4	18.70	119.95	110.60
1	A	758	A	N1-C2-N3	-18.70	119.95	129.30
1	A	1339	A	N1-C2-N3	-18.70	119.95	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1721	A	C2-N3-C4	18.70	119.95	110.60
1	A	2505	A	C2-N3-C4	18.70	119.95	110.60
1	A	2595	A	C2-N3-C4	18.70	119.95	110.60
32	W	209	A	N1-C2-N3	-18.70	119.95	129.30
32	W	1434	A	C2-N3-C4	18.70	119.95	110.60
32	W	1478	A	C2-N3-C4	18.70	119.95	110.60
1	A	830	A	N1-C2-N3	-18.70	119.95	129.30
1	A	888	A	N1-C2-N3	-18.70	119.95	129.30
1	A	1161	A	C2-N3-C4	18.70	119.95	110.60
32	W	271	A	N1-C2-N3	-18.70	119.95	129.30
32	W	357	A	N1-C2-N3	-18.70	119.95	129.30
1	A	140	A	C2-N3-C4	18.70	119.95	110.60
1	A	619	A	N1-C2-N3	-18.70	119.95	129.30
1	A	762	A	N1-C2-N3	-18.70	119.95	129.30
1	A	2778	A	N1-C2-N3	-18.70	119.95	129.30
1	A	653	A	N1-C2-N3	-18.70	119.95	129.30
1	A	1945	A	C2-N3-C4	18.70	119.95	110.60
1	A	1966	A	C2-N3-C4	18.70	119.95	110.60
32	W	129	A	N1-C2-N3	-18.70	119.95	129.30
32	W	947	A	C2-N3-C4	18.70	119.95	110.60
32	W	1238	A	C2-N3-C4	18.70	119.95	110.60
32	W	1260	A	N1-C2-N3	-18.70	119.95	129.30
1	A	421	A	N1-C2-N3	-18.69	119.95	129.30
1	A	517	A	C2-N3-C4	18.69	119.95	110.60
1	A	647	A	C2-N3-C4	18.69	119.95	110.60
1	A	746	A	C2-N3-C4	18.69	119.95	110.60
1	A	1179	A	C2-N3-C4	18.69	119.95	110.60
1	A	2661	A	C2-N3-C4	18.69	119.95	110.60
32	W	232	A	N1-C2-N3	-18.69	119.95	129.30
32	W	679	A	N1-C2-N3	-18.69	119.95	129.30
32	W	928	A	C2-N3-C4	18.69	119.95	110.60
1	A	479	A	N1-C2-N3	-18.69	119.95	129.30
1	A	584	A	C2-N3-C4	18.69	119.95	110.60
1	A	1464	A	N1-C2-N3	-18.69	119.95	129.30
1	A	2365	A	N1-C2-N3	-18.69	119.95	129.30
1	A	2398	A	N1-C2-N3	-18.69	119.95	129.30
32	W	1298	A	N1-C2-N3	-18.69	119.95	129.30
1	A	28	A	N1-C2-N3	-18.69	119.95	129.30
1	A	1791	A	C2-N3-C4	18.69	119.95	110.60
1	A	2542	A	N1-C2-N3	-18.69	119.95	129.30
32	W	53	A	N1-C2-N3	-18.69	119.95	129.30
32	W	616	A	C2-N3-C4	18.69	119.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	801	A	N1-C2-N3	-18.69	119.95	129.30
32	W	1024	A	C2-N3-C4	18.69	119.95	110.60
32	W	1296	A	C2-N3-C4	18.69	119.95	110.60
1	A	94	A	N1-C2-N3	-18.69	119.96	129.30
1	A	1583	A	C2-N3-C4	18.69	119.94	110.60
1	A	2071	A	N1-C2-N3	-18.69	119.96	129.30
32	W	1031	A	C2-N3-C4	18.69	119.94	110.60
32	W	1180	A	C2-N3-C4	18.69	119.94	110.60
1	A	1675	A	N1-C2-N3	-18.69	119.96	129.30
1	A	1967	A	C2-N3-C4	18.69	119.94	110.60
32	W	791	A	N1-C2-N3	-18.69	119.96	129.30
32	W	923	A	N1-C2-N3	-18.69	119.96	129.30
1	A	329	A	C2-N3-C4	18.69	119.94	110.60
1	A	2307	A	C2-N3-C4	18.69	119.94	110.60
1	A	948	A	N1-C2-N3	-18.68	119.96	129.30
1	A	1224	A	N1-C2-N3	-18.68	119.96	129.30
1	A	1335	A	C2-N3-C4	18.68	119.94	110.60
32	W	210	A	N1-C2-N3	-18.68	119.96	129.30
32	W	1140	A	N1-C2-N3	-18.68	119.96	129.30
1	A	1130	A	C2-N3-C4	18.68	119.94	110.60
32	W	568	A	C2-N3-C4	18.68	119.94	110.60
32	W	685	A	N1-C2-N3	-18.68	119.96	129.30
1	A	1149	A	C2-N3-C4	18.68	119.94	110.60
1	A	2762	A	N1-C2-N3	-18.68	119.96	129.30
32	W	236	A	N1-C2-N3	-18.68	119.96	129.30
32	W	296	A	C2-N3-C4	18.68	119.94	110.60
32	W	1133	A	C2-N3-C4	18.68	119.94	110.60
1	A	2497	A	C2-N3-C4	18.68	119.94	110.60
32	W	232	A	C2-N3-C4	18.68	119.94	110.60
32	W	346	A	C2-N3-C4	18.68	119.94	110.60
1	A	500	A	N1-C2-N3	-18.68	119.96	129.30
1	A	646	A	C2-N3-C4	18.68	119.94	110.60
1	A	1593	A	N1-C2-N3	-18.68	119.96	129.30
1	A	2307	A	N1-C2-N3	-18.68	119.96	129.30
32	W	500	A	N1-C2-N3	-18.68	119.96	129.30
32	W	1328	A	N1-C2-N3	-18.68	119.96	129.30
32	W	1366	A	C2-N3-C4	18.68	119.94	110.60
1	A	1056	A	N1-C2-N3	-18.68	119.96	129.30
2	B	20	A	C2-N3-C4	18.68	119.94	110.60
32	W	296	A	N1-C2-N3	-18.68	119.96	129.30
1	A	893	A	N1-C2-N3	-18.68	119.96	129.30
1	A	1066	A	C2-N3-C4	18.68	119.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1743	A	N1-C2-N3	-18.68	119.96	129.30
32	W	202	A	N1-C2-N3	-18.68	119.96	129.30
32	W	974	A	N1-C2-N3	-18.68	119.96	129.30
1	A	1802	A	N1-C2-N3	-18.67	119.96	129.30
1	A	2601	A	N1-C2-N3	-18.67	119.96	129.30
1	A	2787	A	N1-C2-N3	-18.67	119.96	129.30
32	W	1270	A	C2-N3-C4	18.67	119.94	110.60
32	W	1503	A	N1-C2-N3	-18.67	119.96	129.30
1	A	144	A	N1-C2-N3	-18.67	119.96	129.30
1	A	220	A	C2-N3-C4	18.67	119.94	110.60
1	A	325	A	C2-N3-C4	18.67	119.94	110.60
1	A	553	A	C2-N3-C4	18.67	119.94	110.60
1	A	835	A	C2-N3-C4	18.67	119.94	110.60
1	A	1008	A	C2-N3-C4	18.67	119.94	110.60
1	A	1027	A	C2-N3-C4	18.67	119.94	110.60
32	W	142	A	N1-C2-N3	-18.67	119.96	129.30
32	W	474	A	N1-C2-N3	-18.67	119.96	129.30
32	W	758	A	C2-N3-C4	18.67	119.94	110.60
32	W	799	A	C2-N3-C4	18.67	119.94	110.60
1	A	21	A	N1-C2-N3	-18.67	119.97	129.30
1	A	194	A	C2-N3-C4	18.67	119.94	110.60
1	A	1540	A	N1-C2-N3	-18.67	119.97	129.30
1	A	1553	A	N1-C2-N3	-18.67	119.96	129.30
1	A	1895	A	N1-C2-N3	-18.67	119.97	129.30
1	A	2276	A	C2-N3-C4	18.67	119.94	110.60
32	W	879	A	C2-N3-C4	18.67	119.94	110.60
32	W	1271	A	N1-C2-N3	-18.67	119.97	129.30
1	A	354	A	C2-N3-C4	18.67	119.94	110.60
1	A	2362	A	N1-C2-N3	-18.67	119.97	129.30
32	W	727	A	N1-C2-N3	-18.67	119.97	129.30
32	W	828	A	C2-N3-C4	18.67	119.93	110.60
1	A	987	A	C2-N3-C4	18.67	119.93	110.60
1	A	1375	A	N1-C2-N3	-18.67	119.97	129.30
32	W	28	A	N1-C2-N3	-18.67	119.97	129.30
32	W	52	A	N1-C2-N3	-18.67	119.97	129.30
32	W	251	A	N1-C2-N3	-18.67	119.97	129.30
32	W	581	A	N1-C2-N3	-18.67	119.97	129.30
32	W	1128	A	N1-C2-N3	-18.67	119.97	129.30
32	W	1222	A	N1-C2-N3	-18.67	119.97	129.30
52	z	58	A	C2-N3-C4	18.67	119.93	110.60
1	A	244	A	N1-C2-N3	-18.67	119.97	129.30
1	A	1034	A	N1-C2-N3	-18.67	119.97	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1491	A	N1-C2-N3	-18.67	119.97	129.30
1	A	2482	A	C2-N3-C4	18.67	119.93	110.60
1	A	2526	A	C2-N3-C4	18.67	119.93	110.60
32	W	811	A	N1-C2-N3	-18.67	119.97	129.30
1	A	1175	A	C2-N3-C4	18.66	119.93	110.60
1	A	1360	A	N1-C2-N3	-18.66	119.97	129.30
1	A	1381	A	C2-N3-C4	18.66	119.93	110.60
1	A	1813	A	N1-C2-N3	-18.66	119.97	129.30
1	A	2734	A	N1-C2-N3	-18.66	119.97	129.30
1	A	2740	A	N1-C2-N3	-18.66	119.97	129.30
32	W	415	A	C2-N3-C4	18.66	119.93	110.60
32	W	757	A	N1-C2-N3	-18.66	119.97	129.30
1	A	2860	A	N1-C2-N3	-18.66	119.97	129.30
32	W	225	A	N1-C2-N3	-18.66	119.97	129.30
1	A	679	A	C2-N3-C4	18.66	119.93	110.60
1	A	786	A	C2-N3-C4	18.66	119.93	110.60
1	A	2357	A	C2-N3-C4	18.66	119.93	110.60
1	A	2770	A	N1-C2-N3	-18.66	119.97	129.30
32	W	475	A	C2-N3-C4	18.66	119.93	110.60
32	W	738	A	C2-N3-C4	18.66	119.93	110.60
32	W	1121	A	C2-N3-C4	18.66	119.93	110.60
32	W	1341	A	N1-C2-N3	-18.66	119.97	129.30
32	W	1434	A	N1-C2-N3	-18.66	119.97	129.30
1	A	530	A	N1-C2-N3	-18.66	119.97	129.30
2	B	13	A	N1-C2-N3	-18.66	119.97	129.30
32	W	390	A	N1-C2-N3	-18.66	119.97	129.30
32	W	724	A	C2-N3-C4	18.66	119.93	110.60
1	A	494	A	C2-N3-C4	18.66	119.93	110.60
1	A	1113	A	N1-C2-N3	-18.66	119.97	129.30
1	A	1619	A	C2-N3-C4	18.66	119.93	110.60
1	A	2463	A	N1-C2-N3	-18.66	119.97	129.30
2	B	114	A	N1-C2-N3	-18.66	119.97	129.30
32	W	1289	A	C2-N3-C4	18.66	119.93	110.60
32	W	1470	A	N1-C2-N3	-18.66	119.97	129.30
1	A	2619	A	C2-N3-C4	18.66	119.93	110.60
32	W	1147	A	N1-C2-N3	-18.66	119.97	129.30
1	A	1244	A	N1-C2-N3	-18.66	119.97	129.30
1	A	1253	A	C2-N3-C4	18.66	119.93	110.60
1	A	1850	A	C2-N3-C4	18.66	119.93	110.60
1	A	2078	A	N1-C2-N3	-18.66	119.97	129.30
1	A	2364	A	C2-N3-C4	18.66	119.93	110.60
1	A	2848	A	N1-C2-N3	-18.66	119.97	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	281	A	C2-N3-C4	18.66	119.93	110.60
32	W	568	A	N1-C2-N3	-18.66	119.97	129.30
1	A	236	A	C2-N3-C4	18.65	119.93	110.60
1	A	275	A	N1-C2-N3	-18.65	119.97	129.30
1	A	339	A	N1-C2-N3	-18.65	119.97	129.30
1	A	828	A	C2-N3-C4	18.65	119.93	110.60
1	A	2298	A	C2-N3-C4	18.65	119.93	110.60
1	A	198	A	C2-N3-C4	18.65	119.93	110.60
1	A	1142	A	N1-C2-N3	-18.65	119.97	129.30
1	A	1533	A	N1-C2-N3	-18.65	119.97	129.30
1	A	2786	A	N1-C2-N3	-18.65	119.97	129.30
2	B	17	A	C2-N3-C4	18.65	119.93	110.60
32	W	178	A	N1-C2-N3	-18.65	119.97	129.30
32	W	555	A	N1-C2-N3	-18.65	119.97	129.30
32	W	1017	A	C2-N3-C4	18.65	119.93	110.60
32	W	1133	A	N1-C2-N3	-18.65	119.97	129.30
1	A	868	A	N1-C2-N3	-18.65	119.97	129.30
1	A	1339	A	C2-N3-C4	18.65	119.92	110.60
1	A	1432	A	C2-N3-C4	18.65	119.92	110.60
1	A	2080	A	C2-N3-C4	18.65	119.92	110.60
32	W	329	A	C2-N3-C4	18.65	119.92	110.60
32	W	650	A	N1-C2-N3	-18.65	119.97	129.30
32	W	705	A	C2-N3-C4	18.65	119.92	110.60
1	A	1021	A	C2-N3-C4	18.65	119.92	110.60
1	A	2542	A	C2-N3-C4	18.65	119.92	110.60
32	W	171	A	N1-C2-N3	-18.65	119.98	129.30
32	W	423	A	N1-C2-N3	-18.65	119.98	129.30
32	W	496	A	N1-C2-N3	-18.65	119.98	129.30
1	A	229	A	C2-N3-C4	18.65	119.92	110.60
1	A	1092	A	C2-N3-C4	18.65	119.92	110.60
1	A	1235	A	C2-N3-C4	18.65	119.92	110.60
1	A	1254	A	N1-C2-N3	-18.65	119.98	129.30
1	A	1291	A	C2-N3-C4	18.65	119.92	110.60
1	A	1532	A	N1-C2-N3	-18.65	119.98	129.30
1	A	1901	A	N1-C2-N3	-18.65	119.98	129.30
2	B	44	A	N1-C2-N3	-18.65	119.98	129.30
32	W	321	A	C2-N3-C4	18.65	119.92	110.60
32	W	401	A	N1-C2-N3	-18.65	119.98	129.30
32	W	501	A	C2-N3-C4	18.65	119.92	110.60
32	W	923	A	C2-N3-C4	18.65	119.92	110.60
32	W	1092	A	N1-C2-N3	-18.65	119.98	129.30
32	W	81	A	C2-N3-C4	18.64	119.92	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	389	A	N1-C2-N3	-18.64	119.98	129.30
1	A	448	A	N1-C2-N3	-18.64	119.98	129.30
1	A	2440	A	C2-N3-C4	18.64	119.92	110.60
1	A	2317	A	N1-C2-N3	-18.64	119.98	129.30
32	W	120	A	N1-C2-N3	-18.64	119.98	129.30
1	A	216	A	N1-C2-N3	-18.64	119.98	129.30
1	A	373	A	N1-C2-N3	-18.64	119.98	129.30
1	A	1654	A	N1-C2-N3	-18.64	119.98	129.30
1	A	1802	A	C2-N3-C4	18.64	119.92	110.60
2	B	39	A	N1-C2-N3	-18.64	119.98	129.30
32	W	508	A	C2-N3-C4	18.64	119.92	110.60
32	W	1225	A	N1-C2-N3	-18.64	119.98	129.30
1	A	958	A	N1-C2-N3	-18.64	119.98	129.30
1	A	1913	A	N1-C2-N3	-18.64	119.98	129.30
1	A	2405	A	C2-N3-C4	18.64	119.92	110.60
32	W	1289	A	N1-C2-N3	-18.64	119.98	129.30
32	W	501	A	N1-C2-N3	-18.64	119.98	129.30
32	W	1529	A	C2-N3-C4	18.64	119.92	110.60
1	A	584	A	N1-C2-N3	-18.64	119.98	129.30
1	A	999	A	N1-C2-N3	-18.64	119.98	129.30
1	A	2395	A	C2-N3-C4	18.64	119.92	110.60
1	A	2480	A	N1-C2-N3	-18.64	119.98	129.30
32	W	477	A	N1-C2-N3	-18.64	119.98	129.30
32	W	823	A	N1-C2-N3	-18.64	119.98	129.30
32	W	1513	A	C2-N3-C4	18.64	119.92	110.60
1	A	176	A	N1-C2-N3	-18.63	119.98	129.30
1	A	991	A	C2-N3-C4	18.63	119.92	110.60
1	A	1406	A	N1-C2-N3	-18.63	119.98	129.30
1	A	1520	A	N1-C2-N3	-18.63	119.98	129.30
32	W	94	A	N1-C2-N3	-18.63	119.98	129.30
1	A	168	A	C2-N3-C4	18.63	119.92	110.60
1	A	774	A	C2-N3-C4	18.63	119.92	110.60
1	A	2000	A	C2-N3-C4	18.63	119.92	110.60
1	A	2462	A	N1-C2-N3	-18.63	119.98	129.30
1	A	2904	A	C2-N3-C4	18.63	119.92	110.60
1	A	2907	A	N1-C2-N3	-18.63	119.98	129.30
32	W	725	A	C2-N3-C4	18.63	119.92	110.60
32	W	803	A	N1-C2-N3	-18.63	119.98	129.30
32	W	1200	A	N1-C2-N3	-18.63	119.98	129.30
1	A	1585	A	N1-C2-N3	-18.63	119.98	129.30
1	A	1648	A	C2-N3-C4	18.63	119.92	110.60
1	A	1735	A	N1-C2-N3	-18.63	119.98	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2658	A	N1-C2-N3	-18.63	119.98	129.30
1	A	2769	A	N1-C2-N3	-18.63	119.98	129.30
32	W	258	A	N1-C2-N3	-18.63	119.98	129.30
32	W	278	A	C2-N3-C4	18.63	119.92	110.60
32	W	463	A	N1-C2-N3	-18.63	119.98	129.30
32	W	638	A	N1-C2-N3	-18.63	119.98	129.30
32	W	651	A	C2-N3-C4	18.63	119.92	110.60
1	A	302	A	C2-N3-C4	18.63	119.91	110.60
1	A	993	A	C2-N3-C4	18.63	119.91	110.60
1	A	1465	A	N1-C2-N3	-18.63	119.98	129.30
1	A	2819	A	C2-N3-C4	18.63	119.92	110.60
2	B	105	A	C2-N3-C4	18.63	119.92	110.60
32	W	371	A	N1-C2-N3	-18.63	119.98	129.30
32	W	529	A	N1-C2-N3	-18.63	119.98	129.30
32	W	1405	A	C2-N3-C4	18.63	119.92	110.60
32	W	1455	A	N1-C2-N3	-18.63	119.98	129.30
1	A	600	A	N1-C2-N3	-18.63	119.99	129.30
1	A	1265	A	C2-N3-C4	18.63	119.91	110.60
32	W	959	A	C2-N3-C4	18.63	119.91	110.60
32	W	1328	A	C2-N3-C4	18.63	119.91	110.60
1	A	41	A	N1-C2-N3	-18.63	119.99	129.30
1	A	459	A	C2-N3-C4	18.63	119.91	110.60
1	A	1745	A	C2-N3-C4	18.63	119.91	110.60
1	A	1928	A	N1-C2-N3	-18.63	119.99	129.30
32	W	281	A	N1-C2-N3	-18.63	119.99	129.30
1	A	753	A	C2-N3-C4	18.62	119.91	110.60
1	A	1423	A	N1-C2-N3	-18.62	119.99	129.30
32	W	203	A	C2-N3-C4	18.62	119.91	110.60
1	A	355	A	C2-N3-C4	18.62	119.91	110.60
1	A	1412	A	N1-C2-N3	-18.62	119.99	129.30
1	A	1434	A	N1-C2-N3	-18.62	119.99	129.30
1	A	2276	A	N1-C2-N3	-18.62	119.99	129.30
32	W	344	A	N1-C2-N3	-18.62	119.99	129.30
32	W	978	A	N1-C2-N3	-18.62	119.99	129.30
1	A	2837	A	N1-C2-N3	-18.62	119.99	129.30
1	A	2904	A	N1-C2-N3	-18.62	119.99	129.30
32	W	1254	A	N1-C2-N3	-18.62	119.99	129.30
32	W	1466	A	C2-N3-C4	18.62	119.91	110.60
1	A	876	A	N1-C2-N3	-18.62	119.99	129.30
1	A	2869	A	N1-C2-N3	-18.62	119.99	129.30
32	W	569	A	N1-C2-N3	-18.62	119.99	129.30
1	A	322	A	N1-C2-N3	-18.62	119.99	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1967	A	N1-C2-N3	-18.62	119.99	129.30
32	W	975	A	N1-C2-N3	-18.62	119.99	129.30
32	W	1090	A	C2-N3-C4	18.62	119.91	110.60
32	W	1425	A	N1-C2-N3	-18.62	119.99	129.30
1	A	1025	A	C2-N3-C4	18.62	119.91	110.60
1	A	2912	A	N1-C2-N3	-18.62	119.99	129.30
32	W	1283	A	C2-N3-C4	18.62	119.91	110.60
32	W	1327	A	N1-C2-N3	-18.62	119.99	129.30
32	W	1383	A	C2-N3-C4	18.62	119.91	110.60
1	A	1287	A	N1-C2-N3	-18.62	119.99	129.30
32	W	352	A	C2-N3-C4	18.62	119.91	110.60
32	W	671	A	N1-C2-N3	-18.62	119.99	129.30
32	W	1120	A	N1-C2-N3	-18.62	119.99	129.30
1	A	305	A	N1-C2-N3	-18.61	119.99	129.30
1	A	947	A	N1-C2-N3	-18.61	119.99	129.30
1	A	1188	A	C2-N3-C4	18.61	119.91	110.60
1	A	1888	A	C2-N3-C4	18.61	119.91	110.60
1	A	2851	A	N1-C2-N3	-18.61	119.99	129.30
32	W	62	A	N1-C2-N3	-18.61	119.99	129.30
32	W	314	A	N1-C2-N3	-18.61	119.99	129.30
32	W	690	A	N1-C2-N3	-18.61	119.99	129.30
32	W	1333	A	C2-N3-C4	18.61	119.91	110.60
1	A	178	A	C2-N3-C4	18.61	119.91	110.60
1	A	2923	A	N1-C2-N3	-18.61	119.99	129.30
2	B	113	A	N1-C2-N3	-18.61	119.99	129.30
32	W	684	A	N1-C2-N3	-18.61	119.99	129.30
32	W	1315	A	C2-N3-C4	18.61	119.91	110.60
32	W	1403	A	N1-C2-N3	-18.61	119.99	129.30
1	A	202	A	N1-C2-N3	-18.61	119.99	129.30
1	A	470	A	N1-C2-N3	-18.61	119.99	129.30
1	A	1115	A	N1-C2-N3	-18.61	119.99	129.30
1	A	2339	A	N1-C2-N3	-18.61	120.00	129.30
1	A	2924	A	C2-N3-C4	18.61	119.91	110.60
2	B	27	A	N1-C2-N3	-18.61	120.00	129.30
32	W	544	A	N1-C2-N3	-18.61	120.00	129.30
32	W	1176	A	N1-C2-N3	-18.61	119.99	129.30
1	A	333	A	N1-C2-N3	-18.61	120.00	129.30
1	A	337	A	N1-C2-N3	-18.61	120.00	129.30
1	A	1809	A	N1-C2-N3	-18.61	120.00	129.30
1	A	2030	A	N1-C2-N3	-18.61	120.00	129.30
1	A	2405	A	N1-C2-N3	-18.61	120.00	129.30
32	W	308	A	C2-N3-C4	18.61	119.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1197	A	C2-N3-C4	18.61	119.91	110.60
32	W	1236	A	N1-C2-N3	-18.61	120.00	129.30
1	A	199	A	N1-C2-N3	-18.61	120.00	129.30
1	A	1074	A	N1-C2-N3	-18.61	120.00	129.30
32	W	173	A	N1-C2-N3	-18.61	120.00	129.30
1	A	5	A	N1-C2-N3	-18.61	120.00	129.30
1	A	1499	A	N1-C2-N3	-18.61	120.00	129.30
1	A	1697	A	C2-N3-C4	18.61	119.90	110.60
1	A	2454	A	C2-N3-C4	18.61	119.90	110.60
1	A	2793	A	C2-N3-C4	18.61	119.90	110.60
1	A	2826	A	N1-C2-N3	-18.61	120.00	129.30
32	W	919	A	N1-C2-N3	-18.61	120.00	129.30
1	A	661	A	C2-N3-C4	18.61	119.90	110.60
1	A	1302	A	C2-N3-C4	18.61	119.90	110.60
1	A	1699	A	N1-C2-N3	-18.61	120.00	129.30
1	A	1314	A	N1-C2-N3	-18.60	120.00	129.30
1	A	1636	A	N1-C2-N3	-18.60	120.00	129.30
1	A	1797	A	N1-C2-N3	-18.60	120.00	129.30
1	A	2389	A	N1-C2-N3	-18.60	120.00	129.30
1	A	2547	A	N1-C2-N3	-18.60	120.00	129.30
1	A	2683	A	C2-N3-C4	18.60	119.90	110.60
2	B	50	A	N1-C2-N3	-18.60	120.00	129.30
32	W	240	A	N1-C2-N3	-18.60	120.00	129.30
32	W	401	A	C2-N3-C4	18.60	119.90	110.60
32	W	684	A	C2-N3-C4	18.60	119.90	110.60
32	W	1512	A	C2-N3-C4	18.60	119.90	110.60
1	A	225	A	N1-C2-N3	-18.60	120.00	129.30
1	A	1055	A	N1-C2-N3	-18.60	120.00	129.30
32	W	148	A	N1-C2-N3	-18.60	120.00	129.30
1	A	171	A	N1-C2-N3	-18.60	120.00	129.30
1	A	376	A	N1-C2-N3	-18.60	120.00	129.30
1	A	774	A	N1-C2-N3	-18.60	120.00	129.30
1	A	2482	A	N1-C2-N3	-18.60	120.00	129.30
32	W	266	A	N1-C2-N3	-18.60	120.00	129.30
32	W	664	A	N1-C2-N3	-18.60	120.00	129.30
32	W	1014	A	C2-N3-C4	18.60	119.90	110.60
1	A	1504	A	C2-N3-C4	18.60	119.90	110.60
1	A	1663	A	N1-C2-N3	-18.60	120.00	129.30
32	W	367	A	N1-C2-N3	-18.60	120.00	129.30
1	A	199	A	C2-N3-C4	18.60	119.90	110.60
1	A	2296	A	C2-N3-C4	18.60	119.90	110.60
1	A	2846	A	C2-N3-C4	18.60	119.90	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1103	A	C2-N3-C4	18.60	119.90	110.60
1	A	102	A	N1-C2-N3	-18.60	120.00	129.30
1	A	1815	A	N1-C2-N3	-18.60	120.00	129.30
1	A	428	A	C2-N3-C4	18.59	119.90	110.60
1	A	1020	A	N1-C2-N3	-18.59	120.00	129.30
1	A	2407	A	C2-N3-C4	18.59	119.90	110.60
1	A	2810	A	C2-N3-C4	18.59	119.90	110.60
32	W	917	A	N1-C2-N3	-18.59	120.00	129.30
32	W	918	A	C2-N3-C4	18.59	119.90	110.60
32	W	988	A	C2-N3-C4	18.59	119.90	110.60
32	W	1245	A	C2-N3-C4	18.59	119.90	110.60
32	W	1348	A	C2-N3-C4	18.59	119.90	110.60
32	W	1528	A	N1-C2-N3	-18.59	120.00	129.30
1	A	1606	A	N1-C2-N3	-18.59	120.00	129.30
1	A	1839	A	C2-N3-C4	18.59	119.90	110.60
1	A	1850	A	N1-C2-N3	-18.59	120.00	129.30
1	A	1179	A	N1-C2-N3	-18.59	120.00	129.30
1	A	1631	A	N1-C2-N3	-18.59	120.00	129.30
1	A	1734	A	C2-N3-C4	18.59	119.89	110.60
1	A	2571	A	N1-C2-N3	-18.59	120.00	129.30
32	W	1297	A	C2-N3-C4	18.59	119.89	110.60
1	A	302	A	N1-C2-N3	-18.59	120.00	129.30
1	A	1516	A	N1-C2-N3	-18.59	120.00	129.30
1	A	1989	A	C2-N3-C4	18.59	119.89	110.60
1	A	2390	A	N1-C2-N3	-18.59	120.00	129.30
32	W	160	A	C2-N3-C4	18.59	119.89	110.60
1	A	10	A	N1-C2-N3	-18.59	120.01	129.30
1	A	12	A	N1-C2-N3	-18.59	120.00	129.30
1	A	1477	A	C2-N3-C4	18.59	119.89	110.60
1	A	1791	A	N1-C2-N3	-18.59	120.01	129.30
1	A	2417	A	N1-C2-N3	-18.59	120.01	129.30
1	A	2770	A	C2-N3-C4	18.59	119.89	110.60
1	A	2902	A	N1-C2-N3	-18.59	120.01	129.30
1	A	412	A	N1-C2-N3	-18.59	120.01	129.30
1	A	543	A	C2-N3-C4	18.59	119.89	110.60
1	A	1575	A	N1-C2-N3	-18.59	120.01	129.30
1	A	2704	A	N1-C2-N3	-18.59	120.01	129.30
1	A	616	A	N1-C2-N3	-18.59	120.01	129.30
1	A	1027	A	N1-C2-N3	-18.59	120.01	129.30
1	A	1175	A	N1-C2-N3	-18.59	120.01	129.30
1	A	1620	A	N1-C2-N3	-18.59	120.01	129.30
1	A	1966	A	N1-C2-N3	-18.59	120.01	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2030	A	C2-N3-C4	18.59	119.89	110.60
32	W	604	A	C2-N3-C4	18.59	119.89	110.60
32	W	929	A	N1-C2-N3	-18.59	120.01	129.30
32	W	1024	A	N1-C2-N3	-18.58	120.01	129.30
32	W	1509	A	N1-C2-N3	-18.58	120.01	129.30
1	A	110	A	N1-C2-N3	-18.58	120.01	129.30
1	A	247	A	C2-N3-C4	18.58	119.89	110.60
1	A	646	A	N1-C2-N3	-18.58	120.01	129.30
1	A	689	A	N1-C2-N3	-18.58	120.01	129.30
1	A	1190	A	C2-N3-C4	18.58	119.89	110.60
1	A	1580	A	N1-C2-N3	-18.58	120.01	129.30
1	A	1812	A	C2-N3-C4	18.58	119.89	110.60
32	W	335	A	N1-C2-N3	-18.58	120.01	129.30
32	W	987	A	N1-C2-N3	-18.58	120.01	129.30
1	A	811	A	N1-C2-N3	-18.58	120.01	129.30
1	A	1361	A	N1-C2-N3	-18.58	120.01	129.30
1	A	1534	A	N1-C2-N3	-18.58	120.01	129.30
1	A	2835	A	C2-N3-C4	18.58	119.89	110.60
32	W	611	A	C2-N3-C4	18.58	119.89	110.60
32	W	1248	A	N1-C2-N3	-18.58	120.01	129.30
1	A	582	A	N1-C2-N3	-18.58	120.01	129.30
1	A	2087	A	N1-C2-N3	-18.58	120.01	129.30
32	W	419	A	C2-N3-C4	18.58	119.89	110.60
32	W	1259	A	N1-C2-N3	-18.58	120.01	129.30
1	A	786	A	N1-C2-N3	-18.58	120.01	129.30
1	A	1722	A	C2-N3-C4	18.58	119.89	110.60
1	A	1768	A	N1-C2-N3	-18.58	120.01	129.30
1	A	2590	A	C2-N3-C4	18.58	119.89	110.60
2	B	76	A	N1-C2-N3	-18.58	120.01	129.30
32	W	117	A	N1-C2-N3	-18.58	120.01	129.30
32	W	161	A	C2-N3-C4	18.58	119.89	110.60
32	W	630	A	N1-C2-N3	-18.58	120.01	129.30
32	W	911	A	C2-N3-C4	18.58	119.89	110.60
32	W	956	A	N1-C2-N3	-18.58	120.01	129.30
32	W	1176	A	C2-N3-C4	18.58	119.89	110.60
52	z	76	A	C2-N3-C4	18.58	119.89	110.60
1	A	1536	A	N1-C2-N3	-18.58	120.01	129.30
1	A	2468	A	C2-N3-C4	18.58	119.89	110.60
32	W	786	A	N1-C2-N3	-18.58	120.01	129.30
1	A	244	A	C2-N3-C4	18.57	119.89	110.60
1	A	1243	A	N1-C2-N3	-18.57	120.01	129.30
1	A	1592	A	N1-C2-N3	-18.57	120.01	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1648	A	N1-C2-N3	-18.57	120.01	129.30
1	A	1679	A	N1-C2-N3	-18.57	120.01	129.30
1	A	1901	A	C2-N3-C4	18.57	119.89	110.60
32	W	618	A	C2-N3-C4	18.57	119.89	110.60
32	W	924	A	N1-C2-N3	-18.57	120.01	129.30
1	A	1197	A	C2-N3-C4	18.57	119.89	110.60
1	A	2827	A	C2-N3-C4	18.57	119.89	110.60
2	B	43	A	N1-C2-N3	-18.57	120.01	129.30
1	A	117	A	C2-N3-C4	18.57	119.89	110.60
1	A	1569	A	N1-C2-N3	-18.57	120.01	129.30
1	A	2461	A	N1-C2-N3	-18.57	120.02	129.30
32	W	107	A	N1-C2-N3	-18.57	120.01	129.30
1	A	53	A	N1-C2-N3	-18.57	120.02	129.30
1	A	388	A	N1-C2-N3	-18.57	120.02	129.30
1	A	561	A	C2-N3-C4	18.57	119.89	110.60
1	A	2441	A	C2-N3-C4	18.57	119.89	110.60
32	W	1103	A	N1-C2-N3	-18.57	120.02	129.30
1	A	202	A	C2-N3-C4	18.57	119.89	110.60
1	A	325	A	N1-C2-N3	-18.57	120.02	129.30
1	A	1201	A	C2-N3-C4	18.57	119.88	110.60
1	A	1653	A	C2-N3-C4	18.57	119.88	110.60
1	A	1942	A	C2-N3-C4	18.57	119.88	110.60
1	A	1981	A	N1-C2-N3	-18.57	120.02	129.30
1	A	2364	A	N1-C2-N3	-18.57	120.02	129.30
32	W	35	A	N1-C2-N3	-18.57	120.02	129.30
32	W	1179	A	N1-C2-N3	-18.57	120.02	129.30
32	W	1442	A	N1-C2-N3	-18.57	120.02	129.30
1	A	65	A	N1-C2-N3	-18.57	120.02	129.30
1	A	2691	A	C2-N3-C4	18.57	119.88	110.60
1	A	829	A	N1-C2-N3	-18.57	120.02	129.30
1	A	894	A	N1-C2-N3	-18.57	120.02	129.30
1	A	1042	A	C2-N3-C4	18.57	119.88	110.60
1	A	2381	A	C2-N3-C4	18.57	119.88	110.60
1	A	2779	A	N1-C2-N3	-18.57	120.02	129.30
1	A	2782	A	N1-C2-N3	-18.57	120.02	129.30
32	W	825	A	N1-C2-N3	-18.57	120.02	129.30
32	W	1031	A	N1-C2-N3	-18.57	120.02	129.30
1	A	254	A	C2-N3-C4	18.56	119.88	110.60
1	A	459	A	N1-C2-N3	-18.56	120.02	129.30
1	A	922	A	N1-C2-N3	-18.56	120.02	129.30
32	W	1065	A	N1-C2-N3	-18.56	120.02	129.30
1	A	475	A	C2-N3-C4	18.56	119.88	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2059	A	C2-N3-C4	18.56	119.88	110.60
1	A	2885	A	C2-N3-C4	18.56	119.88	110.60
32	W	203	A	N1-C2-N3	-18.56	120.02	129.30
32	W	439	A	N1-C2-N3	-18.56	120.02	129.30
32	W	762	A	N1-C2-N3	-18.56	120.02	129.30
52	z	76	A	N1-C2-N3	-18.56	120.02	129.30
1	A	537	A	C2-N3-C4	18.56	119.88	110.60
1	A	1655	A	N1-C2-N3	-18.56	120.02	129.30
1	A	52	A	C2-N3-C4	18.56	119.88	110.60
1	A	436	A	N1-C2-N3	-18.56	120.02	129.30
1	A	2297	A	C2-N3-C4	18.56	119.88	110.60
1	A	2804	A	C2-N3-C4	18.56	119.88	110.60
1	A	2834	A	N1-C2-N3	-18.56	120.02	129.30
2	B	64	A	N1-C2-N3	-18.56	120.02	129.30
32	W	672	A	C2-N3-C4	18.56	119.88	110.60
32	W	696	A	N1-C2-N3	-18.56	120.02	129.30
32	W	1294	A	N1-C2-N3	-18.56	120.02	129.30
1	A	219	A	N1-C2-N3	-18.56	120.02	129.30
1	A	1014	A	N1-C2-N3	-18.56	120.02	129.30
1	A	1019	A	N1-C2-N3	-18.56	120.02	129.30
1	A	1883	A	C2-N3-C4	18.56	119.88	110.60
1	A	2900	A	N1-C2-N3	-18.56	120.02	129.30
1	A	330	A	N1-C2-N3	-18.56	120.02	129.30
1	A	559	A	C2-N3-C4	18.56	119.88	110.60
2	B	97	A	N1-C2-N3	-18.56	120.02	129.30
32	W	107	A	C2-N3-C4	18.56	119.88	110.60
32	W	1206	A	N1-C2-N3	-18.56	120.02	129.30
32	W	1257	A	N1-C2-N3	-18.56	120.02	129.30
1	A	727	A	N1-C2-N3	-18.55	120.02	129.30
1	A	1260	A	N1-C2-N3	-18.55	120.02	129.30
1	A	162	A	C2-N3-C4	18.55	119.88	110.60
1	A	971	A	N1-C2-N3	-18.55	120.02	129.30
1	A	1073	A	N1-C2-N3	-18.55	120.02	129.30
1	A	1161	A	N1-C2-N3	-18.55	120.02	129.30
1	A	2060	A	N1-C2-N3	-18.55	120.02	129.30
1	A	2643	A	N1-C2-N3	-18.55	120.02	129.30
32	W	1284	A	N1-C2-N3	-18.55	120.02	129.30
32	W	1443	A	C2-N3-C4	18.55	119.88	110.60
1	A	1075	A	C2-N3-C4	18.55	119.88	110.60
1	A	1815	A	C2-N3-C4	18.55	119.88	110.60
1	A	1066	A	N1-C2-N3	-18.55	120.03	129.30
1	A	2327	A	N1-C2-N3	-18.55	120.02	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2526	A	N1-C2-N3	-18.55	120.03	129.30
1	A	2627	A	C2-N3-C4	18.55	119.88	110.60
32	W	452	A	N1-C2-N3	-18.55	120.03	129.30
32	W	617	A	N1-C2-N3	-18.55	120.02	129.30
32	W	969	A	N1-C2-N3	-18.55	120.02	129.30
1	A	67	A	C2-N3-C4	18.55	119.87	110.60
1	A	259	A	N1-C2-N3	-18.55	120.03	129.30
1	A	549	A	N1-C2-N3	-18.55	120.03	129.30
1	A	574	A	N1-C2-N3	-18.55	120.03	129.30
1	A	2511	A	N1-C2-N3	-18.55	120.03	129.30
2	B	18	A	N1-C2-N3	-18.55	120.03	129.30
32	W	18	A	C2-N3-C4	18.55	119.87	110.60
1	A	722	A	C2-N3-C4	18.55	119.87	110.60
32	W	969	A	C2-N3-C4	18.55	119.87	110.60
1	A	1820	A	N1-C2-N3	-18.55	120.03	129.30
32	W	118	A	N1-C2-N3	-18.55	120.03	129.30
32	W	604	A	N1-C2-N3	-18.55	120.03	129.30
32	W	831	A	C2-N3-C4	18.55	119.87	110.60
32	W	1529	A	N1-C2-N3	-18.55	120.03	129.30
1	A	84	A	N1-C2-N3	-18.54	120.03	129.30
1	A	14	A	N1-C2-N3	-18.54	120.03	129.30
32	W	572	A	N1-C2-N3	-18.54	120.03	129.30
32	W	902	A	N1-C2-N3	-18.54	120.03	129.30
52	z	44	A	N1-C2-N3	-18.54	120.03	129.30
1	A	1724	A	C2-N3-C4	18.54	119.87	110.60
32	W	658	A	N1-C2-N3	-18.54	120.03	129.30
32	W	1189	A	N1-C2-N3	-18.54	120.03	129.30
1	A	274	A	N1-C2-N3	-18.54	120.03	129.30
1	A	2750	A	N1-C2-N3	-18.54	120.03	129.30
32	W	1359	A	N1-C2-N3	-18.54	120.03	129.30
1	A	1221	A	C2-N3-C4	18.54	119.87	110.60
1	A	1541	A	N1-C2-N3	-18.54	120.03	129.30
1	A	2595	A	N1-C2-N3	-18.54	120.03	129.30
1	A	752	A	C2-N3-C4	18.54	119.87	110.60
1	A	1445	A	C2-N3-C4	18.54	119.87	110.60
1	A	2629	A	C2-N3-C4	18.54	119.87	110.60
32	W	114	A	N1-C2-N3	-18.54	120.03	129.30
52	z	9	A	C2-N3-C4	18.54	119.87	110.60
1	A	490	A	N1-C2-N3	-18.54	120.03	129.30
1	A	517	A	N1-C2-N3	-18.54	120.03	129.30
1	A	2357	A	N1-C2-N3	-18.54	120.03	129.30
1	A	200	A	N1-C2-N3	-18.53	120.03	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	A	N1-C2-N3	-18.53	120.03	129.30
1	A	355	A	N1-C2-N3	-18.53	120.03	129.30
1	A	746	A	N1-C2-N3	-18.53	120.03	129.30
1	A	1504	A	N1-C2-N3	-18.53	120.03	129.30
1	A	1876	A	N1-C2-N3	-18.53	120.03	129.30
32	W	618	A	N1-C2-N3	-18.53	120.03	129.30
32	W	1143	A	N1-C2-N3	-18.53	120.03	129.30
1	A	917	A	N1-C2-N3	-18.53	120.03	129.30
1	A	2298	A	N1-C2-N3	-18.53	120.03	129.30
1	A	548	A	N1-C2-N3	-18.53	120.03	129.30
1	A	1686	A	N1-C2-N3	-18.53	120.03	129.30
1	A	1721	A	N1-C2-N3	-18.53	120.03	129.30
1	A	1788	A	N1-C2-N3	-18.53	120.03	129.30
32	W	519	A	N1-C2-N3	-18.53	120.03	129.30
32	W	1493	A	N1-C2-N3	-18.53	120.03	129.30
1	A	501	A	N1-C2-N3	-18.53	120.04	129.30
32	W	189	A	C2-N3-C4	18.53	119.86	110.60
32	W	189	A	N1-C2-N3	-18.53	120.04	129.30
1	A	6	A	N1-C2-N3	-18.53	120.04	129.30
1	A	207	A	C2-N3-C4	18.53	119.86	110.60
1	A	1092	A	N1-C2-N3	-18.53	120.04	129.30
1	A	1134	A	N1-C2-N3	-18.53	120.04	129.30
1	A	1210	A	N1-C2-N3	-18.53	120.04	129.30
1	A	2662	A	N1-C2-N3	-18.53	120.04	129.30
32	W	616	A	N1-C2-N3	-18.53	120.04	129.30
32	W	651	A	N1-C2-N3	-18.53	120.04	129.30
32	W	790	A	C2-N3-C4	18.53	119.86	110.60
1	A	835	A	N1-C2-N3	-18.52	120.04	129.30
1	A	1832	A	C2-N3-C4	18.52	119.86	110.60
1	A	2080	A	N1-C2-N3	-18.52	120.04	129.30
1	A	2498	A	C2-N3-C4	18.52	119.86	110.60
32	W	862	A	C2-N3-C4	18.52	119.86	110.60
32	W	1294	A	C2-N3-C4	18.52	119.86	110.60
32	W	491	A	N1-C2-N3	-18.52	120.04	129.30
1	A	882	A	N1-C2-N3	-18.52	120.04	129.30
1	A	2000	A	N1-C2-N3	-18.52	120.04	129.30
1	A	524	A	N1-C2-N3	-18.52	120.04	129.30
1	A	2006	A	C2-N3-C4	18.52	119.86	110.60
32	W	1252	A	N1-C2-N3	-18.52	120.04	129.30
1	A	1746	A	N1-C2-N3	-18.52	120.04	129.30
32	W	1006	A	N1-C2-N3	-18.52	120.04	129.30
52	z	41	A	N1-C2-N3	-18.52	120.04	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	150	A	N1-C2-N3	-18.52	120.04	129.30
1	A	462	A	N1-C2-N3	-18.52	120.04	129.30
1	A	1768	A	C2-N3-C4	18.52	119.86	110.60
32	W	1180	A	N1-C2-N3	-18.52	120.04	129.30
1	A	630	A	C2-N3-C4	18.52	119.86	110.60
1	A	1672	A	N1-C2-N3	-18.52	120.04	129.30
32	W	583	A	N1-C2-N3	-18.52	120.04	129.30
1	A	13	A	C2-N3-C4	18.51	119.86	110.60
1	A	198	A	N1-C2-N3	-18.51	120.04	129.30
1	A	281	A	N1-C2-N3	-18.51	120.04	129.30
1	A	2663	A	N1-C2-N3	-18.51	120.04	129.30
2	B	20	A	N1-C2-N3	-18.51	120.04	129.30
2	B	37	A	C2-N3-C4	18.51	119.86	110.60
32	W	669	A	N1-C2-N3	-18.51	120.04	129.30
32	W	874	A	N1-C2-N3	-18.51	120.04	129.30
1	A	1995	A	N1-C2-N3	-18.51	120.04	129.30
1	A	2670	A	C2-N3-C4	18.51	119.86	110.60
1	A	345	A	N1-C2-N3	-18.51	120.05	129.30
1	A	1542	A	N1-C2-N3	-18.51	120.05	129.30
32	W	1213	A	N1-C2-N3	-18.51	120.05	129.30
32	W	1463	A	N1-C2-N3	-18.51	120.04	129.30
32	W	1155	A	N1-C2-N3	-18.51	120.05	129.30
1	A	126	A	C2-N3-C4	18.51	119.85	110.60
1	A	156	A	N1-C2-N3	-18.51	120.05	129.30
1	A	904	A	N1-C2-N3	-18.51	120.05	129.30
1	A	2593	A	N1-C2-N3	-18.51	120.05	129.30
1	A	991	A	N1-C2-N3	-18.51	120.05	129.30
52	z	23	A	N1-C2-N3	-18.51	120.05	129.30
1	A	678	A	C2-N3-C4	18.50	119.85	110.60
1	A	1556	A	N1-C2-N3	-18.50	120.05	129.30
1	A	1709	A	N1-C2-N3	-18.50	120.05	129.30
1	A	1831	A	C2-N3-C4	18.50	119.85	110.60
1	A	2616	A	C2-N3-C4	18.50	119.85	110.60
1	A	2805	A	C2-N3-C4	18.50	119.85	110.60
32	W	738	A	N1-C2-N3	-18.50	120.05	129.30
1	A	964	A	C2-N3-C4	18.50	119.85	110.60
1	A	2034	A	N1-C2-N3	-18.50	120.05	129.30
1	A	384	A	N1-C2-N3	-18.50	120.05	129.30
1	A	2007	A	N1-C2-N3	-18.50	120.05	129.30
1	A	2059	A	N1-C2-N3	-18.50	120.05	129.30
32	W	204	A	N1-C2-N3	-18.50	120.05	129.30
1	A	1047	A	N1-C2-N3	-18.50	120.05	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1982	A	N1-C2-N3	-18.50	120.05	129.30
32	W	548	A	N1-C2-N3	-18.50	120.05	129.30
1	A	1006	A	C2-N3-C4	18.50	119.85	110.60
1	A	1723	A	N1-C2-N3	-18.50	120.05	129.30
1	A	206	A	N1-C2-N3	-18.50	120.05	129.30
1	A	974	A	C2-N3-C4	18.50	119.85	110.60
1	A	1461	A	N1-C2-N3	-18.50	120.05	129.30
1	A	2441	A	N1-C2-N3	-18.50	120.05	129.30
32	W	611	A	N1-C2-N3	-18.50	120.05	129.30
1	A	622	A	N1-C2-N3	-18.49	120.05	129.30
32	W	975	A	C2-N3-C4	18.49	119.85	110.60
1	A	449	A	N1-C2-N3	-18.49	120.05	129.30
1	A	553	A	N1-C2-N3	-18.49	120.05	129.30
1	A	637	A	N1-C2-N3	-18.49	120.05	129.30
1	A	917	A	C2-N3-C4	18.49	119.85	110.60
1	A	1877	A	N1-C2-N3	-18.49	120.05	129.30
1	A	2830	A	N1-C2-N3	-18.49	120.05	129.30
32	W	1456	A	C2-N3-C4	18.49	119.85	110.60
1	A	1291	A	N1-C2-N3	-18.49	120.05	129.30
1	A	2047	A	N1-C2-N3	-18.49	120.05	129.30
1	A	2601	A	C2-N3-C4	18.49	119.84	110.60
1	A	354	A	N1-C2-N3	-18.49	120.06	129.30
1	A	782	A	N1-C2-N3	-18.49	120.06	129.30
1	A	866	A	C2-N3-C4	18.49	119.84	110.60
1	A	1323	A	N1-C2-N3	-18.49	120.06	129.30
1	A	1722	A	N1-C2-N3	-18.49	120.06	129.30
2	B	105	A	N1-C2-N3	-18.49	120.06	129.30
1	A	1078	A	N1-C2-N3	-18.49	120.06	129.30
1	A	1680	A	N1-C2-N3	-18.49	120.06	129.30
1	A	1845	A	N1-C2-N3	-18.49	120.06	129.30
1	A	117	A	N1-C2-N3	-18.49	120.06	129.30
32	W	139	A	N1-C2-N3	-18.49	120.06	129.30
32	W	793	A	N1-C2-N3	-18.48	120.06	129.30
32	W	1466	A	N1-C2-N3	-18.48	120.06	129.30
1	A	133	A	N1-C2-N3	-18.48	120.06	129.30
1	A	193	A	N1-C2-N3	-18.48	120.06	129.30
1	A	692	A	N1-C2-N3	-18.48	120.06	129.30
1	A	1583	A	N1-C2-N3	-18.48	120.06	129.30
1	A	1588	A	N1-C2-N3	-18.48	120.06	129.30
1	A	1618	A	C2-N3-C4	18.48	119.84	110.60
1	A	2464	A	N1-C2-N3	-18.48	120.06	129.30
1	A	2805	A	N1-C2-N3	-18.48	120.06	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	326	A	N1-C2-N3	-18.48	120.06	129.30
1	A	1054	A	N1-C2-N3	-18.48	120.06	129.30
1	A	1346	A	N1-C2-N3	-18.48	120.06	129.30
1	A	1424	A	N1-C2-N3	-18.48	120.06	129.30
1	A	1818	A	N1-C2-N3	-18.48	120.06	129.30
32	W	1456	A	N1-C2-N3	-18.48	120.06	129.30
1	A	1697	A	N1-C2-N3	-18.48	120.06	129.30
1	A	2111	A	N1-C2-N3	-18.48	120.06	129.30
32	W	352	A	N1-C2-N3	-18.48	120.06	129.30
32	W	504	A	N1-C2-N3	-18.48	120.06	129.30
32	W	583	A	C2-N3-C4	18.48	119.84	110.60
1	A	2340	A	C2-N3-C4	18.48	119.84	110.60
1	A	2498	A	N1-C2-N3	-18.48	120.06	129.30
1	A	2049	A	N1-C2-N3	-18.47	120.06	129.30
1	A	369	A	N1-C2-N3	-18.47	120.06	129.30
1	A	753	A	N1-C2-N3	-18.47	120.06	129.30
1	A	952	A	N1-C2-N3	-18.47	120.06	129.30
1	A	2835	A	N1-C2-N3	-18.47	120.06	129.30
32	W	161	A	N1-C2-N3	-18.47	120.06	129.30
32	W	1121	A	N1-C2-N3	-18.47	120.06	129.30
1	A	518	A	C2-N3-C4	18.47	119.84	110.60
32	W	1513	A	N1-C2-N3	-18.47	120.06	129.30
1	A	1230	A	N1-C2-N3	-18.47	120.06	129.30
1	A	1998	A	N1-C2-N3	-18.47	120.06	129.30
32	W	160	A	N1-C2-N3	-18.47	120.06	129.30
32	W	504	A	C2-N3-C4	18.47	119.83	110.60
1	A	1130	A	N1-C2-N3	-18.47	120.07	129.30
32	W	278	A	N1-C2-N3	-18.47	120.07	129.30
1	A	353	A	N1-C2-N3	-18.47	120.07	129.30
1	A	1008	A	N1-C2-N3	-18.47	120.07	129.30
1	A	2406	A	N1-C2-N3	-18.47	120.07	129.30
32	W	984	A	N1-C2-N3	-18.47	120.07	129.30
32	W	1014	A	N1-C2-N3	-18.47	120.07	129.30
1	A	307	A	N1-C2-N3	-18.46	120.07	129.30
1	A	1774	A	N1-C2-N3	-18.46	120.07	129.30
32	W	799	A	N1-C2-N3	-18.46	120.07	129.30
32	W	1054	A	N1-C2-N3	-18.46	120.07	129.30
32	W	1383	A	N1-C2-N3	-18.46	120.07	129.30
32	W	1437	A	N1-C2-N3	-18.46	120.07	129.30
1	A	1483	A	N1-C2-N3	-18.46	120.07	129.30
1	A	1882	A	N1-C2-N3	-18.46	120.07	129.30
1	A	2694	A	N1-C2-N3	-18.46	120.07	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1335	A	N1-C2-N3	-18.46	120.07	129.30
1	A	537	A	N1-C2-N3	-18.46	120.07	129.30
1	A	993	A	N1-C2-N3	-18.46	120.07	129.30
1	A	2606	A	C2-N3-C4	18.46	119.83	110.60
1	A	236	A	N1-C2-N3	-18.46	120.07	129.30
1	A	507	A	N1-C2-N3	-18.46	120.07	129.30
32	W	1026	A	C2-N3-C4	18.46	119.83	110.60
1	A	183	A	C2-N3-C4	18.46	119.83	110.60
52	z	70	A	N1-C2-N3	-18.46	120.07	129.30
1	A	561	A	N1-C2-N3	-18.45	120.07	129.30
1	A	1812	A	N1-C2-N3	-18.45	120.07	129.30
1	A	2044	A	C2-N3-C4	18.45	119.83	110.60
32	W	290	A	C2-N3-C4	18.45	119.83	110.60
1	A	194	A	N1-C2-N3	-18.45	120.07	129.30
1	A	229	A	N1-C2-N3	-18.45	120.07	129.30
1	A	429	A	N1-C2-N3	-18.45	120.07	129.30
1	A	705	A	N1-C2-N3	-18.45	120.07	129.30
1	A	1221	A	N1-C2-N3	-18.45	120.07	129.30
1	A	1848	A	N1-C2-N3	-18.45	120.07	129.30
1	A	592	A	N1-C2-N3	-18.45	120.07	129.30
1	A	1392	A	N1-C2-N3	-18.45	120.08	129.30
1	A	1838	A	N1-C2-N3	-18.45	120.08	129.30
1	A	2369	A	N1-C2-N3	-18.45	120.08	129.30
1	A	2831	A	N1-C2-N3	-18.45	120.08	129.30
32	W	704	A	N1-C2-N3	-18.45	120.08	129.30
1	A	1100	A	N1-C2-N3	-18.45	120.08	129.30
2	B	56	A	N1-C2-N3	-18.45	120.08	129.30
1	A	2042	A	N1-C2-N3	-18.45	120.08	129.30
1	A	343	A	C2-N3-C4	18.44	119.82	110.60
1	A	490	A	C2-N3-C4	18.44	119.82	110.60
1	A	525	A	N1-C2-N3	-18.44	120.08	129.30
1	A	904	A	C2-N3-C4	18.44	119.82	110.60
1	A	230	A	N1-C2-N3	-18.44	120.08	129.30
1	A	1059	A	N1-C2-N3	-18.44	120.08	129.30
1	A	2381	A	N1-C2-N3	-18.44	120.08	129.30
1	A	2754	A	N1-C2-N3	-18.44	120.08	129.30
32	W	372	A	N1-C2-N3	-18.44	120.08	129.30
32	W	659	A	N1-C2-N3	-18.44	120.08	129.30
1	A	543	A	N1-C2-N3	-18.44	120.08	129.30
32	W	140	A	N1-C2-N3	-18.44	120.08	129.30
32	W	705	A	N1-C2-N3	-18.44	120.08	129.30
1	A	525	A	C2-N3-C4	18.44	119.82	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2454	A	N1-C2-N3	-18.44	120.08	129.30
32	W	1523	A	N1-C2-N3	-18.44	120.08	129.30
1	A	431	A	N1-C2-N3	-18.43	120.08	129.30
1	A	2349	A	N1-C2-N3	-18.43	120.08	129.30
1	A	2560	A	N1-C2-N3	-18.43	120.08	129.30
32	W	1188	A	N1-C2-N3	-18.43	120.08	129.30
32	W	1435	A	N1-C2-N3	-18.43	120.08	129.30
1	A	2794	A	N1-C2-N3	-18.43	120.08	129.30
1	A	173	A	N1-C2-N3	-18.43	120.08	129.30
52	z	58	A	N1-C2-N3	-18.43	120.08	129.30
1	A	1025	A	N1-C2-N3	-18.43	120.09	129.30
1	A	1286	A	N1-C2-N3	-18.43	120.08	129.30
1	A	428	A	N1-C2-N3	-18.43	120.09	129.30
1	A	1999	A	N1-C2-N3	-18.43	120.09	129.30
1	A	987	A	N1-C2-N3	-18.43	120.09	129.30
1	A	1989	A	N1-C2-N3	-18.43	120.09	129.30
32	W	1486	A	N1-C2-N3	-18.42	120.09	129.30
1	A	496	A	N1-C2-N3	-18.42	120.09	129.30
1	A	1426	A	N1-C2-N3	-18.42	120.09	129.30
1	A	1965	A	N1-C2-N3	-18.42	120.09	129.30
1	A	2297	A	N1-C2-N3	-18.42	120.09	129.30
1	A	2387	A	N1-C2-N3	-18.42	120.09	129.30
1	A	329	A	N1-C2-N3	-18.42	120.09	129.30
1	A	2330	A	C2-N3-C4	18.42	119.81	110.60
1	A	456	A	N1-C2-N3	-18.42	120.09	129.30
32	W	677	A	N1-C2-N3	-18.42	120.09	129.30
1	A	896	A	N1-C2-N3	-18.42	120.09	129.30
1	A	265	A	N1-C2-N3	-18.41	120.09	129.30
1	A	1094	A	C2-N3-C4	18.41	119.81	110.60
1	A	1695	A	N1-C2-N3	-18.41	120.09	129.30
32	W	57	A	N1-C2-N3	-18.41	120.09	129.30
32	W	831	A	N1-C2-N3	-18.41	120.09	129.30
32	W	290	A	N1-C2-N3	-18.41	120.09	129.30
32	W	1333	A	N1-C2-N3	-18.41	120.09	129.30
1	A	247	A	N1-C2-N3	-18.41	120.09	129.30
1	A	964	A	N1-C2-N3	-18.41	120.10	129.30
1	A	2006	A	N1-C2-N3	-18.41	120.10	129.30
1	A	2447	A	N1-C2-N3	-18.41	120.09	129.30
1	A	2846	A	N1-C2-N3	-18.41	120.10	129.30
32	W	234	A	N1-C2-N3	-18.41	120.10	129.30
32	W	918	A	N1-C2-N3	-18.41	120.09	129.30
1	A	1312	A	N1-C2-N3	-18.41	120.10	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2343	A	N1-C2-N3	-18.41	120.10	129.30
1	A	2477	A	N1-C2-N3	-18.41	120.10	129.30
2	B	37	A	N1-C2-N3	-18.41	120.10	129.30
1	A	1667	A	N1-C2-N3	-18.40	120.10	129.30
1	A	889	A	N1-C2-N3	-18.40	120.10	129.30
1	A	1357	A	N1-C2-N3	-18.40	120.10	129.30
32	W	1283	A	N1-C2-N3	-18.40	120.10	129.30
32	W	979	A	N1-C2-N3	-18.40	120.10	129.30
1	A	67	A	N1-C2-N3	-18.40	120.10	129.30
1	A	1096	A	N1-C2-N3	-18.40	120.10	129.30
1	A	2387	A	C2-N3-C4	18.40	119.80	110.60
1	A	2459	A	N1-C2-N3	-18.40	120.10	129.30
1	A	140	A	N1-C2-N3	-18.40	120.10	129.30
32	W	828	A	N1-C2-N3	-18.40	120.10	129.30
1	A	2395	A	N1-C2-N3	-18.39	120.10	129.30
32	W	72	A	N1-C2-N3	-18.39	120.10	129.30
1	A	90	A	C2-N3-C4	18.39	119.80	110.60
1	A	623	A	N1-C2-N3	-18.39	120.10	129.30
1	A	690	A	N1-C2-N3	-18.39	120.10	129.30
1	A	1393	A	N1-C2-N3	-18.39	120.10	129.30
32	W	270	A	N1-C2-N3	-18.39	120.10	129.30
32	W	1245	A	N1-C2-N3	-18.39	120.10	129.30
1	A	179	A	N1-C2-N3	-18.39	120.11	129.30
1	A	740	A	N1-C2-N3	-18.39	120.11	129.30
1	A	1284	A	N1-C2-N3	-18.39	120.10	129.30
1	A	125	A	N1-C2-N3	-18.39	120.11	129.30
1	A	1445	A	N1-C2-N3	-18.39	120.11	129.30
32	W	522	A	N1-C2-N3	-18.39	120.11	129.30
32	W	1197	A	N1-C2-N3	-18.39	120.11	129.30
32	W	1384	A	C2-N3-C4	18.39	119.79	110.60
1	A	790	A	N1-C2-N3	-18.39	120.11	129.30
1	A	2804	A	N1-C2-N3	-18.39	120.11	129.30
1	A	2827	A	N1-C2-N3	-18.39	120.11	129.30
1	A	2887	A	N1-C2-N3	-18.39	120.11	129.30
32	W	81	A	N1-C2-N3	-18.39	120.11	129.30
32	W	883	A	C2-N3-C4	18.39	119.79	110.60
1	A	870	A	N1-C2-N3	-18.38	120.11	129.30
1	A	1222	A	N1-C2-N3	-18.38	120.11	129.30
1	A	1381	A	N1-C2-N3	-18.38	120.11	129.30
1	A	2689	A	N1-C2-N3	-18.38	120.11	129.30
1	A	343	A	N1-C2-N3	-18.38	120.11	129.30
32	W	1427	A	N1-C2-N3	-18.38	120.11	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1615	A	N1-C2-N3	-18.38	120.11	129.30
1	A	2700	A	N1-C2-N3	-18.38	120.11	129.30
1	A	2722	A	N1-C2-N3	-18.38	120.11	129.30
1	A	1126	A	N1-C2-N3	-18.38	120.11	129.30
1	A	1627	A	N1-C2-N3	-18.38	120.11	129.30
1	A	2043	A	N1-C2-N3	-18.38	120.11	129.30
32	W	1517	A	N1-C2-N3	-18.38	120.11	129.30
32	W	34	A	N1-C2-N3	-18.38	120.11	129.30
1	A	1233	A	N1-C2-N3	-18.37	120.11	129.30
1	A	1956	A	N1-C2-N3	-18.37	120.11	129.30
32	W	882	A	N1-C2-N3	-18.37	120.11	129.30
32	W	1297	A	N1-C2-N3	-18.37	120.11	129.30
1	A	1734	A	N1-C2-N3	-18.37	120.11	129.30
1	A	2302	A	N1-C2-N3	-18.37	120.11	129.30
32	W	644	A	N1-C2-N3	-18.37	120.11	129.30
1	A	1477	A	N1-C2-N3	-18.37	120.11	129.30
32	W	209	A	C2-N3-C4	18.37	119.78	110.60
1	A	673	A	N1-C2-N3	-18.37	120.12	129.30
32	W	1407	A	C2-N3-C4	18.37	119.78	110.60
32	W	329	A	N1-C2-N3	-18.36	120.12	129.30
1	A	724	A	N1-C2-N3	-18.36	120.12	129.30
1	A	1888	A	N1-C2-N3	-18.36	120.12	129.30
32	W	672	A	N1-C2-N3	-18.36	120.12	129.30
1	A	1727	A	N1-C2-N3	-18.36	120.12	129.30
1	A	2066	A	N1-C2-N3	-18.36	120.12	129.30
1	A	538	A	N1-C2-N3	-18.36	120.12	129.30
32	W	1016	A	N1-C2-N3	-18.36	120.12	129.30
1	A	2383	A	N1-C2-N3	-18.36	120.12	129.30
1	A	390	A	N1-C2-N3	-18.36	120.12	129.30
1	A	1614	A	N1-C2-N3	-18.35	120.12	129.30
1	A	2616	A	N1-C2-N3	-18.35	120.12	129.30
32	W	301	A	N1-C2-N3	-18.35	120.12	129.30
32	W	844	A	N1-C2-N3	-18.35	120.12	129.30
1	A	130	A	N1-C2-N3	-18.35	120.12	129.30
1	A	1253	A	N1-C2-N3	-18.35	120.12	129.30
1	A	2383	A	C2-N3-C4	18.35	119.78	110.60
1	A	278	A	N1-C2-N3	-18.35	120.13	129.30
1	A	722	A	N1-C2-N3	-18.35	120.13	129.30
1	A	1442	A	N1-C2-N3	-18.35	120.13	129.30
1	A	2468	A	N1-C2-N3	-18.35	120.13	129.30
1	A	956	A	N1-C2-N3	-18.35	120.13	129.30
32	W	1490	A	N1-C2-N3	-18.34	120.13	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	A	N1-C2-N3	-18.34	120.13	129.30
1	A	770	A	N1-C2-N3	-18.34	120.13	129.30
32	W	475	A	N1-C2-N3	-18.34	120.13	129.30
32	W	1022	A	N1-C2-N3	-18.34	120.13	129.30
1	A	2790	A	N1-C2-N3	-18.34	120.13	129.30
32	W	1349	A	N1-C2-N3	-18.34	120.13	129.30
1	A	1619	A	N1-C2-N3	-18.34	120.13	129.30
32	W	512	A	N1-C2-N3	-18.34	120.13	129.30
1	A	220	A	N1-C2-N3	-18.33	120.13	129.30
1	A	2106	A	N1-C2-N3	-18.33	120.13	129.30
32	W	911	A	N1-C2-N3	-18.33	120.13	129.30
32	W	518	A	N1-C2-N3	-18.33	120.14	129.30
1	A	518	A	N1-C2-N3	-18.33	120.14	129.30
1	A	1745	A	N1-C2-N3	-18.33	120.14	129.30
32	W	996	A	N1-C2-N3	-18.33	120.14	129.30
32	W	1478	A	N1-C2-N3	-18.33	120.14	129.30
32	W	74	A	N1-C2-N3	-18.33	120.14	129.30
32	W	1272	A	N1-C2-N3	-18.33	120.14	129.30
1	A	1961	A	N1-C2-N3	-18.33	120.14	129.30
1	A	2026	A	N1-C2-N3	-18.32	120.14	129.30
1	A	2497	A	N1-C2-N3	-18.32	120.14	129.30
32	W	875	A	N1-C2-N3	-18.32	120.14	129.30
32	W	913	A	N1-C2-N3	-18.32	120.14	129.30
1	A	279	A	N1-C2-N3	-18.32	120.14	129.30
1	A	2854	A	N1-C2-N3	-18.32	120.14	129.30
32	W	397	A	N1-C2-N3	-18.32	120.14	129.30
32	W	1443	A	N1-C2-N3	-18.31	120.14	129.30
1	A	13	A	N1-C2-N3	-18.31	120.14	129.30
1	A	2296	A	N1-C2-N3	-18.31	120.15	129.30
1	A	44	A	N1-C2-N3	-18.31	120.15	129.30
1	A	2812	A	N1-C2-N3	-18.31	120.15	129.30
1	A	667	A	C2-N3-C4	18.31	119.75	110.60
32	W	721	A	N1-C2-N3	-18.31	120.15	129.30
32	W	1278	A	C2-N3-C4	18.31	119.75	110.60
1	A	1197	A	N1-C2-N3	-18.30	120.15	129.30
1	A	2340	A	N1-C2-N3	-18.30	120.15	129.30
32	W	1384	A	N1-C2-N3	-18.30	120.15	129.30
1	A	1885	A	N1-C2-N3	-18.30	120.15	129.30
1	A	1957	A	C2-N3-C4	18.30	119.75	110.60
32	W	364	A	N1-C2-N3	-18.30	120.15	129.30
32	W	1348	A	N1-C2-N3	-18.30	120.15	129.30
1	A	634	A	N1-C2-N3	-18.30	120.15	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1021	A	N1-C2-N3	-18.30	120.15	129.30
1	A	1485	A	N1-C2-N3	-18.30	120.15	129.30
1	A	1832	A	N1-C2-N3	-18.30	120.15	129.30
1	A	1947	A	N1-C2-N3	-18.30	120.15	129.30
1	A	2505	A	N1-C2-N3	-18.30	120.15	129.30
32	W	1320	A	N1-C2-N3	-18.30	120.15	129.30
1	A	656	A	N1-C2-N3	-18.29	120.15	129.30
1	A	559	A	N1-C2-N3	-18.29	120.15	129.30
1	A	1003	A	N1-C2-N3	-18.29	120.15	129.30
1	A	2924	A	N1-C2-N3	-18.29	120.15	129.30
1	A	258	A	N1-C2-N3	-18.29	120.16	129.30
1	A	2517	A	N1-C2-N3	-18.29	120.16	129.30
32	W	928	A	N1-C2-N3	-18.29	120.16	129.30
1	A	1075	A	N1-C2-N3	-18.29	120.16	129.30
1	A	2052	A	N1-C2-N3	-18.29	120.16	129.30
1	A	2351	A	N1-C2-N3	-18.29	120.16	129.30
32	W	743	A	N1-C2-N3	-18.29	120.16	129.30
1	A	391	A	N1-C2-N3	-18.29	120.16	129.30
1	A	2590	A	N1-C2-N3	-18.29	120.16	129.30
1	A	1194	A	N1-C2-N3	-18.28	120.16	129.30
1	A	769	A	N1-C2-N3	-18.28	120.16	129.30
1	A	2500	A	N1-C2-N3	-18.28	120.16	129.30
32	W	1366	A	N1-C2-N3	-18.28	120.16	129.30
32	W	405	A	N1-C2-N3	-18.28	120.16	129.30
1	A	2629	A	N1-C2-N3	-18.28	120.16	129.30
32	W	346	A	N1-C2-N3	-18.28	120.16	129.30
1	A	2919	A	N1-C2-N3	-18.28	120.16	129.30
32	W	55	A	N1-C2-N3	-18.28	120.16	129.30
1	A	513	A	C2-N3-C4	18.27	119.74	110.60
1	A	1103	A	N1-C2-N3	-18.27	120.16	129.30
1	A	1982	A	C2-N3-C4	18.27	119.74	110.60
1	A	1265	A	N1-C2-N3	-18.26	120.17	129.30
1	A	1258	A	N1-C2-N3	-18.26	120.17	129.30
32	W	649	A	N1-C2-N3	-18.26	120.17	129.30
32	W	790	A	N1-C2-N3	-18.26	120.17	129.30
32	W	1405	A	N1-C2-N3	-18.26	120.17	129.30
32	W	771	A	N1-C2-N3	-18.26	120.17	129.30
1	A	661	A	N1-C2-N3	-18.25	120.17	129.30
1	A	578	A	N1-C2-N3	-18.25	120.17	129.30
1	A	1957	A	N1-C2-N3	-18.25	120.17	129.30
1	A	2100	A	N1-C2-N3	-18.25	120.17	129.30
1	A	913	A	N1-C2-N3	-18.25	120.18	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	630	A	N1-C2-N3	-18.25	120.18	129.30
32	W	945	A	N1-C2-N3	-18.25	120.18	129.30
32	W	433	A	N1-C2-N3	-18.24	120.18	129.30
1	A	486	A	N1-C2-N3	-18.24	120.18	129.30
1	A	2619	A	N1-C2-N3	-18.24	120.18	129.30
1	A	1900	A	N1-C2-N3	-18.24	120.18	129.30
32	W	711	A	N1-C2-N3	-18.24	120.18	129.30
32	W	1315	A	N1-C2-N3	-18.24	120.18	129.30
32	W	1256	A	N1-C2-N3	-18.24	120.18	129.30
1	A	469	A	N1-C2-N3	-18.23	120.18	129.30
1	A	752	A	N1-C2-N3	-18.23	120.18	129.30
1	A	1235	A	N1-C2-N3	-18.23	120.18	129.30
32	W	725	A	N1-C2-N3	-18.23	120.18	129.30
2	B	46	A	N1-C2-N3	-18.23	120.18	129.30
1	A	1710	A	N1-C2-N3	-18.23	120.19	129.30
32	W	404	A	N1-C2-N3	-18.23	120.19	129.30
1	A	1003	A	C2-N3-C4	18.23	119.71	110.60
32	W	838	A	N1-C2-N3	-18.23	120.19	129.30
1	A	1816	A	N1-C2-N3	-18.23	120.19	129.30
1	A	2440	A	N1-C2-N3	-18.22	120.19	129.30
1	A	1776	A	N1-C2-N3	-18.22	120.19	129.30
32	W	758	A	N1-C2-N3	-18.22	120.19	129.30
1	A	2329	A	N1-C2-N3	-18.22	120.19	129.30
1	A	1831	A	N1-C2-N3	-18.21	120.19	129.30
32	W	337	A	N1-C2-N3	-18.21	120.20	129.30
1	A	1858	A	N1-C2-N3	-18.20	120.20	129.30
1	A	1925	A	N1-C2-N3	-18.20	120.20	129.30
1	A	2044	A	N1-C2-N3	-18.20	120.20	129.30
52	z	24	A	N1-C2-N3	-18.20	120.20	129.30
1	A	1724	A	N1-C2-N3	-18.20	120.20	129.30
32	W	282	A	N1-C2-N3	-18.20	120.20	129.30
1	A	910	A	N1-C2-N3	-18.19	120.20	129.30
1	A	1067	A	C2-N3-C4	18.19	119.70	110.60
1	A	970	A	N1-C2-N3	-18.19	120.20	129.30
1	A	1067	A	N1-C2-N3	-18.19	120.21	129.30
1	A	2330	A	N1-C2-N3	-18.19	120.21	129.30
1	A	2691	A	N1-C2-N3	-18.19	120.21	129.30
1	A	168	A	N1-C2-N3	-18.18	120.21	129.30
1	A	1524	A	N1-C2-N3	-18.18	120.21	129.30
1	A	2270	A	N1-C2-N3	-18.18	120.21	129.30
32	W	1112	A	N1-C2-N3	-18.18	120.21	129.30
1	A	1490	A	N1-C2-N3	-18.18	120.21	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	605	A	N1-C2-N3	-18.18	120.21	129.30
32	W	1238	A	N1-C2-N3	-18.18	120.21	129.30
32	W	883	A	N1-C2-N3	-18.17	120.21	129.30
1	A	56	A	N1-C2-N3	-18.17	120.21	129.30
1	A	2436	A	N1-C2-N3	-18.17	120.22	129.30
32	W	715	A	N1-C2-N3	-18.16	120.22	129.30
1	A	2402	A	N1-C2-N3	-18.16	120.22	129.30
32	W	1369	A	N1-C2-N3	-18.16	120.22	129.30
1	A	95	A	N1-C2-N3	-18.15	120.22	129.30
32	W	1160	A	N1-C2-N3	-18.15	120.23	129.30
1	A	1562	A	N1-C2-N3	-18.14	120.23	129.30
52	z	9	A	N1-C2-N3	-18.14	120.23	129.30
1	A	678	A	N1-C2-N3	-18.12	120.24	129.30
1	A	1778	A	N1-C2-N3	-18.12	120.24	129.30
1	A	501	A	C2-N3-C4	18.12	119.66	110.60
1	A	2862	A	N1-C2-N3	-18.12	120.24	129.30
1	A	38	A	N1-C2-N3	-18.11	120.25	129.30
1	A	736	A	N1-C2-N3	-18.11	120.25	129.30
1	A	1883	A	N1-C2-N3	-18.10	120.25	129.30
32	W	308	A	N1-C2-N3	-18.10	120.25	129.30
1	A	90	A	N1-C2-N3	-18.09	120.25	129.30
1	A	52	A	N1-C2-N3	-18.09	120.26	129.30
1	A	679	A	N1-C2-N3	-18.08	120.26	129.30
1	A	1316	A	N1-C2-N3	-18.08	120.26	129.30
32	W	948	A	N1-C2-N3	-18.08	120.26	129.30
1	A	1638	A	N1-C2-N3	-18.07	120.26	129.30
1	A	866	A	N1-C2-N3	-18.07	120.26	129.30
1	A	407	A	N1-C2-N3	-18.07	120.27	129.30
1	A	2358	A	N1-C2-N3	-18.07	120.27	129.30
1	A	1714	A	N1-C2-N3	-18.06	120.27	129.30
1	A	974	A	N1-C2-N3	-18.06	120.27	129.30
1	A	715	A	N1-C2-N3	-18.05	120.27	129.30
1	A	108	A	N1-C2-N3	-18.05	120.28	129.30
1	A	185	A	N1-C2-N3	-18.05	120.28	129.30
1	A	2027	A	N1-C2-N3	-18.04	120.28	129.30
32	W	391	A	N1-C2-N3	-18.04	120.28	129.30
32	W	1278	A	N1-C2-N3	-18.04	120.28	129.30
1	A	178	A	N1-C2-N3	-18.04	120.28	129.30
1	A	2885	A	N1-C2-N3	-18.03	120.28	129.30
1	A	551	A	N1-C2-N3	-18.01	120.30	129.30
1	A	1653	A	N1-C2-N3	-18.01	120.30	129.30
1	A	1839	A	N1-C2-N3	-18.00	120.30	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2735	A	N1-C2-N3	-17.99	120.30	129.30
1	A	1006	A	N1-C2-N3	-17.98	120.31	129.30
32	W	507	A	N1-C2-N3	-17.98	120.31	129.30
32	W	933	A	N1-C2-N3	-17.97	120.32	129.30
1	A	1398	A	N1-C2-N3	-17.96	120.32	129.30
1	A	2407	A	N1-C2-N3	-17.95	120.32	129.30
1	A	1618	A	N1-C2-N3	-17.94	120.33	129.30
32	W	1166	A	N1-C2-N3	-17.91	120.34	129.30
32	W	959	A	N1-C2-N3	-17.90	120.35	129.30
1	A	1094	A	N1-C2-N3	-17.90	120.35	129.30
1	A	2627	A	N1-C2-N3	-17.88	120.36	129.30
1	A	2844	A	N1-C2-N3	-17.88	120.36	129.30
1	A	1190	A	N1-C2-N3	-17.85	120.37	129.30
32	W	1026	A	N1-C2-N3	-17.85	120.37	129.30
1	A	667	A	N1-C2-N3	-17.84	120.38	129.30
1	A	935	A	N1-C2-N3	-17.79	120.40	129.30
1	A	527	A	N1-C2-N3	-17.70	120.45	129.30
1	A	513	A	N1-C2-N3	-17.62	120.49	129.30
32	W	99	A	N1-C2-N3	-17.57	120.51	129.30
1	A	254	A	N1-C2-N3	-17.13	120.73	129.30
2	B	99	A	N1-C2-N3	-17.01	120.79	129.30
1	A	589	G	C4'-C3'-O3'	13.89	140.78	113.00
23	X	69	LYS	C-N-CA	12.96	154.11	121.70
1	A	83	G	C4'-C3'-O3'	-12.66	82.81	109.40
1	A	501	A	N7-C8-N9	-12.17	107.72	113.80
1	A	2807	A	N7-C8-N9	-12.04	107.78	113.80
1	A	2805	A	N7-C8-N9	-12.04	107.78	113.80
1	A	2089	A	N7-C8-N9	-12.03	107.79	113.80
1	A	722	A	N7-C8-N9	-12.00	107.80	113.80
32	W	703	A	N7-C8-N9	-11.97	107.81	113.80
1	A	2750	A	N7-C8-N9	-11.95	107.83	113.80
1	A	1784	A	N7-C8-N9	-11.95	107.83	113.80
32	W	1065	A	N7-C8-N9	-11.95	107.83	113.80
1	A	374	A	N7-C8-N9	-11.92	107.84	113.80
1	A	526	A	N7-C8-N9	-11.92	107.84	113.80
1	A	1084	A	N7-C8-N9	-11.92	107.84	113.80
1	A	2770	A	N7-C8-N9	-11.91	107.84	113.80
1	A	1202	A	N7-C8-N9	-11.90	107.85	113.80
1	A	2683	A	N7-C8-N9	-11.89	107.85	113.80
1	A	774	A	N7-C8-N9	-11.89	107.86	113.80
1	A	2923	A	N7-C8-N9	-11.89	107.85	113.80
1	A	584	A	N7-C8-N9	-11.89	107.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	886	A	N7-C8-N9	-11.88	107.86	113.80
1	A	821	A	N7-C8-N9	-11.87	107.86	113.80
32	W	159	A	N7-C8-N9	-11.87	107.86	113.80
1	A	2417	A	N7-C8-N9	-11.87	107.87	113.80
1	A	1134	A	N3-C4-C5	-11.86	118.50	126.80
32	W	266	A	N7-C8-N9	-11.86	107.87	113.80
1	A	2777	A	N7-C8-N9	-11.86	107.87	113.80
1	A	1224	A	N7-C8-N9	-11.86	107.87	113.80
1	A	2819	A	N7-C8-N9	-11.85	107.88	113.80
1	A	538	A	N7-C8-N9	-11.85	107.88	113.80
1	A	1895	A	N7-C8-N9	-11.84	107.88	113.80
1	A	281	A	N7-C8-N9	-11.84	107.88	113.80
32	W	790	A	N7-C8-N9	-11.84	107.88	113.80
32	W	1355	A	N7-C8-N9	-11.83	107.88	113.80
1	A	1982	A	N7-C8-N9	-11.83	107.88	113.80
1	A	1308	A	N7-C8-N9	-11.83	107.88	113.80
1	A	2364	A	N7-C8-N9	-11.83	107.89	113.80
32	W	452	A	N7-C8-N9	-11.83	107.89	113.80
1	A	207	A	N7-C8-N9	-11.83	107.89	113.80
1	A	71	A	N7-C8-N9	-11.82	107.89	113.80
1	A	2049	A	N7-C8-N9	-11.82	107.89	113.80
1	A	702	A	N7-C8-N9	-11.82	107.89	113.80
32	W	254	A	N7-C8-N9	-11.82	107.89	113.80
1	A	2390	A	N7-C8-N9	-11.82	107.89	113.80
2	B	17	A	N7-C8-N9	-11.81	107.89	113.80
32	W	228	A	N7-C8-N9	-11.81	107.89	113.80
1	A	166	A	N7-C8-N9	-11.81	107.90	113.80
32	W	768	A	N7-C8-N9	-11.81	107.90	113.80
32	W	419	A	N7-C8-N9	-11.80	107.90	113.80
1	A	2876	A	N7-C8-N9	-11.80	107.90	113.80
32	W	650	A	N7-C8-N9	-11.80	107.90	113.80
1	A	2026	A	N7-C8-N9	-11.79	107.90	113.80
1	A	126	A	N7-C8-N9	-11.79	107.90	113.80
1	A	388	A	N7-C8-N9	-11.79	107.91	113.80
1	A	2893	A	N7-C8-N9	-11.79	107.91	113.80
32	W	988	A	N7-C8-N9	-11.78	107.91	113.80
1	A	470	A	N7-C8-N9	-11.78	107.91	113.80
32	W	611	A	N7-C8-N9	-11.78	107.91	113.80
1	A	1555	A	N7-C8-N9	-11.78	107.91	113.80
1	A	1553	A	N7-C8-N9	-11.78	107.91	113.80
1	A	2594	A	N7-C8-N9	-11.78	107.91	113.80
1	A	1189	A	N7-C8-N9	-11.77	107.91	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	824	A	N7-C8-N9	-11.77	107.91	113.80
1	A	1524	A	N7-C8-N9	-11.77	107.92	113.80
1	A	2670	A	N7-C8-N9	-11.77	107.92	113.80
1	A	219	A	N7-C8-N9	-11.77	107.92	113.80
1	A	991	A	N7-C8-N9	-11.77	107.92	113.80
1	A	1809	A	N7-C8-N9	-11.77	107.92	113.80
32	W	1225	A	N7-C8-N9	-11.77	107.92	113.80
1	A	1700	A	N7-C8-N9	-11.76	107.92	113.80
32	W	959	A	N7-C8-N9	-11.76	107.92	113.80
1	A	436	A	N7-C8-N9	-11.76	107.92	113.80
1	A	582	A	N7-C8-N9	-11.76	107.92	113.80
32	W	456	A	N7-C8-N9	-11.76	107.92	113.80
1	A	2315	A	N7-C8-N9	-11.76	107.92	113.80
1	A	1326	A	N7-C8-N9	-11.75	107.92	113.80
32	W	206	A	N7-C8-N9	-11.75	107.92	113.80
1	A	504	A	N7-C8-N9	-11.75	107.93	113.80
1	A	1157	A	N7-C8-N9	-11.75	107.93	113.80
1	A	1461	A	N7-C8-N9	-11.75	107.93	113.80
32	W	862	A	N7-C8-N9	-11.75	107.93	113.80
1	A	553	A	N7-C8-N9	-11.74	107.93	113.80
1	A	575	A	N7-C8-N9	-11.74	107.93	113.80
1	A	1585	A	N7-C8-N9	-11.74	107.93	113.80
32	W	899	A	N7-C8-N9	-11.74	107.93	113.80
1	A	1339	A	N7-C8-N9	-11.73	107.93	113.80
1	A	1532	A	N7-C8-N9	-11.73	107.93	113.80
32	W	1503	A	N7-C8-N9	-11.73	107.93	113.80
1	A	2052	A	N7-C8-N9	-11.73	107.94	113.80
1	A	525	A	N7-C8-N9	-11.73	107.94	113.80
1	A	1417	A	N7-C8-N9	-11.73	107.94	113.80
32	W	364	A	N7-C8-N9	-11.73	107.94	113.80
32	W	1056	A	N7-C8-N9	-11.73	107.94	113.80
32	W	1257	A	N7-C8-N9	-11.73	107.94	113.80
1	A	1066	A	N7-C8-N9	-11.72	107.94	113.80
1	A	1269	A	N7-C8-N9	-11.72	107.94	113.80
1	A	1314	A	N7-C8-N9	-11.72	107.94	113.80
1	A	2601	A	N7-C8-N9	-11.72	107.94	113.80
32	W	1443	A	N7-C8-N9	-11.72	107.94	113.80
32	W	786	A	N7-C8-N9	-11.72	107.94	113.80
32	W	1434	A	N7-C8-N9	-11.72	107.94	113.80
1	A	84	A	N7-C8-N9	-11.71	107.94	113.80
1	A	1473	A	N7-C8-N9	-11.71	107.94	113.80
32	W	1422	A	N7-C8-N9	-11.71	107.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2500	A	N7-C8-N9	-11.71	107.94	113.80
32	W	737	A	N7-C8-N9	-11.71	107.94	113.80
32	W	1456	A	N7-C8-N9	-11.71	107.94	113.80
1	A	1175	A	N7-C8-N9	-11.71	107.95	113.80
1	A	2447	A	N7-C8-N9	-11.71	107.95	113.80
1	A	244	A	N7-C8-N9	-11.71	107.95	113.80
1	A	835	A	N7-C8-N9	-11.71	107.95	113.80
1	A	2812	A	N7-C8-N9	-11.70	107.95	113.80
32	W	148	A	N7-C8-N9	-11.70	107.95	113.80
1	A	1788	A	N7-C8-N9	-11.70	107.95	113.80
1	A	1094	A	N7-C8-N9	-11.70	107.95	113.80
1	A	1813	A	N7-C8-N9	-11.70	107.95	113.80
1	A	2059	A	N7-C8-N9	-11.70	107.95	113.80
1	A	2362	A	N7-C8-N9	-11.70	107.95	113.80
1	A	1061	A	N7-C8-N9	-11.70	107.95	113.80
32	W	10	A	N7-C8-N9	-11.70	107.95	113.80
32	W	811	A	N7-C8-N9	-11.70	107.95	113.80
32	W	923	A	N7-C8-N9	-11.70	107.95	113.80
32	W	1348	A	N7-C8-N9	-11.70	107.95	113.80
1	A	647	A	N7-C8-N9	-11.69	107.95	113.80
32	W	1006	A	N7-C8-N9	-11.69	107.95	113.80
1	A	314	A	N7-C8-N9	-11.69	107.96	113.80
1	A	324	A	N7-C8-N9	-11.69	107.96	113.80
1	A	646	A	N7-C8-N9	-11.69	107.96	113.80
1	A	1483	A	N7-C8-N9	-11.69	107.96	113.80
32	W	18	A	N7-C8-N9	-11.69	107.96	113.80
1	A	717	A	N7-C8-N9	-11.68	107.96	113.80
1	A	999	A	N7-C8-N9	-11.68	107.96	113.80
1	A	2912	A	N7-C8-N9	-11.68	107.96	113.80
1	A	183	A	N7-C8-N9	-11.68	107.96	113.80
1	A	1126	A	N7-C8-N9	-11.68	107.96	113.80
1	A	1672	A	N7-C8-N9	-11.68	107.96	113.80
1	A	2477	A	N7-C8-N9	-11.68	107.96	113.80
1	A	2618	A	N7-C8-N9	-11.68	107.96	113.80
32	W	357	A	N7-C8-N9	-11.68	107.96	113.80
32	W	672	A	N7-C8-N9	-11.68	107.96	113.80
32	W	690	A	N7-C8-N9	-11.68	107.96	113.80
32	W	803	A	N7-C8-N9	-11.68	107.96	113.80
32	W	1210	A	N7-C8-N9	-11.68	107.96	113.80
1	A	2673	A	N7-C8-N9	-11.67	107.96	113.80
32	W	508	A	N7-C8-N9	-11.67	107.96	113.80
32	W	762	A	N7-C8-N9	-11.67	107.96	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	838	A	N7-C8-N9	-11.67	107.96	113.80
32	W	1103	A	N7-C8-N9	-11.67	107.96	113.80
1	A	154	A	N7-C8-N9	-11.67	107.97	113.80
1	A	364	A	N7-C8-N9	-11.67	107.97	113.80
1	A	1284	A	N7-C8-N9	-11.67	107.97	113.80
1	A	150	A	N7-C8-N9	-11.67	107.97	113.80
1	A	389	A	N7-C8-N9	-11.67	107.97	113.80
1	A	572	A	N7-C8-N9	-11.67	107.97	113.80
32	W	189	A	N7-C8-N9	-11.67	107.97	113.80
32	W	651	A	N7-C8-N9	-11.67	107.97	113.80
32	W	975	A	N7-C8-N9	-11.67	107.97	113.80
1	A	345	A	N7-C8-N9	-11.66	107.97	113.80
1	A	1055	A	N7-C8-N9	-11.66	107.97	113.80
1	A	1998	A	N7-C8-N9	-11.66	107.97	113.80
32	W	382	A	N7-C8-N9	-11.66	107.97	113.80
32	W	658	A	N7-C8-N9	-11.66	107.97	113.80
1	A	449	A	N7-C8-N9	-11.66	107.97	113.80
1	A	1179	A	N7-C8-N9	-11.66	107.97	113.80
1	A	1305	A	N7-C8-N9	-11.66	107.97	113.80
1	A	2860	A	N7-C8-N9	-11.66	107.97	113.80
1	A	490	A	N7-C8-N9	-11.66	107.97	113.80
32	W	1090	A	N7-C8-N9	-11.66	107.97	113.80
32	W	1092	A	N7-C8-N9	-11.66	107.97	113.80
1	A	978	A	N7-C8-N9	-11.66	107.97	113.80
1	A	1312	A	N7-C8-N9	-11.66	107.97	113.80
32	W	62	A	N7-C8-N9	-11.66	107.97	113.80
32	W	1048	A	N7-C8-N9	-11.66	107.97	113.80
32	W	1248	A	N7-C8-N9	-11.66	107.97	113.80
1	A	229	A	N7-C8-N9	-11.65	107.97	113.80
1	A	475	A	N7-C8-N9	-11.65	107.97	113.80
1	A	1161	A	N7-C8-N9	-11.65	107.97	113.80
1	A	1504	A	N7-C8-N9	-11.65	107.97	113.80
1	A	2047	A	N7-C8-N9	-11.65	107.97	113.80
1	A	6	A	N7-C8-N9	-11.65	107.97	113.80
1	A	637	A	N7-C8-N9	-11.65	107.97	113.80
1	A	2317	A	N7-C8-N9	-11.65	107.97	113.80
2	B	25	A	N7-C8-N9	-11.65	107.97	113.80
32	W	532	A	N7-C8-N9	-11.65	107.97	113.80
32	W	568	A	N7-C8-N9	-11.65	107.97	113.80
32	W	1298	A	N7-C8-N9	-11.65	107.97	113.80
1	A	847	A	N7-C8-N9	-11.65	107.97	113.80
1	A	2083	A	N7-C8-N9	-11.65	107.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2694	A	N7-C8-N9	-11.65	107.98	113.80
32	W	463	A	N7-C8-N9	-11.65	107.98	113.80
32	W	1383	A	N7-C8-N9	-11.65	107.98	113.80
1	A	888	A	N7-C8-N9	-11.64	107.98	113.80
1	A	1047	A	N7-C8-N9	-11.64	107.98	113.80
1	A	2668	A	N7-C8-N9	-11.64	107.98	113.80
1	A	2846	A	N7-C8-N9	-11.64	107.98	113.80
32	W	139	A	N7-C8-N9	-11.64	107.98	113.80
32	W	251	A	N7-C8-N9	-11.64	107.98	113.80
32	W	569	A	N7-C8-N9	-11.64	107.98	113.80
1	A	2302	A	N7-C8-N9	-11.64	107.98	113.80
32	W	1050	A	N7-C8-N9	-11.64	107.98	113.80
1	A	428	A	N7-C8-N9	-11.64	107.98	113.80
1	A	2837	A	N7-C8-N9	-11.64	107.98	113.80
32	W	924	A	N7-C8-N9	-11.64	107.98	113.80
1	A	1406	A	N7-C8-N9	-11.64	107.98	113.80
1	A	1654	A	N7-C8-N9	-11.64	107.98	113.80
32	W	1160	A	N7-C8-N9	-11.64	107.98	113.80
32	W	1222	A	N7-C8-N9	-11.64	107.98	113.80
32	W	1466	A	N7-C8-N9	-11.64	107.98	113.80
32	W	925	A	N7-C8-N9	-11.64	107.98	113.80
32	W	496	A	N7-C8-N9	-11.63	107.98	113.80
32	W	985	A	N7-C8-N9	-11.63	107.98	113.80
1	A	1735	A	N7-C8-N9	-11.63	107.98	113.80
32	W	777	A	N7-C8-N9	-11.63	107.98	113.80
1	A	193	A	N7-C8-N9	-11.63	107.98	113.80
1	A	1008	A	N7-C8-N9	-11.63	107.98	113.80
1	A	1072	A	N7-C8-N9	-11.63	107.98	113.80
1	A	1914	A	N7-C8-N9	-11.63	107.98	113.80
1	A	2298	A	N7-C8-N9	-11.63	107.98	113.80
1	A	2507	A	N7-C8-N9	-11.63	107.98	113.80
1	A	2908	A	N7-C8-N9	-11.63	107.98	113.80
32	W	190	A	N7-C8-N9	-11.63	107.98	113.80
32	W	730	A	N7-C8-N9	-11.63	107.98	113.80
1	A	1961	A	N7-C8-N9	-11.63	107.98	113.80
1	A	2062	A	N7-C8-N9	-11.63	107.98	113.80
1	A	2700	A	N7-C8-N9	-11.63	107.99	113.80
1	A	1003	A	N7-C8-N9	-11.63	107.99	113.80
1	A	421	A	N7-C8-N9	-11.62	107.99	113.80
52	z	21	A	N7-C8-N9	-11.63	107.99	113.80
1	A	1233	A	N7-C8-N9	-11.62	107.99	113.80
1	A	1925	A	N7-C8-N9	-11.62	107.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2907	A	N7-C8-N9	-11.62	107.99	113.80
32	W	556	A	N7-C8-N9	-11.62	107.99	113.80
32	W	1488	A	N7-C8-N9	-11.62	107.99	113.80
1	A	236	A	N7-C8-N9	-11.62	107.99	113.80
32	W	31	A	N7-C8-N9	-11.62	107.99	113.80
1	A	110	A	N7-C8-N9	-11.62	107.99	113.80
1	A	1287	A	N7-C8-N9	-11.62	107.99	113.80
32	W	1405	A	N7-C8-N9	-11.62	107.99	113.80
32	W	1512	A	N7-C8-N9	-11.62	107.99	113.80
1	A	1034	A	N7-C8-N9	-11.62	107.99	113.80
1	A	2455	A	N7-C8-N9	-11.62	107.99	113.80
1	A	2830	A	N7-C8-N9	-11.62	107.99	113.80
32	W	107	A	N7-C8-N9	-11.62	107.99	113.80
32	W	296	A	N7-C8-N9	-11.62	107.99	113.80
32	W	883	A	N7-C8-N9	-11.62	107.99	113.80
32	W	947	A	N7-C8-N9	-11.62	107.99	113.80
1	A	64	A	N7-C8-N9	-11.62	107.99	113.80
1	A	547	A	N7-C8-N9	-11.62	107.99	113.80
1	A	690	A	N7-C8-N9	-11.62	107.99	113.80
1	A	769	A	N7-C8-N9	-11.61	107.99	113.80
1	A	2307	A	N7-C8-N9	-11.61	107.99	113.80
32	W	1207	A	N7-C8-N9	-11.62	107.99	113.80
32	W	1327	A	N7-C8-N9	-11.62	107.99	113.80
1	A	202	A	N7-C8-N9	-11.61	107.99	113.80
2	B	102	A	N7-C8-N9	-11.61	107.99	113.80
32	W	1254	A	N7-C8-N9	-11.61	107.99	113.80
1	A	1346	A	N7-C8-N9	-11.61	107.99	113.80
1	A	418	A	N7-C8-N9	-11.61	108.00	113.80
32	W	1185	A	N7-C8-N9	-11.61	108.00	113.80
1	A	216	A	N7-C8-N9	-11.61	108.00	113.80
1	A	993	A	N7-C8-N9	-11.61	108.00	113.80
1	A	1115	A	N7-C8-N9	-11.61	108.00	113.80
32	W	281	A	N7-C8-N9	-11.61	108.00	113.80
1	A	2276	A	N7-C8-N9	-11.61	108.00	113.80
1	A	2295	A	N7-C8-N9	-11.61	108.00	113.80
32	W	831	A	N7-C8-N9	-11.61	108.00	113.80
32	W	1102	A	N7-C8-N9	-11.61	108.00	113.80
1	A	1593	A	N7-C8-N9	-11.61	108.00	113.80
1	A	2042	A	N7-C8-N9	-11.61	108.00	113.80
32	W	485	A	N7-C8-N9	-11.61	108.00	113.80
32	W	460	A	N7-C8-N9	-11.61	108.00	113.80
1	A	2088	A	N7-C8-N9	-11.60	108.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	770	A	N7-C8-N9	-11.60	108.00	113.80
1	A	1815	A	N7-C8-N9	-11.60	108.00	113.80
32	W	422	A	N7-C8-N9	-11.60	108.00	113.80
32	W	1407	A	N7-C8-N9	-11.60	108.00	113.80
1	A	1291	A	N7-C8-N9	-11.60	108.00	113.80
1	A	2719	A	N7-C8-N9	-11.60	108.00	113.80
32	W	53	A	N7-C8-N9	-11.60	108.00	113.80
32	W	618	A	N7-C8-N9	-11.60	108.00	113.80
1	A	530	A	N7-C8-N9	-11.60	108.00	113.80
1	A	1445	A	N7-C8-N9	-11.60	108.00	113.80
32	W	704	A	N7-C8-N9	-11.60	108.00	113.80
32	W	1252	A	N7-C8-N9	-11.60	108.00	113.80
1	A	882	A	N7-C8-N9	-11.60	108.00	113.80
1	A	2754	A	N7-C8-N9	-11.60	108.00	113.80
32	W	1328	A	N7-C8-N9	-11.60	108.00	113.80
1	A	1144	A	N7-C8-N9	-11.60	108.00	113.80
32	W	202	A	N7-C8-N9	-11.60	108.00	113.80
1	A	354	A	N7-C8-N9	-11.59	108.00	113.80
1	A	2100	A	N7-C8-N9	-11.59	108.00	113.80
1	A	1174	A	N7-C8-N9	-11.59	108.00	113.80
1	A	2854	A	N7-C8-N9	-11.59	108.00	113.80
32	W	170	A	N7-C8-N9	-11.59	108.00	113.80
32	W	1333	A	N7-C8-N9	-11.59	108.00	113.80
32	W	1541	A	N7-C8-N9	-11.59	108.01	113.80
1	A	2351	A	N7-C8-N9	-11.59	108.01	113.80
1	A	173	A	N7-C8-N9	-11.59	108.01	113.80
1	A	278	A	N7-C8-N9	-11.59	108.01	113.80
1	A	322	A	N7-C8-N9	-11.59	108.01	113.80
1	A	652	A	N7-C8-N9	-11.59	108.01	113.80
1	A	1254	A	N7-C8-N9	-11.59	108.01	113.80
32	W	389	A	N7-C8-N9	-11.59	108.01	113.80
1	A	1948	A	N7-C8-N9	-11.59	108.01	113.80
32	W	150	A	N7-C8-N9	-11.59	108.01	113.80
32	W	204	A	N7-C8-N9	-11.59	108.01	113.80
32	W	506	A	N7-C8-N9	-11.58	108.01	113.80
32	W	1510	A	N7-C8-N9	-11.58	108.01	113.80
1	A	763	A	N7-C8-N9	-11.58	108.01	113.80
1	A	1078	A	N7-C8-N9	-11.58	108.01	113.80
1	A	1325	A	N7-C8-N9	-11.58	108.01	113.80
1	A	10	A	N7-C8-N9	-11.58	108.01	113.80
1	A	1277	A	N7-C8-N9	-11.58	108.01	113.80
32	W	94	A	N7-C8-N9	-11.58	108.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1405	A	N7-C8-N9	-11.58	108.01	113.80
1	A	1592	A	N7-C8-N9	-11.58	108.01	113.80
1	A	2356	A	N7-C8-N9	-11.58	108.01	113.80
2	B	114	A	N7-C8-N9	-11.58	108.01	113.80
32	W	232	A	N7-C8-N9	-11.58	108.01	113.80
32	W	290	A	N7-C8-N9	-11.58	108.01	113.80
32	W	529	A	N7-C8-N9	-11.58	108.01	113.80
32	W	1259	A	N7-C8-N9	-11.58	108.01	113.80
1	A	355	A	N7-C8-N9	-11.57	108.01	113.80
1	A	1313	A	N7-C8-N9	-11.57	108.01	113.80
1	A	1424	A	N7-C8-N9	-11.57	108.01	113.80
1	A	947	A	N7-C8-N9	-11.57	108.02	113.80
1	A	957	A	N7-C8-N9	-11.57	108.02	113.80
1	A	2902	A	N7-C8-N9	-11.57	108.01	113.80
32	W	240	A	N7-C8-N9	-11.57	108.01	113.80
1	A	1918	A	N7-C8-N9	-11.57	108.02	113.80
32	W	1077	A	N7-C8-N9	-11.57	108.02	113.80
32	W	1176	A	N7-C8-N9	-11.57	108.02	113.80
1	A	1648	A	N7-C8-N9	-11.57	108.02	113.80
1	A	2793	A	N7-C8-N9	-11.57	108.02	113.80
2	B	76	A	N7-C8-N9	-11.57	108.02	113.80
1	A	1392	A	N7-C8-N9	-11.56	108.02	113.80
1	A	2087	A	N7-C8-N9	-11.56	108.02	113.80
32	W	57	A	N7-C8-N9	-11.56	108.02	113.80
32	W	512	A	N7-C8-N9	-11.56	108.02	113.80
32	W	776	A	N7-C8-N9	-11.56	108.02	113.80
1	A	224	A	N7-C8-N9	-11.56	108.02	113.80
32	W	775	A	N7-C8-N9	-11.56	108.02	113.80
1	A	1014	A	N7-C8-N9	-11.56	108.02	113.80
1	A	1302	A	N7-C8-N9	-11.56	108.02	113.80
1	A	1580	A	N7-C8-N9	-11.56	108.02	113.80
32	W	211	A	N7-C8-N9	-11.56	108.02	113.80
32	W	541	A	N7-C8-N9	-11.56	108.02	113.80
32	W	671	A	N7-C8-N9	-11.56	108.02	113.80
32	W	1419	A	N7-C8-N9	-11.56	108.02	113.80
1	A	1540	A	N7-C8-N9	-11.56	108.02	113.80
1	A	1746	A	N7-C8-N9	-11.56	108.02	113.80
1	A	2804	A	N7-C8-N9	-11.56	108.02	113.80
32	W	679	A	N7-C8-N9	-11.56	108.02	113.80
32	W	928	A	N7-C8-N9	-11.56	108.02	113.80
1	A	231	A	N7-C8-N9	-11.56	108.02	113.80
1	A	329	A	N7-C8-N9	-11.55	108.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1020	A	N7-C8-N9	-11.55	108.02	113.80
1	A	2369	A	N7-C8-N9	-11.55	108.02	113.80
32	W	258	A	N7-C8-N9	-11.56	108.02	113.80
32	W	996	A	N7-C8-N9	-11.55	108.02	113.80
32	W	1451	A	N7-C8-N9	-11.56	108.02	113.80
1	A	94	A	N7-C8-N9	-11.55	108.02	113.80
1	A	200	A	N7-C8-N9	-11.55	108.02	113.80
2	B	51	A	N7-C8-N9	-11.55	108.02	113.80
32	W	1384	A	N7-C8-N9	-11.55	108.02	113.80
1	A	782	A	N7-C8-N9	-11.55	108.02	113.80
1	A	1685	A	N7-C8-N9	-11.55	108.03	113.80
1	A	1791	A	N7-C8-N9	-11.55	108.02	113.80
1	A	2851	A	N7-C8-N9	-11.55	108.02	113.80
32	W	371	A	N7-C8-N9	-11.55	108.02	113.80
32	W	1386	A	N7-C8-N9	-11.55	108.02	113.80
1	A	965	A	N7-C8-N9	-11.55	108.03	113.80
1	A	179	A	N7-C8-N9	-11.55	108.03	113.80
1	A	1230	A	N7-C8-N9	-11.55	108.03	113.80
1	A	2547	A	N7-C8-N9	-11.55	108.03	113.80
2	B	50	A	N7-C8-N9	-11.55	108.03	113.80
32	W	118	A	N7-C8-N9	-11.55	108.03	113.80
32	W	203	A	N7-C8-N9	-11.55	108.03	113.80
32	W	333	A	N7-C8-N9	-11.55	108.03	113.80
32	W	367	A	N7-C8-N9	-11.55	108.03	113.80
32	W	664	A	N7-C8-N9	-11.55	108.03	113.80
32	W	801	A	N7-C8-N9	-11.55	108.03	113.80
32	W	1529	A	N7-C8-N9	-11.55	108.03	113.80
1	A	1802	A	N7-C8-N9	-11.55	108.03	113.80
1	A	2338	A	N7-C8-N9	-11.54	108.03	113.80
32	W	617	A	N7-C8-N9	-11.55	108.03	113.80
1	A	2834	A	N7-C8-N9	-11.54	108.03	113.80
32	W	321	A	N7-C8-N9	-11.54	108.03	113.80
32	W	160	A	N7-C8-N9	-11.54	108.03	113.80
1	A	974	A	N7-C8-N9	-11.54	108.03	113.80
1	A	1036	A	N7-C8-N9	-11.54	108.03	113.80
32	W	1256	A	N7-C8-N9	-11.54	108.03	113.80
32	W	1528	A	N7-C8-N9	-11.54	108.03	113.80
1	A	140	A	N7-C8-N9	-11.54	108.03	113.80
1	A	273	A	N7-C8-N9	-11.54	108.03	113.80
1	A	1516	A	N7-C8-N9	-11.54	108.03	113.80
52	z	41	A	N7-C8-N9	-11.54	108.03	113.80
1	A	667	A	N7-C8-N9	-11.53	108.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1663	A	N7-C8-N9	-11.54	108.03	113.80
1	A	2782	A	N7-C8-N9	-11.54	108.03	113.80
32	W	142	A	N7-C8-N9	-11.54	108.03	113.80
32	W	386	A	N7-C8-N9	-11.53	108.03	113.80
32	W	956	A	N7-C8-N9	-11.53	108.03	113.80
1	A	49	A	N7-C8-N9	-11.53	108.03	113.80
1	A	1423	A	N7-C8-N9	-11.53	108.03	113.80
1	A	1745	A	N7-C8-N9	-11.53	108.03	113.80
32	W	757	A	N7-C8-N9	-11.53	108.03	113.80
1	A	2686	A	N7-C8-N9	-11.53	108.03	113.80
32	W	401	A	N7-C8-N9	-11.53	108.03	113.80
32	W	816	A	N7-C8-N9	-11.53	108.03	113.80
1	A	1141	A	N7-C8-N9	-11.53	108.03	113.80
1	A	1197	A	N7-C8-N9	-11.53	108.03	113.80
2	B	27	A	N7-C8-N9	-11.53	108.04	113.80
32	W	974	A	N7-C8-N9	-11.53	108.04	113.80
32	W	1437	A	N7-C8-N9	-11.53	108.03	113.80
32	W	1188	A	N7-C8-N9	-11.53	108.04	113.80
52	z	14	A	N7-C8-N9	-11.53	108.04	113.80
1	A	1210	A	N7-C8-N9	-11.53	108.04	113.80
1	A	1375	A	N7-C8-N9	-11.53	108.04	113.80
32	W	715	A	N7-C8-N9	-11.53	108.04	113.80
32	W	677	A	N7-C8-N9	-11.53	108.04	113.80
32	W	823	A	N7-C8-N9	-11.53	108.04	113.80
32	W	1197	A	N7-C8-N9	-11.53	108.04	113.80
1	A	337	A	N7-C8-N9	-11.52	108.04	113.80
1	A	893	A	N7-C8-N9	-11.52	108.04	113.80
1	A	1583	A	N7-C8-N9	-11.52	108.04	113.80
1	A	762	A	N7-C8-N9	-11.52	108.04	113.80
1	A	1201	A	N7-C8-N9	-11.52	108.04	113.80
1	A	1929	A	N7-C8-N9	-11.52	108.04	113.80
32	W	12	A	N7-C8-N9	-11.52	108.04	113.80
1	A	524	A	N7-C8-N9	-11.52	108.04	113.80
1	A	736	A	N7-C8-N9	-11.52	108.04	113.80
32	W	287	A	N7-C8-N9	-11.52	108.04	113.80
1	A	1520	A	N7-C8-N9	-11.52	108.04	113.80
1	A	2398	A	N7-C8-N9	-11.52	108.04	113.80
1	A	230	A	N7-C8-N9	-11.52	108.04	113.80
1	A	876	A	N7-C8-N9	-11.52	108.04	113.80
1	A	1194	A	N7-C8-N9	-11.52	108.04	113.80
32	W	173	A	N7-C8-N9	-11.52	108.04	113.80
1	A	1615	A	N7-C8-N9	-11.52	108.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	329	A	N7-C8-N9	-11.52	108.04	113.80
32	W	649	A	N7-C8-N9	-11.52	108.04	113.80
32	W	917	A	N7-C8-N9	-11.52	108.04	113.80
1	A	125	A	N7-C8-N9	-11.51	108.04	113.80
1	A	1123	A	N7-C8-N9	-11.51	108.04	113.80
1	A	1818	A	N7-C8-N9	-11.51	108.04	113.80
1	A	2365	A	N7-C8-N9	-11.51	108.04	113.80
2	B	39	A	N7-C8-N9	-11.51	108.04	113.80
32	W	910	A	N7-C8-N9	-11.51	108.04	113.80
1	A	412	A	N7-C8-N9	-11.51	108.04	113.80
1	A	870	A	N7-C8-N9	-11.51	108.04	113.80
1	A	2329	A	N7-C8-N9	-11.51	108.05	113.80
1	A	2835	A	N7-C8-N9	-11.51	108.05	113.80
1	A	1347	A	N7-C8-N9	-11.51	108.05	113.80
1	A	2505	A	N7-C8-N9	-11.51	108.05	113.80
32	W	415	A	N7-C8-N9	-11.51	108.05	113.80
32	W	501	A	N7-C8-N9	-11.51	108.05	113.80
32	W	504	A	N7-C8-N9	-11.51	108.05	113.80
32	W	592	A	N7-C8-N9	-11.51	108.05	113.80
32	W	1523	A	N7-C8-N9	-11.51	108.05	113.80
1	A	1434	A	N7-C8-N9	-11.51	108.05	113.80
1	A	2629	A	N7-C8-N9	-11.51	108.05	113.80
32	W	725	A	N7-C8-N9	-11.51	108.05	113.80
32	W	870	A	N7-C8-N9	-11.51	108.05	113.80
32	W	1470	A	N7-C8-N9	-11.51	108.05	113.80
1	A	144	A	N7-C8-N9	-11.50	108.05	113.80
1	A	325	A	N7-C8-N9	-11.50	108.05	113.80
1	A	1631	A	N7-C8-N9	-11.50	108.05	113.80
1	A	1913	A	N7-C8-N9	-11.50	108.05	113.80
1	A	2722	A	N7-C8-N9	-11.50	108.05	113.80
1	A	987	A	N7-C8-N9	-11.50	108.05	113.80
1	A	1638	A	N7-C8-N9	-11.50	108.05	113.80
1	A	65	A	N7-C8-N9	-11.50	108.05	113.80
1	A	459	A	N7-C8-N9	-11.50	108.05	113.80
1	A	543	A	N7-C8-N9	-11.50	108.05	113.80
1	A	2340	A	N7-C8-N9	-11.50	108.05	113.80
32	W	117	A	N7-C8-N9	-11.50	108.05	113.80
32	W	1178	A	N7-C8-N9	-11.50	108.05	113.80
1	A	124	A	N7-C8-N9	-11.50	108.05	113.80
1	A	537	A	N7-C8-N9	-11.50	108.05	113.80
1	A	519	A	N7-C8-N9	-11.50	108.05	113.80
1	A	2000	A	N7-C8-N9	-11.50	108.05	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	44	A	N7-C8-N9	-11.50	108.05	113.80
32	W	638	A	N7-C8-N9	-11.50	108.05	113.80
32	W	1358	A	N7-C8-N9	-11.50	108.05	113.80
32	W	1486	A	N7-C8-N9	-11.50	108.05	113.80
32	W	1490	A	N7-C8-N9	-11.50	108.05	113.80
32	W	721	A	N7-C8-N9	-11.49	108.05	113.80
1	A	28	A	N7-C8-N9	-11.49	108.05	113.80
1	A	500	A	N7-C8-N9	-11.49	108.05	113.80
1	A	752	A	N7-C8-N9	-11.49	108.05	113.80
1	A	1432	A	N7-C8-N9	-11.49	108.05	113.80
1	A	2303	A	N7-C8-N9	-11.49	108.05	113.80
1	A	2590	A	N7-C8-N9	-11.49	108.05	113.80
32	W	440	A	N7-C8-N9	-11.49	108.05	113.80
32	W	837	A	N7-C8-N9	-11.49	108.05	113.80
32	W	1266	A	N7-C8-N9	-11.49	108.05	113.80
1	A	5	A	N7-C8-N9	-11.49	108.06	113.80
1	A	139	A	N7-C8-N9	-11.49	108.06	113.80
1	A	917	A	N7-C8-N9	-11.49	108.06	113.80
1	A	1677	A	N7-C8-N9	-11.49	108.05	113.80
1	A	1989	A	N7-C8-N9	-11.49	108.06	113.80
1	A	2381	A	N7-C8-N9	-11.49	108.06	113.80
1	A	2542	A	N7-C8-N9	-11.49	108.06	113.80
1	A	2919	A	N7-C8-N9	-11.49	108.06	113.80
32	W	234	A	N7-C8-N9	-11.49	108.06	113.80
32	W	404	A	N7-C8-N9	-11.49	108.06	113.80
32	W	522	A	N7-C8-N9	-11.49	108.06	113.80
32	W	1133	A	N7-C8-N9	-11.49	108.06	113.80
32	W	1213	A	N7-C8-N9	-11.49	108.06	113.80
1	A	260	A	N7-C8-N9	-11.49	108.06	113.80
1	A	318	A	N7-C8-N9	-11.49	108.06	113.80
1	A	715	A	N7-C8-N9	-11.49	108.06	113.80
1	A	2034	A	N7-C8-N9	-11.49	108.06	113.80
1	A	2479	A	N7-C8-N9	-11.49	108.06	113.80
32	W	978	A	N7-C8-N9	-11.49	108.06	113.80
1	A	952	A	N7-C8-N9	-11.48	108.06	113.80
1	A	2007	A	N7-C8-N9	-11.48	108.06	113.80
1	A	786	A	N7-C8-N9	-11.48	108.06	113.80
1	A	1844	A	N7-C8-N9	-11.48	108.06	113.80
32	W	81	A	N7-C8-N9	-11.48	108.06	113.80
32	W	1205	A	N7-C8-N9	-11.48	108.06	113.80
32	W	1261	A	N7-C8-N9	-11.48	108.06	113.80
32	W	1320	A	N7-C8-N9	-11.48	108.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	A	N7-C8-N9	-11.48	108.06	113.80
1	A	456	A	N7-C8-N9	-11.48	108.06	113.80
1	A	677	A	N7-C8-N9	-11.48	108.06	113.80
1	A	705	A	N7-C8-N9	-11.48	108.06	113.80
1	A	781	A	N7-C8-N9	-11.48	108.06	113.80
1	A	811	A	N7-C8-N9	-11.48	108.06	113.80
1	A	1722	A	N7-C8-N9	-11.48	108.06	113.80
1	A	1942	A	N7-C8-N9	-11.48	108.06	113.80
2	B	97	A	N7-C8-N9	-11.48	108.06	113.80
32	W	791	A	N7-C8-N9	-11.48	108.06	113.80
32	W	1509	A	N7-C8-N9	-11.48	108.06	113.80
1	A	199	A	N7-C8-N9	-11.48	108.06	113.80
32	W	361	A	N7-C8-N9	-11.48	108.06	113.80
32	W	1296	A	N7-C8-N9	-11.48	108.06	113.80
1	A	1691	A	N3-C4-C5	-11.48	118.77	126.80
1	A	2526	A	N7-C8-N9	-11.48	108.06	113.80
1	A	161	A	N7-C8-N9	-11.47	108.06	113.80
1	A	618	A	N7-C8-N9	-11.47	108.06	113.80
1	A	1116	A	N7-C8-N9	-11.47	108.06	113.80
1	A	2643	A	N7-C8-N9	-11.47	108.06	113.80
32	W	151	A	N7-C8-N9	-11.47	108.06	113.80
32	W	1513	A	N7-C8-N9	-11.47	108.06	113.80
1	A	259	A	N7-C8-N9	-11.47	108.06	113.80
1	A	274	A	N7-C8-N9	-11.47	108.06	113.80
1	A	1845	A	N7-C8-N9	-11.47	108.06	113.80
1	A	1966	A	N7-C8-N9	-11.47	108.06	113.80
2	B	18	A	N7-C8-N9	-11.47	108.06	113.80
1	A	2511	A	N7-C8-N9	-11.47	108.06	113.80
32	W	282	A	N7-C8-N9	-11.47	108.06	113.80
32	W	1289	A	N7-C8-N9	-11.47	108.06	113.80
1	A	333	A	N7-C8-N9	-11.47	108.07	113.80
1	A	723	A	N7-C8-N9	-11.47	108.07	113.80
1	A	1142	A	N7-C8-N9	-11.47	108.07	113.80
32	W	1271	A	N7-C8-N9	-11.47	108.07	113.80
1	A	2663	A	N7-C8-N9	-11.47	108.07	113.80
32	W	475	A	N7-C8-N9	-11.47	108.07	113.80
1	A	866	A	N7-C8-N9	-11.47	108.07	113.80
32	W	1111	A	N7-C8-N9	-11.47	108.07	113.80
32	W	1022	A	N7-C8-N9	-11.46	108.07	113.80
1	A	1092	A	N7-C8-N9	-11.46	108.07	113.80
1	A	1533	A	N7-C8-N9	-11.46	108.07	113.80
1	A	2762	A	N7-C8-N9	-11.46	108.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	278	A	N7-C8-N9	-11.46	108.07	113.80
1	A	1059	A	N7-C8-N9	-11.46	108.07	113.80
1	A	1534	A	N7-C8-N9	-11.46	108.07	113.80
1	A	1901	A	N7-C8-N9	-11.46	108.07	113.80
32	W	178	A	N7-C8-N9	-11.46	108.07	113.80
32	W	346	A	N7-C8-N9	-11.46	108.07	113.80
32	W	1417	A	N7-C8-N9	-11.46	108.07	113.80
1	A	13	A	N7-C8-N9	-11.46	108.07	113.80
1	A	1026	A	N7-C8-N9	-11.46	108.07	113.80
1	A	1335	A	N7-C8-N9	-11.46	108.07	113.80
1	A	330	A	N7-C8-N9	-11.46	108.07	113.80
1	A	1727	A	N7-C8-N9	-11.46	108.07	113.80
1	A	2402	A	N7-C8-N9	-11.46	108.07	113.80
1	A	2464	A	N7-C8-N9	-11.46	108.07	113.80
1	A	2662	A	N7-C8-N9	-11.46	108.07	113.80
32	W	500	A	N7-C8-N9	-11.46	108.07	113.80
32	W	1120	A	N7-C8-N9	-11.46	108.07	113.80
32	W	423	A	N7-C8-N9	-11.46	108.07	113.80
32	W	1284	A	N7-C8-N9	-11.46	108.07	113.80
1	A	2482	A	N7-C8-N9	-11.46	108.07	113.80
32	W	28	A	N7-C8-N9	-11.46	108.07	113.80
32	W	1245	A	N7-C8-N9	-11.46	108.07	113.80
1	A	102	A	N7-C8-N9	-11.45	108.07	113.80
1	A	1235	A	N7-C8-N9	-11.45	108.07	113.80
1	A	1253	A	N7-C8-N9	-11.45	108.07	113.80
1	A	2387	A	N7-C8-N9	-11.46	108.07	113.80
32	W	1425	A	N7-C8-N9	-11.45	108.07	113.80
1	A	275	A	N7-C8-N9	-11.45	108.07	113.80
1	A	2043	A	N7-C8-N9	-11.45	108.08	113.80
32	W	544	A	N7-C8-N9	-11.45	108.07	113.80
32	W	1028	A	N7-C8-N9	-11.45	108.07	113.80
1	A	194	A	N7-C8-N9	-11.45	108.08	113.80
32	W	491	A	N7-C8-N9	-11.45	108.08	113.80
1	A	302	A	N7-C8-N9	-11.45	108.08	113.80
1	A	1906	A	N7-C8-N9	-11.45	108.08	113.80
1	A	2498	A	N7-C8-N9	-11.45	108.08	113.80
1	A	2658	A	N7-C8-N9	-11.45	108.08	113.80
32	W	67	A	N7-C8-N9	-11.45	108.08	113.80
1	A	2767	A	N7-C8-N9	-11.45	108.08	113.80
1	A	2032	A	N7-C8-N9	-11.45	108.08	113.80
2	B	37	A	N7-C8-N9	-11.45	108.08	113.80
1	A	307	A	N7-C8-N9	-11.44	108.08	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	867	A	N7-C8-N9	-11.45	108.08	113.80
32	W	61	A	N7-C8-N9	-11.45	108.08	113.80
32	W	129	A	N7-C8-N9	-11.45	108.08	113.80
32	W	335	A	N7-C8-N9	-11.45	108.08	113.80
32	W	1147	A	N7-C8-N9	-11.45	108.08	113.80
1	A	829	A	N7-C8-N9	-11.44	108.08	113.80
1	A	2383	A	N7-C8-N9	-11.44	108.08	113.80
32	W	738	A	N7-C8-N9	-11.44	108.08	113.80
1	A	922	A	N7-C8-N9	-11.44	108.08	113.80
1	A	1947	A	N7-C8-N9	-11.44	108.08	113.80
1	A	2480	A	N7-C8-N9	-11.44	108.08	113.80
32	W	55	A	N7-C8-N9	-11.44	108.08	113.80
1	A	1709	A	N7-C8-N9	-11.44	108.08	113.80
1	A	1323	A	N7-C8-N9	-11.44	108.08	113.80
1	A	1957	A	N7-C8-N9	-11.44	108.08	113.80
1	A	2421	A	N7-C8-N9	-11.44	108.08	113.80
32	W	696	A	N7-C8-N9	-11.44	108.08	113.80
32	W	919	A	N7-C8-N9	-11.44	108.08	113.80
1	A	206	A	N7-C8-N9	-11.43	108.08	113.80
1	A	619	A	N7-C8-N9	-11.43	108.08	113.80
1	A	1190	A	N7-C8-N9	-11.43	108.08	113.80
1	A	1967	A	N7-C8-N9	-11.43	108.08	113.80
1	A	2018	A	N7-C8-N9	-11.43	108.08	113.80
32	W	507	A	N7-C8-N9	-11.43	108.08	113.80
1	A	1617	A	N7-C8-N9	-11.43	108.08	113.80
1	A	1286	A	N7-C8-N9	-11.43	108.08	113.80
1	A	2375	A	N7-C8-N9	-11.43	108.08	113.80
1	A	1831	A	N7-C8-N9	-11.43	108.08	113.80
1	A	2462	A	N7-C8-N9	-11.43	108.08	113.80
32	W	236	A	N7-C8-N9	-11.43	108.08	113.80
32	W	542	A	N7-C8-N9	-11.43	108.09	113.80
1	A	12	A	N7-C8-N9	-11.43	108.09	113.80
1	A	222	A	N7-C8-N9	-11.43	108.09	113.80
1	A	1713	A	N7-C8-N9	-11.43	108.09	113.80
1	A	518	A	N7-C8-N9	-11.43	108.09	113.80
1	A	1575	A	N7-C8-N9	-11.43	108.09	113.80
1	A	2845	A	N7-C8-N9	-11.43	108.09	113.80
32	W	605	A	N7-C8-N9	-11.43	108.09	113.80
32	W	913	A	N7-C8-N9	-11.43	108.09	113.80
1	A	1743	A	N7-C8-N9	-11.42	108.09	113.80
32	W	1342	A	N7-C8-N9	-11.42	108.09	113.80
1	A	1100	A	N7-C8-N9	-11.42	108.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1517	A	N7-C8-N9	-11.42	108.09	113.80
1	A	2734	A	N7-C8-N9	-11.42	108.09	113.80
1	A	2740	A	N7-C8-N9	-11.42	108.09	113.80
1	A	2889	A	N7-C8-N9	-11.42	108.09	113.80
32	W	344	A	N7-C8-N9	-11.42	108.09	113.80
32	W	306	A	N7-C8-N9	-11.42	108.09	113.80
32	W	799	A	N7-C8-N9	-11.42	108.09	113.80
1	A	1789	A	N7-C8-N9	-11.42	108.09	113.80
1	A	2517	A	N7-C8-N9	-11.42	108.09	113.80
32	W	669	A	N7-C8-N9	-11.42	108.09	113.80
32	W	918	A	N7-C8-N9	-11.42	108.09	113.80
1	A	14	A	N7-C8-N9	-11.42	108.09	113.80
1	A	156	A	N7-C8-N9	-11.42	108.09	113.80
1	A	376	A	N7-C8-N9	-11.42	108.09	113.80
1	A	429	A	N7-C8-N9	-11.42	108.09	113.80
1	A	964	A	N7-C8-N9	-11.42	108.09	113.80
1	A	2708	A	N7-C8-N9	-11.42	108.09	113.80
2	B	64	A	N7-C8-N9	-11.42	108.09	113.80
1	A	176	A	N7-C8-N9	-11.41	108.09	113.80
1	A	727	A	N7-C8-N9	-11.41	108.09	113.80
1	A	746	A	N7-C8-N9	-11.41	108.09	113.80
1	A	1025	A	N7-C8-N9	-11.41	108.09	113.80
1	A	1005	A	N7-C8-N9	-11.41	108.09	113.80
1	A	1636	A	N7-C8-N9	-11.41	108.09	113.80
1	A	1686	A	N7-C8-N9	-11.41	108.09	113.80
1	A	2898	A	N7-C8-N9	-11.41	108.09	113.80
32	W	52	A	N7-C8-N9	-11.41	108.09	113.80
32	W	684	A	N7-C8-N9	-11.41	108.09	113.80
32	W	758	A	N7-C8-N9	-11.41	108.10	113.80
1	A	507	A	N7-C8-N9	-11.41	108.10	113.80
1	A	1357	A	N7-C8-N9	-11.41	108.10	113.80
1	A	2060	A	N7-C8-N9	-11.41	108.10	113.80
1	A	2900	A	N7-C8-N9	-11.41	108.10	113.80
1	A	1149	A	N7-C8-N9	-11.41	108.10	113.80
32	W	72	A	N7-C8-N9	-11.41	108.10	113.80
32	W	879	A	N7-C8-N9	-11.41	108.10	113.80
1	A	659	A	N7-C8-N9	-11.40	108.10	113.80
1	A	753	A	N7-C8-N9	-11.40	108.10	113.80
1	A	2343	A	N7-C8-N9	-11.40	108.10	113.80
1	A	1266	A	N7-C8-N9	-11.40	108.10	113.80
1	A	1588	A	N7-C8-N9	-11.40	108.10	113.80
1	A	1627	A	N7-C8-N9	-11.40	108.10	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1699	A	N7-C8-N9	-11.40	108.10	113.80
32	W	1260	A	N7-C8-N9	-11.40	108.10	113.80
1	A	373	A	N7-C8-N9	-11.40	108.10	113.80
1	A	448	A	N7-C8-N9	-11.40	108.10	113.80
1	A	1119	A	N7-C8-N9	-11.40	108.10	113.80
1	A	1464	A	N7-C8-N9	-11.40	108.10	113.80
1	A	2006	A	N7-C8-N9	-11.40	108.10	113.80
1	A	2769	A	N7-C8-N9	-11.40	108.10	113.80
1	A	549	A	N7-C8-N9	-11.40	108.10	113.80
1	A	692	A	N7-C8-N9	-11.40	108.10	113.80
1	A	2661	A	N7-C8-N9	-11.40	108.10	113.80
1	A	2787	A	N7-C8-N9	-11.40	108.10	113.80
32	W	828	A	N7-C8-N9	-11.40	108.10	113.80
1	A	2080	A	N7-C8-N9	-11.40	108.10	113.80
1	A	2904	A	N7-C8-N9	-11.40	108.10	113.80
1	A	2297	A	N7-C8-N9	-11.40	108.10	113.80
32	W	1054	A	N7-C8-N9	-11.40	108.10	113.80
1	A	2606	A	N7-C8-N9	-11.40	108.10	113.80
32	W	76	A	N7-C8-N9	-11.40	108.10	113.80
32	W	1115	A	N7-C8-N9	-11.40	108.10	113.80
32	W	1247	A	N7-C8-N9	-11.40	108.10	113.80
32	W	1502	A	N7-C8-N9	-11.40	108.10	113.80
1	A	561	A	N7-C8-N9	-11.39	108.10	113.80
1	A	896	A	N7-C8-N9	-11.39	108.10	113.80
1	A	2810	A	N7-C8-N9	-11.39	108.10	113.80
1	A	2875	A	N7-C8-N9	-11.39	108.10	113.80
1	A	130	A	N7-C8-N9	-11.39	108.11	113.80
1	A	1710	A	N7-C8-N9	-11.39	108.11	113.80
1	A	2027	A	N7-C8-N9	-11.39	108.11	113.80
1	A	44	A	N7-C8-N9	-11.39	108.11	113.80
52	z	44	A	N7-C8-N9	-11.39	108.11	113.80
1	A	477	A	N7-C8-N9	-11.39	108.11	113.80
1	A	653	A	N7-C8-N9	-11.39	108.11	113.80
32	W	1479	A	N7-C8-N9	-11.39	108.11	113.80
1	A	118	A	N7-C8-N9	-11.38	108.11	113.80
1	A	1260	A	N7-C8-N9	-11.38	108.11	113.80
1	A	1695	A	N7-C8-N9	-11.38	108.11	113.80
32	W	210	A	N7-C8-N9	-11.38	108.11	113.80
1	A	808	A	N7-C8-N9	-11.38	108.11	113.80
32	W	705	A	N7-C8-N9	-11.38	108.11	113.80
1	A	851	A	N7-C8-N9	-11.38	108.11	113.80
1	A	1734	A	N7-C8-N9	-11.38	108.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2790	A	N7-C8-N9	-11.38	108.11	113.80
1	A	2826	A	N7-C8-N9	-11.38	108.11	113.80
32	W	1121	A	N7-C8-N9	-11.38	108.11	113.80
1	A	2071	A	N7-C8-N9	-11.38	108.11	113.80
2	B	55	A	N7-C8-N9	-11.38	108.11	113.80
1	A	1258	A	N7-C8-N9	-11.38	108.11	113.80
32	W	433	A	N7-C8-N9	-11.38	108.11	113.80
32	W	979	A	N7-C8-N9	-11.38	108.11	113.80
32	W	1024	A	N7-C8-N9	-11.38	108.11	113.80
1	A	1499	A	N7-C8-N9	-11.37	108.11	113.80
1	A	1941	A	N7-C8-N9	-11.37	108.11	113.80
1	A	2924	A	N7-C8-N9	-11.37	108.11	113.80
32	W	875	A	N7-C8-N9	-11.37	108.11	113.80
1	A	1995	A	N7-C8-N9	-11.37	108.11	113.80
32	W	208	A	N7-C8-N9	-11.37	108.11	113.80
1	A	61	A	N7-C8-N9	-11.37	108.12	113.80
1	A	724	A	N7-C8-N9	-11.37	108.12	113.80
1	A	185	A	N7-C8-N9	-11.37	108.12	113.80
1	A	1131	A	N7-C8-N9	-11.37	108.12	113.80
1	A	1490	A	N7-C8-N9	-11.37	108.12	113.80
32	W	604	A	N7-C8-N9	-11.37	108.12	113.80
1	A	178	A	N7-C8-N9	-11.36	108.12	113.80
1	A	1222	A	N7-C8-N9	-11.36	108.12	113.80
32	W	582	A	N7-C8-N9	-11.36	108.12	113.80
32	W	1270	A	N7-C8-N9	-11.36	108.12	113.80
32	W	674	A	N7-C8-N9	-11.36	108.12	113.80
1	A	600	A	N7-C8-N9	-11.36	108.12	113.80
1	A	622	A	N7-C8-N9	-11.36	108.12	113.80
1	A	970	A	N7-C8-N9	-11.36	108.12	113.80
1	A	2570	A	N7-C8-N9	-11.36	108.12	113.80
32	W	120	A	N7-C8-N9	-11.36	108.12	113.80
32	W	337	A	N7-C8-N9	-11.36	108.12	113.80
1	A	578	A	N7-C8-N9	-11.36	108.12	113.80
1	A	1608	A	N7-C8-N9	-11.36	108.12	113.80
32	W	1359	A	N7-C8-N9	-11.36	108.12	113.80
1	A	56	A	N7-C8-N9	-11.35	108.12	113.80
1	A	889	A	N7-C8-N9	-11.35	108.12	113.80
1	A	1103	A	N7-C8-N9	-11.35	108.12	113.80
1	A	1816	A	N7-C8-N9	-11.35	108.12	113.80
32	W	301	A	N7-C8-N9	-11.35	108.12	113.80
32	W	581	A	N7-C8-N9	-11.35	108.12	113.80
32	W	644	A	N7-C8-N9	-11.35	108.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1017	A	N7-C8-N9	-11.35	108.12	113.80
1	A	1054	A	N7-C8-N9	-11.35	108.12	113.80
1	A	1797	A	N7-C8-N9	-11.35	108.12	113.80
1	A	2440	A	N7-C8-N9	-11.35	108.13	113.80
32	W	171	A	N7-C8-N9	-11.35	108.12	113.80
32	W	225	A	N7-C8-N9	-11.35	108.13	113.80
32	W	1004	A	N7-C8-N9	-11.35	108.12	113.80
1	A	1653	A	N7-C8-N9	-11.35	108.13	113.80
1	A	2078	A	N7-C8-N9	-11.35	108.13	113.80
1	A	2270	A	N7-C8-N9	-11.35	108.13	113.80
1	A	2827	A	N7-C8-N9	-11.35	108.13	113.80
32	W	771	A	N7-C8-N9	-11.35	108.13	113.80
32	W	659	A	N7-C8-N9	-11.35	108.13	113.80
52	z	23	A	N7-C8-N9	-11.35	108.13	113.80
1	A	630	A	N7-C8-N9	-11.34	108.13	113.80
1	A	1404	A	N7-C8-N9	-11.34	108.13	113.80
1	A	1675	A	N7-C8-N9	-11.34	108.13	113.80
32	W	1455	A	N7-C8-N9	-11.34	108.13	113.80
1	A	198	A	N7-C8-N9	-11.34	108.13	113.80
1	A	353	A	N7-C8-N9	-11.34	108.13	113.80
32	W	825	A	N7-C8-N9	-11.34	108.13	113.80
1	A	265	A	N7-C8-N9	-11.34	108.13	113.80
1	A	2066	A	N7-C8-N9	-11.34	108.13	113.80
1	A	2330	A	N7-C8-N9	-11.34	108.13	113.80
32	W	438	A	N7-C8-N9	-11.34	108.13	113.80
52	z	58	A	N7-C8-N9	-11.34	108.13	113.80
1	A	476	A	N7-C8-N9	-11.34	108.13	113.80
2	B	56	A	N7-C8-N9	-11.34	108.13	113.80
1	A	548	A	N7-C8-N9	-11.34	108.13	113.80
1	A	592	A	N7-C8-N9	-11.34	108.13	113.80
1	A	1388	A	N7-C8-N9	-11.34	108.13	113.80
1	A	1905	A	N7-C8-N9	-11.34	108.13	113.80
32	W	474	A	N7-C8-N9	-11.34	108.13	113.80
32	W	1031	A	N7-C8-N9	-11.34	108.13	113.80
1	A	225	A	N7-C8-N9	-11.33	108.13	113.80
32	W	874	A	N7-C8-N9	-11.33	108.13	113.80
1	A	486	A	N7-C8-N9	-11.33	108.14	113.80
1	A	623	A	N7-C8-N9	-11.33	108.14	113.80
1	A	1477	A	N7-C8-N9	-11.33	108.14	113.80
32	W	140	A	N7-C8-N9	-11.33	108.14	113.80
32	W	1349	A	N7-C8-N9	-11.33	108.14	113.80
32	W	1493	A	N7-C8-N9	-11.33	108.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	A	N7-C8-N9	-11.33	108.14	113.80
1	A	1113	A	N7-C8-N9	-11.33	108.14	113.80
1	A	2887	A	N7-C8-N9	-11.33	108.14	113.80
1	A	1760	A	N7-C8-N9	-11.33	108.14	113.80
2	B	105	A	N7-C8-N9	-11.33	108.14	113.80
32	W	902	A	N7-C8-N9	-11.33	108.14	113.80
1	A	1243	A	N7-C8-N9	-11.32	108.14	113.80
1	A	1723	A	N7-C8-N9	-11.32	108.14	113.80
32	W	945	A	N7-C8-N9	-11.32	108.14	113.80
52	z	70	A	N7-C8-N9	-11.32	108.14	113.80
1	A	462	A	N7-C8-N9	-11.32	108.14	113.80
1	A	551	A	N7-C8-N9	-11.32	108.14	113.80
1	A	1412	A	N7-C8-N9	-11.32	108.14	113.80
32	W	1206	A	N7-C8-N9	-11.32	108.14	113.80
1	A	1046	A	N7-C8-N9	-11.32	108.14	113.80
1	A	1074	A	N7-C8-N9	-11.32	108.14	113.80
1	A	1542	A	N7-C8-N9	-11.32	108.14	113.80
1	A	41	A	N7-C8-N9	-11.32	108.14	113.80
1	A	758	A	N7-C8-N9	-11.32	108.14	113.80
32	W	1014	A	N7-C8-N9	-11.32	108.14	113.80
1	A	868	A	N7-C8-N9	-11.31	108.14	113.80
1	A	1316	A	N7-C8-N9	-11.31	108.14	113.80
1	A	1721	A	N7-C8-N9	-11.31	108.14	113.80
1	A	2030	A	N7-C8-N9	-11.31	108.14	113.80
32	W	616	A	N7-C8-N9	-11.31	108.14	113.80
1	A	133	A	N7-C8-N9	-11.31	108.14	113.80
1	A	268	A	N7-C8-N9	-11.31	108.14	113.80
1	A	740	A	N7-C8-N9	-11.31	108.14	113.80
1	A	1073	A	N7-C8-N9	-11.31	108.14	113.80
1	A	1393	A	N7-C8-N9	-11.31	108.14	113.80
1	A	305	A	N7-C8-N9	-11.31	108.15	113.80
32	W	34	A	N7-C8-N9	-11.31	108.15	113.80
32	W	323	A	N7-C8-N9	-11.31	108.15	113.80
32	W	372	A	N7-C8-N9	-11.31	108.15	113.80
1	A	407	A	N7-C8-N9	-11.31	108.15	113.80
1	A	894	A	N7-C8-N9	-11.30	108.15	113.80
1	A	2619	A	N7-C8-N9	-11.31	108.15	113.80
1	A	1848	A	N7-C8-N9	-11.30	108.15	113.80
2	B	43	A	N7-C8-N9	-11.30	108.15	113.80
32	W	35	A	N7-C8-N9	-11.30	108.15	113.80
32	W	352	A	N7-C8-N9	-11.30	108.15	113.80
32	W	381	A	N7-C8-N9	-11.30	108.15	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	462	A	N7-C8-N9	-11.30	108.15	113.80
32	W	882	A	N7-C8-N9	-11.30	108.15	113.80
1	A	1029	A	N7-C8-N9	-11.30	108.15	113.80
32	W	685	A	N7-C8-N9	-11.30	108.15	113.80
1	A	1679	A	N7-C8-N9	-11.29	108.15	113.80
1	A	2389	A	N7-C8-N9	-11.30	108.15	113.80
1	A	2571	A	N7-C8-N9	-11.30	108.15	113.80
32	W	1517	A	N7-C8-N9	-11.30	108.15	113.80
32	W	271	A	N7-C8-N9	-11.29	108.15	113.80
1	A	210	A	N7-C8-N9	-11.29	108.15	113.80
1	A	117	A	N7-C8-N9	-11.29	108.16	113.80
1	A	560	A	N7-C8-N9	-11.29	108.16	113.80
32	W	209	A	N7-C8-N9	-11.29	108.16	113.80
1	A	342	A	N7-C8-N9	-11.29	108.16	113.80
1	A	1465	A	N7-C8-N9	-11.29	108.16	113.80
1	A	1838	A	N7-C8-N9	-11.29	108.16	113.80
1	A	1956	A	N7-C8-N9	-11.29	108.16	113.80
1	A	2111	A	N7-C8-N9	-11.29	108.16	113.80
1	A	517	A	N7-C8-N9	-11.29	108.16	113.80
1	A	910	A	N7-C8-N9	-11.29	108.16	113.80
32	W	314	A	N7-C8-N9	-11.28	108.16	113.80
1	A	1606	A	N7-C8-N9	-11.28	108.16	113.80
1	A	1888	A	N7-C8-N9	-11.28	108.16	113.80
1	A	828	A	N7-C8-N9	-11.28	108.16	113.80
1	A	1812	A	N7-C8-N9	-11.28	108.16	113.80
32	W	1297	A	N7-C8-N9	-11.28	108.16	113.80
1	A	162	A	N7-C8-N9	-11.28	108.16	113.80
1	A	1096	A	N7-C8-N9	-11.28	108.16	113.80
1	A	2560	A	N7-C8-N9	-11.28	108.16	113.80
1	A	2862	A	N7-C8-N9	-11.28	108.16	113.80
32	W	1166	A	N7-C8-N9	-11.28	108.16	113.80
32	W	1442	A	N7-C8-N9	-11.28	108.16	113.80
1	A	326	A	N7-C8-N9	-11.27	108.16	113.80
1	A	67	A	N7-C8-N9	-11.27	108.16	113.80
1	A	661	A	N7-C8-N9	-11.27	108.16	113.80
1	A	1541	A	N7-C8-N9	-11.27	108.17	113.80
32	W	128	A	N7-C8-N9	-11.27	108.17	113.80
1	A	479	A	N7-C8-N9	-11.27	108.17	113.80
1	A	1850	A	N7-C8-N9	-11.27	108.17	113.80
2	B	20	A	N7-C8-N9	-11.27	108.17	113.80
32	W	270	A	N7-C8-N9	-11.27	108.17	113.80
32	W	1403	A	N7-C8-N9	-11.27	108.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1308	A	N3-C4-C5	-11.27	118.92	126.80
1	A	247	A	N7-C8-N9	-11.26	108.17	113.80
1	A	469	A	N7-C8-N9	-11.26	108.17	113.80
1	A	1885	A	N7-C8-N9	-11.26	108.17	113.80
32	W	1463	A	N7-C8-N9	-11.26	108.17	113.80
32	W	631	A	N7-C8-N9	-11.26	108.17	113.80
1	A	1778	A	N7-C8-N9	-11.26	108.17	113.80
1	A	2463	A	N7-C8-N9	-11.26	108.17	113.80
32	W	459	A	N7-C8-N9	-11.26	108.17	113.80
32	W	844	A	N7-C8-N9	-11.26	108.17	113.80
1	A	431	A	N7-C8-N9	-11.26	108.17	113.80
1	A	2454	A	N7-C8-N9	-11.26	108.17	113.80
32	W	796	A	N7-C8-N9	-11.26	108.17	113.80
32	W	1128	A	N7-C8-N9	-11.26	108.17	113.80
32	W	1143	A	N7-C8-N9	-11.26	108.17	113.80
1	A	73	A	N7-C8-N9	-11.25	108.17	113.80
1	A	2441	A	N7-C8-N9	-11.25	108.17	113.80
1	A	1130	A	N7-C8-N9	-11.25	108.17	113.80
1	A	1426	A	N7-C8-N9	-11.25	108.17	113.80
1	A	1569	A	N7-C8-N9	-11.25	108.17	113.80
1	A	2497	A	N7-C8-N9	-11.25	108.17	113.80
1	A	2869	A	N7-C8-N9	-11.25	108.17	113.80
1	A	2316	A	N7-C8-N9	-11.25	108.17	113.80
2	B	113	A	N7-C8-N9	-11.25	108.17	113.80
1	A	2395	A	N7-C8-N9	-11.25	108.18	113.80
52	z	24	A	N7-C8-N9	-11.25	108.17	113.80
1	A	258	A	N7-C8-N9	-11.25	108.18	113.80
1	A	1042	A	N7-C8-N9	-11.25	108.18	113.80
1	A	1188	A	N7-C8-N9	-11.25	108.18	113.80
52	z	76	A	N7-C8-N9	-11.25	108.18	113.80
2	B	71	A	N7-C8-N9	-11.25	108.18	113.80
32	W	984	A	N7-C8-N9	-11.25	108.18	113.80
1	A	1724	A	N7-C8-N9	-11.24	108.18	113.80
1	A	1556	A	N7-C8-N9	-11.24	108.18	113.80
1	A	339	A	N7-C8-N9	-11.24	108.18	113.80
1	A	2461	A	N7-C8-N9	-11.24	108.18	113.80
1	A	1714	A	N3-C4-C5	-11.24	118.93	126.80
32	W	793	A	N7-C8-N9	-11.24	108.18	113.80
1	A	38	A	N7-C8-N9	-11.24	108.18	113.80
1	A	1421	A	N7-C8-N9	-11.24	108.18	113.80
32	W	477	A	N7-C8-N9	-11.24	108.18	113.80
32	W	1180	A	N7-C8-N9	-11.24	108.18	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	A	N7-C8-N9	-11.23	108.19	113.80
1	A	1620	A	N7-C8-N9	-11.23	108.18	113.80
32	W	397	A	N7-C8-N9	-11.23	108.18	113.80
1	A	496	A	N7-C8-N9	-11.23	108.19	113.80
32	W	929	A	N7-C8-N9	-11.23	108.19	113.80
1	A	1027	A	N7-C8-N9	-11.22	108.19	113.80
1	A	1858	A	N7-C8-N9	-11.22	108.19	113.80
1	A	2406	A	N7-C8-N9	-11.22	108.19	113.80
1	A	2595	A	N7-C8-N9	-11.22	108.19	113.80
32	W	968	A	N7-C8-N9	-11.22	108.19	113.80
1	A	52	A	N7-C8-N9	-11.22	108.19	113.80
1	A	1601	A	N7-C8-N9	-11.22	108.19	113.80
1	A	1776	A	N7-C8-N9	-11.22	108.19	113.80
1	A	1381	A	N7-C8-N9	-11.21	108.19	113.80
1	A	2106	A	N7-C8-N9	-11.21	108.19	113.80
32	W	630	A	N7-C8-N9	-11.22	108.19	113.80
1	A	2735	A	N7-C8-N9	-11.21	108.19	113.80
2	B	46	A	N7-C8-N9	-11.21	108.19	113.80
1	A	220	A	N7-C8-N9	-11.21	108.19	113.80
32	W	711	A	N7-C8-N9	-11.21	108.19	113.80
32	W	1369	A	N7-C8-N9	-11.21	108.19	113.80
1	A	391	A	N7-C8-N9	-11.21	108.20	113.80
1	A	1361	A	N7-C8-N9	-11.21	108.20	113.80
1	A	904	A	N7-C8-N9	-11.20	108.20	113.80
1	A	1456	A	N7-C8-N9	-11.21	108.20	113.80
32	W	1112	A	N7-C8-N9	-11.20	108.20	113.80
32	W	1140	A	N7-C8-N9	-11.20	108.20	113.80
32	W	1200	A	N7-C8-N9	-11.20	108.20	113.80
1	A	384	A	N7-C8-N9	-11.20	108.20	113.80
32	W	583	A	N7-C8-N9	-11.20	108.20	113.80
1	A	21	A	N7-C8-N9	-11.20	108.20	113.80
1	A	943	A	N7-C8-N9	-11.20	108.20	113.80
2	B	11	A	N7-C8-N9	-11.20	108.20	113.80
1	A	1945	A	N7-C8-N9	-11.19	108.20	113.80
1	A	2358	A	N7-C8-N9	-11.20	108.20	113.80
32	W	1372	A	N7-C8-N9	-11.20	108.20	113.80
1	A	168	A	N7-C8-N9	-11.19	108.20	113.80
32	W	1283	A	N7-C8-N9	-11.19	108.20	113.80
32	W	1478	A	N7-C8-N9	-11.19	108.20	113.80
32	W	743	A	N7-C8-N9	-11.19	108.21	113.80
32	W	993	A	N3-C4-C5	-11.19	118.97	126.80
1	A	1536	A	N7-C8-N9	-11.18	108.21	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1981	A	N7-C8-N9	-11.18	108.21	113.80
32	W	1238	A	N7-C8-N9	-11.18	108.21	113.80
1	A	369	A	N7-C8-N9	-11.18	108.21	113.80
1	A	1221	A	N7-C8-N9	-11.18	108.21	113.80
32	W	724	A	N7-C8-N9	-11.18	108.21	113.80
1	A	343	A	N7-C8-N9	-11.18	108.21	113.80
1	A	1619	A	N7-C8-N9	-11.17	108.21	113.80
32	W	161	A	N7-C8-N9	-11.17	108.21	113.80
1	A	1814	A	N7-C8-N9	-11.17	108.22	113.80
1	A	559	A	N7-C8-N9	-11.17	108.22	113.80
1	A	1480	A	N7-C8-N9	-11.17	108.22	113.80
1	A	2044	A	N7-C8-N9	-11.17	108.22	113.80
1	A	1265	A	N7-C8-N9	-11.16	108.22	113.80
1	A	2327	A	N7-C8-N9	-11.16	108.22	113.80
1	A	2339	A	N7-C8-N9	-11.16	108.22	113.80
1	A	1132	A	N7-C8-N9	-11.16	108.22	113.80
32	W	1435	A	N7-C8-N9	-11.16	108.22	113.80
1	A	279	A	N7-C8-N9	-11.15	108.22	113.80
1	A	437	A	N7-C8-N9	-11.15	108.22	113.80
1	A	2405	A	N7-C8-N9	-11.15	108.22	113.80
1	A	2831	A	N7-C8-N9	-11.15	108.22	113.80
1	A	2436	A	N7-C8-N9	-11.15	108.22	113.80
1	A	226	A	N3-C4-C5	-11.15	119.00	126.80
1	A	699	A	N7-C8-N9	-11.15	108.23	113.80
32	W	713	A	N7-C8-N9	-11.15	108.23	113.80
1	A	1579	A	N7-C8-N9	-11.14	108.23	113.80
32	W	1161	A	N7-C8-N9	-11.14	108.23	113.80
1	A	683	A	N7-C8-N9	-11.14	108.23	113.80
1	A	971	A	N7-C8-N9	-11.14	108.23	113.80
32	W	405	A	N3-C4-C5	-11.14	119.00	126.80
32	W	948	A	N7-C8-N9	-11.14	108.23	113.80
32	W	1366	A	N7-C8-N9	-11.14	108.23	113.80
1	A	1453	A	N7-C8-N9	-11.13	108.23	113.80
32	W	1272	A	N7-C8-N9	-11.14	108.23	113.80
1	A	1882	A	N7-C8-N9	-11.13	108.23	113.80
1	A	1999	A	N7-C8-N9	-11.13	108.23	113.80
1	A	658	A	N7-C8-N9	-11.13	108.24	113.80
1	A	2349	A	N7-C8-N9	-11.12	108.24	113.80
1	A	1244	A	N7-C8-N9	-11.12	108.24	113.80
1	A	1614	A	N7-C8-N9	-11.12	108.24	113.80
1	A	1506	A	N7-C8-N9	-11.12	108.24	113.80
32	W	1179	A	N7-C8-N9	-11.12	108.24	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1360	A	N7-C8-N9	-11.12	108.24	113.80
1	A	1919	A	N7-C8-N9	-11.11	108.25	113.80
2	B	13	A	N7-C8-N9	-11.11	108.24	113.80
1	A	689	A	N7-C8-N9	-11.11	108.25	113.80
1	A	790	A	N7-C8-N9	-11.11	108.25	113.80
1	A	849	A	N7-C8-N9	-11.11	108.25	113.80
1	A	925	A	N7-C8-N9	-11.11	108.25	113.80
1	A	2779	A	N7-C8-N9	-11.11	108.25	113.80
1	A	1876	A	N7-C8-N9	-11.11	108.25	113.80
1	A	2844	A	N7-C8-N9	-11.11	108.25	113.80
1	A	1021	A	N7-C8-N9	-11.10	108.25	113.80
1	A	1680	A	N7-C8-N9	-11.10	108.25	113.80
1	A	1930	A	N7-C8-N9	-11.10	108.25	113.80
1	A	673	A	N7-C8-N9	-11.10	108.25	113.80
1	A	1075	A	N7-C8-N9	-11.09	108.25	113.80
1	A	2916	A	N7-C8-N9	-11.09	108.25	113.80
32	W	911	A	N7-C8-N9	-11.09	108.25	113.80
1	A	1667	A	N7-C8-N9	-11.09	108.26	113.80
1	A	2532	A	N7-C8-N9	-11.08	108.26	113.80
1	A	935	A	N3-C4-C5	-11.08	119.05	126.80
1	A	1767	A	N7-C8-N9	-11.08	108.26	113.80
1	A	1768	A	N7-C8-N9	-11.08	108.26	113.80
1	A	616	A	N7-C8-N9	-11.07	108.26	113.80
1	A	95	A	N7-C8-N9	-11.07	108.26	113.80
1	A	2616	A	N7-C8-N9	-11.07	108.26	113.80
1	A	958	A	N7-C8-N9	-11.07	108.27	113.80
32	W	969	A	N7-C8-N9	-11.06	108.27	113.80
32	W	727	A	N7-C8-N9	-11.06	108.27	113.80
1	A	948	A	N7-C8-N9	-11.06	108.27	113.80
1	A	1697	A	N7-C8-N9	-11.06	108.27	113.80
1	A	2794	A	N7-C8-N9	-11.06	108.27	113.80
1	A	956	A	N7-C8-N9	-11.05	108.27	113.80
52	z	9	A	N7-C8-N9	-11.05	108.27	113.80
32	W	99	A	N7-C8-N9	-11.05	108.28	113.80
1	A	574	A	N7-C8-N9	-11.04	108.28	113.80
1	A	1398	A	N7-C8-N9	-11.04	108.28	113.80
32	W	1294	A	N7-C8-N9	-11.05	108.28	113.80
1	A	2593	A	N7-C8-N9	-11.04	108.28	113.80
32	W	518	A	N7-C8-N9	-11.04	108.28	113.80
32	W	1341	A	N7-C8-N9	-11.04	108.28	113.80
32	W	390	A	N7-C8-N9	-11.04	108.28	113.80
1	A	53	A	N7-C8-N9	-11.03	108.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1900	A	N7-C8-N9	-11.03	108.28	113.80
1	A	1442	A	N7-C8-N9	-11.03	108.29	113.80
1	A	2091	A	N7-C8-N9	-11.03	108.29	113.80
1	A	2296	A	N7-C8-N9	-11.03	108.29	113.80
1	A	1965	A	N7-C8-N9	-11.02	108.29	113.80
1	A	2357	A	N7-C8-N9	-11.02	108.29	113.80
1	A	2407	A	N7-C8-N9	-11.02	108.29	113.80
1	A	2468	A	N7-C8-N9	-11.02	108.29	113.80
32	W	1236	A	N7-C8-N9	-11.02	108.29	113.80
1	A	1485	A	N7-C8-N9	-11.02	108.29	113.80
32	W	548	A	N7-C8-N9	-11.01	108.30	113.80
1	A	1618	A	N7-C8-N9	-11.01	108.30	113.80
1	A	2778	A	N7-C8-N9	-11.01	108.30	113.80
1	A	908	A	N7-C8-N9	-11.01	108.30	113.80
1	A	1056	A	N7-C8-N9	-11.00	108.30	113.80
32	W	74	A	N7-C8-N9	-11.00	108.30	113.80
1	A	1340	A	N7-C8-N9	-10.99	108.30	113.80
1	A	1774	A	N7-C8-N9	-10.99	108.31	113.80
1	A	1839	A	N7-C8-N9	-10.99	108.31	113.80
1	A	765	A	N7-C8-N9	-10.98	108.31	113.80
1	A	830	A	N7-C8-N9	-10.98	108.31	113.80
1	A	656	A	N7-C8-N9	-10.98	108.31	113.80
1	A	2704	A	N7-C8-N9	-10.98	108.31	113.80
1	A	90	A	N7-C8-N9	-10.97	108.31	113.80
1	A	527	A	N7-C8-N9	-10.96	108.32	113.80
32	W	439	A	N7-C8-N9	-10.96	108.32	113.80
1	A	2459	A	N7-C8-N9	-10.96	108.32	113.80
1	A	1832	A	N7-C8-N9	-10.94	108.33	113.80
32	W	987	A	N7-C8-N9	-10.94	108.33	113.80
32	W	1155	A	N7-C8-N9	-10.94	108.33	113.80
1	A	1877	A	N7-C8-N9	-10.93	108.33	113.80
2	B	99	A	N3-C4-C5	-10.93	119.15	126.80
32	W	519	A	N7-C8-N9	-10.93	108.34	113.80
1	A	527	A	N3-C4-C5	-10.92	119.16	126.80
1	A	1655	A	N7-C8-N9	-10.92	108.34	113.80
1	A	1562	A	N7-C8-N9	-10.91	108.34	113.80
32	W	405	A	N7-C8-N9	-10.91	108.34	113.80
1	A	494	A	N7-C8-N9	-10.91	108.34	113.80
1	A	438	A	N7-C8-N9	-10.91	108.35	113.80
1	A	1928	A	N7-C8-N9	-10.90	108.35	113.80
32	W	572	A	N3-C4-C5	-10.90	119.17	126.80
1	A	2689	A	N7-C8-N9	-10.90	108.35	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2786	A	N3-C4-C5	-10.89	119.17	126.80
32	W	1234	A	N3-C4-C5	-10.89	119.17	126.80
1	A	2848	A	N7-C8-N9	-10.89	108.36	113.80
32	W	1288	A	N7-C8-N9	-10.89	108.36	113.80
1	A	678	A	N7-C8-N9	-10.89	108.36	113.80
1	A	1067	A	N7-C8-N9	-10.87	108.37	113.80
1	A	2691	A	N7-C8-N9	-10.86	108.37	113.80
32	W	1234	A	N7-C8-N9	-10.84	108.38	113.80
1	A	390	A	N7-C8-N9	-10.83	108.38	113.80
32	W	1315	A	N7-C8-N9	-10.83	108.39	113.80
1	A	1581	A	N3-C4-C5	-10.82	119.22	126.80
32	W	572	A	N7-C8-N9	-10.82	108.39	113.80
32	W	1016	A	N7-C8-N9	-10.82	108.39	113.80
32	W	1189	A	N7-C8-N9	-10.82	108.39	113.80
1	A	1820	A	N7-C8-N9	-10.82	108.39	113.80
32	W	457	A	N7-C8-N9	-10.81	108.39	113.80
1	A	913	A	N7-C8-N9	-10.81	108.40	113.80
1	A	1097	A	N7-C8-N9	-10.80	108.40	113.80
1	A	254	A	N7-C8-N9	-10.80	108.40	113.80
32	W	195	A	N7-C8-N9	-10.79	108.40	113.80
32	W	1427	A	N7-C8-N9	-10.79	108.41	113.80
32	W	195	A	N3-C4-C5	-10.76	119.27	126.80
32	W	555	A	N7-C8-N9	-10.76	108.42	113.80
32	W	1288	A	N3-C4-C5	-10.76	119.27	126.80
1	A	593	A	N3-C4-C5	-10.76	119.27	126.80
1	A	634	A	N7-C8-N9	-10.75	108.42	113.80
1	A	593	A	N7-C8-N9	-10.74	108.43	113.80
32	W	99	A	N3-C4-C5	-10.74	119.28	126.80
32	W	114	A	N7-C8-N9	-10.72	108.44	113.80
32	W	308	A	N7-C8-N9	-10.72	108.44	113.80
1	A	513	A	N3-C4-C5	-10.72	119.30	126.80
32	W	1026	A	N7-C8-N9	-10.72	108.44	113.80
1	A	1714	A	N7-C8-N9	-10.72	108.44	113.80
1	A	1491	A	N7-C8-N9	-10.71	108.44	113.80
1	A	1883	A	N7-C8-N9	-10.68	108.46	113.80
1	A	1019	A	N7-C8-N9	-10.68	108.46	113.80
1	A	913	A	N3-C4-C5	-10.66	119.34	126.80
32	W	933	A	N7-C8-N9	-10.65	108.47	113.80
1	A	390	A	N3-C4-C5	-10.63	119.36	126.80
32	W	391	A	N7-C8-N9	-10.62	108.49	113.80
1	A	935	A	N7-C8-N9	-10.62	108.49	113.80
1	A	948	A	N3-C4-C5	-10.54	119.42	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2627	A	N3-C4-C5	-10.53	119.43	126.80
32	W	987	A	N3-C4-C5	-10.53	119.43	126.80
1	A	1006	A	N3-C4-C5	-10.51	119.44	126.80
1	A	1581	A	N7-C8-N9	-10.51	108.54	113.80
1	A	254	A	N3-C4-C5	-10.51	119.44	126.80
32	W	1026	A	N3-C4-C5	-10.50	119.45	126.80
1	A	2885	A	N7-C8-N9	-10.48	108.56	113.80
1	A	1667	A	N3-C4-C5	-10.48	119.47	126.80
1	A	2459	A	N3-C4-C5	-10.48	119.47	126.80
1	A	1006	A	N7-C8-N9	-10.47	108.56	113.80
32	W	1341	A	N3-C4-C5	-10.47	119.47	126.80
32	W	114	A	N3-C4-C5	-10.47	119.47	126.80
1	A	732	A	N3-C4-C5	-10.46	119.48	126.80
1	A	1778	A	N3-C4-C5	-10.45	119.49	126.80
1	A	1360	A	N3-C4-C5	-10.45	119.49	126.80
1	A	2786	A	N7-C8-N9	-10.44	108.58	113.80
1	A	108	A	N3-C4-C5	-10.44	119.49	126.80
32	W	727	A	N3-C4-C5	-10.44	119.49	126.80
1	A	437	A	N3-C4-C5	-10.44	119.50	126.80
1	A	2407	A	N3-C4-C5	-10.43	119.50	126.80
1	A	634	A	N3-C4-C5	-10.42	119.51	126.80
32	W	308	A	N3-C4-C5	-10.42	119.51	126.80
32	W	391	A	N3-C4-C5	-10.41	119.51	126.80
2	B	11	A	N3-C4-C5	-10.41	119.51	126.80
1	A	1491	A	N3-C4-C5	-10.40	119.52	126.80
1	A	2844	A	N3-C4-C5	-10.40	119.52	126.80
1	A	2885	A	N3-C4-C5	-10.39	119.53	126.80
1	A	365	U	P-O3'-C3'	-10.39	107.23	119.70
1	A	736	A	N3-C4-C5	-10.39	119.53	126.80
1	A	1073	A	N3-C4-C5	-10.39	119.53	126.80
1	A	2735	A	N3-C4-C5	-10.38	119.53	126.80
1	A	2794	A	N3-C4-C5	-10.38	119.54	126.80
1	A	1562	A	N3-C4-C5	-10.38	119.54	126.80
1	A	2339	A	N3-C4-C5	-10.37	119.54	126.80
1	A	1480	A	N3-C4-C5	-10.37	119.54	126.80
1	A	551	A	N3-C4-C5	-10.36	119.55	126.80
1	A	910	A	N3-C4-C5	-10.36	119.55	126.80
32	W	933	A	N3-C4-C5	-10.36	119.55	126.80
1	A	1877	A	N3-C4-C5	-10.36	119.55	126.80
1	A	1485	A	N3-C4-C5	-10.35	119.55	126.80
32	W	1308	A	N7-C8-N9	-10.35	108.62	113.80
1	A	679	A	N3-C4-C5	-10.35	119.56	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	649	A	N3-C4-C5	-10.33	119.57	126.80
1	A	1398	A	N3-C4-C5	-10.32	119.57	126.80
1	A	679	A	N7-C8-N9	-10.31	108.64	113.80
2	B	46	A	N3-C4-C5	-10.31	119.58	126.80
32	W	1278	A	N7-C8-N9	-10.30	108.65	113.80
1	A	1132	A	N3-C4-C5	-10.30	119.59	126.80
1	A	1638	A	N3-C4-C5	-10.30	119.59	126.80
1	A	130	A	N3-C4-C5	-10.27	119.61	126.80
32	W	74	A	N3-C4-C5	-10.27	119.61	126.80
1	A	1506	A	N3-C4-C5	-10.27	119.61	126.80
1	A	732	A	N7-C8-N9	-10.27	108.67	113.80
1	A	2862	A	N3-C4-C5	-10.27	119.61	126.80
32	W	128	A	N3-C4-C5	-10.27	119.61	126.80
1	A	2402	A	N3-C4-C5	-10.26	119.62	126.80
1	A	2627	A	N7-C8-N9	-10.26	108.67	113.80
1	A	226	A	N7-C8-N9	-10.26	108.67	113.80
1	A	438	A	N3-C4-C5	-10.26	119.62	126.80
32	W	1155	A	N3-C4-C5	-10.25	119.62	126.80
1	A	1096	A	N3-C4-C5	-10.25	119.62	126.80
1	A	513	A	N7-C8-N9	-10.24	108.68	113.80
1	A	656	A	N3-C4-C5	-10.24	119.63	126.80
1	A	1839	A	N3-C4-C5	-10.24	119.63	126.80
1	A	1222	A	N3-C4-C5	-10.23	119.64	126.80
1	A	1900	A	N3-C4-C5	-10.23	119.64	126.80
1	A	1490	A	N3-C4-C5	-10.23	119.64	126.80
32	W	993	A	N7-C8-N9	-10.23	108.69	113.80
32	W	1160	A	N3-C4-C5	-10.23	119.64	126.80
1	A	2532	A	N3-C4-C5	-10.23	119.64	126.80
1	A	1442	A	N3-C4-C5	-10.22	119.64	126.80
32	W	397	A	N3-C4-C5	-10.22	119.64	126.80
1	A	185	A	N3-C4-C5	-10.22	119.65	126.80
1	A	95	A	N3-C4-C5	-10.22	119.65	126.80
32	W	1166	A	N3-C4-C5	-10.22	119.65	126.80
1	A	1858	A	N3-C4-C5	-10.21	119.65	126.80
1	A	1619	A	N3-C4-C5	-10.21	119.65	126.80
1	A	559	A	N3-C4-C5	-10.21	119.65	126.80
1	A	715	A	N3-C4-C5	-10.20	119.66	126.80
2	B	13	A	N3-C4-C5	-10.20	119.66	126.80
1	A	2329	A	N3-C4-C5	-10.20	119.66	126.80
1	A	1103	A	N3-C4-C5	-10.19	119.67	126.80
32	W	1278	A	N3-C4-C5	-10.18	119.67	126.80
52	z	9	A	N3-C4-C5	-10.18	119.67	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2027	A	N3-C4-C5	-10.18	119.67	126.80
1	A	168	A	N3-C4-C5	-10.18	119.67	126.80
1	A	2358	A	N3-C4-C5	-10.18	119.67	126.80
1	A	2689	A	N3-C4-C5	-10.18	119.68	126.80
1	A	1392	A	N3-C4-C5	-10.17	119.68	126.80
1	A	52	A	N3-C4-C5	-10.17	119.68	126.80
1	A	690	A	N3-C4-C5	-10.17	119.68	126.80
1	A	2790	A	N3-C4-C5	-10.16	119.69	126.80
52	z	24	A	N3-C4-C5	-10.16	119.69	126.80
1	A	765	A	N3-C4-C5	-10.16	119.69	126.80
1	A	2111	A	N3-C4-C5	-10.16	119.69	126.80
32	W	337	A	N3-C4-C5	-10.16	119.69	126.80
1	A	2694	A	N3-C4-C5	-10.15	119.69	126.80
32	W	1427	A	N3-C4-C5	-10.15	119.69	126.80
32	W	1517	A	N3-C4-C5	-10.15	119.69	126.80
1	A	2812	A	N3-C4-C5	-10.15	119.69	126.80
1	A	1536	A	N3-C4-C5	-10.15	119.69	126.80
1	A	2106	A	N3-C4-C5	-10.15	119.69	126.80
1	A	560	A	N3-C4-C5	-10.15	119.70	126.80
1	A	1618	A	N3-C4-C5	-10.15	119.70	126.80
1	A	1005	A	N3-C4-C5	-10.15	119.70	126.80
1	A	2691	A	N3-C4-C5	-10.14	119.70	126.80
1	A	44	A	N3-C4-C5	-10.14	119.70	126.80
1	A	689	A	N3-C4-C5	-10.14	119.70	126.80
1	A	2831	A	N3-C4-C5	-10.14	119.70	126.80
1	A	56	A	N3-C4-C5	-10.14	119.70	126.80
1	A	1691	A	N7-C8-N9	-10.13	108.73	113.80
32	W	711	A	N3-C4-C5	-10.13	119.71	126.80
32	W	282	A	N3-C4-C5	-10.13	119.71	126.80
1	A	2343	A	N3-C4-C5	-10.12	119.71	126.80
2	B	71	A	N3-C4-C5	-10.13	119.71	126.80
1	A	1999	A	N3-C4-C5	-10.12	119.71	126.80
32	W	1179	A	N3-C4-C5	-10.12	119.71	126.80
1	A	2026	A	N3-C4-C5	-10.12	119.72	126.80
1	A	2349	A	N3-C4-C5	-10.12	119.72	126.80
1	A	407	A	N3-C4-C5	-10.12	119.72	126.80
1	A	1094	A	N3-C4-C5	-10.12	119.72	126.80
1	A	265	A	N3-C4-C5	-10.11	119.72	126.80
1	A	1709	A	N3-C4-C5	-10.11	119.72	126.80
1	A	970	A	N3-C4-C5	-10.11	119.72	126.80
32	W	913	A	N3-C4-C5	-10.11	119.72	126.80
32	W	507	A	N3-C4-C5	-10.11	119.72	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	391	A	N3-C4-C5	-10.11	119.72	126.80
1	A	1816	A	N3-C4-C5	-10.11	119.72	126.80
32	W	948	A	N3-C4-C5	-10.11	119.72	126.80
32	W	1143	A	N3-C4-C5	-10.11	119.72	126.80
1	A	1820	A	N3-C4-C5	-10.11	119.72	126.80
32	W	57	A	N3-C4-C5	-10.11	119.73	126.80
32	W	1315	A	N3-C4-C5	-10.11	119.73	126.80
1	A	1258	A	N3-C4-C5	-10.10	119.73	126.80
1	A	1524	A	N3-C4-C5	-10.10	119.73	126.80
1	A	1655	A	N3-C4-C5	-10.10	119.73	126.80
32	W	1065	A	N3-C4-C5	-10.10	119.73	126.80
1	A	673	A	N3-C4-C5	-10.10	119.73	126.80
1	A	1286	A	N3-C4-C5	-10.10	119.73	126.80
1	A	2826	A	N3-C4-C5	-10.10	119.73	126.80
1	A	2043	A	N3-C4-C5	-10.10	119.73	126.80
32	W	844	A	N3-C4-C5	-10.10	119.73	126.80
1	A	133	A	N3-C4-C5	-10.09	119.73	126.80
1	A	2560	A	N3-C4-C5	-10.09	119.74	126.80
32	W	911	A	N3-C4-C5	-10.09	119.74	126.80
1	A	574	A	N3-C4-C5	-10.09	119.74	126.80
32	W	945	A	N3-C4-C5	-10.09	119.74	126.80
1	A	38	A	N3-C4-C5	-10.09	119.74	126.80
1	A	1710	A	N3-C4-C5	-10.09	119.74	126.80
1	A	2663	A	N3-C4-C5	-10.09	119.74	126.80
1	A	156	A	N3-C4-C5	-10.08	119.75	126.80
1	A	549	A	N3-C4-C5	-10.08	119.75	126.80
32	W	721	A	N3-C4-C5	-10.08	119.75	126.80
1	A	258	A	N3-C4-C5	-10.07	119.75	126.80
1	A	1019	A	N3-C4-C5	-10.07	119.75	126.80
1	A	1653	A	N3-C4-C5	-10.07	119.75	126.80
32	W	996	A	N3-C4-C5	-10.07	119.75	126.80
32	W	1236	A	N3-C4-C5	-10.07	119.75	126.80
1	A	538	A	N3-C4-C5	-10.07	119.75	126.80
1	A	849	A	N3-C4-C5	-10.07	119.75	126.80
1	A	1695	A	N3-C4-C5	-10.07	119.75	126.80
1	A	353	A	N3-C4-C5	-10.06	119.75	126.80
1	A	1426	A	N3-C4-C5	-10.06	119.75	126.80
1	A	231	A	N3-C4-C5	-10.06	119.76	126.80
1	A	1876	A	N3-C4-C5	-10.06	119.76	126.80
1	A	456	A	N3-C4-C5	-10.06	119.76	126.80
1	A	1046	A	N3-C4-C5	-10.06	119.76	126.80
1	A	2351	A	N3-C4-C5	-10.06	119.76	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	630	A	N3-C4-C5	-10.06	119.76	126.80
32	W	959	A	N3-C4-C5	-10.06	119.76	126.80
1	A	530	A	N3-C4-C5	-10.05	119.76	126.80
1	A	1776	A	N3-C4-C5	-10.05	119.76	126.80
1	A	2049	A	N3-C4-C5	-10.05	119.76	126.80
32	W	140	A	N3-C4-C5	-10.05	119.76	126.80
32	W	605	A	N3-C4-C5	-10.05	119.76	126.80
32	W	1178	A	N3-C4-C5	-10.05	119.76	126.80
1	A	957	A	N3-C4-C5	-10.05	119.77	126.80
1	A	1074	A	N3-C4-C5	-10.05	119.77	126.80
1	A	1316	A	N3-C4-C5	-10.05	119.77	126.80
32	W	1272	A	N3-C4-C5	-10.04	119.77	126.80
32	W	1493	A	N3-C4-C5	-10.05	119.77	126.80
1	A	894	A	N3-C4-C5	-10.04	119.77	126.80
32	W	364	A	N3-C4-C5	-10.04	119.77	126.80
32	W	811	A	N3-C4-C5	-10.04	119.77	126.80
1	A	925	A	N3-C4-C5	-10.04	119.77	126.80
32	W	129	A	N3-C4-C5	-10.04	119.77	126.80
32	W	1016	A	N3-C4-C5	-10.04	119.77	126.80
1	A	1885	A	N3-C4-C5	-10.04	119.78	126.80
32	W	462	A	N3-C4-C5	-10.04	119.78	126.80
32	W	978	A	N3-C4-C5	-10.04	119.77	126.80
32	W	1369	A	N3-C4-C5	-10.03	119.78	126.80
1	A	578	A	N3-C4-C5	-10.03	119.78	126.80
32	W	1256	A	N3-C4-C5	-10.03	119.78	126.80
1	A	661	A	N3-C4-C5	-10.03	119.78	126.80
32	W	1004	A	N3-C4-C5	-10.03	119.78	126.80
1	A	318	A	N3-C4-C5	-10.03	119.78	126.80
1	A	469	A	N3-C4-C5	-10.03	119.78	126.80
1	A	1174	A	N3-C4-C5	-10.03	119.78	126.80
1	A	882	A	N3-C4-C5	-10.02	119.78	126.80
1	A	2662	A	N3-C4-C5	-10.02	119.78	126.80
1	A	2722	A	N3-C4-C5	-10.02	119.78	126.80
1	A	2830	A	N3-C4-C5	-10.02	119.78	126.80
52	z	70	A	N3-C4-C5	-10.02	119.78	126.80
32	W	671	A	N3-C4-C5	-10.02	119.79	126.80
1	A	518	A	N3-C4-C5	-10.02	119.79	126.80
1	A	790	A	N3-C4-C5	-10.02	119.79	126.80
32	W	301	A	N3-C4-C5	-10.02	119.79	126.80
32	W	790	A	N3-C4-C5	-10.02	119.79	126.80
32	W	1478	A	N3-C4-C5	-10.02	119.79	126.80
1	A	1556	A	N3-C4-C5	-10.02	119.79	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	984	A	N3-C4-C5	-10.02	119.79	126.80
32	W	956	A	N3-C4-C5	-10.02	119.79	126.80
1	A	2270	A	N3-C4-C5	-10.01	119.79	126.80
1	A	2395	A	N3-C4-C5	-10.01	119.79	126.80
32	W	72	A	N3-C4-C5	-10.01	119.79	126.80
32	W	76	A	N3-C4-C5	-10.01	119.79	126.80
32	W	838	A	N3-C4-C5	-10.01	119.79	126.80
32	W	1189	A	N3-C4-C5	-10.01	119.79	126.80
1	A	1190	A	N3-C4-C5	-10.01	119.79	126.80
1	A	2700	A	N3-C4-C5	-10.01	119.79	126.80
32	W	1359	A	N3-C4-C5	-10.01	119.79	126.80
1	A	171	A	N3-C4-C5	-10.01	119.79	126.80
1	A	2924	A	N3-C4-C5	-10.01	119.79	126.80
32	W	1435	A	N3-C4-C5	-10.01	119.79	126.80
1	A	275	A	N3-C4-C5	-10.01	119.80	126.80
1	A	866	A	N3-C4-C5	-10.01	119.79	126.80
1	A	943	A	N3-C4-C5	-10.01	119.80	126.80
1	A	1883	A	N3-C4-C5	-10.01	119.80	126.80
1	A	2369	A	N3-C4-C5	-10.01	119.80	126.80
1	A	623	A	N3-C4-C5	-10.00	119.80	126.80
1	A	724	A	N3-C4-C5	-10.00	119.80	126.80
1	A	2317	A	N3-C4-C5	-10.00	119.80	126.80
1	A	2436	A	N3-C4-C5	-10.00	119.80	126.80
2	B	97	A	N3-C4-C5	-10.00	119.80	126.80
1	A	326	A	N3-C4-C5	-10.00	119.80	126.80
32	W	1455	A	N3-C4-C5	-10.00	119.80	126.80
1	A	376	A	N3-C4-C5	-10.00	119.80	126.80
1	A	678	A	N3-C4-C5	-10.00	119.80	126.80
32	W	882	A	N3-C4-C5	-10.00	119.80	126.80
1	A	616	A	N3-C4-C5	-9.99	119.80	126.80
1	A	2461	A	N3-C4-C5	-9.99	119.80	126.80
1	A	41	A	N3-C4-C5	-9.99	119.81	126.80
32	W	335	A	N3-C4-C5	-9.99	119.81	126.80
32	W	902	A	N3-C4-C5	-9.99	119.81	126.80
1	A	1075	A	N3-C4-C5	-9.99	119.81	126.80
1	A	1210	A	N3-C4-C5	-9.99	119.81	126.80
1	A	2769	A	N3-C4-C5	-9.99	119.81	126.80
32	W	55	A	N3-C4-C5	-9.99	119.81	126.80
32	W	793	A	N3-C4-C5	-9.99	119.81	126.80
1	A	1253	A	N3-C4-C5	-9.98	119.81	126.80
1	A	1483	A	N3-C4-C5	-9.98	119.81	126.80
1	A	2066	A	N3-C4-C5	-9.98	119.81	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2500	A	N3-C4-C5	-9.98	119.81	126.80
1	A	2845	A	N3-C4-C5	-9.98	119.81	126.80
1	A	2848	A	N3-C4-C5	-9.98	119.81	126.80
1	A	1357	A	N3-C4-C5	-9.97	119.82	126.80
1	A	1727	A	N3-C4-C5	-9.97	119.82	126.80
1	A	2052	A	N3-C4-C5	-9.97	119.82	126.80
32	W	34	A	N3-C4-C5	-9.97	119.82	126.80
32	W	1112	A	N3-C4-C5	-9.97	119.82	126.80
1	A	2854	A	N3-C4-C5	-9.97	119.82	126.80
32	W	1297	A	N3-C4-C5	-9.97	119.82	126.80
1	A	431	A	N3-C4-C5	-9.97	119.82	126.80
1	A	1361	A	N3-C4-C5	-9.97	119.82	126.80
1	A	1406	A	N3-C4-C5	-9.96	119.82	126.80
1	A	1831	A	N3-C4-C5	-9.97	119.82	126.80
1	A	2919	A	N3-C4-C5	-9.96	119.83	126.80
52	z	41	A	N3-C4-C5	-9.96	119.83	126.80
1	A	384	A	N3-C4-C5	-9.96	119.83	126.80
1	A	1405	A	N3-C4-C5	-9.96	119.83	126.80
2	B	18	A	N3-C4-C5	-9.96	119.83	126.80
1	A	500	A	N3-C4-C5	-9.96	119.83	126.80
1	A	692	A	N3-C4-C5	-9.96	119.83	126.80
1	A	867	A	N3-C4-C5	-9.96	119.83	126.80
1	A	952	A	N3-C4-C5	-9.96	119.83	126.80
1	A	956	A	N3-C4-C5	-9.96	119.83	126.80
1	A	1393	A	N3-C4-C5	-9.96	119.83	126.80
1	A	2643	A	N3-C4-C5	-9.96	119.83	126.80
1	A	2668	A	N3-C4-C5	-9.96	119.83	126.80
32	W	1442	A	N3-C4-C5	-9.96	119.83	126.80
1	A	61	A	N3-C4-C5	-9.96	119.83	126.80
1	A	974	A	N3-C4-C5	-9.96	119.83	126.80
1	A	1945	A	N3-C4-C5	-9.96	119.83	126.80
32	W	1425	A	N3-C4-C5	-9.96	119.83	126.80
1	A	206	A	N3-C4-C5	-9.96	119.83	126.80
1	A	1233	A	N3-C4-C5	-9.96	119.83	126.80
1	A	1532	A	N3-C4-C5	-9.96	119.83	126.80
1	A	1672	A	N3-C4-C5	-9.96	119.83	126.80
1	A	1895	A	N3-C4-C5	-9.96	119.83	126.80
32	W	404	A	N3-C4-C5	-9.96	119.83	126.80
1	A	2517	A	N3-C4-C5	-9.95	119.83	126.80
1	A	179	A	N3-C4-C5	-9.95	119.83	126.80
1	A	592	A	N3-C4-C5	-9.95	119.83	126.80
1	A	1260	A	N3-C4-C5	-9.95	119.83	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2779	A	N3-C4-C5	-9.95	119.83	126.80
1	A	1284	A	N3-C4-C5	-9.95	119.83	126.80
1	A	1774	A	N3-C4-C5	-9.95	119.84	126.80
1	A	2447	A	N3-C4-C5	-9.95	119.84	126.80
32	W	1523	A	N3-C4-C5	-9.95	119.84	126.80
1	A	1126	A	N3-C4-C5	-9.95	119.84	126.80
1	A	1254	A	N3-C4-C5	-9.95	119.84	126.80
32	W	875	A	N3-C4-C5	-9.95	119.84	126.80
1	A	1375	A	N3-C4-C5	-9.94	119.84	126.80
1	A	1461	A	N3-C4-C5	-9.94	119.84	126.80
1	A	1685	A	N3-C4-C5	-9.94	119.84	126.80
1	A	1421	A	N3-C4-C5	-9.94	119.84	126.80
1	A	1424	A	N3-C4-C5	-9.94	119.84	126.80
32	W	522	A	N3-C4-C5	-9.94	119.84	126.80
1	A	1100	A	N3-C4-C5	-9.94	119.84	126.80
1	A	1663	A	N3-C4-C5	-9.94	119.84	126.80
1	A	2754	A	N3-C4-C5	-9.94	119.84	126.80
1	A	2827	A	N3-C4-C5	-9.94	119.84	126.80
2	B	50	A	N3-C4-C5	-9.94	119.84	126.80
1	A	1464	A	N3-C4-C5	-9.94	119.84	126.80
1	A	1767	A	N3-C4-C5	-9.94	119.84	126.80
1	A	2365	A	N3-C4-C5	-9.94	119.85	126.80
32	W	381	A	N3-C4-C5	-9.94	119.84	126.80
32	W	1284	A	N3-C4-C5	-9.94	119.84	126.80
1	A	870	A	N3-C4-C5	-9.93	119.85	126.80
1	A	2302	A	N3-C4-C5	-9.93	119.85	126.80
1	A	2704	A	N3-C4-C5	-9.93	119.85	126.80
1	A	1614	A	N3-C4-C5	-9.93	119.85	126.80
1	A	278	A	N3-C4-C5	-9.93	119.85	126.80
1	A	1388	A	N3-C4-C5	-9.93	119.85	126.80
1	A	2338	A	N3-C4-C5	-9.93	119.85	126.80
32	W	344	A	N3-C4-C5	-9.93	119.85	126.80
32	W	555	A	N3-C4-C5	-9.93	119.85	126.80
32	W	617	A	N3-C4-C5	-9.93	119.85	126.80
32	W	1437	A	N3-C4-C5	-9.93	119.85	126.80
1	A	305	A	N3-C4-C5	-9.93	119.85	126.80
1	A	1029	A	N3-C4-C5	-9.93	119.85	126.80
32	W	496	A	N3-C4-C5	-9.93	119.85	126.80
32	W	743	A	N3-C4-C5	-9.93	119.85	126.80
1	A	964	A	N3-C4-C5	-9.93	119.85	126.80
32	W	979	A	N3-C4-C5	-9.93	119.85	126.80
1	A	91	A	N3-C4-C5	-9.92	119.85	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1269	A	N3-C4-C5	-9.92	119.85	126.80
32	W	771	A	N3-C4-C5	-9.92	119.85	126.80
32	W	333	A	N3-C4-C5	-9.92	119.86	126.80
32	W	1502	A	N3-C4-C5	-9.92	119.85	126.80
1	A	889	A	N3-C4-C5	-9.92	119.86	126.80
1	A	1947	A	N3-C4-C5	-9.92	119.86	126.80
1	A	1813	A	N3-C4-C5	-9.92	119.86	126.80
1	A	1918	A	N3-C4-C5	-9.92	119.86	126.80
1	A	1998	A	N3-C4-C5	-9.92	119.86	126.80
32	W	61	A	N3-C4-C5	-9.92	119.86	126.80
32	W	139	A	N3-C4-C5	-9.92	119.86	126.80
32	W	548	A	N3-C4-C5	-9.92	119.86	126.80
32	W	638	A	N3-C4-C5	-9.92	119.86	126.80
1	A	1520	A	N3-C4-C5	-9.92	119.86	126.80
32	W	758	A	N3-C4-C5	-9.92	119.86	126.80
32	W	1222	A	N3-C4-C5	-9.92	119.86	126.80
1	A	117	A	N3-C4-C5	-9.91	119.86	126.80
1	A	971	A	N3-C4-C5	-9.91	119.86	126.80
1	A	1588	A	N3-C4-C5	-9.91	119.86	126.80
1	A	1845	A	N3-C4-C5	-9.91	119.86	126.80
1	A	2007	A	N3-C4-C5	-9.91	119.86	126.80
1	A	486	A	N3-C4-C5	-9.91	119.86	126.80
1	A	1055	A	N3-C4-C5	-9.91	119.86	126.80
1	A	1848	A	N3-C4-C5	-9.91	119.86	126.80
1	A	1995	A	N3-C4-C5	-9.91	119.86	126.80
2	B	114	A	N3-C4-C5	-9.91	119.86	126.80
1	A	2547	A	N3-C4-C5	-9.91	119.86	126.80
1	A	896	A	N3-C4-C5	-9.91	119.86	126.80
1	A	1235	A	N3-C4-C5	-9.91	119.86	126.80
32	W	659	A	N3-C4-C5	-9.91	119.86	126.80
1	A	2619	A	N3-C4-C5	-9.91	119.87	126.80
32	W	390	A	N3-C4-C5	-9.91	119.87	126.80
32	W	705	A	N3-C4-C5	-9.91	119.86	126.80
32	W	768	A	N3-C4-C5	-9.91	119.87	126.80
32	W	1238	A	N3-C4-C5	-9.91	119.87	126.80
1	A	652	A	N3-C4-C5	-9.90	119.87	126.80
1	A	1981	A	N3-C4-C5	-9.90	119.87	126.80
1	A	2719	A	N3-C4-C5	-9.90	119.87	126.80
32	W	234	A	N3-C4-C5	-9.90	119.87	126.80
32	W	452	A	N3-C4-C5	-9.90	119.87	126.80
32	W	346	A	N3-C4-C5	-9.90	119.87	126.80
32	W	1147	A	N3-C4-C5	-9.90	119.87	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	193	A	N3-C4-C5	-9.90	119.87	126.80
1	A	705	A	N3-C4-C5	-9.90	119.87	126.80
1	A	1636	A	N3-C4-C5	-9.90	119.87	126.80
1	A	2893	A	N3-C4-C5	-9.90	119.87	126.80
1	A	752	A	N3-C4-C5	-9.90	119.87	126.80
32	W	161	A	N3-C4-C5	-9.90	119.87	126.80
32	W	518	A	N3-C4-C5	-9.90	119.87	126.80
32	W	1206	A	N3-C4-C5	-9.90	119.87	126.80
1	A	851	A	N3-C4-C5	-9.90	119.87	126.80
1	A	1838	A	N3-C4-C5	-9.90	119.87	126.80
1	A	470	A	N3-C4-C5	-9.90	119.87	126.80
1	A	1680	A	N3-C4-C5	-9.90	119.87	126.80
1	A	1735	A	N3-C4-C5	-9.90	119.87	126.80
32	W	506	A	N3-C4-C5	-9.90	119.87	126.80
1	A	2091	A	N3-C4-C5	-9.90	119.87	126.80
1	A	2389	A	N3-C4-C5	-9.90	119.87	126.80
32	W	173	A	N3-C4-C5	-9.90	119.87	126.80
1	A	462	A	N3-C4-C5	-9.89	119.88	126.80
1	A	517	A	N3-C4-C5	-9.89	119.87	126.80
1	A	2570	A	N3-C4-C5	-9.89	119.87	126.80
32	W	433	A	N3-C4-C5	-9.89	119.87	126.80
32	W	225	A	N3-C4-C5	-9.89	119.88	126.80
1	A	200	A	N3-C4-C5	-9.89	119.88	126.80
1	A	1194	A	N3-C4-C5	-9.89	119.88	126.80
1	A	1617	A	N3-C4-C5	-9.89	119.88	126.80
2	B	64	A	N3-C4-C5	-9.89	119.88	126.80
1	A	1956	A	N3-C4-C5	-9.89	119.88	126.80
1	A	2100	A	N3-C4-C5	-9.89	119.88	126.80
32	W	1384	A	N3-C4-C5	-9.89	119.88	126.80
1	A	2047	A	N3-C4-C5	-9.89	119.88	126.80
32	W	1510	A	N3-C4-C5	-9.89	119.88	126.80
1	A	260	A	N3-C4-C5	-9.88	119.88	126.80
1	A	600	A	N3-C4-C5	-9.88	119.88	126.80
1	A	1097	A	N3-C4-C5	-9.89	119.88	126.80
32	W	1115	A	N3-C4-C5	-9.89	119.88	126.80
1	A	908	A	N3-C4-C5	-9.88	119.88	126.80
1	A	1627	A	N3-C4-C5	-9.88	119.88	126.80
1	A	1025	A	N3-C4-C5	-9.88	119.88	126.80
1	A	1541	A	N3-C4-C5	-9.88	119.88	126.80
1	A	1686	A	N3-C4-C5	-9.88	119.88	126.80
32	W	423	A	N3-C4-C5	-9.88	119.88	126.80
1	A	2032	A	N3-C4-C5	-9.88	119.88	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	677	A	N3-C4-C5	-9.88	119.88	126.80
32	W	1490	A	N3-C4-C5	-9.88	119.88	126.80
1	A	21	A	N3-C4-C5	-9.88	119.89	126.80
1	A	154	A	N3-C4-C5	-9.88	119.89	126.80
1	A	449	A	N3-C4-C5	-9.88	119.89	126.80
1	A	922	A	N3-C4-C5	-9.88	119.89	126.80
32	W	737	A	N3-C4-C5	-9.88	119.89	126.80
1	A	2044	A	N3-C4-C5	-9.88	119.89	126.80
1	A	94	A	N3-C4-C5	-9.87	119.89	126.80
1	A	1056	A	N3-C4-C5	-9.88	119.89	126.80
1	A	1677	A	N3-C4-C5	-9.87	119.89	126.80
32	W	35	A	N3-C4-C5	-9.88	119.89	126.80
32	W	968	A	N3-C4-C5	-9.88	119.89	126.80
32	W	1259	A	N3-C4-C5	-9.88	119.89	126.80
1	A	830	A	N3-C4-C5	-9.87	119.89	126.80
32	W	1024	A	N3-C4-C5	-9.87	119.89	126.80
1	A	1746	A	N3-C4-C5	-9.87	119.89	126.80
1	A	548	A	N3-C4-C5	-9.87	119.89	126.80
1	A	622	A	N3-C4-C5	-9.87	119.89	126.80
1	A	781	A	N3-C4-C5	-9.87	119.89	126.80
32	W	477	A	N3-C4-C5	-9.87	119.89	126.80
1	A	1965	A	N3-C4-C5	-9.87	119.89	126.80
1	A	2462	A	N3-C4-C5	-9.87	119.89	126.80
32	W	372	A	N3-C4-C5	-9.87	119.89	126.80
32	W	685	A	N3-C4-C5	-9.87	119.89	126.80
32	W	801	A	N3-C4-C5	-9.87	119.89	126.80
32	W	1486	A	N3-C4-C5	-9.87	119.89	126.80
1	A	281	A	N3-C4-C5	-9.87	119.89	126.80
1	A	479	A	N3-C4-C5	-9.87	119.89	126.80
1	A	722	A	N3-C4-C5	-9.87	119.89	126.80
1	A	2087	A	N3-C4-C5	-9.87	119.89	126.80
1	A	2834	A	N3-C4-C5	-9.87	119.89	126.80
1	A	1130	A	N3-C4-C5	-9.86	119.89	126.80
32	W	1366	A	N3-C4-C5	-9.86	119.89	126.80
1	A	412	A	N3-C4-C5	-9.86	119.90	126.80
1	A	1456	A	N3-C4-C5	-9.86	119.90	126.80
1	A	1882	A	N3-C4-C5	-9.86	119.90	126.80
1	A	1404	A	N3-C4-C5	-9.86	119.90	126.80
1	A	1575	A	N3-C4-C5	-9.86	119.90	126.80
1	A	2421	A	N3-C4-C5	-9.86	119.90	126.80
1	A	2805	A	N3-C4-C5	-9.86	119.90	126.80
1	A	2846	A	N3-C4-C5	-9.86	119.90	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	715	A	N3-C4-C5	-9.86	119.90	126.80
1	A	1928	A	N3-C4-C5	-9.86	119.90	126.80
32	W	918	A	N3-C4-C5	-9.86	119.90	126.80
1	A	324	A	N3-C4-C5	-9.86	119.90	126.80
1	A	429	A	N3-C4-C5	-9.86	119.90	126.80
1	A	524	A	N3-C4-C5	-9.86	119.90	126.80
1	A	2034	A	N3-C4-C5	-9.86	119.90	126.80
1	A	2042	A	N3-C4-C5	-9.86	119.90	126.80
1	A	2889	A	N3-C4-C5	-9.86	119.90	126.80
1	A	161	A	N3-C4-C5	-9.85	119.90	126.80
1	A	1059	A	N3-C4-C5	-9.85	119.90	126.80
1	A	2869	A	N3-C4-C5	-9.85	119.90	126.80
1	A	339	A	N3-C4-C5	-9.85	119.91	126.80
1	A	496	A	N3-C4-C5	-9.85	119.90	126.80
1	A	507	A	N3-C4-C5	-9.85	119.90	126.80
1	A	1615	A	N3-C4-C5	-9.85	119.91	126.80
32	W	658	A	N3-C4-C5	-9.85	119.90	126.80
32	W	917	A	N3-C4-C5	-9.85	119.90	126.80
32	W	1128	A	N3-C4-C5	-9.85	119.91	126.80
32	W	1403	A	N3-C4-C5	-9.85	119.90	126.80
1	A	2083	A	N3-C4-C5	-9.85	119.91	126.80
1	A	2464	A	N3-C4-C5	-9.85	119.91	126.80
1	A	259	A	N3-C4-C5	-9.85	119.91	126.80
1	A	330	A	N3-C4-C5	-9.85	119.91	126.80
1	A	699	A	N3-C4-C5	-9.85	119.91	126.80
1	A	868	A	N3-C4-C5	-9.85	119.91	126.80
1	A	1631	A	N3-C4-C5	-9.85	119.91	126.80
32	W	1349	A	N3-C4-C5	-9.85	119.91	126.80
1	A	2497	A	N3-C4-C5	-9.85	119.91	126.80
32	W	361	A	N3-C4-C5	-9.85	119.91	126.80
52	z	21	A	N3-C4-C5	-9.85	119.91	126.80
1	A	1760	A	N3-C4-C5	-9.85	119.91	126.80
2	B	99	A	N7-C8-N9	-9.85	108.88	113.80
32	W	190	A	N3-C4-C5	-9.85	119.91	126.80
32	W	674	A	N3-C4-C5	-9.85	119.91	126.80
32	W	1320	A	N3-C4-C5	-9.85	119.91	126.80
32	W	1348	A	N3-C4-C5	-9.85	119.91	126.80
32	W	270	A	N3-C4-C5	-9.85	119.91	126.80
32	W	382	A	N3-C4-C5	-9.85	119.91	126.80
52	z	58	A	N3-C4-C5	-9.84	119.91	126.80
1	A	307	A	N3-C4-C5	-9.84	119.91	126.80
1	A	418	A	N3-C4-C5	-9.84	119.91	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1745	A	N3-C4-C5	-9.84	119.91	126.80
1	A	2571	A	N3-C4-C5	-9.84	119.91	126.80
1	A	1743	A	N3-C4-C5	-9.84	119.91	126.80
1	A	73	A	N3-C4-C5	-9.84	119.91	126.80
1	A	547	A	N3-C4-C5	-9.84	119.91	126.80
1	A	2887	A	N3-C4-C5	-9.84	119.91	126.80
1	A	2902	A	N3-C4-C5	-9.84	119.91	126.80
32	W	512	A	N3-C4-C5	-9.84	119.91	126.80
32	W	541	A	N3-C4-C5	-9.84	119.91	126.80
1	A	2750	A	N3-C4-C5	-9.84	119.91	126.80
2	B	44	A	N3-C4-C5	-9.84	119.91	126.80
32	W	870	A	N3-C4-C5	-9.84	119.91	126.80
32	W	1451	A	N3-C4-C5	-9.84	119.91	126.80
1	A	65	A	N3-C4-C5	-9.84	119.92	126.80
1	A	1477	A	N3-C4-C5	-9.84	119.92	126.80
1	A	2441	A	N3-C4-C5	-9.84	119.92	126.80
52	z	14	A	N3-C4-C5	-9.84	119.92	126.80
1	A	90	A	N3-C4-C5	-9.83	119.92	126.80
1	A	876	A	N3-C4-C5	-9.83	119.92	126.80
1	A	1346	A	N3-C4-C5	-9.83	119.92	126.80
1	A	2594	A	N3-C4-C5	-9.83	119.92	126.80
32	W	886	A	N3-C4-C5	-9.83	119.92	126.80
1	A	71	A	N3-C4-C5	-9.83	119.92	126.80
1	A	1930	A	N3-C4-C5	-9.83	119.92	126.80
1	A	1265	A	N3-C4-C5	-9.83	119.92	126.80
1	A	1585	A	N3-C4-C5	-9.83	119.92	126.80
1	A	1620	A	N3-C4-C5	-9.83	119.92	126.80
1	A	1608	A	N3-C4-C5	-9.83	119.92	126.80
32	W	928	A	N3-C4-C5	-9.83	119.92	126.80
1	A	1700	A	N3-C4-C5	-9.83	119.92	126.80
32	W	491	A	N3-C4-C5	-9.83	119.92	126.80
32	W	823	A	N3-C4-C5	-9.83	119.92	126.80
52	z	23	A	N3-C4-C5	-9.83	119.92	126.80
1	A	369	A	N3-C4-C5	-9.82	119.92	126.80
32	W	1266	A	N3-C4-C5	-9.82	119.92	126.80
1	A	1606	A	N3-C4-C5	-9.82	119.92	126.80
1	A	2316	A	N3-C4-C5	-9.82	119.92	126.80
1	A	2405	A	N3-C4-C5	-9.82	119.92	126.80
1	A	2511	A	N3-C4-C5	-9.82	119.92	126.80
1	A	1888	A	N3-C4-C5	-9.82	119.92	126.80
2	B	51	A	N3-C4-C5	-9.82	119.92	126.80
32	W	1014	A	N3-C4-C5	-9.82	119.92	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1252	A	N3-C4-C5	-9.82	119.92	126.80
1	A	124	A	N3-C4-C5	-9.82	119.93	126.80
1	A	2356	A	N3-C4-C5	-9.82	119.93	126.80
32	W	475	A	N3-C4-C5	-9.82	119.93	126.80
32	W	1111	A	N3-C4-C5	-9.82	119.93	126.80
32	W	1298	A	N3-C4-C5	-9.82	119.93	126.80
1	A	176	A	N3-C4-C5	-9.82	119.93	126.80
1	A	808	A	N3-C4-C5	-9.82	119.93	126.80
32	W	1056	A	N3-C4-C5	-9.82	119.93	126.80
1	A	12	A	N3-C4-C5	-9.82	119.93	126.80
1	A	28	A	N3-C4-C5	-9.82	119.93	126.80
1	A	178	A	N3-C4-C5	-9.82	119.93	126.80
1	A	758	A	N3-C4-C5	-9.82	119.93	126.80
1	A	1542	A	N3-C4-C5	-9.82	119.93	126.80
1	A	2837	A	N3-C4-C5	-9.82	119.93	126.80
2	B	76	A	N3-C4-C5	-9.82	119.93	126.80
1	A	194	A	N3-C4-C5	-9.81	119.93	126.80
1	A	1230	A	N3-C4-C5	-9.81	119.93	126.80
32	W	258	A	N3-C4-C5	-9.81	119.93	126.80
32	W	616	A	N3-C4-C5	-9.81	119.93	126.80
1	A	102	A	N3-C4-C5	-9.81	119.93	126.80
1	A	1141	A	N3-C4-C5	-9.81	119.93	126.80
1	A	1243	A	N3-C4-C5	-9.81	119.93	126.80
1	A	53	A	N3-C4-C5	-9.81	119.93	126.80
1	A	618	A	N3-C4-C5	-9.81	119.93	126.80
1	A	1047	A	N3-C4-C5	-9.81	119.93	126.80
1	A	1516	A	N3-C4-C5	-9.81	119.93	126.80
1	A	2480	A	N3-C4-C5	-9.81	119.93	126.80
32	W	725	A	N3-C4-C5	-9.81	119.93	126.80
1	A	279	A	N3-C4-C5	-9.81	119.93	126.80
1	A	364	A	N3-C4-C5	-9.81	119.93	126.80
1	A	782	A	N3-C4-C5	-9.81	119.93	126.80
1	A	958	A	N3-C4-C5	-9.81	119.93	126.80
1	A	1553	A	N3-C4-C5	-9.81	119.93	126.80
1	A	2078	A	N3-C4-C5	-9.81	119.93	126.80
1	A	2629	A	N3-C4-C5	-9.81	119.93	126.80
32	W	118	A	N3-C4-C5	-9.81	119.93	126.80
1	A	1925	A	N3-C4-C5	-9.81	119.94	126.80
1	A	428	A	N3-C4-C5	-9.80	119.94	126.80
1	A	829	A	N3-C4-C5	-9.80	119.94	126.80
1	A	835	A	N3-C4-C5	-9.81	119.94	126.80
1	A	978	A	N3-C4-C5	-9.81	119.94	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1313	A	N3-C4-C5	-9.81	119.94	126.80
1	A	2060	A	N3-C4-C5	-9.81	119.94	126.80
2	B	20	A	N3-C4-C5	-9.81	119.94	126.80
1	A	1768	A	N3-C4-C5	-9.80	119.94	126.80
1	A	2381	A	N3-C4-C5	-9.80	119.94	126.80
2	B	56	A	N3-C4-C5	-9.80	119.94	126.80
32	W	52	A	N3-C4-C5	-9.81	119.94	126.80
32	W	81	A	N3-C4-C5	-9.80	119.94	126.80
32	W	1022	A	N3-C4-C5	-9.80	119.94	126.80
32	W	1092	A	N3-C4-C5	-9.80	119.94	126.80
1	A	1287	A	N3-C4-C5	-9.80	119.94	126.80
1	A	2782	A	N3-C4-C5	-9.80	119.94	126.80
32	W	210	A	N3-C4-C5	-9.80	119.94	126.80
1	A	329	A	N3-C4-C5	-9.80	119.94	126.80
1	A	1675	A	N3-C4-C5	-9.80	119.94	126.80
32	W	519	A	N3-C4-C5	-9.80	119.94	126.80
1	A	2593	A	N3-C4-C5	-9.80	119.94	126.80
32	W	459	A	N3-C4-C5	-9.80	119.94	126.80
1	A	140	A	N3-C4-C5	-9.79	119.94	126.80
1	A	1569	A	N3-C4-C5	-9.79	119.94	126.80
1	A	1580	A	N3-C4-C5	-9.79	119.94	126.80
1	A	2463	A	N3-C4-C5	-9.79	119.94	126.80
1	A	2505	A	N3-C4-C5	-9.79	119.94	126.80
32	W	323	A	N3-C4-C5	-9.79	119.94	126.80
32	W	532	A	N3-C4-C5	-9.80	119.94	126.80
32	W	824	A	N3-C4-C5	-9.79	119.94	126.80
1	A	322	A	N3-C4-C5	-9.79	119.95	126.80
1	A	1788	A	N3-C4-C5	-9.79	119.95	126.80
32	W	504	A	N3-C4-C5	-9.79	119.95	126.80
32	W	1213	A	N3-C4-C5	-9.79	119.94	126.80
1	A	219	A	N3-C4-C5	-9.79	119.95	126.80
1	A	1113	A	N3-C4-C5	-9.79	119.95	126.80
1	A	1850	A	N3-C4-C5	-9.79	119.95	126.80
1	A	2900	A	N3-C4-C5	-9.79	119.95	126.80
32	W	669	A	N3-C4-C5	-9.79	119.95	126.80
1	A	144	A	N3-C4-C5	-9.79	119.95	126.80
1	A	216	A	N3-C4-C5	-9.79	119.95	126.80
1	A	769	A	N3-C4-C5	-9.79	119.95	126.80
2	B	113	A	N3-C4-C5	-9.79	119.95	126.80
32	W	53	A	N3-C4-C5	-9.79	119.95	126.80
32	W	251	A	N3-C4-C5	-9.79	119.95	126.80
32	W	529	A	N3-C4-C5	-9.79	119.95	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1528	A	N3-C4-C5	-9.79	119.95	126.80
1	A	1423	A	N3-C4-C5	-9.79	119.95	126.80
1	A	2590	A	N3-C4-C5	-9.79	119.95	126.80
32	W	440	A	N3-C4-C5	-9.79	119.95	126.80
1	A	2762	A	N3-C4-C5	-9.78	119.95	126.80
32	W	604	A	N3-C4-C5	-9.78	119.95	126.80
32	W	1257	A	N3-C4-C5	-9.78	119.95	126.80
32	W	1383	A	N3-C4-C5	-9.79	119.95	126.80
1	A	6	A	N3-C4-C5	-9.78	119.95	126.80
1	A	125	A	N3-C4-C5	-9.78	119.95	126.80
1	A	553	A	N3-C4-C5	-9.78	119.95	126.80
1	A	893	A	N3-C4-C5	-9.78	119.95	126.80
1	A	1054	A	N3-C4-C5	-9.78	119.95	126.80
32	W	271	A	N3-C4-C5	-9.78	119.95	126.80
1	A	2734	A	N3-C4-C5	-9.78	119.95	126.80
1	A	2778	A	N3-C4-C5	-9.78	119.95	126.80
32	W	690	A	N3-C4-C5	-9.78	119.95	126.80
32	W	786	A	N3-C4-C5	-9.78	119.95	126.80
32	W	1054	A	N3-C4-C5	-9.78	119.95	126.80
32	W	1245	A	N3-C4-C5	-9.78	119.95	126.80
1	A	10	A	N3-C4-C5	-9.78	119.95	126.80
1	A	1533	A	N3-C4-C5	-9.78	119.95	126.80
1	A	1312	A	N3-C4-C5	-9.78	119.95	126.80
1	A	1818	A	N3-C4-C5	-9.78	119.95	126.80
1	A	2923	A	N3-C4-C5	-9.78	119.95	126.80
32	W	62	A	N3-C4-C5	-9.78	119.95	126.80
32	W	160	A	N3-C4-C5	-9.78	119.95	126.80
32	W	762	A	N3-C4-C5	-9.78	119.95	126.80
32	W	1260	A	N3-C4-C5	-9.78	119.95	126.80
32	W	796	A	N3-C4-C5	-9.78	119.96	126.80
1	A	173	A	N3-C4-C5	-9.78	119.96	126.80
1	A	345	A	N3-C4-C5	-9.78	119.96	126.80
1	A	753	A	N3-C4-C5	-9.78	119.96	126.80
1	A	1131	A	N3-C4-C5	-9.78	119.96	126.80
1	A	762	A	N3-C4-C5	-9.78	119.96	126.80
1	A	1381	A	N3-C4-C5	-9.78	119.96	126.80
1	A	1453	A	N3-C4-C5	-9.78	119.96	126.80
1	A	1913	A	N3-C4-C5	-9.78	119.96	126.80
32	W	1120	A	N3-C4-C5	-9.78	119.96	126.80
1	A	630	A	N3-C4-C5	-9.77	119.96	126.80
1	A	947	A	N3-C4-C5	-9.77	119.96	126.80
1	A	2303	A	N3-C4-C5	-9.77	119.96	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	704	A	N3-C4-C5	-9.77	119.96	126.80
32	W	883	A	N3-C4-C5	-9.77	119.96	126.80
32	W	1405	A	N3-C4-C5	-9.77	119.96	126.80
1	A	314	A	N3-C4-C5	-9.77	119.96	126.80
32	W	202	A	N3-C4-C5	-9.77	119.96	126.80
32	W	1488	A	N3-C4-C5	-9.77	119.96	126.80
1	A	110	A	N3-C4-C5	-9.77	119.96	126.80
1	A	225	A	N3-C4-C5	-9.77	119.96	126.80
1	A	342	A	N3-C4-C5	-9.77	119.96	126.80
1	A	1036	A	N3-C4-C5	-9.77	119.96	126.80
1	A	1724	A	N3-C4-C5	-9.77	119.96	126.80
1	A	2658	A	N3-C4-C5	-9.77	119.96	126.80
32	W	170	A	N3-C4-C5	-9.77	119.96	126.80
32	W	874	A	N3-C4-C5	-9.77	119.96	126.80
1	A	2708	A	N3-C4-C5	-9.77	119.96	126.80
32	W	208	A	N3-C4-C5	-9.77	119.96	126.80
1	A	2673	A	N3-C4-C5	-9.77	119.96	126.80
32	W	1463	A	N3-C4-C5	-9.77	119.97	126.80
1	A	637	A	N3-C4-C5	-9.76	119.97	126.80
1	A	1465	A	N3-C4-C5	-9.76	119.97	126.80
1	A	1914	A	N3-C4-C5	-9.76	119.97	126.80
1	A	2071	A	N3-C4-C5	-9.76	119.97	126.80
1	A	2454	A	N3-C4-C5	-9.76	119.97	126.80
1	A	2851	A	N3-C4-C5	-9.76	119.97	126.80
32	W	306	A	N3-C4-C5	-9.76	119.97	126.80
32	W	485	A	N3-C4-C5	-9.76	119.97	126.80
32	W	791	A	N3-C4-C5	-9.76	119.97	126.80
32	W	799	A	N3-C4-C5	-9.76	119.97	126.80
32	W	1261	A	N3-C4-C5	-9.76	119.97	126.80
32	W	1161	A	N3-C4-C5	-9.76	119.97	126.80
1	A	1021	A	N3-C4-C5	-9.76	119.97	126.80
1	A	1144	A	N3-C4-C5	-9.76	119.97	126.80
1	A	1906	A	N3-C4-C5	-9.76	119.97	126.80
32	W	650	A	N3-C4-C5	-9.76	119.97	126.80
1	A	2406	A	N3-C4-C5	-9.76	119.97	126.80
1	A	2912	A	N3-C4-C5	-9.76	119.97	126.80
32	W	28	A	N3-C4-C5	-9.76	119.97	126.80
32	W	329	A	N3-C4-C5	-9.76	119.97	126.80
32	W	1180	A	N3-C4-C5	-9.76	119.97	126.80
32	W	1503	A	N3-C4-C5	-9.76	119.97	126.80
1	A	220	A	N3-C4-C5	-9.76	119.97	126.80
1	A	388	A	N3-C4-C5	-9.76	119.97	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	278	A	N3-C4-C5	-9.76	119.97	126.80
32	W	367	A	N3-C4-C5	-9.76	119.97	126.80
32	W	389	A	N3-C4-C5	-9.76	119.97	126.80
1	A	987	A	N3-C4-C5	-9.76	119.97	126.80
1	A	1072	A	N3-C4-C5	-9.76	119.97	126.80
1	A	1116	A	N3-C4-C5	-9.76	119.97	126.80
1	A	2477	A	N3-C4-C5	-9.76	119.97	126.80
32	W	12	A	N3-C4-C5	-9.76	119.97	126.80
32	W	357	A	N3-C4-C5	-9.76	119.97	126.80
32	W	1121	A	N3-C4-C5	-9.76	119.97	126.80
32	W	281	A	N3-C4-C5	-9.76	119.97	126.80
32	W	439	A	N3-C4-C5	-9.76	119.97	126.80
32	W	803	A	N3-C4-C5	-9.76	119.97	126.80
1	A	653	A	N3-C4-C5	-9.75	119.97	126.80
1	A	965	A	N3-C4-C5	-9.75	119.97	126.80
1	A	1654	A	N3-C4-C5	-9.75	119.97	126.80
32	W	94	A	N3-C4-C5	-9.75	119.97	126.80
32	W	240	A	N3-C4-C5	-9.75	119.97	126.80
32	W	314	A	N3-C4-C5	-9.75	119.97	126.80
32	W	544	A	N3-C4-C5	-9.75	119.97	126.80
32	W	672	A	N3-C4-C5	-9.75	119.97	126.80
32	W	1327	A	N3-C4-C5	-9.75	119.97	126.80
32	W	1419	A	N3-C4-C5	-9.75	119.97	126.80
1	A	740	A	N3-C4-C5	-9.75	119.97	126.80
1	A	1179	A	N3-C4-C5	-9.75	119.97	126.80
1	A	1499	A	N3-C4-C5	-9.75	119.97	126.80
1	A	2006	A	N3-C4-C5	-9.75	119.97	126.80
1	A	2417	A	N3-C4-C5	-9.75	119.97	126.80
1	A	2526	A	N3-C4-C5	-9.75	119.97	126.80
1	A	2907	A	N3-C4-C5	-9.75	119.97	126.80
32	W	206	A	N3-C4-C5	-9.75	119.98	126.80
1	A	1115	A	N3-C4-C5	-9.75	119.98	126.80
1	A	1244	A	N3-C4-C5	-9.75	119.98	126.80
1	A	1027	A	N3-C4-C5	-9.75	119.98	126.80
1	A	1224	A	N3-C4-C5	-9.75	119.98	126.80
1	A	2080	A	N3-C4-C5	-9.75	119.98	126.80
32	W	1248	A	N3-C4-C5	-9.75	119.98	126.80
32	W	1417	A	N3-C4-C5	-9.75	119.98	126.80
1	A	2479	A	N3-C4-C5	-9.75	119.98	126.80
2	B	43	A	N3-C4-C5	-9.75	119.98	126.80
1	A	1723	A	N3-C4-C5	-9.74	119.98	126.80
1	A	1901	A	N3-C4-C5	-9.74	119.98	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2440	A	N3-C4-C5	-9.74	119.98	126.80
1	A	1291	A	N3-C4-C5	-9.74	119.98	126.80
1	A	1989	A	N3-C4-C5	-9.74	119.98	126.80
32	W	159	A	N3-C4-C5	-9.74	119.98	126.80
32	W	1509	A	N3-C4-C5	-9.74	119.98	126.80
32	W	1541	A	N3-C4-C5	-9.74	119.98	126.80
1	A	888	A	N3-C4-C5	-9.74	119.98	126.80
32	W	581	A	N3-C4-C5	-9.74	119.98	126.80
1	A	2018	A	N3-C4-C5	-9.74	119.98	126.80
32	W	456	A	N3-C4-C5	-9.74	119.98	126.80
32	W	757	A	N3-C4-C5	-9.74	119.98	126.80
32	W	1200	A	N3-C4-C5	-9.74	119.98	126.80
32	W	1271	A	N3-C4-C5	-9.74	119.98	126.80
1	A	139	A	N3-C4-C5	-9.74	119.98	126.80
1	A	210	A	N3-C4-C5	-9.74	119.98	126.80
1	A	770	A	N3-C4-C5	-9.74	119.98	126.80
1	A	1957	A	N3-C4-C5	-9.74	119.98	126.80
1	A	459	A	N3-C4-C5	-9.73	119.99	126.80
1	A	658	A	N3-C4-C5	-9.73	119.99	126.80
1	A	1809	A	N3-C4-C5	-9.73	119.99	126.80
1	A	2357	A	N3-C4-C5	-9.73	119.99	126.80
1	A	2362	A	N3-C4-C5	-9.73	119.99	126.80
2	B	37	A	N3-C4-C5	-9.73	119.99	126.80
1	A	230	A	N3-C4-C5	-9.73	119.99	126.80
1	A	337	A	N3-C4-C5	-9.73	119.99	126.80
1	A	537	A	N3-C4-C5	-9.73	119.99	126.80
1	A	1734	A	N3-C4-C5	-9.73	119.99	126.80
1	A	2315	A	N3-C4-C5	-9.73	119.99	126.80
1	A	1066	A	N3-C4-C5	-9.73	119.99	126.80
1	A	1679	A	N3-C4-C5	-9.73	119.99	126.80
32	W	1342	A	N3-C4-C5	-9.73	119.99	126.80
32	W	1443	A	N3-C4-C5	-9.73	119.99	126.80
32	W	1185	A	N3-C4-C5	-9.73	119.99	126.80
1	A	229	A	N3-C4-C5	-9.73	119.99	126.80
32	W	228	A	N3-C4-C5	-9.73	119.99	126.80
1	A	198	A	N3-C4-C5	-9.72	119.99	126.80
1	A	2876	A	N3-C4-C5	-9.72	119.99	126.80
1	A	355	A	N3-C4-C5	-9.72	119.99	126.80
1	A	373	A	N3-C4-C5	-9.72	119.99	126.80
1	A	543	A	N3-C4-C5	-9.72	119.99	126.80
32	W	1028	A	N3-C4-C5	-9.72	119.99	126.80
1	A	1042	A	N3-C4-C5	-9.72	119.99	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	831	A	N3-C4-C5	-9.72	120.00	126.80
1	A	1020	A	N3-C4-C5	-9.72	120.00	126.80
1	A	1323	A	N3-C4-C5	-9.72	120.00	126.80
1	A	1721	A	N3-C4-C5	-9.72	120.00	126.80
1	A	2740	A	N3-C4-C5	-9.72	120.00	126.80
32	W	644	A	N3-C4-C5	-9.72	120.00	126.80
32	W	730	A	N3-C4-C5	-9.72	120.00	126.80
1	A	222	A	N3-C4-C5	-9.72	120.00	126.80
1	A	1592	A	N3-C4-C5	-9.72	120.00	126.80
1	A	2307	A	N3-C4-C5	-9.72	120.00	126.80
32	W	1205	A	N3-C4-C5	-9.72	120.00	126.80
32	W	947	A	N3-C4-C5	-9.72	120.00	126.80
32	W	1188	A	N3-C4-C5	-9.72	120.00	126.80
1	A	582	A	N3-C4-C5	-9.71	120.00	126.80
1	A	774	A	N3-C4-C5	-9.72	120.00	126.80
32	W	204	A	N3-C4-C5	-9.72	120.00	126.80
32	W	1283	A	N3-C4-C5	-9.71	120.00	126.80
1	A	763	A	N3-C4-C5	-9.71	120.00	126.80
1	A	1277	A	N3-C4-C5	-9.71	120.00	126.80
32	W	777	A	N3-C4-C5	-9.71	120.00	126.80
32	W	919	A	N3-C4-C5	-9.71	120.00	126.80
1	A	746	A	N3-C4-C5	-9.71	120.00	126.80
1	A	1034	A	N3-C4-C5	-9.71	120.00	126.80
1	A	1789	A	N3-C4-C5	-9.71	120.00	126.80
1	A	2767	A	N3-C4-C5	-9.71	120.00	126.80
1	A	2904	A	N3-C4-C5	-9.71	120.00	126.80
32	W	460	A	N3-C4-C5	-9.71	120.00	126.80
52	z	44	A	N3-C4-C5	-9.71	120.00	126.80
1	A	236	A	N3-C4-C5	-9.71	120.00	126.80
1	A	1175	A	N3-C4-C5	-9.71	120.00	126.80
1	A	2661	A	N3-C4-C5	-9.71	120.00	126.80
32	W	1102	A	N3-C4-C5	-9.71	120.00	126.80
1	A	2616	A	N3-C4-C5	-9.71	120.01	126.80
2	B	105	A	N3-C4-C5	-9.71	120.01	126.80
32	W	287	A	N3-C4-C5	-9.70	120.01	126.80
32	W	321	A	N3-C4-C5	-9.71	120.01	126.80
32	W	1294	A	N3-C4-C5	-9.70	120.01	126.80
32	W	1470	A	N3-C4-C5	-9.71	120.01	126.80
1	A	677	A	N3-C4-C5	-9.70	120.01	126.80
1	A	1540	A	N3-C4-C5	-9.70	120.01	126.80
32	W	776	A	N3-C4-C5	-9.70	120.01	126.80
32	W	1048	A	N3-C4-C5	-9.70	120.01	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1601	A	N3-C4-C5	-9.70	120.01	126.80
1	A	1832	A	N3-C4-C5	-9.70	120.01	126.80
1	A	2327	A	N3-C4-C5	-9.70	120.01	126.80
32	W	925	A	N3-C4-C5	-9.70	120.01	126.80
32	W	1210	A	N3-C4-C5	-9.70	120.01	126.80
32	W	1225	A	N3-C4-C5	-9.70	120.01	126.80
1	A	2875	A	N3-C4-C5	-9.70	120.01	126.80
1	A	247	A	N3-C4-C5	-9.70	120.01	126.80
1	A	1942	A	N3-C4-C5	-9.70	120.01	126.80
1	A	1197	A	N3-C4-C5	-9.70	120.01	126.80
1	A	2398	A	N3-C4-C5	-9.70	120.01	126.80
32	W	67	A	N3-C4-C5	-9.70	120.01	126.80
32	W	1270	A	N3-C4-C5	-9.70	120.01	126.80
1	A	476	A	N3-C4-C5	-9.70	120.01	126.80
1	A	667	A	N3-C4-C5	-9.70	120.01	126.80
32	W	592	A	N3-C4-C5	-9.70	120.01	126.80
32	W	664	A	N3-C4-C5	-9.70	120.01	126.80
1	A	1445	A	N3-C4-C5	-9.70	120.01	126.80
1	A	1697	A	N3-C4-C5	-9.69	120.01	126.80
1	A	2686	A	N3-C4-C5	-9.70	120.01	126.80
2	B	102	A	N3-C4-C5	-9.69	120.01	126.80
52	z	76	A	N3-C4-C5	-9.70	120.01	126.80
1	A	14	A	N3-C4-C5	-9.69	120.02	126.80
1	A	1142	A	N3-C4-C5	-9.69	120.02	126.80
1	A	1266	A	N3-C4-C5	-9.69	120.02	126.80
1	A	1699	A	N3-C4-C5	-9.69	120.02	126.80
1	A	2364	A	N3-C4-C5	-9.69	120.02	126.80
1	A	2860	A	N3-C4-C5	-9.69	120.02	126.80
32	W	474	A	N3-C4-C5	-9.69	120.02	126.80
32	W	542	A	N3-C4-C5	-9.69	120.02	126.80
32	W	618	A	N3-C4-C5	-9.69	120.02	126.80
1	A	1189	A	N3-C4-C5	-9.69	120.02	126.80
32	W	696	A	N3-C4-C5	-9.69	120.02	126.80
1	A	13	A	N3-C4-C5	-9.69	120.02	126.80
1	A	268	A	N3-C4-C5	-9.69	120.02	126.80
1	A	1791	A	N3-C4-C5	-9.69	120.02	126.80
1	A	2296	A	N3-C4-C5	-9.69	120.02	126.80
1	A	2468	A	N3-C4-C5	-9.69	120.02	126.80
32	W	825	A	N3-C4-C5	-9.69	120.02	126.80
1	A	477	A	N3-C4-C5	-9.69	120.02	126.80
1	A	1084	A	N3-C4-C5	-9.69	120.02	126.80
1	A	1119	A	N3-C4-C5	-9.69	120.02	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1534	A	N3-C4-C5	-9.69	120.02	126.80
1	A	274	A	N3-C4-C5	-9.68	120.02	126.80
1	A	999	A	N3-C4-C5	-9.68	120.02	126.80
32	W	1031	A	N3-C4-C5	-9.68	120.02	126.80
1	A	84	A	N3-C4-C5	-9.68	120.02	126.80
1	A	2787	A	N3-C4-C5	-9.68	120.02	126.80
32	W	1289	A	N3-C4-C5	-9.68	120.02	126.80
1	A	727	A	N3-C4-C5	-9.68	120.02	126.80
32	W	236	A	N3-C4-C5	-9.68	120.02	126.80
1	A	49	A	N3-C4-C5	-9.68	120.03	126.80
1	A	1434	A	N3-C4-C5	-9.68	120.03	126.80
1	A	1008	A	N3-C4-C5	-9.68	120.03	126.80
1	A	1583	A	N3-C4-C5	-9.68	120.03	126.80
32	W	148	A	N3-C4-C5	-9.68	120.03	126.80
32	W	828	A	N3-C4-C5	-9.68	120.03	126.80
32	W	1333	A	N3-C4-C5	-9.68	120.03	126.80
1	A	1335	A	N3-C4-C5	-9.67	120.03	126.80
1	A	1593	A	N3-C4-C5	-9.67	120.03	126.80
32	W	974	A	N3-C4-C5	-9.67	120.03	126.80
1	A	325	A	N3-C4-C5	-9.67	120.03	126.80
1	A	519	A	N3-C4-C5	-9.67	120.03	126.80
32	W	500	A	N3-C4-C5	-9.67	120.03	126.80
32	W	1529	A	N3-C4-C5	-9.67	120.03	126.80
32	W	1358	A	N3-C4-C5	-9.67	120.03	126.80
32	W	1386	A	N3-C4-C5	-9.67	120.03	126.80
1	A	683	A	N3-C4-C5	-9.67	120.03	126.80
1	A	2295	A	N3-C4-C5	-9.67	120.03	126.80
1	A	2498	A	N3-C4-C5	-9.67	120.03	126.80
32	W	371	A	N3-C4-C5	-9.67	120.03	126.80
1	A	1961	A	N3-C4-C5	-9.67	120.03	126.80
1	A	821	A	N3-C4-C5	-9.66	120.03	126.80
1	A	1014	A	N3-C4-C5	-9.66	120.03	126.80
1	A	2297	A	N3-C4-C5	-9.66	120.03	126.80
1	A	2030	A	N3-C4-C5	-9.66	120.04	126.80
1	A	2807	A	N3-C4-C5	-9.66	120.03	126.80
2	B	27	A	N3-C4-C5	-9.66	120.03	126.80
2	B	39	A	N3-C4-C5	-9.66	120.04	126.80
32	W	1176	A	N3-C4-C5	-9.66	120.03	126.80
32	W	1296	A	N3-C4-C5	-9.66	120.03	126.80
32	W	178	A	N3-C4-C5	-9.66	120.04	126.80
32	W	611	A	N3-C4-C5	-9.66	120.04	126.80
32	W	969	A	N3-C4-C5	-9.66	120.04	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1513	A	N3-C4-C5	-9.66	120.04	126.80
1	A	67	A	N3-C4-C5	-9.66	120.04	126.80
1	A	646	A	N3-C4-C5	-9.66	120.04	126.80
1	A	2059	A	N3-C4-C5	-9.66	120.04	126.80
32	W	422	A	N3-C4-C5	-9.66	120.04	126.80
32	W	1103	A	N3-C4-C5	-9.66	120.04	126.80
32	W	1328	A	N3-C4-C5	-9.66	120.04	126.80
32	W	1434	A	N3-C4-C5	-9.66	120.04	126.80
1	A	389	A	N3-C4-C5	-9.66	120.04	126.80
1	A	993	A	N3-C4-C5	-9.66	120.04	126.80
1	A	1339	A	N3-C4-C5	-9.66	120.04	126.80
1	A	2542	A	N3-C4-C5	-9.66	120.04	126.80
32	W	910	A	N3-C4-C5	-9.66	120.04	126.80
1	A	1161	A	N3-C4-C5	-9.65	120.04	126.80
32	W	929	A	N3-C4-C5	-9.65	120.04	126.80
32	W	1479	A	N3-C4-C5	-9.65	120.04	126.80
1	A	1325	A	N3-C4-C5	-9.65	120.04	126.80
32	W	1090	A	N3-C4-C5	-9.65	120.04	126.80
1	A	343	A	N3-C4-C5	-9.65	120.05	126.80
1	A	1326	A	N3-C4-C5	-9.65	120.05	126.80
32	W	296	A	N3-C4-C5	-9.65	120.04	126.80
1	A	1308	A	N3-C4-C5	-9.65	120.05	126.80
32	W	569	A	N3-C4-C5	-9.65	120.05	126.80
32	W	582	A	N3-C4-C5	-9.65	120.05	126.80
32	W	1140	A	N3-C4-C5	-9.65	120.05	126.80
1	A	150	A	N3-C4-C5	-9.65	120.05	126.80
32	W	501	A	N3-C4-C5	-9.65	120.05	126.80
1	A	436	A	N3-C4-C5	-9.64	120.05	126.80
1	A	1026	A	N3-C4-C5	-9.64	120.05	126.80
1	A	1812	A	N3-C4-C5	-9.64	120.05	126.80
1	A	2330	A	N3-C4-C5	-9.64	120.05	126.80
32	W	1456	A	N3-C4-C5	-9.64	120.05	126.80
1	A	717	A	N3-C4-C5	-9.64	120.05	126.80
1	A	1929	A	N3-C4-C5	-9.64	120.05	126.80
32	W	142	A	N3-C4-C5	-9.64	120.05	126.80
32	W	211	A	N3-C4-C5	-9.64	120.05	126.80
32	W	266	A	N3-C4-C5	-9.64	120.05	126.80
32	W	352	A	N3-C4-C5	-9.64	120.05	126.80
1	A	572	A	N3-C4-C5	-9.64	120.05	126.80
1	A	702	A	N3-C4-C5	-9.64	120.05	126.80
1	A	2383	A	N3-C4-C5	-9.64	120.05	126.80
2	B	25	A	N3-C4-C5	-9.64	120.05	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1797	A	N3-C4-C5	-9.64	120.05	126.80
1	A	786	A	N3-C4-C5	-9.64	120.05	126.80
1	A	1314	A	N3-C4-C5	-9.64	120.05	126.80
32	W	713	A	N3-C4-C5	-9.64	120.05	126.80
32	W	1466	A	N3-C4-C5	-9.64	120.06	126.80
32	W	290	A	N3-C4-C5	-9.63	120.06	126.80
32	W	724	A	N3-C4-C5	-9.63	120.06	126.80
1	A	273	A	N3-C4-C5	-9.63	120.06	126.80
1	A	1713	A	N3-C4-C5	-9.63	120.06	126.80
1	A	2000	A	N3-C4-C5	-9.63	120.06	126.80
1	A	2340	A	N3-C4-C5	-9.63	120.06	126.80
32	W	386	A	N3-C4-C5	-9.63	120.06	126.80
32	W	1017	A	N3-C4-C5	-9.63	120.06	126.80
1	A	421	A	N3-C4-C5	-9.63	120.06	126.80
1	A	1802	A	N3-C4-C5	-9.63	120.06	126.80
2	B	55	A	N3-C4-C5	-9.63	120.06	126.80
32	W	684	A	N3-C4-C5	-9.63	120.06	126.80
1	A	561	A	N3-C4-C5	-9.63	120.06	126.80
1	A	2835	A	N3-C4-C5	-9.63	120.06	126.80
1	A	1157	A	N3-C4-C5	-9.62	120.06	126.80
1	A	2298	A	N3-C4-C5	-9.62	120.06	126.80
1	A	2390	A	N3-C4-C5	-9.62	120.06	126.80
1	A	2482	A	N3-C4-C5	-9.62	120.07	126.80
1	A	333	A	N3-C4-C5	-9.62	120.07	126.80
1	A	1579	A	N3-C4-C5	-9.62	120.07	126.80
32	W	463	A	N3-C4-C5	-9.62	120.07	126.80
32	W	31	A	N3-C4-C5	-9.61	120.07	126.80
32	W	107	A	N3-C4-C5	-9.61	120.07	126.80
32	W	556	A	N3-C4-C5	-9.61	120.07	126.80
1	A	1722	A	N3-C4-C5	-9.61	120.07	126.80
32	W	120	A	N3-C4-C5	-9.61	120.07	126.80
1	A	1648	A	N3-C4-C5	-9.61	120.07	126.80
32	W	679	A	N3-C4-C5	-9.61	120.08	126.80
1	A	659	A	N3-C4-C5	-9.61	120.08	126.80
1	A	1517	A	N3-C4-C5	-9.61	120.08	126.80
1	A	1948	A	N3-C4-C5	-9.61	120.08	126.80
1	A	5	A	N3-C4-C5	-9.60	120.08	126.80
32	W	117	A	N3-C4-C5	-9.60	120.08	126.80
32	W	151	A	N3-C4-C5	-9.60	120.08	126.80
1	A	302	A	N3-C4-C5	-9.60	120.08	126.80
1	A	1347	A	N3-C4-C5	-9.60	120.08	126.80
1	A	2455	A	N3-C4-C5	-9.60	120.08	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	568	A	N3-C4-C5	-9.60	120.08	126.80
1	A	2770	A	N3-C4-C5	-9.60	120.08	126.80
1	A	166	A	N3-C4-C5	-9.60	120.08	126.80
1	A	619	A	N3-C4-C5	-9.60	120.08	126.80
1	A	1092	A	N3-C4-C5	-9.60	120.08	126.80
1	A	1941	A	N3-C4-C5	-9.60	120.08	126.80
32	W	775	A	N3-C4-C5	-9.60	120.08	126.80
1	A	1967	A	N3-C4-C5	-9.60	120.08	126.80
32	W	738	A	N3-C4-C5	-9.60	120.08	126.80
1	A	199	A	N3-C4-C5	-9.59	120.08	126.80
1	A	584	A	N3-C4-C5	-9.59	120.08	126.80
1	A	917	A	N3-C4-C5	-9.59	120.08	126.80
1	A	2595	A	N3-C4-C5	-9.59	120.08	126.80
32	W	10	A	N3-C4-C5	-9.59	120.09	126.80
32	W	1050	A	N3-C4-C5	-9.59	120.08	126.80
32	W	1254	A	N3-C4-C5	-9.59	120.08	126.80
1	A	723	A	N3-C4-C5	-9.59	120.09	126.80
2	B	17	A	N3-C4-C5	-9.59	120.09	126.80
32	W	651	A	N3-C4-C5	-9.59	120.09	126.80
32	W	924	A	N3-C4-C5	-9.59	120.09	126.80
32	W	1422	A	N3-C4-C5	-9.59	120.09	126.80
1	A	1202	A	N3-C4-C5	-9.59	120.09	126.80
32	W	975	A	N3-C4-C5	-9.59	120.09	126.80
32	W	1133	A	N3-C4-C5	-9.59	120.09	126.80
1	A	2276	A	N3-C4-C5	-9.58	120.09	126.80
1	A	2804	A	N3-C4-C5	-9.58	120.09	126.80
1	A	448	A	N3-C4-C5	-9.58	120.09	126.80
32	W	923	A	N3-C4-C5	-9.58	120.10	126.80
1	A	2088	A	N3-C4-C5	-9.57	120.10	126.80
32	W	203	A	N3-C4-C5	-9.57	120.10	126.80
1	A	904	A	N3-C4-C5	-9.57	120.10	126.80
32	W	171	A	N3-C4-C5	-9.57	120.10	126.80
32	W	583	A	N3-C4-C5	-9.57	120.10	126.80
1	A	1905	A	N3-C4-C5	-9.56	120.11	126.80
32	W	438	A	N3-C4-C5	-9.56	120.11	126.80
32	W	816	A	N3-C4-C5	-9.56	120.10	126.80
1	A	224	A	N3-C4-C5	-9.56	120.11	126.80
1	A	828	A	N3-C4-C5	-9.56	120.11	126.80
1	A	1412	A	N3-C4-C5	-9.56	120.11	126.80
1	A	1432	A	N3-C4-C5	-9.56	120.11	126.80
1	A	1221	A	N3-C4-C5	-9.56	120.11	126.80
1	A	2375	A	N3-C4-C5	-9.56	120.11	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2387	A	N3-C4-C5	-9.56	120.11	126.80
1	A	2810	A	N3-C4-C5	-9.56	120.11	126.80
32	W	189	A	N3-C4-C5	-9.55	120.11	126.80
32	W	1006	A	N3-C4-C5	-9.55	120.11	126.80
32	W	1512	A	N3-C4-C5	-9.55	120.11	126.80
1	A	575	A	N3-C4-C5	-9.55	120.11	126.80
1	A	525	A	N3-C4-C5	-9.55	120.12	126.80
1	A	1504	A	N3-C4-C5	-9.55	120.12	126.80
1	A	991	A	N3-C4-C5	-9.55	120.12	126.80
1	A	1123	A	N3-C4-C5	-9.55	120.12	126.80
32	W	457	A	N3-C4-C5	-9.55	120.11	126.80
1	A	504	A	N3-C4-C5	-9.54	120.12	126.80
1	A	811	A	N3-C4-C5	-9.54	120.12	126.80
32	W	1207	A	N3-C4-C5	-9.54	120.12	126.80
1	A	1784	A	N3-C4-C5	-9.53	120.13	126.80
32	W	837	A	N3-C4-C5	-9.53	120.13	126.80
1	A	1149	A	N3-C4-C5	-9.53	120.13	126.80
1	A	475	A	N3-C4-C5	-9.53	120.13	126.80
1	A	1340	A	N3-C4-C5	-9.53	120.13	126.80
1	A	1815	A	N3-C4-C5	-9.53	120.13	126.80
32	W	1197	A	N3-C4-C5	-9.53	120.13	126.80
1	A	526	A	N3-C4-C5	-9.52	120.14	126.80
1	A	1966	A	N3-C4-C5	-9.52	120.14	126.80
1	A	2683	A	N3-C4-C5	-9.52	120.14	126.80
32	W	988	A	N3-C4-C5	-9.52	120.14	126.80
1	A	1078	A	N3-C4-C5	-9.52	120.14	126.80
1	A	2507	A	N3-C4-C5	-9.52	120.14	126.80
1	A	64	A	N3-C4-C5	-9.51	120.14	126.80
32	W	401	A	N3-C4-C5	-9.51	120.14	126.80
32	W	703	A	N3-C4-C5	-9.51	120.14	126.80
1	A	2898	A	N3-C4-C5	-9.50	120.15	126.80
1	A	2908	A	N3-C4-C5	-9.49	120.16	126.80
1	A	244	A	N3-C4-C5	-9.48	120.16	126.80
32	W	899	A	N3-C4-C5	-9.48	120.16	126.80
1	A	1844	A	N3-C4-C5	-9.48	120.17	126.80
32	W	232	A	N3-C4-C5	-9.48	120.17	126.80
1	A	1555	A	N3-C4-C5	-9.47	120.17	126.80
1	A	354	A	N3-C4-C5	-9.47	120.17	126.80
1	A	1188	A	N3-C4-C5	-9.47	120.17	126.80
1	A	1302	A	N3-C4-C5	-9.46	120.18	126.80
32	W	879	A	N3-C4-C5	-9.46	120.18	126.80
1	A	1919	A	N3-C4-C5	-9.46	120.18	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	150	A	N3-C4-C5	-9.46	120.18	126.80
1	A	202	A	N3-C4-C5	-9.46	120.18	126.80
1	A	118	A	N3-C4-C5	-9.46	120.18	126.80
1	A	2601	A	N3-C4-C5	-9.45	120.18	126.80
1	A	1473	A	N3-C4-C5	-9.45	120.19	126.80
1	A	1061	A	N3-C4-C5	-9.44	120.19	126.80
32	W	18	A	N3-C4-C5	-9.44	120.19	126.80
1	A	162	A	N3-C4-C5	-9.44	120.19	126.80
1	A	2618	A	N3-C4-C5	-9.43	120.20	126.80
1	A	2670	A	N3-C4-C5	-9.43	120.20	126.80
1	A	494	A	N3-C4-C5	-9.43	120.20	126.80
32	W	419	A	N3-C4-C5	-9.43	120.20	126.80
1	A	1134	A	N7-C8-N9	-9.42	109.09	113.80
1	A	490	A	N3-C4-C5	-9.42	120.21	126.80
1	A	2777	A	N3-C4-C5	-9.42	120.21	126.80
1	A	847	A	N3-C4-C5	-9.41	120.21	126.80
1	A	207	A	N3-C4-C5	-9.41	120.21	126.80
32	W	415	A	N3-C4-C5	-9.41	120.21	126.80
1	A	126	A	N3-C4-C5	-9.40	120.22	126.80
32	W	985	A	N3-C4-C5	-9.40	120.22	126.80
1	A	2819	A	N3-C4-C5	-9.39	120.23	126.80
32	W	1077	A	N3-C4-C5	-9.39	120.23	126.80
1	A	1067	A	N3-C4-C5	-9.38	120.24	126.80
1	A	2793	A	N3-C4-C5	-9.37	120.24	126.80
1	A	2089	A	N3-C4-C5	-9.37	120.24	126.80
32	W	1355	A	N3-C4-C5	-9.37	120.24	126.80
32	W	254	A	N3-C4-C5	-9.37	120.24	126.80
32	W	1407	A	N3-C4-C5	-9.37	120.25	126.80
23	X	67	SER	N-CA-C	-9.36	85.73	111.00
32	W	631	A	N3-C4-C5	-9.36	120.25	126.80
1	A	1814	A	N3-C4-C5	-9.36	120.25	126.80
32	W	1247	A	N3-C4-C5	-9.35	120.25	126.80
1	A	2606	A	N3-C4-C5	-9.34	120.26	126.80
1	A	374	A	N3-C4-C5	-9.34	120.27	126.80
1	A	2916	A	N3-C4-C5	-9.33	120.27	126.80
1	A	1417	A	N3-C4-C5	-9.32	120.27	126.80
1	A	1305	A	N3-C4-C5	-9.31	120.28	126.80
1	A	647	A	N3-C4-C5	-9.30	120.29	126.80
32	W	209	A	N3-C4-C5	-9.26	120.32	126.80
1	A	1201	A	N3-C4-C5	-9.26	120.32	126.80
1	A	1003	A	N3-C4-C5	-9.25	120.32	126.80
1	A	82	G	C4'-C3'-O3'	-9.24	89.99	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2487	U	C4'-C3'-O3'	9.24	131.48	113.00
1	A	2062	A	N3-C4-C5	-9.20	120.36	126.80
32	W	862	A	N3-C4-C5	-9.20	120.36	126.80
1	A	1982	A	N3-C4-C5	-9.17	120.38	126.80
1	A	183	A	N3-C4-C5	-9.15	120.39	126.80
1	A	501	A	N3-C4-C5	-9.09	120.43	126.80
32	W	1372	A	N3-C4-C5	-9.07	120.45	126.80
1	A	501	A	C5-N7-C8	8.91	108.35	103.90
1	A	2805	A	C5-N7-C8	8.78	108.29	103.90
1	A	281	A	C5-N7-C8	8.73	108.26	103.90
32	W	508	A	N3-C4-C5	-8.72	120.70	126.80
1	A	1461	A	C5-N7-C8	8.69	108.25	103.90
32	W	1065	A	C5-N7-C8	8.66	108.23	103.90
1	A	2049	A	C5-N7-C8	8.64	108.22	103.90
1	A	527	A	C5-N7-C8	8.62	108.21	103.90
1	A	2364	A	C5-N7-C8	8.61	108.20	103.90
32	W	57	A	C5-N7-C8	8.59	108.20	103.90
32	W	452	A	C5-N7-C8	8.59	108.19	103.90
1	A	2782	A	C5-N7-C8	8.59	108.19	103.90
32	W	768	A	C5-N7-C8	8.57	108.19	103.90
1	A	2670	A	C5-N7-C8	8.57	108.18	103.90
1	A	1084	A	C5-N7-C8	8.56	108.18	103.90
32	W	988	A	C5-N7-C8	8.56	108.18	103.90
1	A	538	A	C5-N7-C8	8.55	108.18	103.90
32	W	886	A	C5-N7-C8	8.54	108.17	103.90
1	A	1809	A	C5-N7-C8	8.53	108.16	103.90
1	A	551	A	C5-N7-C8	8.52	108.16	103.90
1	A	2307	A	C5-N7-C8	8.51	108.16	103.90
1	A	52	A	C5-N7-C8	8.49	108.15	103.90
1	A	1998	A	C5-N7-C8	8.49	108.15	103.90
32	W	803	A	C5-N7-C8	8.49	108.15	103.90
1	A	110	A	C5-N7-C8	8.48	108.14	103.90
1	A	1895	A	C5-N7-C8	8.48	108.14	103.90
1	A	2417	A	C5-N7-C8	8.48	108.14	103.90
1	A	722	A	C5-N7-C8	8.48	108.14	103.90
1	A	449	A	C5-N7-C8	8.48	108.14	103.90
1	A	866	A	C5-N7-C8	8.47	108.14	103.90
1	A	2770	A	C5-N7-C8	8.47	108.14	103.90
32	W	1133	A	C5-N7-C8	8.47	108.14	103.90
32	W	870	A	C5-N7-C8	8.46	108.13	103.90
1	A	2837	A	C5-N7-C8	8.46	108.13	103.90
32	W	703	A	C5-N7-C8	8.46	108.13	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1094	A	C5-N7-C8	8.45	108.13	103.90
1	A	1254	A	C5-N7-C8	8.46	108.13	103.90
32	W	364	A	C5-N7-C8	8.45	108.13	103.90
1	A	2923	A	C5-N7-C8	8.45	108.12	103.90
32	W	1225	A	C5-N7-C8	8.45	108.12	103.90
1	A	1047	A	C5-N7-C8	8.45	108.12	103.90
1	A	1585	A	C5-N7-C8	8.45	108.12	103.90
1	A	2594	A	C5-N7-C8	8.44	108.12	103.90
1	A	1202	A	C5-N7-C8	8.44	108.12	103.90
1	A	1287	A	C5-N7-C8	8.44	108.12	103.90
32	W	228	A	C5-N7-C8	8.44	108.12	103.90
1	A	2351	A	C5-N7-C8	8.44	108.12	103.90
1	A	1524	A	C5-N7-C8	8.43	108.12	103.90
1	A	935	A	C5-N7-C8	8.43	108.11	103.90
1	A	584	A	C5-N7-C8	8.43	108.11	103.90
32	W	206	A	C5-N7-C8	8.43	108.11	103.90
1	A	2464	A	C5-N7-C8	8.43	108.11	103.90
1	A	166	A	C5-N7-C8	8.42	108.11	103.90
1	A	1918	A	C5-N7-C8	8.42	108.11	103.90
1	A	2694	A	C5-N7-C8	8.42	108.11	103.90
32	W	790	A	C5-N7-C8	8.42	108.11	103.90
1	A	690	A	C5-N7-C8	8.42	108.11	103.90
32	W	456	A	C5-N7-C8	8.42	108.11	103.90
1	A	667	A	C5-N7-C8	8.41	108.11	103.90
1	A	1555	A	C5-N7-C8	8.41	108.11	103.90
32	W	422	A	C5-N7-C8	8.41	108.10	103.90
32	W	287	A	C5-N7-C8	8.41	108.10	103.90
23	X	69	LYS	O-C-N	-8.40	109.25	122.70
1	A	1224	A	C5-N7-C8	8.40	108.10	103.90
1	A	526	A	C5-N7-C8	8.40	108.10	103.90
1	A	1685	A	C5-N7-C8	8.40	108.10	103.90
1	A	2673	A	C5-N7-C8	8.40	108.10	103.90
32	W	1004	A	C5-N7-C8	8.40	108.10	103.90
32	W	672	A	C5-N7-C8	8.40	108.10	103.90
1	A	1686	A	C5-N7-C8	8.40	108.10	103.90
1	A	2618	A	C5-N7-C8	8.40	108.10	103.90
32	W	357	A	C5-N7-C8	8.40	108.10	103.90
1	A	1210	A	C5-N7-C8	8.39	108.10	103.90
1	A	1735	A	C5-N7-C8	8.39	108.10	103.90
32	W	12	A	C5-N7-C8	8.39	108.10	103.90
32	W	737	A	C5-N7-C8	8.39	108.09	103.90
1	A	2700	A	C5-N7-C8	8.38	108.09	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2100	A	C5-N7-C8	8.38	108.09	103.90
32	W	1147	A	C5-N7-C8	8.38	108.09	103.90
32	W	811	A	C5-N7-C8	8.37	108.09	103.90
1	A	2907	A	C5-N7-C8	8.37	108.08	103.90
32	W	1103	A	C5-N7-C8	8.37	108.08	103.90
1	A	637	A	C5-N7-C8	8.37	108.08	103.90
1	A	2369	A	C5-N7-C8	8.37	108.08	103.90
32	W	506	A	C5-N7-C8	8.37	108.08	103.90
1	A	957	A	C5-N7-C8	8.36	108.08	103.90
32	W	918	A	C5-N7-C8	8.36	108.08	103.90
1	A	1073	A	C5-N7-C8	8.36	108.08	103.90
1	A	1190	A	C5-N7-C8	8.36	108.08	103.90
1	A	140	A	C5-N7-C8	8.36	108.08	103.90
1	A	1115	A	C5-N7-C8	8.36	108.08	103.90
1	A	1961	A	C5-N7-C8	8.36	108.08	103.90
1	A	622	A	C5-N7-C8	8.36	108.08	103.90
1	A	1648	A	C5-N7-C8	8.36	108.08	103.90
32	W	959	A	C5-N7-C8	8.36	108.08	103.90
32	W	1260	A	C5-N7-C8	8.36	108.08	103.90
32	W	266	A	C5-N7-C8	8.35	108.08	103.90
32	W	611	A	C5-N7-C8	8.35	108.08	103.90
1	A	677	A	C5-N7-C8	8.35	108.08	103.90
1	A	1260	A	C5-N7-C8	8.35	108.08	103.90
32	W	251	A	C5-N7-C8	8.35	108.08	103.90
1	A	763	A	C5-N7-C8	8.35	108.08	103.90
1	A	2812	A	C5-N7-C8	8.35	108.08	103.90
1	A	194	A	C5-N7-C8	8.35	108.07	103.90
1	A	324	A	C5-N7-C8	8.35	108.07	103.90
1	A	2315	A	C5-N7-C8	8.35	108.07	103.90
2	B	97	A	C5-N7-C8	8.35	108.07	103.90
32	W	329	A	C5-N7-C8	8.35	108.07	103.90
1	A	71	A	C5-N7-C8	8.34	108.07	103.90
1	A	2302	A	C5-N7-C8	8.34	108.07	103.90
1	A	353	A	C5-N7-C8	8.34	108.07	103.90
1	A	2447	A	C5-N7-C8	8.34	108.07	103.90
1	A	835	A	C5-N7-C8	8.34	108.07	103.90
1	A	1813	A	C5-N7-C8	8.34	108.07	103.90
1	A	2052	A	C5-N7-C8	8.34	108.07	103.90
1	A	475	A	C5-N7-C8	8.34	108.07	103.90
1	A	1055	A	C5-N7-C8	8.34	108.07	103.90
1	A	2683	A	C5-N7-C8	8.34	108.07	103.90
1	A	2807	A	C5-N7-C8	8.34	108.07	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	532	A	C5-N7-C8	8.34	108.07	103.90
32	W	1178	A	C5-N7-C8	8.34	108.07	103.90
32	W	1259	A	C5-N7-C8	8.34	108.07	103.90
32	W	1320	A	C5-N7-C8	8.34	108.07	103.90
32	W	31	A	C5-N7-C8	8.33	108.07	103.90
32	W	1502	A	C5-N7-C8	8.33	108.07	103.90
1	A	1326	A	C5-N7-C8	8.33	108.06	103.90
1	A	1553	A	C5-N7-C8	8.33	108.07	103.90
32	W	556	A	C5-N7-C8	8.33	108.07	103.90
1	A	2043	A	C5-N7-C8	8.33	108.06	103.90
1	A	2750	A	C5-N7-C8	8.33	108.06	103.90
32	W	1384	A	C5-N7-C8	8.33	108.06	103.90
1	A	2846	A	C5-N7-C8	8.33	108.06	103.90
32	W	1115	A	C5-N7-C8	8.33	108.06	103.90
1	A	1072	A	C5-N7-C8	8.32	108.06	103.90
1	A	2340	A	C5-N7-C8	8.32	108.06	103.90
1	A	2658	A	C5-N7-C8	8.32	108.06	103.90
32	W	189	A	C5-N7-C8	8.32	108.06	103.90
32	W	159	A	C5-N7-C8	8.32	108.06	103.90
32	W	170	A	C5-N7-C8	8.32	108.06	103.90
32	W	496	A	C5-N7-C8	8.32	108.06	103.90
32	W	824	A	C5-N7-C8	8.32	108.06	103.90
1	A	1174	A	C5-N7-C8	8.32	108.06	103.90
1	A	10	A	C5-N7-C8	8.32	108.06	103.90
1	A	1784	A	C5-N7-C8	8.32	108.06	103.90
1	A	572	A	C5-N7-C8	8.32	108.06	103.90
1	A	1046	A	C5-N7-C8	8.32	108.06	103.90
32	W	107	A	C5-N7-C8	8.32	108.06	103.90
1	A	418	A	C5-N7-C8	8.32	108.06	103.90
32	W	658	A	C5-N7-C8	8.32	108.06	103.90
1	A	2303	A	C5-N7-C8	8.32	108.06	103.90
32	W	725	A	C5-N7-C8	8.32	108.06	103.90
32	W	1092	A	C5-N7-C8	8.32	108.06	103.90
32	W	1160	A	C5-N7-C8	8.32	108.06	103.90
32	W	1456	A	C5-N7-C8	8.31	108.06	103.90
1	A	1175	A	C5-N7-C8	8.31	108.06	103.90
1	A	2317	A	C5-N7-C8	8.31	108.06	103.90
32	W	335	A	C5-N7-C8	8.31	108.06	103.90
32	W	1102	A	C5-N7-C8	8.31	108.06	103.90
32	W	1266	A	C5-N7-C8	8.31	108.06	103.90
1	A	278	A	C5-N7-C8	8.31	108.06	103.90
1	A	518	A	C5-N7-C8	8.31	108.06	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1654	A	C5-N7-C8	8.31	108.06	103.90
32	W	148	A	C5-N7-C8	8.31	108.06	103.90
32	W	419	A	C5-N7-C8	8.31	108.06	103.90
32	W	568	A	C5-N7-C8	8.31	108.06	103.90
32	W	704	A	C5-N7-C8	8.31	108.06	103.90
32	W	978	A	C5-N7-C8	8.31	108.06	103.90
1	A	993	A	C5-N7-C8	8.31	108.06	103.90
32	W	1222	A	C5-N7-C8	8.31	108.06	103.90
1	A	888	A	C5-N7-C8	8.31	108.05	103.90
2	B	27	A	C5-N7-C8	8.31	108.05	103.90
1	A	553	A	C5-N7-C8	8.31	108.05	103.90
1	A	1312	A	C5-N7-C8	8.30	108.05	103.90
32	W	638	A	C5-N7-C8	8.30	108.05	103.90
32	W	786	A	C5-N7-C8	8.31	108.05	103.90
32	W	919	A	C5-N7-C8	8.30	108.05	103.90
1	A	1583	A	C5-N7-C8	8.30	108.05	103.90
1	A	231	A	C5-N7-C8	8.30	108.05	103.90
1	A	1161	A	C5-N7-C8	8.30	108.05	103.90
1	A	125	A	C5-N7-C8	8.30	108.05	103.90
1	A	193	A	C5-N7-C8	8.29	108.05	103.90
1	A	1243	A	C5-N7-C8	8.30	108.05	103.90
1	A	1313	A	C5-N7-C8	8.30	108.05	103.90
1	A	1516	A	C5-N7-C8	8.29	108.05	103.90
1	A	2088	A	C5-N7-C8	8.29	108.05	103.90
32	W	923	A	C5-N7-C8	8.29	108.05	103.90
1	A	154	A	C5-N7-C8	8.29	108.05	103.90
1	A	206	A	C5-N7-C8	8.29	108.05	103.90
1	A	1233	A	C5-N7-C8	8.29	108.05	103.90
1	A	1745	A	C5-N7-C8	8.29	108.05	103.90
1	A	753	A	C5-N7-C8	8.29	108.05	103.90
32	W	690	A	C5-N7-C8	8.29	108.05	103.90
32	W	928	A	C5-N7-C8	8.29	108.05	103.90
32	W	1488	A	C5-N7-C8	8.29	108.05	103.90
1	A	2777	A	C5-N7-C8	8.29	108.05	103.90
32	W	1205	A	C5-N7-C8	8.29	108.05	103.90
1	A	44	A	C5-N7-C8	8.29	108.04	103.90
1	A	1445	A	C5-N7-C8	8.29	108.04	103.90
1	A	1672	A	C5-N7-C8	8.29	108.05	103.90
1	A	1580	A	C5-N7-C8	8.29	108.04	103.90
1	A	2390	A	C5-N7-C8	8.29	108.04	103.90
1	A	2830	A	C5-N7-C8	8.29	108.05	103.90
1	A	2876	A	C5-N7-C8	8.29	108.04	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	A	C5-N7-C8	8.29	108.04	103.90
1	A	821	A	C5-N7-C8	8.29	108.04	103.90
1	A	991	A	C5-N7-C8	8.29	108.04	103.90
1	A	1636	A	C5-N7-C8	8.29	108.04	103.90
32	W	1048	A	C5-N7-C8	8.29	108.04	103.90
2	B	76	A	C5-N7-C8	8.28	108.04	103.90
32	W	1185	A	C5-N7-C8	8.29	108.04	103.90
1	A	2383	A	C5-N7-C8	8.28	108.04	103.90
32	W	10	A	C5-N7-C8	8.28	108.04	103.90
1	A	2912	A	C5-N7-C8	8.28	108.04	103.90
2	B	17	A	C5-N7-C8	8.28	108.04	103.90
32	W	501	A	C5-N7-C8	8.28	108.04	103.90
1	A	244	A	C5-N7-C8	8.28	108.04	103.90
1	A	530	A	C5-N7-C8	8.28	108.04	103.90
1	A	1034	A	C5-N7-C8	8.28	108.04	103.90
32	W	202	A	C5-N7-C8	8.28	108.04	103.90
32	W	1443	A	C5-N7-C8	8.28	108.04	103.90
32	W	1510	A	C5-N7-C8	8.28	108.04	103.90
1	A	1189	A	C5-N7-C8	8.28	108.04	103.90
1	A	1302	A	C5-N7-C8	8.28	108.04	103.90
1	A	2854	A	C5-N7-C8	8.28	108.04	103.90
32	W	460	A	C5-N7-C8	8.28	108.04	103.90
1	A	752	A	C5-N7-C8	8.27	108.04	103.90
1	A	1483	A	C5-N7-C8	8.27	108.04	103.90
1	A	1619	A	C5-N7-C8	8.27	108.04	103.90
1	A	2026	A	C5-N7-C8	8.27	108.04	103.90
32	W	477	A	C5-N7-C8	8.27	108.04	103.90
32	W	823	A	C5-N7-C8	8.27	108.04	103.90
32	W	1348	A	C5-N7-C8	8.27	108.04	103.90
32	W	1541	A	C5-N7-C8	8.27	108.04	103.90
52	z	41	A	C5-N7-C8	8.27	108.04	103.90
1	A	1797	A	C5-N7-C8	8.27	108.04	103.90
1	A	1393	A	C5-N7-C8	8.27	108.03	103.90
1	A	1593	A	C5-N7-C8	8.27	108.03	103.90
32	W	397	A	C5-N7-C8	8.27	108.03	103.90
32	W	1333	A	C5-N7-C8	8.27	108.03	103.90
1	A	513	A	C4-C5-C6	8.27	121.13	117.00
1	A	1141	A	C5-N7-C8	8.27	108.03	103.90
1	A	2042	A	C5-N7-C8	8.27	108.03	103.90
32	W	1523	A	C5-N7-C8	8.27	108.03	103.90
1	A	345	A	C5-N7-C8	8.26	108.03	103.90
1	A	987	A	C5-N7-C8	8.26	108.03	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2819	A	C5-N7-C8	8.26	108.03	103.90
32	W	382	A	C5-N7-C8	8.26	108.03	103.90
1	A	1286	A	C5-N7-C8	8.26	108.03	103.90
1	A	1423	A	C5-N7-C8	8.26	108.03	103.90
1	A	1663	A	C5-N7-C8	8.26	108.03	103.90
32	W	522	A	C5-N7-C8	8.26	108.03	103.90
32	W	974	A	C5-N7-C8	8.26	108.03	103.90
52	z	14	A	C5-N7-C8	8.26	108.03	103.90
1	A	364	A	C5-N7-C8	8.26	108.03	103.90
1	A	1025	A	C5-N7-C8	8.26	108.03	103.90
32	W	178	A	C5-N7-C8	8.26	108.03	103.90
32	W	1254	A	C5-N7-C8	8.26	108.03	103.90
32	W	1257	A	C5-N7-C8	8.26	108.03	103.90
1	A	2668	A	C5-N7-C8	8.26	108.03	103.90
32	W	1434	A	C5-N7-C8	8.26	108.03	103.90
1	A	1061	A	C5-N7-C8	8.25	108.03	103.90
32	W	62	A	C5-N7-C8	8.25	108.03	103.90
1	A	1346	A	C5-N7-C8	8.25	108.03	103.90
1	A	2276	A	C5-N7-C8	8.25	108.03	103.90
32	W	762	A	C5-N7-C8	8.25	108.03	103.90
1	A	236	A	C5-N7-C8	8.25	108.03	103.90
1	A	2835	A	C5-N7-C8	8.25	108.03	103.90
32	W	53	A	C5-N7-C8	8.25	108.03	103.90
32	W	1466	A	C5-N7-C8	8.25	108.03	103.90
32	W	232	A	C5-N7-C8	8.25	108.02	103.90
32	W	924	A	C5-N7-C8	8.25	108.02	103.90
32	W	1111	A	C5-N7-C8	8.25	108.03	103.90
32	W	1509	A	C5-N7-C8	8.25	108.03	103.90
1	A	1036	A	C5-N7-C8	8.25	108.02	103.90
32	W	367	A	C5-N7-C8	8.25	108.02	103.90
1	A	102	A	C5-N7-C8	8.24	108.02	103.90
1	A	388	A	C5-N7-C8	8.24	108.02	103.90
52	z	21	A	C5-N7-C8	8.24	108.02	103.90
1	A	717	A	C5-N7-C8	8.24	108.02	103.90
1	A	1608	A	C5-N7-C8	8.24	108.02	103.90
32	W	440	A	C5-N7-C8	8.24	108.02	103.90
32	W	696	A	C5-N7-C8	8.24	108.02	103.90
1	A	715	A	C5-N7-C8	8.24	108.02	103.90
32	W	1405	A	C5-N7-C8	8.24	108.02	103.90
1	A	275	A	C5-N7-C8	8.24	108.02	103.90
32	W	529	A	C5-N7-C8	8.24	108.02	103.90
32	W	956	A	C5-N7-C8	8.24	108.02	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1176	A	C5-N7-C8	8.24	108.02	103.90
1	A	770	A	C5-N7-C8	8.24	108.02	103.90
32	W	1271	A	C5-N7-C8	8.24	108.02	103.90
1	A	273	A	C5-N7-C8	8.24	108.02	103.90
1	A	1314	A	C5-N7-C8	8.24	108.02	103.90
32	W	462	A	C5-N7-C8	8.24	108.02	103.90
1	A	1375	A	C5-N7-C8	8.23	108.02	103.90
1	A	1532	A	C5-N7-C8	8.23	108.02	103.90
1	A	1631	A	C5-N7-C8	8.23	108.02	103.90
1	A	1791	A	C5-N7-C8	8.23	108.02	103.90
32	W	715	A	C5-N7-C8	8.23	108.02	103.90
1	A	2606	A	C5-N7-C8	8.23	108.02	103.90
32	W	831	A	C5-N7-C8	8.23	108.02	103.90
1	A	302	A	C5-N7-C8	8.23	108.02	103.90
1	A	600	A	C5-N7-C8	8.23	108.02	103.90
1	A	2477	A	C5-N7-C8	8.23	108.02	103.90
2	B	102	A	C5-N7-C8	8.23	108.02	103.90
32	W	801	A	C5-N7-C8	8.23	108.02	103.90
1	A	646	A	C5-N7-C8	8.23	108.01	103.90
1	A	705	A	C5-N7-C8	8.23	108.01	103.90
32	W	204	A	C5-N7-C8	8.23	108.01	103.90
32	W	618	A	C5-N7-C8	8.23	108.01	103.90
1	A	330	A	C5-N7-C8	8.23	108.01	103.90
1	A	2500	A	C5-N7-C8	8.23	108.01	103.90
32	W	94	A	C5-N7-C8	8.23	108.01	103.90
32	W	321	A	C5-N7-C8	8.23	108.01	103.90
1	A	1134	A	N3-C4-N9	8.22	133.98	127.40
1	A	1284	A	C5-N7-C8	8.22	108.01	103.90
2	B	43	A	C5-N7-C8	8.22	108.01	103.90
32	W	401	A	C5-N7-C8	8.22	108.01	103.90
1	A	1575	A	C5-N7-C8	8.22	108.01	103.90
1	A	1722	A	C5-N7-C8	8.22	108.01	103.90
1	A	2032	A	C5-N7-C8	8.22	108.01	103.90
32	W	282	A	C5-N7-C8	8.22	108.01	103.90
32	W	1503	A	C5-N7-C8	8.22	108.01	103.90
1	A	84	A	C5-N7-C8	8.22	108.01	103.90
1	A	1700	A	C5-N7-C8	8.22	108.01	103.90
1	A	1838	A	C5-N7-C8	8.22	108.01	103.90
1	A	1325	A	C5-N7-C8	8.22	108.01	103.90
1	A	1778	A	C5-N7-C8	8.22	108.01	103.90
1	A	2111	A	C5-N7-C8	8.22	108.01	103.90
32	W	862	A	C5-N7-C8	8.22	108.01	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	947	A	C5-N7-C8	8.22	108.01	103.90
32	W	1056	A	C5-N7-C8	8.22	108.01	103.90
1	A	178	A	C5-N7-C8	8.21	108.01	103.90
1	A	436	A	C5-N7-C8	8.22	108.01	103.90
1	A	549	A	C5-N7-C8	8.21	108.01	103.90
1	A	1815	A	C5-N7-C8	8.21	108.01	103.90
1	A	2511	A	C5-N7-C8	8.21	108.01	103.90
32	W	18	A	C5-N7-C8	8.21	108.01	103.90
32	W	1213	A	C5-N7-C8	8.21	108.01	103.90
32	W	1478	A	C5-N7-C8	8.22	108.01	103.90
1	A	999	A	C5-N7-C8	8.21	108.01	103.90
1	A	355	A	C5-N7-C8	8.21	108.01	103.90
1	A	578	A	C5-N7-C8	8.21	108.01	103.90
1	A	1008	A	C5-N7-C8	8.21	108.01	103.90
1	A	2087	A	C5-N7-C8	8.21	108.01	103.90
2	B	114	A	C5-N7-C8	8.21	108.00	103.90
32	W	581	A	C5-N7-C8	8.21	108.00	103.90
32	W	828	A	C5-N7-C8	8.21	108.00	103.90
1	A	652	A	C5-N7-C8	8.21	108.00	103.90
1	A	456	A	C5-N7-C8	8.21	108.00	103.90
1	A	1157	A	C5-N7-C8	8.21	108.00	103.90
1	A	1335	A	C5-N7-C8	8.21	108.00	103.90
32	W	1490	A	C5-N7-C8	8.21	108.00	103.90
1	A	2459	A	C5-N7-C8	8.21	108.00	103.90
32	W	651	A	C5-N7-C8	8.21	108.00	103.90
32	W	837	A	C5-N7-C8	8.21	108.00	103.90
1	A	2330	A	C5-N7-C8	8.21	108.00	103.90
1	A	2590	A	C5-N7-C8	8.21	108.00	103.90
1	A	2902	A	C5-N7-C8	8.21	108.00	103.90
1	A	1945	A	C5-N7-C8	8.20	108.00	103.90
1	A	2790	A	C5-N7-C8	8.21	108.00	103.90
32	W	240	A	C5-N7-C8	8.21	108.00	103.90
32	W	1528	A	C5-N7-C8	8.21	108.00	103.90
1	A	618	A	C5-N7-C8	8.20	108.00	103.90
1	A	630	A	C5-N7-C8	8.20	108.00	103.90
1	A	740	A	C5-N7-C8	8.20	108.00	103.90
1	A	1788	A	C5-N7-C8	8.20	108.00	103.90
1	A	2381	A	C5-N7-C8	8.20	108.00	103.90
32	W	669	A	C5-N7-C8	8.20	108.00	103.90
32	W	139	A	C5-N7-C8	8.20	108.00	103.90
32	W	190	A	C5-N7-C8	8.20	108.00	103.90
32	W	791	A	C5-N7-C8	8.20	108.00	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1028	A	C5-N7-C8	8.20	108.00	103.90
32	W	1121	A	C5-N7-C8	8.20	108.00	103.90
1	A	161	A	C5-N7-C8	8.20	108.00	103.90
1	A	1831	A	C5-N7-C8	8.20	108.00	103.90
32	W	160	A	C5-N7-C8	8.20	108.00	103.90
32	W	463	A	C5-N7-C8	8.20	108.00	103.90
32	W	1427	A	C5-N7-C8	8.20	108.00	103.90
32	W	1437	A	C5-N7-C8	8.20	108.00	103.90
1	A	220	A	C5-N7-C8	8.20	108.00	103.90
1	A	225	A	C5-N7-C8	8.20	108.00	103.90
1	A	314	A	C5-N7-C8	8.20	108.00	103.90
1	A	519	A	C5-N7-C8	8.20	108.00	103.90
1	A	575	A	C5-N7-C8	8.20	108.00	103.90
1	A	1235	A	C5-N7-C8	8.20	108.00	103.90
1	A	1818	A	C5-N7-C8	8.20	108.00	103.90
1	A	829	A	C5-N7-C8	8.19	108.00	103.90
1	A	947	A	C5-N7-C8	8.19	108.00	103.90
1	A	1540	A	C5-N7-C8	8.19	108.00	103.90
1	A	2462	A	C5-N7-C8	8.19	108.00	103.90
1	A	2542	A	C5-N7-C8	8.19	108.00	103.90
32	W	76	A	C5-N7-C8	8.19	108.00	103.90
1	A	179	A	C5-N7-C8	8.19	108.00	103.90
1	A	5	A	C5-N7-C8	8.19	108.00	103.90
1	A	219	A	C5-N7-C8	8.19	108.00	103.90
32	W	211	A	C5-N7-C8	8.19	108.00	103.90
1	A	689	A	C5-N7-C8	8.19	108.00	103.90
32	W	838	A	C5-N7-C8	8.19	108.00	103.90
32	W	1284	A	C5-N7-C8	8.19	108.00	103.90
1	A	1347	A	C5-N7-C8	8.19	108.00	103.90
1	A	2007	A	C5-N7-C8	8.19	108.00	103.90
1	A	2338	A	C5-N7-C8	8.19	107.99	103.90
2	B	44	A	C5-N7-C8	8.19	108.00	103.90
32	W	118	A	C5-N7-C8	8.19	107.99	103.90
32	W	883	A	C5-N7-C8	8.19	107.99	103.90
32	W	899	A	C5-N7-C8	8.19	107.99	103.90
32	W	1383	A	C5-N7-C8	8.19	108.00	103.90
1	A	1405	A	C5-N7-C8	8.19	107.99	103.90
1	A	1424	A	C5-N7-C8	8.19	107.99	103.90
32	W	128	A	C5-N7-C8	8.19	107.99	103.90
32	W	1369	A	C5-N7-C8	8.19	107.99	103.90
32	W	1493	A	C5-N7-C8	8.19	107.99	103.90
32	W	475	A	C5-N7-C8	8.19	107.99	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	500	A	C5-N7-C8	8.18	107.99	103.90
1	A	1144	A	C5-N7-C8	8.18	107.99	103.90
1	A	1269	A	C5-N7-C8	8.18	107.99	103.90
1	A	1699	A	C5-N7-C8	8.18	107.99	103.90
32	W	1419	A	C5-N7-C8	8.18	107.99	103.90
1	A	274	A	C5-N7-C8	8.18	107.99	103.90
1	A	421	A	C5-N7-C8	8.18	107.99	103.90
1	A	470	A	C5-N7-C8	8.18	107.99	103.90
1	A	974	A	C5-N7-C8	8.18	107.99	103.90
1	A	1504	A	C5-N7-C8	8.18	107.99	103.90
1	A	1638	A	C5-N7-C8	8.18	107.99	103.90
1	A	1746	A	C5-N7-C8	8.18	107.99	103.90
1	A	2297	A	C5-N7-C8	8.18	107.99	103.90
1	A	2298	A	C5-N7-C8	8.18	107.99	103.90
1	A	2547	A	C5-N7-C8	8.18	107.99	103.90
1	A	2834	A	C5-N7-C8	8.18	107.99	103.90
32	W	664	A	C5-N7-C8	8.18	107.99	103.90
32	W	389	A	C5-N7-C8	8.18	107.99	103.90
1	A	2560	A	C5-N7-C8	8.18	107.99	103.90
1	A	459	A	C5-N7-C8	8.18	107.99	103.90
2	B	11	A	C5-N7-C8	8.18	107.99	103.90
32	W	61	A	C5-N7-C8	8.18	107.99	103.90
32	W	512	A	C5-N7-C8	8.18	107.99	103.90
32	W	1349	A	C5-N7-C8	8.18	107.99	103.90
1	A	38	A	C5-N7-C8	8.17	107.99	103.90
1	A	329	A	C5-N7-C8	8.17	107.99	103.90
1	A	727	A	C5-N7-C8	8.17	107.99	103.90
32	W	129	A	C5-N7-C8	8.17	107.99	103.90
32	W	405	A	C5-N7-C8	8.17	107.99	103.90
32	W	1442	A	C5-N7-C8	8.17	107.99	103.90
32	W	1197	A	C5-N7-C8	8.17	107.99	103.90
1	A	1480	A	C5-N7-C8	8.17	107.98	103.90
1	A	1490	A	C5-N7-C8	8.17	107.98	103.90
1	A	1627	A	C5-N7-C8	8.17	107.98	103.90
1	A	2387	A	C5-N7-C8	8.17	107.98	103.90
1	A	2398	A	C5-N7-C8	8.17	107.98	103.90
32	W	337	A	C5-N7-C8	8.17	107.98	103.90
1	A	13	A	C5-N7-C8	8.17	107.98	103.90
1	A	882	A	C5-N7-C8	8.17	107.98	103.90
1	A	896	A	C5-N7-C8	8.17	107.98	103.90
1	A	2395	A	C5-N7-C8	8.17	107.98	103.90
1	A	412	A	C5-N7-C8	8.17	107.98	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	543	A	C5-N7-C8	8.17	107.98	103.90
1	A	2804	A	C5-N7-C8	8.17	107.98	103.90
2	B	51	A	C5-N7-C8	8.17	107.98	103.90
32	W	917	A	C5-N7-C8	8.17	107.98	103.90
1	A	574	A	C5-N7-C8	8.16	107.98	103.90
1	A	893	A	C5-N7-C8	8.16	107.98	103.90
1	A	1059	A	C5-N7-C8	8.16	107.98	103.90
1	A	1617	A	C5-N7-C8	8.16	107.98	103.90
32	W	582	A	C5-N7-C8	8.16	107.98	103.90
32	W	1248	A	C5-N7-C8	8.16	107.98	103.90
1	A	702	A	C5-N7-C8	8.16	107.98	103.90
1	A	1194	A	C5-N7-C8	8.16	107.98	103.90
1	A	2734	A	C5-N7-C8	8.16	107.98	103.90
32	W	296	A	C5-N7-C8	8.16	107.98	103.90
32	W	346	A	C5-N7-C8	8.16	107.98	103.90
32	W	650	A	C5-N7-C8	8.16	107.98	103.90
32	W	1210	A	C5-N7-C8	8.16	107.98	103.90
1	A	2900	A	C5-N7-C8	8.16	107.98	103.90
1	A	171	A	C5-N7-C8	8.16	107.98	103.90
1	A	1802	A	C5-N7-C8	8.16	107.98	103.90
1	A	2722	A	C5-N7-C8	8.16	107.98	103.90
1	A	376	A	C5-N7-C8	8.16	107.98	103.90
1	A	582	A	C5-N7-C8	8.16	107.98	103.90
1	A	765	A	C5-N7-C8	8.16	107.98	103.90
1	A	1066	A	C5-N7-C8	8.16	107.98	103.90
1	A	428	A	C5-N7-C8	8.15	107.98	103.90
1	A	1230	A	C5-N7-C8	8.15	107.98	103.90
32	W	1513	A	C5-N7-C8	8.15	107.98	103.90
1	A	1392	A	C5-N7-C8	8.15	107.98	103.90
1	A	1592	A	C5-N7-C8	8.15	107.98	103.90
1	A	1914	A	C5-N7-C8	8.15	107.98	103.90
32	W	161	A	C5-N7-C8	8.15	107.98	103.90
32	W	500	A	C5-N7-C8	8.15	107.98	103.90
32	W	649	A	C5-N7-C8	8.15	107.98	103.90
32	W	776	A	C5-N7-C8	8.15	107.98	103.90
32	W	777	A	C5-N7-C8	8.15	107.98	103.90
1	A	325	A	C5-N7-C8	8.15	107.98	103.90
1	A	746	A	C5-N7-C8	8.15	107.98	103.90
1	A	1014	A	C5-N7-C8	8.15	107.98	103.90
1	A	198	A	C5-N7-C8	8.15	107.97	103.90
1	A	1776	A	C5-N7-C8	8.15	107.97	103.90
1	A	2089	A	C5-N7-C8	8.15	107.97	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	203	A	C5-N7-C8	8.15	107.97	103.90
32	W	433	A	C5-N7-C8	8.15	107.97	103.90
32	W	721	A	C5-N7-C8	8.15	107.98	103.90
1	A	925	A	C5-N7-C8	8.15	107.97	103.90
1	A	978	A	C5-N7-C8	8.15	107.97	103.90
1	A	1709	A	C5-N7-C8	8.15	107.97	103.90
1	A	207	A	C5-N7-C8	8.15	107.97	103.90
1	A	762	A	C5-N7-C8	8.15	107.97	103.90
1	A	1406	A	C5-N7-C8	8.15	107.97	103.90
1	A	2505	A	C5-N7-C8	8.15	107.97	103.90
1	A	2663	A	C5-N7-C8	8.15	107.97	103.90
32	W	1252	A	C5-N7-C8	8.15	107.97	103.90
1	A	1534	A	C5-N7-C8	8.14	107.97	103.90
1	A	1989	A	C5-N7-C8	8.14	107.97	103.90
1	A	2827	A	C5-N7-C8	8.14	107.97	103.90
32	W	423	A	C5-N7-C8	8.14	107.97	103.90
52	z	58	A	C5-N7-C8	8.14	107.97	103.90
1	A	2062	A	C5-N7-C8	8.14	107.97	103.90
1	A	2629	A	C5-N7-C8	8.14	107.97	103.90
32	W	1355	A	C5-N7-C8	8.14	107.97	103.90
1	A	1132	A	C5-N7-C8	8.14	107.97	103.90
1	A	1967	A	C5-N7-C8	8.14	107.97	103.90
1	A	2018	A	C5-N7-C8	8.14	107.97	103.90
32	W	604	A	C5-N7-C8	8.14	107.97	103.90
1	A	1653	A	C5-N7-C8	8.14	107.97	103.90
1	A	124	A	C5-N7-C8	8.14	107.97	103.90
1	A	1812	A	C5-N7-C8	8.14	107.97	103.90
1	A	2601	A	C5-N7-C8	8.14	107.97	103.90
32	W	234	A	C5-N7-C8	8.14	107.97	103.90
32	W	825	A	C5-N7-C8	8.14	107.97	103.90
32	W	1245	A	C5-N7-C8	8.14	107.97	103.90
1	A	94	A	C5-N7-C8	8.14	107.97	103.90
1	A	2643	A	C5-N7-C8	8.14	107.97	103.90
1	A	2860	A	C5-N7-C8	8.14	107.97	103.90
1	A	2034	A	C5-N7-C8	8.13	107.97	103.90
32	W	236	A	C5-N7-C8	8.13	107.97	103.90
1	A	851	A	C5-N7-C8	8.13	107.97	103.90
1	A	1253	A	C5-N7-C8	8.13	107.97	103.90
1	A	1677	A	C5-N7-C8	8.13	107.97	103.90
1	A	2059	A	C5-N7-C8	8.13	107.97	103.90
1	A	1473	A	C5-N7-C8	8.13	107.97	103.90
1	A	1679	A	C5-N7-C8	8.13	107.97	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2027	A	C5-N7-C8	8.13	107.97	103.90
32	W	74	A	C5-N7-C8	8.13	107.97	103.90
32	W	1050	A	C5-N7-C8	8.13	107.97	103.90
1	A	322	A	C5-N7-C8	8.13	107.96	103.90
1	A	547	A	C5-N7-C8	8.13	107.96	103.90
1	A	769	A	C5-N7-C8	8.13	107.96	103.90
1	A	965	A	C5-N7-C8	8.13	107.96	103.90
1	A	1078	A	C5-N7-C8	8.13	107.96	103.90
1	A	1308	A	C5-N7-C8	8.13	107.96	103.90
1	A	2762	A	C5-N7-C8	8.13	107.96	103.90
2	B	18	A	C5-N7-C8	8.13	107.96	103.90
32	W	671	A	C5-N7-C8	8.13	107.96	103.90
32	W	1026	A	C5-N7-C8	8.13	107.96	103.90
32	W	1188	A	C5-N7-C8	8.13	107.97	103.90
32	W	1270	A	C5-N7-C8	8.13	107.97	103.90
32	W	1455	A	C5-N7-C8	8.13	107.97	103.90
32	W	542	A	C5-N7-C8	8.13	107.96	103.90
52	z	70	A	C5-N7-C8	8.13	107.96	103.90
1	A	173	A	C5-N7-C8	8.13	107.96	103.90
1	A	374	A	C5-N7-C8	8.12	107.96	103.90
32	W	1128	A	C5-N7-C8	8.13	107.96	103.90
1	A	1562	A	C5-N7-C8	8.12	107.96	103.90
1	A	2047	A	C5-N7-C8	8.12	107.96	103.90
32	W	281	A	C5-N7-C8	8.12	107.96	103.90
32	W	504	A	C5-N7-C8	8.13	107.96	103.90
32	W	333	A	C5-N7-C8	8.12	107.96	103.90
32	W	361	A	C5-N7-C8	8.12	107.96	103.90
32	W	592	A	C5-N7-C8	8.12	107.96	103.90
52	z	76	A	C5-N7-C8	8.12	107.96	103.90
1	A	354	A	C5-N7-C8	8.12	107.96	103.90
1	A	2570	A	C5-N7-C8	8.12	107.96	103.90
1	A	2893	A	C5-N7-C8	8.12	107.96	103.90
1	A	1947	A	C5-N7-C8	8.12	107.96	103.90
1	A	2463	A	C5-N7-C8	8.12	107.96	103.90
1	A	2844	A	C5-N7-C8	8.12	107.96	103.90
32	W	711	A	C5-N7-C8	8.12	107.96	103.90
1	A	117	A	C5-N7-C8	8.12	107.96	103.90
1	A	559	A	C5-N7-C8	8.12	107.96	103.90
1	A	964	A	C5-N7-C8	8.12	107.96	103.90
1	A	2362	A	C5-N7-C8	8.12	107.96	103.90
1	A	2889	A	C5-N7-C8	8.12	107.96	103.90
32	W	72	A	C5-N7-C8	8.12	107.96	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1077	A	C5-N7-C8	8.12	107.96	103.90
32	W	1283	A	C5-N7-C8	8.12	107.96	103.90
1	A	14	A	C5-N7-C8	8.12	107.96	103.90
1	A	28	A	C5-N7-C8	8.12	107.96	103.90
1	A	910	A	C5-N7-C8	8.12	107.96	103.90
32	W	569	A	C5-N7-C8	8.12	107.96	103.90
1	A	343	A	C5-N7-C8	8.11	107.96	103.90
1	A	389	A	C5-N7-C8	8.12	107.96	103.90
1	A	390	A	C5-N7-C8	8.12	107.96	103.90
1	A	724	A	C5-N7-C8	8.12	107.96	103.90
1	A	1615	A	C5-N7-C8	8.12	107.96	103.90
1	A	2787	A	C5-N7-C8	8.12	107.96	103.90
2	B	37	A	C5-N7-C8	8.12	107.96	103.90
1	A	2793	A	C5-N7-C8	8.11	107.96	103.90
32	W	1288	A	C5-N7-C8	8.12	107.96	103.90
32	W	1298	A	C5-N7-C8	8.11	107.96	103.90
1	A	150	A	C5-N7-C8	8.11	107.96	103.90
1	A	876	A	C5-N7-C8	8.11	107.96	103.90
1	A	1126	A	C5-N7-C8	8.11	107.96	103.90
1	A	2810	A	C5-N7-C8	8.11	107.96	103.90
32	W	659	A	C5-N7-C8	8.11	107.96	103.90
32	W	984	A	C5-N7-C8	8.11	107.96	103.90
32	W	1422	A	C5-N7-C8	8.11	107.96	103.90
32	W	1425	A	C5-N7-C8	8.11	107.96	103.90
1	A	199	A	C5-N7-C8	8.11	107.95	103.90
1	A	202	A	C5-N7-C8	8.11	107.95	103.90
1	A	2845	A	C5-N7-C8	8.11	107.95	103.90
2	B	56	A	C5-N7-C8	8.11	107.95	103.90
1	A	867	A	C5-N7-C8	8.11	107.95	103.90
1	A	1464	A	C5-N7-C8	8.11	107.95	103.90
32	W	674	A	C5-N7-C8	8.11	107.95	103.90
32	W	730	A	C5-N7-C8	8.11	107.95	103.90
32	W	996	A	C5-N7-C8	8.11	107.95	103.90
32	W	1341	A	C5-N7-C8	8.11	107.95	103.90
1	A	2619	A	C5-N7-C8	8.11	107.95	103.90
1	A	2754	A	C5-N7-C8	8.11	107.95	103.90
1	A	279	A	C5-N7-C8	8.11	107.95	103.90
32	W	142	A	C5-N7-C8	8.11	107.95	103.90
32	W	254	A	C5-N7-C8	8.11	107.95	103.90
32	W	485	A	C5-N7-C8	8.11	107.95	103.90
32	W	1403	A	C5-N7-C8	8.11	107.95	103.90
1	A	337	A	C5-N7-C8	8.10	107.95	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	476	A	C5-N7-C8	8.10	107.95	103.90
1	A	548	A	C5-N7-C8	8.10	107.95	103.90
1	A	2526	A	C5-N7-C8	8.10	107.95	103.90
32	W	55	A	C5-N7-C8	8.10	107.95	103.90
32	W	195	A	C5-N7-C8	8.10	107.95	103.90
1	A	847	A	C5-N7-C8	8.10	107.95	103.90
1	A	2924	A	C5-N7-C8	8.10	107.95	103.90
32	W	968	A	C5-N7-C8	8.10	107.95	103.90
32	W	799	A	C5-N7-C8	8.10	107.95	103.90
32	W	1112	A	C5-N7-C8	8.10	107.95	103.90
1	A	1197	A	C5-N7-C8	8.10	107.95	103.90
1	A	259	A	C5-N7-C8	8.10	107.95	103.90
1	A	922	A	C5-N7-C8	8.10	107.95	103.90
1	A	1520	A	C5-N7-C8	8.10	107.95	103.90
2	B	71	A	C5-N7-C8	8.10	107.95	103.90
32	W	925	A	C5-N7-C8	8.10	107.95	103.90
32	W	1006	A	C5-N7-C8	8.10	107.95	103.90
32	W	1328	A	C5-N7-C8	8.10	107.95	103.90
1	A	200	A	C5-N7-C8	8.10	107.95	103.90
1	A	786	A	C5-N7-C8	8.10	107.95	103.90
2	B	39	A	C5-N7-C8	8.10	107.95	103.90
32	W	771	A	C5-N7-C8	8.10	107.95	103.90
32	W	1327	A	C5-N7-C8	8.10	107.95	103.90
32	W	1289	A	C5-N7-C8	8.10	107.95	103.90
1	A	1277	A	C5-N7-C8	8.09	107.95	103.90
1	A	1316	A	C5-N7-C8	8.09	107.95	103.90
1	A	1357	A	C5-N7-C8	8.09	107.95	103.90
1	A	1760	A	C5-N7-C8	8.09	107.95	103.90
32	W	386	A	C5-N7-C8	8.09	107.95	103.90
1	A	808	A	C5-N7-C8	8.09	107.94	103.90
1	A	828	A	C5-N7-C8	8.09	107.94	103.90
1	A	2402	A	C5-N7-C8	8.09	107.95	103.90
32	W	945	A	C5-N7-C8	8.09	107.94	103.90
32	W	1359	A	C5-N7-C8	8.09	107.95	103.90
1	A	1727	A	C5-N7-C8	8.09	107.94	103.90
1	A	1877	A	C5-N7-C8	8.09	107.94	103.90
32	W	1512	A	C5-N7-C8	8.09	107.94	103.90
1	A	67	A	C5-N7-C8	8.09	107.94	103.90
1	A	537	A	C5-N7-C8	8.09	107.94	103.90
1	A	952	A	C5-N7-C8	8.09	107.94	103.90
1	A	1499	A	C5-N7-C8	8.09	107.94	103.90
1	A	1588	A	C5-N7-C8	8.09	107.94	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	225	A	C5-N7-C8	8.09	107.94	103.90
32	W	301	A	C5-N7-C8	8.09	107.94	103.90
32	W	617	A	C5-N7-C8	8.09	107.94	103.90
32	W	685	A	C5-N7-C8	8.09	107.94	103.90
32	W	816	A	C5-N7-C8	8.09	107.94	103.90
32	W	1090	A	C5-N7-C8	8.09	107.94	103.90
32	W	1143	A	C5-N7-C8	8.09	107.94	103.90
32	W	1386	A	C5-N7-C8	8.09	107.94	103.90
1	A	661	A	C5-N7-C8	8.09	107.94	103.90
1	A	2295	A	C5-N7-C8	8.09	107.94	103.90
32	W	371	A	C5-N7-C8	8.08	107.94	103.90
1	A	258	A	C5-N7-C8	8.08	107.94	103.90
1	A	260	A	C5-N7-C8	8.08	107.94	103.90
1	A	486	A	C5-N7-C8	8.08	107.94	103.90
1	A	1103	A	C5-N7-C8	8.08	107.94	103.90
1	A	268	A	C5-N7-C8	8.08	107.94	103.90
1	A	1434	A	C5-N7-C8	8.08	107.94	103.90
1	A	1948	A	C5-N7-C8	8.08	107.94	103.90
32	W	758	A	C5-N7-C8	8.08	107.94	103.90
1	A	477	A	C5-N7-C8	8.08	107.94	103.90
1	A	2106	A	C5-N7-C8	8.08	107.94	103.90
1	A	524	A	C5-N7-C8	8.08	107.94	103.90
1	A	1119	A	C5-N7-C8	8.08	107.94	103.90
1	A	1982	A	C5-N7-C8	8.08	107.94	103.90
1	A	2769	A	C5-N7-C8	8.08	107.94	103.90
32	W	913	A	C5-N7-C8	8.08	107.94	103.90
1	A	2869	A	C5-N7-C8	8.08	107.94	103.90
1	A	216	A	C5-N7-C8	8.08	107.94	103.90
1	A	2270	A	C5-N7-C8	8.08	107.94	103.90
1	A	1305	A	C5-N7-C8	8.08	107.94	103.90
1	A	2662	A	C5-N7-C8	8.08	107.94	103.90
32	W	52	A	C5-N7-C8	8.08	107.94	103.90
32	W	1407	A	C5-N7-C8	8.08	107.94	103.90
1	A	6	A	C5-N7-C8	8.07	107.94	103.90
1	A	185	A	C5-N7-C8	8.07	107.94	103.90
1	A	469	A	C5-N7-C8	8.07	107.94	103.90
1	A	781	A	C5-N7-C8	8.07	107.94	103.90
1	A	868	A	C5-N7-C8	8.07	107.94	103.90
1	A	889	A	C5-N7-C8	8.07	107.94	103.90
1	A	1556	A	C5-N7-C8	8.07	107.94	103.90
32	W	644	A	C5-N7-C8	8.07	107.94	103.90
1	A	1360	A	C5-N7-C8	8.07	107.94	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2421	A	C5-N7-C8	8.07	107.94	103.90
32	W	404	A	C5-N7-C8	8.07	107.94	103.90
32	W	544	A	C5-N7-C8	8.07	107.94	103.90
32	W	705	A	C5-N7-C8	8.07	107.94	103.90
1	A	1339	A	C5-N7-C8	8.07	107.94	103.90
32	W	270	A	C5-N7-C8	8.07	107.94	103.90
1	A	130	A	C5-N7-C8	8.07	107.94	103.90
1	A	230	A	C5-N7-C8	8.07	107.94	103.90
1	A	1888	A	C5-N7-C8	8.07	107.93	103.90
1	A	2006	A	C5-N7-C8	8.07	107.93	103.90
1	A	507	A	C5-N7-C8	8.07	107.93	103.90
1	A	49	A	C5-N7-C8	8.07	107.93	103.90
1	A	736	A	C5-N7-C8	8.07	107.93	103.90
1	A	1027	A	C5-N7-C8	8.07	107.93	103.90
1	A	1258	A	C5-N7-C8	8.07	107.93	103.90
1	A	1388	A	C5-N7-C8	8.07	107.93	103.90
1	A	2000	A	C5-N7-C8	8.07	107.93	103.90
1	A	2329	A	C5-N7-C8	8.07	107.93	103.90
32	W	290	A	C5-N7-C8	8.07	107.93	103.90
32	W	679	A	C5-N7-C8	8.07	107.93	103.90
32	W	210	A	C5-N7-C8	8.07	107.93	103.90
1	A	1096	A	C5-N7-C8	8.06	107.93	103.90
1	A	1179	A	C5-N7-C8	8.06	107.93	103.90
1	A	1695	A	C5-N7-C8	8.06	107.93	103.90
1	A	2532	A	C5-N7-C8	8.06	107.93	103.90
1	A	2686	A	C5-N7-C8	8.06	107.93	103.90
32	W	1234	A	C5-N7-C8	8.06	107.93	103.90
1	A	65	A	C5-N7-C8	8.06	107.93	103.90
1	A	307	A	C5-N7-C8	8.06	107.93	103.90
1	A	758	A	C5-N7-C8	8.06	107.93	103.90
1	A	894	A	C5-N7-C8	8.06	107.93	103.90
1	A	2497	A	C5-N7-C8	8.06	107.93	103.90
32	W	306	A	C5-N7-C8	8.06	107.93	103.90
1	A	943	A	C5-N7-C8	8.06	107.93	103.90
1	A	1723	A	C5-N7-C8	8.06	107.93	103.90
1	A	1957	A	C5-N7-C8	8.06	107.93	103.90
1	A	2507	A	C5-N7-C8	8.06	107.93	103.90
32	W	35	A	C5-N7-C8	8.06	107.93	103.90
32	W	1200	A	C5-N7-C8	8.06	107.93	103.90
1	A	61	A	C5-N7-C8	8.06	107.93	103.90
1	A	1020	A	C5-N7-C8	8.06	107.93	103.90
2	B	113	A	C5-N7-C8	8.06	107.93	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	A	C5-N7-C8	8.06	107.93	103.90
1	A	1323	A	C5-N7-C8	8.06	107.93	103.90
1	A	1845	A	C5-N7-C8	8.06	107.93	103.90
1	A	2719	A	C5-N7-C8	8.06	107.93	103.90
32	W	910	A	C5-N7-C8	8.06	107.93	103.90
1	A	12	A	C5-N7-C8	8.05	107.93	103.90
1	A	168	A	C5-N7-C8	8.05	107.93	103.90
1	A	2316	A	C5-N7-C8	8.05	107.93	103.90
32	W	1486	A	C5-N7-C8	8.05	107.93	103.90
52	z	44	A	C5-N7-C8	8.05	107.93	103.90
1	A	2356	A	C5-N7-C8	8.05	107.93	103.90
32	W	34	A	C5-N7-C8	8.05	107.93	103.90
32	W	117	A	C5-N7-C8	8.05	107.93	103.90
32	W	1024	A	C5-N7-C8	8.05	107.93	103.90
32	W	1297	A	C5-N7-C8	8.05	107.93	103.90
1	A	326	A	C5-N7-C8	8.05	107.92	103.90
1	A	673	A	C5-N7-C8	8.05	107.93	103.90
1	A	870	A	C5-N7-C8	8.05	107.93	103.90
32	W	727	A	C5-N7-C8	8.05	107.93	103.90
32	W	1529	A	C5-N7-C8	8.05	107.92	103.90
1	A	108	A	C5-N7-C8	8.05	107.92	103.90
1	A	407	A	C5-N7-C8	8.05	107.92	103.90
1	A	2904	A	C5-N7-C8	8.05	107.92	103.90
32	W	415	A	C5-N7-C8	8.05	107.92	103.90
32	W	1296	A	C5-N7-C8	8.05	107.92	103.90
1	A	183	A	C5-N7-C8	8.04	107.92	103.90
1	A	1026	A	C5-N7-C8	8.04	107.92	103.90
1	A	2066	A	C5-N7-C8	8.05	107.92	103.90
1	A	2375	A	C5-N7-C8	8.05	107.92	103.90
1	A	1116	A	C5-N7-C8	8.04	107.92	103.90
1	A	1965	A	C5-N7-C8	8.04	107.92	103.90
32	W	140	A	C5-N7-C8	8.04	107.92	103.90
32	W	1031	A	C5-N7-C8	8.04	107.92	103.90
1	A	431	A	C5-N7-C8	8.04	107.92	103.90
1	A	2826	A	C5-N7-C8	8.04	107.92	103.90
1	A	1029	A	C5-N7-C8	8.04	107.92	103.90
32	W	985	A	C5-N7-C8	8.04	107.92	103.90
52	z	24	A	C5-N7-C8	8.04	107.92	103.90
1	A	139	A	C5-N7-C8	8.04	107.92	103.90
32	W	975	A	C5-N7-C8	8.04	107.92	103.90
32	W	1120	A	C5-N7-C8	8.04	107.92	103.90
1	A	224	A	C5-N7-C8	8.04	107.92	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1417	A	C5-N7-C8	8.04	107.92	103.90
1	A	2593	A	C5-N7-C8	8.04	107.92	103.90
1	A	970	A	C5-N7-C8	8.04	107.92	103.90
1	A	1885	A	C5-N7-C8	8.04	107.92	103.90
1	A	1942	A	C5-N7-C8	8.04	107.92	103.90
1	A	1981	A	C5-N7-C8	8.04	107.92	103.90
32	W	491	A	C5-N7-C8	8.04	107.92	103.90
1	A	2517	A	C5-N7-C8	8.04	107.92	103.90
1	A	2767	A	C5-N7-C8	8.04	107.92	103.90
32	W	81	A	C5-N7-C8	8.04	107.92	103.90
1	A	1743	A	C5-N7-C8	8.04	107.92	103.90
1	A	1844	A	C5-N7-C8	8.04	107.92	103.90
1	A	1913	A	C5-N7-C8	8.04	107.92	103.90
32	W	208	A	C5-N7-C8	8.04	107.92	103.90
32	W	1451	A	C5-N7-C8	8.04	107.92	103.90
1	A	126	A	C5-N7-C8	8.03	107.92	103.90
1	A	144	A	C5-N7-C8	8.03	107.92	103.90
1	A	1092	A	C5-N7-C8	8.03	107.92	103.90
1	A	2389	A	C5-N7-C8	8.03	107.92	103.90
32	W	1179	A	C5-N7-C8	8.03	107.92	103.90
1	A	369	A	C5-N7-C8	8.03	107.92	103.90
1	A	1005	A	C5-N7-C8	8.03	107.92	103.90
1	A	1536	A	C5-N7-C8	8.03	107.92	103.90
1	A	1054	A	C5-N7-C8	8.03	107.91	103.90
1	A	1222	A	C5-N7-C8	8.03	107.91	103.90
1	A	1734	A	C5-N7-C8	8.03	107.91	103.90
32	W	541	A	C5-N7-C8	8.03	107.91	103.90
32	W	630	A	C5-N7-C8	8.03	107.92	103.90
32	W	738	A	C5-N7-C8	8.03	107.92	103.90
1	A	222	A	C5-N7-C8	8.03	107.91	103.90
1	A	1618	A	C5-N7-C8	8.03	107.91	103.90
1	A	1839	A	C5-N7-C8	8.03	107.91	103.90
1	A	1999	A	C5-N7-C8	8.03	107.91	103.90
32	W	323	A	C5-N7-C8	8.03	107.91	103.90
32	W	1435	A	C5-N7-C8	8.03	107.91	103.90
1	A	438	A	C5-N7-C8	8.02	107.91	103.90
1	A	517	A	C5-N7-C8	8.02	107.91	103.90
32	W	1517	A	C5-N7-C8	8.02	107.91	103.90
1	A	561	A	C5-N7-C8	8.02	107.91	103.90
32	W	929	A	C5-N7-C8	8.02	107.91	103.90
1	A	699	A	C5-N7-C8	8.02	107.91	103.90
32	W	271	A	C5-N7-C8	8.02	107.91	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	619	A	C5-N7-C8	8.02	107.91	103.90
1	A	908	A	C5-N7-C8	8.02	107.91	103.90
1	A	1100	A	C5-N7-C8	8.02	107.91	103.90
1	A	2794	A	C5-N7-C8	8.02	107.91	103.90
32	W	684	A	C5-N7-C8	8.02	107.91	103.90
32	W	1017	A	C5-N7-C8	8.02	107.91	103.90
1	A	1542	A	C5-N7-C8	8.02	107.91	103.90
1	A	2875	A	C5-N7-C8	8.02	107.91	103.90
1	A	2482	A	C5-N7-C8	8.02	107.91	103.90
32	W	979	A	C5-N7-C8	8.02	107.91	103.90
1	A	479	A	C5-N7-C8	8.01	107.91	103.90
1	A	1075	A	C5-N7-C8	8.01	107.91	103.90
32	W	258	A	C5-N7-C8	8.01	107.91	103.90
32	W	278	A	C5-N7-C8	8.01	107.91	103.90
1	A	2407	A	C5-N7-C8	8.01	107.91	103.90
1	A	2455	A	C5-N7-C8	8.01	107.91	103.90
32	W	344	A	C5-N7-C8	8.01	107.91	103.90
32	W	902	A	C5-N7-C8	8.01	107.91	103.90
1	A	1517	A	C5-N7-C8	8.01	107.91	103.90
2	B	25	A	C5-N7-C8	8.01	107.91	103.90
1	A	373	A	C5-N7-C8	8.01	107.90	103.90
1	A	623	A	C5-N7-C8	8.01	107.90	103.90
1	A	653	A	C5-N7-C8	8.01	107.90	103.90
1	A	1149	A	C5-N7-C8	8.01	107.90	103.90
1	A	1724	A	C5-N7-C8	8.01	107.90	103.90
1	A	305	A	C5-N7-C8	8.00	107.90	103.90
1	A	342	A	C5-N7-C8	8.00	107.90	103.90
1	A	384	A	C5-N7-C8	8.00	107.90	103.90
1	A	2357	A	C5-N7-C8	8.00	107.90	103.90
32	W	120	A	C5-N7-C8	8.00	107.90	103.90
32	W	1207	A	C5-N7-C8	8.00	107.90	103.90
1	A	437	A	C5-N7-C8	8.00	107.90	103.90
1	A	490	A	C5-N7-C8	8.00	107.90	103.90
1	A	1966	A	C5-N7-C8	8.00	107.90	103.90
1	A	1477	A	C5-N7-C8	8.00	107.90	103.90
1	A	2436	A	C5-N7-C8	8.00	107.90	103.90
32	W	677	A	C5-N7-C8	8.00	107.90	103.90
1	A	1848	A	C5-N7-C8	8.00	107.90	103.90
1	A	1021	A	C5-N7-C8	8.00	107.90	103.90
1	A	1130	A	C5-N7-C8	8.00	107.90	103.90
1	A	162	A	C5-N7-C8	8.00	107.90	103.90
1	A	1404	A	C5-N7-C8	8.00	107.90	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1906	A	C5-N7-C8	8.00	107.90	103.90
1	A	2441	A	C5-N7-C8	8.00	107.90	103.90
32	W	67	A	C5-N7-C8	8.00	107.90	103.90
32	W	308	A	C5-N7-C8	8.00	107.90	103.90
1	A	917	A	C5-N7-C8	8.00	107.90	103.90
32	W	775	A	C5-N7-C8	7.99	107.90	103.90
32	W	796	A	C5-N7-C8	7.99	107.90	103.90
1	A	2365	A	C5-N7-C8	7.99	107.90	103.90
1	A	1533	A	C5-N7-C8	7.99	107.89	103.90
1	A	1721	A	C5-N7-C8	7.99	107.89	103.90
1	A	1941	A	C5-N7-C8	7.99	107.89	103.90
1	A	2851	A	C5-N7-C8	7.99	107.89	103.90
32	W	1206	A	C5-N7-C8	7.99	107.89	103.90
1	A	525	A	C5-N7-C8	7.99	107.89	103.90
1	A	2661	A	C5-N7-C8	7.99	107.89	103.90
1	A	2908	A	C5-N7-C8	7.99	107.89	103.90
1	A	2343	A	C5-N7-C8	7.99	107.89	103.90
1	A	1569	A	C5-N7-C8	7.99	107.89	103.90
1	A	2030	A	C5-N7-C8	7.99	107.89	103.90
1	A	2339	A	C5-N7-C8	7.99	107.89	103.90
32	W	173	A	C5-N7-C8	7.99	107.89	103.90
32	W	1261	A	C5-N7-C8	7.99	107.89	103.90
1	A	1201	A	C5-N7-C8	7.98	107.89	103.90
1	A	1956	A	C5-N7-C8	7.98	107.89	103.90
32	W	28	A	C5-N7-C8	7.98	107.89	103.90
32	W	1463	A	C5-N7-C8	7.98	107.89	103.90
1	A	64	A	C5-N7-C8	7.98	107.89	103.90
1	A	1832	A	C5-N7-C8	7.98	107.89	103.90
1	A	1995	A	C5-N7-C8	7.98	107.89	103.90
32	W	757	A	C5-N7-C8	7.98	107.89	103.90
32	W	793	A	C5-N7-C8	7.98	107.89	103.90
1	A	2406	A	C5-N7-C8	7.98	107.89	103.90
32	W	583	A	C5-N7-C8	7.98	107.89	103.90
32	W	911	A	C5-N7-C8	7.98	107.89	103.90
1	A	333	A	C5-N7-C8	7.97	107.89	103.90
1	A	1042	A	C5-N7-C8	7.97	107.89	103.90
1	A	1453	A	C5-N7-C8	7.97	107.89	103.90
1	A	1456	A	C5-N7-C8	7.97	107.89	103.90
1	A	156	A	C5-N7-C8	7.97	107.89	103.90
1	A	339	A	C5-N7-C8	7.97	107.89	103.90
1	A	683	A	C5-N7-C8	7.97	107.89	103.90
1	A	2887	A	C5-N7-C8	7.97	107.89	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1054	A	C5-N7-C8	7.97	107.89	103.90
1	A	429	A	C5-N7-C8	7.97	107.89	103.90
1	A	811	A	C5-N7-C8	7.97	107.89	103.90
1	A	1266	A	C5-N7-C8	7.97	107.89	103.90
32	W	314	A	C5-N7-C8	7.97	107.88	103.90
1	A	1876	A	C5-N7-C8	7.97	107.88	103.90
32	W	150	A	C5-N7-C8	7.97	107.88	103.90
32	W	1180	A	C5-N7-C8	7.97	107.88	103.90
32	W	1256	A	C5-N7-C8	7.97	107.88	103.90
1	A	1506	A	C5-N7-C8	7.97	107.88	103.90
1	A	2480	A	C5-N7-C8	7.97	107.88	103.90
1	A	2405	A	C5-N7-C8	7.96	107.88	103.90
32	W	1417	A	C5-N7-C8	7.96	107.88	103.90
1	A	971	A	C5-N7-C8	7.96	107.88	103.90
1	A	1123	A	C5-N7-C8	7.96	107.88	103.90
1	A	1901	A	C5-N7-C8	7.96	107.88	103.90
1	A	41	A	C5-N7-C8	7.96	107.88	103.90
1	A	504	A	C5-N7-C8	7.96	107.88	103.90
1	A	2461	A	C5-N7-C8	7.96	107.88	103.90
32	W	171	A	C5-N7-C8	7.96	107.88	103.90
32	W	151	A	C5-N7-C8	7.96	107.88	103.90
1	A	1768	A	C5-N7-C8	7.96	107.88	103.90
1	A	1929	A	C5-N7-C8	7.96	107.88	103.90
1	A	2708	A	C5-N7-C8	7.96	107.88	103.90
2	B	50	A	C5-N7-C8	7.96	107.88	103.90
32	W	1247	A	C5-N7-C8	7.96	107.88	103.90
1	A	658	A	C5-N7-C8	7.96	107.88	103.90
2	B	55	A	C5-N7-C8	7.96	107.88	103.90
1	A	73	A	C5-N7-C8	7.95	107.88	103.90
1	A	1858	A	C5-N7-C8	7.95	107.88	103.90
1	A	2327	A	C5-N7-C8	7.95	107.88	103.90
1	A	91	A	C5-N7-C8	7.95	107.88	103.90
1	A	592	A	C5-N7-C8	7.95	107.88	103.90
1	A	1905	A	C5-N7-C8	7.95	107.88	103.90
1	A	254	A	C5-N7-C8	7.95	107.88	103.90
1	A	1667	A	C5-N7-C8	7.95	107.88	103.90
1	A	782	A	C5-N7-C8	7.95	107.87	103.90
32	W	605	A	C5-N7-C8	7.95	107.87	103.90
32	W	616	A	C5-N7-C8	7.95	107.87	103.90
1	A	1485	A	C5-N7-C8	7.95	107.87	103.90
1	A	247	A	C5-N7-C8	7.95	107.87	103.90
1	A	1680	A	C5-N7-C8	7.95	107.87	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1900	A	C5-N7-C8	7.95	107.87	103.90
32	W	518	A	C5-N7-C8	7.95	107.87	103.90
32	W	572	A	C5-N7-C8	7.95	107.87	103.90
32	W	1014	A	C5-N7-C8	7.95	107.87	103.90
1	A	2071	A	C5-N7-C8	7.94	107.87	103.90
1	A	2479	A	C5-N7-C8	7.94	107.87	103.90
1	A	2831	A	C5-N7-C8	7.94	107.87	103.90
32	W	352	A	C5-N7-C8	7.94	107.87	103.90
32	W	474	A	C5-N7-C8	7.94	107.87	103.90
52	z	9	A	C5-N7-C8	7.94	107.87	103.90
1	A	678	A	C5-N7-C8	7.94	107.87	103.90
2	B	64	A	C5-N7-C8	7.94	107.87	103.90
1	A	1131	A	C5-N7-C8	7.94	107.87	103.90
1	A	2440	A	C5-N7-C8	7.94	107.87	103.90
32	W	874	A	C5-N7-C8	7.94	107.87	103.90
1	A	2779	A	C5-N7-C8	7.94	107.87	103.90
1	A	723	A	C5-N7-C8	7.93	107.87	103.90
1	A	849	A	C5-N7-C8	7.93	107.87	103.90
1	A	2740	A	C5-N7-C8	7.93	107.87	103.90
32	W	1236	A	C5-N7-C8	7.93	107.87	103.90
1	A	1265	A	C5-N7-C8	7.93	107.87	103.90
1	A	1426	A	C5-N7-C8	7.93	107.87	103.90
1	A	2498	A	C5-N7-C8	7.93	107.87	103.90
2	B	105	A	C5-N7-C8	7.93	107.87	103.90
32	W	390	A	C5-N7-C8	7.93	107.87	103.90
1	A	1221	A	C5-N7-C8	7.93	107.86	103.90
32	W	1155	A	C5-N7-C8	7.93	107.86	103.90
32	W	1308	A	C5-N7-C8	7.93	107.87	103.90
32	W	459	A	C5-N7-C8	7.93	107.86	103.90
32	W	1016	A	C5-N7-C8	7.93	107.86	103.90
32	W	1315	A	C5-N7-C8	7.93	107.86	103.90
1	A	1142	A	C5-N7-C8	7.93	107.86	103.90
32	W	1479	A	C5-N7-C8	7.93	107.86	103.90
1	A	1421	A	C5-N7-C8	7.92	107.86	103.90
1	A	2060	A	C5-N7-C8	7.92	107.86	103.90
1	A	2862	A	C5-N7-C8	7.92	107.86	103.90
32	W	1022	A	C5-N7-C8	7.92	107.86	103.90
52	z	23	A	C5-N7-C8	7.92	107.86	103.90
1	A	1291	A	C5-N7-C8	7.92	107.86	103.90
1	A	1074	A	C5-N7-C8	7.92	107.86	103.90
32	W	381	A	C5-N7-C8	7.92	107.86	103.90
2	B	20	A	C5-N7-C8	7.92	107.86	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1614	A	C5-N7-C8	7.92	107.86	103.90
32	W	209	A	C5-N7-C8	7.92	107.86	103.90
1	A	176	A	C5-N7-C8	7.92	107.86	103.90
1	A	1925	A	C5-N7-C8	7.91	107.86	103.90
1	A	2044	A	C5-N7-C8	7.91	107.86	103.90
1	A	2358	A	C5-N7-C8	7.91	107.86	103.90
1	A	2091	A	C5-N7-C8	7.91	107.85	103.90
1	A	1675	A	C5-N7-C8	7.91	107.85	103.90
32	W	875	A	C5-N7-C8	7.90	107.85	103.90
1	A	2885	A	C5-N7-C8	7.90	107.85	103.90
1	A	2571	A	C5-N7-C8	7.90	107.85	103.90
1	A	593	A	C5-N7-C8	7.90	107.85	103.90
1	A	948	A	C5-N7-C8	7.90	107.85	103.90
32	W	987	A	C5-N7-C8	7.90	107.85	103.90
32	W	1278	A	C5-N7-C8	7.90	107.85	103.90
1	A	692	A	C5-N7-C8	7.89	107.85	103.90
1	A	2078	A	C5-N7-C8	7.89	107.85	103.90
1	A	2919	A	C5-N7-C8	7.89	107.85	103.90
1	A	1882	A	C5-N7-C8	7.89	107.84	103.90
1	A	391	A	C5-N7-C8	7.89	107.84	103.90
1	A	448	A	C5-N7-C8	7.89	107.84	103.90
1	A	1541	A	C5-N7-C8	7.89	107.84	103.90
32	W	724	A	C5-N7-C8	7.89	107.84	103.90
1	A	1465	A	C5-N7-C8	7.88	107.84	103.90
2	B	13	A	C5-N7-C8	7.88	107.84	103.90
32	W	372	A	C5-N7-C8	7.88	107.84	103.90
1	A	2689	A	C5-N7-C8	7.88	107.84	103.90
32	W	1470	A	C5-N7-C8	7.88	107.84	103.90
1	A	1113	A	C5-N7-C8	7.88	107.84	103.90
32	W	844	A	C5-N7-C8	7.88	107.84	103.90
1	A	2595	A	C5-N7-C8	7.88	107.84	103.90
1	A	1710	A	C5-N7-C8	7.87	107.84	103.90
1	A	1432	A	C5-N7-C8	7.87	107.84	103.90
1	A	1442	A	C5-N7-C8	7.87	107.83	103.90
1	A	1850	A	C5-N7-C8	7.87	107.83	103.90
32	W	948	A	C5-N7-C8	7.87	107.83	103.90
1	A	1713	A	C5-N7-C8	7.87	107.83	103.90
1	A	1620	A	C5-N7-C8	7.87	107.83	103.90
1	A	1883	A	C5-N7-C8	7.87	107.83	103.90
32	W	743	A	C5-N7-C8	7.87	107.83	103.90
32	W	969	A	C5-N7-C8	7.86	107.83	103.90
1	A	2080	A	C5-N7-C8	7.86	107.83	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	A	C5-N7-C8	7.86	107.83	103.90
1	A	2735	A	C5-N7-C8	7.86	107.83	103.90
32	W	879	A	C5-N7-C8	7.86	107.83	103.90
1	A	1714	A	C5-N7-C8	7.86	107.83	103.90
1	A	560	A	C5-N7-C8	7.85	107.83	103.90
32	W	1272	A	C5-N7-C8	7.85	107.83	103.90
1	A	1003	A	C5-N7-C8	7.85	107.83	103.90
1	A	1056	A	C5-N7-C8	7.84	107.82	103.90
2	B	46	A	C5-N7-C8	7.84	107.82	103.90
1	A	1381	A	C5-N7-C8	7.84	107.82	103.90
32	W	391	A	C5-N7-C8	7.84	107.82	103.90
1	A	904	A	C5-N7-C8	7.84	107.82	103.90
1	A	1767	A	C5-N7-C8	7.84	107.82	103.90
1	A	2454	A	C5-N7-C8	7.83	107.82	103.90
1	A	2691	A	C5-N7-C8	7.83	107.82	103.90
32	W	548	A	C5-N7-C8	7.83	107.81	103.90
1	A	913	A	C5-N7-C8	7.83	107.81	103.90
1	A	790	A	C5-N7-C8	7.82	107.81	103.90
1	A	2898	A	C5-N7-C8	7.82	107.81	103.90
1	A	21	A	C5-N7-C8	7.82	107.81	103.90
1	A	265	A	C5-N7-C8	7.82	107.81	103.90
1	A	210	A	C5-N7-C8	7.82	107.81	103.90
1	A	1697	A	C5-N7-C8	7.81	107.81	103.90
1	A	226	A	C5-N7-C8	7.81	107.81	103.90
1	A	513	A	C5-N7-C8	7.81	107.80	103.90
1	A	1789	A	C5-N7-C8	7.81	107.80	103.90
1	A	2349	A	C5-N7-C8	7.81	107.80	103.90
1	A	2616	A	C5-N7-C8	7.81	107.80	103.90
32	W	882	A	C5-N7-C8	7.81	107.80	103.90
32	W	1342	A	C5-N7-C8	7.81	107.80	103.90
1	A	1006	A	C5-N7-C8	7.80	107.80	103.90
1	A	956	A	C5-N7-C8	7.80	107.80	103.90
32	W	631	A	C5-N7-C8	7.80	107.80	103.90
1	A	659	A	C5-N7-C8	7.79	107.79	103.90
1	A	2083	A	C5-N7-C8	7.79	107.79	103.90
1	A	1928	A	C5-N7-C8	7.78	107.79	103.90
32	W	519	A	C5-N7-C8	7.78	107.79	103.90
1	A	2468	A	C5-N7-C8	7.77	107.79	103.90
1	A	1606	A	C5-N7-C8	7.77	107.79	103.90
1	A	1601	A	C5-N7-C8	7.77	107.78	103.90
32	W	1140	A	C5-N7-C8	7.77	107.78	103.90
1	A	616	A	C5-N7-C8	7.76	107.78	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	830	A	C5-N7-C8	7.76	107.78	103.90
1	A	1691	A	C5-N7-C8	7.76	107.78	103.90
32	W	1166	A	C5-N7-C8	7.75	107.78	103.90
1	A	1173	A	C5'-C4'-O4'	7.75	118.40	109.10
1	A	2627	A	C5-N7-C8	7.75	107.78	103.90
32	W	555	A	C5-N7-C8	7.75	107.78	103.90
1	A	462	A	C5-N7-C8	7.75	107.77	103.90
1	A	774	A	C5-N7-C8	7.75	107.77	103.90
1	A	1244	A	C5-N7-C8	7.75	107.77	103.90
1	A	2296	A	C5-N7-C8	7.75	107.77	103.90
32	W	438	A	C5-N7-C8	7.75	107.77	103.90
32	W	1161	A	C5-N7-C8	7.75	107.77	103.90
32	W	1294	A	C5-N7-C8	7.75	107.77	103.90
1	A	1930	A	C5-N7-C8	7.74	107.77	103.90
1	A	647	A	C5-N7-C8	7.74	107.77	103.90
32	W	114	A	C5-N7-C8	7.74	107.77	103.90
1	A	1581	A	C5-N7-C8	7.74	107.77	103.90
1	A	958	A	C5-N7-C8	7.74	107.77	103.90
1	A	2848	A	C5-N7-C8	7.74	107.77	103.90
32	W	1189	A	C5-N7-C8	7.74	107.77	103.90
1	A	1097	A	C5-N7-C8	7.74	107.77	103.90
1	A	1655	A	C5-N7-C8	7.74	107.77	103.90
1	A	1774	A	C5-N7-C8	7.73	107.77	103.90
1	A	53	A	C5-N7-C8	7.73	107.76	103.90
1	A	1816	A	C5-N7-C8	7.73	107.76	103.90
32	W	1026	A	C4-C5-C6	7.73	120.86	117.00
1	A	2778	A	C5-N7-C8	7.71	107.75	103.90
32	W	1238	A	C5-N7-C8	7.71	107.75	103.90
1	A	1361	A	C5-N7-C8	7.71	107.75	103.90
32	W	99	A	C5-N7-C8	7.71	107.75	103.90
1	A	90	A	C5-N7-C8	7.70	107.75	103.90
32	W	933	A	C5-N7-C8	7.70	107.75	103.90
1	A	2704	A	C5-N7-C8	7.70	107.75	103.90
1	A	56	A	C5-N7-C8	7.69	107.75	103.90
1	A	1019	A	C5-N7-C8	7.69	107.75	103.90
32	W	1358	A	C5-N7-C8	7.69	107.75	103.90
1	A	1412	A	C5-N7-C8	7.69	107.74	103.90
1	A	496	A	C5-N7-C8	7.68	107.74	103.90
1	A	1491	A	C5-N7-C8	7.68	107.74	103.90
1	A	1814	A	C5-N7-C8	7.68	107.74	103.90
32	W	508	A	C5-N7-C8	7.68	107.74	103.90
1	A	1714	A	N3-C4-N9	7.66	133.53	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	679	A	C5-N7-C8	7.66	107.73	103.90
1	A	118	A	C5-N7-C8	7.66	107.73	103.90
32	W	1366	A	C5-N7-C8	7.66	107.73	103.90
1	A	634	A	C5-N7-C8	7.63	107.72	103.90
1	A	2627	A	C4-C5-C6	7.63	120.81	117.00
32	W	713	A	C5-N7-C8	7.62	107.71	103.90
1	A	95	A	C5-N7-C8	7.62	107.71	103.90
1	A	656	A	C5-N7-C8	7.62	107.71	103.90
1	A	1398	A	C5-N7-C8	7.62	107.71	103.90
1	A	1134	A	C4-C5-C6	7.62	120.81	117.00
1	A	1691	A	N3-C4-N9	7.62	133.49	127.40
32	W	1372	A	C5-N7-C8	7.62	107.71	103.90
1	A	1579	A	C5-N7-C8	7.61	107.70	103.90
1	A	1820	A	C5-N7-C8	7.61	107.70	103.90
1	A	1919	A	C5-N7-C8	7.58	107.69	103.90
32	W	507	A	C5-N7-C8	7.56	107.68	103.90
32	W	993	A	C5-N7-C8	7.56	107.68	103.90
1	A	2916	A	C5-N7-C8	7.55	107.68	103.90
32	W	1308	A	N3-C4-N9	7.52	133.42	127.40
1	A	2786	A	C5-N7-C8	7.50	107.65	103.90
1	A	366	A	C4'-C3'-O3'	7.50	128.00	113.00
1	A	1134	A	C5-N7-C8	7.49	107.65	103.90
1	A	2885	A	C4-C5-C6	7.49	120.74	117.00
1	A	1006	A	C4-C5-C6	7.48	120.74	117.00
1	A	1340	A	C5-N7-C8	7.48	107.64	103.90
32	W	439	A	C5-N7-C8	7.45	107.63	103.90
1	A	478	U	C2-N1-C1'	7.43	126.62	117.70
2	B	99	A	N3-C4-N9	7.42	133.34	127.40
1	A	226	A	N3-C4-N9	7.41	133.33	127.40
32	W	1167	C	C2-N1-C1'	7.40	126.94	118.80
1	A	494	A	C5-N7-C8	7.40	107.60	103.90
32	W	405	A	N3-C4-N9	7.40	133.32	127.40
1	A	935	A	C4-C5-C6	7.38	120.69	117.00
1	A	527	A	C4-C5-C6	7.38	120.69	117.00
1	A	1067	A	C5-N7-C8	7.36	107.58	103.90
1	A	1188	A	C5-N7-C8	7.35	107.57	103.90
1	A	2407	A	C4-C5-C6	7.35	120.67	117.00
32	W	457	A	C5-N7-C8	7.31	107.56	103.90
1	A	1433	U	C2-N1-C1'	7.28	126.43	117.70
1	A	1352	U	C2-N1-C1'	7.27	126.42	117.70
32	W	308	A	C4-C5-C6	7.23	120.62	117.00
1	A	1352	U	N1-C2-O2	7.22	127.85	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	99	A	N3-C4-N9	7.19	133.15	127.40
32	W	391	A	C4-C5-C6	7.18	120.59	117.00
32	W	1278	A	C4-C5-C6	7.18	120.59	117.00
1	A	913	A	N3-C4-N9	7.17	133.13	127.40
2	B	99	A	C4-C5-C6	7.17	120.58	117.00
32	W	507	A	C5-C6-N1	7.16	121.28	117.70
2	B	99	A	C5-N7-C8	7.16	107.48	103.90
32	W	993	A	N3-C4-N9	7.13	133.11	127.40
1	A	527	A	N3-C4-N9	7.13	133.11	127.40
32	W	572	A	N3-C4-N9	7.12	133.09	127.40
1	A	2786	A	N3-C4-N9	7.04	133.03	127.40
1	A	679	A	C4-C5-C6	7.03	120.52	117.00
1	A	551	A	C4-C5-C6	7.02	120.51	117.00
1	A	559	A	C4-C5-C6	7.00	120.50	117.00
1	A	1581	A	N3-C4-N9	6.99	132.99	127.40
1	A	513	A	N3-C4-N9	6.97	132.97	127.40
1	A	2691	A	C4-C5-C6	6.95	120.48	117.00
32	W	1234	A	N3-C4-N9	6.94	132.95	127.40
1	A	52	A	C4-C5-C6	6.92	120.46	117.00
1	A	254	A	C4-C5-C6	6.91	120.46	117.00
1	A	732	A	C5-N7-C8	6.91	107.36	103.90
1	A	1094	A	C4-C5-C6	6.91	120.45	117.00
32	W	99	A	C4-C5-C6	6.90	120.45	117.00
32	W	405	A	C4-C5-C6	6.89	120.44	117.00
1	A	478	U	N1-C2-O2	6.87	127.61	122.80
32	W	993	A	C4-C5-C6	6.87	120.43	117.00
32	W	1288	A	N3-C4-N9	6.87	132.89	127.40
1	A	1618	A	C4-C5-C6	6.86	120.43	117.00
32	W	1026	A	N3-C4-N9	6.86	132.89	127.40
1	A	1691	A	C4-C5-C6	6.86	120.43	117.00
52	z	9	A	C4-C5-C6	6.86	120.43	117.00
1	A	2786	A	C4-C5-C6	6.83	120.42	117.00
1	A	168	A	C4-C5-C6	6.83	120.42	117.00
32	W	911	A	C4-C5-C6	6.83	120.41	117.00
1	A	1433	U	N1-C2-O2	6.82	127.58	122.80
1	A	935	A	N3-C4-N9	6.82	132.85	127.40
1	A	1839	A	C4-C5-C6	6.80	120.40	117.00
1	A	2627	A	N3-C4-N9	6.78	132.83	127.40
1	A	679	A	N3-C4-N9	6.78	132.82	127.40
1	A	2106	A	C4-C5-C6	6.78	120.39	117.00
32	W	572	A	C4-C5-C6	6.76	120.38	117.00
1	A	56	A	N3-C4-N9	6.76	132.81	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	308	A	N3-C4-N9	6.76	132.81	127.40
1	A	2735	A	N3-C4-N9	6.75	132.80	127.40
32	W	790	A	C4-C5-C6	6.75	120.37	117.00
32	W	1166	A	N3-C4-N9	6.75	132.80	127.40
32	W	1167	C	N1-C2-O2	6.75	122.95	118.90
32	W	1427	A	C4-C5-C6	6.75	120.37	117.00
1	A	1619	A	C4-C5-C6	6.74	120.37	117.00
32	W	508	A	N9-C4-C5	6.74	108.50	105.80
32	W	1234	A	C4-C5-C6	6.74	120.37	117.00
32	W	391	A	N3-C4-N9	6.74	132.79	127.40
1	A	2735	A	C4-C5-C6	6.74	120.37	117.00
1	A	1667	A	N3-C4-N9	6.74	132.79	127.40
1	A	1714	A	C4-C5-C6	6.74	120.37	117.00
1	A	390	A	C4-C5-C6	6.73	120.36	117.00
32	W	1308	A	C4-C5-C6	6.72	120.36	117.00
1	A	2407	A	N3-C4-N9	6.71	132.77	127.40
32	W	1315	A	C4-C5-C6	6.71	120.36	117.00
1	A	661	A	C4-C5-C6	6.71	120.35	117.00
32	W	114	A	C4-C5-C6	6.71	120.35	117.00
1	A	390	A	N3-C4-N9	6.70	132.76	127.40
1	A	2459	A	N3-C4-N9	6.70	132.76	127.40
1	A	1638	A	C4-C5-C6	6.69	120.34	117.00
1	A	2395	A	C4-C5-C6	6.69	120.35	117.00
32	W	1384	A	C4-C5-C6	6.69	120.34	117.00
32	W	195	A	N3-C4-N9	6.68	132.74	127.40
32	W	337	A	C4-C5-C6	6.68	120.34	117.00
1	A	108	A	N3-C4-N9	6.68	132.74	127.40
1	A	736	A	N3-C4-N9	6.68	132.74	127.40
1	A	1883	A	C4-C5-C6	6.67	120.34	117.00
1	A	593	A	N3-C4-N9	6.67	132.74	127.40
32	W	987	A	N3-C4-N9	6.67	132.74	127.40
1	A	226	A	C4-C5-C6	6.67	120.33	117.00
32	W	1341	A	N3-C4-N9	6.66	132.73	127.40
32	W	727	A	N3-C4-N9	6.66	132.73	127.40
1	A	673	A	C4-C5-C6	6.65	120.33	117.00
1	A	1398	A	N3-C4-N9	6.65	132.72	127.40
1	A	1006	A	N3-C4-N9	6.65	132.72	127.40
32	W	1065	A	C4-C5-C6	6.64	120.32	117.00
1	A	2885	A	N3-C4-N9	6.64	132.72	127.40
1	A	518	A	C4-C5-C6	6.64	120.32	117.00
1	A	1778	A	N3-C4-N9	6.64	132.71	127.40
1	A	774	A	C8-N9-C4	6.63	108.45	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1816	A	N3-C4-N9	6.63	132.70	127.40
23	X	51	LYS	N-CA-C	-6.63	93.10	111.00
1	A	2459	A	C4-C5-C6	6.63	120.31	117.00
1	A	254	A	N3-C4-N9	6.62	132.70	127.40
1	A	526	A	N9-C4-C5	6.62	108.45	105.80
1	A	1075	A	C4-C5-C6	6.61	120.30	117.00
1	A	1667	A	C4-C5-C6	6.61	120.30	117.00
1	A	2862	A	N3-C4-N9	6.60	132.68	127.40
1	A	2844	A	C4-C5-C6	6.60	120.30	117.00
32	W	397	A	C4-C5-C6	6.60	120.30	117.00
1	A	1442	A	N3-C4-N9	6.60	132.68	127.40
1	A	538	A	C4-C5-C6	6.60	120.30	117.00
1	A	2691	A	N3-C4-N9	6.59	132.67	127.40
32	W	933	A	C4-C5-C6	6.59	120.30	117.00
1	A	948	A	N3-C4-N9	6.59	132.67	127.40
32	W	1166	A	C4-C5-C6	6.59	120.30	117.00
32	W	76	A	C4-C5-C6	6.59	120.29	117.00
1	A	108	A	C4-C5-C6	6.58	120.29	117.00
1	A	95	A	C4-C5-C6	6.57	120.28	117.00
1	A	258	A	C4-C5-C6	6.56	120.28	117.00
1	A	1491	A	N3-C4-N9	6.56	132.65	127.40
1	A	1653	A	C4-C5-C6	6.56	120.28	117.00
1	A	1858	A	C4-C5-C6	6.56	120.28	117.00
1	A	2111	A	N3-C4-N9	6.56	132.65	127.40
32	W	114	A	N3-C4-N9	6.56	132.65	127.40
1	A	910	A	N3-C4-N9	6.55	132.64	127.40
1	A	1831	A	C4-C5-C6	6.55	120.28	117.00
2	B	97	A	C4-C5-C6	6.55	120.28	117.00
1	A	1709	A	C4-C5-C6	6.55	120.28	117.00
1	A	2043	A	C4-C5-C6	6.55	120.28	117.00
1	A	910	A	C4-C5-C6	6.55	120.27	117.00
1	A	1392	A	C4-C5-C6	6.55	120.27	117.00
1	A	2862	A	C4-C5-C6	6.54	120.27	117.00
32	W	1288	A	C4-C5-C6	6.54	120.27	117.00
1	A	2402	A	C4-C5-C6	6.54	120.27	117.00
32	W	948	A	C4-C5-C6	6.54	120.27	117.00
1	A	1618	A	N3-C4-N9	6.53	132.62	127.40
1	A	38	A	C4-C5-C6	6.53	120.26	117.00
1	A	1360	A	N3-C4-N9	6.53	132.62	127.40
1	A	1352	U	N3-C2-O2	-6.53	117.63	122.20
2	B	13	A	C4-C5-C6	6.53	120.26	117.00
32	W	507	A	N3-C4-N9	6.52	132.62	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	437	A	N3-C4-N9	6.52	132.61	127.40
1	A	656	A	C4-C5-C6	6.52	120.26	117.00
1	A	1562	A	N3-C4-N9	6.51	132.61	127.40
1	A	948	A	C4-C5-C6	6.51	120.25	117.00
1	A	1820	A	C4-C5-C6	6.51	120.25	117.00
32	W	649	A	C4-C5-C6	6.51	120.25	117.00
1	A	974	A	C4-C5-C6	6.51	120.25	117.00
1	A	866	A	C4-C5-C6	6.50	120.25	117.00
1	A	752	A	C4-C5-C6	6.49	120.25	117.00
1	A	1638	A	N3-C4-N9	6.49	132.59	127.40
1	A	2111	A	C4-C5-C6	6.49	120.25	117.00
1	A	2844	A	N3-C4-N9	6.49	132.59	127.40
1	A	2339	A	C4-C5-C6	6.49	120.24	117.00
32	W	1478	A	C4-C5-C6	6.49	120.24	117.00
1	A	722	A	C4-C5-C6	6.48	120.24	117.00
1	A	1485	A	C4-C5-C6	6.48	120.24	117.00
1	A	1103	A	C4-C5-C6	6.48	120.24	117.00
1	A	1073	A	N3-C4-N9	6.48	132.58	127.40
1	A	1103	A	N3-C4-N9	6.48	132.58	127.40
1	A	1877	A	C4-C5-C6	6.47	120.24	117.00
1	A	1778	A	C4-C5-C6	6.47	120.24	117.00
32	W	649	A	N3-C4-N9	6.47	132.58	127.40
1	A	913	A	C4-C5-C6	6.47	120.23	117.00
1	A	964	A	C4-C5-C6	6.47	120.23	117.00
1	A	95	A	N3-C4-N9	6.46	132.57	127.40
1	A	1480	A	N3-C4-N9	6.46	132.57	127.40
1	A	2805	A	C4-C5-C6	6.46	120.23	117.00
2	B	13	A	N3-C4-N9	6.46	132.57	127.40
1	A	1253	A	C4-C5-C6	6.46	120.23	117.00
32	W	128	A	N3-C4-N9	6.46	132.57	127.40
32	W	1442	A	C4-C5-C6	6.46	120.23	117.00
2	B	11	A	N3-C4-N9	6.46	132.57	127.40
1	A	117	A	C4-C5-C6	6.46	120.23	117.00
32	W	335	A	C4-C5-C6	6.46	120.23	117.00
1	A	275	A	C4-C5-C6	6.45	120.23	117.00
1	A	1360	A	C4-C5-C6	6.45	120.23	117.00
1	A	551	A	N3-C4-N9	6.45	132.56	127.40
1	A	501	A	C4-C5-N7	-6.45	107.48	110.70
1	A	1999	A	C4-C5-C6	6.45	120.22	117.00
1	A	673	A	N3-C4-N9	6.45	132.56	127.40
1	A	589	G	P-O3'-C3'	6.44	127.43	119.70
1	A	2694	A	C4-C5-C6	6.44	120.22	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	168	A	N3-C4-N9	6.43	132.55	127.40
1	A	2436	A	N3-C4-N9	6.43	132.55	127.40
32	W	1297	A	C4-C5-C6	6.43	120.22	117.00
1	A	1562	A	C4-C5-C6	6.43	120.22	117.00
1	A	634	A	N3-C4-N9	6.43	132.54	127.40
1	A	2027	A	C4-C5-C6	6.43	120.22	117.00
32	W	1160	A	N3-C4-N9	6.43	132.54	127.40
2	B	46	A	N3-C4-N9	6.42	132.54	127.40
1	A	1581	A	C4-C5-C6	6.42	120.21	117.00
1	A	1485	A	N3-C4-N9	6.42	132.54	127.40
1	A	2794	A	N3-C4-N9	6.42	132.54	127.40
32	W	397	A	N3-C4-N9	6.42	132.54	127.40
1	A	1096	A	C4-C5-C6	6.42	120.21	117.00
1	A	1727	A	C4-C5-C6	6.41	120.21	117.00
1	A	559	A	N3-C4-N9	6.41	132.53	127.40
32	W	1133	A	N9-C4-C5	6.41	108.36	105.80
32	W	1179	A	C4-C5-C6	6.41	120.20	117.00
1	A	736	A	C4-C5-C6	6.41	120.20	117.00
1	A	1258	A	C4-C5-C6	6.41	120.20	117.00
1	A	2044	A	C4-C5-C6	6.40	120.20	117.00
32	W	1065	A	N3-C4-N9	6.40	132.52	127.40
1	A	538	A	N3-C4-N9	6.40	132.52	127.40
1	A	1816	A	C4-C5-C6	6.40	120.20	117.00
2	B	46	A	C4-C5-C6	6.40	120.20	117.00
1	A	265	A	C4-C5-C6	6.40	120.20	117.00
1	A	1999	A	N3-C4-N9	6.40	132.52	127.40
32	W	811	A	C4-C5-C6	6.40	120.20	117.00
1	A	130	A	C4-C5-C6	6.39	120.20	117.00
1	A	1695	A	C4-C5-C6	6.39	120.20	117.00
1	A	2402	A	N3-C4-N9	6.39	132.51	127.40
1	A	2689	A	N3-C4-N9	6.39	132.52	127.40
32	W	987	A	C4-C5-C6	6.39	120.20	117.00
32	W	705	A	C4-C5-C6	6.39	120.20	117.00
32	W	790	A	N3-C4-N9	6.39	132.51	127.40
1	A	2339	A	N3-C4-N9	6.39	132.51	127.40
1	A	2790	A	N3-C4-N9	6.39	132.51	127.40
52	z	24	A	N3-C4-N9	6.39	132.51	127.40
1	A	376	A	C4-C5-C6	6.39	120.19	117.00
1	A	689	A	N3-C4-N9	6.39	132.51	127.40
32	W	959	A	C4-C5-C6	6.39	120.19	117.00
1	A	656	A	N3-C4-N9	6.38	132.51	127.40
32	W	1222	A	C4-C5-C6	6.38	120.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	A	N3-C4-N9	6.38	132.50	127.40
1	A	590	U	P-O5'-C5'	6.38	131.11	120.90
1	A	1433	U	N3-C2-O2	-6.38	117.73	122.20
1	A	2831	A	C4-C5-C6	6.38	120.19	117.00
32	W	1341	A	C4-C5-C6	6.38	120.19	117.00
32	W	1517	A	C4-C5-C6	6.38	120.19	117.00
1	A	578	A	N3-C4-N9	6.38	132.50	127.40
1	A	690	A	N3-C4-N9	6.38	132.50	127.40
1	A	2441	A	C4-C5-C6	6.38	120.19	117.00
32	W	337	A	N3-C4-N9	6.38	132.50	127.40
32	W	1517	A	N3-C4-N9	6.38	132.50	127.40
1	A	193	A	C4-C5-C6	6.38	120.19	117.00
1	A	1536	A	C4-C5-C6	6.38	120.19	117.00
32	W	727	A	C4-C5-C6	6.38	120.19	117.00
1	A	1839	A	N3-C4-N9	6.37	132.50	127.40
1	A	2343	A	C4-C5-C6	6.37	120.19	117.00
32	W	1493	A	C4-C5-C6	6.37	120.19	117.00
1	A	1096	A	N3-C4-N9	6.37	132.50	127.40
32	W	996	A	C4-C5-C6	6.37	120.18	117.00
1	A	2924	A	C4-C5-C6	6.37	120.18	117.00
1	A	1556	A	C4-C5-C6	6.37	120.18	117.00
1	A	2270	A	C4-C5-C6	6.37	120.18	117.00
1	A	678	A	C4-C5-C6	6.36	120.18	117.00
1	A	1222	A	N3-C4-N9	6.36	132.49	127.40
1	A	623	A	C4-C5-C6	6.36	120.18	117.00
32	W	838	A	C4-C5-C6	6.36	120.18	117.00
32	W	1155	A	C4-C5-C6	6.36	120.18	117.00
1	A	156	A	C4-C5-C6	6.36	120.18	117.00
1	A	866	A	N3-C4-N9	6.36	132.49	127.40
32	W	344	A	C4-C5-C6	6.36	120.18	117.00
32	W	1238	A	C4-C5-C6	6.36	120.18	117.00
1	A	970	A	C4-C5-C6	6.35	120.18	117.00
1	A	732	A	N3-C4-N9	6.35	132.48	127.40
1	A	1222	A	C4-C5-C6	6.35	120.17	117.00
32	W	918	A	C4-C5-C6	6.35	120.17	117.00
1	A	1957	A	C4-C5-C6	6.35	120.17	117.00
1	A	2794	A	C4-C5-C6	6.35	120.17	117.00
32	W	933	A	N3-C4-N9	6.35	132.48	127.40
1	A	715	A	N3-C4-N9	6.35	132.48	127.40
1	A	1073	A	C4-C5-C6	6.35	120.17	117.00
1	A	1895	A	C4-C5-C6	6.35	120.17	117.00
1	A	2043	A	N3-C4-N9	6.35	132.48	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1272	A	N3-C4-N9	6.35	132.48	127.40
1	A	1901	A	C4-C5-C6	6.35	120.17	117.00
1	A	517	A	C4-C5-C6	6.34	120.17	117.00
1	A	1094	A	N3-C4-N9	6.34	132.48	127.40
1	A	1831	A	N3-C4-N9	6.34	132.48	127.40
1	A	478	U	N3-C2-O2	-6.34	117.76	122.20
1	A	2358	A	N3-C4-N9	6.34	132.47	127.40
32	W	74	A	C4-C5-C6	6.34	120.17	117.00
1	A	1393	A	C4-C5-C6	6.34	120.17	117.00
32	W	1284	A	C4-C5-C6	6.34	120.17	117.00
1	A	2329	A	C4-C5-C6	6.33	120.17	117.00
1	A	1768	A	C4-C5-C6	6.33	120.17	117.00
1	A	1858	A	N3-C4-N9	6.33	132.47	127.40
1	A	1710	A	C4-C5-C6	6.33	120.17	117.00
1	A	1900	A	C4-C5-C6	6.33	120.17	117.00
52	z	9	A	N3-C4-N9	6.33	132.46	127.40
1	A	259	A	C4-C5-C6	6.33	120.16	117.00
1	A	1442	A	C4-C5-C6	6.33	120.16	117.00
1	A	1506	A	N3-C4-N9	6.33	132.46	127.40
32	W	57	A	C4-C5-C6	6.33	120.16	117.00
32	W	1155	A	N3-C4-N9	6.32	132.46	127.40
1	A	2026	A	N3-C4-N9	6.32	132.46	127.40
1	A	456	A	C4-C5-C6	6.32	120.16	117.00
1	A	715	A	C4-C5-C6	6.32	120.16	117.00
1	A	1767	A	C4-C5-C6	6.32	120.16	117.00
1	A	2919	A	C4-C5-C6	6.32	120.16	117.00
32	W	743	A	C4-C5-C6	6.32	120.16	117.00
1	A	1820	A	N3-C4-N9	6.32	132.46	127.40
1	A	2329	A	N3-C4-N9	6.32	132.45	127.40
1	A	2358	A	C4-C5-C6	6.32	120.16	117.00
1	A	692	A	C4-C5-C6	6.32	120.16	117.00
1	A	661	A	N3-C4-N9	6.31	132.45	127.40
1	A	1945	A	C4-C5-C6	6.31	120.15	117.00
32	W	161	A	C4-C5-C6	6.31	120.15	117.00
32	W	875	A	N3-C4-N9	6.31	132.44	127.40
1	A	391	A	C4-C5-C6	6.30	120.15	117.00
1	A	634	A	C4-C5-C6	6.30	120.15	117.00
32	W	882	A	N3-C4-N9	6.30	132.44	127.40
1	A	956	A	N3-C4-N9	6.30	132.44	127.40
32	W	76	A	N3-C4-N9	6.30	132.44	127.40
32	W	301	A	N3-C4-N9	6.30	132.44	127.40
1	A	894	A	C4-C5-C6	6.30	120.15	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	711	A	N3-C4-N9	6.30	132.44	127.40
1	A	2089	A	C8-N9-C4	6.30	108.32	105.80
1	A	2827	A	C4-C5-C6	6.30	120.15	117.00
32	W	984	A	C4-C5-C6	6.30	120.15	117.00
1	A	1877	A	N3-C4-N9	6.30	132.44	127.40
1	A	2351	A	C4-C5-C6	6.30	120.15	117.00
1	A	2532	A	C4-C5-C6	6.29	120.15	117.00
1	A	1361	A	C4-C5-C6	6.29	120.15	117.00
1	A	1480	A	C4-C5-C6	6.29	120.15	117.00
2	B	11	A	C4-C5-C6	6.29	120.15	117.00
32	W	917	A	C4-C5-C6	6.29	120.15	117.00
1	A	1286	A	N3-C4-N9	6.29	132.43	127.40
1	A	526	A	C4-C5-N7	-6.29	107.56	110.70
1	A	1056	A	C4-C5-C6	6.29	120.14	117.00
1	A	1067	A	N9-C4-C5	6.29	108.31	105.80
1	A	2532	A	N3-C4-N9	6.29	132.43	127.40
32	W	1256	A	C4-C5-C6	6.29	120.14	117.00
2	B	50	A	C4-C5-C6	6.28	120.14	117.00
32	W	1478	A	N3-C4-N9	6.28	132.43	127.40
1	A	2663	A	N3-C4-N9	6.28	132.43	127.40
32	W	57	A	N3-C4-N9	6.28	132.43	127.40
1	A	689	A	C4-C5-C6	6.28	120.14	117.00
1	A	90	A	C4-C5-C6	6.28	120.14	117.00
1	A	1900	A	N3-C4-N9	6.28	132.42	127.40
1	A	501	A	N9-C4-C5	6.28	108.31	105.80
1	A	1714	A	C5-C6-N1	6.28	120.84	117.70
1	A	1888	A	C4-C5-C6	6.28	120.14	117.00
32	W	838	A	N3-C4-N9	6.28	132.42	127.40
32	W	844	A	N3-C4-N9	6.28	132.42	127.40
1	A	2349	A	C4-C5-C6	6.28	120.14	117.00
32	W	911	A	N3-C4-N9	6.28	132.42	127.40
32	W	1160	A	C4-C5-C6	6.27	120.14	117.00
32	W	674	A	N9-C4-C5	6.27	108.31	105.80
32	W	883	A	C4-C5-C6	6.27	120.14	117.00
32	W	1366	A	C4-C5-C6	6.27	120.14	117.00
1	A	1190	A	C4-C5-C6	6.27	120.14	117.00
1	A	1210	A	C4-C5-C6	6.27	120.14	117.00
1	A	1316	A	N3-C4-N9	6.27	132.42	127.40
1	A	1655	A	N3-C4-N9	6.27	132.42	127.40
32	W	1016	A	N3-C4-N9	6.27	132.42	127.40
1	A	1426	A	N3-C4-N9	6.27	132.41	127.40
1	A	2049	A	C4-C5-C6	6.27	120.14	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	97	A	N3-C4-N9	6.27	132.41	127.40
32	W	948	A	N3-C4-N9	6.27	132.41	127.40
1	A	699	A	C4-C5-C6	6.27	120.13	117.00
1	A	61	A	C4-C5-C6	6.26	120.13	117.00
1	A	1126	A	N3-C4-N9	6.26	132.41	127.40
1	A	1524	A	N3-C4-N9	6.26	132.41	127.40
1	A	1776	A	N3-C4-N9	6.26	132.41	127.40
32	W	34	A	C4-C5-C6	6.26	120.13	117.00
32	W	882	A	C4-C5-C6	6.26	120.13	117.00
32	W	1143	A	C4-C5-C6	6.26	120.13	117.00
1	A	185	A	N3-C4-N9	6.26	132.41	127.40
32	W	844	A	C4-C5-C6	6.26	120.13	117.00
1	A	438	A	N3-C4-N9	6.26	132.41	127.40
1	A	752	A	N3-C4-N9	6.26	132.41	127.40
32	W	913	A	C4-C5-C6	6.26	120.13	117.00
1	A	724	A	N3-C4-N9	6.26	132.41	127.40
1	A	1490	A	C4-C5-C6	6.26	120.13	117.00
1	A	1620	A	C4-C5-C6	6.26	120.13	117.00
32	W	945	A	N3-C4-N9	6.26	132.41	127.40
1	A	2365	A	C4-C5-C6	6.26	120.13	117.00
32	W	996	A	N3-C4-N9	6.26	132.41	127.40
1	A	156	A	N3-C4-N9	6.26	132.41	127.40
32	W	1143	A	N3-C4-N9	6.26	132.41	127.40
1	A	1709	A	N3-C4-N9	6.25	132.40	127.40
1	A	2026	A	C4-C5-C6	6.25	120.13	117.00
1	A	2571	A	C4-C5-C6	6.25	120.13	117.00
1	A	2643	A	C4-C5-C6	6.25	120.13	117.00
32	W	1024	A	C4-C5-C6	6.25	120.13	117.00
1	A	690	A	C4-C5-C6	6.25	120.13	117.00
1	A	882	A	N3-C4-N9	6.25	132.40	127.40
1	A	2436	A	C4-C5-C6	6.25	120.13	117.00
1	A	2830	A	C4-C5-C6	6.25	120.13	117.00
32	W	462	A	N3-C4-N9	6.25	132.40	127.40
32	W	140	A	C4-C5-C6	6.25	120.12	117.00
1	A	2694	A	N3-C4-N9	6.25	132.40	127.40
1	A	2846	A	C4-C5-C6	6.25	120.12	117.00
1	A	2916	A	N9-C4-C5	6.25	108.30	105.80
32	W	72	A	C4-C5-C6	6.25	120.12	117.00
32	W	335	A	N3-C4-N9	6.25	132.40	127.40
32	W	671	A	C4-C5-C6	6.25	120.12	117.00
1	A	549	A	C4-C5-C6	6.25	120.12	117.00
1	A	616	A	C4-C5-C6	6.25	120.12	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1132	A	N3-C4-N9	6.25	132.40	127.40
1	A	2052	A	C4-C5-C6	6.25	120.12	117.00
1	A	133	A	N3-C4-N9	6.25	132.40	127.40
1	A	1477	A	C4-C5-C6	6.25	120.12	117.00
1	A	943	A	N3-C4-N9	6.24	132.39	127.40
1	A	1291	A	C4-C5-C6	6.24	120.12	117.00
1	A	1885	A	C4-C5-C6	6.24	120.12	117.00
1	A	2395	A	N3-C4-N9	6.24	132.40	127.40
1	A	2790	A	C4-C5-C6	6.24	120.12	117.00
1	A	2349	A	N3-C4-N9	6.24	132.39	127.40
1	A	2704	A	C4-C5-C6	6.24	120.12	117.00
1	A	1426	A	C4-C5-C6	6.24	120.12	117.00
32	W	1315	A	N3-C4-N9	6.24	132.39	127.40
32	W	1383	A	C4-C5-C6	6.24	120.12	117.00
32	W	1425	A	C4-C5-C6	6.24	120.12	117.00
1	A	790	A	C4-C5-C6	6.24	120.12	117.00
1	A	231	A	C4-C5-C6	6.23	120.12	117.00
1	A	1174	A	C4-C5-C6	6.23	120.12	117.00
1	A	2663	A	C4-C5-C6	6.23	120.12	117.00
32	W	605	A	N3-C4-N9	6.23	132.39	127.40
32	W	811	A	N3-C4-N9	6.23	132.38	127.40
1	A	724	A	C4-C5-C6	6.23	120.11	117.00
1	A	1520	A	N3-C4-N9	6.23	132.38	127.40
1	A	2027	A	N3-C4-N9	6.23	132.38	127.40
1	A	133	A	C4-C5-C6	6.23	120.11	117.00
1	A	469	A	C4-C5-C6	6.23	120.11	117.00
1	A	593	A	C4-C5-C6	6.23	120.11	117.00
1	A	1536	A	N3-C4-N9	6.23	132.38	127.40
1	A	1883	A	N3-C4-N9	6.23	132.38	127.40
1	A	958	A	C4-C5-C6	6.23	120.11	117.00
1	A	1235	A	C4-C5-C6	6.23	120.11	117.00
32	W	1272	A	C4-C5-C6	6.23	120.11	117.00
1	A	1357	A	C4-C5-C6	6.23	120.11	117.00
1	A	2365	A	N3-C4-N9	6.23	132.38	127.40
32	W	913	A	N3-C4-N9	6.23	132.38	127.40
1	A	41	A	N3-C4-N9	6.22	132.38	127.40
1	A	2100	A	C4-C5-C6	6.22	120.11	117.00
32	W	346	A	C4-C5-C6	6.22	120.11	117.00
32	W	617	A	C4-C5-C6	6.22	120.11	117.00
32	W	1112	A	C4-C5-C6	6.22	120.11	117.00
1	A	1998	A	N3-C4-N9	6.22	132.38	127.40
1	A	2689	A	C4-C5-C6	6.22	120.11	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	35	A	C4-C5-C6	6.22	120.11	117.00
32	W	721	A	C4-C5-C6	6.22	120.11	117.00
32	W	902	A	C4-C5-C6	6.22	120.11	117.00
1	A	391	A	N3-C4-N9	6.22	132.38	127.40
1	A	1188	A	N9-C4-C5	6.22	108.29	105.80
1	A	2812	A	N3-C4-N9	6.22	132.38	127.40
32	W	129	A	N3-C4-N9	6.22	132.38	127.40
1	A	339	A	C4-C5-C6	6.22	120.11	117.00
1	A	1194	A	N3-C4-N9	6.22	132.37	127.40
1	A	1918	A	C4-C5-C6	6.22	120.11	117.00
1	A	2461	A	C4-C5-C6	6.22	120.11	117.00
32	W	1427	A	N3-C4-N9	6.22	132.37	127.40
1	A	1490	A	N3-C4-N9	6.21	132.37	127.40
1	A	2500	A	C4-C5-C6	6.21	120.11	117.00
1	A	1653	A	N3-C4-N9	6.21	132.37	127.40
1	A	2006	A	C4-C5-C6	6.21	120.11	117.00
1	A	2106	A	N3-C4-N9	6.21	132.37	127.40
32	W	956	A	C4-C5-C6	6.21	120.11	117.00
1	A	41	A	C4-C5-C6	6.21	120.11	117.00
1	A	1392	A	N3-C4-N9	6.21	132.37	127.40
32	W	1133	A	C4-C5-N7	-6.21	107.59	110.70
1	A	431	A	C4-C5-C6	6.21	120.11	117.00
1	A	2812	A	C4-C5-C6	6.21	120.11	117.00
32	W	1435	A	C4-C5-C6	6.21	120.11	117.00
52	z	70	A	C4-C5-C6	6.21	120.11	117.00
1	A	52	A	N3-C4-N9	6.21	132.37	127.40
1	A	179	A	C4-C5-C6	6.21	120.10	117.00
32	W	793	A	C4-C5-C6	6.21	120.10	117.00
1	A	171	A	N3-C4-N9	6.21	132.37	127.40
1	A	1025	A	C4-C5-C6	6.21	120.10	117.00
1	A	1461	A	C4-C5-C6	6.21	120.10	117.00
1	A	1947	A	C4-C5-C6	6.21	120.10	117.00
1	A	2405	A	C4-C5-C6	6.20	120.10	117.00
32	W	1189	A	C4-C5-C6	6.20	120.10	117.00
32	W	1348	A	C4-C5-C6	6.20	120.10	117.00
32	W	1256	A	N3-C4-N9	6.20	132.36	127.40
1	A	2590	A	C4-C5-C6	6.20	120.10	117.00
32	W	140	A	N3-C4-N9	6.20	132.36	127.40
1	A	1074	A	N3-C4-N9	6.20	132.36	127.40
1	A	1661	A	N9-C4-C5	6.20	108.28	105.80
1	A	2302	A	C4-C5-C6	6.20	120.10	117.00
1	A	2779	A	C4-C5-C6	6.20	120.10	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1493	A	N3-C4-N9	6.20	132.36	127.40
1	A	1680	A	C4-C5-C6	6.19	120.10	117.00
1	A	1710	A	N3-C4-N9	6.19	132.35	127.40
1	A	2338	A	C4-C5-C6	6.19	120.10	117.00
1	A	56	A	C4-C5-C6	6.19	120.10	117.00
1	A	91	A	C4-C5-C6	6.19	120.10	117.00
1	A	1190	A	N3-C4-N9	6.19	132.35	127.40
32	W	555	A	C4-C5-C6	6.19	120.10	117.00
32	W	677	A	C4-C5-C6	6.19	120.10	117.00
1	A	692	A	N3-C4-N9	6.19	132.35	127.40
1	A	970	A	N3-C4-N9	6.19	132.35	127.40
1	A	1406	A	C4-C5-C6	6.19	120.10	117.00
1	A	2826	A	N3-C4-N9	6.19	132.35	127.40
32	W	548	A	C4-C5-C6	6.19	120.09	117.00
32	W	1016	A	C4-C5-C6	6.19	120.09	117.00
1	A	1005	A	C4-C5-C6	6.19	120.09	117.00
1	A	1424	A	N3-C4-N9	6.19	132.35	127.40
1	A	1606	A	N3-C4-N9	6.19	132.35	127.40
52	z	24	A	C4-C5-C6	6.19	120.09	117.00
52	z	58	A	C4-C5-C6	6.19	120.09	117.00
1	A	437	A	C4-C5-C6	6.19	120.09	117.00
1	A	2629	A	C4-C5-C6	6.19	120.09	117.00
1	A	2662	A	N3-C4-N9	6.18	132.35	127.40
1	A	130	A	N3-C4-N9	6.18	132.35	127.40
1	A	206	A	C4-C5-C6	6.18	120.09	117.00
1	A	1845	A	N3-C4-N9	6.18	132.34	127.40
32	W	74	A	N3-C4-N9	6.18	132.35	127.40
32	W	685	A	C4-C5-C6	6.18	120.09	117.00
2	B	18	A	C4-C5-C6	6.18	120.09	117.00
1	A	722	A	N3-C4-N9	6.18	132.34	127.40
1	A	1393	A	N3-C4-N9	6.18	132.34	127.40
1	A	2750	A	C8-N9-C4	6.18	108.27	105.80
32	W	1189	A	N3-C4-N9	6.18	132.34	127.40
1	A	1695	A	N3-C4-N9	6.18	132.34	127.40
1	A	1845	A	C4-C5-C6	6.18	120.09	117.00
32	W	364	A	C4-C5-C6	6.18	120.09	117.00
1	A	870	A	N3-C4-N9	6.18	132.34	127.40
1	A	882	A	C4-C5-C6	6.18	120.09	117.00
1	A	1998	A	C4-C5-C6	6.18	120.09	117.00
1	A	2517	A	C4-C5-C6	6.18	120.09	117.00
32	W	225	A	C4-C5-C6	6.18	120.09	117.00
32	W	282	A	N3-C4-N9	6.18	132.34	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	984	A	N3-C4-N9	6.18	132.34	127.40
32	W	1236	A	C4-C5-C6	6.18	120.09	117.00
1	A	265	A	N3-C4-N9	6.17	132.34	127.40
1	A	1619	A	N3-C4-N9	6.17	132.34	127.40
1	A	1850	A	C4-C5-C6	6.17	120.09	117.00
1	A	2381	A	C4-C5-C6	6.17	120.09	117.00
1	A	2848	A	C4-C5-C6	6.17	120.09	117.00
32	W	1372	A	N9-C4-C5	6.17	108.27	105.80
1	A	496	A	N3-C4-N9	6.17	132.34	127.40
1	A	1685	A	C4-C5-C6	6.17	120.09	117.00
32	W	282	A	C4-C5-C6	6.17	120.09	117.00
32	W	1359	A	C4-C5-C6	6.17	120.09	117.00
32	W	605	A	C4-C5-C6	6.17	120.09	117.00
32	W	1014	A	C4-C5-C6	6.17	120.08	117.00
1	A	2750	A	C4-C5-C6	6.17	120.08	117.00
1	A	1258	A	N3-C4-N9	6.17	132.33	127.40
1	A	326	A	C4-C5-C6	6.16	120.08	117.00
1	A	1776	A	C4-C5-C6	6.16	120.08	117.00
1	A	2826	A	C4-C5-C6	6.16	120.08	117.00
32	W	496	A	C4-C5-C6	6.16	120.08	117.00
1	A	1405	A	C4-C5-C6	6.16	120.08	117.00
1	A	194	A	C4-C5-C6	6.16	120.08	117.00
1	A	200	A	C4-C5-C6	6.16	120.08	117.00
1	A	830	A	C4-C5-C6	6.16	120.08	117.00
1	A	2316	A	C4-C5-C6	6.16	120.08	117.00
32	W	333	A	C4-C5-C6	6.16	120.08	117.00
32	W	1278	A	N3-C4-N9	6.16	132.33	127.40
1	A	407	A	C4-C5-C6	6.16	120.08	117.00
1	A	1075	A	N3-C4-N9	6.16	132.33	127.40
1	A	1253	A	N3-C4-N9	6.16	132.33	127.40
1	A	2302	A	N3-C4-N9	6.16	132.33	127.40
1	A	1054	A	C4-C5-C6	6.16	120.08	117.00
32	W	1179	A	N3-C4-N9	6.16	132.33	127.40
1	A	407	A	N3-C4-N9	6.16	132.32	127.40
1	A	943	A	C4-C5-C6	6.16	120.08	117.00
32	W	548	A	N3-C4-N9	6.16	132.32	127.40
32	W	271	A	C4-C5-C6	6.15	120.08	117.00
1	A	765	A	C4-C5-C6	6.15	120.08	117.00
1	A	2854	A	C4-C5-C6	6.15	120.08	117.00
32	W	690	A	C4-C5-C6	6.15	120.08	117.00
32	W	711	A	C4-C5-C6	6.15	120.08	117.00
1	A	260	A	C4-C5-C6	6.15	120.08	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	578	A	C4-C5-C6	6.15	120.08	117.00
1	A	1663	A	C4-C5-C6	6.15	120.08	117.00
1	A	1745	A	C4-C5-C6	6.15	120.08	117.00
1	A	2570	A	C4-C5-C6	6.15	120.08	117.00
1	A	2770	A	C8-N9-C4	6.15	108.26	105.80
32	W	725	A	C4-C5-C6	6.15	120.08	117.00
1	A	517	A	N3-C4-N9	6.15	132.32	127.40
1	A	549	A	N3-C4-N9	6.15	132.32	127.40
1	A	1042	A	C4-C5-C6	6.15	120.08	117.00
1	A	1727	A	N3-C4-N9	6.15	132.32	127.40
1	A	2845	A	C4-C5-C6	6.15	120.08	117.00
1	A	1019	A	C4-C5-C6	6.15	120.07	117.00
1	A	1424	A	C4-C5-C6	6.15	120.07	117.00
1	A	2851	A	C4-C5-C6	6.15	120.07	117.00
32	W	758	A	N3-C4-N9	6.15	132.32	127.40
32	W	1297	A	N3-C4-N9	6.15	132.32	127.40
1	A	185	A	C4-C5-C6	6.14	120.07	117.00
1	A	2722	A	N3-C4-N9	6.14	132.31	127.40
32	W	381	A	N3-C4-N9	6.14	132.31	127.40
32	W	532	A	C4-C5-C6	6.14	120.07	117.00
32	W	1384	A	N3-C4-N9	6.14	132.32	127.40
1	A	2616	A	C4-C5-C6	6.14	120.07	117.00
52	z	41	A	N3-C4-N9	6.14	132.31	127.40
32	W	462	A	C4-C5-C6	6.14	120.07	117.00
32	W	875	A	C4-C5-C6	6.14	120.07	117.00
1	A	90	A	N3-C4-N9	6.14	132.31	127.40
1	A	2032	A	C4-C5-C6	6.14	120.07	117.00
1	A	2351	A	N3-C4-N9	6.14	132.31	127.40
1	A	889	A	C4-C5-C6	6.14	120.07	117.00
1	A	1254	A	C4-C5-C6	6.14	120.07	117.00
1	A	1789	A	C4-C5-C6	6.14	120.07	117.00
1	A	1995	A	C4-C5-C6	6.14	120.07	117.00
1	A	2547	A	N3-C4-N9	6.14	132.31	127.40
32	W	234	A	C4-C5-C6	6.14	120.07	117.00
1	A	1323	A	C4-C5-C6	6.13	120.07	117.00
1	A	1398	A	C4-C5-C6	6.13	120.07	117.00
1	A	1627	A	C4-C5-C6	6.13	120.07	117.00
32	W	1261	A	C4-C5-C6	6.13	120.07	117.00
1	A	353	A	C4-C5-C6	6.13	120.07	117.00
1	A	1814	A	N9-C4-C5	6.13	108.25	105.80
32	W	72	A	N3-C4-N9	6.13	132.31	127.40
1	A	537	A	C4-C5-C6	6.13	120.07	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	829	A	C4-C5-C6	6.13	120.06	117.00
1	A	1532	A	N3-C4-N9	6.13	132.31	127.40
1	A	2876	A	C4-C5-C6	6.13	120.07	117.00
52	z	76	A	C4-C5-C6	6.13	120.06	117.00
1	A	1575	A	C4-C5-C6	6.13	120.06	117.00
1	A	1735	A	C4-C5-C6	6.13	120.06	117.00
1	A	530	A	C4-C5-C6	6.13	120.06	117.00
1	A	574	A	C4-C5-C6	6.13	120.06	117.00
1	A	1284	A	C4-C5-C6	6.13	120.06	117.00
1	A	2317	A	C4-C5-C6	6.13	120.06	117.00
32	W	381	A	C4-C5-C6	6.13	120.06	117.00
32	W	696	A	N3-C4-N9	6.13	132.30	127.40
32	W	790	A	C8-N9-C4	6.13	108.25	105.80
32	W	1238	A	N3-C4-N9	6.13	132.30	127.40
1	A	560	A	N3-C4-N9	6.13	132.30	127.40
1	A	1100	A	C4-C5-C6	6.13	120.06	117.00
1	A	1100	A	N3-C4-N9	6.13	132.30	127.40
1	A	1721	A	C4-C5-C6	6.13	120.06	117.00
2	B	37	A	C4-C5-C6	6.13	120.06	117.00
32	W	173	A	C4-C5-C6	6.13	120.06	117.00
52	z	70	A	N3-C4-N9	6.13	132.30	127.40
1	A	790	A	N3-C4-N9	6.12	132.30	127.40
1	A	1575	A	N3-C4-N9	6.12	132.30	127.40
1	A	1882	A	C4-C5-C6	6.12	120.06	117.00
1	A	2066	A	C4-C5-C6	6.12	120.06	117.00
1	A	2464	A	C4-C5-C6	6.12	120.06	117.00
1	A	518	A	N3-C4-N9	6.12	132.30	127.40
1	A	592	A	N3-C4-N9	6.12	132.30	127.40
1	A	1421	A	C4-C5-C6	6.12	120.06	117.00
1	A	2662	A	C4-C5-C6	6.12	120.06	117.00
32	W	743	A	N3-C4-N9	6.12	132.30	127.40
1	A	1316	A	C4-C5-C6	6.12	120.06	117.00
1	A	1491	A	C4-C5-C6	6.12	120.06	117.00
32	W	254	A	C8-N9-C4	6.12	108.25	105.80
32	W	1004	A	C4-C5-C6	6.12	120.06	117.00
32	W	1210	A	C8-N9-C4	6.12	108.25	105.80
32	W	1490	A	N3-C4-N9	6.12	132.30	127.40
1	A	1541	A	C4-C5-C6	6.12	120.06	117.00
1	A	1981	A	C4-C5-C6	6.12	120.06	117.00
1	A	2369	A	N3-C4-N9	6.12	132.30	127.40
1	A	1876	A	C4-C5-C6	6.12	120.06	117.00
32	W	361	A	N3-C4-N9	6.12	132.29	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2848	A	N3-C4-N9	6.12	132.29	127.40
1	A	616	A	N3-C4-N9	6.12	132.29	127.40
1	A	2819	A	C8-N9-C4	6.12	108.25	105.80
32	W	715	A	C4-C5-C6	6.12	120.06	117.00
1	A	71	A	C4-C5-C6	6.11	120.06	117.00
1	A	774	A	N3-C4-N9	6.11	132.29	127.40
1	A	1346	A	C4-C5-C6	6.11	120.06	117.00
1	A	1672	A	N3-C4-N9	6.11	132.29	127.40
1	A	2560	A	C4-C5-C6	6.11	120.06	117.00
1	A	2719	A	N3-C4-N9	6.11	132.29	127.40
1	A	462	A	C4-C5-C6	6.11	120.06	117.00
1	A	2389	A	C4-C5-C6	6.11	120.06	117.00
1	A	44	A	C4-C5-C6	6.11	120.06	117.00
1	A	429	A	C4-C5-C6	6.11	120.06	117.00
1	A	431	A	N3-C4-N9	6.11	132.29	127.40
1	A	462	A	N3-C4-N9	6.11	132.29	127.40
1	A	667	A	C4-C5-C6	6.11	120.06	117.00
1	A	592	A	C4-C5-C6	6.11	120.05	117.00
32	W	496	A	N3-C4-N9	6.11	132.29	127.40
52	z	21	A	C4-C5-C6	6.11	120.05	117.00
1	A	305	A	N3-C4-N9	6.11	132.28	127.40
1	A	971	A	C4-C5-C6	6.11	120.05	117.00
1	A	1388	A	N3-C4-N9	6.11	132.29	127.40
1	A	1461	A	N3-C4-N9	6.11	132.29	127.40
1	A	2270	A	N3-C4-N9	6.11	132.29	127.40
1	A	2831	A	N3-C4-N9	6.11	132.29	127.40
32	W	671	A	N3-C4-N9	6.11	132.29	127.40
1	A	318	A	C4-C5-C6	6.11	120.05	117.00
1	A	318	A	N3-C4-N9	6.11	132.28	127.40
1	A	722	A	C8-N9-C4	6.11	108.24	105.80
32	W	956	A	N3-C4-N9	6.11	132.28	127.40
32	W	1252	A	C4-C5-C6	6.11	120.05	117.00
1	A	1895	A	N3-C4-N9	6.10	132.28	127.40
1	A	851	A	C4-C5-C6	6.10	120.05	117.00
32	W	190	A	C4-C5-C6	6.10	120.05	117.00
1	A	278	A	C4-C5-C6	6.10	120.05	117.00
1	A	574	A	N3-C4-N9	6.10	132.28	127.40
1	A	2018	A	C4-C5-C6	6.10	120.05	117.00
1	A	2560	A	N3-C4-N9	6.10	132.28	127.40
32	W	978	A	C4-C5-C6	6.10	120.05	117.00
32	W	1437	A	C4-C5-C6	6.10	120.05	117.00
1	A	173	A	C4-C5-C6	6.10	120.05	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	896	A	N3-C4-N9	6.10	132.28	127.40
1	A	956	A	C4-C5-C6	6.10	120.05	117.00
1	A	1375	A	N3-C4-N9	6.10	132.28	127.40
1	A	73	A	C4-C5-C6	6.10	120.05	117.00
1	A	964	A	N3-C4-N9	6.10	132.28	127.40
1	A	1019	A	N3-C4-N9	6.10	132.28	127.40
1	A	2668	A	C4-C5-C6	6.10	120.05	117.00
32	W	1178	A	C4-C5-C6	6.10	120.05	117.00
1	A	56	A	C8-N9-C4	6.09	108.24	105.80
1	A	428	A	C4-C5-C6	6.09	120.05	117.00
1	A	952	A	N3-C4-N9	6.09	132.28	127.40
32	W	323	A	C4-C5-C6	6.09	120.05	117.00
32	W	730	A	C4-C5-C6	6.09	120.05	117.00
1	A	1126	A	C8-N9-C4	6.09	108.24	105.80
1	A	1724	A	C4-C5-C6	6.09	120.05	117.00
1	A	2343	A	N3-C4-N9	6.09	132.27	127.40
32	W	1188	A	N3-C4-N9	6.09	132.27	127.40
32	W	1442	A	N3-C4-N9	6.09	132.27	127.40
1	A	870	A	C4-C5-C6	6.09	120.05	117.00
2	B	20	A	C4-C5-C6	6.09	120.04	117.00
1	A	868	A	C4-C5-C6	6.09	120.04	117.00
1	A	369	A	N3-C4-N9	6.09	132.27	127.40
1	A	896	A	C4-C5-C6	6.09	120.04	117.00
1	A	2517	A	N3-C4-N9	6.09	132.27	127.40
32	W	650	A	C8-N9-C4	6.09	108.23	105.80
1	A	1580	A	C4-C5-C6	6.08	120.04	117.00
1	A	1608	A	N3-C4-N9	6.08	132.27	127.40
32	W	81	A	C4-C5-C6	6.08	120.04	117.00
32	W	1463	A	C4-C5-C6	6.08	120.04	117.00
1	A	630	A	C4-C5-C6	6.08	120.04	117.00
1	A	1047	A	C4-C5-C6	6.08	120.04	117.00
1	A	1569	A	C4-C5-C6	6.08	120.04	117.00
1	A	1615	A	C4-C5-C6	6.08	120.04	117.00
1	A	2044	A	N3-C4-N9	6.08	132.27	127.40
1	A	2362	A	C8-N9-C4	6.08	108.23	105.80
32	W	979	A	C4-C5-C6	6.08	120.04	117.00
32	W	1161	A	N3-C4-N9	6.08	132.27	127.40
1	A	374	A	C8-N9-C4	6.08	108.23	105.80
1	A	589	G	C2'-C3'-O3'	-6.08	96.12	109.50
1	A	925	A	N3-C4-N9	6.08	132.26	127.40
1	A	2417	A	C4-C5-C6	6.08	120.04	117.00
32	W	296	A	C4-C5-C6	6.08	120.04	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	630	A	C4-C5-C6	6.08	120.04	117.00
32	W	1245	A	C4-C5-C6	6.08	120.04	117.00
1	A	329	A	C4-C5-C6	6.08	120.04	117.00
1	A	2060	A	C4-C5-C6	6.08	120.04	117.00
1	A	2383	A	C4-C5-C6	6.08	120.04	117.00
32	W	281	A	C4-C5-C6	6.08	120.04	117.00
1	A	1260	A	C4-C5-C6	6.08	120.04	117.00
32	W	1147	A	C4-C5-C6	6.08	120.04	117.00
32	W	1333	A	C4-C5-C6	6.08	120.04	117.00
32	W	1366	A	N3-C4-N9	6.08	132.26	127.40
1	A	61	A	N3-C4-N9	6.08	132.26	127.40
1	A	622	A	C4-C5-C6	6.08	120.04	117.00
1	A	1265	A	C4-C5-C6	6.08	120.04	117.00
1	A	2734	A	C4-C5-C6	6.08	120.04	117.00
1	A	971	A	N3-C4-N9	6.08	132.26	127.40
1	A	1404	A	N3-C4-N9	6.08	132.26	127.40
1	A	1477	A	N3-C4-N9	6.08	132.26	127.40
1	A	1588	A	C4-C5-C6	6.08	120.04	117.00
1	A	1680	A	N3-C4-N9	6.08	132.26	127.40
1	A	1838	A	C4-C5-C6	6.08	120.04	117.00
1	A	1885	A	N3-C4-N9	6.08	132.26	127.40
32	W	357	A	C4-C5-C6	6.08	120.04	117.00
1	A	171	A	C4-C5-C6	6.07	120.04	117.00
1	A	219	A	C4-C5-C6	6.07	120.04	117.00
1	A	1357	A	N3-C4-N9	6.07	132.26	127.40
1	A	1388	A	C4-C5-C6	6.07	120.04	117.00
1	A	1888	A	N3-C4-N9	6.07	132.26	127.40
2	B	113	A	C4-C5-C6	6.07	120.04	117.00
32	W	862	A	N9-C4-C5	6.07	108.23	105.80
1	A	1230	A	C4-C5-C6	6.07	120.04	117.00
1	A	623	A	N3-C4-N9	6.07	132.26	127.40
1	A	1233	A	N3-C4-N9	6.07	132.26	127.40
1	A	1424	A	C8-N9-C4	6.07	108.23	105.80
1	A	1848	A	N3-C4-N9	6.07	132.26	127.40
1	A	2356	A	C4-C5-C6	6.07	120.04	117.00
32	W	459	A	C4-C5-C6	6.07	120.03	117.00
1	A	2007	A	N3-C4-N9	6.07	132.25	127.40
1	A	2381	A	N3-C4-N9	6.07	132.26	127.40
32	W	504	A	C4-C5-C6	6.07	120.03	117.00
1	A	305	A	C4-C5-C6	6.07	120.03	117.00
1	A	543	A	C4-C5-C6	6.07	120.03	117.00
1	A	1284	A	N3-C4-N9	6.07	132.25	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1286	A	C4-C5-C6	6.07	120.03	117.00
1	A	1620	A	N3-C4-N9	6.07	132.25	127.40
1	A	1675	A	C4-C5-C6	6.07	120.03	117.00
1	A	1925	A	N3-C4-N9	6.07	132.25	127.40
1	A	2454	A	C4-C5-C6	6.07	120.03	117.00
1	A	2670	A	C4-C5-N7	-6.07	107.67	110.70
1	A	2700	A	C4-C5-C6	6.07	120.03	117.00
32	W	616	A	C4-C5-C6	6.07	120.03	117.00
32	W	945	A	C4-C5-C6	6.07	120.03	117.00
32	W	1456	A	C8-N9-C4	6.07	108.23	105.80
1	A	353	A	N3-C4-N9	6.07	132.25	127.40
1	A	922	A	C4-C5-C6	6.07	120.03	117.00
1	A	1059	A	C4-C5-C6	6.07	120.03	117.00
1	A	1614	A	N3-C4-N9	6.07	132.25	127.40
1	A	2497	A	C4-C5-C6	6.07	120.03	117.00
1	A	110	A	C4-C5-C6	6.06	120.03	117.00
1	A	1901	A	N3-C4-N9	6.06	132.25	127.40
1	A	2827	A	N3-C4-N9	6.06	132.25	127.40
32	W	768	A	C4-C5-C6	6.06	120.03	117.00
32	W	1004	A	N3-C4-N9	6.06	132.25	127.40
32	W	1112	A	N3-C4-N9	6.06	132.25	127.40
32	W	1369	A	N3-C4-N9	6.06	132.25	127.40
1	A	230	A	C4-C5-C6	6.06	120.03	117.00
1	A	908	A	C4-C5-C6	6.06	120.03	117.00
1	A	1339	A	C4-C5-C6	6.06	120.03	117.00
32	W	55	A	N3-C4-N9	6.06	132.25	127.40
32	W	234	A	N3-C4-N9	6.06	132.25	127.40
52	z	41	A	C4-C5-C6	6.06	120.03	117.00
1	A	449	A	C4-C5-C6	6.06	120.03	117.00
1	A	525	A	C8-N9-C4	6.06	108.22	105.80
1	A	876	A	C4-C5-C6	6.06	120.03	117.00
1	A	1832	A	C4-C5-C6	6.06	120.03	117.00
1	A	2047	A	C4-C5-C6	6.06	120.03	117.00
1	A	2893	A	C4-C5-C6	6.06	120.03	117.00
32	W	522	A	C4-C5-C6	6.06	120.03	117.00
32	W	918	A	N3-C4-N9	6.06	132.25	127.40
1	A	849	A	N3-C4-N9	6.06	132.25	127.40
2	B	99	A	C5-C6-N1	6.06	120.73	117.70
1	A	1542	A	C4-C5-C6	6.06	120.03	117.00
1	A	1956	A	C4-C5-C6	6.06	120.03	117.00
1	A	2919	A	N3-C4-N9	6.06	132.25	127.40
1	A	753	A	C4-C5-C6	6.06	120.03	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2080	A	N3-C4-N9	6.06	132.25	127.40
32	W	630	A	N3-C4-N9	6.06	132.25	127.40
32	W	1161	A	C4-C5-C6	6.06	120.03	117.00
1	A	376	A	N3-C4-N9	6.05	132.24	127.40
1	A	1005	A	N3-C4-N9	6.05	132.24	127.40
1	A	1233	A	C4-C5-C6	6.05	120.03	117.00
1	A	2769	A	C4-C5-C6	6.05	120.03	117.00
32	W	1092	A	C4-C5-C6	6.05	120.03	117.00
1	A	307	A	C4-C5-C6	6.05	120.03	117.00
1	A	781	A	C4-C5-C6	6.05	120.03	117.00
32	W	61	A	N3-C4-N9	6.05	132.24	127.40
32	W	107	A	C4-C5-C6	6.05	120.03	117.00
32	W	650	A	N3-C4-N9	6.05	132.24	127.40
32	W	786	A	C4-C5-C6	6.05	120.03	117.00
32	W	801	A	C4-C5-C6	6.05	120.03	117.00
32	W	975	A	C4-C5-C6	6.05	120.03	117.00
1	A	21	A	N3-C4-N9	6.05	132.24	127.40
1	A	1434	A	N9-C4-C5	6.05	108.22	105.80
1	A	1606	A	C4-C5-C6	6.05	120.03	117.00
1	A	1672	A	C4-C5-C6	6.05	120.03	117.00
1	A	1774	A	C4-C5-C6	6.05	120.03	117.00
1	A	1361	A	N3-C4-N9	6.05	132.24	127.40
32	W	314	A	C4-C5-C6	6.05	120.03	117.00
32	W	604	A	C4-C5-C6	6.05	120.03	117.00
1	A	2719	A	C4-C5-C6	6.05	120.02	117.00
2	B	64	A	C4-C5-C6	6.05	120.02	117.00
1	A	507	A	C4-C5-C6	6.05	120.02	117.00
1	A	530	A	N3-C4-N9	6.05	132.24	127.40
2	B	64	A	N3-C4-N9	6.05	132.24	127.40
32	W	118	A	N3-C4-N9	6.05	132.24	127.40
32	W	128	A	C4-C5-C6	6.05	120.02	117.00
1	A	1483	A	C4-C5-C6	6.04	120.02	117.00
1	A	2488	A	C5'-C4'-C3'	-6.04	106.33	116.00
1	A	260	A	N3-C4-N9	6.04	132.23	127.40
1	A	835	A	C4-C5-C6	6.04	120.02	117.00
1	A	849	A	C4-C5-C6	6.04	120.02	117.00
1	A	1686	A	C4-C5-C6	6.04	120.02	117.00
1	A	2066	A	N3-C4-N9	6.04	132.23	127.40
32	W	758	A	C4-C5-C6	6.04	120.02	117.00
32	W	1349	A	C4-C5-C6	6.04	120.02	117.00
1	A	229	A	C4-C5-C6	6.04	120.02	117.00
1	A	647	A	C8-N9-C4	6.04	108.22	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2105	U	C2-N1-C1'	6.04	124.95	117.70
32	W	423	A	C4-C5-C6	6.04	120.02	117.00
32	W	433	A	C4-C5-C6	6.04	120.02	117.00
32	W	703	A	C8-N9-C4	6.04	108.22	105.80
32	W	1266	A	C4-C5-C6	6.04	120.02	117.00
1	A	150	A	C8-N9-C4	6.04	108.22	105.80
1	A	1655	A	C4-C5-C6	6.04	120.02	117.00
32	W	173	A	N3-C4-N9	6.04	132.23	127.40
32	W	301	A	C4-C5-C6	6.04	120.02	117.00
1	A	479	A	C4-C5-C6	6.04	120.02	117.00
1	A	2078	A	C4-C5-C6	6.04	120.02	117.00
32	W	53	A	C4-C5-C6	6.04	120.02	117.00
32	W	1333	A	N9-C4-C5	6.04	108.22	105.80
32	W	382	A	C4-C5-C6	6.04	120.02	117.00
32	W	512	A	N3-C4-N9	6.04	132.23	127.40
32	W	1502	A	C4-C5-C6	6.04	120.02	117.00
1	A	12	A	C4-C5-C6	6.04	120.02	117.00
1	A	355	A	C4-C5-C6	6.04	120.02	117.00
1	A	1813	A	N3-C4-N9	6.04	132.23	127.40
1	A	1989	A	C4-C5-C6	6.04	120.02	117.00
1	A	2369	A	C4-C5-C6	6.04	120.02	117.00
1	A	2754	A	N3-C4-N9	6.04	132.23	127.40
1	A	2807	A	N9-C4-C5	6.04	108.21	105.80
2	B	44	A	C4-C5-C6	6.04	120.02	117.00
1	A	71	A	C8-N9-C4	6.03	108.21	105.80
1	A	1029	A	C4-C5-C6	6.03	120.02	117.00
1	A	2500	A	N3-C4-N9	6.03	132.23	127.40
1	A	2805	A	C8-N9-C4	6.03	108.21	105.80
32	W	210	A	C4-C5-C6	6.03	120.02	117.00
32	W	874	A	C4-C5-C6	6.03	120.02	117.00
32	W	1349	A	N3-C4-N9	6.03	132.23	127.40
1	A	507	A	N3-C4-N9	6.03	132.23	127.40
1	A	1046	A	N9-C4-C5	6.03	108.21	105.80
1	A	2869	A	C4-C5-C6	6.03	120.02	117.00
2	B	50	A	N3-C4-N9	6.03	132.23	127.40
32	W	617	A	N3-C4-N9	6.03	132.23	127.40
32	W	1359	A	N3-C4-N9	6.03	132.22	127.40
1	A	459	A	C4-C5-C6	6.03	120.02	117.00
1	A	2542	A	C4-C5-C6	6.03	120.02	117.00
1	A	2700	A	N3-C4-N9	6.03	132.22	127.40
1	A	2830	A	N3-C4-N9	6.03	132.22	127.40
1	A	2887	A	N3-C4-N9	6.03	132.22	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	51	A	C4-C5-C6	6.03	120.02	117.00
32	W	1054	A	C4-C5-C6	6.03	120.02	117.00
32	W	1369	A	C4-C5-C6	6.03	120.02	117.00
32	W	793	A	N3-C4-N9	6.03	132.22	127.40
32	W	1479	A	C4-C5-C6	6.03	120.02	117.00
1	A	486	A	N3-C4-N9	6.03	132.22	127.40
1	A	1072	A	N3-C4-N9	6.03	132.22	127.40
1	A	2462	A	C4-C5-C6	6.03	120.01	117.00
32	W	61	A	C4-C5-C6	6.03	120.01	117.00
32	W	161	A	N3-C4-N9	6.03	132.22	127.40
32	W	1115	A	C4-C5-C6	6.03	120.01	117.00
32	W	1523	A	N3-C4-N9	6.03	132.22	127.40
1	A	769	A	N3-C4-N9	6.03	132.22	127.40
1	A	1784	A	C8-N9-C4	6.03	108.21	105.80
1	A	2087	A	C4-C5-C6	6.03	120.01	117.00
1	A	2904	A	C4-C5-C6	6.03	120.01	117.00
32	W	541	A	C4-C5-C6	6.03	120.01	117.00
1	A	1555	A	C4-C5-N7	-6.02	107.69	110.70
32	W	1065	A	C8-N9-C4	6.02	108.21	105.80
1	A	1302	A	N9-C4-C5	6.02	108.21	105.80
1	A	1700	A	N3-C4-N9	6.02	132.22	127.40
32	W	433	A	N3-C4-N9	6.02	132.22	127.40
32	W	659	A	N3-C4-N9	6.02	132.22	127.40
32	W	988	A	C4-C5-N7	-6.02	107.69	110.70
32	W	1022	A	N3-C4-N9	6.02	132.22	127.40
2	B	114	A	N3-C4-N9	6.02	132.22	127.40
32	W	55	A	C4-C5-C6	6.02	120.01	117.00
1	A	144	A	C4-C5-C6	6.02	120.01	117.00
1	A	705	A	N3-C4-N9	6.02	132.22	127.40
1	A	868	A	N3-C4-N9	6.02	132.22	127.40
1	A	957	A	C4-C5-C6	6.02	120.01	117.00
1	A	1506	A	C4-C5-C6	6.02	120.01	117.00
1	A	2441	A	N3-C4-N9	6.02	132.22	127.40
32	W	278	A	C4-C5-C6	6.02	120.01	117.00
1	A	38	A	N3-C4-N9	6.02	132.21	127.40
1	A	343	A	C4-C5-C6	6.02	120.01	117.00
1	A	364	A	C4-C5-C6	6.02	120.01	117.00
1	A	438	A	C4-C5-C6	6.02	120.01	117.00
1	A	889	A	N3-C4-N9	6.02	132.21	127.40
1	A	1553	A	C8-N9-C4	6.02	108.21	105.80
32	W	404	A	C4-C5-C6	6.02	120.01	117.00
32	W	883	A	N3-C4-N9	6.02	132.21	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1283	A	C4-C5-C6	6.02	120.01	117.00
32	W	1455	A	N3-C4-N9	6.02	132.21	127.40
1	A	582	A	C4-C5-C6	6.02	120.01	117.00
1	A	2421	A	N3-C4-N9	6.02	132.21	127.40
32	W	776	A	C4-C5-C6	6.02	120.01	117.00
1	A	1421	A	N3-C4-N9	6.01	132.21	127.40
32	W	129	A	C4-C5-C6	6.01	120.01	117.00
32	W	344	A	N3-C4-N9	6.01	132.21	127.40
32	W	346	A	N3-C4-N9	6.01	132.21	127.40
1	A	1627	A	N3-C4-N9	6.01	132.21	127.40
1	A	1848	A	C4-C5-C6	6.01	120.01	117.00
1	A	140	A	N3-C4-N9	6.01	132.21	127.40
1	A	1404	A	C4-C5-C6	6.01	120.00	117.00
1	A	1876	A	N3-C4-N9	6.01	132.21	127.40
1	A	1906	A	C4-C5-C6	6.01	120.01	117.00
1	A	2619	A	C4-C5-C6	6.01	120.00	117.00
1	A	2722	A	C4-C5-C6	6.01	120.01	117.00
2	B	71	A	C4-C5-C6	6.01	120.01	117.00
32	W	99	A	C5-C6-N1	6.01	120.71	117.70
32	W	1294	A	C4-C5-C6	6.01	120.00	117.00
1	A	500	A	C4-C5-C6	6.01	120.00	117.00
1	A	1965	A	C4-C5-C6	6.01	120.00	117.00
2	B	105	A	C4-C5-C6	6.01	120.00	117.00
32	W	638	A	C4-C5-C6	6.01	120.00	117.00
32	W	659	A	C4-C5-C6	6.01	120.00	117.00
32	W	1180	A	C4-C5-C6	6.01	120.00	117.00
2	B	51	A	N3-C4-N9	6.01	132.21	127.40
32	W	390	A	N3-C4-N9	6.01	132.21	127.40
1	A	412	A	C4-C5-C6	6.01	120.00	117.00
1	A	1132	A	C4-C5-C6	6.01	120.00	117.00
1	A	1291	A	C8-N9-C4	6.01	108.20	105.80
1	A	1760	A	C4-C5-C6	6.01	120.00	117.00
1	A	456	A	N3-C4-N9	6.00	132.20	127.40
1	A	2052	A	N3-C4-N9	6.00	132.20	127.40
1	A	1254	A	N3-C4-N9	6.00	132.20	127.40
1	A	1524	A	C4-C5-C6	6.00	120.00	117.00
1	A	2316	A	N3-C4-N9	6.00	132.20	127.40
1	A	2390	A	C8-N9-C4	6.00	108.20	105.80
2	B	43	A	C4-C5-C6	6.00	120.00	117.00
32	W	258	A	N3-C4-N9	6.00	132.20	127.40
32	W	506	A	C4-C5-C6	6.00	120.00	117.00
32	W	968	A	C4-C5-C6	6.00	120.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	969	A	C4-C5-C6	6.00	120.00	117.00
1	A	230	A	N3-C4-N9	6.00	132.20	127.40
1	A	2875	A	C4-C5-C6	6.00	120.00	117.00
32	W	928	A	C4-C5-C6	6.00	120.00	117.00
32	W	1296	A	N3-C4-N9	6.00	132.20	127.40
1	A	1556	A	N3-C4-N9	6.00	132.20	127.40
1	A	2683	A	C8-N9-C4	6.00	108.20	105.80
1	A	2719	A	C8-N9-C4	6.00	108.20	105.80
1	A	2834	A	C4-C5-C6	6.00	120.00	117.00
32	W	329	A	C4-C5-C6	6.00	120.00	117.00
1	A	1179	A	C4-C5-C6	6.00	120.00	117.00
1	A	1201	A	N9-C4-C5	6.00	108.20	105.80
1	A	2805	A	N3-C4-N9	6.00	132.20	127.40
1	A	2854	A	N3-C4-N9	6.00	132.20	127.40
1	A	2900	A	N3-C4-N9	6.00	132.20	127.40
32	W	696	A	C4-C5-C6	6.00	120.00	117.00
32	W	1206	A	C4-C5-C6	6.00	120.00	117.00
32	W	1206	A	N3-C4-N9	6.00	132.20	127.40
32	W	1270	A	N3-C4-N9	6.00	132.20	127.40
32	W	1383	A	N3-C4-N9	6.00	132.20	127.40
1	A	178	A	C4-C5-C6	6.00	120.00	117.00
1	A	326	A	N3-C4-N9	6.00	132.20	127.40
1	A	705	A	C4-C5-C6	6.00	120.00	117.00
1	A	952	A	C4-C5-C6	6.00	120.00	117.00
1	A	1260	A	N3-C4-N9	6.00	132.20	127.40
1	A	1913	A	C4-C5-C6	6.00	120.00	117.00
1	A	2477	A	C4-C5-C6	6.00	120.00	117.00
32	W	34	A	N3-C4-N9	6.00	132.20	127.40
32	W	491	A	C4-C5-C6	6.00	120.00	117.00
32	W	803	A	C4-C5-C6	6.00	120.00	117.00
1	A	1464	A	C4-C5-C6	6.00	120.00	117.00
1	A	1743	A	C4-C5-C6	6.00	120.00	117.00
32	W	1405	A	C4-C5-C6	6.00	120.00	117.00
1	A	547	A	C4-C5-C6	5.99	120.00	117.00
1	A	1144	A	C4-C5-C6	5.99	120.00	117.00
1	A	1175	A	C4-C5-C6	5.99	120.00	117.00
1	A	1947	A	N3-C4-N9	5.99	132.20	127.40
1	A	2619	A	N3-C4-N9	5.99	132.19	127.40
1	A	2889	A	N3-C4-N9	5.99	132.19	127.40
32	W	81	A	N3-C4-N9	5.99	132.19	127.40
32	W	352	A	C4-C5-C6	5.99	120.00	117.00
32	W	959	A	N3-C4-N9	5.99	132.19	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1445	A	C4-C5-C6	5.99	120.00	117.00
1	A	2754	A	C4-C5-C6	5.99	120.00	117.00
1	A	2860	A	C8-N9-C4	5.99	108.20	105.80
32	W	475	A	C4-C5-C6	5.99	120.00	117.00
1	A	888	A	C4-C5-C6	5.99	120.00	117.00
1	A	893	A	C4-C5-C6	5.99	120.00	117.00
1	A	1021	A	C4-C5-C6	5.99	120.00	117.00
1	A	1813	A	C4-C5-C6	5.99	120.00	117.00
1	A	2083	A	C8-N9-C4	5.99	108.20	105.80
1	A	2498	A	N3-C4-N9	5.99	132.19	127.40
32	W	721	A	N3-C4-N9	5.99	132.19	127.40
32	W	771	A	N3-C4-N9	5.99	132.19	127.40
32	W	862	A	C4-C5-N7	-5.99	107.70	110.70
32	W	1176	A	C4-C5-C6	5.99	120.00	117.00
32	W	1284	A	N3-C4-N9	5.99	132.19	127.40
1	A	102	A	N3-C4-N9	5.99	132.19	127.40
1	A	525	A	N3-C4-N9	5.99	132.19	127.40
1	A	547	A	N3-C4-N9	5.99	132.19	127.40
1	A	548	A	N3-C4-N9	5.99	132.19	127.40
1	A	1617	A	C4-C5-C6	5.99	119.99	117.00
1	A	2668	A	N3-C4-N9	5.99	132.19	127.40
1	A	2708	A	C4-C5-C6	5.99	120.00	117.00
32	W	142	A	C4-C5-C6	5.99	119.99	117.00
32	W	529	A	C4-C5-C6	5.99	119.99	117.00
32	W	651	A	C8-N9-C4	5.99	108.19	105.80
32	W	1486	A	C4-C5-C6	5.99	119.99	117.00
32	W	1541	A	C4-C5-C6	5.99	119.99	117.00
1	A	139	A	C4-C5-C6	5.99	119.99	117.00
1	A	630	A	N3-C4-N9	5.99	132.19	127.40
1	A	1194	A	C4-C5-C6	5.99	119.99	117.00
2	B	71	A	N3-C4-N9	5.99	132.19	127.40
32	W	372	A	N3-C4-N9	5.99	132.19	127.40
1	A	637	A	C4-C5-C6	5.99	119.99	117.00
1	A	1532	A	C8-N9-C4	5.99	108.19	105.80
1	A	1677	A	C4-C5-C6	5.99	119.99	117.00
1	A	2462	A	N3-C4-N9	5.99	132.19	127.40
32	W	404	A	N3-C4-N9	5.99	132.19	127.40
32	W	917	A	N3-C4-N9	5.99	132.19	127.40
32	W	1120	A	C4-C5-C6	5.99	119.99	117.00
1	A	652	A	N3-C4-N9	5.98	132.19	127.40
1	A	1141	A	C4-C5-C6	5.98	119.99	117.00
1	A	2511	A	N3-C4-N9	5.98	132.19	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	A	C4-C5-C6	5.98	119.99	117.00
1	A	124	A	C4-C5-C6	5.98	119.99	117.00
1	A	384	A	C4-C5-C6	5.98	119.99	117.00
1	A	653	A	C4-C5-C6	5.98	119.99	117.00
1	A	993	A	C4-C5-C6	5.98	119.99	117.00
1	A	1113	A	C4-C5-C6	5.98	119.99	117.00
1	A	1224	A	C4-C5-C6	5.98	119.99	117.00
1	A	2734	A	N3-C4-N9	5.98	132.19	127.40
32	W	786	A	C8-N9-C4	5.98	108.19	105.80
1	A	65	A	C4-C5-C6	5.98	119.99	117.00
1	A	470	A	C8-N9-C4	5.98	108.19	105.80
1	A	1269	A	C4-C5-C6	5.98	119.99	117.00
1	A	1313	A	N3-C4-N9	5.98	132.19	127.40
1	A	1445	A	N3-C4-N9	5.98	132.19	127.40
1	A	1534	A	C4-C5-C6	5.98	119.99	117.00
1	A	1663	A	N3-C4-N9	5.98	132.19	127.40
1	A	2032	A	N3-C4-N9	5.98	132.19	127.40
1	A	2740	A	C4-C5-C6	5.98	119.99	117.00
32	W	644	A	N3-C4-N9	5.98	132.19	127.40
32	W	1405	A	N3-C4-N9	5.98	132.19	127.40
32	W	1455	A	C4-C5-C6	5.98	119.99	117.00
1	A	740	A	C4-C5-C6	5.98	119.99	117.00
1	A	2047	A	N3-C4-N9	5.98	132.18	127.40
32	W	390	A	C4-C5-C6	5.98	119.99	117.00
1	A	947	A	C4-C5-C6	5.98	119.99	117.00
1	A	1456	A	C4-C5-C6	5.98	119.99	117.00
1	A	1533	A	C4-C5-C6	5.98	119.99	117.00
1	A	1791	A	C4-C5-C6	5.98	119.99	117.00
1	A	2769	A	N3-C4-N9	5.98	132.18	127.40
1	A	2807	A	C8-N9-C4	5.98	108.19	105.80
32	W	240	A	C4-C5-C6	5.98	119.99	117.00
32	W	364	A	N3-C4-N9	5.98	132.18	127.40
32	W	611	A	C4-C5-C6	5.98	119.99	117.00
1	A	231	A	N3-C4-N9	5.98	132.18	127.40
1	A	1483	A	N3-C4-N9	5.98	132.18	127.40
1	A	1585	A	C4-C5-C6	5.98	119.99	117.00
32	W	518	A	C4-C5-C6	5.98	119.99	117.00
32	W	1090	A	C4-C5-C6	5.98	119.99	117.00
1	A	1202	A	C8-N9-C4	5.97	108.19	105.80
1	A	1464	A	N3-C4-N9	5.97	132.18	127.40
1	A	1685	A	N3-C4-N9	5.97	132.18	127.40
1	A	1697	A	C4-C5-C6	5.97	119.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1818	A	C4-C5-C6	5.97	119.99	117.00
1	A	2526	A	C4-C5-C6	5.97	119.99	117.00
32	W	1435	A	N3-C4-N9	5.97	132.18	127.40
1	A	273	A	N9-C4-C5	5.97	108.19	105.80
1	A	429	A	N3-C4-N9	5.97	132.18	127.40
1	A	1314	A	C4-C5-C6	5.97	119.99	117.00
1	A	1516	A	C4-C5-C6	5.97	119.99	117.00
1	A	1723	A	C4-C5-C6	5.97	119.99	117.00
1	A	1925	A	C4-C5-C6	5.97	119.99	117.00
1	A	1956	A	N3-C4-N9	5.97	132.18	127.40
32	W	372	A	C4-C5-C6	5.97	119.99	117.00
32	W	568	A	C8-N9-C4	5.97	108.19	105.80
32	W	902	A	N3-C4-N9	5.97	132.18	127.40
52	z	21	A	N3-C4-N9	5.97	132.18	127.40
1	A	144	A	N3-C4-N9	5.97	132.18	127.40
1	A	1066	A	C8-N9-C4	5.97	108.19	105.80
1	A	1423	A	C4-C5-C6	5.97	119.98	117.00
32	W	1528	A	C4-C5-C6	5.97	119.98	117.00
1	A	412	A	N3-C4-N9	5.97	132.18	127.40
1	A	477	A	C4-C5-C6	5.97	119.98	117.00
1	A	763	A	C4-C5-C6	5.97	119.98	117.00
1	A	1532	A	C4-C5-C6	5.97	119.98	117.00
1	A	1767	A	N3-C4-N9	5.97	132.18	127.40
1	A	2463	A	C4-C5-C6	5.97	119.98	117.00
2	B	20	A	N3-C4-N9	5.97	132.18	127.40
32	W	979	A	N3-C4-N9	5.97	132.18	127.40
32	W	1121	A	C4-C5-C6	5.97	119.98	117.00
32	W	1259	A	N3-C4-N9	5.97	132.18	127.40
32	W	1417	A	C4-C5-C6	5.97	119.98	117.00
52	z	37	A	N9-C4-C5	5.97	108.19	105.80
1	A	782	A	N3-C4-N9	5.97	132.17	127.40
1	A	2298	A	C4-C5-C6	5.97	119.98	117.00
1	A	2389	A	N3-C4-N9	5.97	132.17	127.40
1	A	2468	A	N3-C4-N9	5.97	132.17	127.40
1	A	2497	A	N3-C4-N9	5.97	132.17	127.40
2	B	18	A	N9-C4-C5	5.97	108.19	105.80
32	W	672	A	C4-C5-C6	5.97	119.98	117.00
1	A	600	A	N3-C4-N9	5.97	132.17	127.40
1	A	659	A	N3-C4-N9	5.97	132.17	127.40
1	A	876	A	N3-C4-N9	5.97	132.17	127.40
1	A	1174	A	N3-C4-N9	5.97	132.17	127.40
1	A	1453	A	C4-C5-C6	5.97	119.98	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2461	A	N3-C4-N9	5.97	132.17	127.40
32	W	139	A	N3-C4-N9	5.97	132.17	127.40
32	W	542	A	C4-C5-C6	5.97	119.98	117.00
32	W	674	A	C4-C5-N7	-5.97	107.72	110.70
32	W	1248	A	C4-C5-C6	5.97	119.98	117.00
1	A	21	A	C4-C5-C6	5.96	119.98	117.00
1	A	324	A	C4-C5-C6	5.96	119.98	117.00
1	A	373	A	C4-C5-C6	5.96	119.98	117.00
1	A	1055	A	C4-C5-C6	5.96	119.98	117.00
1	A	1617	A	N3-C4-N9	5.96	132.17	127.40
1	A	1636	A	C4-C5-C6	5.96	119.98	117.00
1	A	1768	A	N3-C4-N9	5.96	132.17	127.40
1	A	1774	A	N3-C4-N9	5.96	132.17	127.40
32	W	160	A	C4-C5-C6	5.96	119.98	117.00
32	W	361	A	C4-C5-C6	5.96	119.98	117.00
1	A	44	A	N3-C4-N9	5.96	132.17	127.40
1	A	524	A	N3-C4-N9	5.96	132.17	127.40
1	A	1606	A	C8-N9-C4	5.96	108.19	105.80
32	W	988	A	C4-C5-C6	5.96	119.98	117.00
1	A	94	A	C4-C5-C6	5.96	119.98	117.00
1	A	193	A	N3-C4-N9	5.96	132.17	127.40
1	A	279	A	C4-C5-C6	5.96	119.98	117.00
1	A	578	A	C8-N9-C4	5.96	108.18	105.80
1	A	1405	A	N3-C4-N9	5.96	132.17	127.40
2	B	114	A	C4-C5-C6	5.96	119.98	117.00
32	W	518	A	N3-C4-N9	5.96	132.17	127.40
1	A	330	A	C4-C5-C6	5.96	119.98	117.00
1	A	469	A	N3-C4-N9	5.96	132.17	127.40
1	A	1130	A	C4-C5-C6	5.96	119.98	117.00
1	A	1905	A	N9-C4-C5	5.96	108.18	105.80
32	W	1510	A	C4-C5-C6	5.96	119.98	117.00
1	A	275	A	N3-C4-N9	5.96	132.17	127.40
1	A	1675	A	N3-C4-N9	5.96	132.17	127.40
1	A	1734	A	C4-C5-C6	5.96	119.98	117.00
1	A	2454	A	N3-C4-N9	5.96	132.17	127.40
1	A	2887	A	C4-C5-C6	5.96	119.98	117.00
2	B	56	A	C4-C5-C6	5.96	119.98	117.00
32	W	544	A	C4-C5-C6	5.96	119.98	117.00
32	W	1056	A	C4-C5-C6	5.96	119.98	117.00
32	W	251	A	C4-C5-C6	5.96	119.98	117.00
32	W	507	A	C8-N9-C4	5.96	108.18	105.80
32	W	631	A	N9-C4-C5	5.96	108.18	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	677	A	N3-C4-N9	5.96	132.16	127.40
1	A	524	A	C4-C5-C6	5.95	119.98	117.00
32	W	204	A	C4-C5-C6	5.95	119.98	117.00
32	W	522	A	N3-C4-N9	5.95	132.16	127.40
32	W	618	A	C4-C5-C6	5.95	119.98	117.00
32	W	768	A	N3-C4-N9	5.95	132.16	127.40
32	W	1188	A	C8-N9-C4	5.95	108.18	105.80
32	W	1247	A	N9-C4-C5	5.95	108.18	105.80
32	W	1294	A	N3-C4-N9	5.95	132.16	127.40
1	A	374	A	N9-C4-C5	5.95	108.18	105.80
1	A	1116	A	C4-C5-C6	5.95	119.98	117.00
1	A	1131	A	N3-C4-N9	5.95	132.16	127.40
1	A	1456	A	N9-C4-C5	5.95	108.18	105.80
32	W	1451	A	C4-C5-C6	5.95	119.98	117.00
1	A	1406	A	N3-C4-N9	5.95	132.16	127.40
1	A	1473	A	C8-N9-C4	5.95	108.18	105.80
1	A	1614	A	C4-C5-C6	5.95	119.98	117.00
1	A	1746	A	C4-C5-C6	5.95	119.98	117.00
1	A	2594	A	C4-C5-C6	5.95	119.97	117.00
1	A	2661	A	C4-C5-C6	5.95	119.98	117.00
32	W	715	A	N3-C4-N9	5.95	132.16	127.40
32	W	824	A	C4-C5-C6	5.95	119.97	117.00
1	A	325	A	C4-C5-C6	5.95	119.97	117.00
1	A	867	A	C4-C5-C6	5.95	119.97	117.00
1	A	1569	A	N3-C4-N9	5.95	132.16	127.40
1	A	1636	A	N3-C4-N9	5.95	132.16	127.40
1	A	2330	A	N9-C4-C5	5.95	108.18	105.80
1	A	2511	A	C4-C5-C6	5.95	119.97	117.00
1	A	2851	A	N3-C4-N9	5.95	132.16	127.40
32	W	1014	A	N3-C4-N9	5.95	132.16	127.40
32	W	1486	A	N3-C4-N9	5.95	132.16	127.40
1	A	1277	A	C4-C5-C6	5.95	119.97	117.00
1	A	2307	A	C4-C5-C6	5.95	119.97	117.00
1	A	67	A	C4-C5-C6	5.95	119.97	117.00
1	A	140	A	C4-C5-C6	5.95	119.97	117.00
1	A	717	A	C4-C5-C6	5.95	119.97	117.00
32	W	287	A	C4-C5-C6	5.95	119.97	117.00
32	W	333	A	N3-C4-N9	5.95	132.16	127.40
32	W	1128	A	C4-C5-C6	5.95	119.97	117.00
1	A	194	A	N3-C4-N9	5.94	132.16	127.40
1	A	307	A	N3-C4-N9	5.94	132.16	127.40
1	A	2406	A	N3-C4-N9	5.94	132.16	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2505	A	N3-C4-N9	5.94	132.16	127.40
1	A	470	A	N3-C4-N9	5.94	132.15	127.40
1	A	538	A	C8-N9-C4	5.94	108.18	105.80
1	A	658	A	C4-C5-C6	5.94	119.97	117.00
1	A	765	A	N3-C4-N9	5.94	132.15	127.40
1	A	925	A	C4-C5-C6	5.94	119.97	117.00
1	A	1059	A	N3-C4-N9	5.94	132.15	127.40
1	A	2080	A	C4-C5-C6	5.94	119.97	117.00
1	A	2303	A	C4-C5-C6	5.94	119.97	117.00
32	W	278	A	N3-C4-N9	5.94	132.15	127.40
32	W	786	A	N3-C4-N9	5.94	132.15	127.40
1	A	71	A	N3-C4-N9	5.94	132.15	127.40
1	A	2708	A	N3-C4-N9	5.94	132.15	127.40
1	A	2923	A	C4-C5-C6	5.94	119.97	117.00
32	W	159	A	C8-N9-C4	5.94	108.18	105.80
32	W	1054	A	N3-C4-N9	5.94	132.15	127.40
32	W	1222	A	N3-C4-N9	5.94	132.15	127.40
32	W	1252	A	N3-C4-N9	5.94	132.15	127.40
1	A	1928	A	N3-C4-N9	5.94	132.15	127.40
32	W	1257	A	C8-N9-C4	5.94	108.18	105.80
1	A	65	A	N3-C4-N9	5.94	132.15	127.40
1	A	225	A	N3-C4-N9	5.94	132.15	127.40
1	A	1027	A	C4-C5-C6	5.94	119.97	117.00
1	A	1054	A	N3-C4-N9	5.94	132.15	127.40
1	A	2049	A	N3-C4-N9	5.94	132.15	127.40
1	A	2616	A	N3-C4-N9	5.94	132.15	127.40
32	W	151	A	N9-C4-C5	5.94	108.17	105.80
32	W	159	A	C4-C5-C6	5.94	119.97	117.00
32	W	270	A	N3-C4-N9	5.94	132.15	127.40
32	W	705	A	N3-C4-N9	5.94	132.15	127.40
32	W	757	A	C4-C5-C6	5.94	119.97	117.00
32	W	799	A	C4-C5-C6	5.94	119.97	117.00
1	A	987	A	C4-C5-C6	5.94	119.97	117.00
1	A	1555	A	N9-C4-C5	5.94	108.17	105.80
1	A	2087	A	N3-C4-N9	5.94	132.15	127.40
32	W	704	A	C4-C5-C6	5.94	119.97	117.00
1	A	917	A	C4-C5-C6	5.93	119.97	117.00
1	A	1499	A	C4-C5-C6	5.93	119.97	117.00
1	A	2034	A	N3-C4-N9	5.93	132.15	127.40
1	A	2100	A	N3-C4-N9	5.93	132.15	127.40
2	B	76	A	C4-C5-C6	5.93	119.97	117.00
32	W	290	A	C4-C5-C6	5.93	119.97	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	382	A	N3-C4-N9	5.93	132.15	127.40
32	W	512	A	C4-C5-C6	5.93	119.97	117.00
32	W	555	A	N9-C4-C5	5.93	108.17	105.80
32	W	638	A	N3-C4-N9	5.93	132.15	127.40
32	W	650	A	C4-C5-C6	5.93	119.97	117.00
32	W	669	A	C4-C5-C6	5.93	119.97	117.00
32	W	1503	A	C4-C5-C6	5.93	119.97	117.00
1	A	314	A	C8-N9-C4	5.93	108.17	105.80
1	A	702	A	C8-N9-C4	5.93	108.17	105.80
1	A	904	A	C4-C5-C6	5.93	119.97	117.00
1	A	1269	A	N3-C4-N9	5.93	132.15	127.40
1	A	1592	A	C4-C5-C6	5.93	119.97	117.00
1	A	2482	A	C4-C5-C6	5.93	119.97	117.00
1	A	2770	A	C4-C5-C6	5.93	119.97	117.00
2	B	25	A	C8-N9-C4	5.93	108.17	105.80
32	W	67	A	C4-C5-C6	5.93	119.97	117.00
32	W	270	A	C4-C5-C6	5.93	119.97	117.00
32	W	1092	A	N3-C4-N9	5.93	132.15	127.40
32	W	1245	A	N3-C4-N9	5.93	132.15	127.40
32	W	1403	A	C4-C5-C6	5.93	119.97	117.00
1	A	53	A	N3-C4-N9	5.93	132.15	127.40
1	A	1583	A	C4-C5-C6	5.93	119.97	117.00
32	W	258	A	C8-N9-C4	5.93	108.17	105.80
32	W	658	A	N3-C4-N9	5.93	132.15	127.40
1	A	470	A	C4-C5-C6	5.93	119.97	117.00
1	A	1982	A	C8-N9-C4	5.93	108.17	105.80
1	A	2860	A	N3-C4-N9	5.93	132.14	127.40
32	W	519	A	C4-C5-C6	5.93	119.96	117.00
32	W	583	A	C4-C5-C6	5.93	119.97	117.00
32	W	947	A	C4-C5-C6	5.93	119.97	117.00
32	W	1028	A	C4-C5-C6	5.93	119.97	117.00
1	A	281	A	C4-C5-C6	5.93	119.96	117.00
1	A	782	A	C8-N9-C4	5.93	108.17	105.80
1	A	1072	A	C8-N9-C4	5.93	108.17	105.80
1	A	1812	A	N9-C4-C5	5.93	108.17	105.80
1	A	1961	A	N3-C4-N9	5.93	132.14	127.40
32	W	1298	A	N3-C4-N9	5.93	132.14	127.40
1	A	600	A	C4-C5-C6	5.93	119.96	117.00
1	A	618	A	N9-C4-C5	5.93	108.17	105.80
1	A	781	A	N3-C4-N9	5.93	132.14	127.40
1	A	808	A	N3-C4-N9	5.93	132.14	127.40
1	A	974	A	N3-C4-N9	5.93	132.14	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1265	A	N3-C4-N9	5.93	132.14	127.40
1	A	1930	A	N3-C4-N9	5.93	132.14	127.40
32	W	139	A	C4-C5-C6	5.93	119.96	117.00
32	W	1048	A	C8-N9-C4	5.93	108.17	105.80
32	W	1236	A	N3-C4-N9	5.93	132.14	127.40
52	z	58	A	N3-C4-N9	5.93	132.14	127.40
1	A	330	A	N3-C4-N9	5.92	132.14	127.40
1	A	2026	A	C8-N9-C4	5.92	108.17	105.80
32	W	18	A	C8-N9-C4	5.92	108.17	105.80
32	W	386	A	C4-C5-C6	5.92	119.96	117.00
32	W	874	A	N3-C4-N9	5.92	132.14	127.40
32	W	1147	A	N3-C4-N9	5.92	132.14	127.40
32	W	1327	A	N3-C4-N9	5.92	132.14	127.40
32	W	1523	A	C4-C5-C6	5.92	119.96	117.00
1	A	207	A	C8-N9-C4	5.92	108.17	105.80
1	A	1347	A	N9-C4-C5	5.92	108.17	105.80
1	A	2406	A	C4-C5-C6	5.92	119.96	117.00
32	W	929	A	C4-C5-C6	5.92	119.96	117.00
1	A	324	A	N3-C4-N9	5.92	132.14	127.40
1	A	337	A	C4-C5-C6	5.92	119.96	117.00
1	A	753	A	N3-C4-N9	5.92	132.14	127.40
1	A	867	A	N3-C4-N9	5.92	132.14	127.40
1	A	1074	A	C4-C5-C6	5.92	119.96	117.00
1	A	1901	A	C8-N9-C4	5.92	108.17	105.80
32	W	389	A	C4-C5-C6	5.92	119.96	117.00
32	W	724	A	C4-C5-C6	5.92	119.96	117.00
32	W	1048	A	C4-C5-C6	5.92	119.96	117.00
1	A	2007	A	C4-C5-C6	5.92	119.96	117.00
32	W	1425	A	N3-C4-N9	5.92	132.14	127.40
32	W	1503	A	C8-N9-C4	5.92	108.17	105.80
1	A	150	A	N3-C4-N9	5.92	132.13	127.40
1	A	808	A	C4-C5-C6	5.92	119.96	117.00
1	A	935	A	C4-C5-N7	-5.92	107.74	110.70
1	A	1588	A	N3-C4-N9	5.92	132.13	127.40
1	A	1608	A	C4-C5-C6	5.92	119.96	117.00
1	A	1735	A	N3-C4-N9	5.92	132.13	127.40
1	A	2083	A	N3-C4-N9	5.92	132.13	127.40
1	A	2898	A	N9-C4-C5	5.92	108.17	105.80
32	W	203	A	C4-C5-C6	5.92	119.96	117.00
32	W	1296	A	C4-C5-C6	5.92	119.96	117.00
52	z	14	A	C4-C5-C6	5.92	119.96	117.00
1	A	91	A	N3-C4-N9	5.92	132.13	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	A	N3-C4-N9	5.92	132.13	127.40
1	A	259	A	N3-C4-N9	5.92	132.13	127.40
1	A	746	A	C4-C5-C6	5.92	119.96	117.00
1	A	1036	A	C4-C5-C6	5.92	119.96	117.00
1	A	1339	A	C8-N9-C4	5.92	108.17	105.80
1	A	1929	A	C4-C5-C6	5.92	119.96	117.00
1	A	2421	A	C4-C5-C6	5.92	119.96	117.00
1	A	2468	A	C4-C5-C6	5.92	119.96	117.00
1	A	2570	A	N3-C4-N9	5.92	132.13	127.40
1	A	2670	A	N9-C4-C5	5.92	108.17	105.80
1	A	2846	A	N3-C4-N9	5.92	132.13	127.40
1	A	2907	A	N3-C4-N9	5.92	132.13	127.40
2	B	76	A	N3-C4-N9	5.92	132.13	127.40
32	W	94	A	C4-C5-C6	5.92	119.96	117.00
32	W	919	A	N3-C4-N9	5.92	132.13	127.40
32	W	1210	A	C4-C5-C6	5.92	119.96	117.00
32	W	1348	A	N3-C4-N9	5.92	132.13	127.40
1	A	652	A	C4-C5-C6	5.92	119.96	117.00
1	A	947	A	N3-C4-N9	5.92	132.13	127.40
1	A	1014	A	C4-C5-C6	5.92	119.96	117.00
1	A	1615	A	N3-C4-N9	5.92	132.13	127.40
1	A	2778	A	C4-C5-C6	5.92	119.96	117.00
32	W	1103	A	C4-C5-C6	5.92	119.96	117.00
1	A	161	A	N9-C4-C5	5.91	108.17	105.80
1	A	582	A	C8-N9-C4	5.91	108.17	105.80
1	A	1034	A	C4-C5-C6	5.91	119.96	117.00
1	A	2658	A	C4-C5-C6	5.91	119.96	117.00
32	W	35	A	N3-C4-N9	5.91	132.13	127.40
32	W	452	A	C4-C5-C6	5.91	119.96	117.00
32	W	456	A	C8-N9-C4	5.91	108.17	105.80
32	W	1102	A	C4-C5-C6	5.91	119.96	117.00
1	A	1189	A	C8-N9-C4	5.91	108.17	105.80
1	A	1453	A	N3-C4-N9	5.91	132.13	127.40
1	A	2042	A	N3-C4-N9	5.91	132.13	127.40
1	A	2327	A	C4-C5-C6	5.91	119.96	117.00
1	A	2750	A	N3-C4-N9	5.91	132.13	127.40
1	A	6	A	N3-C4-N9	5.91	132.13	127.40
1	A	958	A	N3-C4-N9	5.91	132.13	127.40
1	A	978	A	C4-C5-C6	5.91	119.95	117.00
1	A	2417	A	C8-N9-C4	5.91	108.16	105.80
32	W	1296	A	C8-N9-C4	5.91	108.16	105.80
32	W	1434	A	C4-C5-C6	5.91	119.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1451	A	N3-C4-N9	5.91	132.13	127.40
32	W	1466	A	C8-N9-C4	5.91	108.16	105.80
52	z	76	A	N3-C4-N9	5.91	132.13	127.40
1	A	6	A	C4-C5-C6	5.91	119.95	117.00
1	A	102	A	C4-C5-C6	5.91	119.95	117.00
1	A	1375	A	C4-C5-C6	5.91	119.95	117.00
1	A	1524	A	C8-N9-C4	5.91	108.16	105.80
1	A	1541	A	N3-C4-N9	5.91	132.13	127.40
1	A	1882	A	N3-C4-N9	5.91	132.13	127.40
1	A	2327	A	N3-C4-N9	5.91	132.13	127.40
1	A	2357	A	C4-C5-C6	5.91	119.95	117.00
1	A	2455	A	C8-N9-C4	5.91	108.16	105.80
32	W	831	A	C4-C5-C6	5.91	119.95	117.00
32	W	899	A	N9-C4-C5	5.91	108.16	105.80
32	W	1205	A	C4-C5-C6	5.91	119.95	117.00
1	A	154	A	C4-C5-C6	5.91	119.95	117.00
1	A	1788	A	N3-C4-N9	5.91	132.13	127.40
1	A	2387	A	C4-C5-C6	5.91	119.95	117.00
1	A	14	A	C4-C5-C6	5.91	119.95	117.00
1	A	200	A	N3-C4-N9	5.91	132.12	127.40
1	A	758	A	N3-C4-N9	5.91	132.12	127.40
1	A	762	A	C4-C5-C6	5.91	119.95	117.00
1	A	1648	A	N3-C4-N9	5.91	132.12	127.40
1	A	1788	A	C4-C5-C6	5.91	119.95	117.00
1	A	1913	A	N3-C4-N9	5.91	132.12	127.40
1	A	2298	A	C8-N9-C4	5.91	108.16	105.80
1	A	2601	A	C8-N9-C4	5.91	108.16	105.80
1	A	2924	A	N3-C4-N9	5.91	132.12	127.40
32	W	771	A	C4-C5-C6	5.91	119.95	117.00
32	W	823	A	N3-C4-N9	5.91	132.12	127.40
32	W	1140	A	C4-C5-C6	5.91	119.95	117.00
52	z	14	A	N3-C4-N9	5.91	132.12	127.40
1	A	281	A	C4-C5-N7	-5.90	107.75	110.70
1	A	384	A	N3-C4-N9	5.90	132.12	127.40
1	A	1686	A	N3-C4-N9	5.90	132.12	127.40
1	A	1844	A	N9-C4-C5	5.90	108.16	105.80
1	A	727	A	C4-C5-C6	5.90	119.95	117.00
1	A	763	A	N3-C4-N9	5.90	132.12	127.40
1	A	1066	A	C4-C5-C6	5.90	119.95	117.00
1	A	1266	A	C4-C5-C6	5.90	119.95	117.00
1	A	2338	A	N3-C4-N9	5.90	132.12	127.40
1	A	2893	A	N3-C4-N9	5.90	132.12	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	532	A	N3-C4-N9	5.90	132.12	127.40
32	W	1022	A	C4-C5-C6	5.90	119.95	117.00
32	W	1210	A	N3-C4-N9	5.90	132.12	127.40
32	W	1456	A	N3-C4-N9	5.90	132.12	127.40
52	z	44	A	C4-C5-C6	5.90	119.95	117.00
1	A	198	A	C4-C5-C6	5.90	119.95	117.00
1	A	500	A	N3-C4-N9	5.90	132.12	127.40
1	A	1269	A	C8-N9-C4	5.90	108.16	105.80
1	A	1654	A	C4-C5-C6	5.90	119.95	117.00
1	A	1721	A	N3-C4-N9	5.90	132.12	127.40
1	A	2440	A	C4-C5-C6	5.90	119.95	117.00
1	A	2498	A	C4-C5-C6	5.90	119.95	117.00
1	A	2807	A	C4-C5-N7	-5.90	107.75	110.70
32	W	367	A	N9-C4-C5	5.90	108.16	105.80
32	W	762	A	C4-C5-C6	5.90	119.95	117.00
32	W	1403	A	N3-C4-N9	5.90	132.12	127.40
32	W	1437	A	N3-C4-N9	5.90	132.12	127.40
1	A	12	A	N3-C4-N9	5.90	132.12	127.40
1	A	1700	A	C8-N9-C4	5.90	108.16	105.80
1	A	2078	A	N3-C4-N9	5.90	132.12	127.40
1	A	2297	A	C4-C5-C6	5.90	119.95	117.00
2	B	39	A	C8-N9-C4	5.90	108.16	105.80
32	W	463	A	C8-N9-C4	5.90	108.16	105.80
1	A	486	A	C4-C5-C6	5.90	119.95	117.00
1	A	560	A	C4-C5-C6	5.90	119.95	117.00
1	A	851	A	N3-C4-N9	5.90	132.12	127.40
1	A	1312	A	C4-C5-C6	5.90	119.95	117.00
2	B	25	A	N3-C4-N9	5.90	132.12	127.40
2	B	39	A	N3-C4-N9	5.90	132.12	127.40
2	B	55	A	C4-C5-C6	5.90	119.95	117.00
2	B	56	A	N3-C4-N9	5.90	132.12	127.40
32	W	118	A	C8-N9-C4	5.90	108.16	105.80
32	W	195	A	C4-C5-C6	5.90	119.95	117.00
32	W	206	A	C4-C5-C6	5.90	119.95	117.00
32	W	287	A	N3-C4-N9	5.90	132.12	127.40
32	W	1259	A	C4-C5-C6	5.90	119.95	117.00
1	A	2708	A	C8-N9-C4	5.90	108.16	105.80
32	W	94	A	N3-C4-N9	5.90	132.12	127.40
32	W	474	A	C4-C5-C6	5.90	119.95	117.00
32	W	823	A	C4-C5-C6	5.90	119.95	117.00
1	A	176	A	N3-C4-N9	5.89	132.12	127.40
1	A	220	A	C4-C5-C6	5.89	119.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1918	A	N3-C4-N9	5.89	132.12	127.40
1	A	2364	A	C4-C5-C6	5.89	119.95	117.00
1	A	2547	A	C4-C5-C6	5.89	119.95	117.00
32	W	211	A	N3-C4-N9	5.89	132.12	127.40
32	W	799	A	N3-C4-N9	5.89	132.12	127.40
32	W	974	A	C4-C5-C6	5.89	119.95	117.00
1	A	496	A	C4-C5-C6	5.89	119.95	117.00
1	A	678	A	N3-C4-N9	5.89	132.11	127.40
1	A	894	A	N9-C4-C5	5.89	108.16	105.80
1	A	1235	A	N3-C4-N9	5.89	132.11	127.40
1	A	1631	A	N3-C4-N9	5.89	132.11	127.40
1	A	1745	A	N3-C4-N9	5.89	132.11	127.40
1	A	2317	A	N3-C4-N9	5.89	132.12	127.40
1	A	2704	A	N3-C4-N9	5.89	132.11	127.40
1	A	2893	A	C8-N9-C4	5.89	108.16	105.80
32	W	737	A	N9-C4-C5	5.89	108.16	105.80
32	W	1257	A	N3-C4-N9	5.89	132.12	127.40
32	W	1419	A	C8-N9-C4	5.89	108.16	105.80
1	A	364	A	N3-C4-N9	5.89	132.11	127.40
1	A	575	A	C8-N9-C4	5.89	108.16	105.80
1	A	618	A	C4-C5-N7	-5.89	107.75	110.70
1	A	2740	A	N3-C4-N9	5.89	132.11	127.40
32	W	62	A	C4-C5-C6	5.89	119.94	117.00
32	W	371	A	C4-C5-C6	5.89	119.95	117.00
32	W	459	A	N3-C4-N9	5.89	132.11	127.40
52	z	41	A	C8-N9-C4	5.89	108.16	105.80
1	A	459	A	N3-C4-N9	5.89	132.11	127.40
1	A	1291	A	N3-C4-N9	5.89	132.11	127.40
1	A	1432	A	C4-C5-C6	5.89	119.94	117.00
1	A	1520	A	C4-C5-C6	5.89	119.94	117.00
1	A	1818	A	N3-C4-N9	5.89	132.11	127.40
1	A	2317	A	C4-C5-N7	-5.89	107.75	110.70
1	A	2330	A	C4-C5-C6	5.89	119.94	117.00
1	A	2447	A	C4-C5-C6	5.89	119.94	117.00
1	A	2593	A	C4-C5-C6	5.89	119.94	117.00
32	W	504	A	N3-C4-N9	5.89	132.11	127.40
32	W	811	A	C8-N9-C4	5.89	108.16	105.80
32	W	870	A	C4-C5-C6	5.89	119.94	117.00
32	W	1328	A	C4-C5-C6	5.89	119.94	117.00
1	A	477	A	N9-C4-C5	5.89	108.16	105.80
1	A	1097	A	N3-C4-N9	5.89	132.11	127.40
1	A	1113	A	N3-C4-N9	5.89	132.11	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1942	A	C4-C5-C6	5.89	119.94	117.00
32	W	266	A	C4-C5-C6	5.89	119.94	117.00
32	W	925	A	C8-N9-C4	5.89	108.16	105.80
1	A	13	A	N3-C4-N9	5.89	132.11	127.40
1	A	278	A	N3-C4-N9	5.89	132.11	127.40
1	A	279	A	N3-C4-N9	5.89	132.11	127.40
1	A	765	A	N9-C4-C5	5.89	108.16	105.80
1	A	1224	A	C8-N9-C4	5.89	108.15	105.80
1	A	1381	A	C4-C5-C6	5.89	119.94	117.00
1	A	1542	A	N3-C4-N9	5.89	132.11	127.40
1	A	1809	A	C4-C5-C6	5.89	119.94	117.00
1	A	1995	A	N3-C4-N9	5.89	132.11	127.40
1	A	2770	A	N3-C4-N9	5.89	132.11	127.40
32	W	883	A	C8-N9-C4	5.89	108.16	105.80
32	W	1178	A	N9-C4-C5	5.89	108.16	105.80
32	W	1510	A	N3-C4-N9	5.89	132.11	127.40
1	A	421	A	C4-C5-C6	5.88	119.94	117.00
1	A	548	A	C4-C5-C6	5.88	119.94	117.00
1	A	1131	A	C4-C5-C6	5.88	119.94	117.00
1	A	1928	A	C4-C5-C6	5.88	119.94	117.00
1	A	2658	A	N3-C4-N9	5.88	132.11	127.40
32	W	1283	A	N3-C4-N9	5.88	132.11	127.40
32	W	1342	A	N3-C4-N9	5.88	132.11	127.40
32	W	1509	A	C4-C5-C6	5.88	119.94	117.00
1	A	1221	A	C4-C5-C6	5.88	119.94	117.00
1	A	2030	A	C4-C5-C6	5.88	119.94	117.00
1	A	2787	A	C4-C5-C6	5.88	119.94	117.00
32	W	314	A	N3-C4-N9	5.88	132.11	127.40
1	A	236	A	N3-C4-N9	5.88	132.10	127.40
1	A	369	A	C4-C5-C6	5.88	119.94	117.00
1	A	547	A	C8-N9-C4	5.88	108.15	105.80
1	A	957	A	N3-C4-N9	5.88	132.10	127.40
1	A	1308	A	C8-N9-C4	5.88	108.15	105.80
1	A	1631	A	C4-C5-C6	5.88	119.94	117.00
32	W	457	A	N9-C4-C5	5.88	108.15	105.80
32	W	491	A	N3-C4-N9	5.88	132.10	127.40
32	W	604	A	N3-C4-N9	5.88	132.10	127.40
32	W	696	A	C8-N9-C4	5.88	108.15	105.80
32	W	828	A	N3-C4-N9	5.88	132.10	127.40
32	W	1031	A	C4-C5-C6	5.88	119.94	117.00
32	W	1259	A	C8-N9-C4	5.88	108.15	105.80
1	A	1533	A	N3-C4-N9	5.88	132.10	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2782	A	C4-C5-C6	5.88	119.94	117.00
32	W	423	A	N3-C4-N9	5.88	132.10	127.40
1	A	13	A	C4-C5-C6	5.88	119.94	117.00
1	A	28	A	N3-C4-N9	5.88	132.10	127.40
1	A	537	A	N3-C4-N9	5.88	132.10	127.40
1	A	1553	A	N3-C4-N9	5.88	132.10	127.40
1	A	2643	A	N3-C4-N9	5.88	132.10	127.40
1	A	2782	A	N9-C4-C5	5.88	108.15	105.80
1	A	2869	A	N3-C4-N9	5.88	132.10	127.40
32	W	460	A	C8-N9-C4	5.88	108.15	105.80
32	W	504	A	C8-N9-C4	5.88	108.15	105.80
32	W	870	A	C4-C5-N7	-5.88	107.76	110.70
1	A	173	A	N3-C4-N9	5.88	132.10	127.40
1	A	1055	A	N3-C4-N9	5.88	132.10	127.40
1	A	1115	A	C4-C5-C6	5.88	119.94	117.00
1	A	1210	A	N3-C4-N9	5.88	132.10	127.40
1	A	1553	A	C4-C5-C6	5.88	119.94	117.00
1	A	1797	A	C4-C5-C6	5.88	119.94	117.00
1	A	1895	A	C8-N9-C4	5.88	108.15	105.80
32	W	1006	A	C8-N9-C4	5.88	108.15	105.80
52	z	23	A	N3-C4-N9	5.88	132.10	127.40
1	A	1813	A	C8-N9-C4	5.88	108.15	105.80
1	A	139	A	N3-C4-N9	5.87	132.10	127.40
1	A	769	A	C4-C5-C6	5.87	119.94	117.00
1	A	1580	A	N3-C4-N9	5.87	132.10	127.40
1	A	1734	A	N3-C4-N9	5.87	132.10	127.40
1	A	2787	A	N3-C4-N9	5.87	132.10	127.40
1	A	2889	A	C4-C5-C6	5.87	119.94	117.00
2	B	43	A	N3-C4-N9	5.87	132.10	127.40
32	W	28	A	C4-C5-C6	5.87	119.94	117.00
32	W	460	A	C4-C5-C6	5.87	119.94	117.00
32	W	978	A	N3-C4-N9	5.87	132.10	127.40
32	W	1513	A	N3-C4-N9	5.87	132.10	127.40
1	A	179	A	N9-C4-C5	5.87	108.15	105.80
1	A	388	A	N3-C4-N9	5.87	132.10	127.40
1	A	1020	A	C8-N9-C4	5.87	108.15	105.80
1	A	1925	A	C8-N9-C4	5.87	108.15	105.80
1	A	2876	A	C8-N9-C4	5.87	108.15	105.80
32	W	477	A	N3-C4-N9	5.87	132.10	127.40
32	W	529	A	N3-C4-N9	5.87	132.10	127.40
32	W	644	A	C4-C5-C6	5.87	119.94	117.00
32	W	737	A	C4-C5-C6	5.87	119.94	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	886	A	C4-C5-C6	5.87	119.94	117.00
32	W	1200	A	C4-C5-C6	5.87	119.94	117.00
1	A	762	A	N3-C4-N9	5.87	132.10	127.40
1	A	1097	A	C4-C5-C6	5.87	119.94	117.00
1	A	1126	A	C4-C5-C6	5.87	119.94	117.00
1	A	2365	A	C8-N9-C4	5.87	108.15	105.80
32	W	506	A	C4-C5-N7	-5.87	107.77	110.70
32	W	762	A	N3-C4-N9	5.87	132.10	127.40
32	W	1327	A	C8-N9-C4	5.87	108.15	105.80
1	A	281	A	N9-C4-C5	5.87	108.15	105.80
1	A	388	A	C4-C5-C6	5.87	119.93	117.00
1	A	1243	A	N3-C4-N9	5.87	132.10	127.40
1	A	1287	A	C4-C5-N7	-5.87	107.77	110.70
1	A	1346	A	N3-C4-N9	5.87	132.09	127.40
1	A	1945	A	N3-C4-N9	5.87	132.09	127.40
1	A	2000	A	C4-C5-C6	5.87	119.94	117.00
1	A	2071	A	C4-C5-C6	5.87	119.93	117.00
1	A	2298	A	N3-C4-N9	5.87	132.09	127.40
1	A	2477	A	N3-C4-N9	5.87	132.09	127.40
1	A	2837	A	C4-C5-C6	5.87	119.93	117.00
32	W	321	A	C4-C5-C6	5.87	119.93	117.00
32	W	569	A	C4-C5-C6	5.87	119.94	117.00
32	W	684	A	N3-C4-N9	5.87	132.09	127.40
32	W	1490	A	C4-C5-C6	5.87	119.93	117.00
32	W	1509	A	N3-C4-N9	5.87	132.10	127.40
1	A	758	A	C4-C5-C6	5.87	119.93	117.00
1	A	1029	A	N3-C4-N9	5.87	132.09	127.40
1	A	1483	A	C8-N9-C4	5.87	108.15	105.80
32	W	1120	A	N3-C4-N9	5.87	132.09	127.40
32	W	1166	A	C8-N9-C4	5.87	108.15	105.80
1	A	10	A	N3-C4-N9	5.87	132.09	127.40
1	A	2062	A	N9-C4-C5	5.87	108.15	105.80
1	A	2777	A	C8-N9-C4	5.87	108.15	105.80
1	A	2845	A	N9-C4-C5	5.87	108.15	105.80
32	W	52	A	C4-C5-C6	5.87	119.93	117.00
32	W	62	A	N3-C4-N9	5.87	132.09	127.40
32	W	568	A	N3-C4-N9	5.87	132.09	127.40
32	W	796	A	C4-C5-C6	5.87	119.93	117.00
32	W	1077	A	C8-N9-C4	5.87	108.15	105.80
1	A	166	A	C8-N9-C4	5.86	108.15	105.80
1	A	216	A	C4-C5-C6	5.86	119.93	117.00
1	A	490	A	C8-N9-C4	5.86	108.14	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	786	A	N3-C4-N9	5.86	132.09	127.40
1	A	1305	A	N9-C4-C5	5.86	108.14	105.80
1	A	1381	A	N3-C4-N9	5.86	132.09	127.40
1	A	2059	A	C4-C5-C6	5.86	119.93	117.00
1	A	2668	A	C8-N9-C4	5.86	108.15	105.80
1	A	2875	A	N3-C4-N9	5.86	132.09	127.40
32	W	208	A	N9-C4-C5	5.86	108.14	105.80
32	W	796	A	N3-C4-N9	5.86	132.09	127.40
32	W	988	A	C8-N9-C4	5.86	108.14	105.80
1	A	110	A	N3-C4-N9	5.86	132.09	127.40
32	W	189	A	C4-C5-C6	5.86	119.93	117.00
32	W	258	A	C4-C5-C6	5.86	119.93	117.00
32	W	1024	A	N3-C4-N9	5.86	132.09	127.40
1	A	1743	A	N3-C4-N9	5.86	132.09	127.40
1	A	1816	A	C8-N9-C4	5.86	108.14	105.80
1	A	2034	A	C4-C5-C6	5.86	119.93	117.00
32	W	190	A	N3-C4-N9	5.86	132.09	127.40
32	W	452	A	C4-C5-N7	-5.86	107.77	110.70
32	W	460	A	N3-C4-N9	5.86	132.09	127.40
32	W	738	A	C4-C5-C6	5.86	119.93	117.00
32	W	768	A	C8-N9-C4	5.86	108.14	105.80
32	W	1502	A	C4-C5-N7	-5.86	107.77	110.70
32	W	1529	A	N3-C4-N9	5.86	132.09	127.40
1	A	247	A	C4-C5-C6	5.86	119.93	117.00
1	A	329	A	N3-C4-N9	5.86	132.09	127.40
1	A	993	A	N3-C4-N9	5.86	132.09	127.40
1	A	1520	A	C8-N9-C4	5.86	108.14	105.80
1	A	2834	A	N3-C4-N9	5.86	132.09	127.40
32	W	500	A	C4-C5-C6	5.86	119.93	117.00
32	W	923	A	C4-C5-C6	5.86	119.93	117.00
32	W	1320	A	N3-C4-N9	5.86	132.09	127.40
32	W	1333	A	C4-C5-N7	-5.86	107.77	110.70
32	W	1383	A	C8-N9-C4	5.86	108.14	105.80
1	A	1697	A	N3-C4-N9	5.86	132.09	127.40
2	B	114	A	C8-N9-C4	5.86	108.14	105.80
32	W	500	A	N9-C4-C5	5.86	108.14	105.80
32	W	685	A	N3-C4-N9	5.86	132.09	127.40
32	W	825	A	C4-C5-C6	5.86	119.93	117.00
32	W	1443	A	C4-C5-C6	5.86	119.93	117.00
1	A	501	A	C8-N9-C4	5.86	108.14	105.80
1	A	622	A	N9-C4-C5	5.86	108.14	105.80
1	A	677	A	N3-C4-N9	5.86	132.09	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1042	A	N3-C4-N9	5.86	132.09	127.40
1	A	1056	A	N9-C4-C5	5.86	108.14	105.80
1	A	1585	A	N3-C4-N9	5.86	132.08	127.40
1	A	2900	A	C4-C5-C6	5.86	119.93	117.00
2	B	44	A	N3-C4-N9	5.86	132.09	127.40
32	W	1031	A	N3-C4-N9	5.86	132.09	127.40
32	W	1355	A	N9-C4-C5	5.86	108.14	105.80
32	W	1419	A	N3-C4-N9	5.86	132.08	127.40
32	W	1463	A	N3-C4-N9	5.86	132.08	127.40
32	W	1479	A	N3-C4-N9	5.86	132.09	127.40
1	A	73	A	N3-C4-N9	5.85	132.08	127.40
1	A	418	A	C4-C5-C6	5.85	119.93	117.00
1	A	519	A	C4-C5-C6	5.85	119.93	117.00
32	W	118	A	C4-C5-C6	5.85	119.93	117.00
32	W	463	A	C4-C5-C6	5.85	119.93	117.00
32	W	679	A	C4-C5-C6	5.85	119.93	117.00
1	A	126	A	C8-N9-C4	5.85	108.14	105.80
1	A	268	A	C4-C5-C6	5.85	119.93	117.00
1	A	770	A	N3-C4-N9	5.85	132.08	127.40
1	A	774	A	C4-C5-C6	5.85	119.93	117.00
1	A	2315	A	C8-N9-C4	5.85	108.14	105.80
1	A	2505	A	C4-C5-C6	5.85	119.93	117.00
1	A	2767	A	C8-N9-C4	5.85	108.14	105.80
1	A	2767	A	N3-C4-N9	5.85	132.08	127.40
1	A	2851	A	C8-N9-C4	5.85	108.14	105.80
32	W	439	A	N9-C4-C5	5.85	108.14	105.80
32	W	1178	A	N3-C4-N9	5.85	132.08	127.40
32	W	1422	A	C8-N9-C4	5.85	108.14	105.80
1	A	428	A	N3-C4-N9	5.85	132.08	127.40
1	A	782	A	C4-C5-C6	5.85	119.92	117.00
1	A	1398	A	C5-C6-N1	5.85	120.62	117.70
32	W	422	A	C4-C5-C6	5.85	119.92	117.00
32	W	569	A	C8-N9-C4	5.85	108.14	105.80
32	W	672	A	N3-C4-N9	5.85	132.08	127.40
32	W	679	A	N3-C4-N9	5.85	132.08	127.40
1	A	84	A	C8-N9-C4	5.85	108.14	105.80
1	A	553	A	N3-C4-N9	5.85	132.08	127.40
1	A	770	A	C4-C5-C6	5.85	119.92	117.00
1	A	1197	A	N3-C4-N9	5.85	132.08	127.40
1	A	1540	A	C4-C5-C6	5.85	119.92	117.00
1	A	1746	A	N3-C4-N9	5.85	132.08	127.40
1	A	1760	A	N3-C4-N9	5.85	132.08	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2480	A	C4-C5-C6	5.85	119.92	117.00
1	A	2767	A	C4-C5-C6	5.85	119.92	117.00
1	A	2912	A	N3-C4-N9	5.85	132.08	127.40
32	W	236	A	C4-C5-C6	5.85	119.92	117.00
32	W	1048	A	N3-C4-N9	5.85	132.08	127.40
32	W	1320	A	C4-C5-C6	5.85	119.92	117.00
32	W	1434	A	C8-N9-C4	5.85	108.14	105.80
1	A	653	A	N3-C4-N9	5.85	132.08	127.40
1	A	908	A	N3-C4-N9	5.85	132.08	127.40
1	A	1020	A	N3-C4-N9	5.85	132.08	127.40
1	A	1197	A	C4-C5-C6	5.85	119.92	117.00
1	A	1516	A	N3-C4-N9	5.85	132.08	127.40
1	A	1918	A	C4-C5-N7	-5.85	107.78	110.70
1	A	2762	A	N3-C4-N9	5.85	132.08	127.40
1	A	2804	A	C4-C5-C6	5.85	119.92	117.00
1	A	2810	A	C4-C5-C6	5.85	119.92	117.00
2	B	64	A	C8-N9-C4	5.85	108.14	105.80
32	W	1090	A	C8-N9-C4	5.85	108.14	105.80
1	A	1142	A	N3-C4-N9	5.85	132.08	127.40
1	A	1326	A	C4-C5-C6	5.85	119.92	117.00
1	A	2295	A	N9-C4-C5	5.85	108.14	105.80
1	A	2297	A	N3-C4-N9	5.85	132.08	127.40
2	B	25	A	C4-C5-C6	5.85	119.92	117.00
1	A	154	A	N3-C4-N9	5.84	132.07	127.40
1	A	274	A	N3-C4-N9	5.84	132.07	127.40
1	A	1047	A	N3-C4-N9	5.84	132.08	127.40
1	A	1845	A	C8-N9-C4	5.84	108.14	105.80
1	A	1941	A	N9-C4-C5	5.84	108.14	105.80
1	A	1942	A	N3-C4-N9	5.84	132.08	127.40
1	A	1961	A	C8-N9-C4	5.84	108.14	105.80
32	W	456	A	N3-C4-N9	5.84	132.08	127.40
32	W	581	A	N3-C4-N9	5.84	132.07	127.40
32	W	1456	A	C4-C5-C6	5.84	119.92	117.00
52	z	44	A	N3-C4-N9	5.84	132.08	127.40
1	A	206	A	N3-C4-N9	5.84	132.07	127.40
1	A	339	A	N3-C4-N9	5.84	132.07	127.40
1	A	987	A	N3-C4-N9	5.84	132.07	127.40
1	A	1008	A	C4-C5-C6	5.84	119.92	117.00
1	A	1967	A	C4-C5-C6	5.84	119.92	117.00
32	W	210	A	N3-C4-N9	5.84	132.07	127.40
32	W	616	A	N3-C4-N9	5.84	132.07	127.40
32	W	824	A	N3-C4-N9	5.84	132.07	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	910	A	C4-C5-C6	5.84	119.92	117.00
32	W	1111	A	C4-C5-C6	5.84	119.92	117.00
32	W	1176	A	N3-C4-N9	5.84	132.07	127.40
32	W	1503	A	N3-C4-N9	5.84	132.07	127.40
1	A	894	A	N3-C4-N9	5.84	132.07	127.40
1	A	2464	A	N3-C4-N9	5.84	132.07	127.40
1	A	2606	A	C4-C5-N7	-5.84	107.78	110.70
32	W	67	A	N3-C4-N9	5.84	132.07	127.40
32	W	556	A	C4-C5-N7	-5.84	107.78	110.70
32	W	1355	A	C8-N9-C4	5.84	108.14	105.80
1	A	322	A	C4-C5-C6	5.84	119.92	117.00
1	A	479	A	N3-C4-N9	5.84	132.07	127.40
1	A	637	A	N3-C4-N9	5.84	132.07	127.40
1	A	829	A	N3-C4-N9	5.84	132.07	127.40
1	A	1142	A	C4-C5-C6	5.84	119.92	117.00
1	A	1312	A	N3-C4-N9	5.84	132.07	127.40
1	A	2060	A	N3-C4-N9	5.84	132.07	127.40
1	A	2447	A	N3-C4-N9	5.84	132.07	127.40
1	A	2601	A	C4-C5-C6	5.84	119.92	117.00
32	W	306	A	C4-C5-C6	5.84	119.92	117.00
32	W	886	A	N3-C4-N9	5.84	132.07	127.40
32	W	1213	A	N9-C4-C5	5.84	108.14	105.80
32	W	1261	A	N3-C4-N9	5.84	132.07	127.40
32	W	1270	A	C4-C5-C6	5.84	119.92	117.00
1	A	139	A	C8-N9-C4	5.84	108.14	105.80
1	A	2762	A	C4-C5-C6	5.84	119.92	117.00
32	W	386	A	C8-N9-C4	5.84	108.14	105.80
32	W	440	A	N3-C4-N9	5.84	132.07	127.40
32	W	474	A	N3-C4-N9	5.84	132.07	127.40
32	W	803	A	N3-C4-N9	5.84	132.07	127.40
1	A	28	A	C4-C5-C6	5.84	119.92	117.00
1	A	84	A	N3-C4-N9	5.84	132.07	127.40
1	A	229	A	N3-C4-N9	5.84	132.07	127.40
1	A	494	A	N9-C4-C5	5.84	108.13	105.80
1	A	618	A	C4-C5-C6	5.84	119.92	117.00
1	A	882	A	C8-N9-C4	5.84	108.13	105.80
1	A	1141	A	C4-C5-N7	-5.84	107.78	110.70
1	A	1679	A	C4-C5-C6	5.84	119.92	117.00
32	W	556	A	C8-N9-C4	5.84	108.13	105.80
32	W	947	A	N3-C4-N9	5.84	132.07	127.40
1	A	619	A	C8-N9-C4	5.83	108.13	105.80
1	A	922	A	N9-C4-C5	5.83	108.13	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1260	A	C4-C5-C6	5.83	119.92	117.00
1	A	835	A	N3-C4-N9	5.83	132.07	127.40
1	A	1116	A	N3-C4-N9	5.83	132.07	127.40
1	A	1194	A	C8-N9-C4	5.83	108.13	105.80
1	A	1831	A	C8-N9-C4	5.83	108.13	105.80
1	A	2629	A	N3-C4-N9	5.83	132.07	127.40
1	A	2908	A	C8-N9-C4	5.83	108.13	105.80
32	W	475	A	N3-C4-N9	5.83	132.07	127.40
32	W	791	A	C4-C5-C6	5.83	119.92	117.00
32	W	1257	A	C4-C5-C6	5.83	119.92	117.00
32	W	1260	A	N3-C4-N9	5.83	132.07	127.40
1	A	5	A	C4-C5-C6	5.83	119.92	117.00
1	A	150	A	C4-C5-C6	5.83	119.92	117.00
1	A	1335	A	C4-C5-C6	5.83	119.92	117.00
1	A	1465	A	C4-C5-C6	5.83	119.92	117.00
1	A	1465	A	N3-C4-N9	5.83	132.07	127.40
1	A	1699	A	C4-C5-C6	5.83	119.92	117.00
1	A	2047	A	C8-N9-C4	5.83	108.13	105.80
1	A	2091	A	N3-C4-N9	5.83	132.06	127.40
1	A	2276	A	C4-C5-C6	5.83	119.92	117.00
1	A	2390	A	C4-C5-C6	5.83	119.92	117.00
1	A	2902	A	N3-C4-N9	5.83	132.06	127.40
1	A	2907	A	C8-N9-C4	5.83	108.13	105.80
32	W	12	A	N3-C4-N9	5.83	132.06	127.40
32	W	120	A	N3-C4-N9	5.83	132.07	127.40
32	W	178	A	C4-C5-C6	5.83	119.92	117.00
32	W	1092	A	C8-N9-C4	5.83	108.13	105.80
1	A	374	A	C4-C5-N7	-5.83	107.78	110.70
1	A	1287	A	C4-C5-C6	5.83	119.92	117.00
32	W	228	A	N3-C4-N9	5.83	132.06	127.40
32	W	592	A	N3-C4-N9	5.83	132.06	127.40
32	W	1115	A	N3-C4-N9	5.83	132.06	127.40
32	W	1512	A	C4-C5-C6	5.83	119.92	117.00
32	W	1513	A	C4-C5-C6	5.83	119.92	117.00
1	A	449	A	N3-C4-N9	5.83	132.06	127.40
1	A	870	A	C8-N9-C4	5.83	108.13	105.80
1	A	2390	A	N3-C4-N9	5.83	132.06	127.40
32	W	202	A	C4-C5-C6	5.83	119.91	117.00
32	W	367	A	C4-C5-C6	5.83	119.91	117.00
32	W	506	A	N9-C4-C5	5.83	108.13	105.80
32	W	569	A	N3-C4-N9	5.83	132.06	127.40
32	W	730	A	C8-N9-C4	5.83	108.13	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	801	A	N3-C4-N9	5.83	132.06	127.40
32	W	1197	A	N3-C4-N9	5.83	132.06	127.40
32	W	1466	A	N3-C4-N9	5.83	132.06	127.40
1	A	337	A	N3-C4-N9	5.83	132.06	127.40
1	A	388	A	C8-N9-C4	5.83	108.13	105.80
1	A	1027	A	N3-C4-N9	5.83	132.06	127.40
1	A	2049	A	C4-C5-N7	-5.83	107.79	110.70
1	A	1008	A	N3-C4-N9	5.83	132.06	127.40
1	A	1335	A	N3-C4-N9	5.83	132.06	127.40
1	A	1699	A	N3-C4-N9	5.83	132.06	127.40
1	A	1815	A	C4-C5-C6	5.83	119.91	117.00
32	W	541	A	N3-C4-N9	5.83	132.06	127.40
32	W	777	A	N3-C4-N9	5.83	132.06	127.40
32	W	1111	A	N3-C4-N9	5.83	132.06	127.40
1	A	220	A	N3-C4-N9	5.82	132.06	127.40
1	A	957	A	N9-C4-C5	5.82	108.13	105.80
1	A	1034	A	C8-N9-C4	5.82	108.13	105.80
1	A	1533	A	C8-N9-C4	5.82	108.13	105.80
1	A	1802	A	C4-C5-C6	5.82	119.91	117.00
1	A	2000	A	N3-C4-N9	5.82	132.06	127.40
1	A	2447	A	C4-C5-N7	-5.82	107.79	110.70
1	A	2902	A	C4-C5-C6	5.82	119.91	117.00
1	A	2923	A	C8-N9-C4	5.82	108.13	105.80
32	W	1342	A	C4-C5-C6	5.82	119.91	117.00
1	A	765	A	C4-C5-N7	-5.82	107.79	110.70
1	A	1593	A	C4-C5-C6	5.82	119.91	117.00
1	A	2673	A	C4-C5-C6	5.82	119.91	117.00
2	B	51	A	C8-N9-C4	5.82	108.13	105.80
2	B	105	A	N3-C4-N9	5.82	132.06	127.40
32	W	117	A	C4-C5-C6	5.82	119.91	117.00
32	W	684	A	C4-C5-C6	5.82	119.91	117.00
32	W	899	A	C4-C5-N7	-5.82	107.79	110.70
1	A	64	A	C4-C5-C6	5.82	119.91	117.00
1	A	124	A	N3-C4-N9	5.82	132.06	127.40
1	A	1308	A	N3-C4-N9	5.82	132.06	127.40
1	A	1517	A	C4-C5-C6	5.82	119.91	117.00
1	A	1815	A	C8-N9-C4	5.82	108.13	105.80
32	W	496	A	C8-N9-C4	5.82	108.13	105.80
32	W	500	A	C4-C5-N7	-5.82	107.79	110.70
32	W	581	A	C4-C5-C6	5.82	119.91	117.00
32	W	862	A	C8-N9-C4	5.82	108.13	105.80
1	A	156	A	C8-N9-C4	5.82	108.13	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	236	A	C4-C5-C6	5.82	119.91	117.00
1	A	342	A	N3-C4-N9	5.82	132.06	127.40
1	A	1066	A	N3-C4-N9	5.82	132.06	127.40
1	A	1423	A	N3-C4-N9	5.82	132.06	127.40
32	W	456	A	C4-C5-C6	5.82	119.91	117.00
32	W	690	A	N9-C4-C5	5.82	108.13	105.80
1	A	140	A	C8-N9-C4	5.82	108.13	105.80
1	A	178	A	N9-C4-C5	5.82	108.13	105.80
1	A	183	A	C8-N9-C4	5.82	108.13	105.80
1	A	222	A	N3-C4-N9	5.82	132.05	127.40
1	A	302	A	C4-C5-C6	5.82	119.91	117.00
1	A	584	A	C8-N9-C4	5.82	108.13	105.80
1	A	1850	A	N3-C4-N9	5.82	132.06	127.40
1	A	2923	A	N3-C4-N9	5.82	132.06	127.40
32	W	371	A	N3-C4-N9	5.82	132.05	127.40
32	W	978	A	N9-C4-C5	5.82	108.13	105.80
1	A	561	A	N3-C4-N9	5.82	132.05	127.40
1	A	1026	A	C4-C5-C6	5.82	119.91	117.00
1	A	1141	A	C8-N9-C4	5.82	108.13	105.80
1	A	1499	A	N3-C4-N9	5.82	132.05	127.40
1	A	1677	A	N3-C4-N9	5.82	132.05	127.40
1	A	2317	A	C8-N9-C4	5.82	108.13	105.80
1	A	2440	A	N3-C4-N9	5.82	132.05	127.40
1	A	2590	A	N3-C4-N9	5.82	132.05	127.40
32	W	52	A	N3-C4-N9	5.82	132.05	127.40
32	W	225	A	N3-C4-N9	5.82	132.05	127.40
32	W	228	A	C8-N9-C4	5.82	108.13	105.80
32	W	463	A	N3-C4-N9	5.82	132.05	127.40
32	W	704	A	N3-C4-N9	5.82	132.05	127.40
1	A	44	A	N9-C4-C5	5.81	108.12	105.80
1	A	94	A	N3-C4-N9	5.81	132.05	127.40
1	A	333	A	C4-C5-C6	5.81	119.91	117.00
1	A	1003	A	C8-N9-C4	5.81	108.13	105.80
1	A	1722	A	N3-C4-N9	5.81	132.05	127.40
1	A	2683	A	C4-C5-C6	5.81	119.91	117.00
1	A	2779	A	N3-C4-N9	5.81	132.05	127.40
32	W	730	A	N3-C4-N9	5.81	132.05	127.40
32	W	1225	A	C4-C5-C6	5.81	119.91	117.00
32	W	1529	A	C8-N9-C4	5.81	108.12	105.80
1	A	314	A	N3-C4-N9	5.81	132.05	127.40
1	A	436	A	C4-C5-C6	5.81	119.91	117.00
1	A	1034	A	N3-C4-N9	5.81	132.05	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1244	A	N3-C4-N9	5.81	132.05	127.40
1	A	1723	A	N3-C4-N9	5.81	132.05	127.40
32	W	117	A	N3-C4-N9	5.81	132.05	127.40
32	W	501	A	C4-C5-C6	5.81	119.91	117.00
32	W	651	A	N3-C4-N9	5.81	132.05	127.40
1	A	619	A	N3-C4-N9	5.81	132.05	127.40
1	A	835	A	C8-N9-C4	5.81	108.12	105.80
1	A	1325	A	C4-C5-C6	5.81	119.91	117.00
32	W	838	A	C8-N9-C4	5.81	108.12	105.80
1	A	412	A	C8-N9-C4	5.81	108.12	105.80
1	A	476	A	N9-C4-C5	5.81	108.12	105.80
1	A	553	A	C4-C5-C6	5.81	119.91	117.00
1	A	821	A	C8-N9-C4	5.81	108.12	105.80
1	A	1722	A	C4-C5-C6	5.81	119.90	117.00
1	A	1802	A	N3-C4-N9	5.81	132.05	127.40
1	A	1989	A	N3-C4-N9	5.81	132.05	127.40
32	W	323	A	N3-C4-N9	5.81	132.05	127.40
32	W	1128	A	N3-C4-N9	5.81	132.05	127.40
1	A	1221	A	N3-C4-N9	5.81	132.04	127.40
1	A	1308	A	C4-C5-C6	5.81	119.90	117.00
1	A	2042	A	C4-C5-C6	5.81	119.90	117.00
1	A	2498	A	C8-N9-C4	5.81	108.12	105.80
32	W	611	A	C8-N9-C4	5.81	108.12	105.80
32	W	777	A	C8-N9-C4	5.81	108.12	105.80
32	W	824	A	C8-N9-C4	5.81	108.12	105.80
32	W	1407	A	C8-N9-C4	5.81	108.12	105.80
32	W	1443	A	C4-C5-N7	-5.81	107.80	110.70
32	W	1529	A	C4-C5-C6	5.81	119.90	117.00
1	A	144	A	C8-N9-C4	5.81	108.12	105.80
1	A	1210	A	C4-C5-N7	-5.81	107.80	110.70
32	W	1502	A	N9-C4-C5	5.81	108.12	105.80
1	A	1141	A	N3-C4-N9	5.80	132.04	127.40
1	A	1417	A	C8-N9-C4	5.80	108.12	105.80
1	A	1417	A	N9-C4-C5	5.80	108.12	105.80
1	A	1555	A	C8-N9-C4	5.80	108.12	105.80
1	A	1981	A	N3-C4-N9	5.80	132.04	127.40
1	A	2526	A	N3-C4-N9	5.80	132.04	127.40
32	W	725	A	N9-C4-C5	5.80	108.12	105.80
32	W	1056	A	C8-N9-C4	5.80	108.12	105.80
32	W	1180	A	N3-C4-N9	5.80	132.04	127.40
1	A	1302	A	C4-C5-N7	-5.80	107.80	110.70
1	A	1583	A	N3-C4-N9	5.80	132.04	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	899	A	C8-N9-C4	5.80	108.12	105.80
32	W	1185	A	N3-C4-N9	5.80	132.04	127.40
1	A	699	A	N3-C4-N9	5.80	132.04	127.40
1	A	876	A	C8-N9-C4	5.80	108.12	105.80
1	A	1405	A	C8-N9-C4	5.80	108.12	105.80
1	A	2030	A	N9-C4-C5	5.80	108.12	105.80
1	A	2362	A	N3-C4-N9	5.80	132.04	127.40
1	A	2876	A	N3-C4-N9	5.80	132.04	127.40
32	W	485	A	C4-C5-C6	5.80	119.90	117.00
32	W	737	A	C4-C5-N7	-5.80	107.80	110.70
32	W	816	A	C4-C5-C6	5.80	119.90	117.00
32	W	1298	A	C8-N9-C4	5.80	108.12	105.80
1	A	199	A	C4-C5-C6	5.80	119.90	117.00
1	A	830	A	N3-C4-N9	5.80	132.04	127.40
1	A	1724	A	N3-C4-N9	5.80	132.04	127.40
32	W	12	A	C4-C5-C6	5.80	119.90	117.00
32	W	53	A	N3-C4-N9	5.80	132.04	127.40
32	W	189	A	N9-C4-C5	5.80	108.12	105.80
32	W	611	A	N3-C4-N9	5.80	132.04	127.40
32	W	828	A	C4-C5-C6	5.80	119.90	117.00
1	A	1189	A	C4-C5-C6	5.80	119.90	117.00
1	A	1727	A	C8-N9-C4	5.80	108.12	105.80
1	A	2845	A	N3-C4-N9	5.80	132.04	127.40
32	W	485	A	N3-C4-N9	5.80	132.04	127.40
32	W	1115	A	C4-C5-N7	-5.80	107.80	110.70
1	A	667	A	C4-C5-N7	-5.80	107.80	110.70
1	A	1230	A	N3-C4-N9	5.80	132.04	127.40
1	A	1592	A	N3-C4-N9	5.80	132.04	127.40
1	A	1593	A	N3-C4-N9	5.80	132.04	127.40
1	A	1791	A	N3-C4-N9	5.80	132.04	127.40
1	A	2463	A	N9-C4-C5	5.80	108.12	105.80
1	A	2594	A	N3-C4-N9	5.80	132.04	127.40
1	A	2782	A	C4-C5-N7	-5.80	107.80	110.70
32	W	605	A	C8-N9-C4	5.80	108.12	105.80
32	W	923	A	C8-N9-C4	5.80	108.12	105.80
32	W	959	A	C8-N9-C4	5.80	108.12	105.80
32	W	968	A	N3-C4-N9	5.80	132.04	127.40
1	A	746	A	N3-C4-N9	5.79	132.04	127.40
1	A	1084	A	C8-N9-C4	5.79	108.12	105.80
1	A	2860	A	C4-C5-C6	5.79	119.90	117.00
32	W	81	A	C8-N9-C4	5.79	108.12	105.80
32	W	1178	A	C4-C5-N7	-5.79	107.80	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	727	A	N3-C4-N9	5.79	132.03	127.40
1	A	978	A	N3-C4-N9	5.79	132.03	127.40
1	A	1036	A	N3-C4-N9	5.79	132.03	127.40
1	A	1123	A	N3-C4-N9	5.79	132.03	127.40
1	A	1534	A	N3-C4-N9	5.79	132.03	127.40
1	A	1838	A	N3-C4-N9	5.79	132.03	127.40
32	W	768	A	C4-C5-N7	-5.79	107.80	110.70
1	A	302	A	N9-C4-C5	5.79	108.12	105.80
1	A	553	A	C8-N9-C4	5.79	108.12	105.80
1	A	723	A	N9-C4-C5	5.79	108.12	105.80
1	A	769	A	C8-N9-C4	5.79	108.12	105.80
1	A	965	A	N3-C4-N9	5.79	132.03	127.40
1	A	1046	A	C4-C5-C6	5.79	119.89	117.00
1	A	1224	A	N3-C4-N9	5.79	132.03	127.40
1	A	1540	A	N3-C4-N9	5.79	132.03	127.40
1	A	1648	A	C4-C5-C6	5.79	119.90	117.00
1	A	1948	A	C8-N9-C4	5.79	108.12	105.80
1	A	2417	A	N3-C4-N9	5.79	132.03	127.40
1	A	2571	A	N3-C4-N9	5.79	132.03	127.40
1	A	2686	A	C4-C5-C6	5.79	119.89	117.00
2	B	76	A	C8-N9-C4	5.79	108.12	105.80
32	W	62	A	C8-N9-C4	5.79	108.12	105.80
32	W	361	A	C8-N9-C4	5.79	108.12	105.80
32	W	669	A	N3-C4-N9	5.79	132.03	127.40
32	W	791	A	N3-C4-N9	5.79	132.03	127.40
32	W	985	A	C8-N9-C4	5.79	108.12	105.80
1	A	125	A	N9-C4-C5	5.79	108.12	105.80
1	A	659	A	C8-N9-C4	5.79	108.12	105.80
1	A	821	A	C4-C5-C6	5.79	119.89	117.00
1	A	828	A	C4-C5-C6	5.79	119.89	117.00
1	A	1406	A	C8-N9-C4	5.79	108.12	105.80
1	A	2507	A	C8-N9-C4	5.79	108.12	105.80
32	W	386	A	N3-C4-N9	5.79	132.03	127.40
32	W	1017	A	C4-C5-C6	5.79	119.89	117.00
1	A	117	A	N9-C4-C5	5.79	108.12	105.80
1	A	421	A	N3-C4-N9	5.79	132.03	127.40
1	A	504	A	N9-C4-C5	5.79	108.11	105.80
1	A	1123	A	C8-N9-C4	5.79	108.12	105.80
1	A	1179	A	N3-C4-N9	5.79	132.03	127.40
1	A	2383	A	C4-C5-N7	-5.79	107.81	110.70
32	W	129	A	C8-N9-C4	5.79	108.11	105.80
32	W	618	A	N3-C4-N9	5.79	132.03	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	975	A	C8-N9-C4	5.79	108.11	105.80
32	W	1056	A	N3-C4-N9	5.79	132.03	127.40
32	W	1248	A	N3-C4-N9	5.79	132.03	127.40
32	W	1342	A	C8-N9-C4	5.79	108.11	105.80
32	W	1443	A	C8-N9-C4	5.79	108.11	105.80
32	W	1466	A	C4-C5-C6	5.79	119.89	117.00
1	A	389	A	C8-N9-C4	5.79	108.11	105.80
1	A	1046	A	N3-C4-N9	5.79	132.03	127.40
32	W	440	A	C4-C5-C6	5.79	119.89	117.00
32	W	452	A	N3-C4-N9	5.79	132.03	127.40
32	W	870	A	N3-C4-N9	5.79	132.03	127.40
32	W	1372	A	C4-C5-N7	-5.79	107.81	110.70
1	A	690	A	C8-N9-C4	5.79	108.11	105.80
1	A	736	A	C5-C6-N1	5.79	120.59	117.70
1	A	1025	A	C4-C5-N7	-5.79	107.81	110.70
1	A	1323	A	N3-C4-N9	5.79	132.03	127.40
1	A	1713	A	C8-N9-C4	5.79	108.11	105.80
1	A	2779	A	N9-C4-C5	5.79	108.11	105.80
2	B	97	A	C8-N9-C4	5.79	108.11	105.80
32	W	107	A	C8-N9-C4	5.79	108.11	105.80
32	W	1254	A	C8-N9-C4	5.79	108.11	105.80
32	W	1327	A	C4-C5-C6	5.79	119.89	117.00
1	A	176	A	C4-C5-C6	5.78	119.89	117.00
1	A	229	A	C8-N9-C4	5.78	108.11	105.80
1	A	325	A	N3-C4-N9	5.78	132.03	127.40
1	A	1130	A	N3-C4-N9	5.78	132.03	127.40
1	A	2091	A	C4-C5-C6	5.78	119.89	117.00
1	A	2593	A	N9-C4-C5	5.78	108.11	105.80
1	A	2740	A	C8-N9-C4	5.78	108.11	105.80
2	B	55	A	N3-C4-N9	5.78	132.03	127.40
32	W	266	A	N9-C4-C5	5.78	108.11	105.80
32	W	1102	A	N3-C4-N9	5.78	132.03	127.40
1	A	210	A	N3-C4-N9	5.78	132.03	127.40
1	A	1445	A	C8-N9-C4	5.78	108.11	105.80
1	A	1965	A	N3-C4-N9	5.78	132.03	127.40
1	A	2302	A	C8-N9-C4	5.78	108.11	105.80
32	W	10	A	C8-N9-C4	5.78	108.11	105.80
32	W	228	A	C4-C5-C6	5.78	119.89	117.00
32	W	1541	A	N3-C4-N9	5.78	132.03	127.40
1	A	64	A	C8-N9-C4	5.78	108.11	105.80
1	A	108	A	C8-N9-C4	5.78	108.11	105.80
1	A	202	A	C4-C5-C6	5.78	119.89	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1305	A	C8-N9-C4	5.78	108.11	105.80
1	A	1788	A	C8-N9-C4	5.78	108.11	105.80
1	A	1957	A	N9-C4-C5	5.78	108.11	105.80
1	A	2330	A	C4-C5-N7	-5.78	107.81	110.70
1	A	2594	A	C4-C5-N7	-5.78	107.81	110.70
1	A	2805	A	C4-C5-N7	-5.78	107.81	110.70
32	W	757	A	N3-C4-N9	5.78	132.02	127.40
32	W	1103	A	N3-C4-N9	5.78	132.02	127.40
32	W	1386	A	C8-N9-C4	5.78	108.11	105.80
1	A	222	A	C4-C5-C6	5.78	119.89	117.00
1	A	2479	A	N3-C4-N9	5.78	132.02	127.40
32	W	190	A	C8-N9-C4	5.78	108.11	105.80
32	W	1502	A	N3-C4-N9	5.78	132.02	127.40
1	A	117	A	N3-C4-N9	5.78	132.02	127.40
1	A	125	A	C4-C5-N7	-5.78	107.81	110.70
1	A	247	A	N3-C4-N9	5.78	132.02	127.40
1	A	418	A	N3-C4-N9	5.78	132.02	127.40
1	A	692	A	C8-N9-C4	5.78	108.11	105.80
1	A	763	A	C8-N9-C4	5.78	108.11	105.80
1	A	1734	A	C8-N9-C4	5.78	108.11	105.80
1	A	2594	A	C8-N9-C4	5.78	108.11	105.80
32	W	879	A	C8-N9-C4	5.78	108.11	105.80
32	W	1271	A	N3-C4-N9	5.78	132.02	127.40
32	W	1328	A	C8-N9-C4	5.78	108.11	105.80
1	A	49	A	N9-C4-C5	5.78	108.11	105.80
1	A	183	A	N9-C4-C5	5.78	108.11	105.80
1	A	224	A	C8-N9-C4	5.78	108.11	105.80
1	A	274	A	C8-N9-C4	5.78	108.11	105.80
1	A	436	A	N3-C4-N9	5.78	132.02	127.40
1	A	504	A	C8-N9-C4	5.78	108.11	105.80
1	A	507	A	C8-N9-C4	5.78	108.11	105.80
1	A	572	A	C4-C5-C6	5.78	119.89	117.00
1	A	1020	A	C4-C5-C6	5.78	119.89	117.00
1	A	1347	A	C4-C5-N7	-5.78	107.81	110.70
32	W	204	A	N3-C4-N9	5.78	132.02	127.40
32	W	290	A	N3-C4-N9	5.78	132.02	127.40
32	W	329	A	N3-C4-N9	5.78	132.02	127.40
32	W	1266	A	N3-C4-N9	5.78	132.02	127.40
32	W	1419	A	C4-C5-C6	5.78	119.89	117.00
32	W	1443	A	N9-C4-C5	5.78	108.11	105.80
1	A	102	A	C8-N9-C4	5.77	108.11	105.80
1	A	475	A	C8-N9-C4	5.77	108.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1967	A	N3-C4-N9	5.77	132.02	127.40
1	A	2307	A	N3-C4-N9	5.77	132.02	127.40
1	A	2480	A	N3-C4-N9	5.77	132.02	127.40
32	W	519	A	N3-C4-N9	5.77	132.02	127.40
32	W	928	A	N3-C4-N9	5.77	132.02	127.40
1	A	179	A	N3-C4-N9	5.77	132.02	127.40
1	A	519	A	N3-C4-N9	5.77	132.02	127.40
1	A	847	A	C8-N9-C4	5.77	108.11	105.80
1	A	893	A	N3-C4-N9	5.77	132.02	127.40
1	A	2080	A	C8-N9-C4	5.77	108.11	105.80
32	W	1022	A	C8-N9-C4	5.77	108.11	105.80
32	W	1200	A	N3-C4-N9	5.77	132.02	127.40
32	W	1205	A	N3-C4-N9	5.77	132.02	127.40
32	W	251	A	N3-C4-N9	5.77	132.02	127.40
1	A	475	A	N3-C4-N9	5.77	132.01	127.40
1	A	561	A	C4-C5-C6	5.77	119.89	117.00
1	A	1314	A	C8-N9-C4	5.77	108.11	105.80
1	A	1942	A	C8-N9-C4	5.77	108.11	105.80
2	B	113	A	N3-C4-N9	5.77	132.02	127.40
32	W	53	A	C8-N9-C4	5.77	108.11	105.80
32	W	240	A	N3-C4-N9	5.77	132.01	127.40
32	W	664	A	N3-C4-N9	5.77	132.01	127.40
32	W	919	A	C4-C5-C6	5.77	119.89	117.00
32	W	1236	A	N9-C4-C5	5.77	108.11	105.80
32	W	1386	A	C4-C5-C6	5.77	119.88	117.00
1	A	333	A	N3-C4-N9	5.77	132.01	127.40
1	A	1021	A	N3-C4-N9	5.77	132.01	127.40
1	A	1313	A	C8-N9-C4	5.77	108.11	105.80
1	A	1648	A	C8-N9-C4	5.77	108.11	105.80
32	W	1328	A	N3-C4-N9	5.77	132.01	127.40
32	W	1407	A	C4-C5-C6	5.77	119.88	117.00
32	W	1488	A	N3-C4-N9	5.77	132.01	127.40
1	A	2303	A	N3-C4-N9	5.77	132.01	127.40
32	W	776	A	N3-C4-N9	5.77	132.01	127.40
32	W	1185	A	C8-N9-C4	5.77	108.11	105.80
1	A	389	A	C4-C5-C6	5.76	119.88	117.00
1	A	1025	A	N9-C4-C5	5.76	108.11	105.80
1	A	1074	A	C8-N9-C4	5.76	108.11	105.80
1	A	1412	A	C8-N9-C4	5.76	108.11	105.80
1	A	1948	A	N3-C4-N9	5.76	132.01	127.40
1	A	2315	A	C4-C5-C6	5.76	119.88	117.00
1	A	2547	A	C8-N9-C4	5.76	108.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2837	A	N3-C4-N9	5.76	132.01	127.40
2	B	37	A	N3-C4-N9	5.76	132.01	127.40
32	W	281	A	N3-C4-N9	5.76	132.01	127.40
32	W	491	A	C8-N9-C4	5.76	108.11	105.80
32	W	762	A	C8-N9-C4	5.76	108.11	105.80
32	W	1028	A	N3-C4-N9	5.76	132.01	127.40
32	W	1405	A	C8-N9-C4	5.76	108.11	105.80
32	W	1513	A	C8-N9-C4	5.76	108.11	105.80
1	A	173	A	C8-N9-C4	5.76	108.11	105.80
1	A	1014	A	N3-C4-N9	5.76	132.01	127.40
1	A	1025	A	N3-C4-N9	5.76	132.01	127.40
1	A	1026	A	N3-C4-N9	5.76	132.01	127.40
1	A	1119	A	C8-N9-C4	5.76	108.11	105.80
1	A	2018	A	N3-C4-N9	5.76	132.01	127.40
1	A	2295	A	C4-C5-C6	5.76	119.88	117.00
1	A	2340	A	N3-C4-N9	5.76	132.01	127.40
32	W	419	A	C8-N9-C4	5.76	108.11	105.80
32	W	582	A	N3-C4-N9	5.76	132.01	127.40
1	A	702	A	N3-C4-N9	5.76	132.01	127.40
1	A	1284	A	C8-N9-C4	5.76	108.11	105.80
1	A	1809	A	C4-C5-N7	-5.76	107.82	110.70
1	A	2296	A	C4-C5-C6	5.76	119.88	117.00
1	A	2362	A	C4-C5-C6	5.76	119.88	117.00
1	A	2673	A	N3-C4-N9	5.76	132.01	127.40
32	W	618	A	C8-N9-C4	5.76	108.11	105.80
32	W	671	A	C8-N9-C4	5.76	108.11	105.80
32	W	910	A	N3-C4-N9	5.76	132.01	127.40
32	W	974	A	C4-C5-N7	-5.76	107.82	110.70
32	W	1271	A	C4-C5-C6	5.76	119.88	117.00
1	A	436	A	C8-N9-C4	5.76	108.10	105.80
1	A	1046	A	C4-C5-N7	-5.76	107.82	110.70
1	A	1277	A	N3-C4-N9	5.76	132.01	127.40
1	A	1287	A	N3-C4-N9	5.76	132.01	127.40
1	A	1340	A	N9-C4-C5	5.76	108.10	105.80
1	A	1375	A	C8-N9-C4	5.76	108.10	105.80
32	W	452	A	N9-C4-C5	5.76	108.10	105.80
1	A	6	A	C8-N9-C4	5.76	108.10	105.80
1	A	952	A	C8-N9-C4	5.76	108.10	105.80
1	A	1601	A	N3-C4-N9	5.76	132.01	127.40
1	A	2919	A	C8-N9-C4	5.76	108.10	105.80
2	B	27	A	C4-C5-C6	5.76	119.88	117.00
32	W	969	A	N3-C4-N9	5.76	132.01	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	41	A	C8-N9-C4	5.76	108.10	105.80
1	A	84	A	C4-C5-C6	5.76	119.88	117.00
1	A	166	A	C4-C5-C6	5.76	119.88	117.00
1	A	231	A	C4-C5-N7	-5.76	107.82	110.70
1	A	260	A	C8-N9-C4	5.76	108.10	105.80
1	A	582	A	N3-C4-N9	5.76	132.00	127.40
1	A	740	A	N3-C4-N9	5.76	132.00	127.40
1	A	1149	A	N3-C4-N9	5.76	132.00	127.40
1	A	1412	A	N3-C4-N9	5.76	132.01	127.40
1	A	2661	A	N3-C4-N9	5.76	132.00	127.40
1	A	2778	A	N9-C4-C5	5.76	108.10	105.80
1	A	2810	A	N3-C4-N9	5.76	132.00	127.40
32	W	236	A	N3-C4-N9	5.76	132.00	127.40
32	W	724	A	N3-C4-N9	5.76	132.01	127.40
32	W	925	A	N3-C4-N9	5.76	132.00	127.40
32	W	1248	A	C8-N9-C4	5.76	108.10	105.80
1	A	225	A	C4-C5-C6	5.75	119.88	117.00
1	A	999	A	C8-N9-C4	5.75	108.10	105.80
1	A	1202	A	N3-C4-N9	5.75	132.00	127.40
1	A	2276	A	C8-N9-C4	5.75	108.10	105.80
1	A	2835	A	C4-C5-C6	5.75	119.88	117.00
1	A	216	A	C8-N9-C4	5.75	108.10	105.80
1	A	314	A	C4-C5-C6	5.75	119.88	117.00
1	A	1078	A	C4-C5-C6	5.75	119.88	117.00
1	A	1078	A	N9-C4-C5	5.75	108.10	105.80
1	A	1464	A	C8-N9-C4	5.75	108.10	105.80
1	A	2307	A	C4-C5-N7	-5.75	107.82	110.70
1	A	2455	A	N3-C4-N9	5.75	132.00	127.40
32	W	107	A	N3-C4-N9	5.75	132.00	127.40
32	W	150	A	N9-C4-C5	5.75	108.10	105.80
32	W	281	A	C8-N9-C4	5.75	108.10	105.80
32	W	306	A	N3-C4-N9	5.75	132.00	127.40
32	W	677	A	C8-N9-C4	5.75	108.10	105.80
32	W	703	A	C4-C5-C6	5.75	119.88	117.00
1	A	67	A	C4-C5-N7	-5.75	107.83	110.70
1	A	345	A	N3-C4-N9	5.75	132.00	127.40
1	A	622	A	C4-C5-N7	-5.75	107.83	110.70
1	A	646	A	C4-C5-C6	5.75	119.88	117.00
1	A	1072	A	C4-C5-C6	5.75	119.88	117.00
1	A	1084	A	C4-C5-C6	5.75	119.88	117.00
1	A	1998	A	C8-N9-C4	5.75	108.10	105.80
1	A	2477	A	C8-N9-C4	5.75	108.10	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	211	A	C8-N9-C4	5.75	108.10	105.80
32	W	405	A	C5-C6-N1	5.75	120.58	117.70
32	W	777	A	C4-C5-C6	5.75	119.88	117.00
32	W	1140	A	N3-C4-N9	5.75	132.00	127.40
1	A	1517	A	N3-C4-N9	5.75	132.00	127.40
1	A	2447	A	C8-N9-C4	5.75	108.10	105.80
32	W	333	A	C8-N9-C4	5.75	108.10	105.80
1	A	957	A	C4-C5-N7	-5.75	107.83	110.70
1	A	1686	A	C4-C5-N7	-5.75	107.83	110.70
1	A	2356	A	N3-C4-N9	5.75	132.00	127.40
2	B	17	A	C4-C5-C6	5.75	119.87	117.00
32	W	947	A	C8-N9-C4	5.75	108.10	105.80
32	W	1386	A	N3-C4-N9	5.75	132.00	127.40
32	W	1512	A	C8-N9-C4	5.75	108.10	105.80
1	A	110	A	C4-C5-N7	-5.75	107.83	110.70
1	A	448	A	C8-N9-C4	5.75	108.10	105.80
1	A	449	A	C4-C5-N7	-5.75	107.83	110.70
1	A	584	A	C4-C5-C6	5.75	119.87	117.00
1	A	991	A	C4-C5-C6	5.75	119.87	117.00
1	A	1713	A	N3-C4-N9	5.75	132.00	127.40
1	A	2854	A	C8-N9-C4	5.75	108.10	105.80
2	B	71	A	N9-C4-C5	5.75	108.10	105.80
32	W	544	A	N3-C4-N9	5.75	132.00	127.40
32	W	583	A	N9-C4-C5	5.75	108.10	105.80
32	W	825	A	N3-C4-N9	5.75	132.00	127.40
32	W	1121	A	N3-C4-N9	5.75	132.00	127.40
32	W	1528	A	N3-C4-N9	5.75	132.00	127.40
1	A	428	A	C8-N9-C4	5.75	108.10	105.80
1	A	1014	A	C8-N9-C4	5.75	108.10	105.80
32	W	506	A	N3-C4-N9	5.75	132.00	127.40
1	A	179	A	C4-C5-N7	-5.74	107.83	110.70
1	A	418	A	C4-C5-N7	-5.74	107.83	110.70
1	A	646	A	C8-N9-C4	5.74	108.10	105.80
1	A	646	A	N3-C4-N9	5.74	131.99	127.40
1	A	1812	A	C4-C5-C6	5.74	119.87	117.00
1	A	2034	A	C8-N9-C4	5.74	108.10	105.80
1	A	2315	A	C4-C5-N7	-5.74	107.83	110.70
32	W	532	A	C8-N9-C4	5.74	108.10	105.80
1	A	244	A	C8-N9-C4	5.74	108.10	105.80
1	A	322	A	N3-C4-N9	5.74	131.99	127.40
1	A	1906	A	N3-C4-N9	5.74	131.99	127.40
32	W	159	A	N3-C4-N9	5.74	131.99	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	371	A	C8-N9-C4	5.74	108.10	105.80
52	z	21	A	C8-N9-C4	5.74	108.10	105.80
1	A	389	A	N3-C4-N9	5.74	131.99	127.40
1	A	935	A	N9-C4-C5	5.74	108.10	105.80
1	A	1473	A	C4-C5-N7	-5.74	107.83	110.70
1	A	2364	A	N3-C4-N9	5.74	131.99	127.40
1	A	2658	A	C8-N9-C4	5.74	108.10	105.80
32	W	367	A	C4-C5-N7	-5.74	107.83	110.70
32	W	1259	A	C4-C5-N7	-5.74	107.83	110.70
1	A	345	A	C4-C5-C6	5.74	119.87	117.00
1	A	717	A	C8-N9-C4	5.74	108.09	105.80
1	A	786	A	C4-C5-C6	5.74	119.87	117.00
1	A	1838	A	N9-C4-C5	5.74	108.09	105.80
1	A	2357	A	N3-C4-N9	5.74	131.99	127.40
32	W	120	A	C4-C5-C6	5.74	119.87	117.00
32	W	1176	A	C8-N9-C4	5.74	108.09	105.80
32	W	1270	A	C8-N9-C4	5.74	108.10	105.80
1	A	206	A	N9-C4-C5	5.74	108.09	105.80
1	A	524	A	C8-N9-C4	5.74	108.09	105.80
1	A	2340	A	C4-C5-C6	5.74	119.87	117.00
32	W	94	A	C8-N9-C4	5.74	108.09	105.80
32	W	148	A	N3-C4-N9	5.74	131.99	127.40
1	A	987	A	C8-N9-C4	5.74	108.09	105.80
1	A	1142	A	C8-N9-C4	5.74	108.09	105.80
1	A	1173	A	N9-C1'-C2'	5.74	121.46	114.00
1	A	1540	A	C8-N9-C4	5.74	108.09	105.80
1	A	1789	A	N3-C4-N9	5.74	131.99	127.40
1	A	1929	A	N3-C4-N9	5.74	131.99	127.40
1	A	2000	A	C8-N9-C4	5.74	108.09	105.80
1	A	2405	A	N3-C4-N9	5.74	131.99	127.40
32	W	352	A	N3-C4-N9	5.74	131.99	127.40
32	W	831	A	N3-C4-N9	5.74	131.99	127.40
32	W	924	A	N3-C4-N9	5.74	131.99	127.40
32	W	1050	A	C4-C5-C6	5.74	119.87	117.00
32	W	1213	A	C4-C5-C6	5.74	119.87	117.00
1	A	14	A	N3-C4-N9	5.73	131.99	127.40
1	A	166	A	N3-C4-N9	5.73	131.99	127.40
1	A	318	A	C8-N9-C4	5.73	108.09	105.80
1	A	1579	A	N3-C4-N9	5.73	131.99	127.40
1	A	2686	A	N3-C4-N9	5.73	131.99	127.40
32	W	357	A	N3-C4-N9	5.73	131.99	127.40
32	W	1213	A	C4-C5-N7	-5.73	107.83	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	A	C4-C5-N7	-5.73	107.83	110.70
1	A	198	A	N3-C4-N9	5.73	131.99	127.40
1	A	658	A	N3-C4-N9	5.73	131.99	127.40
1	A	770	A	C8-N9-C4	5.73	108.09	105.80
1	A	840	A	C5-C6-N1	5.73	120.57	117.70
1	A	1119	A	C4-C5-C6	5.73	119.87	117.00
1	A	1679	A	N3-C4-N9	5.73	131.99	127.40
1	A	2042	A	C8-N9-C4	5.73	108.09	105.80
1	A	2364	A	C4-C5-N7	-5.73	107.83	110.70
1	A	2694	A	C8-N9-C4	5.73	108.09	105.80
2	B	18	A	N3-C4-N9	5.73	131.99	127.40
1	A	110	A	C8-N9-C4	5.73	108.09	105.80
1	A	667	A	N9-C4-C5	5.73	108.09	105.80
1	A	1305	A	C4-C5-N7	-5.73	107.83	110.70
1	A	2447	A	N9-C4-C5	5.73	108.09	105.80
32	W	160	A	N3-C4-N9	5.73	131.99	127.40
32	W	422	A	C4-C5-N7	-5.73	107.83	110.70
1	A	1967	A	C8-N9-C4	5.73	108.09	105.80
1	A	2417	A	C4-C5-N7	-5.73	107.84	110.70
32	W	271	A	N3-C4-N9	5.73	131.98	127.40
32	W	679	A	C8-N9-C4	5.73	108.09	105.80
1	A	219	A	N3-C4-N9	5.73	131.98	127.40
1	A	421	A	C8-N9-C4	5.73	108.09	105.80
1	A	1434	A	C4-C5-N7	-5.73	107.84	110.70
1	A	1654	A	N3-C4-N9	5.73	131.98	127.40
1	A	1812	A	C4-C5-N7	-5.73	107.84	110.70
1	A	2381	A	C8-N9-C4	5.73	108.09	105.80
1	A	2658	A	C4-C5-N7	-5.73	107.84	110.70
1	A	2912	A	C4-C5-C6	5.73	119.86	117.00
1	A	2912	A	C8-N9-C4	5.73	108.09	105.80
32	W	10	A	C4-C5-C6	5.73	119.86	117.00
32	W	189	A	C4-C5-N7	-5.73	107.84	110.70
32	W	321	A	N9-C4-C5	5.73	108.09	105.80
32	W	959	A	C4-C5-N7	-5.73	107.84	110.70
32	W	1470	A	C4-C5-C6	5.73	119.86	117.00
1	A	161	A	C4-C5-N7	-5.73	107.84	110.70
1	A	1149	A	C4-C5-C6	5.73	119.86	117.00
1	A	2837	A	C4-C5-N7	-5.73	107.84	110.70
32	W	837	A	N3-C4-N9	5.73	131.98	127.40
1	A	274	A	C4-C5-C6	5.72	119.86	117.00
1	A	781	A	C8-N9-C4	5.72	108.09	105.80
1	A	847	A	N9-C4-C5	5.72	108.09	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	922	A	N3-C4-N9	5.72	131.98	127.40
1	A	1094	A	C8-N9-C4	5.72	108.09	105.80
1	A	1361	A	C8-N9-C4	5.72	108.09	105.80
32	W	206	A	N3-C4-N9	5.72	131.98	127.40
32	W	879	A	N3-C4-N9	5.72	131.98	127.40
32	W	1188	A	C4-C5-C6	5.72	119.86	117.00
1	A	161	A	C4-C5-C6	5.72	119.86	117.00
1	A	448	A	N3-C4-N9	5.72	131.98	127.40
1	A	1115	A	N3-C4-N9	5.72	131.98	127.40
1	A	1210	A	N9-C4-C5	5.72	108.09	105.80
1	A	2049	A	N9-C4-C5	5.72	108.09	105.80
1	A	2405	A	N9-C4-C5	5.72	108.09	105.80
2	B	102	A	N3-C4-N9	5.72	131.98	127.40
32	W	381	A	C8-N9-C4	5.72	108.09	105.80
32	W	664	A	C4-C5-C6	5.72	119.86	117.00
32	W	924	A	C8-N9-C4	5.72	108.09	105.80
1	A	28	A	C8-N9-C4	5.72	108.09	105.80
1	A	342	A	C4-C5-C6	5.72	119.86	117.00
1	A	1119	A	C4-C5-N7	-5.72	107.84	110.70
1	A	1243	A	C4-C5-C6	5.72	119.86	117.00
1	A	1461	A	C8-N9-C4	5.72	108.09	105.80
1	A	1981	A	N9-C4-C5	5.72	108.09	105.80
1	A	2071	A	N9-C4-C5	5.72	108.09	105.80
1	A	2296	A	N3-C4-N9	5.72	131.98	127.40
1	A	2315	A	N3-C4-N9	5.72	131.98	127.40
32	W	555	A	N3-C4-N9	5.72	131.98	127.40
1	A	1189	A	N3-C4-N9	5.72	131.98	127.40
1	A	1277	A	C8-N9-C4	5.72	108.09	105.80
1	A	2317	A	N9-C4-C5	5.72	108.09	105.80
1	A	2398	A	N9-C4-C5	5.72	108.09	105.80
32	W	139	A	C8-N9-C4	5.72	108.09	105.80
32	W	440	A	C8-N9-C4	5.72	108.09	105.80
32	W	725	A	C4-C5-N7	-5.72	107.84	110.70
32	W	1160	A	C8-N9-C4	5.72	108.09	105.80
32	W	1298	A	C4-C5-C6	5.72	119.86	117.00
32	W	1422	A	C4-C5-C6	5.72	119.86	117.00
1	A	475	A	C4-C5-C6	5.72	119.86	117.00
1	A	1260	A	C4-C5-N7	-5.72	107.84	110.70
1	A	1302	A	C4-C5-C6	5.72	119.86	117.00
1	A	2421	A	C8-N9-C4	5.72	108.09	105.80
32	W	28	A	N3-C4-N9	5.72	131.97	127.40
32	W	344	A	C8-N9-C4	5.72	108.09	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	389	A	N3-C4-N9	5.72	131.97	127.40
32	W	771	A	C8-N9-C4	5.72	108.09	105.80
32	W	925	A	C4-C5-C6	5.72	119.86	117.00
32	W	1451	A	C8-N9-C4	5.72	108.09	105.80
1	A	49	A	C4-C5-C6	5.72	119.86	117.00
1	A	1161	A	N9-C4-C5	5.72	108.09	105.80
32	W	910	A	C8-N9-C4	5.72	108.09	105.80
32	W	1254	A	N3-C4-N9	5.72	131.97	127.40
32	W	1358	A	N3-C4-N9	5.72	131.97	127.40
1	A	278	A	C4-C5-N7	-5.71	107.84	110.70
1	A	811	A	N9-C4-C5	5.71	108.09	105.80
1	A	888	A	N3-C4-N9	5.71	131.97	127.40
1	A	1253	A	C8-N9-C4	5.71	108.09	105.80
1	A	1477	A	C8-N9-C4	5.71	108.09	105.80
1	A	2052	A	C8-N9-C4	5.71	108.09	105.80
1	A	2454	A	C8-N9-C4	5.71	108.09	105.80
1	A	2606	A	C4-C5-C6	5.71	119.86	117.00
2	B	18	A	C4-C5-N7	-5.71	107.84	110.70
32	W	67	A	C8-N9-C4	5.71	108.09	105.80
32	W	287	A	C8-N9-C4	5.71	108.09	105.80
32	W	738	A	N3-C4-N9	5.71	131.97	127.40
32	W	1470	A	N3-C4-N9	5.71	131.97	127.40
1	A	273	A	C4-C5-N7	-5.71	107.84	110.70
1	A	1056	A	N3-C4-N9	5.71	131.97	127.40
1	A	1832	A	N3-C4-N9	5.71	131.97	127.40
1	A	2329	A	C8-N9-C4	5.71	108.08	105.80
1	A	2398	A	C4-C5-C6	5.71	119.86	117.00
1	A	53	A	C4-C5-C6	5.71	119.86	117.00
1	A	652	A	C8-N9-C4	5.71	108.08	105.80
1	A	678	A	N9-C4-C5	5.71	108.08	105.80
1	A	1084	A	N3-C4-N9	5.71	131.97	127.40
1	A	2455	A	C4-C5-C6	5.71	119.86	117.00
32	W	1197	A	C8-N9-C4	5.71	108.08	105.80
32	W	1225	A	N3-C4-N9	5.71	131.97	127.40
32	W	1493	A	C8-N9-C4	5.71	108.08	105.80
1	A	543	A	N3-C4-N9	5.71	131.97	127.40
1	A	1233	A	C8-N9-C4	5.71	108.08	105.80
1	A	1809	A	N3-C4-N9	5.71	131.97	127.40
1	A	2862	A	C8-N9-C4	5.71	108.08	105.80
1	A	355	A	N3-C4-N9	5.71	131.97	127.40
1	A	828	A	N3-C4-N9	5.71	131.97	127.40
1	A	964	A	C8-N9-C4	5.71	108.08	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1144	A	N3-C4-N9	5.71	131.97	127.40
1	A	1175	A	N3-C4-N9	5.71	131.97	127.40
1	A	1179	A	C8-N9-C4	5.71	108.08	105.80
1	A	1254	A	C4-C5-N7	-5.71	107.85	110.70
1	A	1504	A	C4-C5-C6	5.71	119.86	117.00
1	A	2606	A	N9-C4-C5	5.71	108.08	105.80
32	W	206	A	C4-C5-N7	-5.71	107.85	110.70
32	W	672	A	C8-N9-C4	5.71	108.08	105.80
32	W	882	A	C8-N9-C4	5.71	108.08	105.80
32	W	1006	A	N3-C4-N9	5.71	131.97	127.40
1	A	65	A	C8-N9-C4	5.71	108.08	105.80
1	A	622	A	N3-C4-N9	5.71	131.97	127.40
1	A	1119	A	N3-C4-N9	5.71	131.97	127.40
1	A	1161	A	C4-C5-C6	5.71	119.85	117.00
2	B	50	A	C8-N9-C4	5.71	108.08	105.80
32	W	202	A	N9-C4-C5	5.71	108.08	105.80
32	W	1185	A	C4-C5-C6	5.71	119.85	117.00
32	W	1252	A	C8-N9-C4	5.71	108.08	105.80
1	A	1580	A	C8-N9-C4	5.71	108.08	105.80
1	A	2364	A	C8-N9-C4	5.71	108.08	105.80
1	A	2819	A	C4-C5-C6	5.71	119.85	117.00
32	W	142	A	N3-C4-N9	5.71	131.96	127.40
1	A	67	A	N9-C4-C5	5.70	108.08	105.80
1	A	199	A	N3-C4-N9	5.70	131.96	127.40
1	A	210	A	C4-C5-C6	5.70	119.85	117.00
1	A	325	A	C8-N9-C4	5.70	108.08	105.80
1	A	732	A	C5-C6-N1	5.70	120.55	117.70
1	A	1314	A	N3-C4-N9	5.70	131.96	127.40
1	A	1473	A	N9-C4-C5	5.70	108.08	105.80
1	A	1965	A	N9-C4-C5	5.70	108.08	105.80
1	A	2006	A	N3-C4-N9	5.70	131.96	127.40
1	A	2924	A	N9-C4-C5	5.70	108.08	105.80
32	W	178	A	C4-C5-N7	-5.70	107.85	110.70
1	A	219	A	C8-N9-C4	5.70	108.08	105.80
1	A	1067	A	C4-C5-C6	5.70	119.85	117.00
32	W	208	A	C4-C5-C6	5.70	119.85	117.00
32	W	1207	A	C8-N9-C4	5.70	108.08	105.80
32	W	1434	A	C4-C5-N7	-5.70	107.85	110.70
1	A	1084	A	C4-C5-N7	-5.70	107.85	110.70
1	A	2059	A	N3-C4-N9	5.70	131.96	127.40
32	W	170	A	N3-C4-N9	5.70	131.96	127.40
32	W	658	A	C4-C5-C6	5.70	119.85	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	690	A	C4-C5-N7	-5.70	107.85	110.70
32	W	928	A	C4-C5-N7	-5.70	107.85	110.70
32	W	975	A	N3-C4-N9	5.70	131.96	127.40
32	W	1111	A	C4-C5-N7	-5.70	107.85	110.70
32	W	1266	A	C4-C5-N7	-5.70	107.85	110.70
1	A	281	A	N3-C4-N9	5.70	131.96	127.40
1	A	572	A	C8-N9-C4	5.70	108.08	105.80
1	A	888	A	C4-C5-N7	-5.70	107.85	110.70
1	A	1161	A	C4-C5-N7	-5.70	107.85	110.70
1	A	1174	A	C4-C5-N7	-5.70	107.85	110.70
1	A	1313	A	C4-C5-C6	5.70	119.85	117.00
1	A	1483	A	C4-C5-N7	-5.70	107.85	110.70
1	A	1914	A	N3-C4-N9	5.70	131.96	127.40
1	A	2276	A	N3-C4-N9	5.70	131.96	127.40
32	W	638	A	C4-C5-N7	-5.70	107.85	110.70
32	W	703	A	C4-C5-N7	-5.70	107.85	110.70
52	z	37	A	N7-C8-N9	-5.70	110.95	113.80
1	A	2673	A	C4-C5-N7	-5.70	107.85	110.70
32	W	232	A	C8-N9-C4	5.70	108.08	105.80
32	W	1479	A	C8-N9-C4	5.70	108.08	105.80
1	A	1130	A	N9-C4-C5	5.70	108.08	105.80
1	A	1175	A	C8-N9-C4	5.70	108.08	105.80
1	A	1672	A	C8-N9-C4	5.70	108.08	105.80
1	A	2402	A	C8-N9-C4	5.70	108.08	105.80
32	W	202	A	N3-C4-N9	5.70	131.96	127.40
32	W	208	A	C4-C5-N7	-5.70	107.85	110.70
32	W	357	A	C4-C5-N7	-5.70	107.85	110.70
32	W	704	A	C8-N9-C4	5.70	108.08	105.80
32	W	737	A	N3-C4-N9	5.70	131.96	127.40
32	W	1147	A	C4-C5-N7	-5.70	107.85	110.70
32	W	1417	A	N3-C4-N9	5.70	131.96	127.40
1	A	1553	A	C4-C5-N7	-5.69	107.85	110.70
32	W	1222	A	C8-N9-C4	5.69	108.08	105.80
1	A	978	A	C8-N9-C4	5.69	108.08	105.80
1	A	1966	A	N3-C4-N9	5.69	131.96	127.40
32	W	57	A	C8-N9-C4	5.69	108.08	105.80
32	W	170	A	C4-C5-N7	-5.69	107.85	110.70
32	W	508	A	C4-C5-N7	-5.69	107.85	110.70
1	A	736	A	C8-N9-C4	5.69	108.08	105.80
1	A	1266	A	N3-C4-N9	5.69	131.95	127.40
1	A	1914	A	N9-C4-C5	5.69	108.08	105.80
1	A	2088	A	C4-C5-C6	5.69	119.84	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	53	A	C4-C5-N7	-5.69	107.85	110.70
32	W	170	A	N9-C4-C5	5.69	108.08	105.80
32	W	204	A	C8-N9-C4	5.69	108.08	105.80
32	W	462	A	C8-N9-C4	5.69	108.08	105.80
32	W	542	A	N3-C4-N9	5.69	131.95	127.40
32	W	651	A	C4-C5-C6	5.69	119.84	117.00
32	W	886	A	C8-N9-C4	5.69	108.08	105.80
32	W	988	A	N9-C4-C5	5.69	108.08	105.80
32	W	1017	A	N9-C4-C5	5.69	108.08	105.80
32	W	1103	A	C8-N9-C4	5.69	108.08	105.80
1	A	1802	A	C8-N9-C4	5.69	108.08	105.80
23	X	55	LYS	N-CA-C	-5.69	95.64	111.00
1	A	5	A	N3-C4-N9	5.69	131.95	127.40
1	A	206	A	C4-C5-N7	-5.69	107.86	110.70
1	A	373	A	N9-C4-C5	5.69	108.08	105.80
1	A	677	A	C4-C5-C6	5.69	119.84	117.00
1	A	811	A	C4-C5-C6	5.69	119.84	117.00
1	A	1244	A	C4-C5-C6	5.69	119.84	117.00
1	A	1504	A	N3-C4-N9	5.69	131.95	127.40
1	A	1593	A	C8-N9-C4	5.69	108.08	105.80
1	A	1654	A	C4-C5-N7	-5.69	107.86	110.70
1	A	1945	A	N9-C4-C5	5.69	108.08	105.80
1	A	2777	A	C4-C5-C6	5.69	119.84	117.00
2	B	102	A	C8-N9-C4	5.69	108.08	105.80
32	W	508	A	C5-C6-N1	5.69	120.54	117.70
32	W	929	A	N9-C4-C5	5.69	108.08	105.80
32	W	968	A	N9-C4-C5	5.69	108.08	105.80
32	W	1289	A	C8-N9-C4	5.69	108.08	105.80
1	A	324	A	C8-N9-C4	5.69	108.07	105.80
1	A	364	A	C8-N9-C4	5.69	108.08	105.80
1	A	999	A	N3-C4-N9	5.69	131.95	127.40
1	A	1929	A	C8-N9-C4	5.69	108.07	105.80
1	A	2356	A	N9-C4-C5	5.69	108.08	105.80
1	A	2793	A	N9-C4-C5	5.69	108.07	105.80
32	W	440	A	C4-C5-N7	-5.69	107.86	110.70
32	W	974	A	N9-C4-C5	5.69	108.07	105.80
1	A	200	A	C8-N9-C4	5.68	108.07	105.80
1	A	752	A	C8-N9-C4	5.68	108.07	105.80
1	A	786	A	C8-N9-C4	5.68	108.07	105.80
1	A	1627	A	C8-N9-C4	5.68	108.07	105.80
32	W	150	A	C8-N9-C4	5.68	108.07	105.80
32	W	290	A	C8-N9-C4	5.68	108.07	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	617	A	C8-N9-C4	5.68	108.07	105.80
32	W	1320	A	C4-C5-N7	-5.68	107.86	110.70
1	A	1201	A	C4-C5-N7	-5.68	107.86	110.70
1	A	1287	A	C8-N9-C4	5.68	108.07	105.80
1	A	1797	A	N3-C4-N9	5.68	131.95	127.40
1	A	1818	A	C8-N9-C4	5.68	108.07	105.80
1	A	2071	A	N3-C4-N9	5.68	131.95	127.40
1	A	2398	A	C4-C5-N7	-5.68	107.86	110.70
32	W	74	A	C4-C5-N7	-5.68	107.86	110.70
32	W	225	A	N9-C4-C5	5.68	108.07	105.80
32	W	372	A	C8-N9-C4	5.68	108.07	105.80
32	W	501	A	N3-C4-N9	5.68	131.95	127.40
32	W	725	A	N3-C4-N9	5.68	131.95	127.40
1	A	268	A	N9-C4-C5	5.68	108.07	105.80
1	A	1913	A	C8-N9-C4	5.68	108.07	105.80
1	A	2593	A	N3-C4-N9	5.68	131.94	127.40
1	A	2778	A	N3-C4-N9	5.68	131.94	127.40
32	W	57	A	C4-C5-N7	-5.68	107.86	110.70
32	W	423	A	C8-N9-C4	5.68	108.07	105.80
32	W	831	A	C8-N9-C4	5.68	108.07	105.80
1	A	830	A	N9-C4-C5	5.68	108.07	105.80
1	A	2059	A	C8-N9-C4	5.68	108.07	105.80
32	W	31	A	N3-C4-N9	5.68	131.94	127.40
32	W	142	A	C8-N9-C4	5.68	108.07	105.80
32	W	232	A	C4-C5-C6	5.68	119.84	117.00
32	W	757	A	C8-N9-C4	5.68	108.07	105.80
1	A	178	A	N3-C4-N9	5.68	131.94	127.40
1	A	572	A	N3-C4-N9	5.68	131.94	127.40
1	A	1325	A	N3-C4-N9	5.68	131.94	127.40
1	A	1585	A	C8-N9-C4	5.68	108.07	105.80
1	A	2507	A	N3-C4-N9	5.68	131.94	127.40
1	A	219	A	N9-C4-C5	5.68	108.07	105.80
1	A	525	A	C4-C5-C6	5.68	119.84	117.00
1	A	619	A	C4-C5-C6	5.68	119.84	117.00
1	A	683	A	N3-C4-N9	5.68	131.94	127.40
1	A	835	A	C4-C5-N7	-5.68	107.86	110.70
1	A	999	A	C4-C5-C6	5.68	119.84	117.00
1	A	1092	A	C4-C5-C6	5.68	119.84	117.00
1	A	1575	A	C8-N9-C4	5.68	108.07	105.80
1	A	1966	A	C8-N9-C4	5.68	108.07	105.80
1	A	2500	A	C8-N9-C4	5.68	108.07	105.80
1	A	2807	A	C4-C5-C6	5.68	119.84	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	206	A	C8-N9-C4	5.68	108.07	105.80
32	W	522	A	C4-C5-N7	-5.68	107.86	110.70
1	A	548	A	C8-N9-C4	5.67	108.07	105.80
1	A	705	A	C8-N9-C4	5.67	108.07	105.80
1	A	740	A	C4-C5-N7	-5.67	107.86	110.70
1	A	1914	A	C4-C5-C6	5.67	119.84	117.00
1	A	1919	A	N9-C4-C5	5.67	108.07	105.80
1	A	1941	A	C4-C5-N7	-5.67	107.86	110.70
1	A	2007	A	C8-N9-C4	5.67	108.07	105.80
1	A	2383	A	N9-C4-C5	5.67	108.07	105.80
1	A	2387	A	N3-C4-N9	5.67	131.94	127.40
1	A	2643	A	N9-C4-C5	5.67	108.07	105.80
32	W	10	A	N3-C4-N9	5.67	131.94	127.40
32	W	209	A	C4-C5-C6	5.67	119.84	117.00
32	W	456	A	C4-C5-N7	-5.67	107.86	110.70
32	W	837	A	C8-N9-C4	5.67	108.07	105.80
32	W	978	A	C4-C5-N7	-5.67	107.86	110.70
32	W	1014	A	C8-N9-C4	5.67	108.07	105.80
32	W	1090	A	N3-C4-N9	5.67	131.94	127.40
1	A	888	A	C8-N9-C4	5.67	108.07	105.80
1	A	1918	A	C8-N9-C4	5.67	108.07	105.80
32	W	329	A	C4-C5-N7	-5.67	107.86	110.70
32	W	419	A	N9-C4-C5	5.67	108.07	105.80
32	W	917	A	C8-N9-C4	5.67	108.07	105.80
1	A	575	A	C4-C5-N7	-5.67	107.86	110.70
1	A	917	A	N3-C4-N9	5.67	131.94	127.40
1	A	1061	A	C8-N9-C4	5.67	108.07	105.80
1	A	1434	A	C4-C5-C6	5.67	119.84	117.00
1	A	1601	A	C4-C5-C6	5.67	119.83	117.00
1	A	1966	A	C4-C5-C6	5.67	119.84	117.00
1	A	2463	A	N3-C4-N9	5.67	131.94	127.40
1	A	2618	A	N9-C4-C5	5.67	108.07	105.80
2	B	55	A	C8-N9-C4	5.67	108.07	105.80
32	W	592	A	C8-N9-C4	5.67	108.07	105.80
1	A	418	A	N9-C4-C5	5.67	108.07	105.80
1	A	1517	A	C8-N9-C4	5.67	108.07	105.80
1	A	2062	A	C4-C5-N7	-5.67	107.86	110.70
32	W	178	A	N3-C4-N9	5.67	131.94	127.40
32	W	775	A	N3-C4-N9	5.67	131.94	127.40
1	A	56	A	C5-C6-N1	5.67	120.53	117.70
1	A	991	A	N9-C4-C5	5.67	108.07	105.80
1	A	1326	A	C8-N9-C4	5.67	108.07	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1461	A	C4-C5-N7	-5.67	107.87	110.70
1	A	2670	A	C8-N9-C4	5.67	108.07	105.80
2	B	17	A	C8-N9-C4	5.67	108.07	105.80
32	W	232	A	C4-C5-N7	-5.67	107.87	110.70
32	W	477	A	C4-C5-N7	-5.67	107.87	110.70
32	W	582	A	C4-C5-C6	5.67	119.83	117.00
32	W	1348	A	C8-N9-C4	5.67	108.07	105.80
32	W	1417	A	N9-C4-C5	5.67	108.07	105.80
1	A	13	A	C8-N9-C4	5.67	108.07	105.80
1	A	171	A	C8-N9-C4	5.67	108.07	105.80
1	A	1326	A	N3-C4-N9	5.67	131.93	127.40
1	A	1700	A	C4-C5-C6	5.67	119.83	117.00
1	A	2542	A	N3-C4-N9	5.67	131.93	127.40
1	A	2668	A	C4-C5-N7	-5.67	107.87	110.70
32	W	234	A	C8-N9-C4	5.67	108.07	105.80
32	W	415	A	C4-C5-C6	5.67	119.83	117.00
32	W	422	A	N9-C4-C5	5.67	108.07	105.80
32	W	1289	A	N3-C4-N9	5.67	131.93	127.40
1	A	125	A	N3-C4-N9	5.67	131.93	127.40
1	A	161	A	N3-C4-N9	5.67	131.93	127.40
1	A	373	A	N3-C4-N9	5.67	131.93	127.40
1	A	1405	A	C4-C5-N7	-5.67	107.87	110.70
1	A	1945	A	C4-C5-N7	-5.67	107.87	110.70
1	A	2904	A	N3-C4-N9	5.67	131.93	127.40
2	B	17	A	N9-C4-C5	5.67	108.07	105.80
32	W	738	A	C8-N9-C4	5.67	108.07	105.80
32	W	1289	A	C4-C5-N7	-5.67	107.87	110.70
32	W	1355	A	C4-C5-N7	-5.67	107.87	110.70
1	A	117	A	C4-C5-N7	-5.66	107.87	110.70
1	A	1055	A	C4-C5-N7	-5.66	107.87	110.70
1	A	1325	A	C8-N9-C4	5.66	108.06	105.80
1	A	1815	A	N3-C4-N9	5.66	131.93	127.40
32	W	592	A	C4-C5-C6	5.66	119.83	117.00
32	W	1207	A	N3-C4-N9	5.66	131.93	127.40
1	A	965	A	C4-C5-C6	5.66	119.83	117.00
1	A	1003	A	C4-C5-C6	5.66	119.83	117.00
1	A	1404	A	C8-N9-C4	5.66	108.06	105.80
1	A	1464	A	C4-C5-N7	-5.66	107.87	110.70
1	A	2088	A	N3-C4-N9	5.66	131.93	127.40
1	A	2595	A	N3-C4-N9	5.66	131.93	127.40
32	W	271	A	N9-C4-C5	5.66	108.06	105.80
32	W	775	A	C8-N9-C4	5.66	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1144	A	N9-C4-C5	5.66	108.06	105.80
1	A	2904	A	N9-C4-C5	5.66	108.06	105.80
1	A	2907	A	C4-C5-C6	5.66	119.83	117.00
32	W	148	A	C4-C5-C6	5.66	119.83	117.00
32	W	159	A	C4-C5-N7	-5.66	107.87	110.70
32	W	423	A	C4-C5-N7	-5.66	107.87	110.70
32	W	658	A	C8-N9-C4	5.66	108.06	105.80
32	W	1289	A	C4-C5-C6	5.66	119.83	117.00
32	W	1470	A	C8-N9-C4	5.66	108.06	105.80
1	A	231	A	N9-C4-C5	5.66	108.06	105.80
1	A	337	A	C8-N9-C4	5.66	108.06	105.80
1	A	987	A	C4-C5-N7	-5.66	107.87	110.70
1	A	2375	A	N9-C4-C5	5.66	108.06	105.80
1	A	2487	U	C2'-C3'-O3'	-5.66	97.05	109.50
1	A	2507	A	C4-C5-C6	5.66	119.83	117.00
32	W	419	A	C4-C5-N7	-5.66	107.87	110.70
32	W	438	A	N3-C4-N9	5.66	131.93	127.40
32	W	477	A	C4-C5-C6	5.66	119.83	117.00
32	W	801	A	C4-C5-N7	-5.66	107.87	110.70
32	W	1488	A	C4-C5-C6	5.66	119.83	117.00
1	A	1930	A	C4-C5-C6	5.66	119.83	117.00
1	A	2618	A	C4-C5-N7	-5.66	107.87	110.70
32	W	301	A	C8-N9-C4	5.66	108.06	105.80
1	A	584	A	N3-C4-N9	5.66	131.93	127.40
1	A	1316	A	C8-N9-C4	5.66	108.06	105.80
1	A	1347	A	C4-C5-C6	5.66	119.83	117.00
1	A	1947	A	C8-N9-C4	5.66	108.06	105.80
1	A	2006	A	N9-C4-C5	5.66	108.06	105.80
1	A	2091	A	N9-C4-C5	5.66	108.06	105.80
1	A	2479	A	C8-N9-C4	5.66	108.06	105.80
1	A	2830	A	C8-N9-C4	5.66	108.06	105.80
32	W	296	A	N3-C4-N9	5.66	131.93	127.40
32	W	923	A	C4-C5-N7	-5.66	107.87	110.70
1	A	1456	A	N3-C4-N9	5.65	131.92	127.40
1	A	1663	A	C8-N9-C4	5.65	108.06	105.80
1	A	1679	A	C4-C5-N7	-5.65	107.87	110.70
32	W	401	A	N3-C4-N9	5.65	131.92	127.40
1	A	94	A	N9-C4-C5	5.65	108.06	105.80
1	A	476	A	C4-C5-C6	5.65	119.83	117.00
1	A	1254	A	C8-N9-C4	5.65	108.06	105.80
1	A	1654	A	C8-N9-C4	5.65	108.06	105.80
1	A	1905	A	C4-C5-N7	-5.65	107.87	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	160	A	N9-C4-C5	5.65	108.06	105.80
32	W	173	A	C8-N9-C4	5.65	108.06	105.80
32	W	541	A	C8-N9-C4	5.65	108.06	105.80
32	W	913	A	C8-N9-C4	5.65	108.06	105.80
32	W	1207	A	C4-C5-C6	5.65	119.83	117.00
1	A	176	A	C8-N9-C4	5.65	108.06	105.80
1	A	322	A	N9-C4-C5	5.65	108.06	105.80
1	A	847	A	C4-C5-N7	-5.65	107.88	110.70
1	A	1638	A	C8-N9-C4	5.65	108.06	105.80
1	A	2734	A	C8-N9-C4	5.65	108.06	105.80
1	A	2837	A	N9-C4-C5	5.65	108.06	105.80
32	W	690	A	N3-C4-N9	5.65	131.92	127.40
32	W	721	A	N9-C4-C5	5.65	108.06	105.80
32	W	928	A	N9-C4-C5	5.65	108.06	105.80
32	W	1213	A	N3-C4-N9	5.65	131.92	127.40
32	W	1358	A	C8-N9-C4	5.65	108.06	105.80
32	W	1517	A	C8-N9-C4	5.65	108.06	105.80
1	A	501	A	C4-C5-C6	5.65	119.82	117.00
1	A	1131	A	C8-N9-C4	5.65	108.06	105.80
1	A	1677	A	N9-C4-C5	5.65	108.06	105.80
1	A	1914	A	C8-N9-C4	5.65	108.06	105.80
1	A	2032	A	C8-N9-C4	5.65	108.06	105.80
32	W	1434	A	N3-C4-N9	5.65	131.92	127.40
1	A	717	A	C4-C5-N7	-5.65	107.88	110.70
1	A	917	A	C8-N9-C4	5.65	108.06	105.80
1	A	1047	A	C4-C5-N7	-5.65	107.88	110.70
1	A	1055	A	C8-N9-C4	5.65	108.06	105.80
1	A	1189	A	C4-C5-N7	-5.65	107.88	110.70
1	A	1585	A	C4-C5-N7	-5.65	107.88	110.70
1	A	1608	A	C8-N9-C4	5.65	108.06	105.80
1	A	2854	A	C4-C5-N7	-5.65	107.88	110.70
2	B	27	A	N3-C4-N9	5.65	131.92	127.40
32	W	202	A	C4-C5-N7	-5.65	107.88	110.70
32	W	684	A	C8-N9-C4	5.65	108.06	105.80
32	W	704	A	C4-C5-N7	-5.65	107.88	110.70
32	W	1006	A	C4-C5-C6	5.65	119.82	117.00
1	A	904	A	N3-C4-N9	5.65	131.92	127.40
1	A	1339	A	N9-C4-C5	5.65	108.06	105.80
1	A	2083	A	C5-C6-N1	5.65	120.52	117.70
1	A	2673	A	C8-N9-C4	5.65	108.06	105.80
1	A	230	A	C8-N9-C4	5.64	108.06	105.80
1	A	307	A	C8-N9-C4	5.64	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	821	A	N3-C4-N9	5.64	131.92	127.40
1	A	965	A	C8-N9-C4	5.64	108.06	105.80
1	A	1116	A	C8-N9-C4	5.64	108.06	105.80
1	A	1504	A	C8-N9-C4	5.64	108.06	105.80
1	A	1516	A	C4-C5-N7	-5.64	107.88	110.70
1	A	1735	A	C4-C5-N7	-5.64	107.88	110.70
1	A	1838	A	C4-C5-N7	-5.64	107.88	110.70
2	B	105	A	C8-N9-C4	5.64	108.06	105.80
32	W	18	A	N3-C4-N9	5.64	131.91	127.40
32	W	31	A	C4-C5-C6	5.64	119.82	117.00
32	W	1297	A	C8-N9-C4	5.64	108.06	105.80
32	W	1359	A	C8-N9-C4	5.64	108.06	105.80
1	A	183	A	C4-C5-N7	-5.64	107.88	110.70
1	A	1005	A	N9-C4-C5	5.64	108.06	105.80
1	A	1426	A	C8-N9-C4	5.64	108.06	105.80
1	A	2482	A	N3-C4-N9	5.64	131.91	127.40
1	A	2571	A	N9-C4-C5	5.64	108.06	105.80
32	W	28	A	N9-C4-C5	5.64	108.06	105.80
32	W	31	A	C8-N9-C4	5.64	108.06	105.80
32	W	522	A	C8-N9-C4	5.64	108.06	105.80
32	W	1254	A	C4-C5-C6	5.64	119.82	117.00
32	W	1488	A	C8-N9-C4	5.64	108.06	105.80
1	A	1092	A	N3-C4-N9	5.64	131.91	127.40
32	W	870	A	N9-C4-C5	5.64	108.06	105.80
1	A	592	A	C8-N9-C4	5.64	108.06	105.80
1	A	677	A	C8-N9-C4	5.64	108.06	105.80
1	A	683	A	C4-C5-C6	5.64	119.82	117.00
1	A	1312	A	C8-N9-C4	5.64	108.06	105.80
32	W	160	A	C4-C5-N7	-5.64	107.88	110.70
32	W	389	A	N9-C4-C5	5.64	108.06	105.80
32	W	758	A	C8-N9-C4	5.64	108.06	105.80
32	W	1115	A	N9-C4-C5	5.64	108.06	105.80
32	W	1266	A	N9-C4-C5	5.64	108.06	105.80
1	A	724	A	C8-N9-C4	5.64	108.06	105.80
1	A	1809	A	C8-N9-C4	5.64	108.06	105.80
1	A	268	A	N3-C4-N9	5.64	131.91	127.40
1	A	278	A	C8-N9-C4	5.64	108.06	105.80
1	A	314	A	C4-C5-N7	-5.64	107.88	110.70
1	A	333	A	C8-N9-C4	5.64	108.05	105.80
1	A	342	A	C8-N9-C4	5.64	108.05	105.80
1	A	429	A	C8-N9-C4	5.64	108.06	105.80
1	A	947	A	C8-N9-C4	5.64	108.05	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	993	A	C8-N9-C4	5.64	108.05	105.80
1	A	1029	A	N9-C4-C5	5.64	108.06	105.80
1	A	1157	A	N9-C4-C5	5.64	108.06	105.80
1	A	1516	A	C8-N9-C4	5.64	108.06	105.80
1	A	1685	A	C4-C5-N7	-5.64	107.88	110.70
1	A	2782	A	N3-C4-N9	5.64	131.91	127.40
32	W	76	A	C8-N9-C4	5.64	108.06	105.80
32	W	945	A	C8-N9-C4	5.64	108.06	105.80
32	W	1528	A	N9-C4-C5	5.64	108.05	105.80
1	A	526	A	C8-N9-C4	5.63	108.05	105.80
1	A	1115	A	C4-C5-N7	-5.63	107.88	110.70
1	A	1224	A	C4-C5-N7	-5.63	107.88	110.70
1	A	1465	A	C8-N9-C4	5.63	108.05	105.80
1	A	2351	A	C8-N9-C4	5.63	108.05	105.80
1	A	2750	A	C4-C5-N7	-5.63	107.88	110.70
1	A	2762	A	C8-N9-C4	5.63	108.05	105.80
32	W	419	A	C4-C5-C6	5.63	119.82	117.00
32	W	816	A	C8-N9-C4	5.63	108.05	105.80
32	W	1510	A	C8-N9-C4	5.63	108.05	105.80
32	W	1488	A	C4-C5-N7	-5.63	107.88	110.70
1	A	10	A	C8-N9-C4	5.63	108.05	105.80
1	A	185	A	C5-C6-N1	5.63	120.52	117.70
1	A	343	A	N3-C4-N9	5.63	131.91	127.40
1	A	477	A	C4-C5-N7	-5.63	107.89	110.70
1	A	699	A	N9-C4-C5	5.63	108.05	105.80
1	A	1423	A	C8-N9-C4	5.63	108.05	105.80
1	A	1619	A	C4-C5-N7	-5.63	107.89	110.70
1	A	1957	A	N3-C4-N9	5.63	131.90	127.40
1	A	2362	A	C4-C5-N7	-5.63	107.88	110.70
1	A	2601	A	C4-C5-N7	-5.63	107.88	110.70
1	A	2683	A	C4-C5-N7	-5.63	107.89	110.70
32	W	501	A	C4-C5-N7	-5.63	107.88	110.70
32	W	771	A	C4-C5-N7	-5.63	107.88	110.70
1	A	500	A	N9-C4-C5	5.63	108.05	105.80
1	A	653	A	C8-N9-C4	5.63	108.05	105.80
32	W	210	A	C8-N9-C4	5.63	108.05	105.80
32	W	236	A	C8-N9-C4	5.63	108.05	105.80
32	W	1120	A	C8-N9-C4	5.63	108.05	105.80
32	W	1161	A	C8-N9-C4	5.63	108.05	105.80
1	A	449	A	N9-C4-C5	5.63	108.05	105.80
1	A	637	A	C8-N9-C4	5.63	108.05	105.80
1	A	808	A	C8-N9-C4	5.63	108.05	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1287	A	N9-C4-C5	5.63	108.05	105.80
1	A	2087	A	C8-N9-C4	5.63	108.05	105.80
1	A	2480	A	C8-N9-C4	5.63	108.05	105.80
2	B	76	A	C4-C5-N7	-5.63	107.89	110.70
32	W	211	A	C4-C5-C6	5.63	119.81	117.00
32	W	321	A	N3-C4-N9	5.63	131.90	127.40
32	W	649	A	C8-N9-C4	5.63	108.05	105.80
32	W	713	A	N9-C4-C5	5.63	108.05	105.80
32	W	776	A	C8-N9-C4	5.63	108.05	105.80
32	W	886	A	C4-C5-N7	-5.63	107.89	110.70
32	W	1422	A	N3-C4-N9	5.63	131.90	127.40
1	A	133	A	C8-N9-C4	5.63	108.05	105.80
1	A	343	A	N9-C4-C5	5.63	108.05	105.80
1	A	384	A	N9-C4-C5	5.63	108.05	105.80
1	A	418	A	C8-N9-C4	5.63	108.05	105.80
1	A	469	A	N9-C4-C5	5.63	108.05	105.80
1	A	717	A	N3-C4-N9	5.63	131.90	127.40
1	A	1357	A	C8-N9-C4	5.63	108.05	105.80
1	A	2398	A	N3-C4-N9	5.63	131.90	127.40
32	W	240	A	C8-N9-C4	5.63	108.05	105.80
32	W	568	A	C4-C5-C6	5.63	119.81	117.00
32	W	638	A	C8-N9-C4	5.63	108.05	105.80
32	W	642	U	C2-N1-C1'	5.63	124.45	117.70
32	W	1443	A	N3-C4-N9	5.63	131.90	127.40
32	W	1510	A	C4-C5-N7	-5.63	107.89	110.70
32	W	1541	A	C8-N9-C4	5.63	108.05	105.80
1	A	459	A	C8-N9-C4	5.62	108.05	105.80
1	A	572	A	C4-C5-N7	-5.62	107.89	110.70
1	A	908	A	C4-C5-N7	-5.62	107.89	110.70
1	A	1339	A	N3-C4-N9	5.62	131.90	127.40
1	A	717	A	N9-C4-C5	5.62	108.05	105.80
1	A	1026	A	C8-N9-C4	5.62	108.05	105.80
1	A	1113	A	C8-N9-C4	5.62	108.05	105.80
1	A	2088	A	C8-N9-C4	5.62	108.05	105.80
1	A	2887	A	C8-N9-C4	5.62	108.05	105.80
32	W	148	A	C8-N9-C4	5.62	108.05	105.80
32	W	1185	A	C4-C5-N7	-5.62	107.89	110.70
32	W	1247	A	C4-C5-N7	-5.62	107.89	110.70
32	W	1419	A	C4-C5-N7	-5.62	107.89	110.70
1	A	549	A	C8-N9-C4	5.62	108.05	105.80
1	A	702	A	C4-C5-C6	5.62	119.81	117.00
1	A	821	A	N9-C4-C5	5.62	108.05	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1381	A	C8-N9-C4	5.62	108.05	105.80
1	A	1423	A	C4-C5-N7	-5.62	107.89	110.70
1	A	2480	A	N9-C4-C5	5.62	108.05	105.80
1	A	2700	A	C8-N9-C4	5.62	108.05	105.80
1	A	2804	A	N3-C4-N9	5.62	131.90	127.40
2	B	44	A	C8-N9-C4	5.62	108.05	105.80
32	W	203	A	N3-C4-N9	5.62	131.90	127.40
32	W	266	A	C4-C5-N7	-5.62	107.89	110.70
32	W	266	A	C8-N9-C4	5.62	108.05	105.80
32	W	803	A	C4-C5-N7	-5.62	107.89	110.70
32	W	974	A	N3-C4-N9	5.62	131.90	127.40
32	W	1523	A	C8-N9-C4	5.62	108.05	105.80
1	A	302	A	C4-C5-N7	-5.62	107.89	110.70
1	A	575	A	N9-C4-C5	5.62	108.05	105.80
1	A	618	A	N3-C4-N9	5.62	131.90	127.40
1	A	659	A	C4-C5-C6	5.62	119.81	117.00
1	A	1784	A	C4-C5-N7	-5.62	107.89	110.70
32	W	556	A	N3-C4-N9	5.62	131.90	127.40
32	W	713	A	N3-C4-N9	5.62	131.90	127.40
32	W	1128	A	N9-C4-C5	5.62	108.05	105.80
1	A	38	A	N9-C4-C5	5.62	108.05	105.80
1	A	154	A	C8-N9-C4	5.62	108.05	105.80
1	A	667	A	N3-C4-N9	5.62	131.90	127.40
1	A	1008	A	C8-N9-C4	5.62	108.05	105.80
1	A	1175	A	C4-C5-N7	-5.62	107.89	110.70
1	A	1579	A	C8-N9-C4	5.62	108.05	105.80
1	A	1735	A	C8-N9-C4	5.62	108.05	105.80
1	A	1814	A	C4-C5-N7	-5.62	107.89	110.70
1	A	2464	A	C4-C5-N7	-5.62	107.89	110.70
1	A	2845	A	C4-C5-N7	-5.62	107.89	110.70
32	W	120	A	C8-N9-C4	5.62	108.05	105.80
32	W	422	A	N3-C4-N9	5.62	131.90	127.40
32	W	452	A	C8-N9-C4	5.62	108.05	105.80
32	W	1056	A	C4-C5-N7	-5.62	107.89	110.70
1	A	124	A	C8-N9-C4	5.62	108.05	105.80
1	A	888	A	N9-C4-C5	5.62	108.05	105.80
1	A	1948	A	C4-C5-C6	5.62	119.81	117.00
1	A	2835	A	C4-C5-N7	-5.62	107.89	110.70
2	B	27	A	N9-C4-C5	5.62	108.05	105.80
32	W	364	A	N9-C4-C5	5.62	108.05	105.80
32	W	923	A	N3-C4-N9	5.62	131.89	127.40
32	W	1359	A	C4-C5-N7	-5.62	107.89	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1512	A	N3-C4-N9	5.62	131.89	127.40
1	A	224	A	N3-C4-N9	5.62	131.89	127.40
1	A	1115	A	N9-C4-C5	5.62	108.05	105.80
1	A	1654	A	N9-C4-C5	5.62	108.05	105.80
1	A	2601	A	N9-C4-C5	5.62	108.05	105.80
1	A	2700	A	C4-C5-N7	-5.62	107.89	110.70
1	A	2835	A	N3-C4-N9	5.62	131.89	127.40
32	W	801	A	N9-C4-C5	5.62	108.05	105.80
32	W	875	A	C8-N9-C4	5.62	108.05	105.80
32	W	959	A	N9-C4-C5	5.62	108.05	105.80
1	A	52	A	C4-C5-N7	-5.61	107.89	110.70
1	A	193	A	C8-N9-C4	5.61	108.05	105.80
1	A	1174	A	N9-C4-C5	5.61	108.05	105.80
1	A	1432	A	C8-N9-C4	5.61	108.05	105.80
1	A	1809	A	N9-C4-C5	5.61	108.05	105.80
1	A	2351	A	C4-C5-N7	-5.61	107.89	110.70
1	A	2405	A	C4-C5-N7	-5.61	107.89	110.70
1	A	2594	A	N9-C4-C5	5.61	108.05	105.80
1	A	2663	A	C8-N9-C4	5.61	108.05	105.80
1	A	2835	A	N9-C4-C5	5.61	108.05	105.80
32	W	208	A	N3-C4-N9	5.61	131.89	127.40
32	W	346	A	C8-N9-C4	5.61	108.05	105.80
32	W	364	A	C4-C5-N7	-5.61	107.89	110.70
32	W	823	A	C8-N9-C4	5.61	108.05	105.80
32	W	1111	A	C8-N9-C4	5.61	108.05	105.80
32	W	1205	A	C4-C5-N7	-5.61	107.89	110.70
32	W	1437	A	C4-C5-N7	-5.61	107.89	110.70
1	A	456	A	C4-C5-N7	-5.61	107.89	110.70
1	A	1034	A	C4-C5-N7	-5.61	107.89	110.70
32	W	206	A	N9-C4-C5	5.61	108.05	105.80
32	W	357	A	C8-N9-C4	5.61	108.05	105.80
32	W	803	A	C8-N9-C4	5.61	108.05	105.80
32	W	1050	A	C8-N9-C4	5.61	108.05	105.80
1	A	130	A	N9-C4-C5	5.61	108.04	105.80
1	A	345	A	C8-N9-C4	5.61	108.04	105.80
1	A	893	A	C8-N9-C4	5.61	108.04	105.80
1	A	2307	A	C8-N9-C4	5.61	108.04	105.80
1	A	2479	A	C4-C5-C6	5.61	119.81	117.00
1	A	2643	A	C4-C5-N7	-5.61	107.89	110.70
1	A	2662	A	C8-N9-C4	5.61	108.05	105.80
32	W	74	A	N9-C4-C5	5.61	108.04	105.80
32	W	1289	A	N9-C4-C5	5.61	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1490	A	C8-N9-C4	5.61	108.04	105.80
1	A	162	A	C4-C5-C6	5.61	119.80	117.00
1	A	2875	A	C8-N9-C4	5.61	108.04	105.80
32	W	439	A	N3-C4-N9	5.61	131.89	127.40
32	W	1437	A	C8-N9-C4	5.61	108.04	105.80
1	A	231	A	C8-N9-C4	5.61	108.04	105.80
1	A	1149	A	C8-N9-C4	5.61	108.04	105.80
1	A	1157	A	C8-N9-C4	5.61	108.04	105.80
1	A	1432	A	N3-C4-N9	5.61	131.89	127.40
1	A	1580	A	C4-C5-N7	-5.61	107.90	110.70
1	A	2340	A	C8-N9-C4	5.61	108.04	105.80
1	A	2819	A	N3-C4-N9	5.61	131.89	127.40
1	A	2916	A	C4-C5-N7	-5.61	107.90	110.70
2	B	39	A	C4-C5-C6	5.61	119.80	117.00
32	W	287	A	C4-C5-N7	-5.61	107.90	110.70
32	W	504	A	C4-C5-N7	-5.61	107.90	110.70
32	W	556	A	C4-C5-C6	5.61	119.80	117.00
32	W	979	A	C8-N9-C4	5.61	108.04	105.80
32	W	1004	A	C4-C5-N7	-5.61	107.90	110.70
1	A	71	A	C4-C5-N7	-5.61	107.90	110.70
1	A	2526	A	C8-N9-C4	5.61	108.04	105.80
2	B	27	A	C4-C5-N7	-5.61	107.90	110.70
32	W	28	A	C8-N9-C4	5.61	108.04	105.80
32	W	335	A	C8-N9-C4	5.61	108.04	105.80
32	W	357	A	N9-C4-C5	5.61	108.04	105.80
32	W	382	A	C8-N9-C4	5.61	108.04	105.80
32	W	831	A	C4-C5-N7	-5.61	107.90	110.70
32	W	1050	A	N3-C4-N9	5.61	131.88	127.40
32	W	1056	A	N9-C4-C5	5.61	108.04	105.80
32	W	1222	A	C4-C5-N7	-5.61	107.90	110.70
32	W	512	A	C8-N9-C4	5.60	108.04	105.80
32	W	929	A	N3-C4-N9	5.60	131.88	127.40
32	W	1434	A	N9-C4-C5	5.60	108.04	105.80
1	A	67	A	N3-C4-N9	5.60	131.88	127.40
1	A	345	A	N9-C4-C5	5.60	108.04	105.80
1	A	908	A	N9-C4-C5	5.60	108.04	105.80
1	A	1157	A	C4-C5-C6	5.60	119.80	117.00
1	A	1161	A	C8-N9-C4	5.60	108.04	105.80
1	A	2908	A	N3-C4-N9	5.60	131.88	127.40
32	W	171	A	N3-C4-N9	5.60	131.88	127.40
32	W	415	A	C8-N9-C4	5.60	108.04	105.80
32	W	801	A	C8-N9-C4	5.60	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1157	A	N3-C4-N9	5.60	131.88	127.40
32	W	190	A	C4-C5-N7	-5.60	107.90	110.70
32	W	1260	A	C4-C5-N7	-5.60	107.90	110.70
1	A	278	A	N9-C4-C5	5.60	108.04	105.80
1	A	354	A	C8-N9-C4	5.60	108.04	105.80
1	A	490	A	C4-C5-C6	5.60	119.80	117.00
1	A	1417	A	C4-C5-N7	-5.60	107.90	110.70
1	A	1745	A	C8-N9-C4	5.60	108.04	105.80
1	A	2383	A	N3-C4-N9	5.60	131.88	127.40
1	A	2704	A	N9-C4-C5	5.60	108.04	105.80
1	A	2790	A	C8-N9-C4	5.60	108.04	105.80
1	A	2923	A	C4-C5-N7	-5.60	107.90	110.70
32	W	140	A	C8-N9-C4	5.60	108.04	105.80
32	W	321	A	C4-C5-N7	-5.60	107.90	110.70
32	W	644	A	C8-N9-C4	5.60	108.04	105.80
32	W	816	A	N3-C4-N9	5.60	131.88	127.40
32	W	828	A	C8-N9-C4	5.60	108.04	105.80
32	W	974	A	C8-N9-C4	5.60	108.04	105.80
32	W	1284	A	C8-N9-C4	5.60	108.04	105.80
1	A	154	A	N9-C4-C5	5.60	108.04	105.80
1	A	355	A	N9-C4-C5	5.60	108.04	105.80
1	A	517	A	C8-N9-C4	5.60	108.04	105.80
1	A	543	A	N9-C4-C5	5.60	108.04	105.80
1	A	551	A	C4-C5-N7	-5.60	107.90	110.70
1	A	723	A	C4-C5-C6	5.60	119.80	117.00
1	A	1746	A	C8-N9-C4	5.60	108.04	105.80
1	A	2869	A	C4-C5-N7	-5.60	107.90	110.70
32	W	519	A	N9-C4-C5	5.60	108.04	105.80
1	A	126	A	C4-C5-C6	5.60	119.80	117.00
1	A	384	A	C4-C5-N7	-5.60	107.90	110.70
1	A	456	A	N9-C4-C5	5.60	108.04	105.80
1	A	677	A	C4-C5-N7	-5.60	107.90	110.70
1	A	1325	A	C4-C5-N7	-5.60	107.90	110.70
32	W	31	A	C4-C5-N7	-5.60	107.90	110.70
32	W	985	A	N3-C4-N9	5.60	131.88	127.40
32	W	1054	A	C8-N9-C4	5.60	108.04	105.80
32	W	1238	A	C8-N9-C4	5.60	108.04	105.80
1	A	154	A	C4-C5-N7	-5.59	107.90	110.70
1	A	275	A	N9-C4-C5	5.59	108.04	105.80
1	A	732	A	N9-C4-C5	5.59	108.04	105.80
1	A	1174	A	C8-N9-C4	5.59	108.04	105.80
1	A	1675	A	C8-N9-C4	5.59	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1709	A	C8-N9-C4	5.59	108.04	105.80
1	A	1710	A	C8-N9-C4	5.59	108.04	105.80
1	A	1906	A	N9-C4-C5	5.59	108.04	105.80
1	A	1914	A	C4-C5-N7	-5.59	107.90	110.70
1	A	2907	A	C4-C5-N7	-5.59	107.90	110.70
2	B	44	A	C4-C5-N7	-5.59	107.90	110.70
32	W	460	A	C4-C5-N7	-5.59	107.90	110.70
32	W	685	A	C4-C5-N7	-5.59	107.90	110.70
32	W	1048	A	C4-C5-N7	-5.59	107.90	110.70
32	W	1077	A	N3-C4-N9	5.59	131.88	127.40
1	A	469	A	C4-C5-N7	-5.59	107.90	110.70
1	A	999	A	C4-C5-N7	-5.59	107.90	110.70
1	A	1021	A	C4-C5-N7	-5.59	107.90	110.70
1	A	1188	A	C4-C5-C6	5.59	119.80	117.00
1	A	1745	A	C4-C5-N7	-5.59	107.90	110.70
1	A	1961	A	C4-C5-C6	5.59	119.80	117.00
32	W	323	A	C4-C5-N7	-5.59	107.90	110.70
1	A	199	A	C8-N9-C4	5.59	108.04	105.80
1	A	224	A	C4-C5-C6	5.59	119.80	117.00
1	A	518	A	C8-N9-C4	5.59	108.04	105.80
1	A	1055	A	N9-C4-C5	5.59	108.04	105.80
1	A	1339	A	C4-C5-N7	-5.59	107.90	110.70
1	A	1592	A	C8-N9-C4	5.59	108.04	105.80
1	A	1663	A	C4-C5-N7	-5.59	107.90	110.70
1	A	1713	A	C4-C5-C6	5.59	119.80	117.00
1	A	1791	A	C8-N9-C4	5.59	108.04	105.80
1	A	2511	A	C8-N9-C4	5.59	108.04	105.80
1	A	2683	A	N3-C4-N9	5.59	131.87	127.40
32	W	1528	A	C4-C5-N7	-5.59	107.90	110.70
1	A	342	A	C4-C5-N7	-5.59	107.91	110.70
1	A	518	A	C4-C5-N7	-5.59	107.91	110.70
1	A	866	A	C8-N9-C4	5.59	108.04	105.80
1	A	867	A	N9-C4-C5	5.59	108.04	105.80
1	A	1161	A	N3-C4-N9	5.59	131.87	127.40
1	A	1230	A	C8-N9-C4	5.59	108.04	105.80
1	A	1957	A	C4-C5-N7	-5.59	107.91	110.70
1	A	2595	A	C4-C5-C6	5.59	119.79	117.00
2	B	113	A	N9-C4-C5	5.59	108.04	105.80
32	W	919	A	C8-N9-C4	5.59	108.04	105.80
1	A	479	A	N9-C4-C5	5.59	108.03	105.80
1	A	893	A	C4-C5-N7	-5.59	107.91	110.70
1	A	2315	A	N9-C4-C5	5.59	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2560	A	C4-C5-N7	-5.59	107.91	110.70
1	A	202	A	C8-N9-C4	5.59	108.03	105.80
1	A	1130	A	C4-C5-N7	-5.59	107.91	110.70
1	A	1797	A	C4-C5-N7	-5.59	107.91	110.70
1	A	1876	A	N9-C4-C5	5.59	108.03	105.80
1	A	2754	A	C8-N9-C4	5.59	108.03	105.80
32	W	151	A	C4-C5-N7	-5.59	107.91	110.70
32	W	251	A	N9-C4-C5	5.59	108.03	105.80
32	W	367	A	N3-C4-N9	5.59	131.87	127.40
32	W	1225	A	C4-C5-N7	-5.59	107.91	110.70
32	W	1272	A	C8-N9-C4	5.59	108.03	105.80
32	W	1349	A	C8-N9-C4	5.59	108.03	105.80
32	W	1425	A	N9-C4-C5	5.59	108.03	105.80
52	z	23	A	C5-C6-N1	5.59	120.49	117.70
1	A	236	A	C8-N9-C4	5.58	108.03	105.80
1	A	1784	A	C4-C5-C6	5.58	119.79	117.00
1	A	2042	A	C4-C5-N7	-5.58	107.91	110.70
1	A	2810	A	C8-N9-C4	5.58	108.03	105.80
1	A	2846	A	C8-N9-C4	5.58	108.03	105.80
2	B	102	A	C4-C5-N7	-5.58	107.91	110.70
32	W	170	A	C4-C5-C6	5.58	119.79	117.00
32	W	474	A	C8-N9-C4	5.58	108.03	105.80
32	W	1403	A	C4-C5-N7	-5.58	107.91	110.70
1	A	376	A	C8-N9-C4	5.58	108.03	105.80
1	A	448	A	C4-C5-C6	5.58	119.79	117.00
1	A	1269	A	C4-C5-N7	-5.58	107.91	110.70
1	A	2777	A	N3-C4-N9	5.58	131.87	127.40
32	W	107	A	C4-C5-N7	-5.58	107.91	110.70
32	W	401	A	C8-N9-C4	5.58	108.03	105.80
32	W	556	A	N9-C4-C5	5.58	108.03	105.80
32	W	672	A	C4-C5-N7	-5.58	107.91	110.70
32	W	1121	A	N9-C4-C5	5.58	108.03	105.80
1	A	49	A	N3-C4-N9	5.58	131.87	127.40
1	A	210	A	C8-N9-C4	5.58	108.03	105.80
1	A	762	A	C8-N9-C4	5.58	108.03	105.80
1	A	2006	A	C4-C5-N7	-5.58	107.91	110.70
1	A	2043	A	C8-N9-C4	5.58	108.03	105.80
32	W	306	A	N9-C4-C5	5.58	108.03	105.80
32	W	703	A	N3-C4-N9	5.58	131.87	127.40
32	W	791	A	C4-C5-N7	-5.58	107.91	110.70
32	W	1017	A	N3-C4-N9	5.58	131.87	127.40
32	W	1509	A	C8-N9-C4	5.58	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	476	A	N3-C4-N9	5.58	131.86	127.40
1	A	549	A	C4-C5-N7	-5.58	107.91	110.70
1	A	2062	A	C8-N9-C4	5.58	108.03	105.80
1	A	2505	A	C8-N9-C4	5.58	108.03	105.80
1	A	64	A	N3-C4-N9	5.58	131.86	127.40
1	A	1202	A	C4-C5-C6	5.58	119.79	117.00
1	A	1230	A	N9-C4-C5	5.58	108.03	105.80
1	A	1266	A	N9-C4-C5	5.58	108.03	105.80
1	A	2694	A	C4-C5-N7	-5.58	107.91	110.70
1	A	2830	A	C4-C5-N7	-5.58	107.91	110.70
32	W	12	A	C4-C5-N7	-5.58	107.91	110.70
32	W	404	A	C8-N9-C4	5.58	108.03	105.80
32	W	542	A	N9-C4-C5	5.58	108.03	105.80
32	W	1050	A	N9-C4-C5	5.58	108.03	105.80
32	W	1493	A	C4-C5-N7	-5.58	107.91	110.70
1	A	1746	A	N9-C4-C5	5.58	108.03	105.80
1	A	2295	A	C4-C5-N7	-5.58	107.91	110.70
1	A	2338	A	C8-N9-C4	5.58	108.03	105.80
1	A	2735	A	C8-N9-C4	5.58	108.03	105.80
32	W	996	A	C8-N9-C4	5.58	108.03	105.80
1	A	244	A	N3-C4-N9	5.58	131.86	127.40
1	A	893	A	N9-C4-C5	5.58	108.03	105.80
1	A	974	A	N9-C4-C5	5.58	108.03	105.80
1	A	1047	A	C8-N9-C4	5.58	108.03	105.80
1	A	1784	A	N3-C4-N9	5.58	131.86	127.40
1	A	2338	A	N9-C4-C5	5.58	108.03	105.80
32	W	296	A	N9-C4-C5	5.58	108.03	105.80
32	W	323	A	C8-N9-C4	5.58	108.03	105.80
32	W	485	A	C8-N9-C4	5.58	108.03	105.80
32	W	1197	A	C4-C5-C6	5.58	119.79	117.00
52	z	14	A	C8-N9-C4	5.58	108.03	105.80
1	A	345	A	C4-C5-N7	-5.57	107.91	110.70
1	A	462	A	C8-N9-C4	5.57	108.03	105.80
1	A	543	A	C4-C5-N7	-5.57	107.91	110.70
1	A	584	A	C4-C5-N7	-5.57	107.91	110.70
1	A	811	A	C8-N9-C4	5.57	108.03	105.80
1	A	829	A	C4-C5-N7	-5.57	107.91	110.70
1	A	978	A	N9-C4-C5	5.57	108.03	105.80
1	A	999	A	N9-C4-C5	5.57	108.03	105.80
1	A	1061	A	C4-C5-C6	5.57	119.79	117.00
1	A	1078	A	C4-C5-N7	-5.57	107.91	110.70
1	A	1412	A	C4-C5-C6	5.57	119.79	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2340	A	C4-C5-N7	-5.57	107.91	110.70
1	A	2722	A	C8-N9-C4	5.57	108.03	105.80
1	A	2834	A	C8-N9-C4	5.57	108.03	105.80
32	W	542	A	C4-C5-N7	-5.57	107.91	110.70
32	W	544	A	C8-N9-C4	5.57	108.03	105.80
32	W	1225	A	C8-N9-C4	5.57	108.03	105.80
32	W	1541	A	C4-C5-N7	-5.57	107.91	110.70
52	z	41	A	C4-C5-N7	-5.57	107.91	110.70
1	A	1190	A	C8-N9-C4	5.57	108.03	105.80
1	A	1406	A	C4-C5-N7	-5.57	107.91	110.70
1	A	1456	A	C4-C5-N7	-5.57	107.91	110.70
1	A	2303	A	N9-C4-C5	5.57	108.03	105.80
1	A	2517	A	C8-N9-C4	5.57	108.03	105.80
32	W	160	A	C8-N9-C4	5.57	108.03	105.80
32	W	544	A	N9-C4-C5	5.57	108.03	105.80
1	A	140	A	C4-C5-N7	-5.57	107.92	110.70
1	A	527	A	C4-C5-N7	-5.57	107.92	110.70
1	A	658	A	N9-C4-C5	5.57	108.03	105.80
1	A	1813	A	C4-C5-N7	-5.57	107.92	110.70
1	A	1918	A	N9-C4-C5	5.57	108.03	105.80
1	A	1981	A	C4-C5-N7	-5.57	107.92	110.70
1	A	1995	A	N9-C4-C5	5.57	108.03	105.80
1	A	2398	A	C8-N9-C4	5.57	108.03	105.80
32	W	791	A	C8-N9-C4	5.57	108.03	105.80
32	W	1435	A	N9-C4-C5	5.57	108.03	105.80
32	W	1437	A	N9-C4-C5	5.57	108.03	105.80
1	A	1175	A	N9-C4-C5	5.57	108.03	105.80
1	A	2670	A	C4-C5-C6	5.57	119.78	117.00
32	W	282	A	C8-N9-C4	5.57	108.03	105.80
1	A	124	A	C4-C5-N7	-5.57	107.92	110.70
1	A	166	A	C4-C5-N7	-5.57	107.92	110.70
1	A	683	A	N9-C4-C5	5.57	108.03	105.80
1	A	2542	A	N9-C4-C5	5.57	108.03	105.80
32	W	34	A	C4-C5-N7	-5.57	107.92	110.70
32	W	159	A	N9-C4-C5	5.57	108.03	105.80
32	W	178	A	N9-C4-C5	5.57	108.03	105.80
32	W	228	A	C4-C5-N7	-5.57	107.92	110.70
32	W	541	A	N9-C4-C5	5.57	108.03	105.80
32	W	799	A	C8-N9-C4	5.57	108.03	105.80
32	W	1417	A	C8-N9-C4	5.57	108.03	105.80
1	A	125	A	C4-C5-C6	5.57	119.78	117.00
1	A	1615	A	C8-N9-C4	5.57	108.03	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2338	A	C4-C5-N7	-5.57	107.92	110.70
1	A	2570	A	C4-C5-N7	-5.57	107.92	110.70
1	A	2673	A	N9-C4-C5	5.57	108.03	105.80
32	W	1245	A	C8-N9-C4	5.57	108.03	105.80
1	A	102	A	C4-C5-N7	-5.56	107.92	110.70
1	A	162	A	N9-C4-C5	5.56	108.03	105.80
1	A	2089	A	N3-C4-N9	5.56	131.85	127.40
1	A	2297	A	C8-N9-C4	5.56	108.03	105.80
1	A	1679	A	N9-C4-C5	5.56	108.03	105.80
1	A	1746	A	C4-C5-N7	-5.56	107.92	110.70
32	W	10	A	C4-C5-N7	-5.56	107.92	110.70
32	W	34	A	C8-N9-C4	5.56	108.03	105.80
32	W	178	A	C8-N9-C4	5.56	108.03	105.80
32	W	278	A	C8-N9-C4	5.56	108.03	105.80
32	W	786	A	C4-C5-N7	-5.56	107.92	110.70
32	W	824	A	C4-C5-N7	-5.56	107.92	110.70
32	W	1488	A	N9-C4-C5	5.56	108.03	105.80
1	A	222	A	C8-N9-C4	5.56	108.03	105.80
1	A	476	A	C4-C5-N7	-5.56	107.92	110.70
1	A	1141	A	N9-C4-C5	5.56	108.03	105.80
1	A	1888	A	C8-N9-C4	5.56	108.02	105.80
1	A	2375	A	C4-C5-C6	5.56	119.78	117.00
1	A	2542	A	C4-C5-N7	-5.56	107.92	110.70
2	B	71	A	C4-C5-N7	-5.56	107.92	110.70
32	W	240	A	C4-C5-N7	-5.56	107.92	110.70
1	A	118	A	N9-C4-C5	5.56	108.02	105.80
1	A	821	A	C4-C5-N7	-5.56	107.92	110.70
1	A	1677	A	C4-C5-N7	-5.56	107.92	110.70
1	A	2593	A	C4-C5-N7	-5.56	107.92	110.70
1	A	2618	A	C4-C5-C6	5.56	119.78	117.00
1	A	2804	A	C8-N9-C4	5.56	108.02	105.80
2	B	11	A	C4-C5-N7	-5.56	107.92	110.70
2	B	114	A	C4-C5-N7	-5.56	107.92	110.70
32	W	1225	A	N9-C4-C5	5.56	108.02	105.80
32	W	1254	A	C4-C5-N7	-5.56	107.92	110.70
1	A	225	A	C8-N9-C4	5.56	108.02	105.80
1	A	412	A	C4-C5-N7	-5.56	107.92	110.70
1	A	561	A	C8-N9-C4	5.56	108.02	105.80
1	A	1144	A	C4-C5-N7	-5.56	107.92	110.70
1	A	1617	A	C8-N9-C4	5.56	108.02	105.80
1	A	1877	A	C4-C5-N7	-5.56	107.92	110.70
1	A	2032	A	C4-C5-N7	-5.56	107.92	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2461	A	N9-C4-C5	5.56	108.02	105.80
1	A	2826	A	C8-N9-C4	5.56	108.02	105.80
2	B	17	A	N3-C4-N9	5.56	131.85	127.40
32	W	204	A	C4-C5-N7	-5.56	107.92	110.70
32	W	210	A	C4-C5-N7	-5.56	107.92	110.70
32	W	501	A	C8-N9-C4	5.56	108.02	105.80
32	W	1092	A	C4-C5-N7	-5.56	107.92	110.70
1	A	2902	A	N9-C4-C5	5.56	108.02	105.80
1	A	10	A	C4-C5-N7	-5.55	107.92	110.70
1	A	202	A	N3-C4-N9	5.55	131.84	127.40
1	A	925	A	C4-C5-N7	-5.55	107.92	110.70
1	A	1326	A	C4-C5-N7	-5.55	107.92	110.70
1	A	1832	A	C4-C5-N7	-5.55	107.92	110.70
1	A	2030	A	N3-C4-N9	5.55	131.84	127.40
1	A	2357	A	N9-C4-C5	5.55	108.02	105.80
32	W	281	A	C4-C5-N7	-5.55	107.92	110.70
32	W	532	A	C4-C5-N7	-5.55	107.92	110.70
32	W	685	A	N9-C4-C5	5.55	108.02	105.80
32	W	928	A	C8-N9-C4	5.55	108.02	105.80
32	W	956	A	C8-N9-C4	5.55	108.02	105.80
32	W	1121	A	C4-C5-N7	-5.55	107.92	110.70
1	A	339	A	N9-C4-C5	5.55	108.02	105.80
1	A	740	A	N9-C4-C5	5.55	108.02	105.80
1	A	1235	A	N9-C4-C5	5.55	108.02	105.80
1	A	2464	A	N9-C4-C5	5.55	108.02	105.80
32	W	236	A	C4-C5-N7	-5.55	107.92	110.70
32	W	333	A	C4-C5-N7	-5.55	107.92	110.70
32	W	1024	A	N9-C4-C5	5.55	108.02	105.80
32	W	1102	A	C8-N9-C4	5.55	108.02	105.80
32	W	1470	A	N9-C4-C5	5.55	108.02	105.80
1	A	194	A	C4-C5-N7	-5.55	107.92	110.70
1	A	198	A	N9-C4-C5	5.55	108.02	105.80
1	A	354	A	C4-C5-C6	5.55	119.78	117.00
1	A	1042	A	C8-N9-C4	5.55	108.02	105.80
1	A	1100	A	C8-N9-C4	5.55	108.02	105.80
1	A	1144	A	C8-N9-C4	5.55	108.02	105.80
1	A	1326	A	N9-C4-C5	5.55	108.02	105.80
1	A	1832	A	N9-C4-C5	5.55	108.02	105.80
1	A	2406	A	C8-N9-C4	5.55	108.02	105.80
32	W	631	A	C4-C5-N7	-5.55	107.92	110.70
1	A	868	A	C8-N9-C4	5.55	108.02	105.80
1	A	1392	A	C8-N9-C4	5.55	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1906	A	C8-N9-C4	5.55	108.02	105.80
1	A	2482	A	N9-C4-C5	5.55	108.02	105.80
1	A	2606	A	C8-N9-C4	5.55	108.02	105.80
32	W	415	A	N9-C4-C5	5.55	108.02	105.80
32	W	491	A	C4-C5-N7	-5.55	107.92	110.70
32	W	500	A	C8-N9-C4	5.55	108.02	105.80
32	W	669	A	N9-C4-C5	5.55	108.02	105.80
1	A	829	A	C8-N9-C4	5.55	108.02	105.80
1	A	1243	A	C4-C5-N7	-5.55	107.93	110.70
1	A	1323	A	C8-N9-C4	5.55	108.02	105.80
1	A	2034	A	C4-C5-N7	-5.55	107.93	110.70
1	A	2276	A	C4-C5-N7	-5.55	107.93	110.70
32	W	823	A	C4-C5-N7	-5.55	107.93	110.70
32	W	925	A	C4-C5-N7	-5.55	107.93	110.70
32	W	1257	A	C4-C5-N7	-5.55	107.93	110.70
1	A	118	A	C8-N9-C4	5.55	108.02	105.80
1	A	178	A	C4-C5-N7	-5.55	107.93	110.70
1	A	354	A	N3-C4-N9	5.55	131.84	127.40
1	A	575	A	N3-C4-N9	5.55	131.84	127.40
1	A	746	A	C8-N9-C4	5.55	108.02	105.80
1	A	896	A	C8-N9-C4	5.55	108.02	105.80
1	A	1021	A	N9-C4-C5	5.55	108.02	105.80
1	A	2834	A	N9-C4-C5	5.55	108.02	105.80
32	W	171	A	C8-N9-C4	5.55	108.02	105.80
32	W	232	A	N9-C4-C5	5.55	108.02	105.80
32	W	266	A	N3-C4-N9	5.55	131.84	127.40
32	W	664	A	C8-N9-C4	5.55	108.02	105.80
32	W	743	A	C8-N9-C4	5.55	108.02	105.80
32	W	1205	A	C8-N9-C4	5.55	108.02	105.80
1	A	548	A	C4-C5-N7	-5.54	107.93	110.70
1	A	574	A	C4-C5-N7	-5.54	107.93	110.70
1	A	763	A	C4-C5-N7	-5.54	107.93	110.70
1	A	1815	A	C4-C5-N7	-5.54	107.93	110.70
1	A	2357	A	C4-C5-N7	-5.54	107.93	110.70
32	W	438	A	C8-N9-C4	5.54	108.02	105.80
1	A	575	A	C4-C5-C6	5.54	119.77	117.00
1	A	647	A	N3-C4-N9	5.54	131.84	127.40
1	A	1005	A	C4-C5-N7	-5.54	107.93	110.70
1	A	1230	A	C4-C5-N7	-5.54	107.93	110.70
32	W	281	A	N9-C4-C5	5.54	108.02	105.80
32	W	296	A	C8-N9-C4	5.54	108.02	105.80
32	W	831	A	N9-C4-C5	5.54	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	z	58	A	C8-N9-C4	5.54	108.02	105.80
1	A	124	A	N9-C4-C5	5.54	108.02	105.80
1	A	329	A	C8-N9-C4	5.54	108.02	105.80
1	A	637	A	C4-C5-N7	-5.54	107.93	110.70
1	A	1003	A	N9-C4-C5	5.54	108.02	105.80
1	A	1119	A	N9-C4-C5	5.54	108.02	105.80
1	A	1540	A	C4-C5-N7	-5.54	107.93	110.70
1	A	2049	A	C8-N9-C4	5.54	108.02	105.80
1	A	2769	A	C8-N9-C4	5.54	108.02	105.80
1	A	2900	A	C8-N9-C4	5.54	108.02	105.80
32	W	61	A	C8-N9-C4	5.54	108.02	105.80
32	W	337	A	C8-N9-C4	5.54	108.02	105.80
32	W	618	A	C4-C5-N7	-5.54	107.93	110.70
32	W	816	A	N9-C4-C5	5.54	108.02	105.80
32	W	1090	A	C4-C5-N7	-5.54	107.93	110.70
32	W	1090	A	N9-C4-C5	5.54	108.02	105.80
32	W	1284	A	C4-C5-N7	-5.54	107.93	110.70
32	W	1503	A	C4-C5-N7	-5.54	107.93	110.70
32	W	1523	A	C4-C5-N7	-5.54	107.93	110.70
1	A	244	A	C4-C5-C6	5.54	119.77	117.00
1	A	355	A	C4-C5-N7	-5.54	107.93	110.70
1	A	530	A	C8-N9-C4	5.54	108.02	105.80
1	A	1965	A	C4-C5-N7	-5.54	107.93	110.70
1	A	2052	A	C4-C5-N7	-5.54	107.93	110.70
2	B	113	A	C4-C5-N7	-5.54	107.93	110.70
32	W	117	A	C8-N9-C4	5.54	108.02	105.80
1	A	274	A	C4-C5-N7	-5.54	107.93	110.70
1	A	275	A	C4-C5-N7	-5.54	107.93	110.70
1	A	2083	A	C4-C5-C6	5.54	119.77	117.00
32	W	62	A	C4-C5-N7	-5.54	107.93	110.70
32	W	544	A	C4-C5-N7	-5.54	107.93	110.70
1	A	723	A	C8-N9-C4	5.54	108.02	105.80
1	A	1406	A	N9-C4-C5	5.54	108.02	105.80
1	A	1499	A	C8-N9-C4	5.54	108.02	105.80
1	A	2295	A	N3-C4-N9	5.54	131.83	127.40
1	A	2343	A	N9-C4-C5	5.54	108.02	105.80
1	A	2902	A	C8-N9-C4	5.54	108.02	105.80
32	W	189	A	C8-N9-C4	5.54	108.02	105.80
32	W	902	A	N9-C4-C5	5.54	108.02	105.80
52	z	58	A	C4-C5-N7	-5.54	107.93	110.70
1	A	28	A	C4-C5-N7	-5.54	107.93	110.70
1	A	126	A	N3-C4-N9	5.54	131.83	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	A	C4-C5-N7	-5.54	107.93	110.70
1	A	324	A	C4-C5-N7	-5.54	107.93	110.70
1	A	449	A	C8-N9-C4	5.54	108.01	105.80
1	A	490	A	N3-C4-N9	5.54	131.83	127.40
1	A	496	A	C8-N9-C4	5.54	108.01	105.80
1	A	543	A	C8-N9-C4	5.54	108.01	105.80
1	A	1286	A	C8-N9-C4	5.54	108.01	105.80
1	A	1325	A	N9-C4-C5	5.54	108.01	105.80
1	A	1636	A	C4-C5-N7	-5.54	107.93	110.70
1	A	1941	A	C4-C5-C6	5.54	119.77	117.00
1	A	1989	A	C8-N9-C4	5.54	108.01	105.80
1	A	2088	A	C4-C5-N7	-5.54	107.93	110.70
1	A	2389	A	C8-N9-C4	5.54	108.01	105.80
2	B	43	A	C4-C5-N7	-5.54	107.93	110.70
32	W	225	A	C4-C5-N7	-5.54	107.93	110.70
32	W	462	A	C4-C5-N7	-5.54	107.93	110.70
32	W	500	A	N3-C4-N9	5.54	131.83	127.40
32	W	690	A	C8-N9-C4	5.54	108.01	105.80
32	W	1261	A	C8-N9-C4	5.54	108.01	105.80
32	W	1384	A	C8-N9-C4	5.54	108.01	105.80
1	A	91	A	N9-C4-C5	5.53	108.01	105.80
1	A	194	A	C8-N9-C4	5.53	108.01	105.80
1	A	519	A	C8-N9-C4	5.53	108.01	105.80
1	A	553	A	C4-C5-N7	-5.53	107.93	110.70
1	A	922	A	C4-C5-N7	-5.53	107.93	110.70
1	A	991	A	C8-N9-C4	5.53	108.01	105.80
1	A	1132	A	N9-C4-C5	5.53	108.01	105.80
1	A	1335	A	C8-N9-C4	5.53	108.01	105.80
1	A	1388	A	C8-N9-C4	5.53	108.01	105.80
1	A	1627	A	C4-C5-N7	-5.53	107.93	110.70
1	A	1699	A	C8-N9-C4	5.53	108.01	105.80
1	A	1877	A	N9-C4-C5	5.53	108.01	105.80
1	A	2356	A	C8-N9-C4	5.53	108.01	105.80
1	A	2369	A	C8-N9-C4	5.53	108.01	105.80
1	A	2375	A	N3-C4-N9	5.53	131.83	127.40
1	A	2629	A	C8-N9-C4	5.53	108.01	105.80
2	B	17	A	C4-C5-N7	-5.53	107.93	110.70
2	B	56	A	C8-N9-C4	5.53	108.01	105.80
32	W	150	A	C4-C5-N7	-5.53	107.93	110.70
32	W	423	A	N9-C4-C5	5.53	108.01	105.80
32	W	1111	A	N9-C4-C5	5.53	108.01	105.80
1	A	355	A	C8-N9-C4	5.53	108.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	477	A	N3-C4-N9	5.53	131.82	127.40
1	A	910	A	C8-N9-C4	5.53	108.01	105.80
1	A	2834	A	C4-C5-N7	-5.53	107.93	110.70
32	W	53	A	N9-C4-C5	5.53	108.01	105.80
32	W	171	A	N9-C4-C5	5.53	108.01	105.80
32	W	1256	A	C8-N9-C4	5.53	108.01	105.80
1	A	258	A	C8-N9-C4	5.53	108.01	105.80
1	A	470	A	C4-C5-N7	-5.53	107.94	110.70
1	A	1084	A	N9-C4-C5	5.53	108.01	105.80
1	A	1202	A	C4-C5-N7	-5.53	107.93	110.70
1	A	1601	A	C8-N9-C4	5.53	108.01	105.80
1	A	1685	A	C8-N9-C4	5.53	108.01	105.80
1	A	1760	A	N9-C4-C5	5.53	108.01	105.80
1	A	1784	A	N9-C4-C5	5.53	108.01	105.80
32	W	240	A	N9-C4-C5	5.53	108.01	105.80
32	W	329	A	N9-C4-C5	5.53	108.01	105.80
32	W	401	A	C4-C5-C6	5.53	119.77	117.00
32	W	477	A	N9-C4-C5	5.53	108.01	105.80
32	W	506	A	C8-N9-C4	5.53	108.01	105.80
32	W	1372	A	C8-N9-C4	5.53	108.01	105.80
1	A	723	A	C4-C5-N7	-5.53	107.94	110.70
1	A	943	A	C8-N9-C4	5.53	108.01	105.80
1	A	1201	A	C8-N9-C4	5.53	108.01	105.80
1	A	2480	A	C4-C5-N7	-5.53	107.94	110.70
1	A	2769	A	C4-C5-N7	-5.53	107.94	110.70
1	A	219	A	C4-C5-N7	-5.53	107.94	110.70
1	A	847	A	C4-C5-C6	5.53	119.76	117.00
1	A	851	A	N9-C4-C5	5.53	108.01	105.80
1	A	1078	A	C8-N9-C4	5.53	108.01	105.80
1	A	1556	A	N9-C4-C5	5.53	108.01	105.80
1	A	2295	A	C8-N9-C4	5.53	108.01	105.80
1	A	2463	A	C4-C5-N7	-5.53	107.94	110.70
32	W	52	A	N9-C4-C5	5.53	108.01	105.80
32	W	1320	A	C8-N9-C4	5.53	108.01	105.80
32	W	1510	A	N9-C4-C5	5.53	108.01	105.80
1	A	479	A	C4-C5-N7	-5.53	107.94	110.70
1	A	500	A	C4-C5-N7	-5.53	107.94	110.70
1	A	618	A	C8-N9-C4	5.53	108.01	105.80
1	A	2804	A	N9-C4-C5	5.53	108.01	105.80
1	A	2831	A	N9-C4-C5	5.53	108.01	105.80
32	W	28	A	C4-C5-N7	-5.53	107.94	110.70
32	W	55	A	C8-N9-C4	5.53	108.01	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	616	A	C8-N9-C4	5.53	108.01	105.80
32	W	886	A	N9-C4-C5	5.53	108.01	105.80
32	W	1210	A	C4-C5-N7	-5.53	107.94	110.70
32	W	1422	A	N9-C4-C5	5.53	108.01	105.80
1	A	12	A	C8-N9-C4	5.52	108.01	105.80
1	A	2316	A	C8-N9-C4	5.52	108.01	105.80
1	A	2387	A	C8-N9-C4	5.52	108.01	105.80
32	W	923	A	N9-C4-C5	5.52	108.01	105.80
1	A	600	A	C4-C5-N7	-5.52	107.94	110.70
1	A	727	A	C8-N9-C4	5.52	108.01	105.80
1	A	1097	A	N9-C4-C5	5.52	108.01	105.80
1	A	1346	A	C8-N9-C4	5.52	108.01	105.80
1	A	1483	A	N9-C4-C5	5.52	108.01	105.80
1	A	1619	A	N9-C4-C5	5.52	108.01	105.80
1	A	1789	A	C8-N9-C4	5.52	108.01	105.80
1	A	2812	A	C8-N9-C4	5.52	108.01	105.80
1	A	2893	A	N9-C4-C5	5.52	108.01	105.80
2	B	46	A	C8-N9-C4	5.52	108.01	105.80
32	W	329	A	C8-N9-C4	5.52	108.01	105.80
32	W	879	A	C4-C5-C6	5.52	119.76	117.00
32	W	1028	A	C4-C5-N7	-5.52	107.94	110.70
32	W	1103	A	C4-C5-N7	-5.52	107.94	110.70
32	W	1294	A	C8-N9-C4	5.52	108.01	105.80
1	A	244	A	C4-C5-N7	-5.52	107.94	110.70
1	A	582	A	C4-C5-N7	-5.52	107.94	110.70
1	A	1066	A	C4-C5-N7	-5.52	107.94	110.70
1	A	1556	A	C4-C5-N7	-5.52	107.94	110.70
1	A	1789	A	N9-C4-C5	5.52	108.01	105.80
1	A	2570	A	C8-N9-C4	5.52	108.01	105.80
1	A	2769	A	N9-C4-C5	5.52	108.01	105.80
32	W	232	A	N3-C4-N9	5.52	131.82	127.40
1	A	732	A	C4-C5-C6	5.52	119.76	117.00
1	A	956	A	C8-N9-C4	5.52	108.01	105.80
1	A	991	A	N3-C4-N9	5.52	131.81	127.40
1	A	1092	A	C8-N9-C4	5.52	108.01	105.80
1	A	1722	A	C8-N9-C4	5.52	108.01	105.80
1	A	1844	A	C4-C5-N7	-5.52	107.94	110.70
1	A	2876	A	C4-C5-N7	-5.52	107.94	110.70
2	B	102	A	N9-C4-C5	5.52	108.01	105.80
32	W	72	A	C8-N9-C4	5.52	108.01	105.80
32	W	323	A	N9-C4-C5	5.52	108.01	105.80
32	W	1271	A	C4-C5-N7	-5.52	107.94	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1528	A	C8-N9-C4	5.52	108.01	105.80
1	A	38	A	C4-C5-N7	-5.52	107.94	110.70
1	A	572	A	N9-C4-C5	5.52	108.01	105.80
1	A	811	A	C4-C5-N7	-5.52	107.94	110.70
1	A	1189	A	N9-C4-C5	5.52	108.01	105.80
1	A	2018	A	N9-C4-C5	5.52	108.01	105.80
32	W	659	A	C8-N9-C4	5.52	108.01	105.80
32	W	669	A	C4-C5-N7	-5.52	107.94	110.70
32	W	1456	A	C4-C5-N7	-5.52	107.94	110.70
1	A	437	A	C8-N9-C4	5.52	108.01	105.80
1	A	1260	A	C8-N9-C4	5.52	108.01	105.80
1	A	1583	A	C8-N9-C4	5.52	108.01	105.80
1	A	2762	A	C4-C5-N7	-5.52	107.94	110.70
1	A	2793	A	C8-N9-C4	5.52	108.01	105.80
32	W	501	A	N9-C4-C5	5.52	108.01	105.80
32	W	542	A	C8-N9-C4	5.52	108.01	105.80
32	W	1179	A	C4-C5-N7	-5.52	107.94	110.70
1	A	376	A	C4-C5-N7	-5.51	107.94	110.70
1	A	699	A	C4-C5-N7	-5.51	107.94	110.70
1	A	705	A	C4-C5-N7	-5.51	107.94	110.70
1	A	1059	A	C8-N9-C4	5.51	108.00	105.80
1	A	1061	A	N3-C4-N9	5.51	131.81	127.40
1	A	1405	A	N9-C4-C5	5.51	108.01	105.80
1	A	1432	A	N9-C4-C5	5.51	108.01	105.80
1	A	1524	A	C4-C5-N7	-5.51	107.94	110.70
1	A	1541	A	C8-N9-C4	5.51	108.01	105.80
1	A	1588	A	N9-C4-C5	5.51	108.01	105.80
32	W	251	A	C4-C5-N7	-5.51	107.94	110.70
32	W	475	A	N9-C4-C5	5.51	108.01	105.80
1	A	279	A	C4-C5-N7	-5.51	107.94	110.70
1	A	530	A	C4-C5-N7	-5.51	107.94	110.70
1	A	1839	A	C4-C5-N7	-5.51	107.94	110.70
1	A	1895	A	C4-C5-N7	-5.51	107.94	110.70
1	A	2643	A	C8-N9-C4	5.51	108.00	105.80
32	W	1320	A	N9-C4-C5	5.51	108.00	105.80
1	A	322	A	C8-N9-C4	5.51	108.00	105.80
1	A	330	A	C8-N9-C4	5.51	108.00	105.80
1	A	456	A	C8-N9-C4	5.51	108.00	105.80
1	A	1092	A	N9-C4-C5	5.51	108.00	105.80
1	A	1956	A	C8-N9-C4	5.51	108.00	105.80
1	A	2060	A	C8-N9-C4	5.51	108.00	105.80
1	A	2296	A	N9-C4-C5	5.51	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2924	A	C4-C5-N7	-5.51	107.94	110.70
1	A	73	A	N9-C4-C5	5.51	108.00	105.80
1	A	273	A	C4-C5-C6	5.51	119.75	117.00
1	A	391	A	C8-N9-C4	5.51	108.00	105.80
1	A	1631	A	C8-N9-C4	5.51	108.00	105.80
1	A	1695	A	C8-N9-C4	5.51	108.00	105.80
1	A	2327	A	C8-N9-C4	5.51	108.00	105.80
1	A	2793	A	C4-C5-N7	-5.51	107.94	110.70
1	A	2902	A	C4-C5-N7	-5.51	107.94	110.70
32	W	190	A	N9-C4-C5	5.51	108.00	105.80
32	W	203	A	C8-N9-C4	5.51	108.00	105.80
32	W	203	A	N9-C4-C5	5.51	108.00	105.80
32	W	254	A	N3-C4-N9	5.51	131.81	127.40
32	W	737	A	C8-N9-C4	5.51	108.00	105.80
32	W	837	A	C4-C5-C6	5.51	119.75	117.00
32	W	870	A	C8-N9-C4	5.51	108.00	105.80
32	W	1031	A	C8-N9-C4	5.51	108.00	105.80
52	z	14	A	C4-C5-N7	-5.51	107.94	110.70
1	A	781	A	C4-C5-N7	-5.51	107.95	110.70
1	A	2383	A	C8-N9-C4	5.51	108.00	105.80
1	A	978	A	C4-C5-N7	-5.51	107.95	110.70
1	A	1036	A	N9-C4-C5	5.51	108.00	105.80
1	A	2270	A	C8-N9-C4	5.51	108.00	105.80
2	B	37	A	N9-C4-C5	5.51	108.00	105.80
2	B	102	A	C4-C5-C6	5.51	119.75	117.00
32	W	170	A	C8-N9-C4	5.51	108.00	105.80
32	W	1466	A	C4-C5-N7	-5.51	107.95	110.70
1	A	254	A	C5-C6-N1	5.50	120.45	117.70
1	A	259	A	C8-N9-C4	5.50	108.00	105.80
1	A	326	A	N9-C4-C5	5.50	108.00	105.80
1	A	1005	A	C8-N9-C4	5.50	108.00	105.80
1	A	1442	A	C8-N9-C4	5.50	108.00	105.80
1	A	1797	A	N9-C4-C5	5.50	108.00	105.80
1	A	2767	A	C4-C5-N7	-5.50	107.95	110.70
2	B	44	A	N9-C4-C5	5.50	108.00	105.80
1	A	305	A	C8-N9-C4	5.50	108.00	105.80
1	A	560	A	N9-C4-C5	5.50	108.00	105.80
1	A	1269	A	N9-C4-C5	5.50	108.00	105.80
1	A	1312	A	C4-C5-N7	-5.50	107.95	110.70
1	A	1947	A	C4-C5-N7	-5.50	107.95	110.70
1	A	2078	A	C8-N9-C4	5.50	108.00	105.80
32	W	306	A	C4-C5-N7	-5.50	107.95	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1486	A	C8-N9-C4	5.50	108.00	105.80
1	A	224	A	N9-C4-C5	5.50	108.00	105.80
1	A	302	A	N3-C4-N9	5.50	131.80	127.40
1	A	530	A	N9-C4-C5	5.50	108.00	105.80
1	A	715	A	C8-N9-C4	5.50	108.00	105.80
1	A	2542	A	C8-N9-C4	5.50	108.00	105.80
1	A	2618	A	C8-N9-C4	5.50	108.00	105.80
32	W	202	A	C8-N9-C4	5.50	108.00	105.80
32	W	282	A	C4-C5-N7	-5.50	107.95	110.70
32	W	791	A	N9-C4-C5	5.50	108.00	105.80
32	W	1386	A	C4-C5-N7	-5.50	107.95	110.70
32	W	1422	A	C4-C5-N7	-5.50	107.95	110.70
1	A	224	A	C4-C5-N7	-5.50	107.95	110.70
1	A	353	A	C4-C5-N7	-5.50	107.95	110.70
1	A	1631	A	C4-C5-N7	-5.50	107.95	110.70
1	A	1724	A	N9-C4-C5	5.50	108.00	105.80
1	A	1743	A	N9-C4-C5	5.50	108.00	105.80
1	A	1999	A	C8-N9-C4	5.50	108.00	105.80
1	A	179	A	C8-N9-C4	5.50	108.00	105.80
1	A	200	A	N9-C4-C5	5.50	108.00	105.80
1	A	678	A	C4-C5-N7	-5.50	107.95	110.70
1	A	1014	A	C4-C5-N7	-5.50	107.95	110.70
1	A	1222	A	C8-N9-C4	5.50	108.00	105.80
1	A	1314	A	C4-C5-N7	-5.50	107.95	110.70
1	A	1734	A	C4-C5-N7	-5.50	107.95	110.70
1	A	1818	A	C4-C5-N7	-5.50	107.95	110.70
1	A	2375	A	C4-C5-N7	-5.50	107.95	110.70
1	A	2479	A	N9-C4-C5	5.50	108.00	105.80
1	A	2686	A	N9-C4-C5	5.50	108.00	105.80
32	W	306	A	C8-N9-C4	5.50	108.00	105.80
32	W	1248	A	C4-C5-N7	-5.50	107.95	110.70
1	A	207	A	N9-C4-C5	5.50	108.00	105.80
1	A	325	A	C4-C5-N7	-5.50	107.95	110.70
1	A	723	A	N3-C4-N9	5.50	131.80	127.40
1	A	746	A	C4-C5-N7	-5.50	107.95	110.70
1	A	1313	A	C4-C5-N7	-5.50	107.95	110.70
1	A	1677	A	C8-N9-C4	5.50	108.00	105.80
1	A	2027	A	C8-N9-C4	5.50	108.00	105.80
1	A	2059	A	N9-C4-C5	5.50	108.00	105.80
1	A	2619	A	C8-N9-C4	5.50	108.00	105.80
1	A	2629	A	N9-C4-C5	5.50	108.00	105.80
1	A	2770	A	C4-C5-N7	-5.50	107.95	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	583	A	N3-C4-N9	5.50	131.80	127.40
32	W	816	A	C4-C5-N7	-5.50	107.95	110.70
32	W	1200	A	N9-C4-C5	5.50	108.00	105.80
1	A	14	A	N9-C4-C5	5.50	108.00	105.80
52	z	44	A	C8-N9-C4	5.50	108.00	105.80
1	A	118	A	N3-C4-N9	5.49	131.79	127.40
1	A	835	A	N9-C4-C5	5.49	108.00	105.80
1	A	851	A	C4-C5-N7	-5.49	107.95	110.70
1	A	894	A	C4-C5-N7	-5.49	107.95	110.70
1	A	1061	A	N9-C4-C5	5.49	108.00	105.80
1	A	1850	A	C8-N9-C4	5.49	108.00	105.80
1	A	1850	A	N9-C4-C5	5.49	108.00	105.80
1	A	2482	A	C8-N9-C4	5.49	108.00	105.80
1	A	2590	A	N9-C4-C5	5.49	108.00	105.80
1	A	2787	A	C8-N9-C4	5.49	108.00	105.80
32	W	364	A	C8-N9-C4	5.49	108.00	105.80
32	W	568	A	C4-C5-N7	-5.49	107.95	110.70
32	W	630	A	N9-C4-C5	5.49	108.00	105.80
32	W	715	A	C8-N9-C4	5.49	108.00	105.80
32	W	929	A	C4-C5-N7	-5.49	107.95	110.70
32	W	1278	A	N9-C4-C5	5.49	108.00	105.80
32	W	1403	A	C8-N9-C4	5.49	108.00	105.80
1	A	200	A	C4-C5-N7	-5.49	107.95	110.70
1	A	811	A	N3-C4-N9	5.49	131.79	127.40
1	A	849	A	N9-C4-C5	5.49	108.00	105.80
1	A	1103	A	C8-N9-C4	5.49	108.00	105.80
2	B	56	A	C4-C5-N7	-5.49	107.95	110.70
32	W	1417	A	C4-C5-N7	-5.49	107.95	110.70
1	A	770	A	C4-C5-N7	-5.49	107.95	110.70
1	A	1115	A	C8-N9-C4	5.49	108.00	105.80
1	A	1190	A	C4-C5-N7	-5.49	107.95	110.70
1	A	1499	A	C4-C5-N7	-5.49	107.95	110.70
1	A	1585	A	N9-C4-C5	5.49	108.00	105.80
1	A	1760	A	C4-C5-N7	-5.49	107.95	110.70
1	A	2846	A	C4-C5-N7	-5.49	107.95	110.70
32	W	529	A	C8-N9-C4	5.49	108.00	105.80
32	W	762	A	C4-C5-N7	-5.49	107.95	110.70
32	W	1028	A	N9-C4-C5	5.49	108.00	105.80
32	W	1407	A	C4-C5-N7	-5.49	107.95	110.70
1	A	64	A	N9-C4-C5	5.49	108.00	105.80
1	A	330	A	C4-C5-N7	-5.49	107.96	110.70
1	A	965	A	N9-C4-C5	5.49	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1061	A	C4-C5-N7	-5.49	107.96	110.70
1	A	1844	A	C4-C5-C6	5.49	119.74	117.00
1	A	2006	A	C8-N9-C4	5.49	108.00	105.80
1	A	2869	A	N9-C4-C5	5.49	108.00	105.80
32	W	18	A	C4-C5-C6	5.49	119.74	117.00
32	W	422	A	C8-N9-C4	5.49	108.00	105.80
32	W	438	A	C4-C5-C6	5.49	119.74	117.00
32	W	522	A	N9-C4-C5	5.49	108.00	105.80
32	W	582	A	C8-N9-C4	5.49	108.00	105.80
32	W	1200	A	C4-C5-N7	-5.49	107.96	110.70
32	W	1271	A	N9-C4-C5	5.49	108.00	105.80
1	A	582	A	N9-C4-C5	5.49	108.00	105.80
1	A	1876	A	C4-C5-N7	-5.49	107.96	110.70
1	A	1967	A	C4-C5-N7	-5.49	107.96	110.70
1	A	2071	A	C4-C5-N7	-5.49	107.96	110.70
1	A	2111	A	C8-N9-C4	5.49	108.00	105.80
1	A	2904	A	C4-C5-N7	-5.49	107.96	110.70
2	B	37	A	C8-N9-C4	5.49	108.00	105.80
32	W	209	A	N9-C4-C5	5.49	108.00	105.80
32	W	485	A	N9-C4-C5	5.49	108.00	105.80
32	W	616	A	N9-C4-C5	5.49	108.00	105.80
32	W	638	A	N9-C4-C5	5.49	108.00	105.80
32	W	1358	A	N9-C4-C5	5.49	108.00	105.80
1	A	207	A	N3-C4-N9	5.49	131.79	127.40
1	A	225	A	C4-C5-N7	-5.49	107.96	110.70
1	A	593	A	N9-C4-C5	5.49	108.00	105.80
1	A	965	A	C4-C5-N7	-5.49	107.96	110.70
1	A	970	A	C8-N9-C4	5.49	107.99	105.80
1	A	1423	A	N9-C4-C5	5.49	107.99	105.80
1	A	1424	A	C4-C5-N7	-5.49	107.96	110.70
1	A	1617	A	C4-C5-N7	-5.49	107.96	110.70
1	A	1686	A	N9-C4-C5	5.49	107.99	105.80
32	W	142	A	C4-C5-N7	-5.49	107.96	110.70
32	W	658	A	C4-C5-N7	-5.49	107.96	110.70
32	W	988	A	N3-C4-N9	5.49	131.79	127.40
32	W	1102	A	C4-C5-N7	-5.49	107.96	110.70
32	W	1509	A	C4-C5-N7	-5.49	107.96	110.70
32	W	1541	A	N9-C4-C5	5.49	107.99	105.80
52	z	23	A	C4-C5-C6	5.49	119.74	117.00
1	A	1179	A	N9-C4-C5	5.48	107.99	105.80
1	A	1735	A	N9-C4-C5	5.48	107.99	105.80
1	A	1743	A	C8-N9-C4	5.48	107.99	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2912	A	C4-C5-N7	-5.48	107.96	110.70
32	W	254	A	C4-C5-N7	-5.48	107.96	110.70
32	W	390	A	C4-C5-N7	-5.48	107.96	110.70
32	W	711	A	C8-N9-C4	5.48	107.99	105.80
32	W	1425	A	C4-C5-N7	-5.48	107.96	110.70
1	A	652	A	C4-C5-N7	-5.48	107.96	110.70
1	A	1054	A	C8-N9-C4	5.48	107.99	105.80
1	A	1235	A	C4-C5-N7	-5.48	107.96	110.70
1	A	1588	A	C8-N9-C4	5.48	107.99	105.80
1	A	1774	A	N9-C4-C5	5.48	107.99	105.80
1	A	2060	A	N9-C4-C5	5.48	107.99	105.80
1	A	2837	A	C8-N9-C4	5.48	107.99	105.80
32	W	171	A	C4-C5-C6	5.48	119.74	117.00
32	W	757	A	N9-C4-C5	5.48	107.99	105.80
32	W	902	A	C4-C5-N7	-5.48	107.96	110.70
32	W	1248	A	N9-C4-C5	5.48	107.99	105.80
32	W	1478	A	C8-N9-C4	5.48	107.99	105.80
1	A	49	A	C4-C5-N7	-5.48	107.96	110.70
1	A	193	A	C4-C5-N7	-5.48	107.96	110.70
1	A	353	A	N9-C4-C5	5.48	107.99	105.80
1	A	354	A	N9-C4-C5	5.48	107.99	105.80
1	A	991	A	C4-C5-N7	-5.48	107.96	110.70
1	A	1375	A	C4-C5-N7	-5.48	107.96	110.70
1	A	1555	A	C4-C5-C6	5.48	119.74	117.00
1	A	1588	A	C4-C5-N7	-5.48	107.96	110.70
1	A	1593	A	C4-C5-N7	-5.48	107.96	110.70
1	A	1661	A	N7-C8-N9	-5.48	111.06	113.80
1	A	2364	A	N9-C4-C5	5.48	107.99	105.80
1	A	2570	A	N9-C4-C5	5.48	107.99	105.80
1	A	2683	A	N9-C4-C5	5.48	107.99	105.80
1	A	2830	A	N9-C4-C5	5.48	107.99	105.80
1	A	2835	A	C8-N9-C4	5.48	107.99	105.80
32	W	582	A	C4-C5-N7	-5.48	107.96	110.70
32	W	874	A	C8-N9-C4	5.48	107.99	105.80
32	W	1512	A	N9-C4-C5	5.48	107.99	105.80
1	A	829	A	N9-C4-C5	5.48	107.99	105.80
1	A	2497	A	C8-N9-C4	5.48	107.99	105.80
1	A	2923	A	N9-C4-C5	5.48	107.99	105.80
32	W	35	A	C4-C5-N7	-5.48	107.96	110.70
32	W	195	A	C5-C6-N1	5.48	120.44	117.70
32	W	674	A	N3-C4-N9	5.48	131.78	127.40
32	W	1147	A	N9-C4-C5	5.48	107.99	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	A	C8-N9-C4	5.48	107.99	105.80
1	A	162	A	N3-C4-N9	5.48	131.78	127.40
1	A	584	A	N9-C4-C5	5.48	107.99	105.80
1	A	808	A	C4-C5-N7	-5.48	107.96	110.70
1	A	1029	A	C4-C5-N7	-5.48	107.96	110.70
1	A	1047	A	N9-C4-C5	5.48	107.99	105.80
1	A	2417	A	N9-C4-C5	5.48	107.99	105.80
1	A	2619	A	C4-C5-N7	-5.48	107.96	110.70
1	A	2804	A	C4-C5-N7	-5.48	107.96	110.70
1	A	2819	A	C4-C5-N7	-5.48	107.96	110.70
1	A	428	A	C4-C5-N7	-5.48	107.96	110.70
32	W	171	A	C4-C5-N7	-5.48	107.96	110.70
32	W	195	A	N9-C4-C5	5.48	107.99	105.80
32	W	475	A	C4-C5-N7	-5.48	107.96	110.70
32	W	811	A	C4-C5-N7	-5.48	107.96	110.70
32	W	1028	A	C8-N9-C4	5.48	107.99	105.80
1	A	210	A	N9-C4-C5	5.47	107.99	105.80
1	A	314	A	N9-C4-C5	5.47	107.99	105.80
1	A	431	A	C8-N9-C4	5.47	107.99	105.80
1	A	1224	A	N9-C4-C5	5.47	107.99	105.80
1	A	1277	A	N9-C4-C5	5.47	107.99	105.80
1	A	1490	A	N9-C4-C5	5.47	107.99	105.80
1	A	1812	A	N3-C4-N9	5.47	131.78	127.40
1	A	1941	A	C8-N9-C4	5.47	107.99	105.80
1	A	1941	A	N3-C4-N9	5.47	131.78	127.40
1	A	1982	A	N9-C4-C5	5.47	107.99	105.80
1	A	2526	A	C4-C5-N7	-5.47	107.96	110.70
1	A	2661	A	N9-C4-C5	5.47	107.99	105.80
1	A	2869	A	C8-N9-C4	5.47	107.99	105.80
32	W	12	A	C8-N9-C4	5.47	107.99	105.80
32	W	139	A	C4-C5-N7	-5.47	107.96	110.70
32	W	148	A	C4-C5-N7	-5.47	107.96	110.70
32	W	703	A	N9-C4-C5	5.47	107.99	105.80
32	W	704	A	N9-C4-C5	5.47	107.99	105.80
32	W	1147	A	C8-N9-C4	5.47	107.99	105.80
1	A	220	A	C4-C5-N7	-5.47	107.96	110.70
1	A	322	A	C4-C5-N7	-5.47	107.96	110.70
1	A	683	A	C4-C5-N7	-5.47	107.96	110.70
1	A	1277	A	C4-C5-N7	-5.47	107.96	110.70
1	A	1541	A	N9-C4-C5	5.47	107.99	105.80
1	A	2462	A	C8-N9-C4	5.47	107.99	105.80
32	W	333	A	N9-C4-C5	5.47	107.99	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	496	A	C4-C5-N7	-5.47	107.96	110.70
32	W	919	A	C4-C5-N7	-5.47	107.96	110.70
32	W	979	A	C4-C5-N7	-5.47	107.96	110.70
32	W	1455	A	C4-C5-N7	-5.47	107.96	110.70
1	A	265	A	C8-N9-C4	5.47	107.99	105.80
1	A	578	A	C4-C5-N7	-5.47	107.96	110.70
1	A	646	A	C4-C5-N7	-5.47	107.96	110.70
1	A	974	A	C4-C5-N7	-5.47	107.96	110.70
1	A	1533	A	C4-C5-N7	-5.47	107.97	110.70
32	W	1180	A	N9-C4-C5	5.47	107.99	105.80
32	W	1222	A	N9-C4-C5	5.47	107.99	105.80
1	A	1123	A	C4-C5-C6	5.47	119.73	117.00
1	A	1346	A	N9-C4-C5	5.47	107.99	105.80
1	A	1516	A	N9-C4-C5	5.47	107.99	105.80
1	A	1982	A	C4-C5-C6	5.47	119.73	117.00
1	A	2389	A	C4-C5-N7	-5.47	107.97	110.70
32	W	796	A	C8-N9-C4	5.47	107.99	105.80
32	W	862	A	C4-C5-C6	5.47	119.73	117.00
1	A	1686	A	C8-N9-C4	5.47	107.99	105.80
32	W	439	A	C4-C5-C6	5.47	119.73	117.00
32	W	825	A	C4-C5-N7	-5.47	107.97	110.70
1	A	504	A	C4-C5-N7	-5.47	107.97	110.70
1	A	1393	A	C8-N9-C4	5.47	107.99	105.80
1	A	1653	A	C8-N9-C4	5.47	107.99	105.80
1	A	2018	A	C4-C5-N7	-5.47	107.97	110.70
1	A	2087	A	C4-C5-N7	-5.47	107.97	110.70
1	A	2590	A	C4-C5-N7	-5.47	107.97	110.70
32	W	925	A	N9-C4-C5	5.47	107.99	105.80
32	W	1407	A	N9-C4-C5	5.47	107.99	105.80
1	A	67	A	C8-N9-C4	5.46	107.99	105.80
1	A	2091	A	C4-C5-N7	-5.46	107.97	110.70
1	A	2303	A	C4-C5-N7	-5.46	107.97	110.70
1	A	2330	A	N3-C4-N9	5.46	131.77	127.40
1	A	2595	A	N9-C4-C5	5.46	107.98	105.80
1	A	2601	A	N3-C4-N9	5.46	131.77	127.40
1	A	2893	A	C4-C5-N7	-5.46	107.97	110.70
2	B	37	A	C4-C5-N7	-5.46	107.97	110.70
2	B	97	A	C4-C5-N7	-5.46	107.97	110.70
32	W	34	A	N9-C4-C5	5.46	107.99	105.80
32	W	142	A	N9-C4-C5	5.46	107.99	105.80
32	W	415	A	C4-C5-N7	-5.46	107.97	110.70
32	W	611	A	C4-C5-N7	-5.46	107.97	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1435	A	C4-C5-N7	-5.46	107.97	110.70
32	W	1455	A	N9-C4-C5	5.46	107.99	105.80
1	A	198	A	C4-C5-N7	-5.46	107.97	110.70
1	A	974	A	C8-N9-C4	5.46	107.98	105.80
1	A	1233	A	C4-C5-N7	-5.46	107.97	110.70
1	A	1906	A	C4-C5-N7	-5.46	107.97	110.70
2	B	43	A	C8-N9-C4	5.46	107.98	105.80
32	W	129	A	C4-C5-N7	-5.46	107.97	110.70
32	W	389	A	C4-C5-N7	-5.46	107.97	110.70
32	W	825	A	N9-C4-C5	5.46	107.98	105.80
1	A	94	A	C4-C5-N7	-5.46	107.97	110.70
1	A	390	A	C4-C5-N7	-5.46	107.97	110.70
1	A	1601	A	N9-C4-C5	5.46	107.98	105.80
1	A	2560	A	N9-C4-C5	5.46	107.98	105.80
1	A	2629	A	C4-C5-N7	-5.46	107.97	110.70
32	W	31	A	N9-C4-C5	5.46	107.98	105.80
32	W	210	A	N9-C4-C5	5.46	107.98	105.80
32	W	705	A	N9-C4-C5	5.46	107.98	105.80
32	W	947	A	C4-C5-N7	-5.46	107.97	110.70
32	W	1205	A	N9-C4-C5	5.46	107.98	105.80
1	A	2030	A	C4-C5-N7	-5.46	107.97	110.70
32	W	189	A	N3-C4-N9	5.46	131.77	127.40
32	W	902	A	C8-N9-C4	5.46	107.98	105.80
32	W	1407	A	N3-C4-N9	5.46	131.77	127.40
1	A	574	A	N9-C4-C5	5.46	107.98	105.80
1	A	623	A	C8-N9-C4	5.46	107.98	105.80
1	A	634	A	C5-C6-N1	5.46	120.43	117.70
1	A	690	A	C4-C5-N7	-5.46	107.97	110.70
1	A	727	A	C4-C5-N7	-5.46	107.97	110.70
1	A	1314	A	N9-C4-C5	5.46	107.98	105.80
1	A	1340	A	N3-C4-N9	5.46	131.77	127.40
1	A	2307	A	N9-C4-C5	5.46	107.98	105.80
1	A	2700	A	N9-C4-C5	5.46	107.98	105.80
32	W	94	A	C4-C5-N7	-5.46	107.97	110.70
32	W	148	A	N9-C4-C5	5.46	107.98	105.80
32	W	415	A	N3-C4-N9	5.46	131.77	127.40
32	W	713	A	C4-C5-C6	5.46	119.73	117.00
32	W	985	A	C4-C5-C6	5.46	119.73	117.00
1	A	207	A	C4-C5-N7	-5.46	107.97	110.70
1	A	342	A	N9-C4-C5	5.46	107.98	105.80
1	A	428	A	N9-C4-C5	5.46	107.98	105.80
1	A	504	A	N3-C4-N9	5.46	131.76	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	876	A	C4-C5-N7	-5.46	107.97	110.70
1	A	1056	A	C4-C5-N7	-5.46	107.97	110.70
1	A	1073	A	C4-C5-N7	-5.46	107.97	110.70
1	A	1157	A	C4-C5-N7	-5.46	107.97	110.70
1	A	1679	A	C8-N9-C4	5.46	107.98	105.80
1	A	2441	A	C8-N9-C4	5.46	107.98	105.80
1	A	2908	A	C4-C5-C6	5.46	119.73	117.00
32	W	18	A	C4-C5-N7	-5.46	107.97	110.70
32	W	459	A	C8-N9-C4	5.46	107.98	105.80
32	W	604	A	C8-N9-C4	5.46	107.98	105.80
32	W	630	A	C4-C5-N7	-5.46	107.97	110.70
32	W	651	A	C4-C5-N7	-5.46	107.97	110.70
32	W	1266	A	C8-N9-C4	5.46	107.98	105.80
32	W	1359	A	N9-C4-C5	5.46	107.98	105.80
1	A	1961	A	C4-C5-N7	-5.46	107.97	110.70
1	A	2668	A	N9-C4-C5	5.46	107.98	105.80
1	A	2854	A	N9-C4-C5	5.46	107.98	105.80
32	W	824	A	N9-C4-C5	5.46	107.98	105.80
1	A	139	A	C4-C5-N7	-5.45	107.97	110.70
1	A	407	A	C8-N9-C4	5.45	107.98	105.80
1	A	753	A	C4-C5-N7	-5.45	107.97	110.70
1	A	904	A	N9-C4-C5	5.45	107.98	105.80
1	A	1036	A	C4-C5-N7	-5.45	107.97	110.70
1	A	1697	A	C8-N9-C4	5.45	107.98	105.80
1	A	1699	A	C4-C5-N7	-5.45	107.97	110.70
1	A	2526	A	N9-C4-C5	5.45	107.98	105.80
1	A	2827	A	C8-N9-C4	5.45	107.98	105.80
32	W	35	A	N9-C4-C5	5.45	107.98	105.80
32	W	775	A	N9-C4-C5	5.45	107.98	105.80
32	W	1442	A	C4-C5-N7	-5.45	107.97	110.70
32	W	1512	A	C4-C5-N7	-5.45	107.97	110.70
1	A	1020	A	C4-C5-N7	-5.45	107.97	110.70
1	A	1583	A	C4-C5-N7	-5.45	107.97	110.70
1	A	2356	A	C4-C5-N7	-5.45	107.97	110.70
32	W	204	A	N9-C4-C5	5.45	107.98	105.80
32	W	685	A	C8-N9-C4	5.45	107.98	105.80
32	W	721	A	C4-C5-N7	-5.45	107.97	110.70
32	W	1349	A	C4-C5-N7	-5.45	107.97	110.70
1	A	125	A	C8-N9-C4	5.45	107.98	105.80
1	A	494	A	C4-C5-C6	5.45	119.72	117.00
1	A	758	A	C8-N9-C4	5.45	107.98	105.80
1	A	1210	A	C8-N9-C4	5.45	107.98	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1631	A	N9-C4-C5	5.45	107.98	105.80
1	A	1685	A	N9-C4-C5	5.45	107.98	105.80
1	A	1848	A	C8-N9-C4	5.45	107.98	105.80
1	A	2369	A	C4-C5-N7	-5.45	107.97	110.70
1	A	2898	A	C4-C5-N7	-5.45	107.97	110.70
32	W	389	A	C8-N9-C4	5.45	107.98	105.80
32	W	404	A	N9-C4-C5	5.45	107.98	105.80
32	W	440	A	N9-C4-C5	5.45	107.98	105.80
32	W	776	A	C4-C5-N7	-5.45	107.97	110.70
32	W	1271	A	C8-N9-C4	5.45	107.98	105.80
32	W	1283	A	C4-C5-N7	-5.45	107.97	110.70
1	A	1072	A	C4-C5-N7	-5.45	107.98	110.70
1	A	1078	A	N3-C4-N9	5.45	131.76	127.40
1	A	2343	A	C8-N9-C4	5.45	107.98	105.80
32	W	35	A	C8-N9-C4	5.45	107.98	105.80
32	W	386	A	C4-C5-N7	-5.45	107.97	110.70
32	W	776	A	N9-C4-C5	5.45	107.98	105.80
1	A	1534	A	C8-N9-C4	5.45	107.98	105.80
1	A	2066	A	C8-N9-C4	5.45	107.98	105.80
1	A	2590	A	C8-N9-C4	5.45	107.98	105.80
32	W	1260	A	N9-C4-C5	5.45	107.98	105.80
32	W	1333	A	N3-C4-N9	5.45	131.76	127.40
32	W	1442	A	C8-N9-C4	5.45	107.98	105.80
1	A	91	A	C4-C5-N7	-5.45	107.98	110.70
1	A	94	A	C8-N9-C4	5.45	107.98	105.80
1	A	364	A	C4-C5-N7	-5.45	107.98	110.70
1	A	486	A	C8-N9-C4	5.45	107.98	105.80
1	A	600	A	C8-N9-C4	5.45	107.98	105.80
1	A	917	A	N9-C4-C5	5.45	107.98	105.80
1	A	1767	A	N9-C4-C5	5.45	107.98	105.80
1	A	2052	A	N9-C4-C5	5.45	107.98	105.80
32	W	541	A	C4-C5-N7	-5.45	107.98	110.70
32	W	616	A	C4-C5-N7	-5.45	107.98	110.70
32	W	1358	A	C5-C6-N1	5.45	120.42	117.70
32	W	1425	A	C8-N9-C4	5.45	107.98	105.80
52	z	21	A	C4-C5-N7	-5.45	107.98	110.70
1	A	2375	A	C8-N9-C4	5.44	107.98	105.80
32	W	271	A	C4-C5-N7	-5.44	107.98	110.70
32	W	433	A	C8-N9-C4	5.44	107.98	105.80
32	W	777	A	C4-C5-N7	-5.44	107.98	110.70
32	W	1115	A	C8-N9-C4	5.44	107.98	105.80
1	A	339	A	C4-C5-N7	-5.44	107.98	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	437	A	C4-C5-N7	-5.44	107.98	110.70
1	A	867	A	C4-C5-N7	-5.44	107.98	110.70
1	A	1323	A	N9-C4-C5	5.44	107.98	105.80
1	A	1347	A	C8-N9-C4	5.44	107.98	105.80
1	A	1421	A	C8-N9-C4	5.44	107.98	105.80
1	A	1464	A	N9-C4-C5	5.44	107.98	105.80
1	A	1791	A	C4-C5-N7	-5.44	107.98	110.70
1	A	1882	A	N9-C4-C5	5.44	107.98	105.80
1	A	2661	A	C8-N9-C4	5.44	107.98	105.80
32	W	705	A	C8-N9-C4	5.44	107.98	105.80
32	W	730	A	C4-C5-N7	-5.44	107.98	110.70
32	W	1050	A	C4-C5-N7	-5.44	107.98	110.70
52	z	23	A	N9-C4-C5	5.44	107.98	105.80
1	A	202	A	N9-C4-C5	5.44	107.98	105.80
1	A	244	A	N9-C4-C5	5.44	107.98	105.80
1	A	273	A	N3-C4-N9	5.44	131.75	127.40
1	A	753	A	C8-N9-C4	5.44	107.98	105.80
1	A	1465	A	C4-C5-N7	-5.44	107.98	110.70
1	A	1745	A	N9-C4-C5	5.44	107.98	105.80
32	W	1176	A	C4-C5-N7	-5.44	107.98	110.70
32	W	1369	A	C4-C5-N7	-5.44	107.98	110.70
32	W	1403	A	N9-C4-C5	5.44	107.98	105.80
32	W	296	A	C4-C5-N7	-5.44	107.98	110.70
32	W	918	A	C8-N9-C4	5.44	107.97	105.80
1	A	1347	A	N3-C4-N9	5.44	131.75	127.40
1	A	1434	A	N3-C4-N9	5.44	131.75	127.40
1	A	1919	A	N3-C4-N9	5.44	131.75	127.40
1	A	2686	A	C8-N9-C4	5.44	107.97	105.80
1	A	2807	A	N3-C4-N9	5.44	131.75	127.40
32	W	10	A	N9-C4-C5	5.44	107.97	105.80
32	W	99	A	C8-N9-C4	5.44	107.97	105.80
32	W	344	A	C4-C5-N7	-5.44	107.98	110.70
32	W	837	A	C4-C5-N7	-5.44	107.98	110.70
32	W	1333	A	C8-N9-C4	5.44	107.97	105.80
1	A	95	A	C8-N9-C4	5.44	107.97	105.80
1	A	2100	A	C4-C5-N7	-5.44	107.98	110.70
32	W	151	A	C8-N9-C4	5.44	107.97	105.80
1	A	173	A	C4-C5-N7	-5.43	107.98	110.70
1	A	470	A	N9-C4-C5	5.43	107.97	105.80
1	A	1019	A	N9-C4-C5	5.43	107.97	105.80
1	A	1244	A	N9-C4-C5	5.43	107.97	105.80
1	A	1346	A	C4-C5-N7	-5.43	107.98	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2018	A	C8-N9-C4	5.43	107.97	105.80
1	A	2779	A	C4-C5-N7	-5.43	107.98	110.70
32	W	314	A	C8-N9-C4	5.43	107.97	105.80
32	W	475	A	C8-N9-C4	5.43	107.97	105.80
32	W	491	A	N9-C4-C5	5.43	107.97	105.80
32	W	671	A	C4-C5-N7	-5.43	107.98	110.70
32	W	793	A	C8-N9-C4	5.43	107.97	105.80
32	W	924	A	C4-C5-N7	-5.43	107.98	110.70
32	W	979	A	N9-C4-C5	5.43	107.97	105.80
1	A	889	A	C8-N9-C4	5.43	107.97	105.80
1	A	1243	A	N9-C4-C5	5.43	107.97	105.80
1	A	1357	A	C4-C5-N7	-5.43	107.98	110.70
1	A	1499	A	N9-C4-C5	5.43	107.97	105.80
1	A	1858	A	C8-N9-C4	5.43	107.97	105.80
1	A	1989	A	N9-C4-C5	5.43	107.97	105.80
1	A	1995	A	C8-N9-C4	5.43	107.97	105.80
1	A	2088	A	N9-C4-C5	5.43	107.97	105.80
1	A	2362	A	N9-C4-C5	5.43	107.97	105.80
1	A	2387	A	C4-C5-N7	-5.43	107.98	110.70
32	W	151	A	N3-C4-N9	5.43	131.75	127.40
32	W	346	A	C4-C5-N7	-5.43	107.98	110.70
1	A	1126	A	C5-C6-N1	5.43	120.42	117.70
1	A	1636	A	N9-C4-C5	5.43	107.97	105.80
1	A	2071	A	C8-N9-C4	5.43	107.97	105.80
1	A	2100	A	N9-C4-C5	5.43	107.97	105.80
1	A	2497	A	C4-C5-N7	-5.43	107.98	110.70
32	W	1369	A	N9-C4-C5	5.43	107.97	105.80
1	A	5	A	N9-C4-C5	5.43	107.97	105.80
1	A	220	A	N9-C4-C5	5.43	107.97	105.80
1	A	369	A	C8-N9-C4	5.43	107.97	105.80
1	A	519	A	C4-C5-N7	-5.43	107.98	110.70
1	A	1312	A	N9-C4-C5	5.43	107.97	105.80
1	A	1663	A	N9-C4-C5	5.43	107.97	105.80
1	A	1723	A	N9-C4-C5	5.43	107.97	105.80
1	A	1989	A	C4-C5-N7	-5.43	107.98	110.70
32	W	236	A	N9-C4-C5	5.43	107.97	105.80
32	W	463	A	C4-C5-N7	-5.43	107.99	110.70
32	W	664	A	N9-C4-C5	5.43	107.97	105.80
32	W	1077	A	C4-C5-C6	5.43	119.72	117.00
32	W	1077	A	C4-C5-N7	-5.43	107.98	110.70
32	W	1348	A	C4-C5-N7	-5.43	107.98	110.70
1	A	2708	A	C4-C5-N7	-5.43	107.99	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	604	A	C4-C5-N7	-5.43	107.99	110.70
32	W	828	A	C4-C5-N7	-5.43	107.99	110.70
32	W	1133	A	C4-C5-C6	5.43	119.71	117.00
32	W	1283	A	C8-N9-C4	5.43	107.97	105.80
1	A	329	A	N9-C4-C5	5.43	107.97	105.80
1	A	740	A	C8-N9-C4	5.43	107.97	105.80
1	A	1381	A	C4-C5-N7	-5.43	107.99	110.70
1	A	1490	A	C5-C6-N1	5.43	120.41	117.70
1	A	1608	A	C4-C5-N7	-5.43	107.99	110.70
1	A	1957	A	C8-N9-C4	5.43	107.97	105.80
1	A	2105	U	N1-C2-O2	5.43	126.60	122.80
1	A	2762	A	N9-C4-C5	5.43	107.97	105.80
1	A	2846	A	N9-C4-C5	5.43	107.97	105.80
32	W	139	A	N9-C4-C5	5.43	107.97	105.80
32	W	457	A	C4-C5-C6	5.43	119.71	117.00
32	W	768	A	N9-C4-C5	5.43	107.97	105.80
32	W	933	A	N9-C4-C5	5.43	107.97	105.80
1	A	438	A	N9-C4-C5	5.42	107.97	105.80
1	A	507	A	C4-C5-N7	-5.42	107.99	110.70
1	A	1260	A	N9-C4-C5	5.42	107.97	105.80
1	A	1885	A	C4-C5-N7	-5.42	107.99	110.70
1	A	2027	A	C4-C5-N7	-5.42	107.99	110.70
1	A	2477	A	C4-C5-N7	-5.42	107.99	110.70
1	A	2571	A	C4-C5-N7	-5.42	107.99	110.70
32	W	208	A	C8-N9-C4	5.42	107.97	105.80
32	W	401	A	C4-C5-N7	-5.42	107.99	110.70
32	W	1004	A	N9-C4-C5	5.42	107.97	105.80
32	W	1065	A	C4-C5-N7	-5.42	107.99	110.70
32	W	1386	A	N9-C4-C5	5.42	107.97	105.80
32	W	1513	A	C4-C5-N7	-5.42	107.99	110.70
1	A	1096	A	C8-N9-C4	5.42	107.97	105.80
1	A	2440	A	N9-C4-C5	5.42	107.97	105.80
32	W	251	A	C8-N9-C4	5.42	107.97	105.80
32	W	793	A	C4-C5-N7	-5.42	107.99	110.70
1	A	318	A	C4-C5-N7	-5.42	107.99	110.70
1	A	537	A	C8-N9-C4	5.42	107.97	105.80
1	A	653	A	C4-C5-N7	-5.42	107.99	110.70
1	A	913	A	C8-N9-C4	5.42	107.97	105.80
1	A	1258	A	C8-N9-C4	5.42	107.97	105.80
1	A	1465	A	N9-C4-C5	5.42	107.97	105.80
1	A	2042	A	N9-C4-C5	5.42	107.97	105.80
1	A	2436	A	C8-N9-C4	5.42	107.97	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	968	A	C4-C5-N7	-5.42	107.99	110.70
32	W	1102	A	N9-C4-C5	5.42	107.97	105.80
32	W	1213	A	C8-N9-C4	5.42	107.97	105.80
1	A	5	A	C8-N9-C4	5.42	107.97	105.80
1	A	28	A	N9-C4-C5	5.42	107.97	105.80
1	A	781	A	N9-C4-C5	5.42	107.97	105.80
1	A	1036	A	C8-N9-C4	5.42	107.97	105.80
32	W	793	A	N9-C4-C5	5.42	107.97	105.80
32	W	796	A	C4-C5-N7	-5.42	107.99	110.70
32	W	984	A	C8-N9-C4	5.42	107.97	105.80
32	W	1112	A	C4-C5-N7	-5.42	107.99	110.70
32	W	1185	A	N9-C4-C5	5.42	107.97	105.80
1	A	130	A	C4-C5-N7	-5.42	107.99	110.70
1	A	407	A	C4-C5-N7	-5.42	107.99	110.70
1	A	553	A	N9-C4-C5	5.42	107.97	105.80
1	A	1244	A	C8-N9-C4	5.42	107.97	105.80
1	A	1532	A	C4-C5-N7	-5.42	107.99	110.70
1	A	1839	A	C8-N9-C4	5.42	107.97	105.80
1	A	2390	A	C4-C5-N7	-5.42	107.99	110.70
1	A	2618	A	N3-C4-N9	5.42	131.73	127.40
32	W	52	A	C4-C5-N7	-5.42	107.99	110.70
32	W	118	A	C4-C5-N7	-5.42	107.99	110.70
32	W	203	A	C4-C5-N7	-5.42	107.99	110.70
32	W	390	A	C8-N9-C4	5.42	107.97	105.80
32	W	438	A	N9-C4-C5	5.42	107.97	105.80
32	W	705	A	C4-C5-N7	-5.42	107.99	110.70
32	W	1024	A	C4-C5-N7	-5.42	107.99	110.70
32	W	1180	A	C4-C5-N7	-5.42	107.99	110.70
1	A	247	A	N9-C4-C5	5.42	107.97	105.80
1	A	559	A	C8-N9-C4	5.42	107.97	105.80
1	A	646	A	N9-C4-C5	5.42	107.97	105.80
1	A	667	A	C8-N9-C4	5.42	107.97	105.80
1	A	1221	A	C8-N9-C4	5.42	107.97	105.80
1	A	1398	A	C8-N9-C4	5.42	107.97	105.80
1	A	1473	A	N3-C4-N9	5.42	131.73	127.40
1	A	1579	A	C4-C5-C6	5.42	119.71	117.00
2	B	11	A	C8-N9-C4	5.42	107.97	105.80
32	W	321	A	C8-N9-C4	5.42	107.97	105.80
32	W	910	A	C4-C5-N7	-5.42	107.99	110.70
32	W	1328	A	C4-C5-N7	-5.42	107.99	110.70
52	z	76	A	C8-N9-C4	5.42	107.97	105.80
1	A	389	A	N9-C4-C5	5.42	107.97	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2876	A	N9-C4-C5	5.42	107.97	105.80
32	W	419	A	N3-C4-N9	5.42	131.73	127.40
32	W	457	A	N3-C4-N9	5.42	131.73	127.40
32	W	583	A	C4-C5-N7	-5.42	107.99	110.70
32	W	659	A	C4-C5-N7	-5.42	107.99	110.70
32	W	664	A	C4-C5-N7	-5.42	107.99	110.70
1	A	21	A	C8-N9-C4	5.41	107.97	105.80
1	A	162	A	C4-C5-N7	-5.41	107.99	110.70
1	A	500	A	C8-N9-C4	5.41	107.97	105.80
1	A	1025	A	C8-N9-C4	5.41	107.97	105.80
1	A	1132	A	C4-C5-N7	-5.41	107.99	110.70
1	A	1323	A	C4-C5-N7	-5.41	107.99	110.70
1	A	1724	A	C4-C5-N7	-5.41	107.99	110.70
1	A	2297	A	C4-C5-N7	-5.41	107.99	110.70
2	B	27	A	C8-N9-C4	5.41	107.97	105.80
32	W	352	A	C8-N9-C4	5.41	107.97	105.80
32	W	581	A	C4-C5-N7	-5.41	107.99	110.70
32	W	1427	A	C4-C5-N7	-5.41	107.99	110.70
1	A	326	A	C4-C5-N7	-5.41	107.99	110.70
1	A	1097	A	C4-C5-N7	-5.41	107.99	110.70
1	A	1340	A	C4-C5-C6	5.41	119.71	117.00
2	B	51	A	C4-C5-N7	-5.41	107.99	110.70
32	W	52	A	C8-N9-C4	5.41	107.97	105.80
32	W	1297	A	C4-C5-N7	-5.41	107.99	110.70
1	A	199	A	C4-C5-N7	-5.41	108.00	110.70
1	A	389	A	C4-C5-N7	-5.41	108.00	110.70
1	A	475	A	C4-C5-N7	-5.41	108.00	110.70
1	A	490	A	N9-C4-C5	5.41	107.96	105.80
1	A	524	A	C4-C5-N7	-5.41	108.00	110.70
1	A	547	A	C4-C5-N7	-5.41	107.99	110.70
1	A	593	A	C4-C5-N7	-5.41	108.00	110.70
1	A	1042	A	C4-C5-N7	-5.41	108.00	110.70
1	A	1995	A	C4-C5-N7	-5.41	108.00	110.70
1	A	2007	A	C4-C5-N7	-5.41	108.00	110.70
1	A	2047	A	C4-C5-N7	-5.41	108.00	110.70
32	W	12	A	N9-C4-C5	5.41	107.96	105.80
32	W	439	A	C5-C6-N1	5.41	120.41	117.70
32	W	738	A	C4-C5-N7	-5.41	107.99	110.70
32	W	1284	A	N9-C4-C5	5.41	107.96	105.80
1	A	637	A	N9-C4-C5	5.41	107.96	105.80
1	A	964	A	C4-C5-N7	-5.41	108.00	110.70
1	A	1116	A	C4-C5-N7	-5.41	108.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1592	A	N9-C4-C5	5.41	107.96	105.80
1	A	1615	A	N9-C4-C5	5.41	107.96	105.80
1	A	1767	A	C4-C5-N7	-5.41	108.00	110.70
1	A	1885	A	N9-C4-C5	5.41	107.96	105.80
1	A	49	A	C8-N9-C4	5.41	107.96	105.80
1	A	324	A	N9-C4-C5	5.41	107.96	105.80
1	A	337	A	C4-C5-N7	-5.41	108.00	110.70
1	A	1453	A	C8-N9-C4	5.41	107.96	105.80
1	A	1541	A	C4-C5-N7	-5.41	108.00	110.70
1	A	1620	A	C8-N9-C4	5.41	107.96	105.80
1	A	1882	A	C4-C5-N7	-5.41	108.00	110.70
32	W	404	A	C4-C5-N7	-5.41	108.00	110.70
32	W	1261	A	N9-C4-C5	5.41	107.96	105.80
1	A	281	A	C8-N9-C4	5.41	107.96	105.80
1	A	925	A	N9-C4-C5	5.41	107.96	105.80
1	A	952	A	C4-C5-N7	-5.41	108.00	110.70
1	A	1542	A	N9-C4-C5	5.41	107.96	105.80
1	A	1553	A	N9-C4-C5	5.41	107.96	105.80
1	A	1648	A	C4-C5-N7	-5.41	108.00	110.70
1	A	1776	A	C8-N9-C4	5.41	107.96	105.80
2	B	13	A	C8-N9-C4	5.41	107.96	105.80
32	W	128	A	C8-N9-C4	5.41	107.96	105.80
32	W	352	A	N9-C4-C5	5.41	107.96	105.80
32	W	518	A	N9-C4-C5	5.41	107.96	105.80
32	W	917	A	C4-C5-N7	-5.41	108.00	110.70
1	A	1885	A	C8-N9-C4	5.40	107.96	105.80
1	A	1929	A	N9-C4-C5	5.40	107.96	105.80
1	A	2812	A	C5-C6-N1	5.40	120.40	117.70
32	W	592	A	C4-C5-N7	-5.40	108.00	110.70
32	W	713	A	C8-N9-C4	5.40	107.96	105.80
1	A	84	A	C4-C5-N7	-5.40	108.00	110.70
1	A	193	A	N9-C4-C5	5.40	107.96	105.80
1	A	259	A	N9-C4-C5	5.40	107.96	105.80
1	A	438	A	C4-C5-N7	-5.40	108.00	110.70
1	A	1116	A	N9-C4-C5	5.40	107.96	105.80
1	A	1542	A	C8-N9-C4	5.40	107.96	105.80
1	A	2026	A	C5-C6-N1	5.40	120.40	117.70
1	A	2461	A	C4-C5-N7	-5.40	108.00	110.70
1	A	2500	A	N9-C4-C5	5.40	107.96	105.80
32	W	956	A	C4-C5-N7	-5.40	108.00	110.70
32	W	1014	A	C4-C5-N7	-5.40	108.00	110.70
1	A	307	A	C4-C5-N7	-5.40	108.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	746	A	N9-C4-C5	5.40	107.96	105.80
1	A	758	A	C4-C5-N7	-5.40	108.00	110.70
1	A	1027	A	N9-C4-C5	5.40	107.96	105.80
1	A	1059	A	C4-C5-N7	-5.40	108.00	110.70
1	A	1930	A	C8-N9-C4	5.40	107.96	105.80
1	A	1942	A	C4-C5-N7	-5.40	108.00	110.70
1	A	2889	A	C8-N9-C4	5.40	107.96	105.80
32	W	150	A	N3-C4-N9	5.40	131.72	127.40
32	W	367	A	C8-N9-C4	5.40	107.96	105.80
32	W	711	A	C4-C5-N7	-5.40	108.00	110.70
32	W	1179	A	N9-C4-C5	5.40	107.96	105.80
32	W	1366	A	C8-N9-C4	5.40	107.96	105.80
1	A	840	A	C6-N1-C2	-5.40	115.36	118.60
1	A	1743	A	C4-C5-N7	-5.40	108.00	110.70
1	A	2083	A	N9-C4-C5	5.40	107.96	105.80
32	W	918	A	C4-C5-N7	-5.40	108.00	110.70
52	z	14	A	N9-C4-C5	5.40	107.96	105.80
1	A	1254	A	N9-C4-C5	5.40	107.96	105.80
1	A	1335	A	C4-C5-N7	-5.40	108.00	110.70
1	A	1540	A	N9-C4-C5	5.40	107.96	105.80
1	A	2908	A	N9-C4-C5	5.40	107.96	105.80
32	W	1348	A	N9-C4-C5	5.40	107.96	105.80
1	A	65	A	C4-C5-N7	-5.40	108.00	110.70
1	A	851	A	C8-N9-C4	5.40	107.96	105.80
1	A	1092	A	C4-C5-N7	-5.40	108.00	110.70
1	A	2560	A	C8-N9-C4	5.40	107.96	105.80
32	W	1451	A	N9-C4-C5	5.40	107.96	105.80
1	A	1580	A	N9-C4-C5	5.39	107.96	105.80
1	A	1727	A	C4-C5-N7	-5.39	108.00	110.70
1	A	1850	A	C4-C5-N7	-5.39	108.00	110.70
1	A	1956	A	C4-C5-N7	-5.39	108.00	110.70
1	A	2482	A	C4-C5-N7	-5.39	108.00	110.70
1	A	2511	A	C4-C5-N7	-5.39	108.00	110.70
32	W	803	A	N9-C4-C5	5.39	107.96	105.80
1	A	329	A	C4-C5-N7	-5.39	108.00	110.70
1	A	354	A	C4-C5-N7	-5.39	108.00	110.70
1	A	407	A	N9-C4-C5	5.39	107.96	105.80
1	A	619	A	C4-C5-N7	-5.39	108.00	110.70
1	A	1636	A	C8-N9-C4	5.39	107.96	105.80
1	A	2087	A	N9-C4-C5	5.39	107.96	105.80
1	A	2421	A	C4-C5-N7	-5.39	108.00	110.70
1	A	2750	A	N9-C4-C5	5.39	107.96	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	39	A	C4-C5-N7	-5.39	108.00	110.70
2	B	105	A	C4-C5-N7	-5.39	108.00	110.70
32	W	924	A	C4-C5-C6	5.39	119.70	117.00
32	W	969	A	N9-C4-C5	5.39	107.96	105.80
32	W	1455	A	C8-N9-C4	5.39	107.96	105.80
32	W	1503	A	N9-C4-C5	5.39	107.96	105.80
1	A	268	A	C4-C5-N7	-5.39	108.00	110.70
1	A	343	A	C4-C5-N7	-5.39	108.00	110.70
1	A	1453	A	C4-C5-N7	-5.39	108.00	110.70
1	A	176	A	N9-C4-C5	5.39	107.96	105.80
1	A	207	A	C4-C5-C6	5.39	119.69	117.00
1	A	279	A	N9-C4-C5	5.39	107.96	105.80
1	A	479	A	C8-N9-C4	5.39	107.96	105.80
1	A	616	A	C8-N9-C4	5.39	107.96	105.80
1	A	1066	A	N9-C4-C5	5.39	107.96	105.80
1	A	1393	A	C4-C5-N7	-5.39	108.01	110.70
1	A	1667	A	C8-N9-C4	5.39	107.96	105.80
32	W	715	A	C4-C5-N7	-5.39	108.00	110.70
32	W	1180	A	C8-N9-C4	5.39	107.95	105.80
1	A	330	A	N9-C4-C5	5.39	107.95	105.80
1	A	673	A	C8-N9-C4	5.39	107.95	105.80
1	A	849	A	C4-C5-N7	-5.39	108.01	110.70
1	A	1905	A	N3-C4-N9	5.39	131.71	127.40
1	A	2066	A	N9-C4-C5	5.39	107.95	105.80
32	W	945	A	C4-C5-N7	-5.39	108.01	110.70
32	W	1140	A	C8-N9-C4	5.39	107.95	105.80
1	A	1284	A	C4-C5-N7	-5.39	108.01	110.70
1	A	2904	A	C8-N9-C4	5.39	107.95	105.80
32	W	771	A	N9-C4-C5	5.39	107.95	105.80
1	A	10	A	N9-C4-C5	5.38	107.95	105.80
1	A	13	A	C4-C5-N7	-5.38	108.01	110.70
1	A	364	A	N9-C4-C5	5.38	107.95	105.80
1	A	376	A	N9-C4-C5	5.38	107.95	105.80
1	A	762	A	C4-C5-N7	-5.38	108.01	110.70
1	A	867	A	C8-N9-C4	5.38	107.95	105.80
1	A	971	A	C8-N9-C4	5.38	107.95	105.80
1	A	987	A	N9-C4-C5	5.38	107.95	105.80
1	A	1014	A	N9-C4-C5	5.38	107.95	105.80
1	A	2100	A	C8-N9-C4	5.38	107.95	105.80
1	A	2571	A	C8-N9-C4	5.38	107.95	105.80
32	W	62	A	N9-C4-C5	5.38	107.95	105.80
32	W	529	A	N9-C4-C5	5.38	107.95	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	677	A	C4-C5-N7	-5.38	108.01	110.70
32	W	823	A	N9-C4-C5	5.38	107.95	105.80
32	W	1120	A	C4-C5-N7	-5.38	108.01	110.70
52	z	9	A	C8-N9-C4	5.38	107.95	105.80
1	A	388	A	C4-C5-N7	-5.38	108.01	110.70
1	A	1617	A	N9-C4-C5	5.38	107.95	105.80
1	A	2270	A	C4-C5-N7	-5.38	108.01	110.70
1	A	2302	A	C4-C5-N7	-5.38	108.01	110.70
1	A	2462	A	C4-C5-N7	-5.38	108.01	110.70
32	W	618	A	N9-C4-C5	5.38	107.95	105.80
1	A	5	A	C4-C5-N7	-5.38	108.01	110.70
1	A	126	A	N9-C4-C5	5.38	107.95	105.80
1	A	519	A	N9-C4-C5	5.38	107.95	105.80
1	A	715	A	C5-C6-N1	5.38	120.39	117.70
1	A	1434	A	C8-N9-C4	5.38	107.95	105.80
1	A	1788	A	C4-C5-N7	-5.38	108.01	110.70
1	A	2034	A	N9-C4-C5	5.38	107.95	105.80
1	A	2059	A	C4-C5-N7	-5.38	108.01	110.70
1	A	2089	A	C4-C5-N7	-5.38	108.01	110.70
1	A	2389	A	N9-C4-C5	5.38	107.95	105.80
32	W	254	A	C4-C5-C6	5.38	119.69	117.00
32	W	730	A	N9-C4-C5	5.38	107.95	105.80
32	W	796	A	N9-C4-C5	5.38	107.95	105.80
32	W	1140	A	N9-C4-C5	5.38	107.95	105.80
32	W	1478	A	C4-C5-N7	-5.38	108.01	110.70
1	A	12	A	N9-C4-C5	5.38	107.95	105.80
1	A	199	A	N9-C4-C5	5.38	107.95	105.80
1	A	459	A	C4-C5-N7	-5.38	108.01	110.70
1	A	1615	A	C4-C5-N7	-5.38	108.01	110.70
1	A	2734	A	C4-C5-N7	-5.38	108.01	110.70
32	W	518	A	C4-C5-N7	-5.38	108.01	110.70
1	A	64	A	C4-C5-N7	-5.38	108.01	110.70
1	A	73	A	C4-C5-N7	-5.38	108.01	110.70
1	A	917	A	C4-C5-N7	-5.38	108.01	110.70
1	A	1381	A	N9-C4-C5	5.38	107.95	105.80
1	A	2500	A	C4-C5-N7	-5.38	108.01	110.70
1	A	2912	A	N9-C4-C5	5.38	107.95	105.80
32	W	658	A	N9-C4-C5	5.38	107.95	105.80
32	W	677	A	N9-C4-C5	5.38	107.95	105.80
1	A	847	A	N3-C4-N9	5.38	131.70	127.40
1	A	913	A	C5-C6-N1	5.38	120.39	117.70
1	A	1592	A	C4-C5-N7	-5.38	108.01	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1928	A	N9-C4-C5	5.38	107.95	105.80
1	A	2066	A	C4-C5-N7	-5.38	108.01	110.70
1	A	2479	A	C4-C5-N7	-5.38	108.01	110.70
1	A	2898	A	C8-N9-C4	5.38	107.95	105.80
32	W	254	A	N9-C4-C5	5.38	107.95	105.80
32	W	825	A	C8-N9-C4	5.38	107.95	105.80
32	W	1288	A	C4-C5-N7	-5.38	108.01	110.70
32	W	1463	A	N9-C4-C5	5.38	107.95	105.80
1	A	1253	A	C4-C5-N7	-5.38	108.01	110.70
1	A	1392	A	N9-C4-C5	5.38	107.95	105.80
1	A	2387	A	N9-C4-C5	5.38	107.95	105.80
1	A	2777	A	C4-C5-N7	-5.38	108.01	110.70
32	W	757	A	C4-C5-N7	-5.38	108.01	110.70
1	A	52	A	N9-C4-C5	5.37	107.95	105.80
1	A	91	A	C8-N9-C4	5.37	107.95	105.80
1	A	110	A	N9-C4-C5	5.37	107.95	105.80
1	A	337	A	N9-C4-C5	5.37	107.95	105.80
1	A	630	A	C8-N9-C4	5.37	107.95	105.80
1	A	634	A	N9-C4-C5	5.37	107.95	105.80
1	A	1760	A	C8-N9-C4	5.37	107.95	105.80
1	A	2276	A	N9-C4-C5	5.37	107.95	105.80
2	B	64	A	C4-C5-N7	-5.37	108.01	110.70
32	W	382	A	C4-C5-N7	-5.37	108.01	110.70
32	W	762	A	N9-C4-C5	5.37	107.95	105.80
32	W	910	A	N9-C4-C5	5.37	107.95	105.80
32	W	913	A	C4-C5-N7	-5.37	108.01	110.70
32	W	975	A	N9-C4-C5	5.37	107.95	105.80
32	W	1017	A	C4-C5-N7	-5.37	108.01	110.70
32	W	1024	A	C8-N9-C4	5.37	107.95	105.80
32	W	1120	A	N9-C4-C5	5.37	107.95	105.80
52	z	58	A	N9-C4-C5	5.37	107.95	105.80
1	A	210	A	C4-C5-N7	-5.37	108.01	110.70
1	A	653	A	N9-C4-C5	5.37	107.95	105.80
1	A	957	A	C8-N9-C4	5.37	107.95	105.80
1	A	1235	A	C8-N9-C4	5.37	107.95	105.80
1	A	1562	A	C4-C5-N7	-5.37	108.02	110.70
1	A	1947	A	N9-C4-C5	5.37	107.95	105.80
1	A	1982	A	C4-C5-N7	-5.37	108.01	110.70
1	A	2343	A	C4-C5-N7	-5.37	108.01	110.70
1	A	2459	A	C4-C5-N7	-5.37	108.02	110.70
1	A	2827	A	C4-C5-N7	-5.37	108.01	110.70
32	W	507	A	C4-C5-C6	5.37	119.69	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1247	A	C8-N9-C4	5.37	107.95	105.80
32	W	1451	A	C4-C5-N7	-5.37	108.02	110.70
32	W	1486	A	N9-C4-C5	5.37	107.95	105.80
1	A	758	A	N9-C4-C5	5.37	107.95	105.80
1	A	1618	A	C8-N9-C4	5.37	107.95	105.80
32	W	270	A	C4-C5-N7	-5.37	108.02	110.70
52	z	24	A	C5-C6-N1	5.37	120.39	117.70
1	A	168	A	C8-N9-C4	5.37	107.95	105.80
1	A	222	A	N9-C4-C5	5.37	107.95	105.80
1	A	260	A	C4-C5-N7	-5.37	108.02	110.70
1	A	486	A	C5-C6-N1	5.37	120.39	117.70
1	A	1026	A	C4-C5-N7	-5.37	108.02	110.70
1	A	1034	A	N9-C4-C5	5.37	107.95	105.80
1	A	1074	A	C4-C5-N7	-5.37	108.02	110.70
1	A	1421	A	N9-C4-C5	5.37	107.95	105.80
1	A	1517	A	C4-C5-N7	-5.37	108.02	110.70
1	A	1882	A	C8-N9-C4	5.37	107.95	105.80
1	A	2078	A	N9-C4-C5	5.37	107.95	105.80
1	A	2316	A	C4-C5-N7	-5.37	108.02	110.70
32	W	61	A	C4-C5-N7	-5.37	108.02	110.70
32	W	282	A	N9-C4-C5	5.37	107.95	105.80
32	W	669	A	C8-N9-C4	5.37	107.95	105.80
32	W	799	A	C4-C5-N7	-5.37	108.02	110.70
1	A	373	A	C4-C5-N7	-5.37	108.02	110.70
1	A	762	A	N9-C4-C5	5.37	107.95	105.80
1	A	600	A	N9-C4-C5	5.37	107.95	105.80
1	A	623	A	N9-C4-C5	5.37	107.95	105.80
1	A	652	A	N9-C4-C5	5.37	107.95	105.80
1	A	1534	A	N9-C4-C5	5.37	107.95	105.80
1	A	2339	A	N9-C4-C5	5.37	107.95	105.80
32	W	55	A	C4-C5-N7	-5.37	108.02	110.70
32	W	161	A	C4-C5-N7	-5.37	108.02	110.70
32	W	672	A	N9-C4-C5	5.37	107.95	105.80
32	W	674	A	C4-C5-C6	5.37	119.68	117.00
32	W	738	A	N9-C4-C5	5.37	107.95	105.80
32	W	1260	A	C8-N9-C4	5.37	107.95	105.80
32	W	1298	A	C4-C5-N7	-5.37	108.02	110.70
32	W	1328	A	N9-C4-C5	5.37	107.95	105.80
1	A	702	A	C4-C5-N7	-5.36	108.02	110.70
1	A	948	A	C8-N9-C4	5.36	107.95	105.80
1	A	2395	A	C8-N9-C4	5.36	107.95	105.80
2	B	56	A	N9-C4-C5	5.36	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	459	A	N9-C4-C5	5.36	107.94	105.80
32	W	529	A	C4-C5-N7	-5.36	108.02	110.70
32	W	775	A	C4-C5-C6	5.36	119.68	117.00
32	W	1207	A	N9-C4-C5	5.36	107.94	105.80
32	W	1236	A	C4-C5-N7	-5.36	108.02	110.70
1	A	661	A	C8-N9-C4	5.36	107.94	105.80
1	A	1520	A	C5-C6-N1	5.36	120.38	117.70
1	A	1524	A	C5-C6-N1	5.36	120.38	117.70
1	A	1767	A	C8-N9-C4	5.36	107.94	105.80
1	A	2704	A	C4-C5-N7	-5.36	108.02	110.70
32	W	519	A	C4-C5-N7	-5.36	108.02	110.70
1	A	384	A	C8-N9-C4	5.36	107.94	105.80
1	A	490	A	C4-C5-N7	-5.36	108.02	110.70
1	A	1197	A	C8-N9-C4	5.36	107.94	105.80
1	A	1713	A	C4-C5-N7	-5.36	108.02	110.70
1	A	1713	A	N9-C4-C5	5.36	107.94	105.80
1	A	1791	A	N9-C4-C5	5.36	107.94	105.80
1	A	1956	A	N9-C4-C5	5.36	107.94	105.80
1	A	1998	A	C4-C5-N7	-5.36	108.02	110.70
32	W	209	A	N3-C4-N9	5.36	131.69	127.40
32	W	228	A	N9-C4-C5	5.36	107.94	105.80
32	W	382	A	N9-C4-C5	5.36	107.94	105.80
1	A	421	A	C4-C5-N7	-5.36	108.02	110.70
1	A	2785	U	P-O3'-C3'	5.36	126.13	119.70
1	A	2793	A	N3-C4-N9	5.36	131.69	127.40
32	W	508	A	C8-N9-C4	5.36	107.94	105.80
32	W	581	A	N9-C4-C5	5.36	107.94	105.80
32	W	1252	A	C4-C5-N7	-5.36	108.02	110.70
1	A	185	A	N9-C4-C5	5.36	107.94	105.80
1	A	868	A	C4-C5-N7	-5.36	108.02	110.70
1	A	1059	A	N9-C4-C5	5.36	107.94	105.80
1	A	1179	A	C4-C5-N7	-5.36	108.02	110.70
1	A	1579	A	N9-C4-C5	5.36	107.94	105.80
1	A	1721	A	C8-N9-C4	5.36	107.94	105.80
32	W	504	A	N9-C4-C5	5.36	107.94	105.80
32	W	582	A	N9-C4-C5	5.36	107.94	105.80
32	W	604	A	N9-C4-C5	5.36	107.94	105.80
32	W	715	A	N9-C4-C5	5.36	107.94	105.80
1	A	325	A	N9-C4-C5	5.36	107.94	105.80
1	A	904	A	C8-N9-C4	5.36	107.94	105.80
1	A	1948	A	C4-C5-N7	-5.36	108.02	110.70
32	W	371	A	C4-C5-N7	-5.36	108.02	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	1254	A	N9-C4-C5	5.36	107.94	105.80
32	W	1327	A	C4-C5-N7	-5.36	108.02	110.70
32	W	1419	A	N9-C4-C5	5.36	107.94	105.80
32	W	1523	A	N9-C4-C5	5.36	107.94	105.80
52	z	70	A	C8-N9-C4	5.36	107.94	105.80
1	A	727	A	N9-C4-C5	5.35	107.94	105.80
1	A	1361	A	C4-C5-N7	-5.35	108.02	110.70
1	A	2027	A	N9-C4-C5	5.35	107.94	105.80
1	A	2298	A	C4-C5-N7	-5.35	108.02	110.70
2	B	18	A	C8-N9-C4	5.35	107.94	105.80
32	W	140	A	C4-C5-N7	-5.35	108.02	110.70
32	W	209	A	C8-N9-C4	5.35	107.94	105.80
32	W	270	A	N9-C4-C5	5.35	107.94	105.80
32	W	372	A	C4-C5-N7	-5.35	108.02	110.70
1	A	12	A	C4-C5-N7	-5.35	108.02	110.70
1	A	173	A	N9-C4-C5	5.35	107.94	105.80
1	A	259	A	C4-C5-N7	-5.35	108.02	110.70
1	A	947	A	C4-C5-N7	-5.35	108.02	110.70
1	A	993	A	C4-C5-N7	-5.35	108.02	110.70
1	A	1026	A	N9-C4-C5	5.35	107.94	105.80
1	A	1113	A	N9-C4-C5	5.35	107.94	105.80
1	A	1130	A	C8-N9-C4	5.35	107.94	105.80
1	A	1533	A	N9-C4-C5	5.35	107.94	105.80
1	A	1569	A	C8-N9-C4	5.35	107.94	105.80
1	A	1680	A	C8-N9-C4	5.35	107.94	105.80
1	A	1930	A	N9-C4-C5	5.35	107.94	105.80
1	A	2455	A	C4-C5-N7	-5.35	108.02	110.70
1	A	2810	A	C4-C5-N7	-5.35	108.02	110.70
1	A	2844	A	C4-C5-N7	-5.35	108.02	110.70
1	A	2898	A	N3-C4-N9	5.35	131.68	127.40
32	W	55	A	N9-C4-C5	5.35	107.94	105.80
32	W	270	A	C8-N9-C4	5.35	107.94	105.80
32	W	456	A	N9-C4-C5	5.35	107.94	105.80
32	W	1179	A	C8-N9-C4	5.35	107.94	105.80
52	z	23	A	C8-N9-C4	5.35	107.94	105.80
1	A	469	A	C8-N9-C4	5.35	107.94	105.80
1	A	702	A	N9-C4-C5	5.35	107.94	105.80
32	W	1016	A	C4-C5-N7	-5.35	108.03	110.70
1	A	247	A	C8-N9-C4	5.35	107.94	105.80
1	A	265	A	N9-C4-C5	5.35	107.94	105.80
1	A	1258	A	N9-C4-C5	5.35	107.94	105.80
1	A	1802	A	C4-C5-N7	-5.35	108.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2406	A	C4-C5-N7	-5.35	108.03	110.70
1	A	2619	A	N9-C4-C5	5.35	107.94	105.80
32	W	67	A	C4-C5-N7	-5.35	108.03	110.70
32	W	234	A	C4-C5-N7	-5.35	108.03	110.70
32	W	485	A	C4-C5-N7	-5.35	108.03	110.70
32	W	1006	A	C4-C5-N7	-5.35	108.03	110.70
32	W	1143	A	C8-N9-C4	5.35	107.94	105.80
32	W	1502	A	C8-N9-C4	5.35	107.94	105.80
1	A	229	A	N9-C4-C5	5.35	107.94	105.80
1	A	1094	A	C4-C5-N7	-5.35	108.03	110.70
1	A	1900	A	N9-C4-C5	5.35	107.94	105.80
1	A	2106	A	C4-C5-N7	-5.35	108.03	110.70
2	B	76	A	N9-C4-C5	5.35	107.94	105.80
32	W	433	A	C4-C5-N7	-5.35	108.03	110.70
32	W	777	A	N9-C4-C5	5.35	107.94	105.80
32	W	1470	A	C4-C5-N7	-5.35	108.03	110.70
1	A	1265	A	N9-C4-C5	5.35	107.94	105.80
1	A	1361	A	N9-C4-C5	5.35	107.94	105.80
32	W	724	A	N9-C4-C5	5.35	107.94	105.80
32	W	1206	A	C8-N9-C4	5.35	107.94	105.80
32	W	1405	A	C4-C5-N7	-5.35	108.03	110.70
1	A	958	A	N9-C4-C5	5.34	107.94	105.80
1	A	1542	A	C4-C5-N7	-5.34	108.03	110.70
1	A	1575	A	C4-C5-N7	-5.34	108.03	110.70
1	A	1601	A	C4-C5-N7	-5.34	108.03	110.70
1	A	1815	A	N9-C4-C5	5.34	107.94	105.80
1	A	2860	A	C4-C5-N7	-5.34	108.03	110.70
32	W	344	A	N9-C4-C5	5.34	107.94	105.80
32	W	721	A	C8-N9-C4	5.34	107.94	105.80
32	W	1103	A	N9-C4-C5	5.34	107.94	105.80
1	A	222	A	C4-C5-N7	-5.34	108.03	110.70
1	A	275	A	C8-N9-C4	5.34	107.94	105.80
1	A	2691	A	C8-N9-C4	5.34	107.94	105.80
32	W	984	A	C4-C5-N7	-5.34	108.03	110.70
1	A	431	A	C4-C5-N7	-5.34	108.03	110.70
1	A	486	A	C4-C5-N7	-5.34	108.03	110.70
1	A	496	A	C5-C6-N1	5.34	120.37	117.70
1	A	1291	A	C4-C5-N7	-5.34	108.03	110.70
1	A	1844	A	N3-C4-N9	5.34	131.67	127.40
1	A	2047	A	N9-C4-C5	5.34	107.94	105.80
1	A	2908	A	C4-C5-N7	-5.34	108.03	110.70
2	B	55	A	C4-C5-N7	-5.34	108.03	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	899	A	N3-C4-N9	5.34	131.67	127.40
32	W	1259	A	N9-C4-C5	5.34	107.94	105.80
32	W	1315	A	C4-C5-N7	-5.34	108.03	110.70
32	W	1369	A	C5-C6-N1	5.34	120.37	117.70
1	A	73	A	C8-N9-C4	5.34	107.94	105.80
1	A	1316	A	C4-C5-N7	-5.34	108.03	110.70
1	A	1709	A	C4-C5-N7	-5.34	108.03	110.70
1	A	2826	A	C4-C5-N7	-5.34	108.03	110.70
32	W	335	A	C4-C5-N7	-5.34	108.03	110.70
32	W	532	A	N9-C4-C5	5.34	107.94	105.80
32	W	617	A	C4-C5-N7	-5.34	108.03	110.70
32	W	1270	A	C4-C5-N7	-5.34	108.03	110.70
32	W	1427	A	N9-C4-C5	5.34	107.94	105.80
1	A	2719	A	C4-C5-N7	-5.34	108.03	110.70
32	W	569	A	C4-C5-N7	-5.34	108.03	110.70
1	A	65	A	N9-C4-C5	5.34	107.93	105.80
1	A	161	A	C8-N9-C4	5.34	107.94	105.80
1	A	307	A	N9-C4-C5	5.34	107.93	105.80
1	A	339	A	C8-N9-C4	5.34	107.93	105.80
1	A	448	A	C4-C5-N7	-5.34	108.03	110.70
1	A	770	A	N9-C4-C5	5.34	107.93	105.80
1	A	948	A	C4-C5-N7	-5.34	108.03	110.70
1	A	1266	A	C8-N9-C4	5.34	107.94	105.80
1	A	1302	A	C8-N9-C4	5.34	107.94	105.80
1	A	1421	A	C4-C5-N7	-5.34	108.03	110.70
1	A	2106	A	N9-C4-C5	5.34	107.93	105.80
1	A	2477	A	N9-C4-C5	5.34	107.94	105.80
32	W	581	A	C8-N9-C4	5.34	107.94	105.80
32	W	883	A	C4-C5-N7	-5.34	108.03	110.70
32	W	1245	A	C4-C5-N7	-5.34	108.03	110.70
1	A	95	A	C5-C6-N1	5.33	120.37	117.70
1	A	176	A	C4-C5-N7	-5.33	108.03	110.70
1	A	623	A	C4-C5-N7	-5.33	108.03	110.70
1	A	1286	A	C4-C5-N7	-5.33	108.03	110.70
1	A	1504	A	N9-C4-C5	5.33	107.93	105.80
1	A	1593	A	N9-C4-C5	5.33	107.93	105.80
1	A	2532	A	C4-C5-N7	-5.33	108.03	110.70
2	B	105	A	N9-C4-C5	5.33	107.93	105.80
32	W	258	A	C4-C5-N7	-5.33	108.03	110.70
32	W	548	A	C8-N9-C4	5.33	107.93	105.80
32	W	1257	A	N9-C4-C5	5.33	107.93	105.80
1	A	549	A	N9-C4-C5	5.33	107.93	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1534	A	C4-C5-N7	-5.33	108.03	110.70
1	A	1723	A	C4-C5-N7	-5.33	108.03	110.70
1	A	1818	A	N9-C4-C5	5.33	107.93	105.80
1	A	1905	A	C8-N9-C4	5.33	107.93	105.80
32	W	401	A	N9-C4-C5	5.33	107.93	105.80
1	A	318	A	N9-C4-C5	5.33	107.93	105.80
1	A	388	A	N9-C4-C5	5.33	107.93	105.80
1	A	494	A	N3-C4-N9	5.33	131.67	127.40
1	A	1113	A	C4-C5-N7	-5.33	108.03	110.70
1	A	1556	A	C8-N9-C4	5.33	107.93	105.80
32	W	72	A	C4-C5-N7	-5.33	108.03	110.70
32	W	195	A	C4-C5-N7	-5.33	108.03	110.70
32	W	725	A	C8-N9-C4	5.33	107.93	105.80
32	W	947	A	N9-C4-C5	5.33	107.93	105.80
32	W	1121	A	C8-N9-C4	5.33	107.93	105.80
1	A	1900	A	C4-C5-N7	-5.33	108.03	110.70
32	W	1383	A	C4-C5-N7	-5.33	108.03	110.70
1	A	118	A	C4-C5-C6	5.33	119.66	117.00
1	A	436	A	C4-C5-N7	-5.33	108.04	110.70
1	A	808	A	N9-C4-C5	5.33	107.93	105.80
1	A	889	A	C4-C5-N7	-5.33	108.04	110.70
1	A	1392	A	C4-C5-N7	-5.33	108.03	110.70
1	A	1583	A	N9-C4-C5	5.33	107.93	105.80
1	A	1653	A	C4-C5-N7	-5.33	108.04	110.70
1	A	2032	A	N9-C4-C5	5.33	107.93	105.80
1	A	2340	A	N9-C4-C5	5.33	107.93	105.80
1	A	2812	A	C4-C5-N7	-5.33	108.04	110.70
1	A	2812	A	N9-C4-C5	5.33	107.93	105.80
2	B	50	A	N9-C4-C5	5.33	107.93	105.80
32	W	459	A	C4-C5-N7	-5.33	108.03	110.70
32	W	1112	A	C8-N9-C4	5.33	107.93	105.80
1	A	889	A	N9-C4-C5	5.33	107.93	105.80
1	A	1672	A	C4-C5-N7	-5.33	108.04	110.70
1	A	1797	A	C8-N9-C4	5.33	107.93	105.80
2	B	113	A	C8-N9-C4	5.33	107.93	105.80
32	W	1298	A	N9-C4-C5	5.33	107.93	105.80
52	z	9	A	C4-C5-N7	-5.33	108.04	110.70
1	A	166	A	N9-C4-C5	5.33	107.93	105.80
1	A	436	A	N9-C4-C5	5.33	107.93	105.80
1	A	896	A	C4-C5-N7	-5.33	108.04	110.70
1	A	1003	A	N3-C4-N9	5.33	131.66	127.40
1	A	2000	A	C4-C5-N7	-5.33	108.04	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2327	A	C4-C5-N7	-5.33	108.04	110.70
1	A	2402	A	C4-C5-N7	-5.33	108.04	110.70
1	A	2595	A	C8-N9-C4	5.33	107.93	105.80
1	A	2658	A	N9-C4-C5	5.33	107.93	105.80
32	W	775	A	C4-C5-N7	-5.33	108.04	110.70
32	W	1206	A	N9-C4-C5	5.33	107.93	105.80
52	z	76	A	C4-C5-N7	-5.33	108.04	110.70
1	A	71	A	N9-C4-C5	5.32	107.93	105.80
1	A	970	A	C4-C5-N7	-5.32	108.04	110.70
1	A	1360	A	C4-C5-N7	-5.32	108.04	110.70
1	A	1774	A	C4-C5-N7	-5.32	108.04	110.70
1	A	1816	A	C5-C6-N1	5.32	120.36	117.70
1	A	2351	A	N9-C4-C5	5.32	107.93	105.80
1	A	2532	A	N9-C4-C5	5.32	107.93	105.80
1	A	2754	A	N9-C4-C5	5.32	107.93	105.80
32	W	81	A	C4-C5-N7	-5.32	108.04	110.70
32	W	1112	A	N9-C4-C5	5.32	107.93	105.80
1	A	524	A	N9-C4-C5	5.32	107.93	105.80
1	A	559	A	C4-C5-N7	-5.32	108.04	110.70
1	A	782	A	C4-C5-N7	-5.32	108.04	110.70
1	A	866	A	C4-C5-N7	-5.32	108.04	110.70
1	A	2661	A	C4-C5-N7	-5.32	108.04	110.70
1	A	2740	A	C4-C5-N7	-5.32	108.04	110.70
1	A	2919	A	N9-C4-C5	5.32	107.93	105.80
32	W	397	A	C4-C5-N7	-5.32	108.04	110.70
1	A	53	A	C8-N9-C4	5.32	107.93	105.80
1	A	144	A	C4-C5-N7	-5.32	108.04	110.70
1	A	1490	A	C4-C5-N7	-5.32	108.04	110.70
1	A	1506	A	N9-C4-C5	5.32	107.93	105.80
1	A	1555	A	N3-C4-N9	5.32	131.66	127.40
1	A	1723	A	C8-N9-C4	5.32	107.93	105.80
1	A	2043	A	C4-C5-N7	-5.32	108.04	110.70
1	A	2329	A	C5-C6-N1	5.32	120.36	117.70
1	A	2794	A	N9-C4-C5	5.32	107.93	105.80
32	W	671	A	N9-C4-C5	5.32	107.93	105.80
52	z	70	A	C4-C5-N7	-5.32	108.04	110.70
1	A	1021	A	C8-N9-C4	5.32	107.93	105.80
1	A	1788	A	N9-C4-C5	5.32	107.93	105.80
1	A	202	A	C4-C5-N7	-5.32	108.04	110.70
1	A	412	A	N9-C4-C5	5.32	107.93	105.80
1	A	448	A	N9-C4-C5	5.32	107.93	105.80
1	A	970	A	N9-C4-C5	5.32	107.93	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1697	A	C4-C5-N7	-5.32	108.04	110.70
1	A	2089	A	C4-C5-C6	5.32	119.66	117.00
1	A	2606	A	N3-C4-N9	5.32	131.65	127.40
1	A	2722	A	C4-C5-N7	-5.32	108.04	110.70
32	W	390	A	N9-C4-C5	5.32	107.93	105.80
32	W	631	A	C8-N9-C4	5.32	107.93	105.80
32	W	933	A	C5-C6-N1	5.32	120.36	117.70
32	W	1529	A	C4-C5-N7	-5.32	108.04	110.70
1	A	1445	A	C4-C5-N7	-5.32	108.04	110.70
1	A	1506	A	C4-C5-N7	-5.32	108.04	110.70
1	A	1778	A	C8-N9-C4	5.32	107.93	105.80
1	A	1913	A	C4-C5-N7	-5.32	108.04	110.70
1	A	2296	A	C4-C5-N7	-5.32	108.04	110.70
2	B	20	A	C8-N9-C4	5.32	107.93	105.80
32	W	107	A	N9-C4-C5	5.32	107.93	105.80
32	W	956	A	N9-C4-C5	5.32	107.93	105.80
1	A	279	A	C8-N9-C4	5.31	107.92	105.80
1	A	828	A	C8-N9-C4	5.31	107.93	105.80
1	A	1020	A	N9-C4-C5	5.31	107.93	105.80
1	A	2831	A	C4-C5-N7	-5.31	108.04	110.70
1	A	130	A	C8-N9-C4	5.31	107.92	105.80
1	A	150	A	C4-C5-N7	-5.31	108.04	110.70
1	A	156	A	C4-C5-N7	-5.31	108.04	110.70
1	A	828	A	C4-C5-N7	-5.31	108.04	110.70
1	A	828	A	N9-C4-C5	5.31	107.92	105.80
1	A	1265	A	C8-N9-C4	5.31	107.92	105.80
1	A	1724	A	C8-N9-C4	5.31	107.92	105.80
1	A	1929	A	C4-C5-N7	-5.31	108.04	110.70
1	A	2060	A	C4-C5-N7	-5.31	108.04	110.70
1	A	2777	A	N9-C4-C5	5.31	107.92	105.80
1	A	2790	A	C4-C5-N7	-5.31	108.04	110.70
32	W	225	A	C8-N9-C4	5.31	107.92	105.80
32	W	617	A	N9-C4-C5	5.31	107.92	105.80
32	W	1509	A	N9-C4-C5	5.31	107.92	105.80
1	A	1699	A	N9-C4-C5	5.31	107.92	105.80
1	A	1776	A	C4-C5-N7	-5.31	108.05	110.70
32	W	630	A	C8-N9-C4	5.31	107.92	105.80
1	A	216	A	C4-C5-N7	-5.31	108.05	110.70
1	A	538	A	C4-C5-N7	-5.31	108.05	110.70
1	A	790	A	C8-N9-C4	5.31	107.92	105.80
1	A	1003	A	C4-C5-N7	-5.31	108.05	110.70
1	A	1244	A	C4-C5-N7	-5.31	108.05	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1504	A	C4-C5-N7	-5.31	108.05	110.70
1	A	2875	A	C4-C5-N7	-5.31	108.05	110.70
2	B	43	A	N9-C4-C5	5.31	107.92	105.80
32	W	592	A	N9-C4-C5	5.31	107.92	105.80
32	W	611	A	N9-C4-C5	5.31	107.92	105.80
32	W	844	A	C8-N9-C4	5.31	107.92	105.80
32	W	1178	A	C8-N9-C4	5.31	107.92	105.80
1	A	943	A	C4-C5-N7	-5.31	108.05	110.70
1	A	1258	A	C4-C5-N7	-5.31	108.05	110.70
1	A	1357	A	N9-C4-C5	5.31	107.92	105.80
1	A	1517	A	N9-C4-C5	5.31	107.92	105.80
1	A	1536	A	N9-C4-C5	5.31	107.92	105.80
1	A	2270	A	N9-C4-C5	5.31	107.92	105.80
1	A	2381	A	C4-C5-N7	-5.31	108.05	110.70
1	A	2505	A	C4-C5-N7	-5.31	108.05	110.70
1	A	2616	A	C8-N9-C4	5.31	107.92	105.80
2	B	11	A	N9-C4-C5	5.31	107.92	105.80
32	W	290	A	N9-C4-C5	5.31	107.92	105.80
32	W	924	A	N9-C4-C5	5.31	107.92	105.80
32	W	1252	A	N9-C4-C5	5.31	107.92	105.80
52	z	44	A	C4-C5-N7	-5.31	108.05	110.70
1	A	1722	A	C4-C5-N7	-5.31	108.05	110.70
32	W	713	A	C4-C5-N7	-5.31	108.05	110.70
32	W	993	A	N9-C4-C5	5.31	107.92	105.80
1	A	53	A	N9-C4-C5	5.30	107.92	105.80
1	A	1188	A	C4-C5-N7	-5.30	108.05	110.70
1	A	2329	A	C4-C5-N7	-5.30	108.05	110.70
32	W	211	A	C4-C5-N7	-5.30	108.05	110.70
32	W	474	A	C4-C5-N7	-5.30	108.05	110.70
52	z	44	A	N9-C4-C5	5.30	107.92	105.80
1	A	14	A	C4-C5-N7	-5.30	108.05	110.70
1	A	429	A	C4-C5-N7	-5.30	108.05	110.70
1	A	1844	A	C8-N9-C4	5.30	107.92	105.80
32	W	1031	A	C4-C5-N7	-5.30	108.05	110.70
1	A	162	A	C8-N9-C4	5.30	107.92	105.80
1	A	429	A	N9-C4-C5	5.30	107.92	105.80
1	A	658	A	C4-C5-N7	-5.30	108.05	110.70
1	A	1008	A	C4-C5-N7	-5.30	108.05	110.70
1	A	1027	A	C4-C5-N7	-5.30	108.05	110.70
1	A	1042	A	N9-C4-C5	5.30	107.92	105.80
1	A	2845	A	C8-N9-C4	5.30	107.92	105.80
2	B	114	A	N9-C4-C5	5.30	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	314	A	N9-C4-C5	5.30	107.92	105.80
32	W	346	A	N9-C4-C5	5.30	107.92	105.80
32	W	397	A	C8-N9-C4	5.30	107.92	105.80
32	W	975	A	C4-C5-N7	-5.30	108.05	110.70
1	A	830	A	C4-C5-N7	-5.30	108.05	110.70
1	A	1265	A	C4-C5-N7	-5.30	108.05	110.70
1	A	1266	A	C4-C5-N7	-5.30	108.05	110.70
1	A	1695	A	C4-C5-N7	-5.30	108.05	110.70
1	A	1700	A	C4-C5-N7	-5.30	108.05	110.70
1	A	1919	A	C8-N9-C4	5.30	107.92	105.80
1	A	2462	A	N9-C4-C5	5.30	107.92	105.80
1	A	2497	A	N9-C4-C5	5.30	107.92	105.80
1	A	2507	A	C4-C5-N7	-5.30	108.05	110.70
1	A	2898	A	C5-C6-N1	5.30	120.35	117.70
32	W	209	A	C4-C5-N7	-5.30	108.05	110.70
32	W	1006	A	N9-C4-C5	5.30	107.92	105.80
1	A	6	A	N9-C4-C5	5.30	107.92	105.80
1	A	206	A	C8-N9-C4	5.30	107.92	105.80
1	A	247	A	C4-C5-N7	-5.30	108.05	110.70
1	A	333	A	N9-C4-C5	5.30	107.92	105.80
1	A	548	A	N9-C4-C5	5.30	107.92	105.80
1	A	1913	A	N9-C4-C5	5.30	107.92	105.80
1	A	1966	A	C4-C5-N7	-5.30	108.05	110.70
1	A	2547	A	C4-C5-N7	-5.30	108.05	110.70
32	W	1155	A	N9-C4-C5	5.30	107.92	105.80
1	A	1480	A	C4-C5-N7	-5.29	108.05	110.70
1	A	2507	A	N9-C4-C5	5.29	107.92	105.80
1	A	2670	A	N3-C4-N9	5.29	131.64	127.40
32	W	1247	A	C4-C5-C6	5.29	119.65	117.00
1	A	171	A	C4-C5-N7	-5.29	108.05	110.70
1	A	216	A	N9-C4-C5	5.29	107.92	105.80
1	A	273	A	C8-N9-C4	5.29	107.92	105.80
1	A	2358	A	C8-N9-C4	5.29	107.92	105.80
1	A	2461	A	C8-N9-C4	5.29	107.92	105.80
32	W	352	A	C4-C5-N7	-5.29	108.05	110.70
32	W	659	A	N9-C4-C5	5.29	107.92	105.80
32	W	799	A	N9-C4-C5	5.29	107.92	105.80
32	W	1014	A	N9-C4-C5	5.29	107.92	105.80
32	W	1092	A	N9-C4-C5	5.29	107.92	105.80
1	A	139	A	N9-C4-C5	5.29	107.92	105.80
1	A	1477	A	C4-C5-N7	-5.29	108.05	110.70
1	A	2062	A	C4-C5-C6	5.29	119.65	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2455	A	N9-C4-C5	5.29	107.92	105.80
1	A	2862	A	C5-C6-N1	5.29	120.35	117.70
32	W	372	A	N9-C4-C5	5.29	107.92	105.80
1	A	61	A	C4-C5-N7	-5.29	108.06	110.70
1	A	326	A	C8-N9-C4	5.29	107.92	105.80
1	A	722	A	C4-C5-N7	-5.29	108.06	110.70
1	A	1096	A	C4-C5-N7	-5.29	108.06	110.70
1	A	1982	A	N3-C4-N9	5.29	131.63	127.40
1	A	2767	A	N9-C4-C5	5.29	107.92	105.80
1	A	2900	A	C4-C5-N7	-5.29	108.06	110.70
32	W	1160	A	C4-C5-N7	-5.29	108.06	110.70
32	W	1200	A	C8-N9-C4	5.29	107.92	105.80
32	W	1272	A	C5-C6-N1	5.29	120.34	117.70
52	z	21	A	N9-C4-C5	5.29	107.92	105.80
1	A	391	A	C4-C5-N7	-5.29	108.06	110.70
1	A	486	A	N9-C4-C5	5.29	107.92	105.80
1	A	971	A	C4-C5-N7	-5.29	108.06	110.70
1	A	1243	A	C8-N9-C4	5.29	107.92	105.80
1	A	1316	A	C5-C6-N1	5.29	120.34	117.70
1	A	1388	A	C4-C5-N7	-5.29	108.06	110.70
1	A	2826	A	N9-C4-C5	5.29	107.92	105.80
32	W	67	A	N9-C4-C5	5.29	107.92	105.80
1	A	518	A	N9-C4-C5	5.29	107.92	105.80
1	A	715	A	C4-C5-N7	-5.29	108.06	110.70
1	A	1813	A	N9-C4-C5	5.29	107.92	105.80
1	A	194	A	N9-C4-C5	5.29	107.91	105.80
1	A	705	A	N9-C4-C5	5.29	107.91	105.80
1	A	1073	A	C8-N9-C4	5.29	107.92	105.80
1	A	1188	A	C8-N9-C4	5.29	107.91	105.80
1	A	1942	A	N9-C4-C5	5.29	107.91	105.80
1	A	2454	A	C4-C5-N7	-5.29	108.06	110.70
32	W	290	A	C4-C5-N7	-5.29	108.06	110.70
32	W	371	A	N9-C4-C5	5.29	107.91	105.80
32	W	474	A	N9-C4-C5	5.29	107.91	105.80
52	z	70	A	N9-C4-C5	5.29	107.91	105.80
1	A	477	A	C8-N9-C4	5.28	107.91	105.80
1	A	1008	A	N9-C4-C5	5.28	107.91	105.80
1	A	1453	A	N9-C4-C5	5.28	107.91	105.80
1	A	1734	A	N9-C4-C5	5.28	107.91	105.80
1	A	2595	A	C4-C5-N7	-5.28	108.06	110.70
32	W	1128	A	C4-C5-N7	-5.28	108.06	110.70
32	W	1155	A	C4-C5-N7	-5.28	108.06	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	904	A	C4-C5-N7	-5.28	108.06	110.70
1	A	1029	A	C8-N9-C4	5.28	107.91	105.80
1	A	1233	A	N9-C4-C5	5.28	107.91	105.80
1	A	41	A	C4-C5-N7	-5.28	108.06	110.70
1	A	790	A	N9-C4-C5	5.28	107.91	105.80
1	A	1190	A	C5-C6-N1	5.28	120.34	117.70
1	A	1432	A	C4-C5-N7	-5.28	108.06	110.70
1	A	1814	A	C5-C6-N1	5.28	120.34	117.70
1	A	1948	A	N9-C4-C5	5.28	107.91	105.80
1	A	2405	A	C8-N9-C4	5.28	107.91	105.80
1	A	2686	A	C4-C5-N7	-5.28	108.06	110.70
2	B	55	A	N9-C4-C5	5.28	107.91	105.80
32	W	114	A	C4-C5-N7	-5.28	108.06	110.70
32	W	790	A	C4-C5-N7	-5.28	108.06	110.70
32	W	1048	A	N9-C4-C5	5.28	107.91	105.80
1	A	1284	A	N9-C4-C5	5.28	107.91	105.80
1	A	108	A	C4-C5-N7	-5.28	108.06	110.70
1	A	183	A	C4-C5-C6	5.28	119.64	117.00
1	A	910	A	C4-C5-N7	-5.28	108.06	110.70
1	A	1134	A	C5-C6-N1	5.28	120.34	117.70
1	A	1335	A	N9-C4-C5	5.28	107.91	105.80
1	A	1485	A	N9-C4-C5	5.28	107.91	105.80
32	W	361	A	C4-C5-N7	-5.28	108.06	110.70
32	W	1016	A	C8-N9-C4	5.28	107.91	105.80
32	W	1166	A	C5-C6-N1	5.28	120.34	117.70
52	z	24	A	C8-N9-C4	5.28	107.91	105.80
1	A	185	A	C8-N9-C4	5.28	107.91	105.80
1	A	236	A	C4-C5-N7	-5.28	108.06	110.70
1	A	421	A	N9-C4-C5	5.28	107.91	105.80
1	A	947	A	N9-C4-C5	5.28	107.91	105.80
1	A	1966	A	N9-C4-C5	5.28	107.91	105.80
32	W	94	A	N9-C4-C5	5.28	107.91	105.80
32	W	460	A	N9-C4-C5	5.28	107.91	105.80
32	W	948	A	C8-N9-C4	5.28	107.91	105.80
1	A	61	A	N9-C4-C5	5.27	107.91	105.80
1	A	226	A	C5-C6-N1	5.27	120.34	117.70
1	A	786	A	C4-C5-N7	-5.27	108.06	110.70
1	A	1627	A	N9-C4-C5	5.27	107.91	105.80
1	A	2694	A	N9-C4-C5	5.27	107.91	105.80
1	A	2794	A	C4-C5-N7	-5.27	108.06	110.70
32	W	696	A	C4-C5-N7	-5.27	108.06	110.70
1	A	90	A	C8-N9-C4	5.27	107.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	876	A	N9-C4-C5	5.27	107.91	105.80
1	A	1197	A	N9-C4-C5	5.27	107.91	105.80
1	A	1536	A	C4-C5-N7	-5.27	108.06	110.70
1	A	2517	A	C4-C5-N7	-5.27	108.06	110.70
1	A	2924	A	C8-N9-C4	5.27	107.91	105.80
32	W	128	A	C4-C5-N7	-5.27	108.06	110.70
32	W	282	A	C5-C6-N1	5.27	120.34	117.70
32	W	314	A	C4-C5-N7	-5.27	108.06	110.70
32	W	381	A	C4-C5-N7	-5.27	108.06	110.70
32	W	386	A	N9-C4-C5	5.27	107.91	105.80
32	W	433	A	N9-C4-C5	5.27	107.91	105.80
32	W	917	A	N9-C4-C5	5.27	107.91	105.80
32	W	1355	A	N3-C4-N9	5.27	131.62	127.40
1	A	1888	A	C4-C5-N7	-5.27	108.06	110.70
1	A	2026	A	C4-C5-N7	-5.27	108.06	110.70
1	A	2089	A	N9-C4-C5	5.27	107.91	105.80
32	W	161	A	N9-C4-C5	5.27	107.91	105.80
1	A	84	A	N9-C4-C5	5.27	107.91	105.80
1	A	537	A	N9-C4-C5	5.27	107.91	105.80
1	A	560	A	C5-C6-N1	5.27	120.33	117.70
1	A	882	A	C4-C5-N7	-5.27	108.06	110.70
1	A	1291	A	N9-C4-C5	5.27	107.91	105.80
1	A	1302	A	N3-C4-N9	5.27	131.62	127.40
1	A	1700	A	C5-C6-N1	5.27	120.33	117.70
1	A	2436	A	C5-C6-N1	5.27	120.33	117.70
1	A	2787	A	C4-C5-N7	-5.27	108.06	110.70
1	A	2851	A	C4-C5-N7	-5.27	108.06	110.70
1	A	2887	A	C4-C5-N7	-5.27	108.06	110.70
1	A	2919	A	C4-C5-N7	-5.27	108.06	110.70
32	W	1004	A	C8-N9-C4	5.27	107.91	105.80
1	A	6	A	C4-C5-N7	-5.27	108.07	110.70
1	A	198	A	C8-N9-C4	5.27	107.91	105.80
1	A	677	A	N9-C4-C5	5.27	107.91	105.80
1	A	753	A	N9-C4-C5	5.27	107.91	105.80
1	A	1142	A	N9-C4-C5	5.27	107.91	105.80
1	A	1202	A	N9-C4-C5	5.27	107.91	105.80
1	A	1404	A	C4-C5-N7	-5.27	108.07	110.70
1	A	2369	A	N9-C4-C5	5.27	107.91	105.80
1	A	2440	A	C8-N9-C4	5.27	107.91	105.80
32	W	969	A	C4-C5-N7	-5.27	108.07	110.70
1	A	2844	A	C5-C6-N1	5.27	120.33	117.70
32	W	120	A	C4-C5-N7	-5.27	108.07	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	373	A	C8-N9-C4	5.26	107.91	105.80
1	A	551	A	C8-N9-C4	5.26	107.91	105.80
1	A	592	A	C4-C5-N7	-5.26	108.07	110.70
1	A	630	A	C4-C5-N7	-5.26	108.07	110.70
1	A	1201	A	C4-C5-C6	5.26	119.63	117.00
1	A	1710	A	N9-C4-C5	5.26	107.91	105.80
1	A	2106	A	C8-N9-C4	5.26	107.91	105.80
1	A	2889	A	N9-C4-C5	5.26	107.91	105.80
32	W	724	A	C8-N9-C4	5.26	107.91	105.80
1	A	1506	A	C8-N9-C4	5.26	107.91	105.80
1	A	2827	A	N9-C4-C5	5.26	107.91	105.80
2	B	46	A	C5-C6-N1	5.26	120.33	117.70
32	W	911	A	C8-N9-C4	5.26	107.91	105.80
1	A	948	A	N9-C4-C5	5.26	107.90	105.80
1	A	1142	A	C4-C5-N7	-5.26	108.07	110.70
1	A	1294	A	C4'-C3'-O3'	-5.26	98.35	109.40
1	A	1680	A	C4-C5-N7	-5.26	108.07	110.70
1	A	1695	A	N9-C4-C5	5.26	107.91	105.80
32	W	605	A	C4-C5-N7	-5.26	108.07	110.70
32	W	1517	A	C4-C5-N7	-5.26	108.07	110.70
1	A	14	A	C8-N9-C4	5.26	107.90	105.80
1	A	274	A	N9-C4-C5	5.26	107.90	105.80
1	A	616	A	N9-C4-C5	5.26	107.90	105.80
1	A	1054	A	C4-C5-N7	-5.26	108.07	110.70
1	A	2464	A	C8-N9-C4	5.26	107.90	105.80
1	A	2790	A	C5-C6-N1	5.26	120.33	117.70
1	A	2805	A	N9-C4-C5	5.26	107.90	105.80
32	W	477	A	C8-N9-C4	5.26	107.90	105.80
32	W	985	A	N9-C4-C5	5.26	107.90	105.80
1	A	1131	A	C4-C5-N7	-5.26	108.07	110.70
32	W	1342	A	N9-C4-C5	5.26	107.90	105.80
1	A	459	A	N9-C4-C5	5.26	107.90	105.80
1	A	922	A	C8-N9-C4	5.26	107.90	105.80
1	A	1075	A	C8-N9-C4	5.26	107.90	105.80
1	A	1417	A	N3-C4-N9	5.26	131.60	127.40
32	W	72	A	N9-C4-C5	5.26	107.90	105.80
32	W	308	A	C4-C5-N7	-5.26	108.07	110.70
32	W	337	A	C4-C5-N7	-5.26	108.07	110.70
32	W	1167	C	C6-N1-C1'	-5.26	114.49	120.80
32	W	1308	A	C5-C6-N1	5.26	120.33	117.70
32	W	1486	A	C4-C5-N7	-5.26	108.07	110.70
1	A	117	A	C8-N9-C4	5.25	107.90	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1075	A	C4-C5-N7	-5.25	108.07	110.70
1	A	1426	A	C4-C5-N7	-5.25	108.07	110.70
32	W	61	A	N9-C4-C5	5.25	107.90	105.80
32	W	1261	A	C4-C5-N7	-5.25	108.07	110.70
1	A	302	A	C8-N9-C4	5.25	107.90	105.80
1	A	2722	A	N9-C4-C5	5.25	107.90	105.80
32	W	1245	A	N9-C4-C5	5.25	107.90	105.80
1	A	333	A	C4-C5-N7	-5.25	108.07	110.70
1	A	1919	A	C4-C5-N7	-5.25	108.07	110.70
1	A	2505	A	N9-C4-C5	5.25	107.90	105.80
32	W	308	A	C8-N9-C4	5.25	107.90	105.80
32	W	649	A	C5-C6-N1	5.25	120.33	117.70
32	W	1143	A	C4-C5-N7	-5.25	108.07	110.70
1	A	391	A	N9-C4-C5	5.25	107.90	105.80
1	A	1768	A	C4-C5-N7	-5.25	108.08	110.70
1	A	1845	A	C4-C5-N7	-5.25	108.08	110.70
1	A	2083	A	C4-C5-N7	-5.25	108.08	110.70
32	W	1442	A	N9-C4-C5	5.25	107.90	105.80
1	A	1614	A	N9-C4-C5	5.25	107.90	105.80
1	A	1697	A	N9-C4-C5	5.25	107.90	105.80
1	A	2875	A	N9-C4-C5	5.25	107.90	105.80
32	W	674	A	C8-N9-C4	5.25	107.90	105.80
32	W	985	A	C4-C5-N7	-5.25	108.08	110.70
32	W	1189	A	C4-C5-N7	-5.25	108.08	110.70
1	A	1308	A	N9-C4-C5	5.25	107.90	105.80
1	A	1814	A	C8-N9-C4	5.25	107.90	105.80
1	A	1858	A	C4-C5-N7	-5.25	108.08	110.70
1	A	1930	A	C4-C5-N7	-5.25	108.08	110.70
1	A	2078	A	C4-C5-N7	-5.25	108.08	110.70
1	A	2441	A	C4-C5-N7	-5.25	108.08	110.70
1	A	2517	A	N9-C4-C5	5.25	107.90	105.80
1	A	2662	A	C4-C5-N7	-5.25	108.08	110.70
1	A	724	A	C4-C5-N7	-5.25	108.08	110.70
1	A	1579	A	C4-C5-N7	-5.25	108.08	110.70
32	W	913	A	N9-C4-C5	5.25	107.90	105.80
1	A	561	A	C4-C5-N7	-5.24	108.08	110.70
1	A	952	A	N9-C4-C5	5.24	107.90	105.80
1	A	1054	A	N9-C4-C5	5.24	107.90	105.80
1	A	1569	A	N9-C4-C5	5.24	107.90	105.80
1	A	1967	A	N9-C4-C5	5.24	107.90	105.80
32	W	76	A	C4-C5-N7	-5.24	108.08	110.70
1	A	2907	A	C5-C6-N1	5.24	120.32	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	50	A	C4-C5-N7	-5.24	108.08	110.70
32	W	644	A	C4-C5-N7	-5.24	108.08	110.70
32	W	874	A	N9-C4-C5	5.24	107.90	105.80
32	W	978	A	C8-N9-C4	5.24	107.90	105.80
32	W	1054	A	C4-C5-N7	-5.24	108.08	110.70
32	W	1490	A	C4-C5-N7	-5.24	108.08	110.70
1	A	547	A	N9-C4-C5	5.24	107.90	105.80
1	A	1442	A	C5-C6-N1	5.24	120.32	117.70
1	A	1581	A	C5-C6-N1	5.24	120.32	117.70
1	A	2663	A	C4-C5-N7	-5.24	108.08	110.70
32	W	173	A	N9-C4-C5	5.24	107.90	105.80
32	W	649	A	C4-C5-N7	-5.24	108.08	110.70
32	W	1189	A	C8-N9-C4	5.24	107.90	105.80
32	W	1207	A	C4-C5-N7	-5.24	108.08	110.70
32	W	1479	A	C4-C5-N7	-5.24	108.08	110.70
1	A	656	A	C8-N9-C4	5.24	107.89	105.80
1	A	1774	A	C8-N9-C4	5.24	107.89	105.80
1	A	1831	A	C4-C5-N7	-5.24	108.08	110.70
1	A	2395	A	C4-C5-N7	-5.24	108.08	110.70
32	W	1054	A	N9-C4-C5	5.24	107.89	105.80
1	A	2754	A	C4-C5-N7	-5.24	108.08	110.70
1	A	2296	A	C8-N9-C4	5.24	107.89	105.80
32	W	18	A	N9-C4-C5	5.24	107.89	105.80
32	W	664	A	C5-C6-N1	5.24	120.32	117.70
32	W	1031	A	N9-C4-C5	5.24	107.89	105.80
32	W	1077	A	N9-C4-C5	5.24	107.89	105.80
1	A	551	A	N9-C4-C5	5.23	107.89	105.80
1	A	2358	A	C5-C6-N1	5.23	120.32	117.70
32	W	271	A	C8-N9-C4	5.23	107.89	105.80
32	W	786	A	N9-C4-C5	5.23	107.89	105.80
1	A	689	A	C4-C5-N7	-5.23	108.08	110.70
1	A	925	A	C8-N9-C4	5.23	107.89	105.80
1	A	1360	A	C8-N9-C4	5.23	107.89	105.80
1	A	1768	A	C8-N9-C4	5.23	107.89	105.80
1	A	1802	A	N9-C4-C5	5.23	107.89	105.80
1	A	1999	A	C4-C5-N7	-5.23	108.08	110.70
32	W	758	A	C4-C5-N7	-5.23	108.08	110.70
1	A	517	A	C4-C5-N7	-5.23	108.08	110.70
1	A	560	A	C8-N9-C4	5.23	107.89	105.80
1	A	683	A	C8-N9-C4	5.23	107.89	105.80
1	A	1067	A	C4-C5-N7	-5.23	108.08	110.70
1	A	1638	A	C4-C5-N7	-5.23	108.08	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2303	A	C8-N9-C4	5.23	107.89	105.80
32	W	837	A	N9-C4-C5	5.23	107.89	105.80
1	A	126	A	C4-C5-N7	-5.23	108.09	110.70
1	A	647	A	C5-C6-N1	5.23	120.31	117.70
1	A	958	A	C8-N9-C4	5.23	107.89	105.80
1	A	1768	A	N9-C4-C5	5.23	107.89	105.80
1	A	2349	A	N9-C4-C5	5.23	107.89	105.80
1	A	2740	A	N9-C4-C5	5.23	107.89	105.80
1	A	2907	A	N9-C4-C5	5.23	107.89	105.80
32	W	457	A	C4-C5-N7	-5.23	108.09	110.70
32	W	569	A	N9-C4-C5	5.23	107.89	105.80
1	A	305	A	C4-C5-N7	-5.23	108.09	110.70
1	A	782	A	N9-C4-C5	5.23	107.89	105.80
1	A	1473	A	C4-C5-C6	5.23	119.61	117.00
1	A	1675	A	N9-C4-C5	5.23	107.89	105.80
1	A	2848	A	N9-C4-C5	5.23	107.89	105.80
32	W	1283	A	N9-C4-C5	5.23	107.89	105.80
1	A	44	A	C8-N9-C4	5.23	107.89	105.80
1	A	437	A	N9-C4-C5	5.23	107.89	105.80
1	A	2421	A	N9-C4-C5	5.23	107.89	105.80
1	A	2844	A	N9-C4-C5	5.23	107.89	105.80
32	W	74	A	C5-C6-N1	5.23	120.31	117.70
32	W	1176	A	N9-C4-C5	5.23	107.89	105.80
32	W	1341	A	C4-C5-N7	-5.23	108.09	110.70
1	A	236	A	N9-C4-C5	5.22	107.89	105.80
1	A	494	A	C4-C5-N7	-5.22	108.09	110.70
1	A	870	A	C4-C5-N7	-5.22	108.09	110.70
1	A	1360	A	N9-C4-C5	5.22	107.89	105.80
1	A	2889	A	C4-C5-N7	-5.22	108.09	110.70
2	B	20	A	N9-C4-C5	5.22	107.89	105.80
32	W	1197	A	C4-C5-N7	-5.22	108.09	110.70
1	A	1073	A	N9-C4-C5	5.22	107.89	105.80
1	A	1536	A	C8-N9-C4	5.22	107.89	105.80
1	A	2044	A	C8-N9-C4	5.22	107.89	105.80
1	A	2297	A	N9-C4-C5	5.22	107.89	105.80
1	A	2407	A	C8-N9-C4	5.22	107.89	105.80
1	A	2511	A	N9-C4-C5	5.22	107.89	105.80
32	W	875	A	C5-C6-N1	5.22	120.31	117.70
32	W	1296	A	C4-C5-N7	-5.22	108.09	110.70
1	A	1149	A	C4-C5-N7	-5.22	108.09	110.70
32	W	1342	A	C4-C5-N7	-5.22	108.09	110.70
1	A	225	A	N9-C4-C5	5.22	107.89	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	431	A	N9-C4-C5	5.22	107.89	105.80
1	A	689	A	C8-N9-C4	5.22	107.89	105.80
1	A	1675	A	C4-C5-N7	-5.22	108.09	110.70
1	A	1789	A	C4-C5-N7	-5.22	108.09	110.70
32	W	684	A	C4-C5-N7	-5.22	108.09	110.70
32	W	1327	A	N9-C4-C5	5.22	107.89	105.80
1	A	1848	A	C4-C5-N7	-5.22	108.09	110.70
1	A	2468	A	C8-N9-C4	5.22	107.89	105.80
32	W	1188	A	C4-C5-N7	-5.22	108.09	110.70
1	A	185	A	C4-C5-N7	-5.22	108.09	110.70
1	A	254	A	C4-C5-N7	-5.22	108.09	110.70
1	A	504	A	C5-C6-N1	5.22	120.31	117.70
1	A	1412	A	N9-C4-C5	5.22	107.89	105.80
1	A	1778	A	C4-C5-N7	-5.22	108.09	110.70
1	A	2329	A	N9-C4-C5	5.22	107.89	105.80
1	A	2754	A	C5-C6-N1	5.22	120.31	117.70
1	A	2848	A	C8-N9-C4	5.22	107.89	105.80
2	B	64	A	N9-C4-C5	5.22	107.89	105.80
32	W	743	A	C4-C5-N7	-5.22	108.09	110.70
1	A	1194	A	C4-C5-N7	-5.21	108.09	110.70
1	A	2459	A	C8-N9-C4	5.21	107.89	105.80
1	A	2819	A	N9-C4-C5	5.21	107.89	105.80
32	W	650	A	C4-C5-N7	-5.21	108.09	110.70
52	z	23	A	C4-C5-N7	-5.21	108.09	110.70
1	A	561	A	N9-C4-C5	5.21	107.89	105.80
1	A	1480	A	N9-C4-C5	5.21	107.89	105.80
1	A	1895	A	N9-C4-C5	5.21	107.89	105.80
32	W	1384	A	C4-C5-N7	-5.21	108.09	110.70
1	A	369	A	C4-C5-N7	-5.21	108.09	110.70
1	A	1305	A	N3-C4-N9	5.21	131.57	127.40
1	A	1858	A	N9-C4-C5	5.21	107.88	105.80
1	A	2708	A	N9-C4-C5	5.21	107.89	105.80
1	A	2778	A	C4-C5-N7	-5.21	108.09	110.70
32	W	512	A	C4-C5-N7	-5.21	108.09	110.70
32	W	1234	A	C4-C5-N7	-5.21	108.09	110.70
1	A	260	A	N9-C4-C5	5.21	107.88	105.80
1	A	769	A	C4-C5-N7	-5.21	108.09	110.70
1	A	1222	A	C4-C5-N7	-5.21	108.09	110.70
1	A	1569	A	C4-C5-N7	-5.21	108.09	110.70
32	W	234	A	N9-C4-C5	5.21	107.88	105.80
32	W	631	A	N3-C4-N9	5.21	131.57	127.40
1	A	616	A	C4-C5-N7	-5.21	108.09	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1655	A	C8-N9-C4	5.21	107.88	105.80
1	A	1721	A	N9-C4-C5	5.21	107.88	105.80
1	A	2007	A	N9-C4-C5	5.21	107.88	105.80
1	A	2704	A	C8-N9-C4	5.21	107.88	105.80
1	A	2810	A	N9-C4-C5	5.21	107.88	105.80
32	W	161	A	C8-N9-C4	5.21	107.88	105.80
1	A	870	A	C5-C6-N1	5.21	120.30	117.70
1	A	2000	A	N9-C4-C5	5.21	107.88	105.80
1	A	2848	A	C4-C5-N7	-5.21	108.10	110.70
2	B	46	A	C4-C5-N7	-5.21	108.10	110.70
32	W	1206	A	C4-C5-N7	-5.21	108.10	110.70
32	W	1247	A	N3-C4-N9	5.21	131.56	127.40
32	W	1315	A	N9-C4-C5	5.21	107.88	105.80
32	W	1466	A	N9-C4-C5	5.21	107.88	105.80
1	A	1126	A	C4-C5-N7	-5.21	108.10	110.70
1	A	1131	A	N9-C4-C5	5.21	107.88	105.80
1	A	1286	A	C5-C6-N1	5.21	120.30	117.70
1	A	1375	A	N9-C4-C5	5.21	107.88	105.80
1	A	1905	A	C4-C5-C6	5.21	119.60	117.00
32	W	114	A	N9-C4-C5	5.21	107.88	105.80
32	W	1529	A	N9-C4-C5	5.21	107.88	105.80
1	A	849	A	C8-N9-C4	5.20	107.88	105.80
1	A	1096	A	N9-C4-C5	5.20	107.88	105.80
1	A	1614	A	C8-N9-C4	5.20	107.88	105.80
32	W	301	A	C4-C5-N7	-5.20	108.10	110.70
1	A	525	A	C5-C6-N1	5.20	120.30	117.70
1	A	1653	A	N9-C4-C5	5.20	107.88	105.80
1	A	1848	A	N9-C4-C5	5.20	107.88	105.80
1	A	2339	A	C4-C5-N7	-5.20	108.10	110.70
32	W	140	A	N9-C4-C5	5.20	107.88	105.80
32	W	1341	A	C8-N9-C4	5.20	107.88	105.80
1	A	390	A	N9-C4-C5	5.20	107.88	105.80
1	A	1308	A	C4-C5-N7	-5.20	108.10	110.70
1	A	1313	A	N9-C4-C5	5.20	107.88	105.80
1	A	1672	A	N9-C4-C5	5.20	107.88	105.80
1	A	2787	A	N9-C4-C5	5.20	107.88	105.80
2	B	46	A	N9-C4-C5	5.20	107.88	105.80
32	W	724	A	C4-C5-N7	-5.20	108.10	110.70
1	A	868	A	N9-C4-C5	5.20	107.88	105.80
1	A	1340	A	C4-C5-N7	-5.20	108.10	110.70
32	W	463	A	N9-C4-C5	5.20	107.88	105.80
1	A	53	A	C4-C5-N7	-5.20	108.10	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	841	A	C4-C5-N7	-5.20	108.10	110.70
1	A	971	A	N9-C4-C5	5.20	107.88	105.80
1	A	2844	A	C8-N9-C4	5.20	107.88	105.80
32	W	1463	A	C8-N9-C4	5.20	107.88	105.80
1	A	1074	A	N9-C4-C5	5.19	107.88	105.80
1	A	1901	A	C4-C5-N7	-5.19	108.10	110.70
32	W	969	A	C8-N9-C4	5.19	107.88	105.80
1	A	102	A	N9-C4-C5	5.19	107.88	105.80
1	A	374	A	N3-C4-N9	5.19	131.55	127.40
1	A	647	A	N9-C4-C5	5.19	107.88	105.80
1	A	763	A	N9-C4-C5	5.19	107.88	105.80
1	A	1876	A	C8-N9-C4	5.19	107.88	105.80
1	A	2330	A	C8-N9-C4	5.19	107.88	105.80
32	W	278	A	N9-C4-C5	5.19	107.88	105.80
32	W	1017	A	C8-N9-C4	5.19	107.88	105.80
32	W	1234	A	N9-C4-C5	5.19	107.88	105.80
32	W	1493	A	N9-C4-C5	5.19	107.88	105.80
1	A	1722	A	N9-C4-C5	5.19	107.88	105.80
1	A	2406	A	N9-C4-C5	5.19	107.88	105.80
1	A	1709	A	N9-C4-C5	5.19	107.88	105.80
1	A	2349	A	C8-N9-C4	5.19	107.88	105.80
1	A	133	A	C4-C5-N7	-5.19	108.11	110.70
1	A	2851	A	N9-C4-C5	5.19	107.88	105.80
32	W	287	A	N9-C4-C5	5.19	107.88	105.80
32	W	439	A	C4-C5-N7	-5.19	108.11	110.70
32	W	518	A	C8-N9-C4	5.19	107.88	105.80
32	W	758	A	C5-C6-N1	5.19	120.29	117.70
32	W	844	A	C5-C6-N1	5.19	120.29	117.70
1	A	144	A	N9-C4-C5	5.19	107.87	105.80
1	A	790	A	C4-C5-N7	-5.19	108.11	110.70
1	A	2916	A	C8-N9-C4	5.19	107.87	105.80
1	A	21	A	N9-C4-C5	5.18	107.87	105.80
1	A	476	A	C8-N9-C4	5.18	107.87	105.80
1	A	1006	A	C4-C5-N7	-5.18	108.11	110.70
1	A	1461	A	N9-C4-C5	5.18	107.87	105.80
1	A	2030	A	C8-N9-C4	5.18	107.87	105.80
32	W	679	A	C4-C5-N7	-5.18	108.11	110.70
32	W	874	A	C4-C5-N7	-5.18	108.11	110.70
32	W	911	A	C4-C5-N7	-5.18	108.11	110.70
32	W	1490	A	C5-C6-N1	5.18	120.29	117.70
1	A	1123	A	C4-C5-N7	-5.18	108.11	110.70
1	A	1222	A	N9-C4-C5	5.18	107.87	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1520	A	C4-C5-N7	-5.18	108.11	110.70
1	A	2042	A	C5-C6-N1	5.18	120.29	117.70
1	A	2316	A	N9-C4-C5	5.18	107.87	105.80
1	A	2390	A	N9-C4-C5	5.18	107.87	105.80
32	W	173	A	C4-C5-N7	-5.18	108.11	110.70
32	W	1133	A	N3-C4-N9	5.18	131.55	127.40
32	W	1140	A	C4-C5-N7	-5.18	108.11	110.70
32	W	933	A	C4-C5-N7	-5.18	108.11	110.70
32	W	945	A	C5-C6-N1	5.18	120.29	117.70
32	W	1463	A	C4-C5-N7	-5.18	108.11	110.70
32	W	1479	A	N9-C4-C5	5.18	107.87	105.80
1	A	13	A	N9-C4-C5	5.18	107.87	105.80
1	A	220	A	C8-N9-C4	5.18	107.87	105.80
1	A	993	A	N9-C4-C5	5.18	107.87	105.80
32	W	929	A	C8-N9-C4	5.18	107.87	105.80
1	A	507	A	N9-C4-C5	5.18	107.87	105.80
1	A	1221	A	C4-C5-N7	-5.18	108.11	110.70
1	A	1778	A	C5-C6-N1	5.18	120.29	117.70
32	W	438	A	C4-C5-N7	-5.18	108.11	110.70
32	W	899	A	C4-C5-C6	5.18	119.59	117.00
1	A	374	A	C4-C5-C6	5.18	119.59	117.00
32	W	117	A	N9-C4-C5	5.18	107.87	105.80
32	W	984	A	N9-C4-C5	5.18	107.87	105.80
32	W	1143	A	N9-C4-C5	5.18	107.87	105.80
32	W	1210	A	N9-C4-C5	5.18	107.87	105.80
32	W	1294	A	C4-C5-N7	-5.18	108.11	110.70
32	W	1435	A	C8-N9-C4	5.18	107.87	105.80
1	A	964	A	N9-C4-C5	5.17	107.87	105.80
1	A	1188	A	N3-C4-N9	5.17	131.54	127.40
1	A	1243	A	C5-C6-N1	5.17	120.29	117.70
1	A	2441	A	N9-C4-C5	5.17	107.87	105.80
1	A	1490	A	C8-N9-C4	5.17	107.87	105.80
1	A	1839	A	N9-C4-C5	5.17	107.87	105.80
1	A	2662	A	N9-C4-C5	5.17	107.87	105.80
2	B	51	A	N9-C4-C5	5.17	107.87	105.80
32	W	1188	A	C5-C6-N1	5.17	120.29	117.70
1	A	133	A	N9-C4-C5	5.17	107.87	105.80
1	A	526	A	C5-C6-N1	5.17	120.28	117.70
1	A	619	A	N9-C4-C5	5.17	107.87	105.80
1	A	752	A	C4-C5-N7	-5.17	108.11	110.70
1	A	1027	A	C8-N9-C4	5.17	107.87	105.80
1	A	1672	A	C5-C6-N1	5.17	120.29	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1710	A	C4-C5-N7	-5.17	108.11	110.70
1	A	1900	A	C8-N9-C4	5.17	107.87	105.80
1	A	2454	A	N9-C4-C5	5.17	107.87	105.80
32	W	1349	A	N9-C4-C5	5.17	107.87	105.80
1	A	2402	A	N9-C4-C5	5.17	107.87	105.80
32	W	727	A	C8-N9-C4	5.17	107.87	105.80
32	W	828	A	N9-C4-C5	5.17	107.87	105.80
1	A	504	A	C4-C5-C6	5.17	119.58	117.00
1	A	592	A	N9-C4-C5	5.17	107.87	105.80
32	W	81	A	N9-C4-C5	5.17	107.87	105.80
32	W	1167	C	N3-C2-O2	-5.17	118.28	121.90
1	A	699	A	C8-N9-C4	5.17	107.87	105.80
1	A	1149	A	N9-C4-C5	5.17	107.87	105.80
1	A	1680	A	N9-C4-C5	5.17	107.87	105.80
2	B	25	A	C4-C5-N7	-5.17	108.12	110.70
32	W	258	A	N9-C4-C5	5.17	107.87	105.80
32	W	1022	A	C4-C5-N7	-5.17	108.12	110.70
1	A	1981	A	C8-N9-C4	5.17	107.87	105.80
32	W	919	A	N9-C4-C5	5.17	107.87	105.80
32	W	1189	A	N9-C4-C5	5.17	107.87	105.80
32	W	1513	A	N9-C4-C5	5.17	107.87	105.80
1	A	1710	A	C5-C6-N1	5.16	120.28	117.70
1	A	2662	A	C5-C6-N1	5.16	120.28	117.70
1	A	2916	A	C5-C6-N1	5.16	120.28	117.70
32	W	507	A	C5-C6-N6	-5.16	119.57	123.70
32	W	879	A	C4-C5-N7	-5.16	108.12	110.70
1	A	1388	A	N9-C4-C5	5.16	107.86	105.80
52	z	9	A	N9-C4-C5	5.16	107.86	105.80
1	A	118	A	C4-C5-N7	-5.16	108.12	110.70
1	A	692	A	C4-C5-N7	-5.16	108.12	110.70
1	A	715	A	N9-C4-C5	5.16	107.86	105.80
1	A	908	A	C8-N9-C4	5.16	107.86	105.80
1	A	1075	A	N9-C4-C5	5.16	107.86	105.80
1	A	1417	A	C4-C5-C6	5.16	119.58	117.00
1	A	2887	A	N9-C4-C5	5.16	107.86	105.80
1	A	305	A	N9-C4-C5	5.16	107.86	105.80
1	A	1532	A	N9-C4-C5	5.16	107.86	105.80
1	A	1614	A	C4-C5-N7	-5.16	108.12	110.70
1	A	1691	A	C5-C6-N1	5.16	120.28	117.70
1	A	2327	A	N9-C4-C5	5.16	107.86	105.80
1	A	2735	A	C5-C6-N1	5.16	120.28	117.70
1	A	44	A	C5-C6-N1	5.16	120.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	656	A	N9-C4-C5	5.16	107.86	105.80
1	A	2793	A	C4-C5-C6	5.16	119.58	117.00
32	W	120	A	N9-C4-C5	5.16	107.86	105.80
32	W	651	A	N9-C4-C5	5.16	107.86	105.80
32	W	1278	A	C4-C5-N7	-5.16	108.12	110.70
1	A	1253	A	N9-C4-C5	5.16	107.86	105.80
1	A	1727	A	N9-C4-C5	5.16	107.86	105.80
1	A	1812	A	C8-N9-C4	5.16	107.86	105.80
1	A	2793	A	C5-C6-N1	5.16	120.28	117.70
32	W	496	A	N9-C4-C5	5.16	107.86	105.80
1	A	593	A	C5-C6-N1	5.15	120.28	117.70
1	A	1412	A	C4-C5-N7	-5.15	108.12	110.70
1	A	1524	A	N9-C4-C5	5.15	107.86	105.80
52	z	41	A	N9-C4-C5	5.15	107.86	105.80
1	A	1480	A	C8-N9-C4	5.15	107.86	105.80
1	A	1838	A	C8-N9-C4	5.15	107.86	105.80
32	W	278	A	C4-C5-N7	-5.15	108.12	110.70
32	W	1256	A	N9-C4-C5	5.15	107.86	105.80
32	W	1297	A	N9-C4-C5	5.15	107.86	105.80
1	A	258	A	C4-C5-N7	-5.15	108.12	110.70
1	A	560	A	C4-C5-N7	-5.15	108.12	110.70
1	A	1100	A	C4-C5-N7	-5.15	108.12	110.70
1	A	1161	A	C5-C6-N1	5.15	120.28	117.70
1	A	1700	A	N9-C4-C5	5.15	107.86	105.80
1	A	2734	A	N9-C4-C5	5.15	107.86	105.80
1	A	2357	A	C8-N9-C4	5.15	107.86	105.80
32	W	674	A	C5-C6-N1	5.15	120.27	117.70
32	W	948	A	N9-C4-C5	5.15	107.86	105.80
32	W	1517	A	C5-C6-N1	5.15	120.27	117.70
1	A	171	A	C5-C6-N1	5.15	120.27	117.70
32	W	1369	A	C8-N9-C4	5.15	107.86	105.80
32	W	512	A	N9-C4-C5	5.15	107.86	105.80
52	z	76	A	N9-C4-C5	5.15	107.86	105.80
1	A	537	A	C4-C5-N7	-5.14	108.13	110.70
32	W	838	A	C4-C5-N7	-5.14	108.13	110.70
1	A	896	A	N9-C4-C5	5.14	107.86	105.80
1	A	2440	A	C4-C5-N7	-5.14	108.13	110.70
32	W	899	A	C5-C6-N1	5.14	120.27	117.70
32	W	1405	A	N9-C4-C5	5.14	107.86	105.80
1	A	254	A	N9-C4-C5	5.14	107.86	105.80
1	A	786	A	N9-C4-C5	5.14	107.86	105.80
1	A	1619	A	C8-N9-C4	5.14	107.86	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	151	A	C5-C6-N1	5.14	120.27	117.70
32	W	555	A	C4-C5-N7	-5.14	108.13	110.70
1	A	1100	A	N9-C4-C5	5.14	107.86	105.80
32	W	993	A	C5-C6-N1	5.14	120.27	117.70
1	A	265	A	C4-C5-N7	-5.14	108.13	110.70
1	A	1655	A	N9-C4-C5	5.14	107.86	105.80
32	W	945	A	N9-C4-C5	5.14	107.86	105.80
1	A	353	A	C8-N9-C4	5.14	107.86	105.80
2	B	71	A	C8-N9-C4	5.14	107.86	105.80
1	A	108	A	C5-C6-N1	5.13	120.27	117.70
1	A	281	A	C5-C6-N1	5.13	120.27	117.70
1	A	475	A	N9-C4-C5	5.13	107.85	105.80
1	A	1019	A	C4-C5-N7	-5.13	108.13	110.70
1	A	2358	A	N9-C4-C5	5.13	107.85	105.80
32	W	918	A	N9-C4-C5	5.13	107.85	105.80
1	A	1190	A	N9-C4-C5	5.13	107.85	105.80
1	A	133	A	C5-C6-N1	5.13	120.27	117.70
1	A	958	A	C4-C5-N7	-5.13	108.13	110.70
1	A	1103	A	C5-C6-N1	5.13	120.27	117.70
1	A	1562	A	N9-C4-C5	5.13	107.85	105.80
1	A	1721	A	C4-C5-N7	-5.13	108.13	110.70
1	A	2900	A	N9-C4-C5	5.13	107.85	105.80
32	W	129	A	N9-C4-C5	5.13	107.85	105.80
32	W	171	A	C5-C6-N1	5.13	120.27	117.70
32	W	924	A	C5-C6-N1	5.13	120.27	117.70
1	A	630	A	N9-C4-C5	5.13	107.85	105.80
1	A	1340	A	C8-N9-C4	5.13	107.85	105.80
1	A	2831	A	C8-N9-C4	5.13	107.85	105.80
32	W	711	A	N9-C4-C5	5.13	107.85	105.80
32	W	1358	A	C4-C5-C6	5.13	119.56	117.00
1	A	1945	A	C8-N9-C4	5.13	107.85	105.80
32	W	1133	A	C8-N9-C4	5.13	107.85	105.80
32	W	1383	A	N9-C4-C5	5.13	107.85	105.80
1	A	156	A	N9-C4-C5	5.13	107.85	105.80
1	A	273	A	C5-C6-N1	5.13	120.26	117.70
32	W	117	A	C4-C5-N7	-5.13	108.14	110.70
32	W	1160	A	C5-C6-N1	5.13	120.26	117.70
32	W	605	A	N9-C4-C5	5.12	107.85	105.80
32	W	649	A	N9-C4-C5	5.12	107.85	105.80
32	W	548	A	C4-C5-N7	-5.12	108.14	110.70
32	W	743	A	N9-C4-C5	5.12	107.85	105.80
1	A	125	A	C5-C6-N1	5.12	120.26	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	183	A	N3-C4-N9	5.12	131.50	127.40
1	A	1123	A	N9-C4-C5	5.12	107.85	105.80
1	A	2365	A	C4-C5-N7	-5.12	108.14	110.70
1	A	2663	A	C5-C6-N1	5.12	120.26	117.70
32	W	57	A	N9-C4-C5	5.12	107.85	105.80
1	A	1008	A	C5-C6-N1	5.12	120.26	117.70
1	A	1506	A	C5-C6-N1	5.12	120.26	117.70
1	A	118	A	C5-C6-N1	5.12	120.26	117.70
1	A	1814	A	N3-C4-N9	5.12	131.50	127.40
1	A	2062	A	N3-C4-N9	5.12	131.50	127.40
1	A	2532	A	C8-N9-C4	5.12	107.85	105.80
32	W	658	A	C5-C6-N1	5.12	120.26	117.70
1	A	140	A	N9-C4-C5	5.12	107.85	105.80
1	A	1941	A	C5-C6-N1	5.12	120.26	117.70
32	W	114	A	C8-N9-C4	5.12	107.85	105.80
1	A	1776	A	C5-C6-N1	5.12	120.26	117.70
32	W	684	A	N9-C4-C5	5.12	107.85	105.80
1	A	526	A	C4-C5-C6	5.11	119.56	117.00
1	A	1221	A	N9-C4-C5	5.11	107.84	105.80
1	A	2044	A	N9-C4-C5	5.11	107.85	105.80
2	B	39	A	N9-C4-C5	5.11	107.84	105.80
32	W	1298	A	C5-C6-N1	5.11	120.26	117.70
1	A	168	A	C4-C5-N7	-5.11	108.14	110.70
32	W	572	A	C8-N9-C4	5.11	107.84	105.80
32	W	1022	A	N9-C4-C5	5.11	107.84	105.80
1	A	1606	A	C4-C5-N7	-5.11	108.14	110.70
1	A	1820	A	C8-N9-C4	5.11	107.84	105.80
1	A	2616	A	N9-C4-C5	5.11	107.84	105.80
32	W	679	A	N9-C4-C5	5.11	107.84	105.80
32	W	844	A	N9-C4-C5	5.11	107.84	105.80
32	W	1026	A	C4-C5-N7	-5.11	108.14	110.70
32	W	811	A	N9-C4-C5	5.11	107.84	105.80
32	W	911	A	N9-C4-C5	5.11	107.84	105.80
1	A	38	A	C8-N9-C4	5.11	107.84	105.80
1	A	2885	A	C4-C5-N7	-5.11	108.15	110.70
32	W	879	A	N9-C4-C5	5.11	107.84	105.80
32	W	1358	A	C4-C5-N7	-5.11	108.15	110.70
1	A	21	A	C4-C5-N7	-5.11	108.15	110.70
1	A	1404	A	N9-C4-C5	5.11	107.84	105.80
32	W	55	A	C5-C6-N1	5.11	120.25	117.70
32	W	1288	A	N9-C4-C5	5.11	107.84	105.80
32	W	1366	A	N9-C4-C5	5.11	107.84	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	318	A	C5-C6-N1	5.10	120.25	117.70
1	A	1244	A	C5-C6-N1	5.10	120.25	117.70
1	A	2719	A	N9-C4-C5	5.10	107.84	105.80
1	A	2898	A	C4-C5-C6	5.10	119.55	117.00
32	W	996	A	N9-C4-C5	5.10	107.84	105.80
32	W	1022	A	C5-C6-N1	5.10	120.25	117.70
1	A	171	A	N9-C4-C5	5.10	107.84	105.80
1	A	1006	A	N9-C4-C5	5.10	107.84	105.80
1	A	2298	A	N9-C4-C5	5.10	107.84	105.80
1	A	2339	A	C8-N9-C4	5.10	107.84	105.80
32	W	1470	A	C5-C6-N1	5.10	120.25	117.70
1	A	6	A	C5-C6-N1	5.10	120.25	117.70
1	A	1131	A	C5-C6-N1	5.10	120.25	117.70
1	A	1201	A	N3-C4-N9	5.10	131.48	127.40
1	A	1928	A	C4-C5-N7	-5.10	108.15	110.70
1	A	2722	A	C5-C6-N1	5.10	120.25	117.70
1	A	2860	A	N9-C4-C5	5.10	107.84	105.80
32	W	381	A	N9-C4-C5	5.10	107.84	105.80
32	W	996	A	C4-C5-N7	-5.10	108.15	110.70
1	A	647	A	C4-C5-C6	5.10	119.55	117.00
1	A	1832	A	C8-N9-C4	5.10	107.84	105.80
32	W	94	A	C5-C6-N1	5.10	120.25	117.70
1	A	53	A	C5-C6-N1	5.09	120.25	117.70
1	A	268	A	C8-N9-C4	5.09	107.84	105.80
1	A	1286	A	N9-C4-C5	5.09	107.84	105.80
1	A	1655	A	C4-C5-N7	-5.09	108.15	110.70
1	A	2027	A	C5-C6-N1	5.09	120.25	117.70
32	W	1272	A	C4-C5-N7	-5.09	108.15	110.70
1	A	2908	A	C5-C6-N1	5.09	120.25	117.70
32	W	1315	A	C8-N9-C4	5.09	107.84	105.80
1	A	230	A	C4-C5-N7	-5.09	108.16	110.70
1	A	1074	A	C5-C6-N1	5.09	120.25	117.70
1	A	2351	A	C5-C6-N1	5.09	120.25	117.70
1	A	462	A	N9-C4-C5	5.09	107.84	105.80
1	A	673	A	C4-C5-N7	-5.09	108.16	110.70
1	A	1491	A	C4-C5-N7	-5.09	108.16	110.70
32	W	211	A	N9-C4-C5	5.09	107.84	105.80
32	W	572	A	C4-C5-N7	-5.09	108.16	110.70
32	W	605	A	C5-C6-N1	5.09	120.25	117.70
1	A	910	A	C5-C6-N1	5.09	120.24	117.70
15	O	22	LEU	CA-CB-CG	5.09	127.00	115.30
32	W	987	A	C4-C5-N7	-5.09	108.16	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	622	A	C8-N9-C4	5.08	107.83	105.80
1	A	2663	A	N9-C4-C5	5.08	107.83	105.80
32	W	987	A	C8-N9-C4	5.08	107.83	105.80
32	W	1288	A	C8-N9-C4	5.08	107.83	105.80
1	A	690	A	C5-C6-N1	5.08	120.24	117.70
1	A	2498	A	C4-C5-N7	-5.08	108.16	110.70
2	B	20	A	C4-C5-N7	-5.08	108.16	110.70
32	W	150	A	C4-C5-C6	5.08	119.54	117.00
32	W	631	A	C5-C6-N1	5.08	120.24	117.70
1	A	956	A	C5-C6-N1	5.08	120.24	117.70
1	A	1655	A	C5-C6-N6	-5.08	119.64	123.70
32	W	1238	A	N9-C4-C5	5.08	107.83	105.80
1	A	494	A	C8-N9-C4	5.08	107.83	105.80
1	A	769	A	N9-C4-C5	5.08	107.83	105.80
1	A	1491	A	N9-C4-C5	5.08	107.83	105.80
32	W	987	A	N9-C4-C5	5.08	107.83	105.80
32	W	1355	A	C5-C6-N1	5.08	120.24	117.70
1	A	1485	A	C4-C5-N7	-5.08	108.16	110.70
32	W	727	A	C4-C5-N7	-5.08	108.16	110.70
1	A	774	A	C5-C6-N1	5.08	120.24	117.70
1	A	1197	A	C4-C5-N7	-5.08	108.16	110.70
1	A	1618	A	C4-C5-N7	-5.08	108.16	110.70
1	A	2719	A	C5-C6-N1	5.08	120.24	117.70
2	B	25	A	N9-C4-C5	5.08	107.83	105.80
1	A	1393	A	N9-C4-C5	5.07	107.83	105.80
1	A	1426	A	N9-C4-C5	5.07	107.83	105.80
1	A	2091	A	C8-N9-C4	5.07	107.83	105.80
32	W	74	A	C8-N9-C4	5.07	107.83	105.80
32	W	118	A	N9-C4-C5	5.07	107.83	105.80
32	W	948	A	C4-C5-N7	-5.07	108.16	110.70
32	W	1294	A	N9-C4-C5	5.07	107.83	105.80
32	W	1456	A	N9-C4-C5	5.07	107.83	105.80
1	A	1480	A	C5-C6-N1	5.07	120.24	117.70
1	A	574	A	C8-N9-C4	5.07	107.83	105.80
1	A	634	A	C4-C5-N7	-5.07	108.17	110.70
1	A	1097	A	C8-N9-C4	5.07	107.83	105.80
1	A	2616	A	C4-C5-N7	-5.07	108.17	110.70
1	A	2794	A	C8-N9-C4	5.07	107.83	105.80
32	W	883	A	N9-C4-C5	5.07	107.83	105.80
32	W	1155	A	C8-N9-C4	5.07	107.83	105.80
1	A	1667	A	C4-C5-N7	-5.07	108.17	110.70
32	W	1238	A	C4-C5-N7	-5.07	108.17	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	841	A	N9-C4-C5	5.07	107.83	105.80
1	A	1417	A	C5-C6-N1	5.07	120.23	117.70
1	A	1620	A	N9-C4-C5	5.07	107.83	105.80
1	A	1776	A	N9-C4-C5	5.07	107.83	105.80
1	A	2026	A	N9-C4-C5	5.07	107.83	105.80
1	A	2302	A	N9-C4-C5	5.07	107.83	105.80
1	A	2547	A	N9-C4-C5	5.07	107.83	105.80
32	W	568	A	N9-C4-C5	5.07	107.83	105.80
1	A	1491	A	C8-N9-C4	5.07	107.83	105.80
1	A	1562	A	C8-N9-C4	5.07	107.83	105.80
1	A	1814	A	C4-C5-C6	5.07	119.53	117.00
1	A	1883	A	C4-C5-N7	-5.07	108.17	110.70
32	W	391	A	C4-C5-N7	-5.07	108.17	110.70
32	W	1355	A	C4-C5-C6	5.07	119.53	117.00
1	A	2402	A	C5-C6-N1	5.06	120.23	117.70
32	W	364	A	C5-C6-N1	5.06	120.23	117.70
1	A	1067	A	N3-C4-N9	5.06	131.45	127.40
1	A	1961	A	N9-C4-C5	5.06	107.83	105.80
1	A	236	A	C5-C6-N6	-5.06	119.65	123.70
1	A	1477	A	N9-C4-C5	5.06	107.82	105.80
32	W	391	A	C8-N9-C4	5.06	107.82	105.80
1	A	462	A	C5-C6-N1	5.06	120.23	117.70
32	W	433	A	C5-C6-N1	5.06	120.23	117.70
32	W	462	A	N9-C4-C5	5.06	107.82	105.80
32	W	758	A	N9-C4-C5	5.06	107.82	105.80
1	A	1579	A	C5-C6-N1	5.06	120.23	117.70
1	A	2358	A	C4-C5-N7	-5.06	108.17	110.70
1	A	1305	A	C5-C6-N1	5.06	120.23	117.70
32	W	128	A	C5-C6-N6	-5.06	119.66	123.70
1	A	1258	A	C5-C6-N1	5.05	120.23	117.70
1	A	2782	A	C8-N9-C4	5.05	107.82	105.80
32	W	397	A	N9-C4-C5	5.05	107.82	105.80
1	A	1667	A	C5-C6-N1	5.05	120.23	117.70
1	A	2447	A	C5-C6-N1	5.05	120.23	117.70
1	A	2689	A	C8-N9-C4	5.05	107.82	105.80
1	A	692	A	N9-C4-C5	5.05	107.82	105.80
1	A	769	A	C5-C6-N1	5.05	120.22	117.70
1	A	1883	A	N9-C4-C5	5.05	107.82	105.80
32	W	1143	A	C5-C6-N1	5.05	120.23	117.70
32	W	1486	A	C5-C6-N1	5.05	120.23	117.70
32	W	1490	A	N9-C4-C5	5.05	107.82	105.80
1	A	527	A	C8-N9-C4	5.05	107.82	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	656	A	C5-C6-N1	5.05	120.22	117.70
1	A	1197	A	C5-C6-N1	5.05	120.22	117.70
1	A	1820	A	N9-C4-C5	5.05	107.82	105.80
1	A	2111	A	C4-C5-N7	-5.05	108.17	110.70
32	W	592	A	C5-C6-N1	5.05	120.22	117.70
32	W	715	A	C5-C6-N1	5.05	120.22	117.70
32	W	1513	A	C5-C6-N1	5.05	120.22	117.70
1	A	559	A	N9-C4-C5	5.05	107.82	105.80
1	A	661	A	C4-C5-N7	-5.05	108.18	110.70
1	A	1456	A	C8-N9-C4	5.05	107.82	105.80
1	A	1638	A	C5-C6-N1	5.05	120.22	117.70
32	W	583	A	C8-N9-C4	5.05	107.82	105.80
32	W	644	A	N9-C4-C5	5.05	107.82	105.80
1	A	52	A	C8-N9-C4	5.05	107.82	105.80
1	A	1714	A	C8-N9-C4	5.05	107.82	105.80
32	W	548	A	N9-C4-C5	5.05	107.82	105.80
32	W	1197	A	C5-C6-N1	5.04	120.22	117.70
1	A	150	A	N9-C4-C5	5.04	107.82	105.80
1	A	1316	A	N9-C4-C5	5.04	107.82	105.80
1	A	2270	A	C5-C6-N1	5.04	120.22	117.70
32	W	1488	A	C5-C6-N1	5.04	120.22	117.70
1	A	1888	A	N9-C4-C5	5.04	107.82	105.80
1	A	2627	A	C4-C5-N7	-5.04	108.18	110.70
1	A	2689	A	C4-C5-N7	-5.04	108.18	110.70
32	W	128	A	N9-C4-C5	5.04	107.82	105.80
32	W	1160	A	N9-C4-C5	5.04	107.82	105.80
1	A	1638	A	N9-C4-C5	5.04	107.82	105.80
1	A	1928	A	C5-C6-N1	5.04	120.22	117.70
1	A	647	A	C4-C5-N7	-5.04	108.18	110.70
1	A	882	A	N9-C4-C5	5.04	107.81	105.80
1	A	2080	A	C4-C5-N7	-5.04	108.18	110.70
1	A	2916	A	N3-C4-N9	5.04	131.43	127.40
32	W	913	A	C5-C6-N1	5.04	120.22	117.70
32	W	1161	A	C4-C5-N7	-5.04	108.18	110.70
2	B	13	A	C4-C5-N7	-5.04	108.18	110.70
32	W	1349	A	C5-C6-N1	5.04	120.22	117.70
1	A	41	A	N9-C4-C5	5.04	107.81	105.80
1	A	178	A	C8-N9-C4	5.04	107.81	105.80
1	A	207	A	C5-C6-N1	5.04	120.22	117.70
1	A	1812	A	C5-C6-N1	5.04	120.22	117.70
1	A	2463	A	C8-N9-C4	5.04	107.81	105.80
1	A	2479	A	C5-C6-N1	5.04	120.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	W	519	A	C8-N9-C4	5.04	107.81	105.80
1	A	619	A	C5-C6-N1	5.03	120.22	117.70
1	A	690	A	N9-C4-C5	5.03	107.81	105.80
1	A	1919	A	C4-C5-C6	5.03	119.52	117.00
1	A	2395	A	N9-C4-C5	5.03	107.81	105.80
1	A	2837	A	C5-C6-N1	5.03	120.22	117.70
32	W	211	A	C5-C6-N1	5.03	120.22	117.70
32	W	1206	A	C5-C6-N1	5.03	120.22	117.70
1	A	2066	A	C5-C6-N1	5.03	120.22	117.70
1	A	2407	A	C4-C5-N7	-5.03	108.19	110.70
32	W	1256	A	C5-C6-N1	5.03	120.22	117.70
1	A	894	A	C8-N9-C4	5.03	107.81	105.80
1	A	2907	A	C5-C6-N6	-5.03	119.68	123.70
1	A	870	A	N9-C4-C5	5.03	107.81	105.80
1	A	1340	A	C5-C6-N1	5.03	120.21	117.70
1	A	1608	A	N9-C4-C5	5.03	107.81	105.80
1	A	2349	A	C5-C6-N1	5.03	120.21	117.70
32	W	151	A	C4-C5-C6	5.03	119.51	117.00
32	W	401	A	C5-C6-N6	-5.03	119.68	123.70
32	W	886	A	C5-C6-N1	5.03	120.21	117.70
32	W	993	A	C4-C5-N7	-5.03	108.19	110.70
1	A	910	A	N9-C4-C5	5.03	107.81	105.80
1	A	943	A	N9-C4-C5	5.03	107.81	105.80
1	A	1925	A	N9-C4-C5	5.03	107.81	105.80
1	A	2505	A	C5-C6-N1	5.03	120.21	117.70
1	A	2770	A	N9-C4-C5	5.03	107.81	105.80
1	A	2827	A	C5-C6-N6	-5.03	119.68	123.70
32	W	658	A	C5-C6-N6	-5.03	119.68	123.70
32	W	775	A	C5-C6-N1	5.03	120.21	117.70
32	W	1016	A	N9-C4-C5	5.03	107.81	105.80
1	A	230	A	N9-C4-C5	5.02	107.81	105.80
1	A	1103	A	C4-C5-N7	-5.02	108.19	110.70
32	W	372	A	C5-C6-N1	5.02	120.21	117.70
1	A	390	A	C8-N9-C4	5.02	107.81	105.80
1	A	956	A	C4-C5-N7	-5.02	108.19	110.70
1	A	1858	A	C5-C6-N1	5.02	120.21	117.70
1	A	2500	A	C5-C6-N1	5.02	120.21	117.70
1	A	2619	A	C5-C6-N6	-5.02	119.68	123.70
1	A	2629	A	C5-C6-N1	5.02	120.21	117.70
32	W	150	A	C5-C6-N1	5.02	120.21	117.70
32	W	457	A	C8-N9-C4	5.02	107.81	105.80
32	W	512	A	C5-C6-N1	5.02	120.21	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	517	A	C5-C6-N6	-5.02	119.68	123.70
1	A	2468	A	N9-C4-C5	5.02	107.81	105.80
1	A	2862	A	C4-C5-N7	-5.02	108.19	110.70
52	z	24	A	C4-C5-N7	-5.02	108.19	110.70
1	A	369	A	N9-C4-C5	5.02	107.81	105.80
1	A	526	A	N3-C4-N9	5.02	131.41	127.40
1	A	658	A	C8-N9-C4	5.02	107.81	105.80
1	A	1483	A	C5-C6-N1	5.02	120.21	117.70
1	A	2349	A	C4-C5-N7	-5.02	108.19	110.70
32	W	617	A	C5-C6-N1	5.02	120.21	117.70
32	W	1372	A	C5-C6-N1	5.02	120.21	117.70
1	A	517	A	N9-C4-C5	5.02	107.81	105.80
1	A	1072	A	N9-C4-C5	5.02	107.81	105.80
1	A	1424	A	N9-C4-C5	5.02	107.81	105.80
1	A	1961	A	C5-C6-N1	5.02	120.21	117.70
1	A	2381	A	N9-C4-C5	5.02	107.81	105.80
1	A	2689	A	N9-C4-C5	5.02	107.81	105.80
32	W	278	A	C5-C6-N1	5.02	120.21	117.70
32	W	1517	A	N9-C4-C5	5.02	107.81	105.80
1	A	553	A	C5-C6-N6	-5.01	119.69	123.70
1	A	1094	A	N9-C4-C5	5.01	107.81	105.80
32	W	337	A	N9-C4-C5	5.01	107.81	105.80
32	W	439	A	C8-N9-C4	5.01	107.81	105.80
1	A	965	A	C5-C6-N1	5.01	120.21	117.70
1	A	1620	A	C4-C5-N7	-5.01	108.19	110.70
1	A	2044	A	C4-C5-N7	-5.01	108.19	110.70
1	A	2369	A	C5-C6-N1	5.01	120.21	117.70
32	W	1197	A	N9-C4-C5	5.01	107.81	105.80
32	W	1384	A	N9-C4-C5	5.01	107.81	105.80
1	A	407	A	C5-C6-N1	5.01	120.21	117.70
1	A	724	A	C5-C6-N1	5.01	120.21	117.70
1	A	1636	A	C5-C6-N1	5.01	120.21	117.70
1	A	2594	A	C5-C6-N6	-5.01	119.69	123.70
1	A	1305	A	C4-C5-C6	5.01	119.50	117.00
1	A	1778	A	N9-C4-C5	5.01	107.80	105.80
1	A	1925	A	C4-C5-N7	-5.01	108.20	110.70
32	W	862	A	N3-C4-N9	5.01	131.41	127.40
32	W	1200	A	C5-C6-N1	5.01	120.20	117.70
1	A	2790	A	N9-C4-C5	5.01	107.80	105.80
52	z	24	A	N9-C4-C5	5.01	107.80	105.80
1	A	1157	A	C5-C6-N1	5.01	120.20	117.70
1	A	1575	A	N9-C4-C5	5.01	107.80	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1614	A	C5-C6-N1	5.01	120.20	117.70
1	A	2673	A	C5-C6-N6	-5.00	119.70	123.70
1	A	1132	A	C8-N9-C4	5.00	107.80	105.80
1	A	1445	A	N9-C4-C5	5.00	107.80	105.80
1	A	1648	A	N9-C4-C5	5.00	107.80	105.80
1	A	2887	A	C5-C6-N1	5.00	120.20	117.70
1	A	1888	A	C5-C6-N6	-5.00	119.70	123.70
32	W	150	A	C5-C6-N6	-5.00	119.70	123.70
32	W	306	A	C5-C6-N6	-5.00	119.70	123.70
32	W	404	A	C5-C6-N1	5.00	120.20	117.70
32	W	1435	A	C5-C6-N1	5.00	120.20	117.70

There are no chirality outliers.

All (121) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1006	A	Sidechain
1	A	1042	A	Sidechain
1	A	1075	A	Sidechain
1	A	1078	A	Sidechain
1	A	1094	A	Sidechain
1	A	1097	A	Sidechain
1	A	1172	A	Sidechain
1	A	1173	A	Sidechain
1	A	1253	A	Sidechain
1	A	126	A	Sidechain
1	A	1293	A	Sidechain
1	A	1294	A	Sidechain
1	A	1302	A	Sidechain
1	A	1393	A	Sidechain
1	A	1555	A	Sidechain
1	A	1618	A	Sidechain
1	A	1619	A	Sidechain
1	A	1659	A	Sidechain
1	A	1661	A	Sidechain
1	A	168	A	Sidechain
1	A	1686	A	Sidechain
1	A	1724	A	Sidechain
1	A	183	A	Sidechain
1	A	1831	A	Sidechain
1	A	1839	A	Sidechain
1	A	1848	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1883	A	Sidechain
1	A	1888	A	Sidechain
1	A	1957	A	Sidechain
1	A	1998	A	Sidechain
1	A	2006	A	Sidechain
1	A	2010	A	Sidechain
1	A	2062	A	Sidechain
1	A	2111	A	Sidechain
1	A	2316	A	Sidechain
1	A	2364	A	Sidechain
1	A	2383	A	Sidechain
1	A	2395	A	Sidechain
1	A	2407	A	Sidechain
1	A	2488	A	Sidechain
1	A	259	A	Sidechain
1	A	2601	A	Sidechain
1	A	2606	A	Sidechain
1	A	2616	A	Sidechain
1	A	2627	A	Sidechain
1	A	2631	A	Sidechain
1	A	2670	A	Sidechain
1	A	2691	A	Sidechain
1	A	2708	A	Sidechain
1	A	2805	A	Sidechain
1	A	2819	A	Sidechain
1	A	2827	A	Sidechain
1	A	2885	A	Sidechain
1	A	366	A	Sidechain
1	A	477	A	Sidechain
1	A	501	A	Sidechain
1	A	513	A	Sidechain
1	A	517	A	Sidechain
1	A	518	A	Sidechain
1	A	52	A	Sidechain
1	A	538	A	Sidechain
1	A	551	A	Sidechain
1	A	559	A	Sidechain
1	A	64	A	Sidechain
1	A	661	A	Sidechain
1	A	67	A	Sidechain
1	A	679	A	Sidechain
1	A	692	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	699	A	Sidechain
1	A	752	A	Sidechain
1	A	765	A	Sidechain
1	A	796	A	Sidechain
1	A	797	A	Sidechain
1	A	798	A	Sidechain
1	A	799	A	Sidechain
1	A	836	A	Sidechain
1	A	841	A	Sidechain
1	A	866	A	Sidechain
1	A	904	A	Sidechain
2	B	55	A	Sidechain
2	B	97	A	Sidechain
5	E	66	ARG	Sidechain
19	S	86	ARG	Sidechain
19	S	88	ARG	Sidechain
32	W	1026	A	Sidechain
32	W	1065	A	Sidechain
32	W	1261	A	Sidechain
32	W	1278	A	Sidechain
32	W	1297	A	Sidechain
32	W	1384	A	Sidechain
32	W	1407	A	Sidechain
32	W	1427	A	Sidechain
32	W	1442	A	Sidechain
32	W	1478	A	Sidechain
32	W	209	A	Sidechain
32	W	308	A	Sidechain
32	W	335	A	Sidechain
32	W	391	A	Sidechain
32	W	401	A	Sidechain
32	W	415	A	Sidechain
32	W	419	A	Sidechain
32	W	496	A	Sidechain
32	W	500	A	Sidechain
32	W	53	A	Sidechain
32	W	532	A	Sidechain
32	W	583	A	Sidechain
32	W	696	A	Sidechain
32	W	790	A	Sidechain
32	W	811	A	Sidechain
32	W	862	A	Sidechain

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Mol	Chain	Res	Type	Group
32	W	879	A	Sidechain
32	W	883	A	Sidechain
32	W	911	A	Sidechain
32	W	918	A	Sidechain
32	W	969	A	Sidechain
32	W	975	A	Sidechain
32	W	988	A	Sidechain
23	X	69	LYS	Peptide,Mainchain
52	z	37	A	Sidechain
52	z	9	A	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
3	C	273/277 (99%)	264 (97%)	8 (3%)	1 (0%)	34	72
4	D	205/208 (99%)	189 (92%)	11 (5%)	5 (2%)	6	35
5	E	203/207 (98%)	185 (91%)	15 (7%)	3 (2%)	10	46
6	F	176/179 (98%)	154 (88%)	18 (10%)	4 (2%)	6	36
7	G	173/179 (97%)	164 (95%)	8 (5%)	1 (1%)	25	65
8	H	121/166 (73%)	97 (80%)	14 (12%)	10 (8%)	1	13
9	I	131/141 (93%)	122 (93%)	7 (5%)	2 (2%)	10	46
10	J	140/145 (97%)	130 (93%)	9 (6%)	1 (1%)	22	62
11	K	120/122 (98%)	112 (93%)	6 (5%)	2 (2%)	9	43
12	L	144/146 (99%)	132 (92%)	10 (7%)	2 (1%)	11	47
13	M	136/144 (94%)	129 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	17	56
15	O	118/120 (98%)	106 (90%)	7 (6%)	5 (4%)	3	25
16	P	112/115 (97%)	100 (89%)	12 (11%)	0	100	100
17	Q	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
18	R	99/102 (97%)	82 (83%)	15 (15%)	2 (2%)	7	39
19	S	107/113 (95%)	96 (90%)	8 (8%)	3 (3%)	5	33
20	T	91/95 (96%)	86 (94%)	5 (6%)	0	100	100
21	U	98/103 (95%)	87 (89%)	8 (8%)	3 (3%)	4	30
22	V	80/94 (85%)	77 (96%)	3 (4%)	0	100	100
23	X	147/149 (99%)	83 (56%)	42 (29%)	22 (15%)	0	4
24	Y	56/62 (90%)	53 (95%)	1 (2%)	2 (4%)	3	28
25	Z	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
26	a	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	8	41
27	b	52/59 (88%)	47 (90%)	4 (8%)	1 (2%)	8	40
28	c	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	d	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
30	e	62/66 (94%)	56 (90%)	5 (8%)	1 (2%)	9	45
31	f	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
33	g	222/246 (90%)	204 (92%)	13 (6%)	5 (2%)	6	36
34	h	208/218 (95%)	193 (93%)	14 (7%)	1 (0%)	29	68
35	i	197/200 (98%)	191 (97%)	4 (2%)	2 (1%)	15	54
36	j	163/166 (98%)	150 (92%)	9 (6%)	4 (2%)	5	35
37	k	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	6	37
38	l	151/156 (97%)	144 (95%)	6 (4%)	1 (1%)	22	62
39	m	129/132 (98%)	123 (95%)	5 (4%)	1 (1%)	19	60
40	n	128/130 (98%)	113 (88%)	10 (8%)	5 (4%)	3	26
41	o	100/102 (98%)	88 (88%)	8 (8%)	4 (4%)	3	25
42	p	116/131 (88%)	106 (91%)	9 (8%)	1 (1%)	17	56
43	q	135/138 (98%)	119 (88%)	9 (7%)	7 (5%)	2	22
44	r	117/121 (97%)	94 (80%)	13 (11%)	10 (8%)	1	13
45	s	58/61 (95%)	51 (88%)	4 (7%)	3 (5%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	t	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	6	36
47	u	87/90 (97%)	82 (94%)	3 (3%)	2 (2%)	6	36
48	v	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
49	w	69/79 (87%)	64 (93%)	2 (3%)	3 (4%)	2	24
50	x	82/92 (89%)	75 (92%)	5 (6%)	2 (2%)	6	35
51	y	84/88 (96%)	77 (92%)	6 (7%)	1 (1%)	13	50
53	2	22/95 (23%)	17 (77%)	2 (9%)	3 (14%)	0	5
54	3	43/66 (65%)	37 (86%)	4 (9%)	2 (5%)	2	23
All	All	5691/6068 (94%)	5180 (91%)	378 (7%)	133 (2%)	9	36

All (133) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	93	ALA
9	I	19	ASN
15	O	26	ALA
21	U	87	ASP
23	X	29	PHE
23	X	41	ALA
23	X	68	LEU
23	X	70	GLU
23	X	88	ARG
23	X	107	ASN
23	X	130	PRO
23	X	135	PRO
36	j	4	ILE
37	k	70	ALA
43	q	127	ARG
44	r	101	ASN
53	2	78	PHE
53	2	84	VAL
4	D	18	GLU
4	D	78	ARG
4	D	90	ALA
4	D	99	VAL
6	F	42	ASP
8	H	48	ALA
8	H	72	LEU
8	H	89	VAL

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Mol	Chain	Res	Type
8	H	108	ILE
8	H	124	LYS
15	O	68	THR
15	O	91	SER
19	S	8	ARG
23	X	8	ASP
23	X	38	GLU
33	g	18	HIS
33	g	36	ASN
33	g	104	PHE
36	j	163	GLU
37	k	54	ASP
38	l	54	THR
39	m	71	GLU
40	n	106	ARG
40	n	122	ARG
43	q	38	VAL
44	r	41	GLU
44	r	46	ARG
44	r	65	VAL
44	r	102	SER
44	r	112	PRO
54	3	49	PHE
5	E	4	VAL
8	H	55	TYR
8	H	90	VAL
8	H	113	ILE
11	K	89	ASP
15	O	63	LEU
18	R	28	GLU
19	S	41	ARG
19	S	65	ASP
21	U	74	LYS
21	U	89	LYS
23	X	20	ASN
23	X	44	ILE
23	X	69	LYS
23	X	85	GLU
23	X	126	TYR
23	X	127	THR
30	e	31	HIS
34	h	60	ALA

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Mol	Chain	Res	Type
35	i	5	THR
40	n	57	THR
41	o	35	SER
43	q	32	LYS
43	q	39	SER
43	q	115	LEU
44	r	42	ASP
44	r	66	GLU
46	t	88	ARG
50	x	84	ALA
53	2	77	VAL
3	C	245	SER
4	D	54	ASP
5	E	128	ASP
6	F	112	ARG
6	F	147	THR
7	G	13	SER
11	K	34	ASN
15	O	71	THR
23	X	12	LYS
23	X	42	SER
23	X	118	PRO
26	a	29	LYS
27	b	45	ALA
33	g	37	GLY
35	i	142	ARG
41	o	44	THR
43	q	25	ASN
44	r	10	PRO
47	u	44	ALA
47	u	47	ALA
49	w	28	TYR
5	E	89	VAL
8	H	107	GLU
10	J	22	ALA
12	L	107	ALA
14	N	110	ASP
18	R	52	THR
23	X	75	LEU
24	Y	44	PRO
41	o	36	VAL
43	q	16	VAL

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Mol	Chain	Res	Type
45	s	31	HIS
45	s	56	VAL
50	x	30	VAL
51	y	69	LYS
54	3	60	ASN
24	Y	40	VAL
36	j	162	GLU
40	n	104	LEU
40	n	107	ASP
42	p	120	HIS
49	w	16	CYS
36	j	109	GLY
12	L	88	GLY
44	r	84	GLY
45	s	51	GLY
23	X	34	GLY
41	o	80	THR
46	t	24	SER
49	w	23	ILE
23	X	9	VAL
33	g	201	PRO
6	F	25	VAL
9	I	24	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	223/225 (99%)	223 (100%)	0	100	100
4	D	168/169 (99%)	168 (100%)	0	100	100
5	E	169/170 (99%)	168 (99%)	1 (1%)	86	92
6	F	153/154 (99%)	153 (100%)	0	100	100
7	G	148/151 (98%)	148 (100%)	0	100	100
8	H	105/139 (76%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	103/110 (94%)	103 (100%)	0	100	100
10	J	120/123 (98%)	120 (100%)	0	100	100
11	K	101/101 (100%)	101 (100%)	0	100	100
12	L	110/110 (100%)	110 (100%)	0	100	100
13	M	111/116 (96%)	111 (100%)	0	100	100
14	N	99/100 (99%)	99 (100%)	0	100	100
15	O	93/93 (100%)	93 (100%)	0	100	100
16	P	99/100 (99%)	99 (100%)	0	100	100
17	Q	96/98 (98%)	96 (100%)	0	100	100
18	R	83/84 (99%)	83 (100%)	0	100	100
19	S	90/93 (97%)	89 (99%)	1 (1%)	73	85
20	T	84/85 (99%)	84 (100%)	0	100	100
21	U	84/87 (97%)	84 (100%)	0	100	100
22	V	64/74 (86%)	64 (100%)	0	100	100
24	Y	47/50 (94%)	47 (100%)	0	100	100
25	Z	56/57 (98%)	56 (100%)	0	100	100
26	a	52/53 (98%)	52 (100%)	0	100	100
27	b	48/53 (91%)	48 (100%)	0	100	100
28	c	46/47 (98%)	46 (100%)	0	100	100
29	d	39/39 (100%)	39 (100%)	0	100	100
30	e	54/56 (96%)	54 (100%)	0	100	100
31	f	34/35 (97%)	34 (100%)	0	100	100
53	2	6/87 (7%)	4 (67%)	2 (33%)	0	2
54	3	39/55 (71%)	39 (100%)	0	100	100
All	All	2724/2914 (94%)	2720 (100%)	4 (0%)	93	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	66	ARG
19	S	90	MET
53	2	81	ASN
53	2	86	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	194	GLN
3	C	199	GLN
3	C	264	ASN
4	D	50	GLN
4	D	152	ASN
4	D	172	GLN
4	D	191	ASN
5	E	29	ASN
5	E	67	GLN
5	E	82	GLN
6	F	37	ASN
6	F	135	GLN
7	G	62	HIS
7	G	107	ASN
9	I	93	ASN
10	J	59	ASN
12	L	78	ASN
14	N	27	ASN
16	P	15	GLN
16	P	80	HIS
17	Q	37	GLN
17	Q	91	ASN
18	R	65	GLN
19	S	60	HIS
19	S	102	HIS
21	U	2	HIS
21	U	39	ASN
21	U	64	HIS
22	V	37	GLN
24	Y	23	ASN
24	Y	34	GLN
26	a	37	HIS
26	a	40	ASN
27	b	40	HIS
28	c	25	ASN
29	d	9	ASN
30	e	31	HIS
30	e	35	ASN
31	f	36	GLN
53	2	81	ASN
54	3	60	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2922/2928 (99%)	828 (28%)	85 (2%)
2	B	111/119 (93%)	32 (28%)	4 (3%)
32	W	1543/1555 (99%)	235 (15%)	17 (1%)
52	z	76/77 (98%)	15 (19%)	0
All	All	4652/4679 (99%)	1110 (23%)	106 (2%)

All (1110) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	10	A
1	A	13	A
1	A	27	G
1	A	28	A
1	A	31	C
1	A	34	U
1	A	35	G
1	A	38	A
1	A	44	A
1	A	45	G
1	A	46	C
1	A	48	G
1	A	49	A
1	A	51	G
1	A	55	G
1	A	59	G
1	A	60	G
1	A	61	A
1	A	63	G
1	A	70	G
1	A	71	A
1	A	75	G
1	A	76	C
1	A	84	A
1	A	87	U
1	A	90	A
1	A	91	A
1	A	94	A
1	A	101	G
1	A	102	A

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Mol	Chain	Res	Type
1	A	109	G
1	A	118	A
1	A	119	U
1	A	124	A
1	A	125	A
1	A	126	A
1	A	127	C
1	A	130	A
1	A	133	A
1	A	156	A
1	A	161	A
1	A	162	A
1	A	163	U
1	A	164	U
1	A	176	A
1	A	177	G
1	A	179	A
1	A	183	A
1	A	184	G
1	A	185	A
1	A	188	C
1	A	199	A
1	A	202	A
1	A	203	U
1	A	207	A
1	A	208	G
1	A	215	G
1	A	216	A
1	A	217	G
1	A	218	G
1	A	219	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	230	A
1	A	231	A
1	A	232	U
1	A	233	G
1	A	236	A
1	A	245	G
1	A	248	G
1	A	251	G

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Mol	Chain	Res	Type
1	A	252	C
1	A	253	G
1	A	258	A
1	A	267	C
1	A	268	A
1	A	272	C
1	A	275	A
1	A	282	G
1	A	283	G
1	A	289	C
1	A	290	U
1	A	291	C
1	A	299	U
1	A	300	G
1	A	301	U
1	A	302	A
1	A	310	C
1	A	312	G
1	A	313	U
1	A	314	A
1	A	315	C
1	A	321	U
1	A	322	A
1	A	324	A
1	A	326	A
1	A	327	G
1	A	328	G
1	A	337	A
1	A	338	G
1	A	345	A
1	A	346	G
1	A	349	C
1	A	354	A
1	A	355	A
1	A	360	C
1	A	367	G
1	A	368	G
1	A	373	A
1	A	375	C
1	A	376	A
1	A	378	C
1	A	379	C

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Mol	Chain	Res	Type
1	A	380	C
1	A	387	C
1	A	390	A
1	A	393	U
1	A	394	U
1	A	405	U
1	A	406	G
1	A	407	A
1	A	411	G
1	A	418	A
1	A	419	G
1	A	420	U
1	A	430	C
1	A	433	G
1	A	434	U
1	A	435	G
1	A	438	A
1	A	453	G
1	A	459	A
1	A	474	U
1	A	478	U
1	A	481	U
1	A	485	U
1	A	489	G
1	A	490	A
1	A	494	A
1	A	502	C
1	A	503	C
1	A	504	A
1	A	525	A
1	A	526	A
1	A	527	A
1	A	528	G
1	A	537	A
1	A	538	A
1	A	544	G
1	A	548	A
1	A	550	G
1	A	551	A
1	A	553	A
1	A	555	C
1	A	556	C

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Mol	Chain	Res	Type
1	A	558	G
1	A	559	A
1	A	561	A
1	A	562	C
1	A	564	G
1	A	575	A
1	A	576	G
1	A	577	U
1	A	578	A
1	A	589	G
1	A	591	U
1	A	592	A
1	A	594	C
1	A	595	G
1	A	599	G
1	A	606	U
1	A	607	G
1	A	616	A
1	A	618	A
1	A	619	A
1	A	634	A
1	A	637	A
1	A	647	A
1	A	648	G
1	A	649	G
1	A	650	U
1	A	651	U
1	A	655	C
1	A	656	A
1	A	657	G
1	A	658	A
1	A	660	G
1	A	663	G
1	A	664	C
1	A	665	G
1	A	666	G
1	A	667	A
1	A	668	G
1	A	673	A
1	A	674	G
1	A	684	G
1	A	691	U

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Mol	Chain	Res	Type
1	A	692	A
1	A	698	C
1	A	700	U
1	A	711	U
1	A	718	C
1	A	722	A
1	A	732	A
1	A	733	U
1	A	734	C
1	A	736	A
1	A	746	A
1	A	764	C
1	A	769	A
1	A	774	A
1	A	775	G
1	A	777	C
1	A	785	C
1	A	786	A
1	A	787	C
1	A	788	G
1	A	794	U
1	A	795	G
1	A	799	A
1	A	811	A
1	A	812	G
1	A	822	G
1	A	823	G
1	A	829	A
1	A	830	A
1	A	831	U
1	A	832	G
1	A	836	A
1	A	837	U
1	A	838	C
1	A	840	A
1	A	841	A
1	A	843	C
1	A	847	A
1	A	848	G
1	A	851	A
1	A	852	G
1	A	853	C

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Mol	Chain	Res	Type
1	A	858	U
1	A	859	C
1	A	866	A
1	A	872	C
1	A	874	U
1	A	875	U
1	A	878	G
1	A	880	C
1	A	882	A
1	A	892	U
1	A	893	A
1	A	894	A
1	A	895	G
1	A	896	A
1	A	900	U
1	A	908	A
1	A	910	A
1	A	912	C
1	A	913	A
1	A	914	C
1	A	915	U
1	A	916	G
1	A	918	U
1	A	924	U
1	A	925	A
1	A	928	G
1	A	931	C
1	A	932	C
1	A	933	C
1	A	934	U
1	A	935	A
1	A	937	C
1	A	942	U
1	A	943	A
1	A	944	C
1	A	948	A
1	A	952	A
1	A	956	A
1	A	957	A
1	A	959	C
1	A	964	A
1	A	970	A

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Mol	Chain	Res	Type
1	A	972	U
1	A	974	A
1	A	976	U
1	A	977	U
1	A	978	A
1	A	981	C
1	A	987	A
1	A	992	G
1	A	998	G
1	A	1005	A
1	A	1007	G
1	A	1019	A
1	A	1020	A
1	A	1025	A
1	A	1027	A
1	A	1030	G
1	A	1031	C
1	A	1034	A
1	A	1035	G
1	A	1037	C
1	A	1042	A
1	A	1055	A
1	A	1058	U
1	A	1059	A
1	A	1063	G
1	A	1067	A
1	A	1068	G
1	A	1071	G
1	A	1072	A
1	A	1073	A
1	A	1079	U
1	A	1093	G
1	A	1096	A
1	A	1097	A
1	A	1100	A
1	A	1102	G
1	A	1103	A
1	A	1104	U
1	A	1107	U
1	A	1108	G
1	A	1111	U
1	A	1113	A

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Mol	Chain	Res	Type
1	A	1115	A
1	A	1116	A
1	A	1117	G
1	A	1118	C
1	A	1121	C
1	A	1122	C
1	A	1123	A
1	A	1124	C
1	A	1126	A
1	A	1128	U
1	A	1129	U
1	A	1130	A
1	A	1131	A
1	A	1134	A
1	A	1135	G
1	A	1136	U
1	A	1138	C
1	A	1139	G
1	A	1141	A
1	A	1145	G
1	A	1148	C
1	A	1150	C
1	A	1152	G
1	A	1158	G
1	A	1177	G
1	A	1178	U
1	A	1179	A
1	A	1181	C
1	A	1182	G
1	A	1188	A
1	A	1189	A
1	A	1194	A
1	A	1197	A
1	A	1201	A
1	A	1202	A
1	A	1209	G
1	A	1218	U
1	A	1219	C
1	A	1220	G
1	A	1222	A
1	A	1236	G
1	A	1244	A

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Mol	Chain	Res	Type
1	A	1246	G
1	A	1247	G
1	A	1248	C
1	A	1249	U
1	A	1250	G
1	A	1251	U
1	A	1268	G
1	A	1269	A
1	A	1278	G
1	A	1286	A
1	A	1289	U
1	A	1293	A
1	A	1295	U
1	A	1296	G
1	A	1305	A
1	A	1306	G
1	A	1312	A
1	A	1313	A
1	A	1314	A
1	A	1315	G
1	A	1319	G
1	A	1327	U
1	A	1339	A
1	A	1340	A
1	A	1341	U
1	A	1344	C
1	A	1345	U
1	A	1346	A
1	A	1352	U
1	A	1360	A
1	A	1363	G
1	A	1364	C
1	A	1375	A
1	A	1376	G
1	A	1380	U
1	A	1381	A
1	A	1382	G
1	A	1384	C
1	A	1388	A
1	A	1404	A
1	A	1417	A
1	A	1418	U

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Mol	Chain	Res	Type
1	A	1423	A
1	A	1424	A
1	A	1426	A
1	A	1432	A
1	A	1433	U
1	A	1434	A
1	A	1435	U
1	A	1436	U
1	A	1439	U
1	A	1441	U
1	A	1442	A
1	A	1450	C
1	A	1456	A
1	A	1459	U
1	A	1460	G
1	A	1464	A
1	A	1473	A
1	A	1474	C
1	A	1495	C
1	A	1496	G
1	A	1497	G
1	A	1498	U
1	A	1499	A
1	A	1504	A
1	A	1507	U
1	A	1513	U
1	A	1516	A
1	A	1517	A
1	A	1519	C
1	A	1520	A
1	A	1521	G
1	A	1523	U
1	A	1524	A
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1536	A
1	A	1539	C
1	A	1543	U
1	A	1553	A
1	A	1555	A
1	A	1558	C

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Mol	Chain	Res	Type
1	A	1561	G
1	A	1562	A
1	A	1572	G
1	A	1573	C
1	A	1578	G
1	A	1581	A
1	A	1582	U
1	A	1583	A
1	A	1584	U
1	A	1585	A
1	A	1596	U
1	A	1600	G
1	A	1601	A
1	A	1607	C
1	A	1608	A
1	A	1615	A
1	A	1617	A
1	A	1626	U
1	A	1631	A
1	A	1632	G
1	A	1638	A
1	A	1640	G
1	A	1647	U
1	A	1648	A
1	A	1651	G
1	A	1652	C
1	A	1653	A
1	A	1655	A
1	A	1657	C
1	A	1658	G
1	A	1660	C
1	A	1667	A
1	A	1674	G
1	A	1679	A
1	A	1680	A
1	A	1688	G
1	A	1691	A
1	A	1693	C
1	A	1695	A
1	A	1696	G
1	A	1697	A
1	A	1707	U

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Mol	Chain	Res	Type
1	A	1708	U
1	A	1712	G
1	A	1713	A
1	A	1719	G
1	A	1727	A
1	A	1728	C
1	A	1739	C
1	A	1744	G
1	A	1745	A
1	A	1752	G
1	A	1756	U
1	A	1757	G
1	A	1758	U
1	A	1759	U
1	A	1767	A
1	A	1769	G
1	A	1771	C
1	A	1774	A
1	A	1776	A
1	A	1777	G
1	A	1778	A
1	A	1780	C
1	A	1781	C
1	A	1782	G
1	A	1785	G
1	A	1787	G
1	A	1788	A
1	A	1790	U
1	A	1791	A
1	A	1792	G
1	A	1793	G
1	A	1796	C
1	A	1802	A
1	A	1810	G
1	A	1811	C
1	A	1814	A
1	A	1829	C
1	A	1830	G
1	A	1831	A
1	A	1832	A
1	A	1834	C
1	A	1839	A

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Mol	Chain	Res	Type
1	A	1858	A
1	A	1862	C
1	A	1876	A
1	A	1877	A
1	A	1882	A
1	A	1897	C
1	A	1900	A
1	A	1901	A
1	A	1902	G
1	A	1910	G
1	A	1912	G
1	A	1913	A
1	A	1916	U
1	A	1918	A
1	A	1919	A
1	A	1925	A
1	A	1930	A
1	A	1935	G
1	A	1942	A
1	A	1943	C
1	A	1944	U
1	A	1948	A
1	A	1954	C
1	A	1959	G
1	A	1960	U
1	A	1966	A
1	A	1967	A
1	A	1968	U
1	A	1969	U
1	A	1972	U
1	A	1981	A
1	A	1984	U
1	A	1992	C
1	A	1995	A
1	A	1996	C
1	A	1999	A
1	A	2000	A
1	A	2001	G
1	A	2010	A
1	A	2011	U
1	A	2012	C
1	A	2020	U

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Mol	Chain	Res	Type
1	A	2024	U
1	A	2026	A
1	A	2027	A
1	A	2033	G
1	A	2042	A
1	A	2047	A
1	A	2052	A
1	A	2059	A
1	A	2060	A
1	A	2062	A
1	A	2072	C
1	A	2084	C
1	A	2085	G
1	A	2088	A
1	A	2089	A
1	A	2090	G
1	A	2091	A
1	A	2092	C
1	A	2098	G
1	A	2111	A
1	A	2116	G
1	A	2117	A
1	A	2119	A
1	A	2121	U
1	A	2123	A
1	A	2124	A
1	A	2125	U
1	A	2126	G
1	A	2130	G
1	A	2131	U
1	A	2132	A
1	A	2139	G
1	A	2140	U
1	A	2142	C
1	A	2143	A
1	A	2145	G
1	A	2147	U
1	A	2148	A
1	A	2149	G
1	A	2155	A
1	A	2156	G
1	A	2157	C

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Mol	Chain	Res	Type
1	A	2158	C
1	A	2160	U
1	A	2161	G
1	A	2162	G
1	A	2163	A
1	A	2164	A
1	A	2166	C
1	A	2167	C
1	A	2168	G
1	A	2170	A
1	A	2174	C
1	A	2175	C
1	A	2176	A
1	A	2177	G
1	A	2183	G
1	A	2186	G
1	A	2187	A
1	A	2188	G
1	A	2190	C
1	A	2192	U
1	A	2195	G
1	A	2196	U
1	A	2197	G
1	A	2199	G
1	A	2201	U
1	A	2202	A
1	A	2203	C
1	A	2212	C
1	A	2216	A
1	A	2218	U
1	A	2220	A
1	A	2221	C
1	A	2222	C
1	A	2223	U
1	A	2226	U
1	A	2227	A
1	A	2228	A
1	A	2231	C
1	A	2232	G
1	A	2233	C
1	A	2235	G
1	A	2239	U

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Mol	Chain	Res	Type
1	A	2240	U
1	A	2241	A
1	A	2242	U
1	A	2243	C
1	A	2245	G
1	A	2246	G
1	A	2247	C
1	A	2248	G
1	A	2252	A
1	A	2253	G
1	A	2254	A
1	A	2255	C
1	A	2256	A
1	A	2260	U
1	A	2267	G
1	A	2268	G
1	A	2279	G
1	A	2295	A
1	A	2296	A
1	A	2308	G
1	A	2312	C
1	A	2315	A
1	A	2333	G
1	A	2334	U
1	A	2335	U
1	A	2336	G
1	A	2337	G
1	A	2339	A
1	A	2340	A
1	A	2343	A
1	A	2345	U
1	A	2346	C
1	A	2347	G
1	A	2348	C
1	A	2349	A
1	A	2350	G
1	A	2351	A
1	A	2352	G
1	A	2356	A
1	A	2357	A
1	A	2362	A
1	A	2363	C

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Mol	Chain	Res	Type
1	A	2364	A
1	A	2369	A
1	A	2376	C
1	A	2377	U
1	A	2379	C
1	A	2387	A
1	A	2390	A
1	A	2400	G
1	A	2411	G
1	A	2412	G
1	A	2414	C
1	A	2420	G
1	A	2421	A
1	A	2431	U
1	A	2435	C
1	A	2453	C
1	A	2454	A
1	A	2455	A
1	A	2456	C
1	A	2458	G
1	A	2459	A
1	A	2460	U
1	A	2463	A
1	A	2464	A
1	A	2468	A
1	A	2469	C
1	A	2470	C
1	A	2477	A
1	A	2483	G
1	A	2505	A
1	A	2513	G
1	A	2523	G
1	A	2528	C
1	A	2531	G
1	A	2532	A
1	A	2533	U
1	A	2534	G
1	A	2536	C
1	A	2541	C
1	A	2542	A
1	A	2543	U
1	A	2546	C

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Mol	Chain	Res	Type
1	A	2547	A
1	A	2558	G
1	A	2569	C
1	A	2570	A
1	A	2571	A
1	A	2572	G
1	A	2575	U
1	A	2576	U
1	A	2583	U
1	A	2594	A
1	A	2595	A
1	A	2596	G
1	A	2601	A
1	A	2602	C
1	A	2610	G
1	A	2611	G
1	A	2614	U
1	A	2619	A
1	A	2630	C
1	A	2631	A
1	A	2638	U
1	A	2639	C
1	A	2642	U
1	A	2648	U
1	A	2658	A
1	A	2661	A
1	A	2663	A
1	A	2668	A
1	A	2680	C
1	A	2683	A
1	A	2684	G
1	A	2711	G
1	A	2714	G
1	A	2717	G
1	A	2718	U
1	A	2720	C
1	A	2730	U
1	A	2731	G
1	A	2743	G
1	A	2754	A
1	A	2755	U
1	A	2766	G

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Mol	Chain	Res	Type
1	A	2773	G
1	A	2779	A
1	A	2780	G
1	A	2784	C
1	A	2785	U
1	A	2786	A
1	A	2787	A
1	A	2790	A
1	A	2794	A
1	A	2795	G
1	A	2797	C
1	A	2798	C
1	A	2800	C
1	A	2804	A
1	A	2807	A
1	A	2808	U
1	A	2809	G
1	A	2813	U
1	A	2818	C
1	A	2819	A
1	A	2820	U
1	A	2825	C
1	A	2826	A
1	A	2843	G
1	A	2855	G
1	A	2858	U
1	A	2859	G
1	A	2860	A
1	A	2869	A
1	A	2873	G
1	A	2874	G
1	A	2892	G
1	A	2897	G
1	A	2898	A
1	A	2899	C
1	A	2902	A
1	A	2905	C
1	A	2909	U
1	A	2918	G
1	A	2919	A
2	B	10	G
2	B	11	A

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Mol	Chain	Res	Type
2	B	12	U
2	B	13	A
2	B	20	A
2	B	23	U
2	B	28	C
2	B	37	A
2	B	39	A
2	B	40	C
2	B	41	C
2	B	42	G
2	B	46	A
2	B	48	G
2	B	49	G
2	B	50	A
2	B	51	A
2	B	55	A
2	B	59	U
2	B	60	C
2	B	61	U
2	B	63	C
2	B	64	A
2	B	81	G
2	B	85	U
2	B	86	U
2	B	87	U
2	B	88	C
2	B	96	G
2	B	97	A
2	B	107	G
2	B	110	G
32	W	10	A
32	W	11	G
32	W	34	A
32	W	41	G
32	W	49	C
32	W	50	C
32	W	52	A
32	W	53	A
32	W	83	C
32	W	85	U
32	W	87	C
32	W	88	U

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Mol	Chain	Res	Type
32	W	99	A
32	W	114	A
32	W	118	A
32	W	119	C
32	W	120	A
32	W	127	U
32	W	129	A
32	W	130	C
32	W	140	A
32	W	142	A
32	W	143	C
32	W	151	A
32	W	158	G
32	W	162	C
32	W	163	C
32	W	182	U
32	W	183	U
32	W	194	C
32	W	195	A
32	W	197	G
32	W	210	A
32	W	222	G
32	W	249	G
32	W	255	G
32	W	258	A
32	W	259	G
32	W	274	G
32	W	275	C
32	W	287	A
32	W	288	C
32	W	297	G
32	W	336	C
32	W	337	A
32	W	338	C
32	W	340	G
32	W	355	G
32	W	360	C
32	W	362	G
32	W	375	U
32	W	380	C
32	W	405	A
32	W	414	G

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Mol	Chain	Res	Type
32	W	419	A
32	W	420	U
32	W	421	G
32	W	422	A
32	W	429	U
32	W	430	C
32	W	432	G
32	W	437	U
32	W	456	A
32	W	457	A
32	W	460	A
32	W	472	C
32	W	474	A
32	W	475	A
32	W	476	U
32	W	477	A
32	W	488	U
32	W	490	G
32	W	491	A
32	W	494	G
32	W	506	A
32	W	507	A
32	W	518	A
32	W	520	C
32	W	527	C
32	W	528	C
32	W	533	G
32	W	536	G
32	W	541	A
32	W	556	A
32	W	568	A
32	W	572	A
32	W	581	A
32	W	582	A
32	W	585	G
32	W	586	G
32	W	605	A
32	W	642	U
32	W	643	C
32	W	651	A
32	W	662	U
32	W	674	A

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Mol	Chain	Res	Type
32	W	696	A
32	W	704	A
32	W	711	A
32	W	727	A
32	W	728	C
32	W	729	C
32	W	730	A
32	W	732	U
32	W	740	G
32	W	741	C
32	W	756	U
32	W	757	A
32	W	764	G
32	W	786	A
32	W	793	A
32	W	802	U
32	W	803	A
32	W	823	A
32	W	824	A
32	W	826	C
32	W	830	G
32	W	837	A
32	W	838	A
32	W	843	U
32	W	849	G
32	W	856	C
32	W	865	G
32	W	874	A
32	W	880	U
32	W	881	U
32	W	882	A
32	W	883	A
32	W	924	A
32	W	936	G
32	W	944	C
32	W	945	A
32	W	948	A
32	W	970	U
32	W	974	A
32	W	979	A
32	W	981	G
32	W	984	A

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Mol	Chain	Res	Type
32	W	985	A
32	W	986	G
32	W	987	A
32	W	992	U
32	W	993	A
32	W	1003	G
32	W	1004	A
32	W	1012	U
32	W	1014	A
32	W	1018	U
32	W	1027	U
32	W	1028	A
32	W	1033	G
32	W	1036	C
32	W	1040	U
32	W	1042	G
32	W	1044	G
32	W	1046	G
32	W	1053	G
32	W	1054	A
32	W	1060	G
32	W	1064	C
32	W	1075	U
32	W	1104	G
32	W	1105	U
32	W	1111	A
32	W	1112	A
32	W	1143	A
32	W	1148	G
32	W	1149	U
32	W	1150	U
32	W	1151	G
32	W	1155	A
32	W	1161	A
32	W	1168	U
32	W	1169	G
32	W	1170	C
32	W	1177	C
32	W	1191	G
32	W	1192	U
32	W	1193	G
32	W	1200	A

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Mol	Chain	Res	Type
32	W	1205	A
32	W	1206	A
32	W	1210	A
32	W	1211	U
32	W	1221	U
32	W	1222	A
32	W	1223	U
32	W	1230	G
32	W	1237	C
32	W	1247	A
32	W	1250	G
32	W	1266	A
32	W	1269	G
32	W	1289	A
32	W	1295	C
32	W	1296	A
32	W	1308	A
32	W	1313	G
32	W	1314	G
32	W	1326	C
32	W	1329	C
32	W	1331	C
32	W	1332	G
32	W	1341	A
32	W	1343	G
32	W	1345	U
32	W	1346	G
32	W	1355	A
32	W	1373	U
32	W	1377	G
32	W	1407	A
32	W	1435	A
32	W	1451	A
32	W	1452	G
32	W	1455	A
32	W	1461	U
32	W	1462	U
32	W	1463	A
32	W	1464	G
32	W	1490	A
32	W	1502	A
32	W	1503	A

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Mol	Chain	Res	Type
32	W	1504	G
32	W	1509	A
32	W	1513	A
32	W	1515	G
32	W	1516	U
32	W	1527	G
32	W	1539	G
32	W	1540	G
32	W	1541	A
32	W	1544	A
32	W	1545	C
32	W	1547	U
32	W	1548	C
52	z	9	A
52	z	18	G
52	z	19	U
52	z	21	A
52	z	34	G
52	z	35	U
52	z	36	C
52	z	48	C
52	z	49	G
52	z	55	U
52	z	56	C
52	z	57	G
52	z	70	A
52	z	73	G
52	z	76	A

All (106) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	43	G
1	A	58	G
1	A	90	A
1	A	118	A
1	A	124	A
1	A	163	U
1	A	175	G
1	A	183	A
1	A	207	A
1	A	229	A

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Mol	Chain	Res	Type
1	A	252	C
1	A	271	C
1	A	288	C
1	A	298	U
1	A	366	A
1	A	377	G
1	A	405	U
1	A	419	G
1	A	526	A
1	A	549	A
1	A	647	A
1	A	649	G
1	A	666	G
1	A	683	A
1	A	717	A
1	A	785	C
1	A	837	U
1	A	847	A
1	A	934	U
1	A	936	C
1	A	1019	A
1	A	1066	A
1	A	1092	A
1	A	1103	A
1	A	1107	U
1	A	1117	G
1	A	1173	A
1	A	1245	G
1	A	1250	G
1	A	1305	A
1	A	1339	A
1	A	1351	U
1	A	1434	A
1	A	1438	C
1	A	1455	C
1	A	1527	C
1	A	1535	U
1	A	1581	A
1	A	1595	U
1	A	1630	G
1	A	1652	C
1	A	1679	A

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Mol	Chain	Res	Type
1	A	1755	C
1	A	1779	G
1	A	1784	A
1	A	1813	A
1	A	1876	A
1	A	1965	A
1	A	2122	G
1	A	2139	G
1	A	2155	A
1	A	2174	C
1	A	2187	A
1	A	2226	U
1	A	2241	A
1	A	2254	A
1	A	2267	G
1	A	2278	U
1	A	2295	A
1	A	2334	U
1	A	2348	C
1	A	2351	A
1	A	2454	A
1	A	2468	A
1	A	2504	C
1	A	2595	A
1	A	2631	A
1	A	2683	A
1	A	2710	C
1	A	2716	U
1	A	2779	A
1	A	2784	C
1	A	2785	U
1	A	2807	A
1	A	2812	A
2	B	38	U
2	B	47	C
2	B	54	U
2	B	59	U
32	W	98	U
32	W	113	G
32	W	119	C
32	W	126	G
32	W	436	G

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Mol	Chain	Res	Type
32	W	641	G
32	W	842	U
32	W	848	G
32	W	855	G
32	W	864	U
32	W	873	U
32	W	1111	A
32	W	1154	C
32	W	1210	A
32	W	1461	U
32	W	1501	G
32	W	1544	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

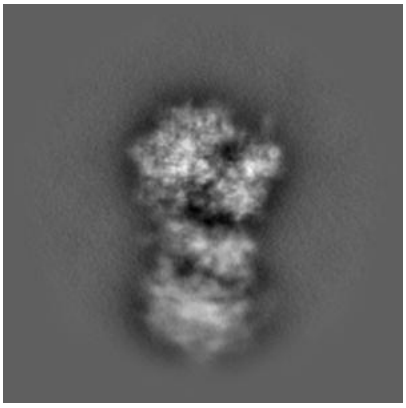
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13959. These allow visual inspection of the internal detail of the map and identification of artifacts.

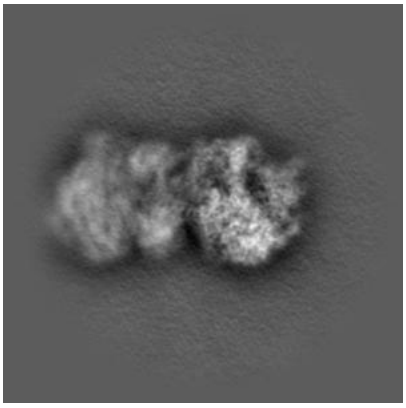
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

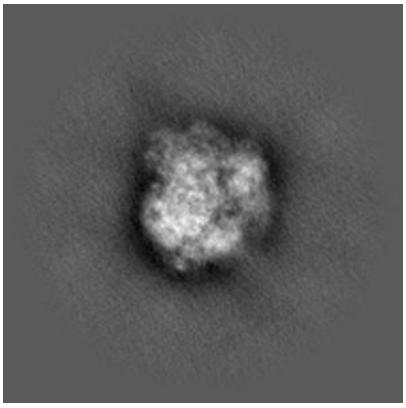
6.1.1 Primary map



X



Y

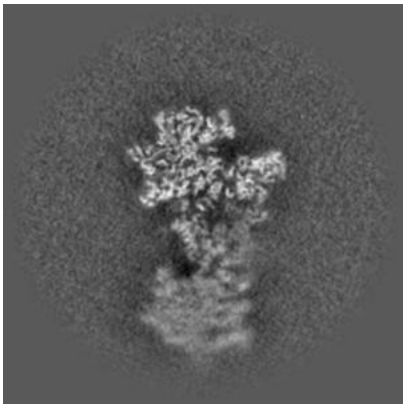


Z

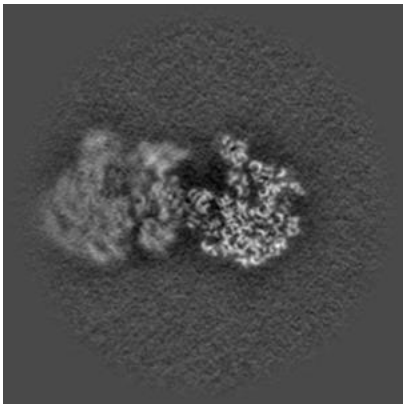
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

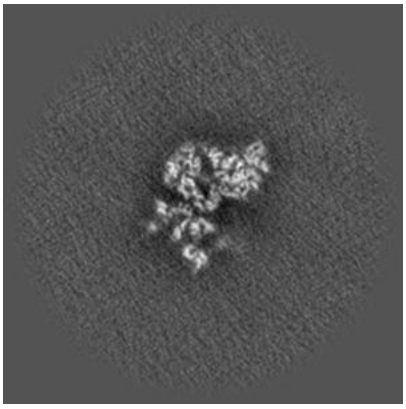
6.2.1 Primary map



X Index: 300



Y Index: 300

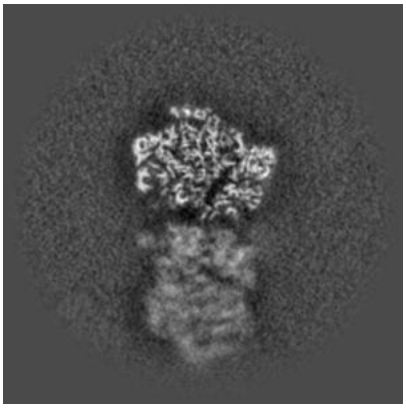


Z Index: 300

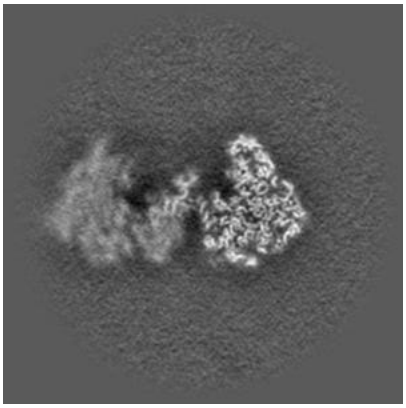
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

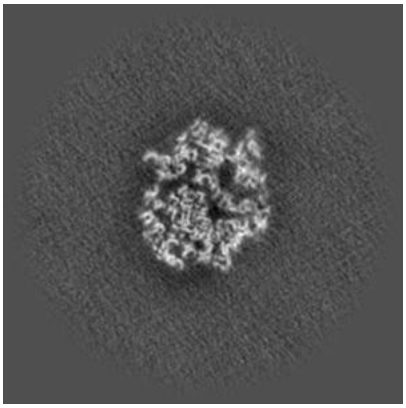
6.3.1 Primary map



X Index: 267



Y Index: 275



Z Index: 349

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

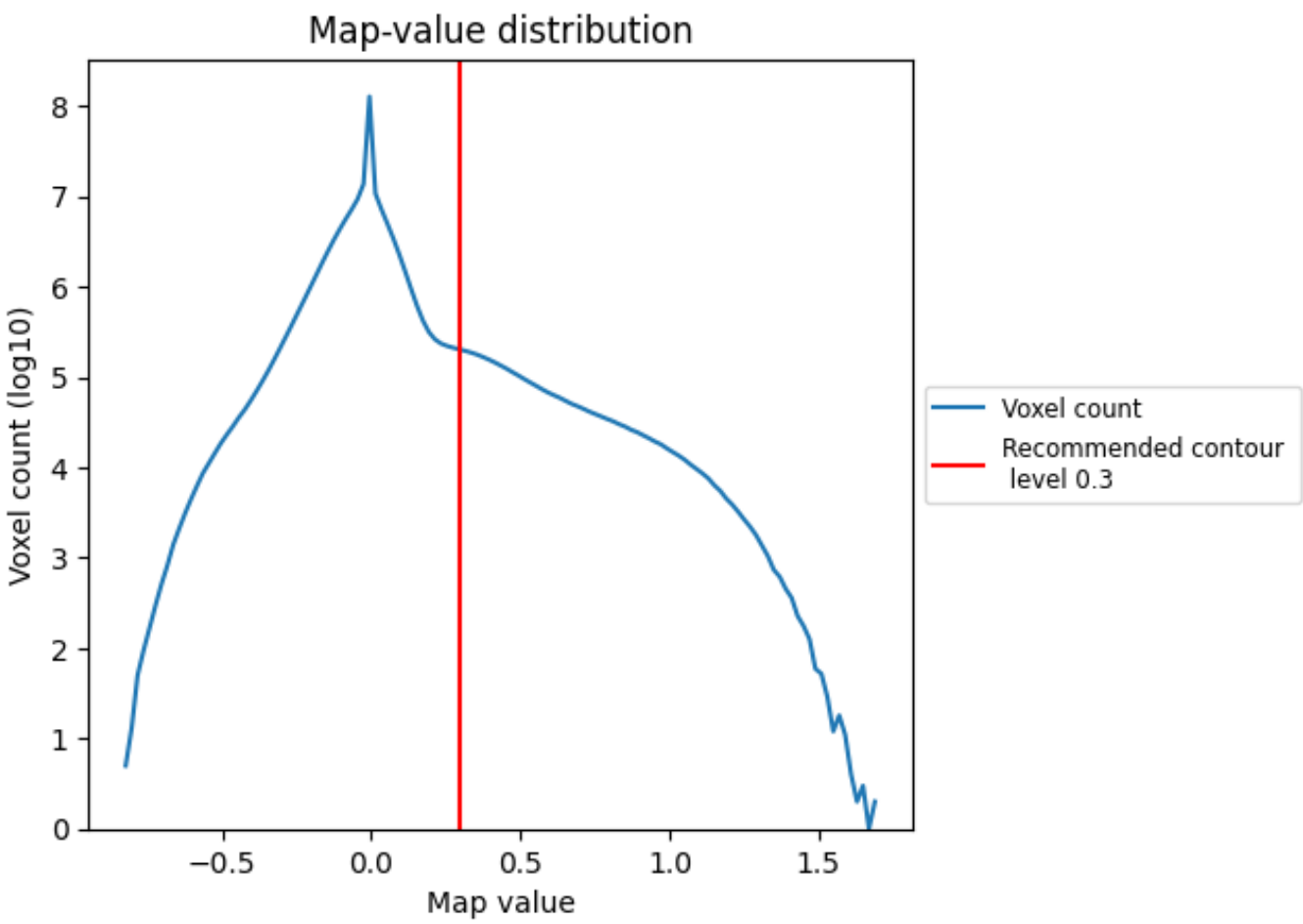
6.5 Mask visualisation (i)

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

7 Map analysis (i)

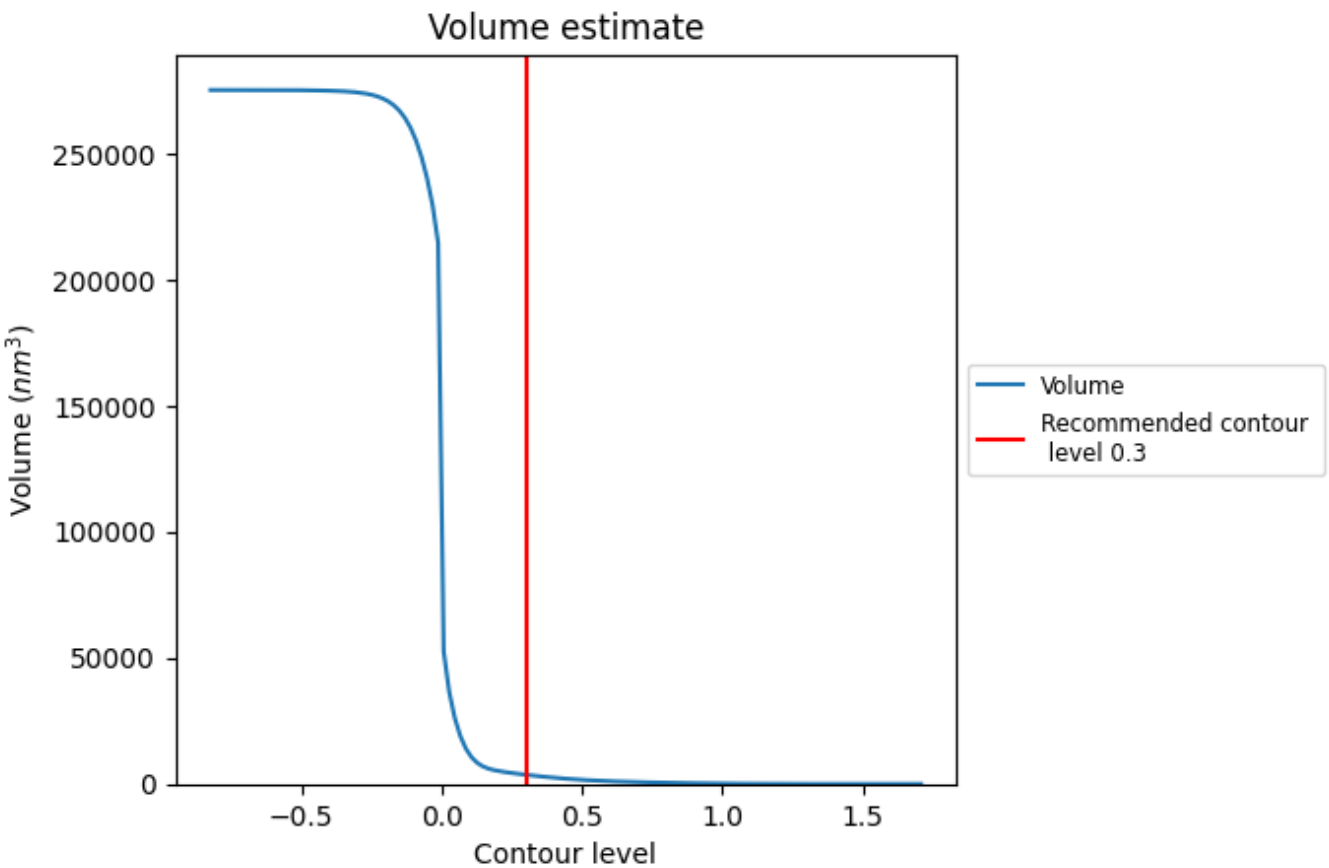
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

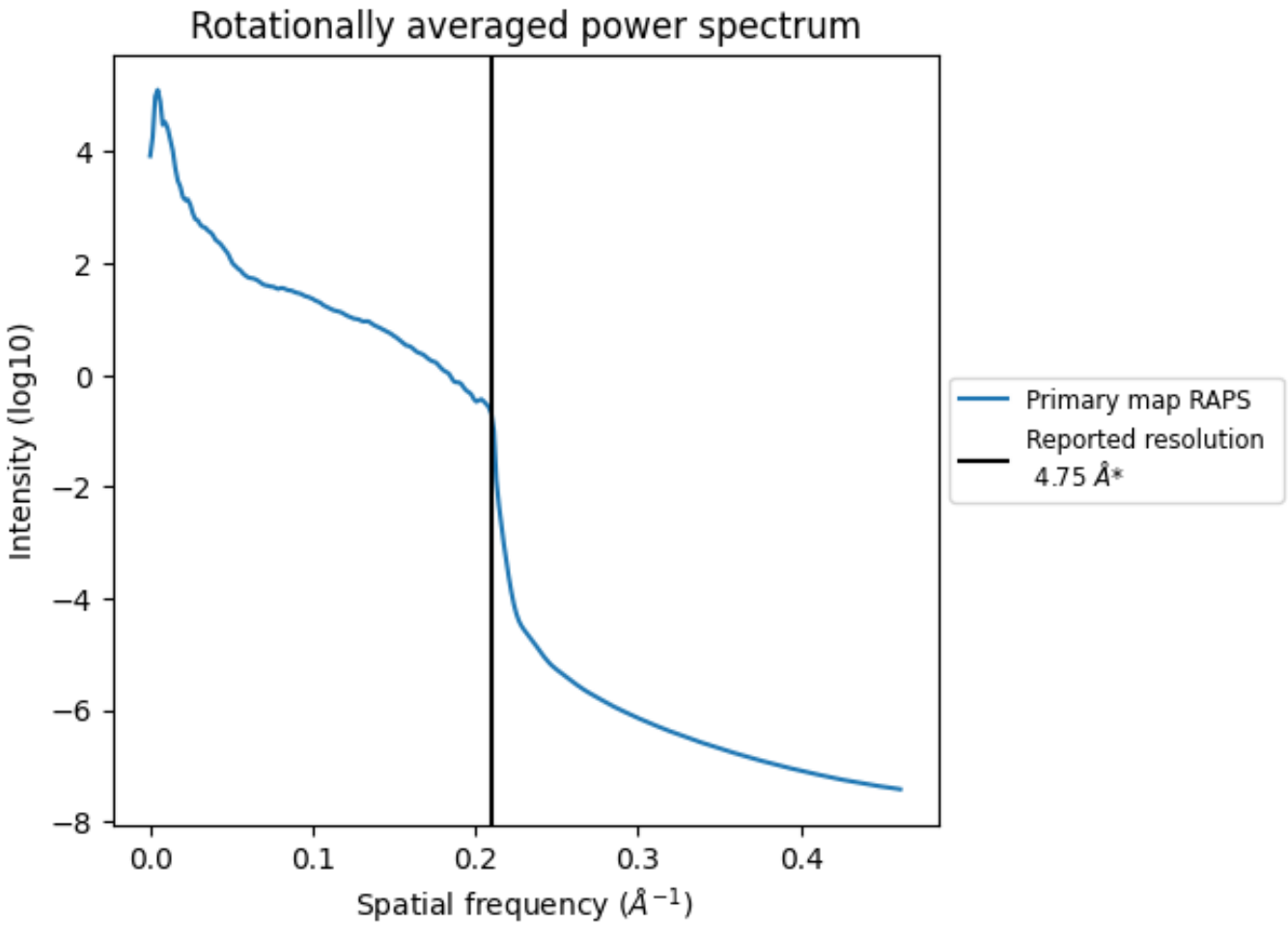
7.2 Volume estimate (i)



The volume at the recommended contour level is 3652 nm^3; this corresponds to an approximate mass of 3299 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.211 Å^{-1}

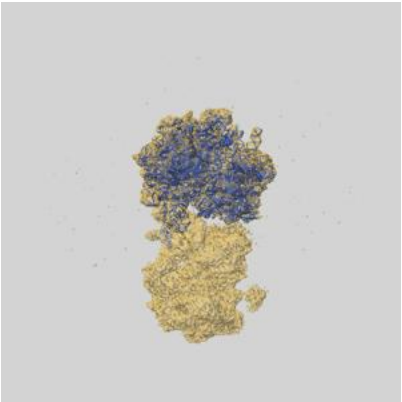
8 Fourier-Shell correlation (i)

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

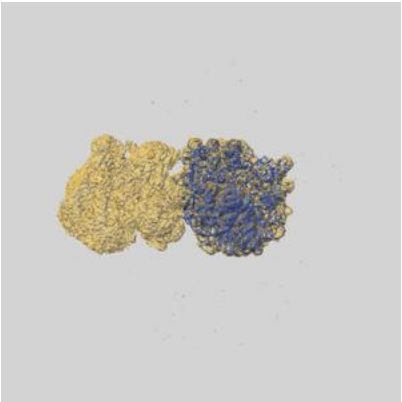
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13959 and PDB model 7QGU. Per-residue inclusion information can be found in section 3 on page 14.

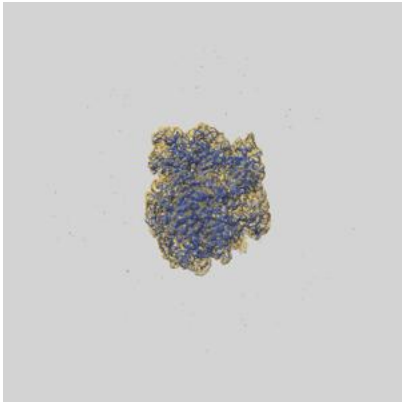
9.1 Map-model overlay (i)



X



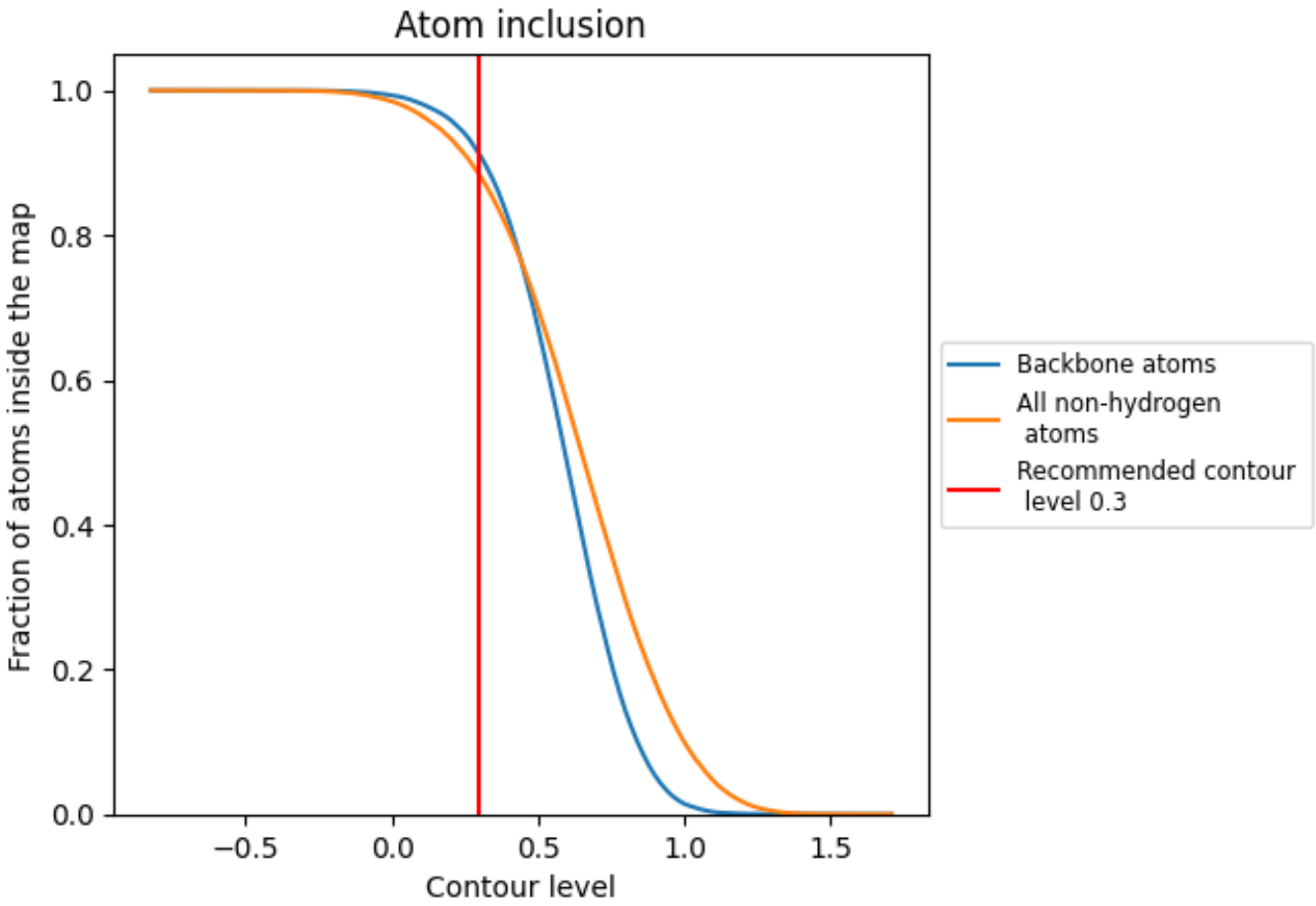
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.