



Full wwPDB EM Validation Report ⓘ

Apr 16, 2024 – 02:51 am BST

PDB ID : 7Q4K
EMDB ID : EMD-13805
Title : Erythromycin-stalled Escherichia coli 70S ribosome with streptococcal MsrDL nascent chain
Authors : Fostier, C.R.; Ousalem, F.; Soufari, H.; Leroy, E.C.; Ngo, S.; Innis, A.; Hashem, Y.; Boel, G.
Deposited on : 2021-10-31
Resolution : 3.00 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 ⓘ symbol.

The types of validation reports are described at

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

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

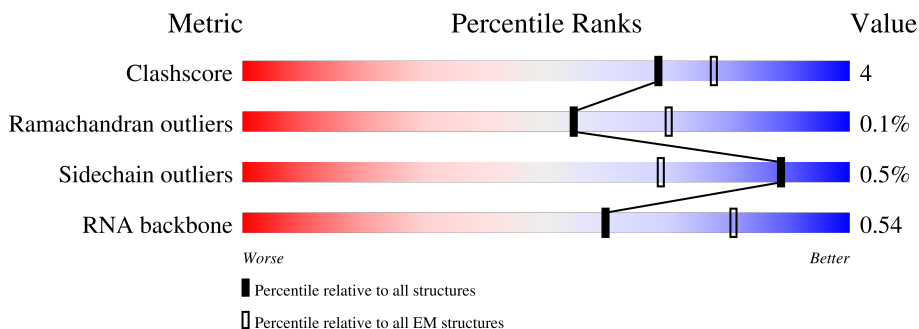
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.00 Å.

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



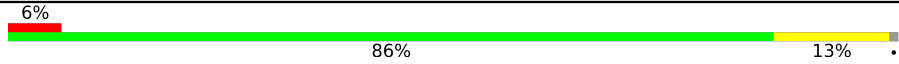
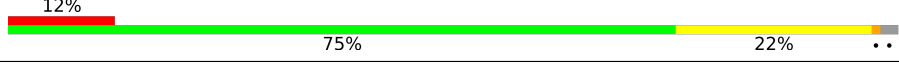
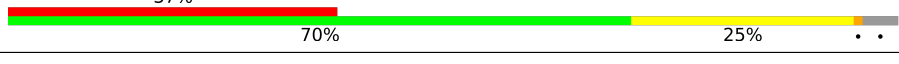


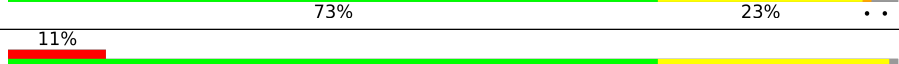
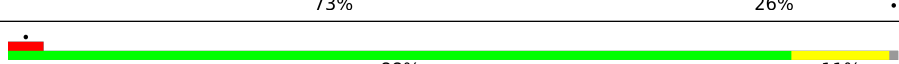
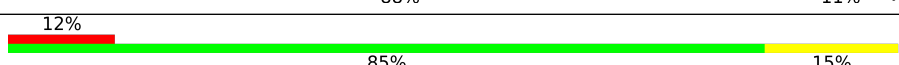
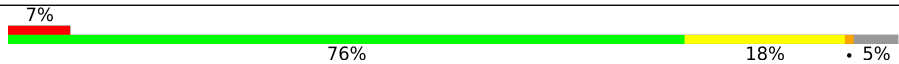


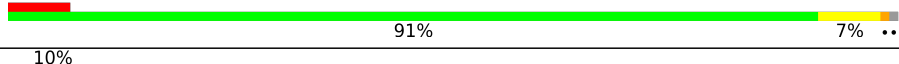
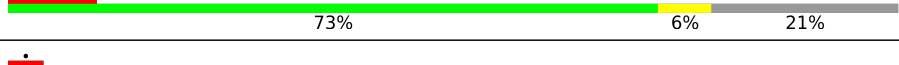

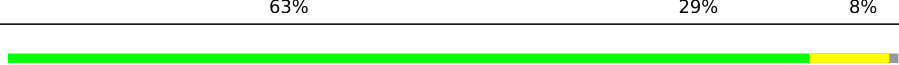
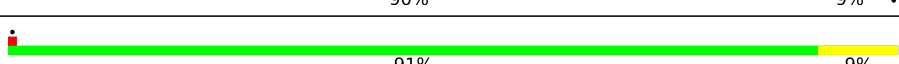


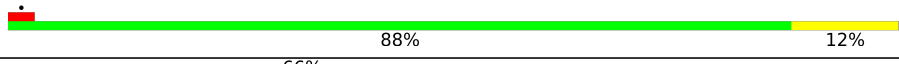
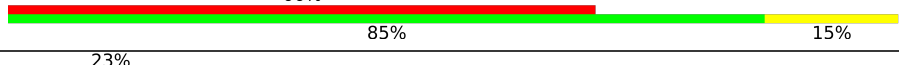

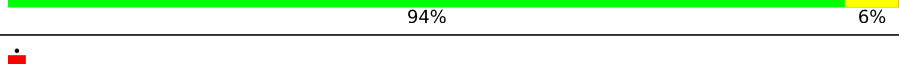
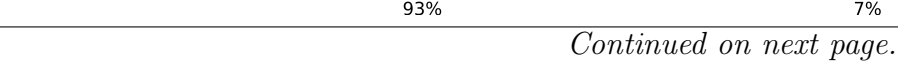


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AA	1534	
2	AB	241	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	

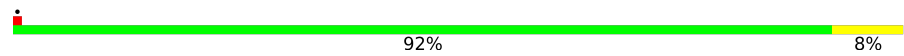


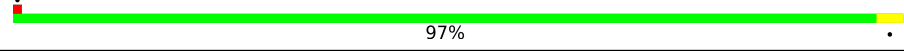
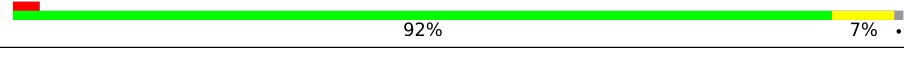
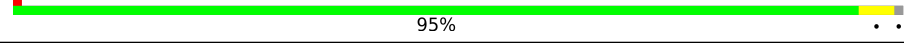
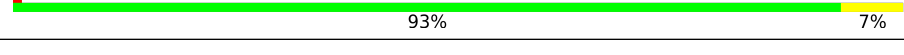
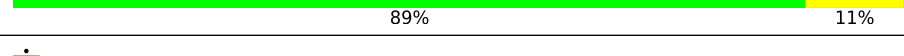

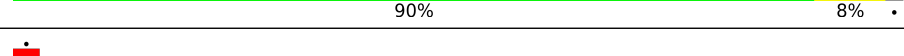
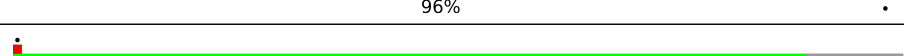
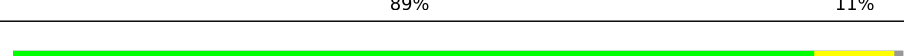
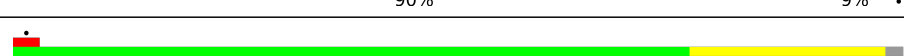
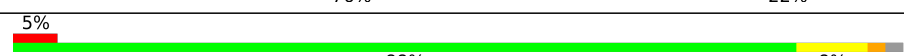

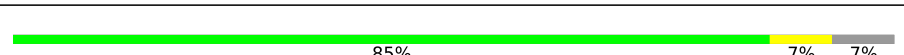
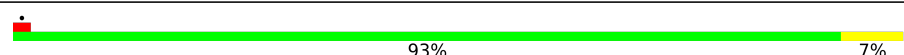





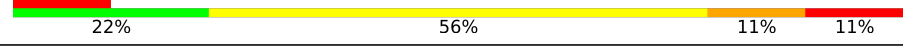

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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2903	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	
28	BG	177	
29	BH	149	
30	BI	70	
31	BJ	142	
32	BK	123	

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Mol	Chain	Length	Quality of chain
33	BL	144	 92% 8%
34	BM	136	 86% 13%
35	BN	127	 86% 7% 7%
36	BO	117	 97%
37	BP	115	 92% 7%
38	BQ	118	 95%
39	BR	103	 93% 7%
40	BS	110	 89% 11%
41	BT	100	 80% 13% 7%
42	BU	104	 90% 8%
43	BV	94	 96%
44	BW	85	 89% 11%
45	BX	78	 90% 9%
46	BY	63	 76% 22%
47	BZ	59	 5% 88% 8%
48	B0	57	 89% 9%
49	B1	55	 85% 7% 7%
50	B2	46	 93% 7%
51	B3	65	 83% 12%
52	B4	38	 82% 18%
53	D1	6	 50% 33% 17%
54	D2	77	 43% 34% 17% 5%
55	D3	76	 26% 30% 32% 11%
56	D4	9	 11% 22% 56% 11%

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 146607 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 16S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP C3SR07

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a protein called MsrDL: FME-TYR-LEU-ILE-PHE-MET.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	D1	6	57	41	6	8	2	0	0

- Molecule 54 is a RNA chain called Met-tRNA (P site).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
54	D2	76	1634	733	290	534	76	1	0	0

- Molecule 55 is a RNA chain called Phe-tRNA (E site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	P			S
55	D3	75	1604	715	288	525	75	1	0	0

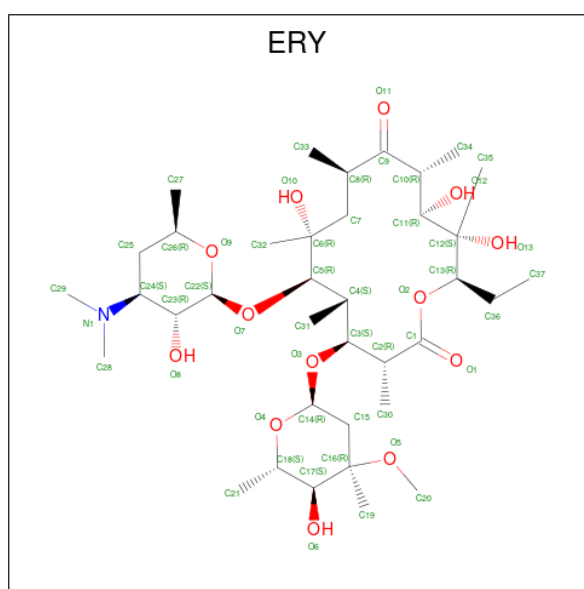
- Molecule 56 is a RNA chain called MsrDL mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	D4	9	189	85	31	64	9	0	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	AA	35	35	35	0
57	BA	134	134	134	0
57	BC	1	1	1	0
57	BD	1	1	1	0
57	D2	1	1	1	0

- Molecule 58 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C₃₇H₆₇NO₁₃).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
58	BA	1	51	37	1	13	0

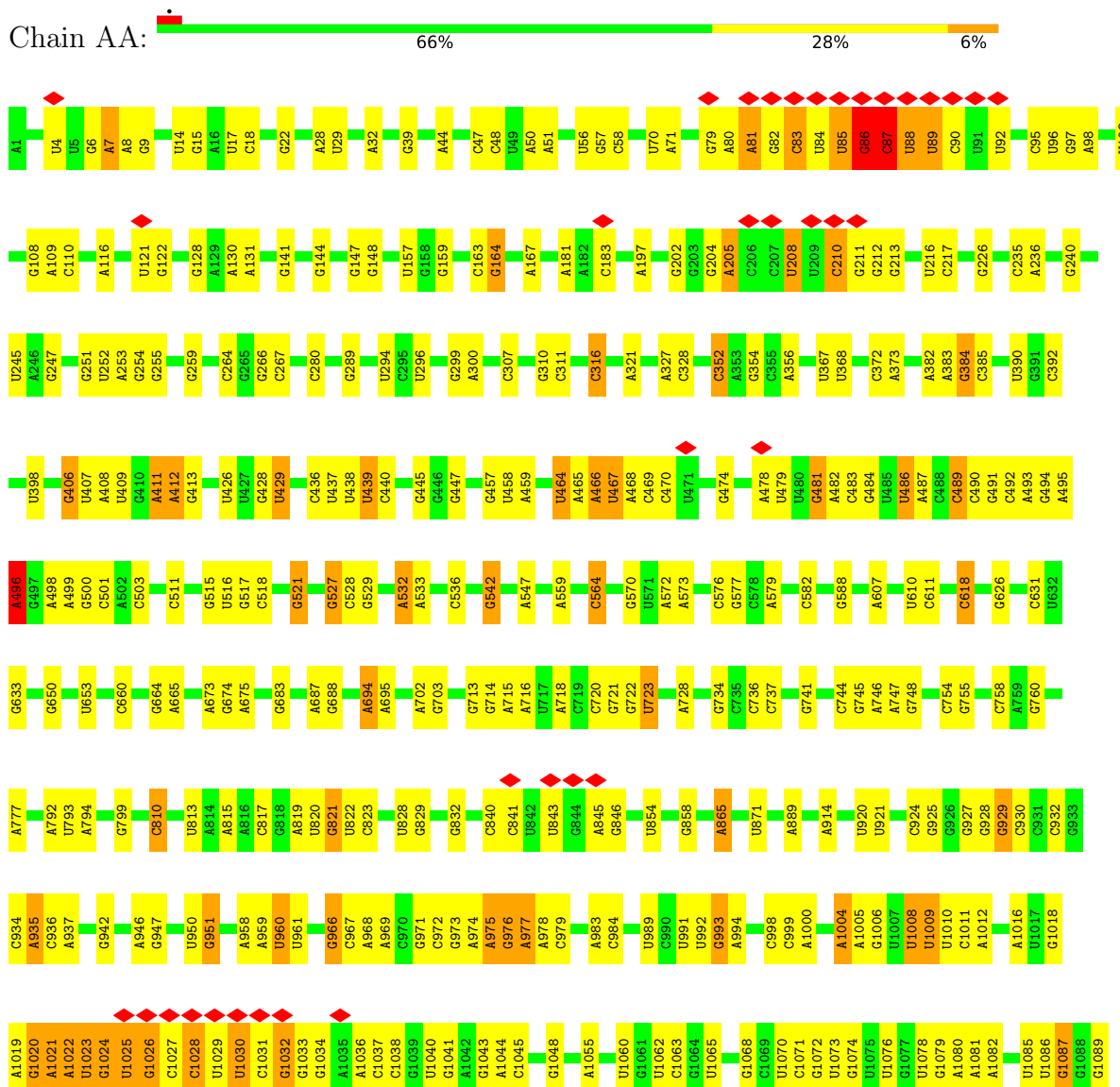
- Molecule 59 is water.

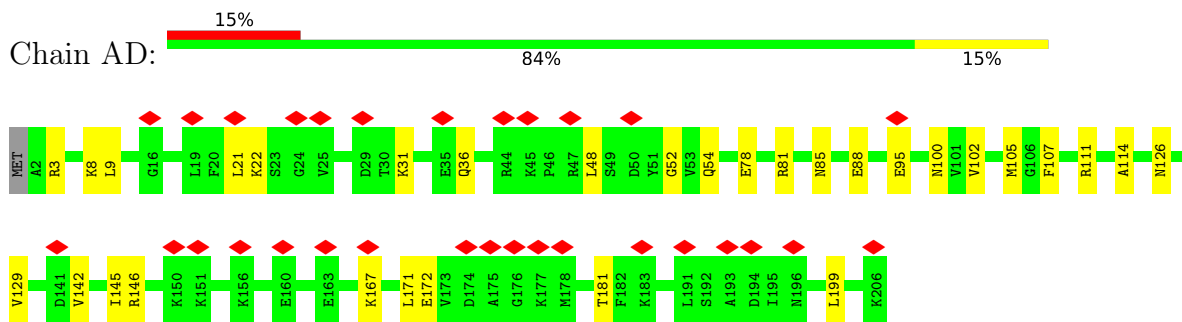
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
59	AA	166	166	166	0
59	AK	2	2	2	0
59	AM	1	1	1	0
59	AN	2	2	2	0
59	AQ	1	1	1	0
59	BA	614	614	614	0
59	BC	6	6	6	0
59	BD	3	3	3	0
59	BE	1	1	1	0
59	BJ	1	1	1	0
59	BL	1	1	1	0
59	BN	2	2	2	0

3 Residue-property plots [i](#)

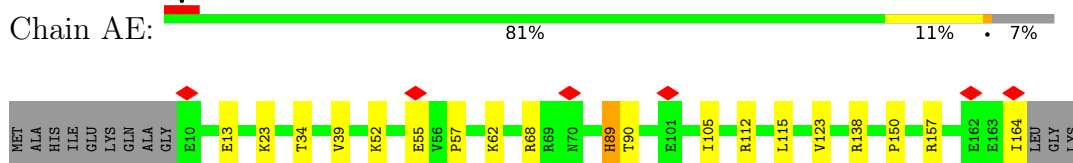
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

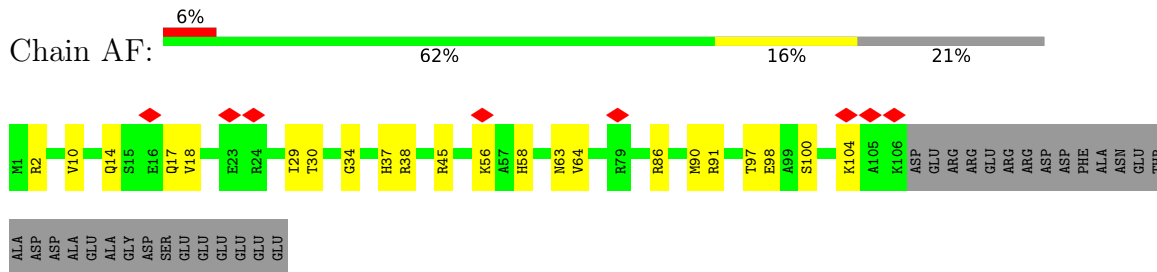




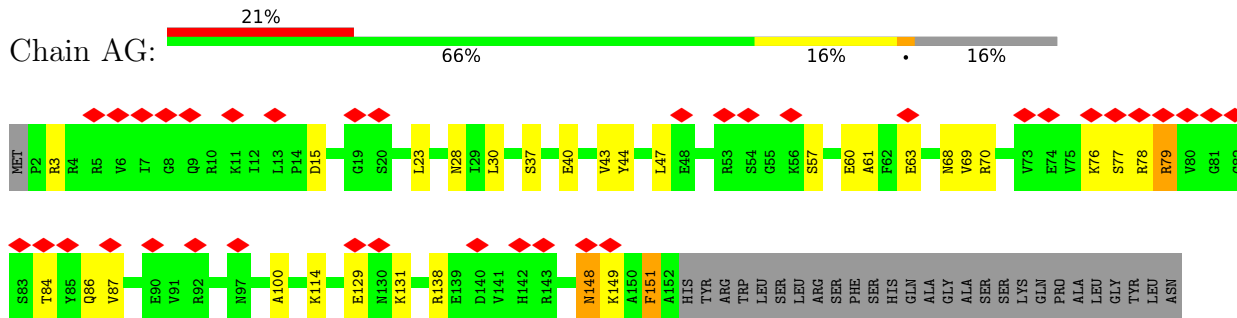
• Molecule 5: 30S ribosomal protein S5



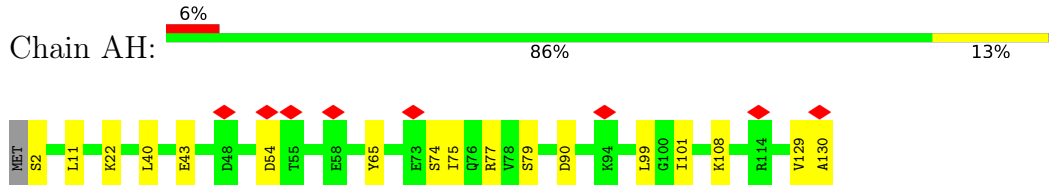
• Molecule 6: 30S ribosomal protein S6



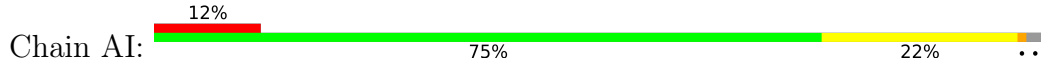
• Molecule 7: 30S ribosomal protein S7

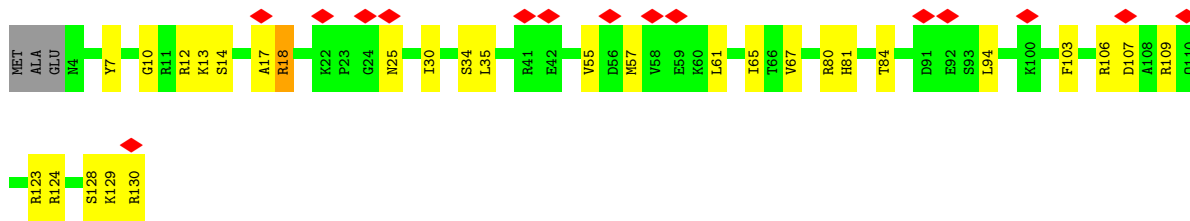


• Molecule 8: 30S ribosomal protein S8

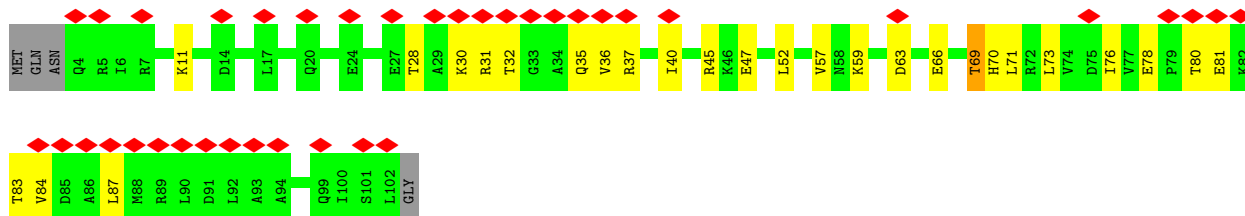


• Molecule 9: 30S ribosomal protein S9

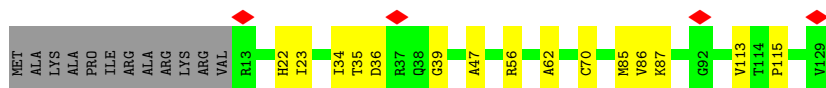
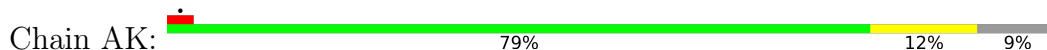




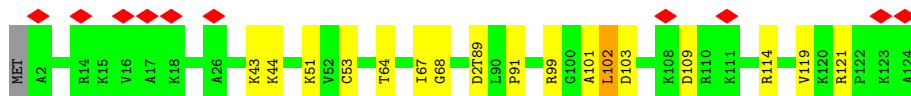
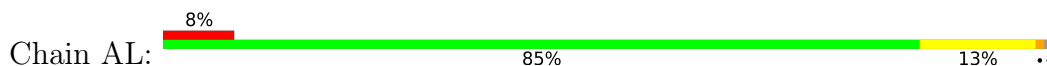
- Molecule 10: 30S ribosomal protein S10



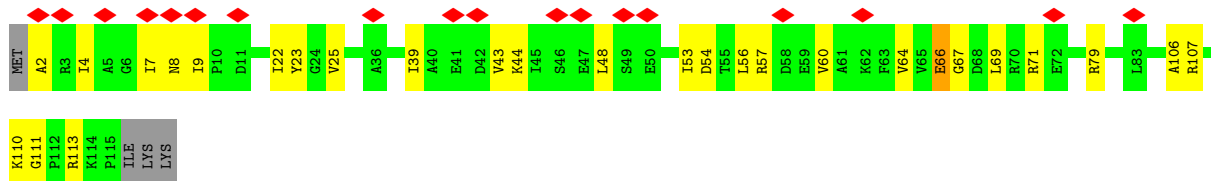
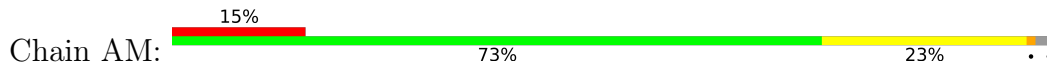
- Molecule 11: 30S ribosomal protein S11



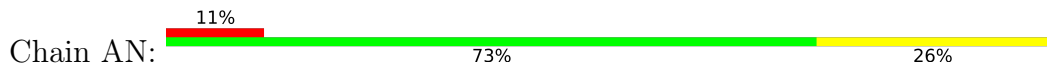
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

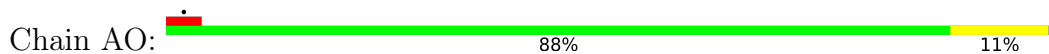


- Molecule 14: 30S ribosomal protein S14

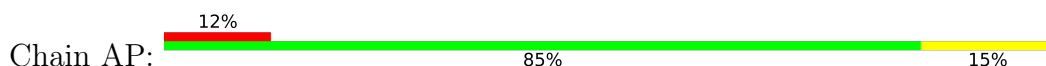




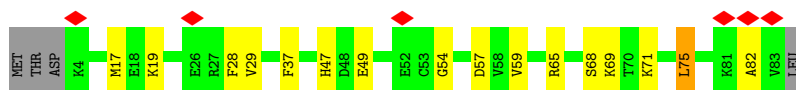
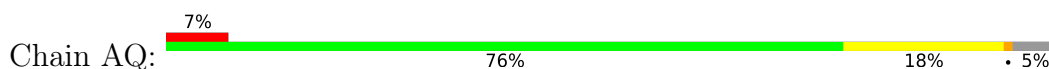
- Molecule 15: 30S ribosomal protein S15



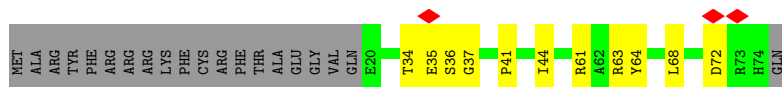
- Molecule 16: 30S ribosomal protein S16



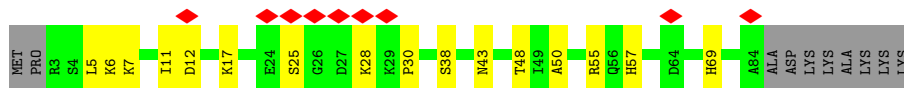
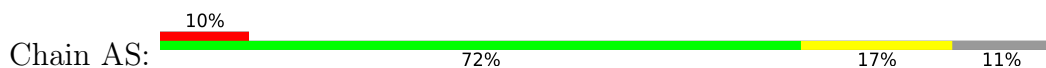
- Molecule 17: 30S ribosomal protein S17



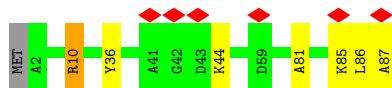
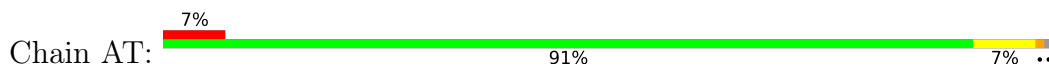
- Molecule 18: 30S ribosomal protein S18



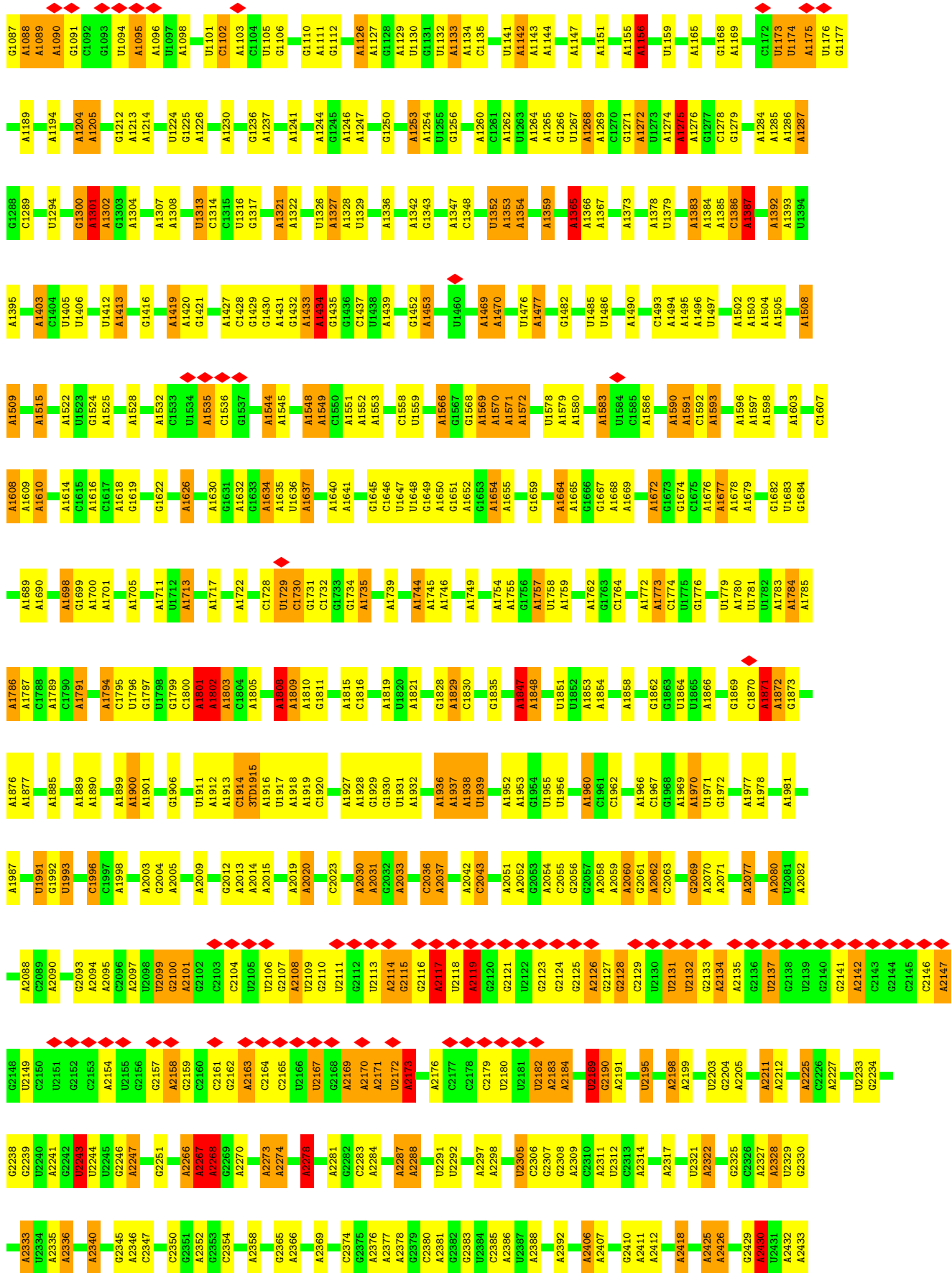
- Molecule 19: 30S ribosomal protein S19

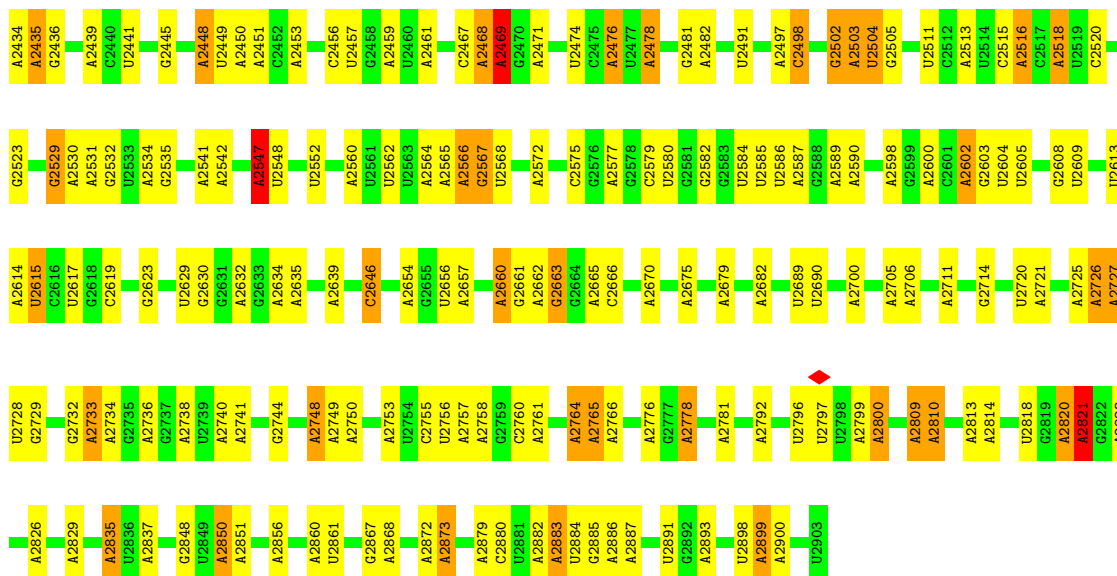


- Molecule 20: 30S ribosomal protein S20

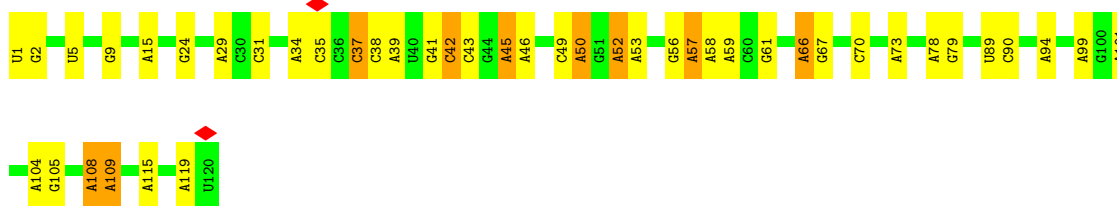


- Molecule 21: 30S ribosomal protein S21





• Molecule 23: 5S rRNA



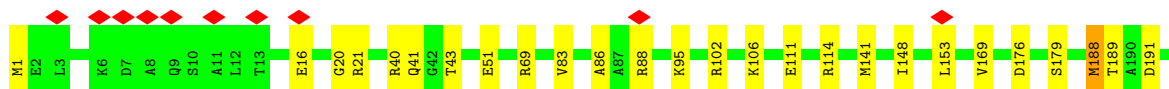
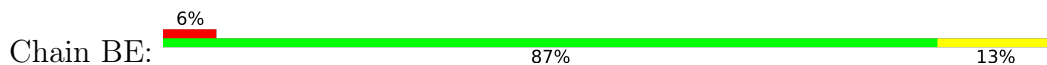
• Molecule 24: 50S ribosomal protein L2



• Molecule 25: 50S ribosomal protein L3

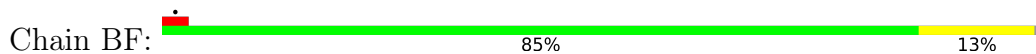


• Molecule 26: 50S ribosomal protein L4

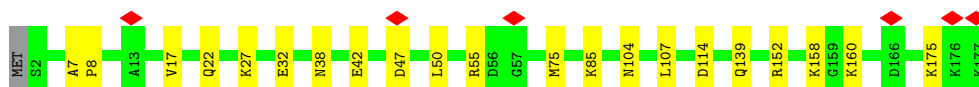




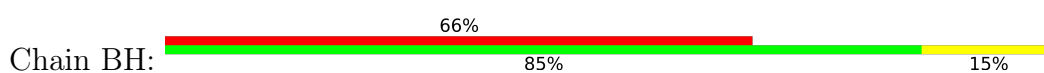
- Molecule 27: 50S ribosomal protein L5



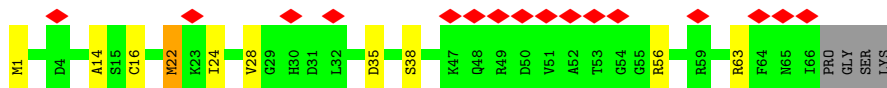
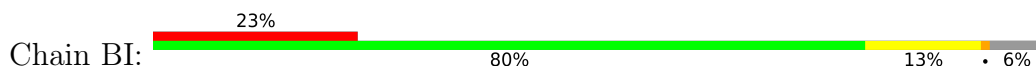
- Molecule 28: 50S ribosomal protein L6



- Molecule 29: 50S ribosomal protein L9



- Molecule 30: 50S ribosomal protein L31

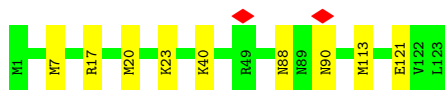


- Molecule 31: 50S ribosomal protein L13



- Molecule 32: 50S ribosomal protein L14

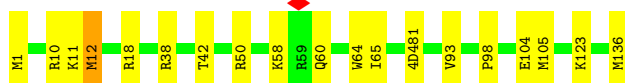
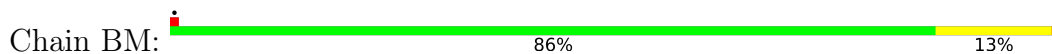




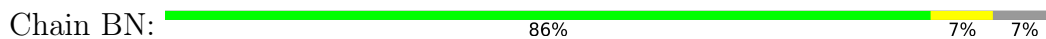
- Molecule 33: 50S ribosomal protein L15



- Molecule 34: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L18



- Molecule 37: 50S ribosomal protein L19



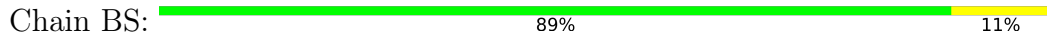
- Molecule 38: 50S ribosomal protein L20



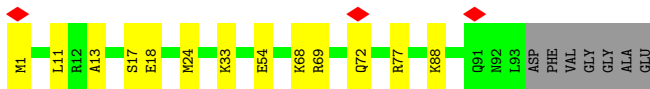
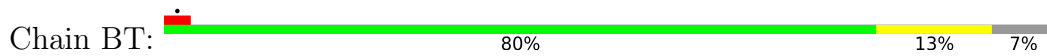
- Molecule 39: 50S ribosomal protein L21



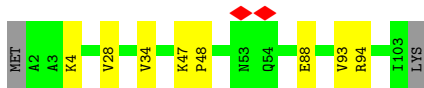
- Molecule 40: 50S ribosomal protein L22



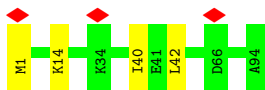
- Molecule 41: 50S ribosomal protein L23



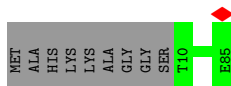
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25




- Molecule 44: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L28




- Molecule 46: 50S ribosomal protein L29

Chain BY:  76% 22%




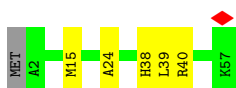
- Molecule 47: 50S ribosomal protein L30

Chain BZ:  5% 88% 8%




- Molecule 48: 50S ribosomal protein L32

Chain B0:  89% 9%



- Molecule 49: 50S ribosomal protein L33

Chain B1:  85% 7% 7%




- Molecule 50: 50S ribosomal protein L34

Chain B2:  93% 7%




- Molecule 51: 50S ribosomal protein L35

Chain B3:  83% 12%



- Molecule 52: 50S ribosomal protein L36

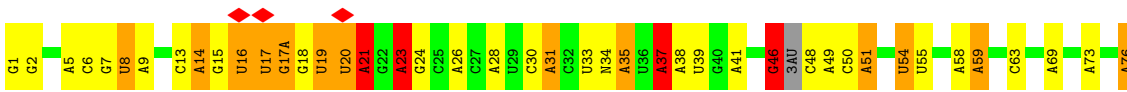
Chain B4:  82% 18%



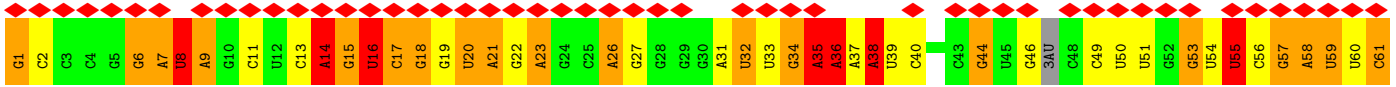
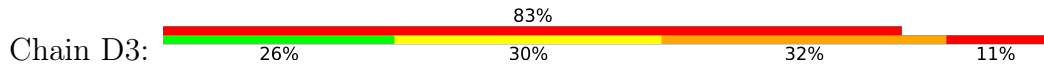
- Molecule 53: MsrDL: FME-TYR-LEU-ILE-PHE-MET



- Molecule 54: Met-tRNA (P site)



- Molecule 55: Phe-tRNA (E site)



- Molecule 56: MsrDL mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	23.089	Depositor
Minimum map value	-11.414	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.85	Depositor
Map size (Å)	414.0, 414.0, 414.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 2MG, PSU, 3TD, D2T, MA6, 1MG, OMG, G7M, MEQ, T6A, 2MA, FME, 4AC, 4D4, 4OC, 6MZ, H2U, 5MU, 5MC, UR3, ERY, OMC, MG, 4SU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	1.42	48/36593 (0.1%)	1.10	110/57081 (0.2%)
2	AB	0.41	0/1784	0.57	0/2403
3	AC	0.70	0/1651	0.64	0/2225
4	AD	0.59	0/1665	0.59	0/2227
5	AE	0.58	0/1157	0.59	0/1557
6	AF	0.50	0/881	0.60	0/1189
7	AG	0.55	0/1195	0.62	0/1602
8	AH	0.57	0/989	0.57	0/1326
9	AI	0.77	0/1034	0.70	0/1375
10	AJ	0.68	0/805	0.68	0/1089
11	AK	0.51	0/893	0.58	0/1205
12	AL	0.62	0/960	0.78	5/1286 (0.4%)
13	AM	0.62	0/892	0.70	0/1193
14	AN	0.74	0/811	0.67	0/1081
15	AO	0.49	0/722	0.53	0/964
16	AP	0.60	0/659	0.72	1/884 (0.1%)
17	AQ	0.57	0/657	0.61	1/881 (0.1%)
18	AR	0.60	0/462	0.60	0/621
19	AS	0.75	0/672	0.67	0/904
20	AT	0.44	0/676	0.54	1/895 (0.1%)
21	AU	0.50	0/472	0.52	0/627
22	BA	2.27	2742/69099 (4.0%)	3.49	8699/107794 (8.1%)
23	BB	1.94	90/2872 (3.1%)	3.02	275/4478 (6.1%)
24	BC	0.41	0/2121	0.59	5/2852 (0.2%)
25	BD	0.41	0/1576	0.57	3/2119 (0.1%)
26	BE	0.35	0/1571	0.58	5/2113 (0.2%)
27	BF	0.31	0/1434	0.57	2/1926 (0.1%)
28	BG	0.32	0/1343	0.49	1/1816 (0.1%)
29	BH	0.30	0/1121	0.63	2/1515 (0.1%)
30	BI	0.31	0/531	0.61	2/709 (0.3%)
31	BJ	0.38	0/1152	0.55	3/1551 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BK	0.38	0/955	0.61	3/1279 (0.2%)
33	BL	0.36	0/1062	0.57	2/1413 (0.1%)
34	BM	0.39	0/1081	0.60	4/1443 (0.3%)
35	BN	0.36	0/958	0.60	3/1281 (0.2%)
36	BO	0.33	0/910	0.49	1/1219 (0.1%)
37	BP	0.39	0/929	0.52	1/1242 (0.1%)
38	BQ	0.42	0/960	0.46	0/1278
39	BR	0.39	0/829	0.57	1/1107 (0.1%)
40	BS	0.35	0/864	0.58	3/1156 (0.3%)
41	BT	0.36	0/744	0.57	2/994 (0.2%)
42	BU	0.34	0/787	0.50	0/1051
43	BV	0.34	0/766	0.56	1/1025 (0.1%)
44	BW	0.39	0/587	0.46	0/776
45	BX	0.39	0/635	0.57	1/848 (0.1%)
46	BY	0.28	0/502	0.48	1/667 (0.1%)
47	BZ	0.35	0/453	0.61	2/605 (0.3%)
48	B0	0.40	0/450	0.55	1/599 (0.2%)
49	B1	0.34	0/421	0.51	0/561
50	B2	0.37	0/380	0.64	2/498 (0.4%)
51	B3	0.36	0/513	0.67	1/676 (0.1%)
52	B4	0.39	0/303	0.57	1/397 (0.3%)
53	D1	0.62	0/48	0.74	0/63
54	D2	2.31	72/1531 (4.7%)	3.60	211/2380 (8.9%)
55	D3	2.07	54/1636 (3.3%)	3.39	194/2547 (7.6%)
56	D4	0.89	0/210	1.35	7/324 (2.2%)
All	All	1.72	3006/156964 (1.9%)	2.53	9557/234917 (4.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AC	0	1
5	AE	0	1
29	BH	0	1
51	B3	0	1
All	All	0	4

All (3006) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1872	A	C6-N6	17.23	1.47	1.33
55	D3	23	A	C6-N6	17.03	1.47	1.33
22	BA	1086	A	C6-N6	17.01	1.47	1.33
22	BA	2101	A	C6-N6	16.98	1.47	1.33
22	BA	1420	A	C6-N6	16.97	1.47	1.33
22	BA	1089	A	C6-N6	16.95	1.47	1.33
22	BA	2170	A	C6-N6	16.95	1.47	1.33
22	BA	2158	A	C6-N6	16.95	1.47	1.33
22	BA	2126	A	C6-N6	16.94	1.47	1.33
22	BA	1096	A	C6-N6	16.92	1.47	1.33
22	BA	1098	A	C6-N6	16.92	1.47	1.33
22	BA	1077	A	C6-N6	16.90	1.47	1.33
22	BA	1048	A	C6-N6	16.90	1.47	1.33
22	BA	896	A	C6-N6	16.89	1.47	1.33
22	BA	1175	A	C6-N6	16.88	1.47	1.33
22	BA	1084	A	C6-N6	16.88	1.47	1.33
22	BA	2163	A	C6-N6	16.87	1.47	1.33
22	BA	1871	A	C6-N6	16.87	1.47	1.33
22	BA	2602	A	C6-N6	16.86	1.47	1.33
22	BA	1095	A	C6-N6	16.84	1.47	1.33
22	BA	1046	A	C6-N6	16.84	1.47	1.33
55	D3	37	A	C6-N6	16.84	1.47	1.33
22	BA	877	A	C6-N6	16.83	1.47	1.33
22	BA	2134	A	C6-N6	16.82	1.47	1.33
22	BA	547	A	C6-N6	16.81	1.47	1.33
22	BA	2108	A	C6-N6	16.80	1.47	1.33
22	BA	1103	A	C6-N6	16.79	1.47	1.33
22	BA	2176	A	C6-N6	16.79	1.47	1.33
22	BA	1027	A	C6-N6	16.79	1.47	1.33
22	BA	362	A	C6-N6	16.78	1.47	1.33
22	BA	1528	A	C6-N6	16.78	1.47	1.33
22	BA	2082	A	C6-N6	16.78	1.47	1.33
22	BA	2171	A	C6-N6	16.77	1.47	1.33
22	BA	614	A	C6-N6	16.77	1.47	1.33
22	BA	94	A	C6-N6	16.77	1.47	1.33
22	BA	1069	A	C6-N6	16.77	1.47	1.33
55	D3	9	A	C6-N6	16.77	1.47	1.33
22	BA	1067	A	C6-N6	16.76	1.47	1.33
55	D3	58	A	C6-N6	16.75	1.47	1.33
22	BA	1057	A	C6-N6	16.74	1.47	1.33
22	BA	1085	A	C6-N6	16.74	1.47	1.33
22	BA	613	A	C6-N6	16.74	1.47	1.33
22	BA	1080	A	C6-N6	16.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	D3	73	A	C6-N6	16.73	1.47	1.33
22	BA	2117	A	C6-N6	16.72	1.47	1.33
22	BA	1070	A	C6-N6	16.72	1.47	1.33
22	BA	718	A	C6-N6	16.72	1.47	1.33
22	BA	2211	A	C6-N6	16.72	1.47	1.33
22	BA	1913	A	C6-N6	16.71	1.47	1.33
54	D2	73	A	C6-N6	16.71	1.47	1.33
22	BA	1490	A	C6-N6	16.70	1.47	1.33
22	BA	716	A	C6-N6	16.70	1.47	1.33
22	BA	1810	A	C6-N6	16.69	1.47	1.33
22	BA	1535	A	C6-N6	16.69	1.47	1.33
22	BA	1508	A	C6-N6	16.68	1.47	1.33
22	BA	2412	A	C6-N6	16.68	1.47	1.33
55	D3	38	A	C6-N6	16.68	1.47	1.33
22	BA	278	A	C6-N6	16.66	1.47	1.33
22	BA	1111	A	C6-N6	16.66	1.47	1.33
22	BA	2142	A	C6-N6	16.66	1.47	1.33
22	BA	1073	A	C6-N6	16.64	1.47	1.33
22	BA	1722	A	C6-N6	16.64	1.47	1.33
54	D2	51	A	C6-N6	16.63	1.47	1.33
22	BA	1866	A	C6-N6	16.63	1.47	1.33
54	D2	9	A	C6-N6	16.63	1.47	1.33
22	BA	95	A	C6-N6	16.62	1.47	1.33
22	BA	1937	A	C6-N6	16.61	1.47	1.33
22	BA	213	A	C6-N6	16.61	1.47	1.33
22	BA	1745	A	C6-N6	16.61	1.47	1.33
22	BA	1735	A	C6-N6	16.61	1.47	1.33
55	D3	35	A	C6-N6	16.61	1.47	1.33
22	BA	1373	A	C6-N6	16.60	1.47	1.33
22	BA	165	A	C6-N6	16.60	1.47	1.33
22	BA	878	A	C6-N6	16.60	1.47	1.33
22	BA	892	A	C6-N6	16.60	1.47	1.33
22	BA	354	A	C6-N6	16.59	1.47	1.33
22	BA	2042	A	C6-N6	16.59	1.47	1.33
22	BA	1580	A	C6-N6	16.59	1.47	1.33
22	BA	2814	A	C6-N6	16.59	1.47	1.33
55	D3	31	A	C6-N6	16.59	1.47	1.33
22	BA	1916	A	C6-N6	16.58	1.47	1.33
22	BA	1509	A	C6-N6	16.58	1.47	1.33
22	BA	251	A	C6-N6	16.58	1.47	1.33
22	BA	2820	A	C6-N6	16.57	1.47	1.33
22	BA	101	A	C6-N6	16.57	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2184	A	C6-N6	16.57	1.47	1.33
22	BA	2733	A	C6-N6	16.57	1.47	1.33
22	BA	2665	A	C6-N6	16.57	1.47	1.33
22	BA	2800	A	C6-N6	16.57	1.47	1.33
22	BA	633	A	C6-N6	16.56	1.47	1.33
22	BA	1395	A	C6-N6	16.56	1.47	1.33
22	BA	2662	A	C6-N6	16.56	1.47	1.33
22	BA	2309	A	C6-N6	16.56	1.47	1.33
54	D2	49	A	C6-N6	16.56	1.47	1.33
22	BA	1029	A	C6-N6	16.55	1.47	1.33
54	D2	14	A	C6-N6	16.55	1.47	1.33
22	BA	2781	A	C6-N6	16.55	1.47	1.33
22	BA	1090	A	C6-N6	16.55	1.47	1.33
22	BA	1586	A	C6-N6	16.55	1.47	1.33
22	BA	332	A	C6-N6	16.55	1.47	1.33
22	BA	2872	A	C6-N6	16.54	1.47	1.33
54	D2	69	A	C6-N6	16.54	1.47	1.33
22	BA	1532	A	C6-N6	16.54	1.47	1.33
54	D2	59	A	C6-N6	16.54	1.47	1.33
54	D2	58	A	C6-N6	16.54	1.47	1.33
22	BA	480	A	C6-N6	16.53	1.47	1.33
22	BA	2887	A	C6-N6	16.53	1.47	1.33
22	BA	2660	A	C6-N6	16.53	1.47	1.33
22	BA	508	A	C6-N6	16.53	1.47	1.33
22	BA	2154	A	C6-N6	16.53	1.47	1.33
22	BA	111	A	C6-N6	16.52	1.47	1.33
22	BA	749	A	C6-N6	16.52	1.47	1.33
22	BA	142	A	C6-N6	16.52	1.47	1.33
22	BA	279	A	C6-N6	16.51	1.47	1.33
22	BA	1583	A	C6-N6	16.51	1.47	1.33
22	BA	2748	A	C6-N6	16.51	1.47	1.33
22	BA	1054	A	C6-N6	16.51	1.47	1.33
22	BA	504	A	C6-N6	16.51	1.47	1.33
22	BA	1050	A	C6-N6	16.51	1.47	1.33
22	BA	1156	A	C6-N6	16.51	1.47	1.33
22	BA	265	A	C6-N6	16.50	1.47	1.33
22	BA	1434	A	C6-N6	16.50	1.47	1.33
22	BA	2879	A	C6-N6	16.50	1.47	1.33
23	BB	15	A	C6-N6	16.50	1.47	1.33
55	D3	36	A	C6-N6	16.50	1.47	1.33
23	BB	29	A	C6-N6	16.49	1.47	1.33
22	BA	2212	A	C6-N6	16.49	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D2	26	A	C6-N6	16.49	1.47	1.33
22	BA	2191	A	C6-N6	16.49	1.47	1.33
23	BB	52	A	C6-N6	16.49	1.47	1.33
23	BB	108	A	C6-N6	16.49	1.47	1.33
22	BA	1367	A	C6-N6	16.48	1.47	1.33
54	D2	21	A	C6-N6	16.48	1.47	1.33
22	BA	975	A	C6-N6	16.47	1.47	1.33
22	BA	2287	A	C6-N6	16.47	1.47	1.33
22	BA	849	A	C6-N6	16.47	1.47	1.33
22	BA	345	A	C6-N6	16.47	1.47	1.33
22	BA	2173	A	C6-N6	16.47	1.47	1.33
54	D2	35	A	C6-N6	16.47	1.47	1.33
22	BA	2135	A	C6-N6	16.46	1.47	1.33
22	BA	2297	A	C6-N6	16.46	1.47	1.33
22	BA	739	A	C6-N6	16.46	1.47	1.33
22	BA	2468	A	C6-N6	16.46	1.47	1.33
22	BA	960	A	C6-N6	16.46	1.47	1.33
22	BA	71	A	C6-N6	16.45	1.47	1.33
22	BA	900	A	C6-N6	16.45	1.47	1.33
23	BB	53	A	C6-N6	16.45	1.47	1.33
22	BA	1690	A	C6-N6	16.45	1.47	1.33
22	BA	1919	A	C6-N6	16.45	1.47	1.33
23	BB	34	A	C6-N6	16.45	1.47	1.33
22	BA	91	A	C6-N6	16.45	1.47	1.33
22	BA	104	A	C6-N6	16.45	1.47	1.33
22	BA	2513	A	C6-N6	16.45	1.47	1.33
22	BA	2886	A	C6-N6	16.45	1.47	1.33
22	BA	2406	A	C6-N6	16.44	1.47	1.33
22	BA	1755	A	C6-N6	16.44	1.47	1.33
22	BA	2750	A	C6-N6	16.44	1.47	1.33
23	BB	39	A	C6-N6	16.43	1.47	1.33
22	BA	990	A	C6-N6	16.43	1.47	1.33
22	BA	1284	A	C6-N6	16.43	1.47	1.33
22	BA	347	A	C6-N6	16.43	1.47	1.33
22	BA	1328	A	C6-N6	16.43	1.47	1.33
22	BA	2119	A	C6-N6	16.43	1.47	1.33
22	BA	1039	A	C6-N6	16.42	1.47	1.33
22	BA	502	A	C6-N6	16.42	1.47	1.33
23	BB	119	A	C6-N6	16.42	1.47	1.33
22	BA	1593	A	C6-N6	16.42	1.47	1.33
22	BA	655	A	C6-N6	16.42	1.47	1.33
22	BA	1876	A	C6-N6	16.42	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D2	31	A	C6-N6	16.42	1.47	1.33
54	D2	38	A	C6-N6	16.42	1.47	1.33
22	BA	155	A	C6-N6	16.42	1.47	1.33
22	BA	270	A	C6-N6	16.42	1.47	1.33
22	BA	344	A	C6-N6	16.41	1.47	1.33
22	BA	2335	A	C6-N6	16.41	1.47	1.33
22	BA	2377	A	C6-N6	16.41	1.47	1.33
22	BA	2547	A	C6-N6	16.41	1.47	1.33
22	BA	83	A	C6-N6	16.41	1.47	1.33
22	BA	167	A	C6-N6	16.41	1.47	1.33
22	BA	1453	A	C6-N6	16.41	1.47	1.33
22	BA	282	A	C6-N6	16.40	1.47	1.33
22	BA	1413	A	C6-N6	16.40	1.47	1.33
22	BA	1744	A	C6-N6	16.40	1.47	1.33
22	BA	2541	A	C6-N6	16.40	1.47	1.33
22	BA	330	A	C6-N6	16.40	1.47	1.33
23	BB	66	A	C6-N6	16.40	1.47	1.33
22	BA	294	A	C6-N6	16.40	1.47	1.33
22	BA	1544	A	C6-N6	16.40	1.47	1.33
22	BA	2378	A	C6-N6	16.40	1.47	1.33
22	BA	626	A	C6-N6	16.40	1.47	1.33
22	BA	2169	A	C6-N6	16.39	1.47	1.33
22	BA	2721	A	C6-N6	16.39	1.47	1.33
22	BA	2657	A	C6-N6	16.39	1.47	1.33
22	BA	342	A	C6-N6	16.39	1.47	1.33
22	BA	352	A	C6-N6	16.39	1.47	1.33
22	BA	538	A	C6-N6	16.39	1.47	1.33
22	BA	1952	A	C6-N6	16.39	1.47	1.33
22	BA	2205	A	C6-N6	16.39	1.47	1.33
22	BA	1626	A	C6-N6	16.39	1.47	1.33
22	BA	2893	A	C6-N6	16.39	1.47	1.33
22	BA	1591	A	C6-N6	16.38	1.47	1.33
22	BA	2376	A	C6-N6	16.38	1.47	1.33
22	BA	1502	A	C6-N6	16.38	1.47	1.33
22	BA	2033	A	C6-N6	16.38	1.47	1.33
23	BB	45	A	C6-N6	16.38	1.47	1.33
22	BA	933	A	C6-N6	16.38	1.47	1.33
22	BA	2478	A	C6-N6	16.38	1.47	1.33
22	BA	782	A	C6-N6	16.38	1.47	1.33
22	BA	2298	A	C6-N6	16.38	1.47	1.33
22	BA	2598	A	C6-N6	16.38	1.47	1.33
22	BA	2850	A	C6-N6	16.38	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2821	A	C6-N6	16.38	1.47	1.33
23	BB	50	A	C6-N6	16.38	1.47	1.33
22	BA	1009	A	C6-N6	16.37	1.47	1.33
54	D2	76	A	C6-N6	16.37	1.47	1.33
22	BA	218	A	C6-N6	16.37	1.47	1.33
22	BA	2753	A	C6-N6	16.37	1.47	1.33
22	BA	2439	A	C6-N6	16.37	1.47	1.33
22	BA	996	A	C6-N6	16.36	1.47	1.33
55	D3	7	A	C6-N6	16.36	1.47	1.33
22	BA	1598	A	C6-N6	16.36	1.47	1.33
22	BA	2757	A	C6-N6	16.36	1.47	1.33
22	BA	482	A	C6-N6	16.35	1.47	1.33
22	BA	1495	A	C6-N6	16.35	1.47	1.33
22	BA	1503	A	C6-N6	16.35	1.47	1.33
22	BA	2311	A	C6-N6	16.35	1.47	1.33
22	BA	2654	A	C6-N6	16.35	1.47	1.33
22	BA	401	A	C6-N6	16.35	1.47	1.33
22	BA	983	A	C6-N6	16.35	1.47	1.33
22	BA	1927	A	C6-N6	16.35	1.47	1.33
22	BA	1205	A	C6-N6	16.35	1.47	1.33
22	BA	227	A	C6-N6	16.34	1.47	1.33
22	BA	64	A	C6-N6	16.34	1.47	1.33
22	BA	156	A	C6-N6	16.34	1.47	1.33
22	BA	391	A	C6-N6	16.34	1.47	1.33
55	D3	64	A	C6-N6	16.34	1.47	1.33
22	BA	802	A	C6-N6	16.34	1.47	1.33
22	BA	1353	A	C6-N6	16.34	1.47	1.33
22	BA	1383	A	C6-N6	16.34	1.47	1.33
22	BA	1545	A	C6-N6	16.34	1.47	1.33
22	BA	1632	A	C6-N6	16.34	1.47	1.33
22	BA	2482	A	C6-N6	16.34	1.47	1.33
22	BA	2381	A	C6-N6	16.33	1.47	1.33
22	BA	833	A	C6-N6	16.33	1.47	1.33
22	BA	125	A	C6-N6	16.33	1.47	1.33
22	BA	299	A	C6-N6	16.33	1.47	1.33
22	BA	2432	A	C6-N6	16.33	1.47	1.33
22	BA	1640	A	C6-N6	16.32	1.47	1.33
23	BB	59	A	C6-N6	16.32	1.47	1.33
22	BA	2632	A	C6-N6	16.32	1.47	1.33
22	BA	1272	A	C6-N6	16.32	1.47	1.33
22	BA	1901	A	C6-N6	16.32	1.47	1.33
22	BA	721	A	C6-N6	16.32	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2738	A	C6-N6	16.32	1.47	1.33
55	D3	21	A	C6-N6	16.32	1.47	1.33
22	BA	2198	A	C6-N6	16.32	1.47	1.33
22	BA	221	A	C6-N6	16.32	1.47	1.33
22	BA	2873	A	C6-N6	16.32	1.47	1.33
22	BA	608	A	C6-N6	16.31	1.47	1.33
22	BA	1739	A	C6-N6	16.31	1.47	1.33
22	BA	2080	A	C6-N6	16.31	1.47	1.33
22	BA	2741	A	C6-N6	16.31	1.47	1.33
22	BA	1322	A	C6-N6	16.31	1.47	1.33
22	BA	2453	A	C6-N6	16.31	1.47	1.33
22	BA	899	A	C6-N6	16.31	1.47	1.33
22	BA	2705	A	C6-N6	16.30	1.47	1.33
22	BA	428	A	C6-N6	16.30	1.47	1.33
22	BA	1385	A	C6-N6	16.30	1.47	1.33
22	BA	1590	A	C6-N6	16.30	1.47	1.33
54	D2	5	A	C6-N6	16.30	1.47	1.33
22	BA	715	A	C6-N6	16.30	1.47	1.33
22	BA	311	A	C6-N6	16.30	1.47	1.33
22	BA	2392	A	C6-N6	16.30	1.47	1.33
22	BA	637	A	C6-N6	16.30	1.47	1.33
23	BB	57	A	C6-N6	16.30	1.47	1.33
22	BA	654	A	C6-N6	16.29	1.47	1.33
54	D2	41	A	C6-N6	16.29	1.47	1.33
22	BA	2813	A	C6-N6	16.29	1.47	1.33
22	BA	63	A	C6-N6	16.29	1.47	1.33
22	BA	1393	A	C6-N6	16.29	1.47	1.33
22	BA	2856	A	C6-N6	16.29	1.47	1.33
22	BA	1504	A	C6-N6	16.29	1.47	1.33
55	D3	14	A	C6-N6	16.28	1.47	1.33
22	BA	84	A	C6-N6	16.28	1.47	1.33
22	BA	752	A	C6-N6	16.28	1.47	1.33
22	BA	2900	A	C6-N6	16.28	1.47	1.33
22	BA	503	A	C6-N6	16.28	1.47	1.33
22	BA	2114	A	C6-N6	16.27	1.47	1.33
22	BA	172	A	C6-N6	16.27	1.47	1.33
22	BA	2199	A	C6-N6	16.27	1.47	1.33
22	BA	309	A	C6-N6	16.27	1.47	1.33
22	BA	1928	A	C6-N6	16.27	1.47	1.33
22	BA	644	A	C6-N6	16.27	1.47	1.33
22	BA	1877	A	C6-N6	16.27	1.47	1.33
22	BA	44	A	C6-N6	16.27	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	322	A	C6-N6	16.27	1.47	1.33
22	BA	1307	A	C6-N6	16.27	1.47	1.33
22	BA	1900	A	C6-N6	16.27	1.47	1.33
22	BA	2476	A	C6-N6	16.27	1.47	1.33
22	BA	2761	A	C6-N6	16.27	1.47	1.33
22	BA	1147	A	C6-N6	16.27	1.47	1.33
22	BA	430	A	C6-N6	16.27	1.47	1.33
22	BA	905	A	C6-N6	16.27	1.47	1.33
22	BA	1609	A	C6-N6	16.27	1.47	1.33
22	BA	2097	A	C6-N6	16.27	1.47	1.33
22	BA	1912	A	C6-N6	16.26	1.47	1.33
22	BA	1134	A	C6-N6	16.26	1.47	1.33
22	BA	541	A	C6-N6	16.26	1.47	1.33
22	BA	2147	A	C6-N6	16.26	1.47	1.33
22	BA	2758	A	C6-N6	16.26	1.47	1.33
22	BA	340	A	C6-N6	16.26	1.47	1.33
22	BA	829	A	C6-N6	16.26	1.47	1.33
22	BA	1978	A	C6-N6	16.26	1.47	1.33
22	BA	89	A	C6-N6	16.26	1.47	1.33
22	BA	501	A	C6-N6	16.26	1.47	1.33
22	BA	1553	A	C6-N6	16.26	1.47	1.33
22	BA	1847	A	C6-N6	16.26	1.47	1.33
22	BA	2183	A	C6-N6	16.26	1.47	1.33
22	BA	1634	A	C6-N6	16.26	1.47	1.33
22	BA	1918	A	C6-N6	16.26	1.47	1.33
22	BA	1040	A	C6-N6	16.25	1.47	1.33
22	BA	2792	A	C6-N6	16.25	1.47	1.33
23	BB	109	A	C6-N6	16.25	1.47	1.33
22	BA	477	A	C6-N6	16.25	1.47	1.33
22	BA	507	A	C6-N6	16.25	1.47	1.33
22	BA	2314	A	C6-N6	16.25	1.47	1.33
22	BA	1204	A	C6-N6	16.25	1.47	1.33
22	BA	1885	A	C6-N6	16.25	1.47	1.33
54	D2	23	A	C6-N6	16.25	1.47	1.33
22	BA	2288	A	C6-N6	16.24	1.47	1.33
22	BA	1608	A	C6-N6	16.24	1.47	1.33
22	BA	2860	A	C6-N6	16.24	1.47	1.33
23	BB	73	A	C6-N6	16.24	1.47	1.33
22	BA	1304	A	C6-N6	16.24	1.47	1.33
22	BA	1287	A	C6-N6	16.24	1.47	1.33
22	BA	2734	A	C6-N6	16.24	1.47	1.33
22	BA	14	A	C6-N6	16.24	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	429	A	C6-N6	16.24	1.47	1.33
22	BA	616	A	C6-N6	16.24	1.47	1.33
22	BA	1155	A	C6-N6	16.23	1.47	1.33
22	BA	1551	A	C6-N6	16.23	1.47	1.33
22	BA	1596	A	C6-N6	16.23	1.47	1.33
22	BA	2530	A	C6-N6	16.23	1.47	1.33
22	BA	73	A	C6-N6	16.23	1.47	1.33
22	BA	1241	A	C6-N6	16.23	1.47	1.33
22	BA	1773	A	C6-N6	16.23	1.47	1.33
22	BA	2776	A	C6-N6	16.23	1.47	1.33
22	BA	1783	A	C6-N6	16.23	1.47	1.33
22	BA	368	A	C6-N6	16.23	1.47	1.33
22	BA	2322	A	C6-N6	16.23	1.47	1.33
22	BA	320	A	C6-N6	16.23	1.47	1.33
22	BA	734	A	C6-N6	16.23	1.47	1.33
22	BA	2572	A	C6-N6	16.23	1.47	1.33
22	BA	1678	A	C6-N6	16.22	1.47	1.33
22	BA	2366	A	C6-N6	16.22	1.47	1.33
22	BA	526	A	C6-N6	16.22	1.47	1.33
22	BA	1327	A	C6-N6	16.22	1.47	1.33
22	BA	602	A	C6-N6	16.22	1.47	1.33
23	BB	115	A	C6-N6	16.22	1.47	1.33
22	BA	988	A	C6-N6	16.22	1.47	1.33
22	BA	2531	A	C6-N6	16.22	1.47	1.33
22	BA	945	A	C6-N6	16.21	1.47	1.33
22	BA	478	A	C6-N6	16.21	1.47	1.33
22	BA	603	A	C6-N6	16.21	1.47	1.33
22	BA	1347	A	C6-N6	16.21	1.47	1.33
22	BA	1780	A	C6-N6	16.21	1.47	1.33
22	BA	497	A	C6-N6	16.21	1.47	1.33
22	BA	404	A	C6-N6	16.21	1.47	1.33
22	BA	1757	A	C6-N6	16.21	1.47	1.33
22	BA	2587	A	C6-N6	16.21	1.47	1.33
22	BA	1000	A	C6-N6	16.21	1.47	1.33
22	BA	1433	A	C6-N6	16.20	1.47	1.33
22	BA	196	A	C6-N6	16.20	1.47	1.33
22	BA	244	A	C6-N6	16.20	1.47	1.33
22	BA	412	A	C6-N6	16.20	1.47	1.33
22	BA	182	A	C6-N6	16.20	1.47	1.33
22	BA	384	A	C6-N6	16.20	1.47	1.33
22	BA	866	A	C6-N6	16.20	1.47	1.33
22	BA	1470	A	C6-N6	16.20	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2095	A	C6-N6	16.20	1.47	1.33
22	BA	1133	A	C6-N6	16.20	1.47	1.33
22	BA	2799	A	C6-N6	16.20	1.47	1.33
22	BA	819	A	C6-N6	16.19	1.47	1.33
22	BA	2336	A	C6-N6	16.19	1.47	1.33
22	BA	146	A	C6-N6	16.19	1.47	1.33
22	BA	447	A	C6-N6	16.19	1.47	1.33
22	BA	643	A	C6-N6	16.19	1.47	1.33
22	BA	675	A	C6-N6	16.19	1.47	1.33
22	BA	1384	A	C6-N6	16.19	1.47	1.33
22	BA	1597	A	C6-N6	16.19	1.47	1.33
22	BA	980	A	C6-N6	16.19	1.47	1.33
22	BA	1759	A	C6-N6	16.19	1.47	1.33
22	BA	2430	A	C6-N6	16.19	1.47	1.33
22	BA	219	A	C6-N6	16.19	1.46	1.33
22	BA	1165	A	C6-N6	16.19	1.46	1.33
23	BB	46	A	C6-N6	16.19	1.46	1.33
22	BA	927	A	C6-N6	16.18	1.46	1.33
22	BA	1672	A	C6-N6	16.18	1.46	1.33
22	BA	1253	A	C6-N6	16.18	1.46	1.33
22	BA	1746	A	C6-N6	16.18	1.46	1.33
22	BA	2051	A	C6-N6	16.18	1.46	1.33
22	BA	2077	A	C6-N6	16.18	1.46	1.33
22	BA	1525	A	C6-N6	16.18	1.46	1.33
22	BA	460	A	C6-N6	16.18	1.46	1.33
22	BA	1969	A	C6-N6	16.18	1.46	1.33
22	BA	789	A	C6-N6	16.17	1.46	1.33
22	BA	2518	A	C6-N6	16.17	1.46	1.33
22	BA	609	A	C6-N6	16.17	1.46	1.33
22	BA	2835	A	C6-N6	16.17	1.46	1.33
22	BA	979	A	C6-N6	16.17	1.46	1.33
22	BA	2829	A	C6-N6	16.17	1.46	1.33
22	BA	1981	A	C6-N6	16.17	1.46	1.33
22	BA	943	A	C6-N6	16.17	1.46	1.33
22	BA	936	A	C6-N6	16.16	1.46	1.33
22	BA	1635	A	C6-N6	16.16	1.46	1.33
22	BA	2534	A	C6-N6	16.16	1.46	1.33
22	BA	1641	A	C6-N6	16.16	1.46	1.33
22	BA	917	A	C6-N6	16.16	1.46	1.33
22	BA	1321	A	C6-N6	16.16	1.46	1.33
22	BA	2450	A	C6-N6	16.16	1.46	1.33
22	BA	126	A	C6-N6	16.16	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1274	A	C6-N6	16.16	1.46	1.33
22	BA	1494	A	C6-N6	16.16	1.46	1.33
22	BA	2317	A	C6-N6	16.16	1.46	1.33
22	BA	2706	A	C6-N6	16.16	1.46	1.33
22	BA	2899	A	C6-N6	16.16	1.46	1.33
22	BA	173	A	C6-N6	16.16	1.46	1.33
22	BA	1754	A	C6-N6	16.15	1.46	1.33
22	BA	2227	A	C6-N6	16.15	1.46	1.33
22	BA	127	A	C6-N6	16.15	1.46	1.33
22	BA	2851	A	C6-N6	16.15	1.46	1.33
22	BA	1664	A	C6-N6	16.15	1.46	1.33
22	BA	1717	A	C6-N6	16.15	1.46	1.33
22	BA	984	A	C6-N6	16.15	1.46	1.33
22	BA	1469	A	C6-N6	16.15	1.46	1.33
22	BA	751	A	C6-N6	16.15	1.46	1.33
22	BA	223	A	C6-N6	16.15	1.46	1.33
22	BA	2425	A	C6-N6	16.14	1.46	1.33
22	BA	1654	A	C6-N6	16.14	1.46	1.33
22	BA	471	A	C6-N6	16.14	1.46	1.33
22	BA	256	A	C6-N6	16.14	1.46	1.33
22	BA	699	A	C6-N6	16.14	1.46	1.33
22	BA	1010	A	C6-N6	16.14	1.46	1.33
22	BA	928	A	C6-N6	16.14	1.46	1.33
22	BA	1268	A	C6-N6	16.14	1.46	1.33
22	BA	1571	A	C6-N6	16.14	1.46	1.33
22	BA	1713	A	C6-N6	16.14	1.46	1.33
22	BA	2727	A	C6-N6	16.14	1.46	1.33
22	BA	2764	A	C6-N6	16.14	1.46	1.33
22	BA	781	A	C6-N6	16.14	1.46	1.33
22	BA	42	A	C6-N6	16.14	1.46	1.33
22	BA	160	A	C6-N6	16.14	1.46	1.33
22	BA	272	A	C6-N6	16.14	1.46	1.33
22	BA	556	A	C6-N6	16.14	1.46	1.33
22	BA	2019	A	C6-N6	16.13	1.46	1.33
22	BA	2352	A	C6-N6	16.13	1.46	1.33
22	BA	1970	A	C6-N6	16.13	1.46	1.33
23	BB	104	A	C6-N6	16.13	1.46	1.33
22	BA	181	A	C6-N6	16.13	1.46	1.33
22	BA	454	A	C6-N6	16.13	1.46	1.33
22	BA	1226	A	C6-N6	16.13	1.46	1.33
22	BA	1275	A	C6-N6	16.13	1.46	1.33
22	BA	149	A	C6-N6	16.12	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	492	A	C6-N6	16.12	1.46	1.33
22	BA	1808	A	C6-N6	16.12	1.46	1.33
22	BA	1020	A	C6-N6	16.12	1.46	1.33
22	BA	1403	A	C6-N6	16.12	1.46	1.33
22	BA	2003	A	C6-N6	16.12	1.46	1.33
22	BA	666	A	C6-N6	16.12	1.46	1.33
22	BA	131	A	C6-N6	16.12	1.46	1.33
22	BA	483	A	C6-N6	16.11	1.46	1.33
22	BA	2418	A	C6-N6	16.11	1.46	1.33
22	BA	2434	A	C6-N6	16.11	1.46	1.33
22	BA	2566	A	C6-N6	16.11	1.46	1.33
22	BA	2823	A	C6-N6	16.11	1.46	1.33
22	BA	1794	A	C6-N6	16.11	1.46	1.33
22	BA	1194	A	C6-N6	16.11	1.46	1.33
22	BA	2060	A	C6-N6	16.11	1.46	1.33
22	BA	470	A	C6-N6	16.11	1.46	1.33
22	BA	1427	A	C6-N6	16.10	1.46	1.33
22	BA	1821	A	C6-N6	16.10	1.46	1.33
22	BA	627	A	C6-N6	16.10	1.46	1.33
22	BA	2328	A	C6-N6	16.10	1.46	1.33
22	BA	2542	A	C6-N6	16.10	1.46	1.33
22	BA	825	A	C6-N6	16.10	1.46	1.33
22	BA	1579	A	C6-N6	16.10	1.46	1.33
22	BA	1785	A	C6-N6	16.10	1.46	1.33
22	BA	49	A	C6-N6	16.10	1.46	1.33
22	BA	1214	A	C6-N6	16.10	1.46	1.33
22	BA	1566	A	C6-N6	16.10	1.46	1.33
22	BA	2031	A	C6-N6	16.10	1.46	1.33
22	BA	2340	A	C6-N6	16.10	1.46	1.33
22	BA	300	A	C6-N6	16.10	1.46	1.33
22	BA	443	A	C6-N6	16.10	1.46	1.33
22	BA	513	A	C6-N6	16.10	1.46	1.33
22	BA	1143	A	C6-N6	16.10	1.46	1.33
22	BA	310	A	C6-N6	16.09	1.46	1.33
22	BA	783	A	C6-N6	16.09	1.46	1.33
22	BA	1762	A	C6-N6	16.09	1.46	1.33
22	BA	1987	A	C6-N6	16.09	1.46	1.33
54	D2	28	A	C6-N6	16.09	1.46	1.33
22	BA	217	A	C6-N6	16.09	1.46	1.33
22	BA	1630	A	C6-N6	16.09	1.46	1.33
22	BA	2411	A	C6-N6	16.09	1.46	1.33
22	BA	2058	A	C6-N6	16.09	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	161	A	C6-N6	16.09	1.46	1.33
22	BA	1285	A	C6-N6	16.09	1.46	1.33
22	BA	1786	A	C6-N6	16.09	1.46	1.33
22	BA	592	A	C6-N6	16.08	1.46	1.33
22	BA	941	A	C6-N6	16.08	1.46	1.33
22	BA	1342	A	C6-N6	16.08	1.46	1.33
22	BA	735	A	C6-N6	16.08	1.46	1.33
22	BA	1614	A	C6-N6	16.08	1.46	1.33
22	BA	1014	A	C6-N6	16.08	1.46	1.33
22	BA	1548	A	C6-N6	16.08	1.46	1.33
22	BA	1552	A	C6-N6	16.08	1.46	1.33
22	BA	2273	A	C6-N6	16.08	1.46	1.33
22	BA	574	A	C6-N6	16.07	1.46	1.33
22	BA	1260	A	C6-N6	16.07	1.46	1.33
22	BA	1366	A	C6-N6	16.07	1.46	1.33
22	BA	1749	A	C6-N6	16.07	1.46	1.33
22	BA	2560	A	C6-N6	16.07	1.46	1.33
22	BA	1854	A	C6-N6	16.07	1.46	1.33
22	BA	2274	A	C6-N6	16.07	1.46	1.33
22	BA	2448	A	C6-N6	16.07	1.46	1.33
22	BA	792	A	C6-N6	16.07	1.46	1.33
22	BA	1698	A	C6-N6	16.07	1.46	1.33
22	BA	1809	A	C6-N6	16.07	1.46	1.33
22	BA	1496	A	C6-N6	16.07	1.46	1.33
22	BA	1610	A	C6-N6	16.07	1.46	1.33
22	BA	2810	A	C6-N6	16.07	1.46	1.33
22	BA	422	A	C6-N6	16.06	1.46	1.33
22	BA	103	A	C6-N6	16.06	1.46	1.33
22	BA	1276	A	C6-N6	16.06	1.46	1.33
22	BA	1701	A	C6-N6	16.06	1.46	1.33
22	BA	2094	A	C6-N6	16.06	1.46	1.33
22	BA	1572	A	C6-N6	16.06	1.46	1.33
22	BA	1549	A	C6-N6	16.06	1.46	1.33
22	BA	1144	A	C6-N6	16.06	1.46	1.33
22	BA	1890	A	C6-N6	16.06	1.46	1.33
22	BA	255	A	C6-N6	16.05	1.46	1.33
22	BA	1772	A	C6-N6	16.05	1.46	1.33
22	BA	2670	A	C6-N6	16.05	1.46	1.33
22	BA	346	A	C6-N6	16.05	1.46	1.33
22	BA	529	A	C6-N6	16.05	1.46	1.33
22	BA	1265	A	C6-N6	16.05	1.46	1.33
22	BA	1953	A	C6-N6	16.05	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2778	A	C6-N6	16.05	1.46	1.33
23	BB	58	A	C6-N6	16.05	1.46	1.33
22	BA	972	A	C6-N6	16.05	1.46	1.33
22	BA	1127	A	C6-N6	16.04	1.46	1.33
22	BA	706	A	C6-N6	16.04	1.46	1.33
22	BA	2015	A	C6-N6	16.04	1.46	1.33
22	BA	1603	A	C6-N6	16.04	1.46	1.33
22	BA	432	A	C6-N6	16.04	1.46	1.33
22	BA	1677	A	C6-N6	16.04	1.46	1.33
22	BA	1439	A	C6-N6	16.03	1.46	1.33
22	BA	631	A	C6-N6	16.03	1.46	1.33
22	BA	1189	A	C6-N6	16.03	1.46	1.33
22	BA	1679	A	C6-N6	16.03	1.46	1.33
22	BA	2564	A	C6-N6	16.03	1.46	1.33
23	BB	99	A	C6-N6	16.03	1.46	1.33
22	BA	13	A	C6-N6	16.03	1.46	1.33
22	BA	1008	A	C6-N6	16.03	1.46	1.33
22	BA	1169	A	C6-N6	16.02	1.46	1.33
22	BA	1711	A	C6-N6	16.02	1.46	1.33
22	BA	528	A	C6-N6	16.02	1.46	1.33
22	BA	532	A	C6-N6	16.02	1.46	1.33
22	BA	2635	A	C6-N6	16.02	1.46	1.33
22	BA	371	A	C6-N6	16.02	1.46	1.33
22	BA	505	A	C6-N6	16.02	1.46	1.33
55	D3	26	A	C6-N6	16.02	1.46	1.33
22	BA	1998	A	C6-N6	16.02	1.46	1.33
22	BA	191	A	C6-N6	16.02	1.46	1.33
22	BA	1431	A	C6-N6	16.02	1.46	1.33
22	BA	1264	A	C6-N6	16.02	1.46	1.33
22	BA	1419	A	C6-N6	16.01	1.46	1.33
22	BA	668	A	C6-N6	16.01	1.46	1.33
22	BA	586	A	C6-N6	16.01	1.46	1.33
22	BA	1477	A	C6-N6	16.01	1.46	1.33
22	BA	820	A	C6-N6	16.00	1.46	1.33
22	BA	1286	A	C6-N6	16.00	1.46	1.33
22	BA	241	A	C6-N6	16.00	1.46	1.33
22	BA	226	A	C6-N6	16.00	1.46	1.33
22	BA	1784	A	C6-N6	16.00	1.46	1.33
22	BA	1853	A	C6-N6	16.00	1.46	1.33
22	BA	2711	A	C6-N6	16.00	1.46	1.33
22	BA	74	A	C6-N6	16.00	1.46	1.33
22	BA	1700	A	C6-N6	16.00	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2433	A	C6-N6	16.00	1.46	1.33
22	BA	2600	A	C6-N6	16.00	1.46	1.33
22	BA	2682	A	C6-N6	16.00	1.46	1.33
22	BA	925	A	C6-N6	16.00	1.46	1.33
22	BA	1668	A	C6-N6	16.00	1.46	1.33
22	BA	1889	A	C6-N6	16.00	1.46	1.33
22	BA	910	A	C6-N6	15.99	1.46	1.33
22	BA	1522	A	C6-N6	15.99	1.46	1.33
22	BA	2059	A	C6-N6	15.99	1.46	1.33
22	BA	1308	A	C6-N6	15.99	1.46	1.33
22	BA	423	A	C6-N6	15.99	1.46	1.33
22	BA	415	A	C6-N6	15.99	1.46	1.33
22	BA	1230	A	C6-N6	15.99	1.46	1.33
22	BA	1336	A	C6-N6	15.99	1.46	1.33
22	BA	1848	A	C6-N6	15.98	1.46	1.33
22	BA	1789	A	C6-N6	15.98	1.46	1.33
22	BA	144	A	C6-N6	15.98	1.46	1.33
22	BA	1129	A	C6-N6	15.98	1.46	1.33
22	BA	262	A	C6-N6	15.98	1.46	1.33
22	BA	1676	A	C6-N6	15.98	1.46	1.33
22	BA	1936	A	C6-N6	15.98	1.46	1.33
22	BA	2749	A	C6-N6	15.98	1.46	1.33
22	BA	1787	A	C6-N6	15.98	1.46	1.33
22	BA	1803	A	C6-N6	15.98	1.46	1.33
22	BA	981	A	C6-N6	15.98	1.46	1.33
22	BA	5	A	C6-N6	15.97	1.46	1.33
22	BA	233	A	C6-N6	15.97	1.46	1.33
22	BA	1669	A	C6-N6	15.97	1.46	1.33
22	BA	6	A	C6-N6	15.97	1.46	1.33
22	BA	753	A	C6-N6	15.97	1.46	1.33
22	BA	1247	A	C6-N6	15.96	1.46	1.33
22	BA	1354	A	C6-N6	15.96	1.46	1.33
22	BA	1244	A	C6-N6	15.96	1.46	1.33
22	BA	1365	A	C6-N6	15.96	1.46	1.33
22	BA	2071	A	C6-N6	15.96	1.46	1.33
22	BA	861	A	C6-N6	15.96	1.46	1.33
22	BA	1262	A	C6-N6	15.96	1.46	1.33
22	BA	10	A	C6-N6	15.95	1.46	1.33
22	BA	449	A	C6-N6	15.95	1.46	1.33
22	BA	2740	A	C6-N6	15.96	1.46	1.33
22	BA	1570	A	C6-N6	15.95	1.46	1.33
22	BA	2868	A	C6-N6	15.95	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	207	A	C6-N6	15.95	1.46	1.33
22	BA	2700	A	C6-N6	15.95	1.46	1.33
22	BA	2088	A	C6-N6	15.95	1.46	1.33
22	BA	2388	A	C6-N6	15.95	1.46	1.33
22	BA	2883	A	C6-N6	15.95	1.46	1.33
22	BA	661	A	C6-N6	15.95	1.46	1.33
22	BA	920	A	C6-N6	15.95	1.46	1.33
22	BA	1505	A	C6-N6	15.95	1.46	1.33
22	BA	1301	A	C6-N6	15.95	1.46	1.33
22	BA	2459	A	C6-N6	15.95	1.46	1.33
22	BA	670	A	C6-N6	15.94	1.46	1.33
22	BA	909	A	C6-N6	15.94	1.46	1.33
22	BA	844	A	C6-N6	15.94	1.46	1.33
22	BA	1515	A	C6-N6	15.94	1.46	1.33
22	BA	2009	A	C6-N6	15.94	1.46	1.33
22	BA	2589	A	C6-N6	15.94	1.46	1.33
22	BA	231	A	C6-N6	15.93	1.46	1.33
22	BA	466	A	C6-N6	15.93	1.46	1.33
22	BA	2426	A	C6-N6	15.93	1.46	1.33
22	BA	1032	A	C6-N6	15.93	1.46	1.33
22	BA	2725	A	C6-N6	15.93	1.46	1.33
22	BA	1088	A	C6-N6	15.93	1.46	1.33
22	BA	761	A	C6-N6	15.93	1.46	1.33
22	BA	1966	A	C6-N6	15.93	1.46	1.33
22	BA	52	A	C6-N6	15.92	1.46	1.33
22	BA	599	A	C6-N6	15.92	1.46	1.33
22	BA	2270	A	C6-N6	15.92	1.46	1.33
22	BA	911	A	C6-N6	15.92	1.46	1.33
22	BA	2451	A	C6-N6	15.92	1.46	1.33
22	BA	199	A	C6-N6	15.92	1.46	1.33
22	BA	563	A	C6-N6	15.92	1.46	1.33
22	BA	1213	A	C6-N6	15.92	1.46	1.33
22	BA	2386	A	C6-N6	15.92	1.46	1.33
22	BA	793	A	C6-N6	15.91	1.46	1.33
22	BA	804	A	C6-N6	15.91	1.46	1.33
22	BA	152	A	C6-N6	15.91	1.46	1.33
22	BA	197	A	C6-N6	15.91	1.46	1.33
22	BA	845	A	C6-N6	15.91	1.46	1.33
22	BA	2565	A	C6-N6	15.91	1.46	1.33
22	BA	2037	A	C6-N6	15.90	1.46	1.33
22	BA	2247	A	C6-N6	15.90	1.46	1.33
22	BA	402	A	C6-N6	15.90	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	216	A	C6-N6	15.89	1.46	1.33
22	BA	348	A	C6-N6	15.89	1.46	1.33
22	BA	590	A	C6-N6	15.89	1.46	1.33
22	BA	2241	A	C6-N6	15.89	1.46	1.33
22	BA	2278	A	C6-N6	15.89	1.46	1.33
22	BA	53	A	C6-N6	15.88	1.46	1.33
22	BA	918	A	C6-N6	15.89	1.46	1.33
22	BA	756	A	C6-N6	15.88	1.46	1.33
22	BA	190	A	C6-N6	15.88	1.46	1.33
22	BA	1650	A	C6-N6	15.88	1.46	1.33
22	BA	2358	A	C6-N6	15.88	1.46	1.33
22	BA	21	A	C6-N6	15.88	1.46	1.33
22	BA	730	A	C6-N6	15.87	1.46	1.33
22	BA	19	A	C6-N6	15.87	1.46	1.33
22	BA	472	A	C6-N6	15.87	1.46	1.33
23	BB	94	A	C6-N6	15.87	1.46	1.33
22	BA	1269	A	C6-N6	15.87	1.46	1.33
22	BA	1801	A	C6-N6	15.87	1.46	1.33
22	BA	2435	A	C6-N6	15.87	1.46	1.33
22	BA	1938	A	C6-N6	15.87	1.46	1.33
22	BA	2013	A	C6-N6	15.86	1.46	1.33
22	BA	2497	A	C6-N6	15.86	1.46	1.33
22	BA	947	A	C6-N6	15.86	1.46	1.33
22	BA	2281	A	C6-N6	15.85	1.46	1.33
22	BA	1359	A	C6-N6	15.85	1.46	1.33
22	BA	453	A	C6-N6	15.85	1.46	1.33
22	BA	515	A	C6-N6	15.85	1.46	1.33
22	BA	2346	A	C6-N6	15.85	1.46	1.33
22	BA	203	A	C6-N6	15.85	1.46	1.33
22	BA	382	A	C6-N6	15.85	1.46	1.33
22	BA	689	A	C6-N6	15.85	1.46	1.33
55	D3	76	A	C6-N6	15.85	1.46	1.33
22	BA	800	A	C6-N6	15.84	1.46	1.33
22	BA	1665	A	C6-N6	15.84	1.46	1.33
22	BA	1829	A	C6-N6	15.84	1.46	1.33
22	BA	1151	A	C6-N6	15.84	1.46	1.33
22	BA	195	A	C6-N6	15.84	1.46	1.33
22	BA	1126	A	C6-N6	15.84	1.46	1.33
22	BA	1805	A	C6-N6	15.84	1.46	1.33
22	BA	2634	A	C6-N6	15.83	1.46	1.33
22	BA	2516	A	C6-N6	15.83	1.46	1.33
22	BA	1960	A	C6-N6	15.83	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2327	A	C6-N6	15.83	1.46	1.33
23	BB	101	A	C6-N6	15.82	1.46	1.33
22	BA	788	A	C6-N6	15.82	1.46	1.33
22	BA	2266	A	C6-N6	15.82	1.46	1.33
22	BA	722	A	C6-N6	15.82	1.46	1.33
22	BA	1652	A	C6-N6	15.82	1.46	1.33
22	BA	2225	A	C6-N6	15.81	1.46	1.33
22	BA	56	A	C6-N6	15.81	1.46	1.33
22	BA	2471	A	C6-N6	15.81	1.46	1.33
22	BA	374	A	C6-N6	15.81	1.46	1.33
22	BA	2675	A	C6-N6	15.81	1.46	1.33
22	BA	632	A	C6-N6	15.81	1.46	1.33
22	BA	794	A	C6-N6	15.81	1.46	1.33
22	BA	2726	A	C6-N6	15.81	1.46	1.33
22	BA	2070	A	C6-N6	15.80	1.46	1.33
22	BA	2590	A	C6-N6	15.80	1.46	1.33
22	BA	1802	A	C6-N6	15.80	1.46	1.33
22	BA	2826	A	C6-N6	15.80	1.46	1.33
22	BA	1977	A	C6-N6	15.79	1.46	1.33
22	BA	2882	A	C6-N6	15.79	1.46	1.33
22	BA	176	A	C6-N6	15.79	1.46	1.33
22	BA	1932	A	C6-N6	15.79	1.46	1.33
22	BA	621	A	C6-N6	15.79	1.46	1.33
22	BA	2736	A	C6-N6	15.79	1.46	1.33
22	BA	2765	A	C6-N6	15.79	1.46	1.33
22	BA	572	A	C6-N6	15.79	1.46	1.33
22	BA	959	A	C6-N6	15.79	1.46	1.33
22	BA	118	A	C6-N6	15.78	1.46	1.33
22	BA	28	A	C6-N6	15.77	1.46	1.33
22	BA	676	A	C6-N6	15.77	1.46	1.33
22	BA	119	A	C6-N6	15.77	1.46	1.33
22	BA	2614	A	C6-N6	15.76	1.46	1.33
22	BA	2461	A	C6-N6	15.75	1.46	1.33
22	BA	1569	A	C6-N6	15.74	1.46	1.33
22	BA	38	A	C6-N6	15.74	1.46	1.33
22	BA	2268	A	C6-N6	15.74	1.46	1.33
22	BA	2090	A	C6-N6	15.74	1.46	1.33
22	BA	1392	A	C6-N6	15.73	1.46	1.33
22	BA	1689	A	C6-N6	15.73	1.46	1.33
22	BA	2369	A	C6-N6	15.73	1.46	1.33
22	BA	439	A	C6-N6	15.71	1.46	1.33
22	BA	1378	A	C6-N6	15.71	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1246	A	C6-N6	15.70	1.46	1.33
22	BA	2679	A	C6-N6	15.69	1.46	1.33
22	BA	2020	A	C6-N6	15.69	1.46	1.33
22	BA	2014	A	C6-N6	15.68	1.46	1.33
22	BA	1001	A	C6-N6	15.68	1.46	1.33
22	BA	677	A	C6-N6	15.68	1.46	1.33
22	BA	1387	A	C6-N6	15.67	1.46	1.33
22	BA	1899	A	C6-N6	15.67	1.46	1.33
22	BA	2333	A	C6-N6	15.67	1.46	1.33
22	BA	693	A	C6-N6	15.66	1.46	1.33
22	BA	1302	A	C6-N6	15.66	1.46	1.33
22	BA	1858	A	C6-N6	15.66	1.46	1.33
22	BA	1616	A	C6-N6	15.66	1.46	1.33
22	BA	2809	A	C6-N6	15.65	1.46	1.33
22	BA	685	A	C6-N6	15.65	1.46	1.33
22	BA	1705	A	C6-N6	15.65	1.46	1.33
22	BA	2639	A	C6-N6	15.65	1.46	1.33
22	BA	2062	A	C6-N6	15.63	1.46	1.33
22	BA	2407	A	C6-N6	15.60	1.46	1.33
22	BA	821	A	C6-N6	15.60	1.46	1.33
22	BA	1637	A	C6-N6	15.59	1.46	1.33
22	BA	1655	A	C6-N6	15.59	1.46	1.33
22	BA	2577	A	C6-N6	15.57	1.46	1.33
22	BA	1815	A	C6-N6	15.56	1.46	1.33
22	BA	863	A	C6-N6	15.56	1.46	1.33
22	BA	743	A	C6-N6	15.55	1.46	1.33
22	BA	1791	A	C6-N6	15.55	1.46	1.33
22	BA	727	A	C6-N6	15.52	1.46	1.33
22	BA	742	A	C6-N6	15.52	1.46	1.33
22	BA	2284	A	C6-N6	15.51	1.46	1.33
22	BA	2837	A	C6-N6	15.51	1.46	1.33
22	BA	204	A	C6-N6	15.50	1.46	1.33
22	BA	522	A	C6-N6	15.50	1.46	1.33
22	BA	705	A	C6-N6	15.49	1.46	1.33
22	BA	1254	A	C6-N6	15.48	1.46	1.33
22	BA	222	A	C6-N6	15.46	1.46	1.33
22	BA	457	A	C6-N6	15.46	1.46	1.33
22	BA	582	A	C6-N6	15.46	1.46	1.33
22	BA	973	A	C6-N6	15.46	1.46	1.33
22	BA	575	A	C6-N6	15.45	1.46	1.33
22	BA	764	A	C6-N6	15.44	1.46	1.33
23	BB	78	A	C6-N6	15.41	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	479	A	C6-N6	15.40	1.46	1.33
22	BA	2766	A	C6-N6	15.39	1.46	1.33
22	BA	1819	A	C6-N6	15.38	1.46	1.33
22	BA	2005	A	C6-N6	15.37	1.46	1.33
22	BA	2469	A	C6-N6	15.37	1.46	1.33
22	BA	1237	A	C6-N6	15.34	1.46	1.33
22	BA	324	A	C6-N6	15.29	1.46	1.33
22	BA	2054	A	C6-N6	15.21	1.46	1.33
22	BA	1142	A	C6-N6	15.20	1.46	1.33
22	BA	1021	A	C6-N6	15.16	1.46	1.33
22	BA	2267	A	C6-N6	15.12	1.46	1.33
22	BA	1028	A	C6-N6	15.11	1.46	1.33
22	BA	750	A	C6-N6	15.10	1.46	1.33
22	BA	2052	A	C6-N6	14.84	1.45	1.33
22	BA	514	A	C6-N6	14.82	1.45	1.33
55	D3	1	G	OP3-P	-10.60	1.48	1.61
22	BA	1070	A	C8-N7	7.88	1.37	1.31
22	BA	2119	A	C8-N7	7.81	1.37	1.31
22	BA	1668	A	C5-C4	-7.77	1.33	1.38
22	BA	2134	A	C8-N7	7.77	1.36	1.31
22	BA	354	A	C8-N7	7.72	1.36	1.31
22	BA	896	A	C8-N7	7.68	1.36	1.31
22	BA	1069	A	C8-N7	7.65	1.36	1.31
22	BA	1583	A	C8-N7	7.64	1.36	1.31
22	BA	1535	A	C8-N7	7.64	1.36	1.31
55	D3	21	A	C8-N7	7.64	1.36	1.31
22	BA	1046	A	C8-N7	7.61	1.36	1.31
54	D2	9	A	C8-N7	7.57	1.36	1.31
22	BA	2154	A	C8-N7	7.57	1.36	1.31
22	BA	1913	A	C8-N7	7.56	1.36	1.31
22	BA	2170	A	C8-N7	7.56	1.36	1.31
22	BA	84	A	C8-N7	7.56	1.36	1.31
22	BA	10	A	C8-N7	7.55	1.36	1.31
22	BA	2126	A	C8-N7	7.54	1.36	1.31
22	BA	1515	A	C8-N7	7.53	1.36	1.31
22	BA	1419	A	C8-N7	7.52	1.36	1.31
22	BA	2009	A	C5-C4	-7.51	1.33	1.38
22	BA	1088	A	N3-C4	7.51	1.39	1.34
22	BA	2758	A	C8-N7	7.51	1.36	1.31
22	BA	1504	A	C8-N7	7.50	1.36	1.31
22	BA	613	A	N3-C4	7.50	1.39	1.34
23	BB	119	A	C8-N7	7.49	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1871	A	C8-N7	7.48	1.36	1.31
22	BA	547	A	C8-N7	7.48	1.36	1.31
22	BA	2108	A	C8-N7	7.46	1.36	1.31
22	BA	2792	A	C8-N7	7.46	1.36	1.31
55	D3	23	A	C8-N7	7.46	1.36	1.31
22	BA	1111	A	C8-N7	7.45	1.36	1.31
55	D3	76	A	C8-N7	7.44	1.36	1.31
22	BA	2211	A	C8-N7	7.44	1.36	1.31
22	BA	899	A	C8-N7	7.43	1.36	1.31
54	D2	58	A	C8-N7	7.43	1.36	1.31
22	BA	195	A	C8-N7	7.42	1.36	1.31
22	BA	352	A	C8-N7	7.42	1.36	1.31
22	BA	1089	A	C8-N7	7.41	1.36	1.31
55	D3	7	A	C8-N7	7.41	1.36	1.31
22	BA	2176	A	C8-N7	7.40	1.36	1.31
22	BA	1175	A	C8-N7	7.39	1.36	1.31
22	BA	2052	A	C5-C4	-7.39	1.33	1.38
22	BA	1420	A	C8-N7	7.38	1.36	1.31
22	BA	322	A	C8-N7	7.37	1.36	1.31
22	BA	1090	A	C8-N7	7.36	1.36	1.31
54	D2	14	A	C8-N7	7.36	1.36	1.31
1	AA	978	A	N3-C4	-7.36	1.30	1.34
22	BA	2173	A	C8-N7	7.36	1.36	1.31
22	BA	1385	A	C8-N7	7.35	1.36	1.31
22	BA	2163	A	C8-N7	7.35	1.36	1.31
22	BA	1095	A	C8-N7	7.35	1.36	1.31
22	BA	1077	A	C8-N7	7.33	1.36	1.31
23	BB	115	A	C8-N7	7.33	1.36	1.31
22	BA	1453	A	C8-N7	7.33	1.36	1.31
54	D2	23	A	C8-N7	7.32	1.36	1.31
22	BA	125	A	C8-N7	7.32	1.36	1.31
22	BA	155	A	C8-N7	7.32	1.36	1.31
22	BA	2147	A	C8-N7	7.32	1.36	1.31
22	BA	181	A	C8-N7	7.31	1.36	1.31
54	D2	69	A	C8-N7	7.31	1.36	1.31
22	BA	504	A	C8-N7	7.30	1.36	1.31
22	BA	1080	A	C8-N7	7.29	1.36	1.31
22	BA	2142	A	C8-N7	7.29	1.36	1.31
22	BA	310	A	C8-N7	7.29	1.36	1.31
22	BA	1509	A	C8-N7	7.29	1.36	1.31
22	BA	1067	A	C8-N7	7.29	1.36	1.31
22	BA	2158	A	C8-N7	7.28	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	D3	26	A	C8-N7	7.28	1.36	1.31
22	BA	344	A	C8-N7	7.28	1.36	1.31
54	D2	38	A	C8-N7	7.28	1.36	1.31
55	D3	37	A	C8-N7	7.28	1.36	1.31
22	BA	1073	A	C8-N7	7.27	1.36	1.31
22	BA	2184	A	C8-N7	7.26	1.36	1.31
1	AA	1227	A	N9-C4	-7.25	1.33	1.37
22	BA	1503	A	C8-N7	7.25	1.36	1.31
23	BB	109	A	C8-N7	7.25	1.36	1.31
22	BA	2163	A	N3-C4	7.25	1.39	1.34
22	BA	1353	A	C8-N7	7.24	1.36	1.31
55	D3	58	A	C8-N7	7.24	1.36	1.31
22	BA	1247	A	C8-N7	7.23	1.36	1.31
22	BA	1347	A	C8-N7	7.22	1.36	1.31
22	BA	1040	A	C8-N7	7.21	1.36	1.31
22	BA	1597	A	C8-N7	7.21	1.36	1.31
22	BA	2314	A	C8-N7	7.21	1.36	1.31
22	BA	526	A	C8-N7	7.21	1.36	1.31
22	BA	603	A	C8-N7	7.20	1.36	1.31
22	BA	844	A	C8-N7	7.20	1.36	1.31
22	BA	1744	A	C8-N7	7.20	1.36	1.31
22	BA	83	A	C8-N7	7.20	1.36	1.31
22	BA	1205	A	C8-N7	7.20	1.36	1.31
22	BA	905	A	C8-N7	7.19	1.36	1.31
22	BA	1085	A	C8-N7	7.19	1.36	1.31
22	BA	2602	A	N3-C4	7.19	1.39	1.34
22	BA	1505	A	C8-N7	7.19	1.36	1.31
22	BA	1590	A	C8-N7	7.19	1.36	1.31
54	D2	59	A	C8-N7	7.19	1.36	1.31
55	D3	9	A	C8-N7	7.19	1.36	1.31
55	D3	73	A	C8-N7	7.19	1.36	1.31
22	BA	172	A	C8-N7	7.18	1.36	1.31
22	BA	347	A	C8-N7	7.18	1.36	1.31
22	BA	508	A	C8-N7	7.18	1.36	1.31
22	BA	111	A	C8-N7	7.18	1.36	1.31
54	D2	51	A	C8-N7	7.18	1.36	1.31
54	D2	73	A	C8-N7	7.18	1.36	1.31
22	BA	2761	A	C8-N7	7.18	1.36	1.31
55	D3	14	A	C8-N7	7.17	1.36	1.31
22	BA	2171	A	C8-N7	7.17	1.36	1.31
22	BA	161	A	C8-N7	7.16	1.36	1.31
22	BA	878	A	C8-N7	7.16	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D2	49	A	C8-N7	7.16	1.36	1.31
22	BA	2298	A	C8-N7	7.15	1.36	1.31
22	BA	2654	A	C8-N7	7.15	1.36	1.31
22	BA	529	A	C8-N7	7.15	1.36	1.31
55	D3	26	A	N3-C4	7.15	1.39	1.34
1	AA	1362	A	N9-C4	-7.14	1.33	1.37
22	BA	1532	A	C8-N7	7.14	1.36	1.31
22	BA	1096	A	C8-N7	7.14	1.36	1.31
22	BA	2736	A	C8-N7	7.14	1.36	1.31
22	BA	430	A	C8-N7	7.13	1.36	1.31
22	BA	1630	A	C5-C4	-7.13	1.33	1.38
22	BA	2311	A	C8-N7	7.13	1.36	1.31
22	BA	272	A	C8-N7	7.13	1.36	1.31
22	BA	900	A	C8-N7	7.13	1.36	1.31
22	BA	1039	A	C8-N7	7.13	1.36	1.31
22	BA	282	A	C8-N7	7.12	1.36	1.31
22	BA	1169	A	C8-N7	7.12	1.36	1.31
22	BA	1129	A	C8-N7	7.12	1.36	1.31
22	BA	1552	A	C8-N7	7.11	1.36	1.31
22	BA	1050	A	C8-N7	7.11	1.36	1.31
22	BA	2534	A	C8-N7	7.11	1.36	1.31
22	BA	1285	A	C8-N7	7.11	1.36	1.31
22	BA	1508	A	C8-N7	7.11	1.36	1.31
22	BA	2309	A	C8-N7	7.10	1.36	1.31
22	BA	213	A	C8-N7	7.10	1.36	1.31
22	BA	2406	A	C8-N7	7.10	1.36	1.31
22	BA	2882	A	C8-N7	7.10	1.36	1.31
22	BA	119	A	C8-N7	7.10	1.36	1.31
54	D2	21	A	C8-N7	7.10	1.36	1.31
23	BB	29	A	C8-N7	7.10	1.36	1.31
22	BA	1321	A	C8-N7	7.09	1.36	1.31
22	BA	1745	A	C8-N7	7.09	1.36	1.31
22	BA	2169	A	C8-N7	7.09	1.36	1.31
22	BA	1652	A	C5-C4	-7.08	1.33	1.38
22	BA	1749	A	C8-N7	7.08	1.36	1.31
22	BA	348	A	C8-N7	7.08	1.36	1.31
22	BA	877	A	C8-N7	7.08	1.36	1.31
22	BA	2297	A	C8-N7	7.08	1.36	1.31
22	BA	2660	A	C8-N7	7.08	1.36	1.31
22	BA	2602	A	C8-N7	7.07	1.36	1.31
22	BA	1383	A	C8-N7	7.07	1.36	1.31
22	BA	2435	A	C5-C4	-7.07	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	483	A	C8-N7	7.07	1.36	1.31
22	BA	265	A	C8-N7	7.07	1.36	1.31
22	BA	761	A	C8-N7	7.06	1.36	1.31
22	BA	1877	A	C8-N7	7.06	1.36	1.31
23	BB	108	A	C8-N7	7.06	1.36	1.31
22	BA	1103	A	C8-N7	7.06	1.36	1.31
22	BA	2369	A	C5-C4	-7.06	1.33	1.38
22	BA	382	A	C8-N7	7.06	1.36	1.31
22	BA	362	A	C8-N7	7.06	1.36	1.31
23	BB	45	A	C8-N7	7.06	1.36	1.31
22	BA	1808	A	C8-N7	7.05	1.36	1.31
22	BA	637	A	C8-N7	7.05	1.36	1.31
22	BA	2566	A	C8-N7	7.05	1.36	1.31
22	BA	528	A	C8-N7	7.05	1.36	1.31
22	BA	1395	A	C8-N7	7.05	1.36	1.31
22	BA	1502	A	C8-N7	7.04	1.36	1.31
22	BA	71	A	C8-N7	7.04	1.36	1.31
22	BA	514	A	C5-C4	-7.04	1.33	1.38
22	BA	2173	A	N3-C4	7.04	1.39	1.34
22	BA	2191	A	C8-N7	7.04	1.36	1.31
23	BB	58	A	C8-N7	7.04	1.36	1.31
22	BA	2288	A	C8-N7	7.04	1.36	1.31
22	BA	1916	A	C8-N7	7.03	1.36	1.31
22	BA	2117	A	C8-N7	7.03	1.36	1.31
22	BA	479	A	C8-N7	7.03	1.36	1.31
55	D3	64	A	C8-N7	7.03	1.36	1.31
22	BA	749	A	C8-N7	7.03	1.36	1.31
22	BA	1579	A	C8-N7	7.03	1.36	1.31
22	BA	1937	A	C8-N7	7.02	1.36	1.31
22	BA	2033	A	C8-N7	7.02	1.36	1.31
22	BA	320	A	C8-N7	7.02	1.36	1.31
22	BA	2101	A	C8-N7	7.02	1.36	1.31
22	BA	1057	A	C8-N7	7.02	1.36	1.31
22	BA	1580	A	C8-N7	7.01	1.36	1.31
22	BA	89	A	C8-N7	7.01	1.36	1.31
22	BA	2095	A	C8-N7	7.01	1.36	1.31
22	BA	479	A	C5-C4	-7.01	1.33	1.38
22	BA	2090	A	C5-C4	-7.01	1.33	1.38
22	BA	979	A	C8-N7	7.01	1.36	1.31
22	BA	1378	A	C8-N7	7.01	1.36	1.31
22	BA	126	A	C8-N7	7.00	1.36	1.31
22	BA	2114	A	C8-N7	7.00	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	756	A	C5-C4	-7.00	1.33	1.38
22	BA	1785	A	C8-N7	7.00	1.36	1.31
22	BA	1805	A	C8-N7	7.00	1.36	1.31
22	BA	2114	A	N3-C4	7.00	1.39	1.34
22	BA	689	A	C5-C4	-7.00	1.33	1.38
22	BA	1086	A	C8-N7	7.00	1.36	1.31
22	BA	345	A	C8-N7	7.00	1.36	1.31
22	BA	1000	A	C5-C4	-6.99	1.33	1.38
22	BA	2900	A	C8-N7	6.99	1.36	1.31
22	BA	2471	A	C8-N7	6.99	1.36	1.31
23	BB	53	A	C8-N7	6.98	1.36	1.31
22	BA	743	A	C5-C4	-6.98	1.33	1.38
22	BA	2054	A	C5-C4	-6.98	1.33	1.38
22	BA	165	A	C8-N7	6.97	1.36	1.31
22	BA	655	A	C8-N7	6.97	1.36	1.31
22	BA	1088	A	C8-N7	6.96	1.36	1.31
22	BA	1098	A	C8-N7	6.96	1.36	1.31
22	BA	1392	A	C8-N7	6.96	1.36	1.31
22	BA	2800	A	C8-N7	6.96	1.36	1.31
22	BA	1490	A	N3-C4	6.96	1.39	1.34
22	BA	2764	A	C8-N7	6.95	1.36	1.31
22	BA	402	A	C8-N7	6.95	1.36	1.31
22	BA	1596	A	C8-N7	6.95	1.36	1.31
22	BA	1885	A	C8-N7	6.94	1.36	1.31
22	BA	2317	A	C8-N7	6.94	1.36	1.31
23	BB	39	A	C8-N7	6.94	1.36	1.31
23	BB	59	A	C8-N7	6.94	1.36	1.31
22	BA	342	A	C8-N7	6.94	1.36	1.31
22	BA	2014	A	C5-C4	-6.94	1.33	1.38
22	BA	833	A	C5-C4	-6.93	1.33	1.38
22	BA	718	A	C8-N7	6.93	1.36	1.31
22	BA	2097	A	C8-N7	6.93	1.36	1.31
55	D3	38	A	C8-N7	6.93	1.36	1.31
22	BA	332	A	C8-N7	6.93	1.36	1.31
22	BA	199	A	C8-N7	6.92	1.36	1.31
22	BA	1204	A	C8-N7	6.92	1.36	1.31
22	BA	1434	A	C8-N7	6.92	1.36	1.31
22	BA	654	A	C8-N7	6.92	1.36	1.31
22	BA	2542	A	C8-N7	6.92	1.36	1.31
55	D3	31	A	N3-C4	6.92	1.39	1.34
22	BA	2020	A	C5-C4	-6.91	1.33	1.38
22	BA	1403	A	C8-N7	6.91	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2670	A	C8-N7	6.91	1.36	1.31
23	BB	15	A	C8-N7	6.91	1.36	1.31
22	BA	1098	A	N3-C4	6.90	1.39	1.34
22	BA	2328	A	C8-N7	6.90	1.36	1.31
22	BA	764	A	C8-N7	6.90	1.36	1.31
23	BB	34	A	C8-N7	6.89	1.36	1.31
22	BA	1746	A	C8-N7	6.89	1.36	1.31
22	BA	2060	A	C5-C4	-6.89	1.33	1.38
54	D2	5	A	C8-N7	6.89	1.36	1.31
22	BA	616	A	C8-N7	6.89	1.36	1.31
22	BA	1014	A	C8-N7	6.89	1.36	1.31
22	BA	1912	A	C8-N7	6.89	1.36	1.31
22	BA	146	A	C8-N7	6.89	1.36	1.31
22	BA	270	A	C8-N7	6.88	1.36	1.31
22	BA	2381	A	C8-N7	6.88	1.36	1.31
22	BA	311	A	C8-N7	6.88	1.36	1.31
22	BA	1302	A	C8-N7	6.88	1.36	1.31
22	BA	63	A	C8-N7	6.87	1.36	1.31
22	BA	1586	A	C8-N7	6.87	1.36	1.31
22	BA	13	A	C8-N7	6.87	1.36	1.31
22	BA	627	A	C8-N7	6.87	1.36	1.31
22	BA	2478	A	C8-N7	6.87	1.36	1.31
22	BA	933	A	C8-N7	6.87	1.36	1.31
22	BA	346	A	C8-N7	6.87	1.36	1.31
22	BA	972	A	C5-C4	-6.86	1.33	1.38
22	BA	644	A	C8-N7	6.86	1.36	1.31
54	D2	76	A	C8-N7	6.86	1.36	1.31
22	BA	1095	A	N3-C4	6.86	1.39	1.34
22	BA	1783	A	C5-C4	-6.86	1.33	1.38
55	D3	36	A	C8-N7	6.86	1.36	1.31
55	D3	73	A	N3-C4	6.86	1.39	1.34
22	BA	1525	A	C8-N7	6.85	1.36	1.31
22	BA	2005	A	C8-N7	6.85	1.36	1.31
55	D3	64	A	N3-C4	6.85	1.39	1.34
22	BA	1247	A	C5-C4	-6.85	1.33	1.38
22	BA	2560	A	C8-N7	6.85	1.36	1.31
54	D2	41	A	C8-N7	6.85	1.36	1.31
22	BA	1230	A	C8-N7	6.85	1.36	1.31
22	BA	1264	A	C5-C4	-6.84	1.33	1.38
22	BA	404	A	C8-N7	6.84	1.36	1.31
22	BA	626	A	C8-N7	6.84	1.36	1.31
22	BA	2734	A	C8-N7	6.84	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1253	A	C8-N7	6.84	1.36	1.31
22	BA	2705	A	C8-N7	6.84	1.36	1.31
22	BA	142	A	C8-N7	6.83	1.36	1.31
22	BA	614	A	C8-N7	6.83	1.36	1.31
22	BA	1616	A	C8-N7	6.83	1.36	1.31
22	BA	1640	A	C8-N7	6.83	1.36	1.31
22	BA	1966	A	C8-N7	6.83	1.36	1.31
22	BA	241	A	C8-N7	6.83	1.36	1.31
22	BA	160	A	C8-N7	6.83	1.36	1.31
22	BA	2134	A	N3-C4	6.83	1.39	1.34
22	BA	2750	A	C8-N7	6.83	1.36	1.31
22	BA	1858	A	C8-N7	6.83	1.36	1.31
22	BA	715	A	C8-N7	6.82	1.36	1.31
22	BA	1701	A	C8-N7	6.82	1.36	1.31
22	BA	1819	A	C5-C4	-6.82	1.33	1.38
23	BB	78	A	C5-C4	-6.82	1.33	1.38
22	BA	2799	A	N3-C4	6.82	1.39	1.34
22	BA	1367	A	C8-N7	6.82	1.36	1.31
22	BA	1545	A	C8-N7	6.82	1.36	1.31
22	BA	1609	A	C8-N7	6.82	1.36	1.31
22	BA	621	A	C8-N7	6.82	1.36	1.31
22	BA	1413	A	C8-N7	6.82	1.36	1.31
22	BA	1711	A	C8-N7	6.82	1.36	1.31
22	BA	103	A	C8-N7	6.82	1.36	1.31
22	BA	1655	A	C5-C4	-6.81	1.33	1.38
22	BA	371	A	C8-N7	6.81	1.36	1.31
22	BA	892	A	N3-C4	6.81	1.39	1.34
22	BA	1496	A	C8-N7	6.81	1.36	1.31
22	BA	526	A	C5-C4	-6.81	1.33	1.38
22	BA	613	A	C8-N7	6.81	1.36	1.31
22	BA	2448	A	C8-N7	6.81	1.36	1.31
22	BA	1147	A	C8-N7	6.81	1.36	1.31
22	BA	1359	A	C8-N7	6.81	1.36	1.31
22	BA	1630	A	C8-N7	6.81	1.36	1.31
22	BA	1876	A	C8-N7	6.80	1.36	1.31
22	BA	2386	A	C5-C4	-6.80	1.33	1.38
22	BA	2632	A	C8-N7	6.80	1.36	1.31
22	BA	1918	A	C8-N7	6.80	1.36	1.31
22	BA	2829	A	C8-N7	6.80	1.36	1.31
22	BA	1165	A	C5-C4	-6.80	1.33	1.38
22	BA	1268	A	C5-C4	-6.80	1.33	1.38
22	BA	1342	A	C8-N7	6.80	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2547	A	C8-N7	6.80	1.36	1.31
22	BA	538	A	C8-N7	6.79	1.36	1.31
22	BA	1032	A	C8-N7	6.79	1.36	1.31
22	BA	1551	A	C8-N7	6.79	1.36	1.31
22	BA	821	A	C5-C4	-6.79	1.33	1.38
22	BA	1591	A	C8-N7	6.79	1.36	1.31
22	BA	294	A	C8-N7	6.79	1.36	1.31
22	BA	1155	A	C8-N7	6.79	1.36	1.31
22	BA	2657	A	C8-N7	6.79	1.36	1.31
23	BB	50	A	C8-N7	6.79	1.36	1.31
22	BA	1151	A	C8-N7	6.79	1.36	1.31
22	BA	1214	A	C8-N7	6.79	1.36	1.31
22	BA	2062	A	C8-N7	6.79	1.36	1.31
54	D2	26	A	C8-N7	6.79	1.36	1.31
22	BA	1008	A	C8-N7	6.78	1.36	1.31
22	BA	1755	A	C8-N7	6.78	1.36	1.31
22	BA	104	A	C8-N7	6.78	1.36	1.31
22	BA	632	A	C8-N7	6.78	1.36	1.31
22	BA	1304	A	C8-N7	6.77	1.36	1.31
22	BA	742	A	C5-C4	-6.77	1.34	1.38
22	BA	1286	A	C8-N7	6.77	1.36	1.31
22	BA	1495	A	C8-N7	6.77	1.36	1.31
22	BA	2776	A	C8-N7	6.77	1.36	1.31
22	BA	2198	A	C8-N7	6.77	1.36	1.31
22	BA	2809	A	C8-N7	6.77	1.36	1.31
22	BA	845	A	C8-N7	6.76	1.36	1.31
22	BA	928	A	C8-N7	6.76	1.36	1.31
22	BA	1439	A	C8-N7	6.76	1.36	1.31
22	BA	1494	A	C8-N7	6.75	1.36	1.31
22	BA	1522	A	C8-N7	6.75	1.36	1.31
22	BA	1544	A	C8-N7	6.75	1.36	1.31
22	BA	2070	A	C8-N7	6.75	1.36	1.31
22	BA	2469	A	C8-N7	6.75	1.36	1.31
22	BA	278	A	C8-N7	6.75	1.36	1.31
22	BA	439	A	C8-N7	6.74	1.36	1.31
22	BA	2205	A	C8-N7	6.74	1.36	1.31
22	BA	1593	A	C8-N7	6.74	1.36	1.31
22	BA	1253	A	C5-C4	-6.74	1.34	1.38
22	BA	1722	A	C8-N7	6.74	1.36	1.31
22	BA	167	A	C8-N7	6.74	1.36	1.31
22	BA	892	A	C8-N7	6.74	1.36	1.31
22	BA	2887	A	C8-N7	6.74	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1772	A	C5-C4	-6.73	1.34	1.38
22	BA	64	A	C8-N7	6.73	1.36	1.31
22	BA	1194	A	C8-N7	6.73	1.36	1.31
22	BA	227	A	C8-N7	6.73	1.36	1.31
22	BA	1001	A	C5-C4	-6.73	1.34	1.38
22	BA	1275	A	C5-C4	-6.73	1.34	1.38
22	BA	1735	A	C8-N7	6.73	1.36	1.31
22	BA	1393	A	C8-N7	6.73	1.36	1.31
22	BA	2665	A	C8-N7	6.73	1.36	1.31
22	BA	1901	A	C8-N7	6.72	1.36	1.31
22	BA	38	A	C8-N7	6.72	1.36	1.31
22	BA	340	A	C8-N7	6.72	1.36	1.31
22	BA	504	A	N3-C4	6.72	1.38	1.34
22	BA	1490	A	C8-N7	6.72	1.36	1.31
22	BA	1853	A	C5-C4	-6.72	1.34	1.38
22	BA	222	A	C8-N7	6.72	1.36	1.31
22	BA	2003	A	C8-N7	6.72	1.36	1.31
22	BA	502	A	C8-N7	6.72	1.36	1.31
22	BA	800	A	C5-C4	-6.72	1.34	1.38
22	BA	1244	A	C8-N7	6.72	1.36	1.31
22	BA	2241	A	C8-N7	6.71	1.36	1.31
22	BA	670	A	C8-N7	6.71	1.36	1.31
22	BA	1084	A	C8-N7	6.71	1.36	1.31
22	BA	1226	A	C5-C4	-6.71	1.34	1.38
22	BA	2340	A	C8-N7	6.71	1.36	1.31
22	BA	2635	A	C8-N7	6.71	1.36	1.31
22	BA	1054	A	N3-C4	6.71	1.38	1.34
22	BA	1938	A	C8-N7	6.71	1.36	1.31
22	BA	2015	A	C5-C4	-6.71	1.34	1.38
22	BA	927	A	C8-N7	6.70	1.36	1.31
22	BA	368	A	C8-N7	6.70	1.36	1.31
22	BA	1385	A	C5-C4	-6.70	1.34	1.38
22	BA	2721	A	C5-C4	-6.70	1.34	1.38
22	BA	1147	A	C5-C4	-6.70	1.34	1.38
22	BA	2733	A	C8-N7	6.70	1.36	1.31
22	BA	734	A	C8-N7	6.69	1.36	1.31
22	BA	1805	A	C5-C4	-6.69	1.34	1.38
22	BA	412	A	C8-N7	6.69	1.36	1.31
22	BA	574	A	C8-N7	6.69	1.36	1.31
22	BA	2749	A	C8-N7	6.69	1.36	1.31
22	BA	1801	A	C8-N7	6.68	1.36	1.31
22	BA	2835	A	C8-N7	6.68	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2135	A	C8-N7	6.68	1.36	1.31
22	BA	1981	A	C8-N7	6.68	1.36	1.31
22	BA	5	A	C8-N7	6.68	1.36	1.31
22	BA	149	A	C8-N7	6.67	1.36	1.31
22	BA	1469	A	C8-N7	6.67	1.36	1.31
22	BA	219	A	C8-N7	6.67	1.36	1.31
22	BA	861	A	C5-C4	-6.67	1.34	1.38
22	BA	941	A	C8-N7	6.67	1.36	1.31
22	BA	1632	A	C8-N7	6.67	1.36	1.31
22	BA	2738	A	C8-N7	6.67	1.36	1.31
22	BA	2267	A	C5-C4	-6.67	1.34	1.38
22	BA	1241	A	C8-N7	6.67	1.36	1.31
22	BA	300	A	C8-N7	6.66	1.36	1.31
22	BA	643	A	C8-N7	6.66	1.36	1.31
22	BA	761	A	C5-C4	-6.66	1.34	1.38
22	BA	2565	A	C5-C4	-6.66	1.34	1.38
22	BA	503	A	C8-N7	6.66	1.36	1.31
22	BA	2058	A	C8-N7	6.66	1.36	1.31
22	BA	182	A	C8-N7	6.66	1.36	1.31
22	BA	2358	A	C5-C4	-6.66	1.34	1.38
22	BA	556	A	C8-N7	6.66	1.36	1.31
22	BA	756	A	C8-N7	6.66	1.36	1.31
22	BA	631	A	C5-C4	-6.66	1.34	1.38
22	BA	2033	A	C5-C4	-6.66	1.34	1.38
22	BA	2476	A	C8-N7	6.66	1.36	1.31
54	D2	28	A	C8-N7	6.66	1.36	1.31
22	BA	432	A	C8-N7	6.65	1.36	1.31
22	BA	91	A	C8-N7	6.65	1.36	1.31
22	BA	2147	A	N3-C4	6.65	1.38	1.34
22	BA	2837	A	C8-N7	6.65	1.36	1.31
22	BA	95	A	C8-N7	6.65	1.36	1.31
22	BA	127	A	C5-C4	-6.65	1.34	1.38
22	BA	449	A	C5-C4	-6.65	1.34	1.38
22	BA	1847	A	C8-N7	6.65	1.36	1.31
22	BA	466	A	C5-C4	-6.65	1.34	1.38
22	BA	1322	A	C8-N7	6.65	1.36	1.31
22	BA	2212	A	C8-N7	6.65	1.36	1.31
22	BA	2426	A	C8-N7	6.65	1.36	1.31
22	BA	1960	A	C5-C4	-6.65	1.34	1.38
22	BA	42	A	C8-N7	6.64	1.36	1.31
22	BA	217	A	C8-N7	6.64	1.36	1.31
22	BA	721	A	C8-N7	6.64	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1366	A	C8-N7	6.64	1.36	1.31
22	BA	1598	A	C8-N7	6.64	1.36	1.31
22	BA	2378	A	C8-N7	6.64	1.36	1.31
22	BA	2764	A	C5-C4	-6.64	1.34	1.38
22	BA	706	A	C8-N7	6.64	1.36	1.31
22	BA	1784	A	C5-C4	-6.64	1.34	1.38
22	BA	454	A	C8-N7	6.64	1.36	1.31
22	BA	2753	A	C8-N7	6.64	1.36	1.31
22	BA	1566	A	C5-C4	-6.64	1.34	1.38
22	BA	44	A	C8-N7	6.63	1.36	1.31
22	BA	602	A	C8-N7	6.63	1.36	1.31
22	BA	1077	A	N3-C4	6.63	1.38	1.34
22	BA	1932	A	C8-N7	6.63	1.36	1.31
22	BA	131	A	C8-N7	6.63	1.36	1.31
22	BA	457	A	C5-C4	-6.63	1.34	1.38
22	BA	457	A	C8-N7	6.63	1.36	1.31
22	BA	1246	A	C8-N7	6.63	1.36	1.31
22	BA	1262	A	C5-C4	-6.63	1.34	1.38
22	BA	1960	A	C8-N7	6.63	1.36	1.31
22	BA	2893	A	C8-N7	6.63	1.36	1.31
55	D3	31	A	C8-N7	6.63	1.36	1.31
22	BA	362	A	N3-C4	6.63	1.38	1.34
22	BA	2411	A	C8-N7	6.63	1.36	1.31
22	BA	119	A	C5-C4	-6.62	1.34	1.38
22	BA	1566	A	C8-N7	6.62	1.36	1.31
22	BA	279	A	C8-N7	6.62	1.36	1.31
22	BA	794	A	C5-C4	-6.62	1.34	1.38
22	BA	2820	A	C8-N7	6.62	1.36	1.31
22	BA	2873	A	C8-N7	6.62	1.36	1.31
22	BA	1717	A	C8-N7	6.62	1.36	1.31
22	BA	2531	A	C8-N7	6.62	1.36	1.31
22	BA	739	A	C8-N7	6.62	1.36	1.31
22	BA	1165	A	C8-N7	6.62	1.36	1.31
22	BA	1780	A	C8-N7	6.62	1.36	1.31
22	BA	2564	A	C8-N7	6.62	1.36	1.31
22	BA	2266	A	C5-C4	-6.62	1.34	1.38
22	BA	309	A	C5-C4	-6.62	1.34	1.38
22	BA	661	A	C5-C4	-6.62	1.34	1.38
22	BA	668	A	C5-C4	-6.62	1.34	1.38
22	BA	2369	A	C8-N7	6.62	1.36	1.31
22	BA	752	A	C8-N7	6.61	1.36	1.31
22	BA	144	A	C8-N7	6.61	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	223	A	C8-N7	6.61	1.36	1.31
22	BA	988	A	C8-N7	6.61	1.36	1.31
22	BA	2560	A	C5-C4	-6.61	1.34	1.38
22	BA	925	A	C8-N7	6.60	1.36	1.31
22	BA	2530	A	C8-N7	6.60	1.36	1.31
22	BA	936	A	C8-N7	6.60	1.36	1.31
22	BA	2377	A	C8-N7	6.60	1.36	1.31
22	BA	2418	A	C5-C4	-6.60	1.34	1.38
22	BA	94	A	C8-N7	6.60	1.36	1.31
22	BA	2388	A	C5-C4	-6.59	1.34	1.38
22	BA	262	A	C8-N7	6.59	1.36	1.31
22	BA	472	A	C8-N7	6.58	1.36	1.31
22	BA	1336	A	C8-N7	6.58	1.36	1.31
22	BA	1477	A	C8-N7	6.58	1.36	1.31
22	BA	829	A	C8-N7	6.58	1.36	1.31
22	BA	1067	A	N3-C4	6.58	1.38	1.34
22	BA	2225	A	C8-N7	6.58	1.36	1.31
22	BA	2060	A	C8-N7	6.58	1.36	1.31
22	BA	2270	A	C8-N7	6.58	1.36	1.31
22	BA	2814	A	C8-N7	6.58	1.36	1.31
22	BA	176	A	C8-N7	6.58	1.36	1.31
22	BA	2482	A	C8-N7	6.58	1.36	1.31
22	BA	2883	A	C5-C4	-6.58	1.34	1.38
22	BA	204	A	C8-N7	6.57	1.36	1.31
22	BA	241	A	C5-C4	-6.57	1.34	1.38
22	BA	453	A	C8-N7	6.57	1.36	1.31
22	BA	482	A	C8-N7	6.57	1.36	1.31
23	BB	46	A	C8-N7	6.57	1.36	1.31
22	BA	256	A	C8-N7	6.57	1.36	1.31
22	BA	899	A	N3-C4	6.57	1.38	1.34
22	BA	833	A	C8-N7	6.57	1.36	1.31
22	BA	2542	A	C5-C4	-6.57	1.34	1.38
22	BA	2741	A	C5-C4	-6.57	1.34	1.38
22	BA	792	A	C8-N7	6.57	1.36	1.31
22	BA	863	A	C5-C4	-6.57	1.34	1.38
22	BA	2516	A	C5-C4	-6.57	1.34	1.38
22	BA	233	A	C8-N7	6.56	1.36	1.31
22	BA	1569	A	C5-C4	-6.56	1.34	1.38
22	BA	1927	A	C8-N7	6.56	1.36	1.31
22	BA	2813	A	C8-N7	6.56	1.36	1.31
22	BA	764	A	C5-C4	-6.56	1.34	1.38
22	BA	1634	A	C8-N7	6.56	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1672	A	C8-N7	6.56	1.36	1.31
22	BA	2346	A	C8-N7	6.56	1.36	1.31
22	BA	2572	A	C5-C4	-6.56	1.34	1.38
22	BA	84	A	C5-C4	-6.56	1.34	1.38
22	BA	152	A	C8-N7	6.56	1.36	1.31
22	BA	599	A	C8-N7	6.56	1.36	1.31
22	BA	1020	A	C8-N7	6.56	1.36	1.31
22	BA	449	A	C8-N7	6.55	1.36	1.31
22	BA	750	A	C5-C4	-6.55	1.34	1.38
22	BA	792	A	C5-C4	-6.55	1.34	1.38
22	BA	1652	A	C8-N7	6.55	1.36	1.31
22	BA	2126	A	N3-C4	6.55	1.38	1.34
22	BA	2227	A	C8-N7	6.55	1.36	1.31
22	BA	2634	A	C8-N7	6.55	1.36	1.31
22	BA	204	A	C5-C4	-6.55	1.34	1.38
22	BA	788	A	C8-N7	6.55	1.36	1.31
22	BA	1133	A	C8-N7	6.55	1.36	1.31
22	BA	222	A	C5-C4	-6.55	1.34	1.38
22	BA	1821	A	C8-N7	6.55	1.36	1.31
22	BA	2810	A	C8-N7	6.55	1.36	1.31
22	BA	2327	A	C8-N7	6.54	1.36	1.31
22	BA	454	A	C5-C4	-6.54	1.34	1.38
22	BA	804	A	C5-C4	-6.54	1.34	1.38
22	BA	2278	A	C8-N7	6.54	1.36	1.31
22	BA	2748	A	C8-N7	6.54	1.36	1.31
22	BA	19	A	C5-C4	-6.54	1.34	1.38
22	BA	207	A	C8-N7	6.54	1.36	1.31
22	BA	2598	A	C5-C4	-6.54	1.34	1.38
22	BA	2899	A	C8-N7	6.54	1.36	1.31
22	BA	541	A	C8-N7	6.54	1.36	1.31
22	BA	1650	A	C5-C4	-6.54	1.34	1.38
22	BA	2725	A	C5-C4	-6.54	1.34	1.38
22	BA	73	A	C8-N7	6.54	1.36	1.31
22	BA	1274	A	C5-C4	-6.54	1.34	1.38
22	BA	1853	A	C8-N7	6.54	1.36	1.31
22	BA	216	A	C8-N7	6.53	1.36	1.31
22	BA	401	A	C8-N7	6.53	1.36	1.31
22	BA	1791	A	C5-C4	-6.53	1.34	1.38
22	BA	2281	A	C8-N7	6.53	1.36	1.31
22	BA	2639	A	C8-N7	6.53	1.36	1.31
22	BA	2837	A	C5-C4	-6.53	1.34	1.38
22	BA	2199	A	C8-N7	6.53	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	661	A	C8-N7	6.53	1.36	1.31
22	BA	716	A	C8-N7	6.53	1.36	1.31
22	BA	1762	A	C8-N7	6.53	1.36	1.31
22	BA	1634	A	C5-C4	-6.53	1.34	1.38
22	BA	2376	A	C8-N7	6.53	1.36	1.31
23	BB	78	A	C8-N7	6.53	1.36	1.31
22	BA	2868	A	C8-N7	6.53	1.36	1.31
22	BA	2882	A	C5-C4	-6.53	1.34	1.38
22	BA	866	A	C8-N7	6.52	1.36	1.31
22	BA	1919	A	C8-N7	6.52	1.36	1.31
22	BA	2589	A	C5-C4	-6.52	1.34	1.38
54	D2	35	A	C8-N7	6.52	1.36	1.31
22	BA	1057	A	N3-C4	6.52	1.38	1.34
22	BA	2614	A	C8-N7	6.52	1.36	1.31
23	BB	104	A	C8-N7	6.52	1.36	1.31
22	BA	821	A	C8-N7	6.51	1.36	1.31
22	BA	592	A	C8-N7	6.51	1.36	1.31
22	BA	1089	A	N3-C4	6.51	1.38	1.34
22	BA	2821	A	C8-N7	6.51	1.36	1.31
55	D3	35	A	C8-N7	6.51	1.36	1.31
22	BA	443	A	C8-N7	6.51	1.36	1.31
22	BA	1665	A	C8-N7	6.51	1.36	1.31
22	BA	429	A	C8-N7	6.51	1.36	1.31
22	BA	1815	A	C5-C4	-6.51	1.34	1.38
22	BA	1134	A	C8-N7	6.51	1.36	1.31
22	BA	2757	A	C8-N7	6.50	1.36	1.31
22	BA	1700	A	C5-C4	-6.50	1.34	1.38
22	BA	676	A	C5-C4	-6.50	1.34	1.38
22	BA	330	A	C8-N7	6.50	1.36	1.31
22	BA	1569	A	C8-N7	6.50	1.36	1.31
22	BA	2333	A	C8-N7	6.50	1.36	1.31
22	BA	563	A	C8-N7	6.50	1.36	1.31
22	BA	1054	A	C8-N7	6.50	1.36	1.31
22	BA	1650	A	C8-N7	6.50	1.36	1.31
22	BA	1987	A	C8-N7	6.50	1.36	1.31
22	BA	1803	A	C8-N7	6.49	1.36	1.31
22	BA	1890	A	C8-N7	6.49	1.36	1.31
22	BA	2241	A	C5-C4	-6.49	1.34	1.38
22	BA	2322	A	C8-N7	6.49	1.36	1.31
22	BA	730	A	C8-N7	6.49	1.36	1.31
22	BA	677	A	C5-C4	-6.49	1.34	1.38
22	BA	945	A	C8-N7	6.49	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2513	A	C8-N7	6.49	1.36	1.31
22	BA	299	A	C8-N7	6.49	1.36	1.31
22	BA	990	A	C5-C4	-6.49	1.34	1.38
22	BA	2450	A	C8-N7	6.49	1.36	1.31
22	BA	221	A	C8-N7	6.48	1.36	1.31
22	BA	391	A	C8-N7	6.48	1.36	1.31
22	BA	2418	A	C8-N7	6.48	1.36	1.31
22	BA	2778	A	C8-N7	6.48	1.36	1.31
22	BA	547	A	N3-C4	6.48	1.38	1.34
22	BA	599	A	C5-C4	-6.48	1.34	1.38
22	BA	1272	A	C8-N7	6.48	1.36	1.31
22	BA	2003	A	C5-C4	-6.48	1.34	1.38
22	BA	1610	A	C8-N7	6.47	1.36	1.31
22	BA	1626	A	C8-N7	6.47	1.36	1.31
22	BA	1175	A	N3-C4	6.47	1.38	1.34
22	BA	1698	A	C5-C4	-6.47	1.34	1.38
22	BA	2883	A	C8-N7	6.47	1.36	1.31
22	BA	1365	A	C8-N7	6.47	1.36	1.31
22	BA	896	A	N3-C4	6.47	1.38	1.34
22	BA	1641	A	C8-N7	6.47	1.36	1.31
22	BA	2711	A	C5-C4	-6.47	1.34	1.38
22	BA	482	A	C5-C4	-6.47	1.34	1.38
22	BA	173	A	C8-N7	6.46	1.36	1.31
22	BA	74	A	C8-N7	6.46	1.36	1.31
22	BA	1308	A	C5-C4	-6.46	1.34	1.38
22	BA	675	A	C5-C4	-6.46	1.34	1.38
22	BA	1274	A	C8-N7	6.46	1.36	1.31
22	BA	1427	A	C8-N7	6.46	1.36	1.31
22	BA	1786	A	C8-N7	6.46	1.36	1.31
22	BA	2042	A	C8-N7	6.46	1.36	1.31
22	BA	2101	A	N3-C4	6.46	1.38	1.34
22	BA	2600	A	C5-C4	-6.46	1.34	1.38
22	BA	53	A	C8-N7	6.46	1.36	1.31
22	BA	972	A	C8-N7	6.45	1.36	1.31
22	BA	1759	A	C8-N7	6.45	1.36	1.31
22	BA	2856	A	C8-N7	6.45	1.36	1.31
22	BA	478	A	C8-N7	6.45	1.36	1.31
22	BA	1096	A	N3-C4	6.45	1.38	1.34
23	BB	57	A	C8-N7	6.45	1.36	1.31
22	BA	2268	A	C5-C4	-6.45	1.34	1.38
22	BA	1635	A	C8-N7	6.45	1.36	1.31
22	BA	118	A	C8-N7	6.45	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	203	A	C8-N7	6.45	1.36	1.31
22	BA	2037	A	C5-C4	-6.45	1.34	1.38
22	BA	2117	A	N3-C4	6.44	1.38	1.34
22	BA	2439	A	C8-N7	6.44	1.36	1.31
22	BA	1705	A	C8-N7	6.44	1.36	1.31
22	BA	2094	A	C8-N7	6.44	1.36	1.31
1	AA	1362	A	C5-C4	-6.44	1.34	1.38
22	BA	1321	A	N3-C4	6.44	1.38	1.34
22	BA	1713	A	C8-N7	6.44	1.36	1.31
22	BA	28	A	C5-C4	-6.44	1.34	1.38
22	BA	492	A	C8-N7	6.44	1.36	1.31
22	BA	1260	A	C5-C4	-6.44	1.34	1.38
23	BB	99	A	C8-N7	6.44	1.36	1.31
22	BA	56	A	C8-N7	6.43	1.36	1.31
22	BA	753	A	C5-C4	-6.43	1.34	1.38
22	BA	1570	A	C8-N7	6.43	1.36	1.31
22	BA	423	A	C8-N7	6.43	1.36	1.31
22	BA	920	A	C8-N7	6.43	1.36	1.31
22	BA	2031	A	C8-N7	6.43	1.36	1.31
22	BA	1129	A	C5-C4	-6.43	1.34	1.38
22	BA	1155	A	C5-C4	-6.43	1.34	1.38
22	BA	1689	A	C5-C4	-6.43	1.34	1.38
22	BA	2497	A	C5-C4	-6.43	1.34	1.38
22	BA	1664	A	C8-N7	6.43	1.36	1.31
22	BA	1254	A	C5-C4	-6.43	1.34	1.38
22	BA	1384	A	C8-N7	6.43	1.36	1.31
22	BA	2600	A	C8-N7	6.43	1.36	1.31
22	BA	2851	A	C8-N7	6.43	1.36	1.31
22	BA	820	A	C8-N7	6.42	1.36	1.31
22	BA	1142	A	C5-C4	-6.42	1.34	1.38
22	BA	1244	A	C5-C4	-6.42	1.34	1.38
22	BA	1265	A	C5-C4	-6.42	1.34	1.38
22	BA	2005	A	C5-C4	-6.42	1.34	1.38
22	BA	1678	A	C8-N7	6.42	1.36	1.31
22	BA	2388	A	C8-N7	6.42	1.36	1.31
22	BA	1866	A	C8-N7	6.42	1.36	1.31
22	BA	2468	A	C5-C4	-6.42	1.34	1.38
22	BA	21	A	C5-C4	-6.42	1.34	1.38
22	BA	1966	A	C5-C4	-6.42	1.34	1.38
22	BA	722	A	C8-N7	6.41	1.36	1.31
22	BA	1551	A	C5-C4	-6.41	1.34	1.38
22	BA	2639	A	C5-C4	-6.41	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	582	A	C5-C4	-6.41	1.34	1.38
22	BA	428	A	C8-N7	6.41	1.36	1.31
22	BA	590	A	C5-C4	-6.41	1.34	1.38
22	BA	2381	A	C5-C4	-6.41	1.34	1.38
22	BA	309	A	C8-N7	6.41	1.36	1.31
22	BA	2432	A	C8-N7	6.41	1.36	1.31
22	BA	190	A	C5-C4	-6.40	1.34	1.38
22	BA	1977	A	C5-C4	-6.40	1.34	1.38
22	BA	2169	A	N3-C4	6.40	1.38	1.34
22	BA	2336	A	C5-C4	-6.40	1.34	1.38
22	BA	2872	A	C5-C4	-6.40	1.34	1.38
22	BA	878	A	N3-C4	6.40	1.38	1.34
22	BA	2459	A	C5-C4	-6.40	1.34	1.38
22	BA	1757	A	C8-N7	6.40	1.36	1.31
22	BA	2267	A	C8-N7	6.40	1.36	1.31
22	BA	203	A	C5-C4	-6.39	1.34	1.38
22	BA	1027	A	C8-N7	6.39	1.36	1.31
22	BA	2736	A	C5-C4	-6.39	1.34	1.38
22	BA	918	A	C5-C4	-6.39	1.34	1.38
22	BA	1936	A	N3-C4	6.39	1.38	1.34
22	BA	666	A	C8-N7	6.39	1.36	1.31
22	BA	1549	A	C8-N7	6.39	1.36	1.31
22	BA	2340	A	C5-C4	-6.39	1.34	1.38
22	BA	2572	A	C8-N7	6.39	1.36	1.31
22	BA	804	A	C8-N7	6.39	1.36	1.31
22	BA	1069	A	N3-C4	6.39	1.38	1.34
22	BA	2577	A	C5-C4	-6.39	1.34	1.38
22	BA	2727	A	C5-C4	-6.39	1.34	1.38
54	D2	31	A	C8-N7	6.39	1.36	1.31
22	BA	1987	A	C5-C4	-6.39	1.34	1.38
22	BA	127	A	C8-N7	6.39	1.36	1.31
22	BA	477	A	C8-N7	6.39	1.36	1.31
22	BA	689	A	C8-N7	6.38	1.36	1.31
22	BA	1070	A	N3-C4	6.38	1.38	1.34
22	BA	1237	A	C5-C4	-6.38	1.34	1.38
22	BA	1269	A	C5-C4	-6.38	1.34	1.38
22	BA	1342	A	C5-C4	-6.38	1.34	1.38
22	BA	563	A	C5-C4	-6.38	1.34	1.38
22	BA	324	A	C8-N7	6.38	1.36	1.31
22	BA	1028	A	C5-C4	-6.38	1.34	1.38
22	BA	575	A	C5-C4	-6.38	1.34	1.38
22	BA	2873	A	C5-C4	-6.38	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1871	A	N3-C4	6.38	1.38	1.34
22	BA	2886	A	C8-N7	6.38	1.36	1.31
1	AA	978	A	N9-C4	-6.37	1.34	1.37
22	BA	1548	A	C8-N7	6.37	1.36	1.31
22	BA	2725	A	C8-N7	6.37	1.36	1.31
22	BA	2469	A	C5-C4	-6.37	1.34	1.38
23	BB	66	A	C8-N7	6.37	1.36	1.31
22	BA	6	A	C8-N7	6.37	1.36	1.31
22	BA	1387	A	C5-C4	-6.37	1.34	1.38
22	BA	2451	A	C8-N7	6.37	1.36	1.31
54	D2	76	A	C5-C4	-6.37	1.34	1.38
22	BA	196	A	C8-N7	6.36	1.36	1.31
22	BA	514	A	C8-N7	6.36	1.36	1.31
22	BA	900	A	N3-C4	6.36	1.38	1.34
22	BA	218	A	C8-N7	6.36	1.36	1.31
22	BA	668	A	C8-N7	6.36	1.36	1.31
22	BA	735	A	C5-C4	-6.36	1.34	1.38
22	BA	422	A	C8-N7	6.36	1.36	1.31
22	BA	447	A	C8-N7	6.36	1.36	1.31
22	BA	844	A	C5-C4	-6.36	1.34	1.38
22	BA	1701	A	C5-C4	-6.36	1.34	1.38
22	BA	231	A	C8-N7	6.36	1.35	1.31
22	BA	2158	A	N3-C4	6.36	1.38	1.34
22	BA	789	A	C8-N7	6.35	1.35	1.31
22	BA	2518	A	C5-C4	-6.35	1.34	1.38
22	BA	654	A	N3-C4	6.35	1.38	1.34
22	BA	1048	A	C8-N7	6.35	1.35	1.31
22	BA	10	A	C5-C4	-6.35	1.34	1.38
22	BA	21	A	C8-N7	6.35	1.35	1.31
22	BA	983	A	C5-C4	-6.35	1.34	1.38
22	BA	1889	A	C8-N7	6.35	1.35	1.31
22	BA	1378	A	C5-C4	-6.35	1.34	1.38
22	BA	2450	A	C5-C4	-6.35	1.34	1.38
22	BA	2590	A	C8-N7	6.35	1.35	1.31
23	BB	52	A	C8-N7	6.35	1.35	1.31
23	BB	73	A	C8-N7	6.35	1.35	1.31
22	BA	637	A	C5-C4	-6.34	1.34	1.38
22	BA	2435	A	C8-N7	6.34	1.35	1.31
22	BA	1637	A	C5-C4	-6.34	1.34	1.38
22	BA	2278	A	C5-C4	-6.34	1.34	1.38
22	BA	2726	A	C8-N7	6.34	1.35	1.31
22	BA	943	A	C5-C4	-6.34	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1610	A	C5-C4	-6.34	1.34	1.38
22	BA	2020	A	C8-N7	6.34	1.35	1.31
22	BA	1978	A	C8-N7	6.34	1.35	1.31
22	BA	693	A	C5-C4	-6.33	1.34	1.38
22	BA	2171	A	N3-C4	6.33	1.38	1.34
22	BA	2799	A	C8-N7	6.33	1.35	1.31
55	D3	14	A	N3-C4	6.33	1.38	1.34
22	BA	156	A	C8-N7	6.33	1.35	1.31
54	D2	69	A	N3-C4	6.33	1.38	1.34
22	BA	666	A	C5-C4	-6.33	1.34	1.38
22	BA	501	A	C5-C4	-6.33	1.34	1.38
22	BA	2059	A	C5-C4	-6.33	1.34	1.38
22	BA	1572	A	C5-C4	-6.33	1.34	1.38
22	BA	2071	A	C5-C4	-6.33	1.34	1.38
22	BA	2700	A	C8-N7	6.33	1.35	1.31
1	AA	1287	A	N9-C4	-6.32	1.34	1.37
22	BA	1690	A	C8-N7	6.32	1.35	1.31
22	BA	2077	A	C5-C4	-6.32	1.34	1.38
22	BA	1304	A	C5-C4	-6.32	1.34	1.38
22	BA	2088	A	C5-C4	-6.32	1.34	1.38
22	BA	2170	A	N3-C4	6.32	1.38	1.34
22	BA	197	A	C5-C4	-6.32	1.34	1.38
22	BA	1669	A	C8-N7	6.32	1.35	1.31
22	BA	223	A	C5-C4	-6.32	1.34	1.38
22	BA	2270	A	C5-C4	-6.32	1.34	1.38
55	D3	37	A	N3-C4	6.32	1.38	1.34
22	BA	1046	A	N3-C4	6.31	1.38	1.34
22	BA	1189	A	C8-N7	6.31	1.35	1.31
22	BA	501	A	C8-N7	6.31	1.35	1.31
22	BA	1080	A	N3-C4	6.31	1.38	1.34
22	BA	2013	A	C8-N7	6.31	1.35	1.31
22	BA	1262	A	C8-N7	6.31	1.35	1.31
22	BA	783	A	C8-N7	6.31	1.35	1.31
22	BA	909	A	C8-N7	6.31	1.35	1.31
22	BA	2281	A	C5-C4	-6.31	1.34	1.38
22	BA	2336	A	C8-N7	6.31	1.35	1.31
22	BA	2461	A	C5-C4	-6.31	1.34	1.38
22	BA	2471	A	C5-C4	-6.31	1.34	1.38
22	BA	1433	A	C8-N7	6.31	1.35	1.31
22	BA	255	A	C8-N7	6.30	1.35	1.31
22	BA	2183	A	N3-C4	6.30	1.38	1.34
54	D2	5	A	N3-C4	6.30	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1144	A	C8-N7	6.30	1.35	1.31
22	BA	199	A	C5-C4	-6.30	1.34	1.38
22	BA	1307	A	C8-N7	6.30	1.35	1.31
22	BA	1603	A	C8-N7	6.30	1.35	1.31
22	BA	2019	A	C5-C4	-6.30	1.34	1.38
22	BA	497	A	C8-N7	6.30	1.35	1.31
22	BA	505	A	C8-N7	6.30	1.35	1.31
22	BA	1937	A	C5-C4	-6.30	1.34	1.38
22	BA	1419	A	C5-C4	-6.30	1.34	1.38
23	BB	104	A	C5-C4	-6.30	1.34	1.38
22	BA	1126	A	C8-N7	6.29	1.35	1.31
22	BA	470	A	C8-N7	6.29	1.35	1.31
22	BA	947	A	C5-C4	-6.29	1.34	1.38
22	BA	1226	A	C8-N7	6.29	1.35	1.31
22	BA	1854	A	C5-C4	-6.29	1.34	1.38
22	BA	2766	A	N3-C4	6.29	1.38	1.34
22	BA	2778	A	C5-C4	-6.29	1.34	1.38
22	BA	1998	A	C5-C4	-6.29	1.34	1.38
22	BA	1754	A	C8-N7	6.29	1.35	1.31
22	BA	332	A	C5-C4	-6.29	1.34	1.38
22	BA	996	A	C5-C4	-6.29	1.34	1.38
22	BA	608	A	C8-N7	6.28	1.35	1.31
22	BA	1308	A	C8-N7	6.28	1.35	1.31
22	BA	1580	A	N3-C4	6.28	1.38	1.34
22	BA	699	A	C5-C4	-6.28	1.34	1.38
22	BA	1133	A	C5-C4	-6.28	1.34	1.38
22	BA	52	A	C8-N7	6.28	1.35	1.31
22	BA	1009	A	C8-N7	6.28	1.35	1.31
22	BA	1808	A	N3-C4	6.28	1.38	1.34
22	BA	2013	A	C5-C4	-6.28	1.34	1.38
22	BA	2274	A	C8-N7	6.28	1.35	1.31
54	D2	14	A	N3-C4	6.28	1.38	1.34
22	BA	789	A	C5-C4	-6.28	1.34	1.38
22	BA	1276	A	C8-N7	6.28	1.35	1.31
22	BA	1705	A	C5-C4	-6.28	1.34	1.38
22	BA	1927	A	C5-C4	-6.28	1.34	1.38
22	BA	2587	A	C5-C4	-6.28	1.34	1.38
22	BA	825	A	C5-C4	-6.27	1.34	1.38
22	BA	423	A	C5-C4	-6.27	1.34	1.38
22	BA	959	A	C5-C4	-6.27	1.34	1.38
22	BA	1090	A	N3-C4	6.27	1.38	1.34
22	BA	2741	A	C8-N7	6.27	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	735	A	C8-N7	6.27	1.35	1.31
22	BA	2191	A	N3-C4	6.27	1.38	1.34
22	BA	2266	A	C8-N7	6.27	1.35	1.31
22	BA	324	A	C5-C4	-6.27	1.34	1.38
22	BA	244	A	C8-N7	6.26	1.35	1.31
22	BA	1189	A	C5-C4	-6.26	1.34	1.38
22	BA	1928	A	C8-N7	6.26	1.35	1.31
22	BA	2014	A	C8-N7	6.26	1.35	1.31
22	BA	2287	A	C8-N7	6.26	1.35	1.31
22	BA	1327	A	C5-C4	-6.26	1.34	1.38
22	BA	609	A	C8-N7	6.26	1.35	1.31
22	BA	988	A	C5-C4	-6.26	1.34	1.38
22	BA	1008	A	C5-C4	-6.26	1.34	1.38
22	BA	1073	A	N3-C4	6.26	1.38	1.34
22	BA	6	A	C5-C4	-6.26	1.34	1.38
22	BA	739	A	C5-C4	-6.26	1.34	1.38
22	BA	2059	A	C8-N7	6.26	1.35	1.31
22	BA	1676	A	C8-N7	6.26	1.35	1.31
22	BA	621	A	C5-C4	-6.25	1.34	1.38
22	BA	2135	A	N3-C4	6.25	1.38	1.34
22	BA	574	A	C5-C4	-6.25	1.34	1.38
23	BB	101	A	C8-N7	6.25	1.35	1.31
22	BA	1001	A	C8-N7	6.25	1.35	1.31
22	BA	1214	A	C5-C4	-6.25	1.34	1.38
22	BA	1981	A	C5-C4	-6.25	1.34	1.38
22	BA	2541	A	C8-N7	6.25	1.35	1.31
22	BA	522	A	C5-C4	-6.25	1.34	1.38
22	BA	1237	A	C8-N7	6.25	1.35	1.31
22	BA	2879	A	C8-N7	6.25	1.35	1.31
22	BA	2634	A	C5-C4	-6.25	1.34	1.38
22	BA	502	A	C5-C4	-6.24	1.34	1.38
22	BA	820	A	C5-C4	-6.24	1.34	1.38
22	BA	2590	A	C5-C4	-6.24	1.34	1.38
22	BA	1373	A	C8-N7	6.24	1.35	1.31
22	BA	1794	A	C5-C4	-6.24	1.34	1.38
22	BA	1872	A	C8-N7	6.24	1.35	1.31
22	BA	278	A	N3-C4	6.24	1.38	1.34
22	BA	2829	A	C5-C4	-6.24	1.34	1.38
22	BA	541	A	C5-C4	-6.24	1.34	1.38
22	BA	990	A	C8-N7	6.24	1.35	1.31
22	BA	1010	A	C5-C4	-6.24	1.34	1.38
22	BA	2682	A	C8-N7	6.24	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	507	A	C8-N7	6.23	1.35	1.31
22	BA	917	A	C5-C4	-6.23	1.34	1.38
22	BA	480	A	C8-N7	6.23	1.35	1.31
22	BA	515	A	C8-N7	6.23	1.35	1.31
22	BA	1028	A	C8-N7	6.23	1.35	1.31
22	BA	1086	A	N3-C4	6.23	1.38	1.34
22	BA	1427	A	C5-C4	-6.23	1.34	1.38
22	BA	1535	A	N3-C4	6.23	1.38	1.34
55	D3	35	A	N3-C4	6.23	1.38	1.34
22	BA	161	A	C5-C4	-6.23	1.34	1.38
22	BA	975	A	C8-N7	6.23	1.35	1.31
22	BA	1048	A	N3-C4	6.23	1.38	1.34
22	BA	2566	A	C5-C4	-6.23	1.34	1.38
22	BA	226	A	C8-N7	6.23	1.35	1.31
22	BA	374	A	C5-C4	-6.23	1.34	1.38
22	BA	384	A	C8-N7	6.23	1.35	1.31
22	BA	1515	A	C5-C4	-6.23	1.34	1.38
22	BA	2082	A	C8-N7	6.23	1.35	1.31
22	BA	2273	A	C8-N7	6.23	1.35	1.31
22	BA	2407	A	C5-C4	-6.23	1.34	1.38
22	BA	2587	A	C8-N7	6.23	1.35	1.31
22	BA	1301	A	C8-N7	6.23	1.35	1.31
22	BA	14	A	C8-N7	6.22	1.35	1.31
22	BA	943	A	C8-N7	6.22	1.35	1.31
22	BA	508	A	N3-C4	6.22	1.38	1.34
22	BA	1431	A	C8-N7	6.22	1.35	1.31
22	BA	2176	A	N3-C4	6.22	1.38	1.34
22	BA	38	A	C5-C4	-6.22	1.34	1.38
22	BA	2392	A	C8-N7	6.22	1.35	1.31
22	BA	1395	A	C5-C4	-6.22	1.34	1.38
22	BA	1784	A	C8-N7	6.22	1.35	1.31
22	BA	1969	A	C5-C4	-6.22	1.34	1.38
22	BA	2358	A	C8-N7	6.22	1.35	1.31
22	BA	2776	A	C5-C4	-6.22	1.34	1.38
22	BA	101	A	N3-C4	6.21	1.38	1.34
22	BA	705	A	C5-C4	-6.21	1.34	1.38
22	BA	1254	A	C8-N7	6.21	1.35	1.31
22	BA	609	A	C5-C4	-6.21	1.34	1.38
22	BA	1021	A	C8-N7	6.21	1.35	1.31
22	BA	453	A	C5-C4	-6.21	1.34	1.38
22	BA	575	A	C8-N7	6.21	1.35	1.31
22	BA	693	A	C8-N7	6.21	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1789	A	C5-C4	-6.21	1.34	1.38
22	BA	2211	A	N3-C4	6.21	1.38	1.34
22	BA	2434	A	C8-N7	6.21	1.35	1.31
22	BA	1143	A	C5-C4	-6.21	1.34	1.38
22	BA	101	A	C8-N7	6.21	1.35	1.31
22	BA	980	A	C5-C4	-6.21	1.34	1.38
22	BA	2434	A	C5-C4	-6.20	1.34	1.38
22	BA	608	A	C5-C4	-6.20	1.34	1.38
22	BA	2425	A	C8-N7	6.20	1.35	1.31
22	BA	2781	A	C8-N7	6.20	1.35	1.31
22	BA	947	A	C8-N7	6.20	1.35	1.31
22	BA	981	A	C8-N7	6.20	1.35	1.31
22	BA	1809	A	C5-C4	-6.20	1.34	1.38
22	BA	2019	A	C8-N7	6.20	1.35	1.31
22	BA	49	A	C8-N7	6.20	1.35	1.31
22	BA	244	A	C5-C4	-6.20	1.34	1.38
23	BB	99	A	C5-C4	-6.20	1.34	1.38
22	BA	1698	A	C8-N7	6.19	1.35	1.31
22	BA	19	A	C8-N7	6.19	1.35	1.31
22	BA	221	A	C5-C4	-6.19	1.34	1.38
22	BA	1285	A	C5-C4	-6.19	1.34	1.38
22	BA	1608	A	C8-N7	6.19	1.35	1.31
22	BA	1654	A	C8-N7	6.19	1.35	1.31
22	BA	1786	A	C5-C4	-6.19	1.34	1.38
22	BA	2711	A	C8-N7	6.19	1.35	1.31
22	BA	191	A	C8-N7	6.19	1.35	1.31
22	BA	905	A	C5-C4	-6.19	1.34	1.38
22	BA	1126	A	C5-C4	-6.19	1.34	1.38
22	BA	2821	A	C5-C4	-6.19	1.34	1.38
22	BA	196	A	C5-C4	-6.19	1.34	1.38
22	BA	2051	A	C5-C4	-6.19	1.34	1.38
22	BA	2451	A	C5-C4	-6.19	1.34	1.38
22	BA	742	A	C8-N7	6.19	1.35	1.31
22	BA	861	A	C8-N7	6.19	1.35	1.31
22	BA	1809	A	C8-N7	6.18	1.35	1.31
22	BA	460	A	C8-N7	6.18	1.35	1.31
22	BA	1127	A	C5-C4	-6.18	1.34	1.38
22	BA	1265	A	C8-N7	6.18	1.35	1.31
22	BA	1952	A	C8-N7	6.18	1.35	1.31
54	D2	9	A	N3-C4	6.18	1.38	1.34
22	BA	1528	A	C8-N7	6.18	1.35	1.31
22	BA	1532	A	N3-C4	6.18	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	279	A	N3-C4	6.18	1.38	1.34
22	BA	920	A	C5-C4	-6.18	1.34	1.38
22	BA	1583	A	N3-C4	6.18	1.38	1.34
22	BA	1655	A	C8-N7	6.18	1.35	1.31
22	BA	74	A	C5-C4	-6.18	1.34	1.38
22	BA	849	A	C8-N7	6.18	1.35	1.31
22	BA	1275	A	C8-N7	6.18	1.35	1.31
22	BA	1387	A	C8-N7	6.17	1.35	1.31
22	BA	322	A	C5-C4	-6.17	1.34	1.38
22	BA	1021	A	C5-C4	-6.17	1.34	1.38
22	BA	1384	A	C5-C4	-6.17	1.34	1.38
22	BA	1762	A	C5-C4	-6.17	1.34	1.38
22	BA	213	A	C5-C4	-6.16	1.34	1.38
22	BA	1571	A	C5-C4	-6.16	1.34	1.38
22	BA	1548	A	C5-C4	-6.16	1.34	1.38
22	BA	2247	A	C5-C4	-6.16	1.34	1.38
22	BA	1354	A	C8-N7	6.16	1.35	1.31
22	BA	2433	A	C8-N7	6.16	1.35	1.31
22	BA	727	A	C5-C4	-6.15	1.34	1.38
22	BA	632	A	C5-C4	-6.15	1.34	1.38
22	BA	1815	A	C8-N7	6.15	1.35	1.31
22	BA	2497	A	C8-N7	6.15	1.35	1.31
22	BA	197	A	C8-N7	6.15	1.35	1.31
22	BA	371	A	C5-C4	-6.15	1.34	1.38
22	BA	631	A	C8-N7	6.15	1.35	1.31
22	BA	2453	A	C8-N7	6.15	1.35	1.31
22	BA	2564	A	C5-C4	-6.15	1.34	1.38
22	BA	2670	A	C5-C4	-6.15	1.34	1.38
22	BA	2757	A	N3-C4	6.15	1.38	1.34
22	BA	2826	A	C8-N7	6.15	1.35	1.31
22	BA	2758	A	C5-C4	-6.14	1.34	1.38
23	BB	94	A	C8-N7	6.14	1.35	1.31
22	BA	909	A	C5-C4	-6.14	1.34	1.38
22	BA	1637	A	C8-N7	6.14	1.35	1.31
22	BA	430	A	C5-C4	-6.14	1.34	1.38
22	BA	911	A	C8-N7	6.14	1.35	1.31
22	BA	1307	A	C5-C4	-6.14	1.34	1.38
22	BA	825	A	C8-N7	6.14	1.35	1.31
22	BA	1156	A	C8-N7	6.14	1.35	1.31
22	BA	1508	A	N3-C4	6.14	1.38	1.34
22	BA	1336	A	C5-C4	-6.13	1.34	1.38
22	BA	685	A	C5-C4	-6.13	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1632	A	C5-C4	-6.13	1.34	1.38
22	BA	1739	A	C8-N7	6.13	1.35	1.31
22	BA	1677	A	C5-C4	-6.13	1.34	1.38
22	BA	1678	A	C5-C4	-6.13	1.34	1.38
22	BA	2094	A	C5-C4	-6.13	1.34	1.38
22	BA	1246	A	C5-C4	-6.13	1.34	1.38
22	BA	2740	A	C8-N7	6.13	1.35	1.31
22	BA	56	A	C5-C4	-6.13	1.34	1.38
22	BA	1302	A	C5-C4	-6.13	1.34	1.38
22	BA	1802	A	C5-C4	-6.13	1.34	1.38
22	BA	2366	A	C5-C4	-6.13	1.34	1.38
22	BA	1553	A	C8-N7	6.12	1.35	1.31
22	BA	633	A	C8-N7	6.12	1.35	1.31
22	BA	1260	A	C8-N7	6.12	1.35	1.31
22	BA	1608	A	C5-C4	-6.12	1.34	1.38
22	BA	1889	A	C5-C4	-6.12	1.34	1.38
22	BA	1899	A	C8-N7	6.12	1.35	1.31
22	BA	1953	A	C5-C4	-6.12	1.34	1.38
54	D2	26	A	N3-C4	6.12	1.38	1.34
22	BA	53	A	C5-C4	-6.12	1.34	1.38
22	BA	262	A	C5-C4	-6.12	1.34	1.38
22	BA	699	A	C8-N7	6.12	1.35	1.31
22	BA	877	A	N3-C4	6.12	1.38	1.34
22	BA	980	A	C8-N7	6.12	1.35	1.31
22	BA	1392	A	C5-C4	-6.12	1.34	1.38
22	BA	1603	A	C5-C4	-6.12	1.34	1.38
22	BA	1772	A	C8-N7	6.12	1.35	1.31
22	BA	1872	A	N3-C4	6.12	1.38	1.34
22	BA	2632	A	C5-C4	-6.12	1.34	1.38
22	BA	195	A	C5-C4	-6.12	1.34	1.38
22	BA	478	A	C5-C4	-6.12	1.34	1.38
22	BA	572	A	C8-N7	6.12	1.35	1.31
22	BA	1284	A	C8-N7	6.12	1.35	1.31
22	BA	528	A	C5-C4	-6.11	1.34	1.38
22	BA	1969	A	C8-N7	6.11	1.35	1.31
22	BA	918	A	C8-N7	6.11	1.35	1.31
22	BA	2453	A	C5-C4	-6.11	1.34	1.38
54	D2	31	A	N3-C4	6.11	1.38	1.34
55	D3	21	A	N3-C4	6.11	1.38	1.34
22	BA	1142	A	C8-N7	6.11	1.35	1.31
22	BA	1477	A	C5-C4	-6.11	1.34	1.38
22	BA	1829	A	C8-N7	6.11	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2119	A	N3-C4	6.11	1.38	1.34
22	BA	2352	A	C5-C4	-6.11	1.34	1.38
22	BA	1029	A	C5-C4	-6.11	1.34	1.38
22	BA	1354	A	C5-C4	-6.11	1.34	1.38
22	BA	1359	A	C5-C4	-6.11	1.34	1.38
22	BA	2031	A	C5-C4	-6.11	1.34	1.38
22	BA	2142	A	N3-C4	6.11	1.38	1.34
22	BA	819	A	C5-C4	-6.10	1.34	1.38
22	BA	471	A	C8-N7	6.10	1.35	1.31
22	BA	1614	A	C8-N7	6.10	1.35	1.31
22	BA	1700	A	C8-N7	6.10	1.35	1.31
22	BA	2679	A	C5-C4	-6.10	1.34	1.38
22	BA	1679	A	C8-N7	6.10	1.35	1.31
22	BA	1711	A	C5-C4	-6.10	1.34	1.38
22	BA	793	A	C8-N7	6.10	1.35	1.31
22	BA	1264	A	C8-N7	6.10	1.35	1.31
22	BA	2287	A	C5-C4	-6.09	1.34	1.38
22	BA	190	A	C8-N7	6.09	1.35	1.31
22	BA	984	A	N3-C4	6.09	1.38	1.34
22	BA	443	A	C5-C4	-6.09	1.34	1.38
22	BA	374	A	C8-N7	6.09	1.35	1.31
22	BA	781	A	C5-C4	-6.09	1.34	1.38
22	BA	2058	A	C5-C4	-6.09	1.34	1.38
22	BA	2309	A	N3-C4	6.09	1.38	1.34
22	BA	685	A	C8-N7	6.09	1.35	1.31
22	BA	910	A	C5-C4	-6.09	1.34	1.38
22	BA	1722	A	N3-C4	6.09	1.38	1.34
22	BA	2062	A	C5-C4	-6.09	1.34	1.38
22	BA	2541	A	C5-C4	-6.09	1.34	1.38
22	BA	428	A	C5-C4	-6.08	1.34	1.38
22	BA	1689	A	C8-N7	6.08	1.35	1.31
22	BA	265	A	C5-C4	-6.08	1.34	1.38
22	BA	2184	A	N3-C4	6.08	1.38	1.34
22	BA	2765	A	C5-C4	-6.08	1.34	1.38
55	D3	7	A	N3-C4	6.08	1.38	1.34
22	BA	2090	A	C8-N7	6.08	1.35	1.31
22	BA	2761	A	C5-C4	-6.08	1.34	1.38
55	D3	58	A	N3-C4	6.08	1.38	1.34
22	BA	1431	A	C5-C4	-6.08	1.34	1.38
22	BA	2284	A	C5-C4	-6.08	1.34	1.38
22	BA	1084	A	N3-C4	6.07	1.38	1.34
22	BA	1744	A	N3-C4	6.07	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1773	A	C5-C4	-6.07	1.34	1.38
22	BA	1000	A	C8-N7	6.07	1.35	1.31
22	BA	2088	A	C8-N7	6.07	1.35	1.31
22	BA	2860	A	C8-N7	6.07	1.35	1.31
22	BA	1268	A	C8-N7	6.07	1.35	1.31
22	BA	207	A	C5-C4	-6.07	1.34	1.38
22	BA	1286	A	C5-C4	-6.07	1.34	1.38
22	BA	2198	A	C5-C4	-6.07	1.34	1.38
22	BA	2518	A	C8-N7	6.07	1.35	1.31
22	BA	1785	A	C5-C4	-6.06	1.34	1.38
22	BA	1810	A	C5-C4	-6.06	1.34	1.38
22	BA	1522	A	C5-C4	-6.06	1.34	1.38
22	BA	1677	A	C8-N7	6.06	1.35	1.31
22	BA	2062	A	N3-C4	6.06	1.38	1.34
23	BB	101	A	C5-C4	-6.06	1.34	1.38
22	BA	1928	A	C5-C4	-6.06	1.34	1.38
22	BA	2284	A	C8-N7	6.06	1.35	1.31
22	BA	866	A	N3-C4	6.06	1.38	1.34
22	BA	1032	A	C5-C4	-6.06	1.34	1.38
22	BA	1571	A	C8-N7	6.06	1.35	1.31
22	BA	2726	A	C5-C4	-6.06	1.34	1.38
22	BA	391	A	C5-C4	-6.05	1.34	1.38
22	BA	863	A	C8-N7	6.05	1.35	1.31
22	BA	2705	A	C5-C4	-6.05	1.34	1.38
22	BA	233	A	C5-C4	-6.05	1.34	1.38
22	BA	505	A	C5-C4	-6.05	1.34	1.38
22	BA	1789	A	C8-N7	6.05	1.35	1.31
22	BA	1821	A	C5-C4	-6.05	1.34	1.38
22	BA	1854	A	C8-N7	6.05	1.35	1.31
22	BA	2183	A	C8-N7	6.05	1.35	1.31
22	BA	2614	A	C5-C4	-6.05	1.34	1.38
54	D2	28	A	N3-C4	6.05	1.38	1.34
22	BA	1614	A	C5-C4	-6.05	1.34	1.38
22	BA	1848	A	C8-N7	6.05	1.35	1.31
22	BA	227	A	C5-C4	-6.04	1.34	1.38
22	BA	959	A	C8-N7	6.04	1.35	1.31
22	BA	2327	A	C5-C4	-6.04	1.34	1.38
22	BA	753	A	C8-N7	6.04	1.35	1.31
22	BA	981	A	C5-C4	-6.04	1.34	1.38
22	BA	1912	A	C5-C4	-6.04	1.34	1.38
22	BA	2070	A	C5-C4	-6.04	1.34	1.38
22	BA	941	A	C5-C4	-6.04	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2335	A	C8-N7	6.04	1.35	1.31
22	BA	1143	A	C8-N7	6.04	1.35	1.31
22	BA	614	A	N3-C4	6.04	1.38	1.34
22	BA	1616	A	C5-C4	-6.04	1.34	1.38
22	BA	1890	A	C5-C4	-6.04	1.34	1.38
22	BA	2738	A	C5-C4	-6.03	1.34	1.38
22	BA	2352	A	C8-N7	6.03	1.35	1.31
22	BA	2765	A	C8-N7	6.03	1.35	1.31
22	BA	1276	A	C5-C4	-6.03	1.34	1.38
22	BA	2700	A	C5-C4	-6.03	1.34	1.38
22	BA	960	A	C5-C4	-6.03	1.34	1.38
22	BA	2412	A	C8-N7	6.03	1.35	1.31
22	BA	2682	A	C5-C4	-6.03	1.34	1.38
22	BA	676	A	C8-N7	6.03	1.35	1.31
22	BA	751	A	C8-N7	6.03	1.35	1.31
22	BA	1366	A	C5-C4	-6.03	1.34	1.38
22	BA	529	A	C5-C4	-6.03	1.34	1.38
22	BA	1103	A	N3-C4	6.03	1.38	1.34
22	BA	1204	A	C5-C4	-6.03	1.34	1.38
22	BA	1749	A	C5-C4	-6.03	1.34	1.38
22	BA	2530	A	C5-C4	-6.03	1.34	1.38
22	BA	483	A	N3-C4	6.02	1.38	1.34
22	BA	734	A	C5-C4	-6.02	1.34	1.38
22	BA	996	A	C8-N7	6.02	1.35	1.31
22	BA	1801	A	N3-C4	6.02	1.38	1.34
23	BB	94	A	C5-C4	-6.02	1.34	1.38
22	BA	1932	A	C5-C4	-6.02	1.34	1.38
22	BA	2872	A	C8-N7	6.02	1.35	1.31
22	BA	1287	A	C8-N7	6.02	1.35	1.31
22	BA	2810	A	C5-C4	-6.02	1.34	1.38
22	BA	1665	A	C5-C4	-6.02	1.34	1.38
22	BA	1900	A	C8-N7	6.02	1.35	1.31
22	BA	2734	A	C5-C4	-6.02	1.34	1.38
22	BA	2740	A	C5-C4	-6.02	1.34	1.38
22	BA	1641	A	C5-C4	-6.02	1.34	1.38
22	BA	2781	A	C5-C4	-6.02	1.34	1.38
22	BA	1327	A	C8-N7	6.01	1.35	1.31
22	BA	2366	A	C8-N7	6.01	1.35	1.31
22	BA	627	A	C5-C4	-6.01	1.34	1.38
22	BA	1802	A	C8-N7	6.01	1.35	1.31
22	BA	1953	A	C8-N7	6.01	1.35	1.31
22	BA	1085	A	N3-C4	6.01	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	800	A	C8-N7	6.01	1.35	1.31
22	BA	945	A	C5-C4	-6.01	1.34	1.38
22	BA	2823	A	C5-C4	-6.01	1.34	1.38
22	BA	911	A	C5-C4	-6.00	1.34	1.38
22	BA	782	A	C5-C4	-6.00	1.34	1.38
22	BA	1010	A	C8-N7	6.00	1.35	1.31
22	BA	2154	A	N3-C4	6.00	1.38	1.34
22	BA	471	A	C5-C4	-6.00	1.34	1.38
22	BA	1151	A	C5-C4	-6.00	1.34	1.38
22	BA	2273	A	C5-C4	-6.00	1.34	1.38
22	BA	2077	A	C8-N7	6.00	1.35	1.31
22	BA	515	A	C5-C4	-6.00	1.34	1.38
22	BA	670	A	C5-C4	-6.00	1.34	1.38
22	BA	1470	A	C8-N7	6.00	1.35	1.31
22	BA	1549	A	C5-C4	-5.99	1.34	1.38
22	BA	1672	A	C5-C4	-5.99	1.34	1.38
22	BA	2589	A	C8-N7	5.99	1.35	1.31
22	BA	2635	A	C5-C4	-5.99	1.34	1.38
22	BA	2227	A	C5-C4	-5.99	1.34	1.38
22	BA	2792	A	C5-C4	-5.99	1.34	1.38
22	BA	368	A	N3-C4	5.99	1.38	1.34
22	BA	1913	A	N3-C4	5.99	1.38	1.34
22	BA	788	A	C5-C4	-5.99	1.34	1.38
22	BA	1635	A	C5-C4	-5.99	1.34	1.38
22	BA	28	A	C8-N7	5.99	1.35	1.31
22	BA	251	A	C5-C4	-5.99	1.34	1.38
22	BA	310	A	C5-C4	-5.99	1.34	1.38
22	BA	1284	A	C5-C4	-5.99	1.34	1.38
22	BA	1754	A	C5-C4	-5.99	1.34	1.38
22	BA	925	A	C5-C4	-5.98	1.34	1.38
22	BA	1877	A	N3-C4	5.98	1.38	1.34
22	BA	1938	A	C5-C4	-5.98	1.34	1.38
22	BA	2733	A	N3-C4	5.98	1.38	1.34
22	BA	2835	A	C5-C4	-5.98	1.34	1.38
22	BA	1194	A	C5-C4	-5.98	1.34	1.38
22	BA	2097	A	N3-C4	5.98	1.38	1.34
22	BA	586	A	C8-N7	5.98	1.35	1.31
22	BA	2448	A	C5-C4	-5.98	1.34	1.38
22	BA	1545	A	C5-C4	-5.98	1.34	1.38
22	BA	460	A	C5-C4	-5.98	1.34	1.38
22	BA	973	A	C5-C4	-5.98	1.34	1.38
22	BA	1230	A	C5-C4	-5.98	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1791	A	C8-N7	5.98	1.35	1.31
54	D2	41	A	C5-C4	-5.98	1.34	1.38
22	BA	2721	A	C8-N7	5.98	1.35	1.31
22	BA	155	A	C5-C4	-5.97	1.34	1.38
22	BA	1420	A	N3-C4	5.97	1.38	1.34
22	BA	439	A	C5-C4	-5.97	1.34	1.38
22	BA	2432	A	C5-C4	-5.97	1.34	1.38
1	AA	1180	A	N7-C5	-5.97	1.35	1.39
22	BA	1328	A	C8-N7	5.97	1.35	1.31
22	BA	2346	A	C5-C4	-5.97	1.34	1.38
22	BA	2459	A	C8-N7	5.97	1.35	1.31
22	BA	2547	A	C5-C4	-5.97	1.34	1.38
23	BB	109	A	N3-C4	5.97	1.38	1.34
23	BB	73	A	N3-C4	5.97	1.38	1.34
22	BA	1970	A	C5-C4	-5.97	1.34	1.38
22	BA	917	A	C8-N7	5.96	1.35	1.31
22	BA	42	A	C5-C4	-5.96	1.34	1.38
22	BA	1668	A	C8-N7	5.96	1.35	1.31
22	BA	2297	A	C5-C4	-5.96	1.34	1.38
22	BA	2823	A	C8-N7	5.96	1.35	1.31
22	BA	2042	A	C5-C4	-5.96	1.34	1.38
22	BA	1570	A	C5-C4	-5.96	1.34	1.38
22	BA	1783	A	C8-N7	5.96	1.35	1.31
22	BA	2850	A	C8-N7	5.96	1.35	1.31
22	BA	586	A	C5-C4	-5.95	1.34	1.38
22	BA	845	A	N3-C4	5.95	1.38	1.34
22	BA	1127	A	C8-N7	5.95	1.35	1.31
22	BA	2856	A	C5-C4	-5.95	1.34	1.38
22	BA	2887	A	C5-C4	-5.95	1.34	1.38
22	BA	1794	A	C8-N7	5.95	1.35	1.31
22	BA	2430	A	C8-N7	5.95	1.35	1.31
22	BA	466	A	C8-N7	5.95	1.35	1.31
22	BA	626	A	N3-C4	5.95	1.38	1.34
55	D3	38	A	N3-C4	5.95	1.38	1.34
22	BA	415	A	C5-C4	-5.95	1.34	1.38
22	BA	422	A	C5-C4	-5.94	1.34	1.38
22	BA	1952	A	C5-C4	-5.94	1.34	1.38
22	BA	2386	A	C8-N7	5.94	1.35	1.31
22	BA	299	A	C5-C4	-5.94	1.34	1.38
22	BA	572	A	C5-C4	-5.94	1.34	1.38
22	BA	1713	A	N3-C4	5.94	1.38	1.34
23	BB	57	A	N3-C4	5.94	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	216	A	N3-C4	5.94	1.38	1.34
22	BA	1876	A	N3-C4	5.94	1.38	1.34
22	BA	1780	A	C5-C4	-5.94	1.34	1.38
22	BA	1970	A	N3-C4	5.94	1.38	1.34
22	BA	391	A	N3-C4	5.93	1.38	1.34
22	BA	497	A	C5-C4	-5.93	1.34	1.38
22	BA	1272	A	C5-C4	-5.93	1.34	1.38
22	BA	1347	A	C5-C4	-5.93	1.34	1.38
22	BA	655	A	C5-C4	-5.93	1.34	1.38
22	BA	2009	A	C8-N7	5.93	1.35	1.31
22	BA	2407	A	C8-N7	5.93	1.35	1.31
22	BA	1213	A	C5-C4	-5.92	1.34	1.38
22	BA	2333	A	C5-C4	-5.92	1.34	1.38
22	BA	2513	A	C5-C4	-5.92	1.34	1.38
22	BA	52	A	C5-C4	-5.92	1.34	1.38
22	BA	216	A	C5-C4	-5.92	1.34	1.38
22	BA	2461	A	C8-N7	5.92	1.35	1.31
22	BA	781	A	C8-N7	5.91	1.35	1.31
1	AA	1360	A	N7-C5	-5.91	1.35	1.39
22	BA	182	A	C5-C4	-5.91	1.34	1.38
22	BA	1156	A	C5-C4	-5.91	1.34	1.38
22	BA	384	A	C5-C4	-5.91	1.34	1.38
22	BA	1039	A	N3-C4	5.91	1.38	1.34
22	BA	1342	A	N3-C4	5.91	1.38	1.34
22	BA	1676	A	C5-C4	-5.91	1.34	1.38
22	BA	2080	A	C8-N7	5.91	1.35	1.31
22	BA	144	A	N3-C4	5.91	1.38	1.34
22	BA	1144	A	C5-C4	-5.91	1.34	1.38
22	BA	125	A	N3-C4	5.90	1.38	1.34
22	BA	1009	A	C5-C4	-5.90	1.34	1.38
22	BA	1597	A	C5-C4	-5.90	1.34	1.38
22	BA	2860	A	C5-C4	-5.90	1.34	1.38
22	BA	282	A	N3-C4	5.90	1.38	1.34
22	BA	402	A	C5-C4	-5.90	1.34	1.38
22	BA	721	A	N3-C4	5.90	1.38	1.34
22	BA	2727	A	C8-N7	5.90	1.35	1.31
22	BA	447	A	C5-C4	-5.90	1.34	1.38
22	BA	340	A	C5-C4	-5.89	1.34	1.38
22	BA	330	A	N3-C4	5.89	1.38	1.34
22	BA	1900	A	C5-C4	-5.89	1.34	1.38
22	BA	802	A	C5-C4	-5.89	1.34	1.38
22	BA	2054	A	C8-N7	5.89	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2675	A	C8-N7	5.89	1.35	1.31
22	BA	2809	A	C5-C4	-5.89	1.34	1.38
22	BA	2766	A	C5-C4	-5.88	1.34	1.38
22	BA	415	A	C8-N7	5.88	1.35	1.31
22	BA	633	A	C5-C4	-5.88	1.34	1.38
22	BA	1977	A	C8-N7	5.88	1.35	1.31
22	BA	89	A	C5-C4	-5.88	1.34	1.38
22	BA	749	A	C5-C4	-5.88	1.34	1.38
23	BB	108	A	C5-C4	-5.88	1.34	1.38
22	BA	590	A	C8-N7	5.88	1.35	1.31
22	BA	616	A	N3-C4	5.88	1.38	1.34
22	BA	2516	A	C8-N7	5.88	1.35	1.31
22	BA	715	A	N3-C4	5.87	1.38	1.34
22	BA	675	A	C8-N7	5.87	1.35	1.31
22	BA	532	A	C5-C4	-5.87	1.34	1.38
22	BA	2335	A	C5-C4	-5.87	1.34	1.38
22	BA	231	A	C5-C4	-5.86	1.34	1.38
22	BA	983	A	C8-N7	5.86	1.35	1.31
23	BB	59	A	N3-C4	5.86	1.38	1.34
22	BA	1544	A	C5-C4	-5.86	1.34	1.38
22	BA	1819	A	C8-N7	5.86	1.35	1.31
22	BA	794	A	C8-N7	5.86	1.35	1.31
22	BA	1287	A	C5-C4	-5.86	1.34	1.38
22	BA	1367	A	C5-C4	-5.86	1.34	1.38
22	BA	1509	A	N3-C4	5.86	1.38	1.34
22	BA	1773	A	C8-N7	5.86	1.35	1.31
22	BA	910	A	C8-N7	5.86	1.35	1.31
22	BA	1505	A	N3-C4	5.86	1.38	1.34
22	BA	984	A	C8-N7	5.86	1.35	1.31
22	BA	219	A	C5-C4	-5.85	1.34	1.38
22	BA	480	A	C5-C4	-5.85	1.34	1.38
22	BA	2879	A	C5-C4	-5.85	1.34	1.38
22	BA	538	A	N3-C4	5.85	1.38	1.34
22	BA	2052	A	C8-N7	5.85	1.35	1.31
22	BA	538	A	C5-C4	-5.85	1.34	1.38
22	BA	125	A	C5-C4	-5.85	1.34	1.38
54	D2	49	A	N3-C4	5.85	1.38	1.34
22	BA	2826	A	C5-C4	-5.85	1.34	1.38
22	BA	2886	A	C5-C4	-5.85	1.34	1.38
22	BA	845	A	C5-C4	-5.84	1.34	1.38
22	BA	352	A	N3-C4	5.84	1.38	1.34
22	BA	432	A	C5-C4	-5.84	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	782	A	C8-N7	5.84	1.35	1.31
22	BA	344	A	N3-C4	5.84	1.38	1.34
22	BA	925	A	N3-C4	5.84	1.38	1.34
22	BA	2080	A	C5-C4	-5.84	1.34	1.38
22	BA	2412	A	C5-C4	-5.84	1.34	1.38
22	BA	2406	A	N3-C4	5.83	1.38	1.34
23	BB	53	A	N3-C4	5.83	1.38	1.34
22	BA	1858	A	C5-C4	-5.83	1.34	1.38
22	BA	1901	A	C5-C4	-5.83	1.34	1.38
22	BA	2322	A	C5-C4	-5.83	1.34	1.38
22	BA	2665	A	C5-C4	-5.83	1.34	1.38
23	BB	50	A	C5-C4	-5.83	1.34	1.38
22	BA	1029	A	C8-N7	5.83	1.35	1.31
22	BA	1803	A	C5-C4	-5.83	1.34	1.38
22	BA	2433	A	C5-C4	-5.83	1.34	1.38
22	BA	2478	A	C5-C4	-5.83	1.34	1.38
22	BA	49	A	C5-C4	-5.82	1.34	1.38
22	BA	793	A	C5-C4	-5.82	1.34	1.38
22	BA	1690	A	C5-C4	-5.82	1.34	1.38
22	BA	2565	A	C8-N7	5.82	1.35	1.31
22	BA	2706	A	C8-N7	5.82	1.35	1.31
22	BA	2706	A	C5-C4	-5.82	1.34	1.38
55	D3	9	A	N3-C4	5.82	1.38	1.34
22	BA	1504	A	C5-C4	-5.82	1.34	1.38
22	BA	2675	A	C5-C4	-5.82	1.34	1.38
22	BA	1635	A	N3-C4	5.81	1.38	1.34
22	BA	2851	A	C5-C4	-5.81	1.34	1.38
22	BA	191	A	C5-C4	-5.81	1.34	1.38
22	BA	2051	A	C8-N7	5.81	1.35	1.31
22	BA	14	A	C5-C4	-5.81	1.34	1.38
22	BA	1787	A	C5-C4	-5.81	1.34	1.38
22	BA	1433	A	C5-C4	-5.81	1.34	1.38
22	BA	716	A	N3-C4	5.80	1.38	1.34
22	BA	1040	A	C5-C4	-5.80	1.34	1.38
22	BA	1735	A	N3-C4	5.80	1.38	1.34
22	BA	1978	A	C5-C4	-5.80	1.34	1.38
22	BA	118	A	C5-C4	-5.80	1.34	1.38
22	BA	324	A	N3-C4	5.80	1.38	1.34
22	BA	1759	A	N3-C4	5.80	1.38	1.34
22	BA	492	A	C5-C4	-5.80	1.34	1.38
22	BA	513	A	C5-C4	-5.80	1.34	1.38
22	BA	751	A	C5-C4	-5.80	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1469	A	C5-C4	-5.80	1.34	1.38
22	BA	156	A	N3-C4	5.79	1.38	1.34
22	BA	522	A	C8-N7	5.79	1.35	1.31
22	BA	973	A	C8-N7	5.79	1.35	1.31
22	BA	1403	A	C5-C4	-5.79	1.34	1.38
22	BA	118	A	N3-C4	5.79	1.38	1.34
22	BA	849	A	C5-C4	-5.79	1.34	1.38
22	BA	2893	A	N3-C4	5.79	1.38	1.34
23	BB	29	A	C5-C4	-5.79	1.34	1.38
22	BA	1413	A	C5-C4	-5.79	1.34	1.38
22	BA	718	A	N3-C4	5.79	1.38	1.34
22	BA	706	A	C5-C4	-5.79	1.34	1.38
22	BA	1502	A	C5-C4	-5.79	1.34	1.38
22	BA	160	A	C5-C4	-5.78	1.34	1.38
22	BA	1301	A	C5-C4	-5.78	1.34	1.38
22	BA	1654	A	C5-C4	-5.78	1.34	1.38
1	AA	977	A	N7-C5	-5.78	1.35	1.39
22	BA	2425	A	C5-C4	-5.78	1.34	1.38
22	BA	472	A	C5-C4	-5.78	1.34	1.38
22	BA	1393	A	C5-C4	-5.78	1.34	1.38
22	BA	1353	A	C5-C4	-5.78	1.34	1.38
22	BA	1579	A	N3-C4	5.78	1.38	1.34
22	BA	1998	A	C8-N7	5.78	1.35	1.31
22	BA	131	A	C5-C4	-5.78	1.34	1.38
22	BA	1213	A	C8-N7	5.78	1.35	1.31
22	BA	1503	A	C5-C4	-5.78	1.34	1.38
22	BA	2037	A	C8-N7	5.78	1.35	1.31
22	BA	2268	A	C8-N7	5.78	1.35	1.31
22	BA	71	A	C5-C4	-5.77	1.34	1.38
22	BA	401	A	C5-C4	-5.77	1.34	1.38
22	BA	1626	A	C5-C4	-5.77	1.34	1.38
54	D2	51	A	N3-C4	5.77	1.38	1.34
22	BA	2015	A	C8-N7	5.77	1.35	1.31
22	BA	2095	A	C5-C4	-5.77	1.34	1.38
22	BA	743	A	C8-N7	5.77	1.35	1.31
22	BA	167	A	C5-C4	-5.76	1.34	1.38
22	BA	1134	A	C5-C4	-5.76	1.34	1.38
22	BA	2411	A	C5-C4	-5.76	1.34	1.38
54	D2	21	A	N3-C4	5.76	1.38	1.34
22	BA	1496	A	C5-C4	-5.76	1.34	1.38
22	BA	2080	A	N3-C4	5.76	1.38	1.34
22	BA	2820	A	N3-C4	5.76	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1318	A	N9-C4	-5.75	1.34	1.37
22	BA	2753	A	C5-C4	-5.75	1.34	1.38
22	BA	2247	A	N3-C4	5.75	1.38	1.34
22	BA	1713	A	C5-C4	-5.75	1.34	1.38
22	BA	1373	A	C5-C4	-5.75	1.34	1.38
22	BA	111	A	C5-C4	-5.74	1.34	1.38
22	BA	1746	A	N3-C4	5.74	1.38	1.34
22	BA	2247	A	C8-N7	5.74	1.35	1.31
22	BA	2750	A	N3-C4	5.74	1.38	1.34
22	BA	979	A	C5-C4	-5.74	1.34	1.38
22	BA	1014	A	C5-C4	-5.74	1.34	1.38
22	BA	1759	A	C5-C4	-5.74	1.34	1.38
22	BA	507	A	C5-C4	-5.74	1.34	1.38
22	BA	2660	A	N3-C4	5.74	1.38	1.34
55	D3	36	A	N3-C4	5.74	1.38	1.34
22	BA	144	A	C5-C4	-5.73	1.34	1.38
22	BA	1365	A	C5-C4	-5.73	1.34	1.38
54	D2	73	A	N3-C4	5.73	1.38	1.34
22	BA	984	A	C5-C4	-5.73	1.34	1.38
22	BA	256	A	C5-C4	-5.73	1.34	1.38
22	BA	2288	A	N3-C4	5.73	1.38	1.34
22	BA	783	A	N3-C4	5.73	1.38	1.34
22	BA	255	A	C5-C4	-5.72	1.34	1.38
22	BA	218	A	C5-C4	-5.72	1.34	1.38
22	BA	439	A	N3-C4	5.72	1.38	1.34
22	BA	602	A	C5-C4	-5.72	1.34	1.38
22	BA	1453	A	N3-C4	5.72	1.38	1.34
22	BA	2376	A	C5-C4	-5.72	1.34	1.38
22	BA	342	A	C5-C4	-5.72	1.34	1.38
22	BA	1899	A	C5-C4	-5.72	1.34	1.38
22	BA	644	A	C5-C4	-5.71	1.34	1.38
22	BA	1525	A	C5-C4	-5.71	1.34	1.38
22	BA	1829	A	C5-C4	-5.71	1.34	1.38
22	BA	2598	A	C8-N7	5.71	1.35	1.31
23	BB	34	A	C5-C4	-5.71	1.34	1.38
23	BB	45	A	N3-C4	5.71	1.38	1.34
22	BA	1050	A	N3-C4	5.71	1.38	1.34
22	BA	1552	A	C5-C4	-5.71	1.34	1.38
1	AA	959	A	N9-C4	-5.71	1.34	1.37
22	BA	471	A	N3-C4	5.71	1.38	1.34
22	BA	2662	A	N3-C4	5.71	1.38	1.34
22	BA	1885	A	C5-C4	-5.71	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	866	A	C5-C4	-5.70	1.34	1.38
22	BA	2662	A	C8-N7	5.70	1.35	1.31
22	BA	1640	A	C5-C4	-5.70	1.34	1.38
22	BA	131	A	N3-C4	5.70	1.38	1.34
22	BA	213	A	N3-C4	5.70	1.38	1.34
22	BA	2071	A	C8-N7	5.70	1.35	1.31
22	BA	429	A	C5-C4	-5.70	1.34	1.38
22	BA	2288	A	C5-C4	-5.70	1.34	1.38
22	BA	382	A	C5-C4	-5.70	1.34	1.38
22	BA	470	A	N3-C4	5.70	1.38	1.34
22	BA	270	A	C5-C4	-5.69	1.34	1.38
22	BA	477	A	C5-C4	-5.69	1.34	1.38
22	BA	1787	A	C8-N7	5.69	1.35	1.31
1	AA	1234	C	N1-C6	-5.69	1.33	1.37
22	BA	1328	A	C5-C4	-5.69	1.34	1.38
22	BA	2314	A	C5-C4	-5.69	1.34	1.38
22	BA	2706	A	N3-C4	5.69	1.38	1.34
22	BA	1020	A	C5-C4	-5.68	1.34	1.38
22	BA	1204	A	N3-C4	5.68	1.38	1.34
22	BA	2654	A	C5-C4	-5.68	1.34	1.38
23	BB	94	A	N3-C4	5.68	1.38	1.34
22	BA	310	A	N3-C4	5.68	1.38	1.34
22	BA	2082	A	C5-C4	-5.68	1.34	1.38
22	BA	1241	A	N3-C4	5.67	1.38	1.34
22	BA	1572	A	C8-N7	5.67	1.35	1.31
22	BA	1596	A	C5-C4	-5.67	1.34	1.38
22	BA	1009	A	N3-C4	5.67	1.38	1.34
22	BA	470	A	C5-C4	-5.67	1.34	1.38
22	BA	300	A	C5-C4	-5.67	1.34	1.38
22	BA	2225	A	N3-C4	5.67	1.38	1.34
22	BA	2850	A	N3-C4	5.67	1.38	1.34
22	BA	1470	A	C5-C4	-5.67	1.34	1.38
22	BA	2726	A	N3-C4	5.67	1.38	1.34
22	BA	1548	A	N3-C4	5.66	1.38	1.34
22	BA	1717	A	C5-C4	-5.66	1.34	1.38
22	BA	1739	A	N3-C4	5.66	1.38	1.34
22	BA	1439	A	C5-C4	-5.66	1.34	1.38
22	BA	1598	A	C5-C4	-5.66	1.34	1.38
23	BB	39	A	C5-C4	-5.66	1.34	1.38
22	BA	975	A	C5-C4	-5.66	1.34	1.38
22	BA	614	A	C5-C4	-5.66	1.34	1.38
22	BA	1383	A	C5-C4	-5.66	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1664	A	C5-C4	-5.66	1.34	1.38
22	BA	2531	A	C5-C4	-5.66	1.34	1.38
23	BB	115	A	C5-C4	-5.66	1.34	1.38
22	BA	503	A	C5-C4	-5.65	1.34	1.38
22	BA	2377	A	C5-C4	-5.65	1.34	1.38
22	BA	64	A	C5-C4	-5.65	1.34	1.38
22	BA	73	A	C5-C4	-5.65	1.34	1.38
22	BA	556	A	C5-C4	-5.65	1.34	1.38
22	BA	1936	A	C2-N3	5.65	1.38	1.33
22	BA	730	A	C5-C4	-5.65	1.34	1.38
22	BA	1522	A	N3-C4	5.65	1.38	1.34
22	BA	2439	A	C5-C4	-5.65	1.34	1.38
22	BA	2679	A	C8-N7	5.65	1.35	1.31
22	BA	483	A	C5-C4	-5.64	1.34	1.38
22	BA	2893	A	C5-C4	-5.64	1.34	1.38
22	BA	802	A	C8-N7	5.64	1.35	1.31
22	BA	1858	A	N3-C4	5.64	1.38	1.34
22	BA	226	A	C5-C4	-5.64	1.34	1.38
22	BA	1591	A	N3-C4	5.64	1.38	1.34
22	BA	2468	A	C8-N7	5.64	1.35	1.31
22	BA	2850	A	C5-C4	-5.63	1.34	1.38
22	BA	126	A	C5-C4	-5.63	1.34	1.38
22	BA	750	A	C8-N7	5.63	1.35	1.31
54	D2	35	A	C5-C4	-5.63	1.34	1.38
22	BA	1866	A	N3-C4	5.63	1.38	1.34
22	BA	217	A	C5-C4	-5.63	1.34	1.38
22	BA	1169	A	N3-C4	5.62	1.38	1.34
22	BA	727	A	C8-N7	5.62	1.35	1.31
22	BA	2225	A	C5-C4	-5.62	1.34	1.38
22	BA	13	A	C5-C4	-5.62	1.34	1.38
22	BA	176	A	C5-C4	-5.62	1.34	1.38
22	BA	374	A	N3-C4	5.62	1.38	1.34
22	BA	1936	A	C8-N7	5.62	1.35	1.31
22	BA	2284	A	N3-C4	5.62	1.38	1.34
23	BB	58	A	C5-C4	-5.62	1.34	1.38
22	BA	927	A	C5-C4	-5.61	1.34	1.38
22	BA	1039	A	C5-C4	-5.61	1.34	1.38
22	BA	2212	A	C5-C4	-5.61	1.34	1.38
22	BA	1745	A	N3-C4	5.61	1.38	1.34
22	BA	1977	A	N3-C4	5.61	1.38	1.34
22	BA	2750	A	C5-C4	-5.61	1.34	1.38
22	BA	103	A	C5-C4	-5.61	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2879	A	N3-C4	5.61	1.38	1.34
22	BA	513	A	C8-N7	5.60	1.35	1.31
22	BA	294	A	N3-C4	5.60	1.38	1.34
22	BA	1590	A	N3-C4	5.60	1.38	1.34
22	BA	2426	A	C5-C4	-5.60	1.34	1.38
22	BA	1755	A	C5-C4	-5.60	1.34	1.38
22	BA	165	A	N3-C4	5.60	1.38	1.34
22	BA	320	A	C5-C4	-5.60	1.34	1.38
22	BA	602	A	N3-C4	5.60	1.38	1.34
22	BA	1579	A	C5-C4	-5.59	1.34	1.38
22	BA	91	A	C5-C4	-5.59	1.34	1.38
22	BA	44	A	C5-C4	-5.59	1.34	1.38
22	BA	705	A	C8-N7	5.59	1.35	1.31
1	AA	728	A	N7-C5	-5.59	1.35	1.39
22	BA	217	A	N3-C4	5.59	1.38	1.34
22	BA	829	A	C5-C4	-5.59	1.34	1.38
22	BA	1505	A	C5-C4	-5.59	1.34	1.38
22	BA	2476	A	C5-C4	-5.59	1.34	1.38
23	BB	52	A	C5-C4	-5.59	1.34	1.38
22	BA	311	A	C5-C4	-5.58	1.34	1.38
22	BA	677	A	C8-N7	5.58	1.35	1.31
22	BA	752	A	C5-C4	-5.58	1.34	1.38
1	AA	1236	A	N9-C4	-5.58	1.34	1.37
22	BA	172	A	C5-C4	-5.58	1.34	1.38
22	BA	1553	A	C5-C4	-5.58	1.34	1.38
22	BA	2205	A	C5-C4	-5.58	1.34	1.38
22	BA	532	A	C8-N7	5.58	1.35	1.31
22	BA	1609	A	C5-C4	-5.58	1.34	1.38
23	BB	99	A	N3-C4	5.58	1.38	1.34
22	BA	936	A	C5-C4	-5.58	1.34	1.38
22	BA	1669	A	C5-C4	-5.58	1.34	1.38
55	D3	64	A	C2-N3	5.58	1.38	1.33
22	BA	1717	A	N3-C4	5.58	1.38	1.34
22	BA	1757	A	C5-C4	-5.58	1.34	1.38
22	BA	1746	A	C5-C4	-5.57	1.34	1.38
22	BA	2534	A	C5-C4	-5.57	1.34	1.38
22	BA	83	A	C5-C4	-5.57	1.34	1.38
22	BA	311	A	N3-C4	5.57	1.38	1.34
22	BA	722	A	C5-C4	-5.57	1.34	1.38
22	BA	2199	A	C5-C4	-5.57	1.34	1.38
22	BA	2274	A	C5-C4	-5.57	1.34	1.38
23	BB	59	A	C5-C4	-5.57	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	95	A	C5-C4	-5.57	1.34	1.38
22	BA	2900	A	N3-C4	5.57	1.38	1.34
22	BA	149	A	N3-C4	5.57	1.38	1.34
22	BA	1050	A	C5-C4	-5.57	1.34	1.38
22	BA	1453	A	C5-C4	-5.57	1.34	1.38
54	D2	59	A	N3-C4	5.57	1.38	1.34
22	BA	64	A	N3-C4	5.57	1.38	1.34
22	BA	928	A	C5-C4	-5.57	1.34	1.38
22	BA	2577	A	C8-N7	5.57	1.35	1.31
22	BA	820	A	N3-C4	5.56	1.38	1.34
22	BA	71	A	N3-C4	5.56	1.38	1.34
22	BA	152	A	C5-C4	-5.56	1.34	1.38
22	BA	1916	A	N3-C4	5.56	1.38	1.34
22	BA	2749	A	N3-C4	5.56	1.38	1.34
22	BA	94	A	N3-C4	5.56	1.38	1.34
22	BA	2531	A	N3-C4	5.56	1.38	1.34
22	BA	1847	A	N3-C4	5.56	1.38	1.34
22	BA	2392	A	C5-C4	-5.56	1.34	1.38
22	BA	2899	A	C5-C4	-5.56	1.34	1.38
22	BA	167	A	N3-C4	5.55	1.38	1.34
22	BA	603	A	C5-C4	-5.55	1.34	1.38
22	BA	742	A	N3-C4	5.55	1.38	1.34
22	BA	74	A	N3-C4	5.55	1.38	1.34
22	BA	2587	A	N3-C4	5.55	1.38	1.34
22	BA	2657	A	C5-C4	-5.55	1.34	1.38
22	BA	272	A	C5-C4	-5.55	1.34	1.38
22	BA	1829	A	N3-C4	5.55	1.38	1.34
22	BA	2868	A	N3-C4	5.55	1.38	1.34
22	BA	2800	A	C5-C4	-5.55	1.34	1.38
22	BA	1936	A	C5-C4	-5.55	1.34	1.38
22	BA	927	A	N3-C4	5.55	1.38	1.34
22	BA	1494	A	N3-C4	5.55	1.38	1.34
22	BA	428	A	N3-C4	5.54	1.38	1.34
22	BA	1590	A	C5-C4	-5.54	1.34	1.38
22	BA	2108	A	N3-C4	5.54	1.38	1.34
22	BA	197	A	N3-C4	5.54	1.38	1.34
54	D2	38	A	C5-C4	-5.54	1.34	1.38
22	BA	1919	A	C5-C4	-5.54	1.34	1.38
22	BA	404	A	N3-C4	5.54	1.38	1.34
23	BB	66	A	N3-C4	5.54	1.38	1.34
22	BA	173	A	N3-C4	5.53	1.38	1.34
22	BA	532	A	N3-C4	5.53	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1495	A	C5-C4	-5.53	1.34	1.38
54	D2	58	A	C5-C4	-5.53	1.34	1.38
22	BA	1504	A	N3-C4	5.53	1.38	1.34
22	BA	2856	A	N3-C4	5.53	1.38	1.34
22	BA	94	A	C5-C4	-5.53	1.34	1.38
22	BA	819	A	C8-N7	5.53	1.35	1.31
23	BB	58	A	N3-C4	5.53	1.38	1.34
22	BA	2748	A	C5-C4	-5.53	1.34	1.38
22	BA	1142	A	N3-C4	5.52	1.38	1.34
22	BA	1593	A	C5-C4	-5.52	1.34	1.38
22	BA	2298	A	C5-C4	-5.52	1.34	1.38
22	BA	1938	A	N3-C4	5.52	1.38	1.34
54	D2	23	A	N3-C4	5.51	1.38	1.34
55	D3	23	A	N3-C4	5.51	1.38	1.34
22	BA	722	A	N3-C4	5.51	1.38	1.34
22	BA	2376	A	N3-C4	5.51	1.38	1.34
22	BA	1387	A	N3-C4	5.51	1.38	1.34
22	BA	2183	A	C2-N3	5.51	1.38	1.33
22	BA	2317	A	N3-C4	5.51	1.38	1.34
22	BA	56	A	N3-C4	5.50	1.38	1.34
22	BA	2749	A	C5-C4	-5.50	1.34	1.38
22	BA	146	A	C5-C4	-5.50	1.34	1.38
22	BA	643	A	C5-C4	-5.50	1.34	1.38
22	BA	2900	A	C5-C4	-5.50	1.34	1.38
22	BA	83	A	N3-C4	5.50	1.38	1.34
22	BA	1705	A	N3-C4	5.50	1.38	1.34
54	D2	38	A	N3-C4	5.50	1.38	1.34
22	BA	10	A	N3-C4	5.50	1.38	1.34
22	BA	294	A	C5-C4	-5.50	1.34	1.38
22	BA	1040	A	N3-C4	5.50	1.38	1.34
22	BA	2328	A	C5-C4	-5.50	1.34	1.38
22	BA	1494	A	C5-C4	-5.49	1.34	1.38
22	BA	1503	A	N3-C4	5.49	1.38	1.34
22	BA	2482	A	C5-C4	-5.49	1.34	1.38
23	BB	15	A	C5-C4	-5.49	1.34	1.38
22	BA	429	A	N3-C4	5.49	1.38	1.34
22	BA	1269	A	C8-N7	5.49	1.35	1.31
54	D2	28	A	C5-C4	-5.49	1.34	1.38
22	BA	1403	A	N3-C4	5.48	1.38	1.34
23	BB	52	A	N3-C4	5.48	1.38	1.34
22	BA	340	A	N3-C4	5.48	1.38	1.34
22	BA	345	A	C5-C4	-5.48	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	643	A	N3-C4	5.48	1.38	1.34
22	BA	945	A	N3-C4	5.48	1.38	1.34
22	BA	1927	A	N3-C4	5.48	1.38	1.34
22	BA	582	A	N3-C4	5.48	1.38	1.34
22	BA	1586	A	N3-C4	5.48	1.38	1.34
23	BB	119	A	C5-C4	-5.48	1.34	1.38
54	D2	73	A	C5-C4	-5.48	1.34	1.38
22	BA	332	A	N3-C4	5.48	1.38	1.34
22	BA	592	A	C5-C4	-5.47	1.34	1.38
22	BA	1365	A	N3-C4	5.47	1.38	1.34
22	BA	1616	A	N3-C4	5.47	1.38	1.34
22	BA	2298	A	N3-C4	5.47	1.38	1.34
22	BA	2766	A	C8-N7	5.47	1.35	1.31
22	BA	1672	A	N3-C4	5.47	1.38	1.34
22	BA	1027	A	N3-C4	5.47	1.38	1.34
22	BA	2748	A	N3-C4	5.46	1.38	1.34
22	BA	348	A	C5-C4	-5.46	1.34	1.38
22	BA	1413	A	N3-C4	5.46	1.38	1.34
23	BB	57	A	C5-C4	-5.46	1.34	1.38
22	BA	2482	A	N3-C4	5.46	1.38	1.34
22	BA	172	A	N3-C4	5.46	1.38	1.34
22	BA	165	A	C5-C4	-5.45	1.34	1.38
22	BA	181	A	C5-C4	-5.45	1.34	1.38
22	BA	1819	A	N3-C4	5.45	1.38	1.34
23	BB	45	A	C5-C4	-5.45	1.34	1.38
1	AA	1223	C	N1-C6	-5.45	1.33	1.37
22	BA	492	A	N3-C4	5.45	1.38	1.34
22	BA	44	A	N3-C4	5.45	1.38	1.34
22	BA	2733	A	C5-C4	-5.45	1.34	1.38
22	BA	1205	A	C5-C4	-5.45	1.34	1.38
22	BA	1970	A	C8-N7	5.45	1.35	1.31
23	BB	46	A	N3-C4	5.45	1.38	1.34
22	BA	734	A	N3-C4	5.45	1.38	1.34
22	BA	447	A	N3-C4	5.44	1.38	1.34
22	BA	2094	A	N3-C4	5.44	1.38	1.34
23	BB	53	A	C5-C4	-5.44	1.34	1.38
22	BA	52	A	N3-C4	5.44	1.38	1.34
22	BA	1679	A	C5-C4	-5.44	1.34	1.38
22	BA	2518	A	N3-C4	5.44	1.38	1.34
22	BA	412	A	C5-C4	-5.43	1.34	1.38
1	AA	973	G	N7-C5	-5.43	1.35	1.39
22	BA	616	A	C5-C4	-5.43	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D2	23	A	C5-C4	-5.43	1.34	1.38
22	BA	666	A	N3-C4	5.43	1.38	1.34
22	BA	789	A	N3-C4	5.43	1.38	1.34
22	BA	1301	A	N3-C4	5.43	1.38	1.34
22	BA	1890	A	N3-C4	5.43	1.38	1.34
22	BA	342	A	N3-C4	5.43	1.38	1.34
22	BA	348	A	N3-C4	5.43	1.38	1.34
22	BA	1134	A	N3-C4	5.43	1.38	1.34
22	BA	1609	A	N3-C4	5.43	1.38	1.34
22	BA	1634	A	N3-C4	5.43	1.38	1.34
22	BA	2886	A	N3-C4	5.43	1.38	1.34
54	D2	58	A	N3-C4	5.42	1.38	1.34
22	BA	354	A	C5-C4	-5.42	1.34	1.38
22	BA	793	A	N3-C4	5.42	1.38	1.34
22	BA	1885	A	N3-C4	5.42	1.38	1.34
22	BA	1111	A	N3-C4	5.42	1.38	1.34
22	BA	2199	A	N3-C4	5.42	1.38	1.34
22	BA	2657	A	N3-C4	5.42	1.38	1.34
22	BA	2679	A	N3-C4	5.42	1.38	1.34
22	BA	1553	A	N3-C4	5.41	1.38	1.34
22	BA	63	A	C5-C4	-5.41	1.34	1.38
22	BA	1151	A	N3-C4	5.41	1.38	1.34
22	BA	1545	A	N3-C4	5.41	1.38	1.34
22	BA	2227	A	N3-C4	5.41	1.38	1.34
22	BA	2868	A	C5-C4	-5.41	1.34	1.38
22	BA	173	A	C5-C4	-5.41	1.34	1.38
22	BA	1419	A	N3-C4	5.41	1.38	1.34
22	BA	2799	A	C2-N3	5.41	1.38	1.33
22	BA	1286	A	N3-C4	5.41	1.38	1.34
23	BB	119	A	N3-C4	5.41	1.38	1.34
22	BA	1889	A	N3-C4	5.40	1.38	1.34
22	BA	2317	A	C5-C4	-5.40	1.34	1.38
22	BA	412	A	N3-C4	5.40	1.38	1.34
22	BA	2287	A	N3-C4	5.40	1.38	1.34
55	D3	76	A	C5-C4	-5.40	1.34	1.38
22	BA	104	A	N3-C4	5.40	1.38	1.34
22	BA	142	A	N3-C4	5.40	1.38	1.34
22	BA	1284	A	N3-C4	5.40	1.38	1.34
22	BA	2377	A	N3-C4	5.40	1.38	1.34
1	AA	1362	A	N3-C4	-5.40	1.31	1.34
1	AA	1368	A	N9-C4	-5.40	1.34	1.37
22	BA	344	A	C5-C4	-5.40	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1899	A	N3-C4	5.39	1.38	1.34
22	BA	829	A	N3-C4	5.39	1.38	1.34
22	BA	910	A	N3-C4	5.39	1.38	1.34
22	BA	1978	A	N3-C4	5.39	1.38	1.34
22	BA	1637	A	N3-C4	5.39	1.38	1.34
22	BA	1237	A	N3-C4	5.39	1.38	1.34
22	BA	2665	A	N3-C4	5.39	1.38	1.34
23	BB	104	A	N3-C4	5.38	1.38	1.34
22	BA	522	A	N3-C4	5.38	1.38	1.34
22	BA	1268	A	N3-C4	5.38	1.38	1.34
22	BA	1998	A	N3-C4	5.38	1.38	1.34
1	AA	1239	A	N9-C4	-5.38	1.34	1.37
22	BA	637	A	N3-C4	5.38	1.38	1.34
22	BA	2814	A	N3-C4	5.38	1.38	1.34
22	BA	1640	A	N3-C4	5.38	1.38	1.34
22	BA	2461	A	N3-C4	5.37	1.38	1.34
1	AA	951	G	N7-C5	-5.37	1.36	1.39
22	BA	1913	A	C5-C4	-5.37	1.34	1.38
22	BA	2311	A	N3-C4	5.37	1.38	1.34
22	BA	2534	A	N3-C4	5.37	1.38	1.34
54	D2	35	A	N3-C4	5.37	1.38	1.34
22	BA	1111	A	C5-C4	-5.37	1.34	1.38
22	BA	1801	A	C5-C4	-5.37	1.34	1.38
22	BA	2476	A	N3-C4	5.37	1.38	1.34
1	AA	979	C	N1-C6	-5.36	1.33	1.37
22	BA	1918	A	C5-C4	-5.36	1.34	1.38
22	BA	2835	A	N3-C4	5.36	1.38	1.34
54	D2	76	A	N3-C4	5.36	1.38	1.34
1	AA	1361	G	C5-C4	-5.36	1.34	1.38
22	BA	1912	A	N3-C4	5.36	1.38	1.34
22	BA	2060	A	N3-C4	5.36	1.38	1.34
22	BA	2654	A	N3-C4	5.36	1.38	1.34
22	BA	2776	A	N3-C4	5.36	1.38	1.34
22	BA	207	A	N3-C4	5.36	1.38	1.34
22	BA	270	A	N3-C4	5.36	1.38	1.34
22	BA	911	A	N3-C4	5.36	1.38	1.34
22	BA	2378	A	N3-C4	5.35	1.38	1.34
22	BA	1027	A	C5-C4	-5.35	1.35	1.38
1	AA	974	A	N7-C5	-5.35	1.36	1.39
22	BA	2800	A	N3-C4	5.35	1.38	1.34
22	BA	2820	A	C5-C4	-5.35	1.35	1.38
22	BA	49	A	N3-C4	5.35	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2851	A	N3-C4	5.35	1.38	1.34
22	BA	1525	A	N3-C4	5.35	1.38	1.34
22	BA	609	A	N3-C4	5.34	1.38	1.34
54	D2	9	A	C5-C4	-5.34	1.35	1.38
22	BA	63	A	N3-C4	5.34	1.38	1.34
22	BA	947	A	N3-C4	5.34	1.38	1.34
22	BA	1528	A	N3-C4	5.34	1.38	1.34
22	BA	849	A	N3-C4	5.34	1.38	1.34
22	BA	917	A	N3-C4	5.34	1.38	1.34
23	BB	109	A	C5-C4	-5.34	1.35	1.38
54	D2	5	A	C5-C4	-5.34	1.35	1.38
22	BA	2761	A	N3-C4	5.34	1.38	1.34
22	BA	2639	A	N3-C4	5.33	1.38	1.34
1	AA	1087	G	N9-C8	-5.33	1.34	1.37
22	BA	53	A	N3-C4	5.33	1.38	1.34
22	BA	1126	A	N3-C4	5.33	1.38	1.34
22	BA	1336	A	N3-C4	5.33	1.38	1.34
22	BA	5	A	C5-C4	-5.33	1.35	1.38
22	BA	1918	A	N3-C4	5.33	1.38	1.34
22	BA	2082	A	N3-C4	5.32	1.38	1.34
22	BA	2311	A	C5-C4	-5.32	1.35	1.38
22	BA	2426	A	N3-C4	5.32	1.38	1.34
22	BA	91	A	N3-C4	5.32	1.38	1.34
22	BA	1677	A	N3-C4	5.32	1.38	1.34
22	BA	2469	A	N3-C4	5.32	1.38	1.34
22	BA	960	A	C8-N7	5.32	1.35	1.31
22	BA	103	A	N3-C4	5.32	1.38	1.34
22	BA	161	A	N3-C4	5.32	1.38	1.34
22	BA	1815	A	N3-C4	5.32	1.38	1.34
22	BA	320	A	N3-C4	5.31	1.38	1.34
1	AA	1323	G	C5-C4	-5.31	1.34	1.38
22	BA	149	A	C5-C4	-5.31	1.35	1.38
22	BA	347	A	C5-C4	-5.31	1.35	1.38
22	BA	941	A	N3-C4	5.31	1.38	1.34
22	BA	156	A	C5-C4	-5.30	1.35	1.38
22	BA	330	A	C5-C4	-5.30	1.35	1.38
22	BA	282	A	C5-C4	-5.30	1.35	1.38
22	BA	2634	A	N3-C4	5.30	1.38	1.34
22	BA	256	A	N3-C4	5.30	1.38	1.34
22	BA	582	A	C8-N7	5.30	1.35	1.31
22	BA	352	A	C5-C4	-5.30	1.35	1.38
22	BA	1509	A	C5-C4	-5.30	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2378	A	C5-C4	-5.30	1.35	1.38
23	BB	34	A	N3-C4	5.30	1.38	1.34
22	BA	2432	A	N3-C4	5.30	1.38	1.34
23	BB	46	A	C5-C4	-5.30	1.35	1.38
22	BA	804	A	N3-C4	5.29	1.38	1.34
22	BA	2590	A	N3-C4	5.29	1.38	1.34
22	BA	2439	A	N3-C4	5.29	1.38	1.34
22	BA	404	A	C5-C4	-5.29	1.35	1.38
22	BA	371	A	N3-C4	5.29	1.38	1.34
22	BA	933	A	C5-C4	-5.29	1.35	1.38
54	D2	59	A	C5-C4	-5.29	1.35	1.38
22	BA	272	A	N3-C4	5.28	1.38	1.34
22	BA	603	A	N3-C4	5.28	1.38	1.34
22	BA	1322	A	N3-C4	5.28	1.38	1.34
22	BA	1496	A	N3-C4	5.28	1.38	1.34
22	BA	2019	A	N3-C4	5.28	1.38	1.34
22	BA	2425	A	N3-C4	5.28	1.38	1.34
22	BA	2270	A	N3-C4	5.28	1.38	1.34
22	BA	95	A	N3-C4	5.28	1.38	1.34
22	BA	142	A	C5-C4	-5.28	1.35	1.38
22	BA	346	A	C5-C4	-5.28	1.35	1.38
22	BA	572	A	N3-C4	5.28	1.38	1.34
22	BA	1433	A	N3-C4	5.28	1.38	1.34
22	BA	2198	A	N3-C4	5.28	1.38	1.34
22	BA	2322	A	N3-C4	5.28	1.38	1.34
22	BA	345	A	N3-C4	5.27	1.38	1.34
22	BA	1098	A	C2-N3	5.27	1.38	1.33
22	BA	1876	A	C5-C4	-5.27	1.35	1.38
22	BA	878	A	C5-C4	-5.27	1.35	1.38
22	BA	2753	A	N3-C4	5.27	1.38	1.34
1	AA	1357	A	N9-C4	-5.27	1.34	1.37
22	BA	233	A	N3-C4	5.27	1.38	1.34
22	BA	1549	A	N3-C4	5.27	1.38	1.34
22	BA	2335	A	N3-C4	5.27	1.38	1.34
22	BA	2660	A	C5-C4	-5.27	1.35	1.38
22	BA	2799	A	C5-C4	-5.27	1.35	1.38
22	BA	2814	A	C5-C4	-5.27	1.35	1.38
22	BA	928	A	N3-C4	5.27	1.38	1.34
22	BA	2205	A	N3-C4	5.27	1.38	1.34
22	BA	181	A	N3-C4	5.26	1.38	1.34
22	BA	2734	A	N3-C4	5.26	1.38	1.34
22	BA	1866	A	C5-C4	-5.26	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	608	A	N3-C4	5.26	1.38	1.34
22	BA	2542	A	N3-C4	5.26	1.38	1.34
22	BA	111	A	N3-C4	5.25	1.38	1.34
22	BA	513	A	N7-C5	-5.25	1.36	1.39
22	BA	1552	A	N3-C4	5.25	1.38	1.34
22	BA	705	A	N3-C4	5.25	1.38	1.34
22	BA	1932	A	N3-C4	5.25	1.38	1.34
22	BA	2670	A	N3-C4	5.25	1.38	1.34
22	BA	1169	A	C5-C4	-5.25	1.35	1.38
22	BA	2809	A	N3-C4	5.25	1.38	1.34
22	BA	1241	A	C5-C4	-5.25	1.35	1.38
22	BA	1722	A	C5-C4	-5.25	1.35	1.38
22	BA	2266	A	N3-C4	5.25	1.38	1.34
22	BA	176	A	N3-C4	5.25	1.38	1.34
22	BA	979	A	N3-C4	5.25	1.38	1.34
22	BA	1155	A	N3-C4	5.25	1.38	1.34
22	BA	721	A	C5-C4	-5.24	1.35	1.38
22	BA	1871	A	C5-C4	-5.24	1.35	1.38
54	D2	28	A	C2-N3	5.24	1.38	1.33
54	D2	49	A	C5-C4	-5.24	1.35	1.38
22	BA	513	A	N3-C4	5.24	1.38	1.34
1	AA	1252	A	N9-C4	-5.24	1.34	1.37
22	BA	1272	A	N3-C4	5.24	1.38	1.34
22	BA	14	A	N3-C4	5.24	1.38	1.34
22	BA	152	A	N3-C4	5.24	1.38	1.34
22	BA	255	A	N3-C4	5.23	1.38	1.34
22	BA	1147	A	N3-C4	5.23	1.38	1.34
22	BA	2154	A	C5-C4	-5.23	1.35	1.38
22	BA	1528	A	C5-C4	-5.23	1.35	1.38
22	BA	1690	A	N3-C4	5.23	1.38	1.34
22	BA	1735	A	C5-C4	-5.23	1.35	1.38
22	BA	2042	A	N3-C4	5.23	1.38	1.34
22	BA	346	A	N3-C4	5.23	1.38	1.34
22	BA	1322	A	C5-C4	-5.23	1.35	1.38
22	BA	2757	A	C5-C4	-5.23	1.35	1.38
22	BA	661	A	N3-C4	5.22	1.38	1.34
22	BA	2135	A	C2-N3	5.22	1.38	1.33
22	BA	146	A	N3-C4	5.22	1.38	1.34
22	BA	1328	A	N3-C4	5.22	1.38	1.34
22	BA	182	A	N3-C4	5.22	1.38	1.34
22	BA	1608	A	N3-C4	5.22	1.38	1.34
22	BA	2183	A	C5-C4	-5.22	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1320	C	N1-C6	-5.22	1.34	1.37
22	BA	1744	A	C5-C4	-5.22	1.35	1.38
22	BA	2738	A	N3-C4	5.22	1.38	1.34
22	BA	1502	A	N3-C4	5.21	1.38	1.34
22	BA	1848	A	N3-C4	5.21	1.38	1.34
22	BA	2406	A	C5-C4	-5.21	1.35	1.38
1	AA	1234	C	N3-C4	-5.21	1.30	1.33
22	BA	626	A	C5-C4	-5.21	1.35	1.38
22	BA	751	A	N3-C4	5.21	1.38	1.34
22	BA	2171	A	C5-C4	-5.21	1.35	1.38
22	BA	2682	A	N3-C4	5.21	1.38	1.34
22	BA	1205	A	N3-C4	5.21	1.38	1.34
22	BA	1477	A	N3-C4	5.21	1.38	1.34
22	BA	1937	A	N3-C4	5.21	1.38	1.34
22	BA	2727	A	N3-C4	5.21	1.38	1.34
23	BB	66	A	C5-C4	-5.21	1.35	1.38
22	BA	38	A	N3-C4	5.21	1.38	1.34
22	BA	1021	A	N3-C4	5.21	1.38	1.34
22	BA	2778	A	N3-C4	5.21	1.38	1.34
22	BA	477	A	N3-C4	5.21	1.38	1.34
22	BA	2826	A	N3-C4	5.20	1.38	1.34
1	AA	1221	G	C5-C4	-5.20	1.34	1.38
22	BA	13	A	N3-C4	5.20	1.38	1.34
22	BA	1269	A	N3-C4	5.20	1.38	1.34
1	AA	1371	G	C5-C4	-5.20	1.34	1.38
22	BA	716	A	C5-C4	-5.20	1.35	1.38
22	BA	718	A	C5-C4	-5.20	1.35	1.38
22	BA	1383	A	N3-C4	5.20	1.38	1.34
22	BA	2119	A	C5-C4	-5.20	1.35	1.38
22	BA	1669	A	N3-C4	5.19	1.38	1.34
22	BA	877	A	C5-C4	-5.19	1.35	1.38
22	BA	2792	A	N3-C4	5.19	1.38	1.34
22	BA	322	A	N3-C4	5.19	1.38	1.34
22	BA	783	A	C5-C4	-5.19	1.35	1.38
22	BA	423	A	N3-C4	5.19	1.38	1.34
22	BA	28	A	N3-C4	5.19	1.38	1.34
22	BA	231	A	N3-C4	5.19	1.38	1.34
22	BA	497	A	N3-C4	5.18	1.38	1.34
22	BA	2314	A	N3-C4	5.18	1.38	1.34
22	BA	368	A	C5-C4	-5.18	1.35	1.38
22	BA	1214	A	N3-C4	5.18	1.38	1.34
22	BA	2430	A	C5-C4	-5.18	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2451	A	N3-C4	5.18	1.38	1.34
22	BA	479	A	N3-C4	5.18	1.38	1.34
22	BA	2813	A	C5-C4	-5.18	1.35	1.38
22	BA	1213	A	N3-C4	5.18	1.38	1.34
22	BA	1054	A	C2-N3	5.18	1.38	1.33
22	BA	2058	A	N3-C4	5.18	1.38	1.34
22	BA	1495	A	N3-C4	5.17	1.38	1.34
22	BA	1532	A	C5-C4	-5.17	1.35	1.38
22	BA	933	A	N3-C4	5.17	1.38	1.34
22	BA	1054	A	C5-C4	-5.17	1.35	1.38
23	BB	108	A	N3-C4	5.17	1.38	1.34
54	D2	21	A	C5-C4	-5.17	1.35	1.38
1	AA	1361	G	N9-C4	-5.17	1.33	1.38
22	BA	2191	A	C5-C4	-5.17	1.35	1.38
23	BB	29	A	N3-C4	5.17	1.38	1.34
22	BA	1745	A	C5-C4	-5.17	1.35	1.38
22	BA	2392	A	N3-C4	5.17	1.38	1.34
22	BA	155	A	N3-C4	5.17	1.38	1.34
22	BA	460	A	N3-C4	5.17	1.38	1.34
22	BA	654	A	C2-N3	5.17	1.38	1.33
22	BA	1755	A	N3-C4	5.17	1.38	1.34
1	AA	1252	A	N3-C4	-5.16	1.31	1.34
22	BA	2101	A	C5-C4	-5.16	1.35	1.38
22	BA	501	A	N3-C4	5.16	1.38	1.34
22	BA	2031	A	N3-C4	5.16	1.38	1.34
55	D3	9	A	C2-N3	5.16	1.38	1.33
22	BA	655	A	N3-C4	5.16	1.38	1.34
22	BA	1420	A	C5-C4	-5.16	1.35	1.38
22	BA	633	A	N3-C4	5.15	1.38	1.34
22	BA	1593	A	N3-C4	5.15	1.38	1.34
55	D3	14	A	C5-C4	-5.15	1.35	1.38
22	BA	1032	A	N3-C4	5.15	1.38	1.34
22	BA	1096	A	C2-N3	5.15	1.38	1.33
22	BA	1434	A	N3-C4	5.15	1.38	1.34
22	BA	2135	A	C5-C4	-5.15	1.35	1.38
22	BA	223	A	N3-C4	5.15	1.38	1.34
22	BA	693	A	N3-C4	5.15	1.38	1.34
22	BA	2095	A	N3-C4	5.15	1.38	1.34
22	BA	1916	A	C5-C4	-5.14	1.35	1.38
22	BA	104	A	C5-C4	-5.14	1.35	1.38
22	BA	190	A	N3-C4	5.14	1.38	1.34
22	BA	251	A	C8-N7	5.14	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	101	A	N3-C4	5.14	1.38	1.34
54	D2	69	A	C2-N3	5.14	1.38	1.33
22	BA	2433	A	N3-C4	5.14	1.38	1.34
22	BA	2541	A	N3-C4	5.14	1.38	1.34
22	BA	715	A	C5-C4	-5.14	1.35	1.38
1	AA	1318	A	C5-C6	-5.14	1.36	1.41
22	BA	2184	A	C2-N3	5.14	1.38	1.33
1	AA	984	C	N1-C6	-5.13	1.34	1.37
22	BA	300	A	N3-C4	5.13	1.38	1.34
22	BA	2765	A	N3-C4	5.13	1.38	1.34
22	BA	504	A	C2-N3	5.13	1.38	1.33
22	BA	508	A	C5-C4	-5.13	1.35	1.38
22	BA	1580	A	C5-C4	-5.13	1.35	1.38
22	BA	1641	A	N3-C4	5.13	1.38	1.34
22	BA	2758	A	N3-C4	5.13	1.38	1.34
22	BA	592	A	N3-C4	5.13	1.38	1.34
22	BA	1586	A	C5-C4	-5.13	1.35	1.38
22	BA	5	A	N3-C4	5.13	1.38	1.34
22	BA	354	A	N3-C4	5.13	1.38	1.34
1	AA	1223	C	N3-C4	-5.12	1.30	1.33
22	BA	1156	A	N3-C4	5.12	1.38	1.34
22	BA	2823	A	N3-C4	5.12	1.38	1.34
22	BA	1373	A	N3-C4	5.12	1.38	1.34
22	BA	422	A	N3-C4	5.12	1.38	1.34
22	BA	1739	A	C2-N3	5.12	1.38	1.33
1	AA	1314	C	N1-C6	-5.12	1.34	1.37
22	BA	1583	A	C5-C4	-5.12	1.35	1.38
22	BA	1535	A	C2-N3	5.11	1.38	1.33
22	BA	2097	A	C5-C4	-5.11	1.35	1.38
22	BA	1508	A	C5-C4	-5.11	1.35	1.38
22	BA	2097	A	C2-N3	5.11	1.38	1.33
22	BA	126	A	N3-C4	5.11	1.38	1.34
22	BA	1085	A	C2-N3	5.11	1.38	1.33
22	BA	1469	A	N3-C4	5.11	1.38	1.34
22	BA	2211	A	C5-C4	-5.11	1.35	1.38
55	D3	21	A	C5-C4	-5.11	1.35	1.38
1	AA	977	A	C5-C4	-5.11	1.35	1.38
1	AA	1352	C	N1-C6	-5.11	1.34	1.37
54	D2	14	A	C5-C4	-5.11	1.35	1.38
22	BA	347	A	N3-C4	5.11	1.38	1.34
22	BA	1230	A	N3-C4	5.11	1.38	1.34
22	BA	1901	A	N3-C4	5.11	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	199	A	N3-C4	5.10	1.38	1.34
22	BA	825	A	N3-C4	5.10	1.38	1.34
22	BA	1746	A	C2-N3	5.10	1.38	1.33
22	BA	2003	A	N3-C4	5.10	1.38	1.34
22	BA	1810	A	C8-N7	5.10	1.35	1.31
1	AA	1221	G	C6-N1	-5.10	1.35	1.39
23	BB	15	A	N3-C4	5.10	1.38	1.34
22	BA	670	A	N3-C4	5.10	1.38	1.34
22	BA	2530	A	N3-C4	5.10	1.38	1.34
22	BA	2577	A	N3-C4	5.10	1.38	1.34
22	BA	2781	A	N3-C4	5.09	1.38	1.34
54	D2	41	A	N3-C4	5.09	1.38	1.34
55	D3	7	A	C5-C4	-5.09	1.35	1.38
55	D3	26	A	C2-N3	5.09	1.38	1.33
22	BA	507	A	N3-C4	5.09	1.38	1.34
22	BA	2478	A	N3-C4	5.09	1.38	1.34
22	BA	1571	A	N3-C4	5.08	1.38	1.34
23	BB	78	A	N3-C4	5.08	1.38	1.34
22	BA	480	A	N3-C4	5.08	1.37	1.34
22	BA	1528	A	C2-N3	5.08	1.38	1.33
22	BA	251	A	N3-C4	5.08	1.37	1.34
1	AA	1280	A	N9-C4	-5.08	1.34	1.37
22	BA	749	A	N3-C4	5.08	1.37	1.34
22	BA	1591	A	C5-C4	-5.08	1.35	1.38
22	BA	2662	A	C2-N3	5.08	1.38	1.33
22	BA	1175	A	C2-N3	5.07	1.38	1.33
22	BA	1785	A	N3-C4	5.07	1.37	1.34
1	AA	865	A	N7-C5	-5.07	1.36	1.39
1	AA	1371	G	N9-C8	-5.07	1.34	1.37
54	D2	69	A	C5-C4	-5.07	1.35	1.38
22	BA	1067	A	C2-N3	5.06	1.38	1.33
22	BA	1069	A	C2-N3	5.06	1.38	1.33
22	BA	2126	A	C2-N3	5.06	1.38	1.33
22	BA	84	A	N3-C4	5.06	1.37	1.34
22	BA	279	A	C5-C4	-5.06	1.35	1.38
22	BA	1080	A	C2-N3	5.06	1.38	1.33
22	BA	1470	A	N3-C4	5.06	1.37	1.34
22	BA	899	A	C2-N3	5.06	1.38	1.33
22	BA	960	A	N3-C4	5.06	1.37	1.34
22	BA	574	A	N3-C4	5.06	1.37	1.34
1	AA	994	A	N7-C5	-5.05	1.36	1.39
22	BA	218	A	N3-C4	5.05	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1302	A	N3-C4	5.05	1.37	1.34
22	BA	1384	A	N3-C4	5.05	1.37	1.34
22	BA	453	A	N3-C4	5.05	1.37	1.34
22	BA	1665	A	N3-C4	5.05	1.37	1.34
22	BA	556	A	N3-C4	5.05	1.37	1.34
22	BA	920	A	N3-C4	5.05	1.37	1.34
22	BA	265	A	N3-C4	5.05	1.37	1.34
22	BA	1784	A	N3-C4	5.05	1.37	1.34
1	AA	975	A	N3-C4	-5.05	1.31	1.34
22	BA	1532	A	C2-N3	5.05	1.38	1.33
22	BA	1762	A	N3-C4	5.05	1.37	1.34
22	BA	2191	A	C2-N3	5.05	1.38	1.33
22	BA	1569	A	N3-C4	5.04	1.37	1.34
55	D3	76	A	N3-C4	5.04	1.37	1.34
22	BA	1392	A	N3-C4	5.04	1.37	1.34
22	BA	2333	A	N3-C4	5.04	1.37	1.34
22	BA	2366	A	N3-C4	5.04	1.37	1.34
22	BA	1287	A	N3-C4	5.04	1.37	1.34
22	BA	900	A	C5-C4	-5.04	1.35	1.38
22	BA	983	A	N3-C4	5.04	1.37	1.34
22	BA	1676	A	N3-C4	5.04	1.37	1.34
22	BA	2088	A	N3-C4	5.04	1.37	1.34
22	BA	2267	A	N3-C4	5.04	1.37	1.34
22	BA	644	A	N3-C4	5.04	1.37	1.34
22	BA	1919	A	N3-C4	5.04	1.37	1.34
22	BA	2340	A	N3-C4	5.04	1.37	1.34
22	BA	2856	A	C2-N3	5.04	1.38	1.33
22	BA	1029	A	N3-C4	5.03	1.37	1.34
22	BA	2090	A	N3-C4	5.03	1.37	1.34
1	AA	1355	G	N7-C5	-5.03	1.36	1.39
22	BA	1872	A	C2-N3	5.03	1.38	1.33
22	BA	160	A	N3-C4	5.03	1.37	1.34
22	BA	529	A	N3-C4	5.03	1.37	1.34
22	BA	892	A	C2-N3	5.03	1.38	1.33
22	BA	1439	A	N3-C4	5.03	1.37	1.34
22	BA	1591	A	C2-N3	5.03	1.38	1.33
22	BA	1810	A	N7-C5	-5.03	1.36	1.39
22	BA	1020	A	N3-C4	5.03	1.37	1.34
22	BA	1080	A	C5-C4	-5.03	1.35	1.38
22	BA	203	A	N3-C4	5.02	1.37	1.34
22	BA	503	A	N3-C4	5.02	1.37	1.34
22	BA	1877	A	C5-C4	-5.02	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2675	A	N3-C4	5.02	1.37	1.34
54	D2	5	A	C2-N3	5.02	1.38	1.33
55	D3	31	A	C2-N3	5.02	1.38	1.33
22	BA	863	A	N3-C4	5.02	1.37	1.34
1	AA	951	G	C5-C4	-5.02	1.34	1.38
22	BA	196	A	N3-C4	5.02	1.37	1.34
22	BA	547	A	C5-C4	-5.02	1.35	1.38
22	BA	727	A	N3-C4	5.02	1.37	1.34
22	BA	936	A	N3-C4	5.01	1.37	1.34
22	BA	1679	A	N3-C4	5.01	1.37	1.34
22	BA	1169	A	C2-N3	5.01	1.38	1.33
22	BA	2147	A	C2-N3	5.01	1.38	1.33
23	BB	39	A	N3-C4	5.01	1.37	1.34
1	AA	951	G	N9-C8	-5.01	1.34	1.37
22	BA	1749	A	N3-C4	5.01	1.37	1.34
22	BA	1808	A	C5-C4	-5.01	1.35	1.38
22	BA	1848	A	C5-C4	-5.01	1.35	1.38
22	BA	382	A	N3-C4	5.01	1.37	1.34
22	BA	925	A	C2-N3	5.01	1.38	1.33
22	BA	2430	A	N7-C5	-5.00	1.36	1.39
22	BA	204	A	N3-C4	5.00	1.37	1.34
22	BA	2706	A	C2-N3	5.00	1.38	1.33
23	BB	73	A	C5-C4	-5.00	1.35	1.38

All (9557) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1021	A	C2-N3-C4	22.58	121.89	110.60
22	BA	783	A	C2-N3-C4	22.43	121.82	110.60
22	BA	1515	A	N1-C6-N6	-22.17	105.30	118.60
22	BA	2765	A	C2-N3-C4	21.64	121.42	110.60
22	BA	1392	A	C2-N3-C4	21.64	121.42	110.60
22	BA	621	A	N1-C6-N6	-21.60	105.64	118.60
22	BA	613	A	C2-N3-C4	21.54	121.37	110.60
22	BA	764	A	N1-C6-N6	-21.46	105.72	118.60
22	BA	1901	A	C2-N3-C4	21.35	121.27	110.60
22	BA	514	A	C2-N3-C4	21.34	121.27	110.60
22	BA	1088	A	C2-N3-C4	21.27	121.23	110.60
22	BA	1490	A	C2-N3-C4	21.25	121.23	110.60
22	BA	2267	A	N1-C6-N6	-21.25	105.85	118.60
22	BA	2060	A	N1-C2-N3	-21.21	118.70	129.30
22	BA	2602	A	C2-N3-C4	21.12	121.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1001	A	N1-C6-N6	-21.06	105.97	118.60
22	BA	984	A	C2-N3-C4	21.05	121.12	110.60
22	BA	2518	A	C2-N3-C4	20.97	121.09	110.60
22	BA	2758	A	N1-C6-N6	-20.92	106.05	118.60
22	BA	84	A	N1-C2-N3	-20.89	118.85	129.30
22	BA	1378	A	N1-C6-N6	-20.87	106.08	118.60
22	BA	1086	A	C2-N3-C4	20.87	121.03	110.60
22	BA	1652	A	N1-C6-N6	-20.86	106.08	118.60
22	BA	529	A	N1-C6-N6	-20.83	106.10	118.60
22	BA	1000	A	C2-N3-C4	20.80	121.00	110.60
22	BA	278	A	C2-N3-C4	20.75	120.98	110.60
22	BA	1392	A	N1-C6-N6	-20.75	106.15	118.60
22	BA	2450	A	N1-C2-N3	-20.75	118.93	129.30
22	BA	1701	A	N1-C6-N6	-20.74	106.16	118.60
22	BA	1365	A	C2-N3-C4	20.71	120.95	110.60
22	BA	675	A	C2-N3-C4	20.70	120.95	110.60
22	BA	892	A	C2-N3-C4	20.70	120.95	110.60
22	BA	160	A	C2-N3-C4	20.66	120.93	110.60
22	BA	1668	A	N1-C2-N3	-20.64	118.98	129.30
22	BA	1155	A	N1-C6-N6	-20.62	106.23	118.60
22	BA	1668	A	N1-C6-N6	-20.60	106.24	118.60
22	BA	1669	A	C2-N3-C4	20.59	120.90	110.60
22	BA	1744	A	C2-N3-C4	20.56	120.88	110.60
22	BA	1028	A	C2-N3-C4	20.56	120.88	110.60
22	BA	739	A	C2-N3-C4	20.55	120.87	110.60
22	BA	1668	A	C2-N3-C4	20.55	120.87	110.60
22	BA	1214	A	C2-N3-C4	20.49	120.84	110.60
22	BA	119	A	N1-C2-N3	-20.48	119.06	129.30
22	BA	514	A	N1-C6-N6	-20.46	106.33	118.60
22	BA	532	A	C2-N3-C4	20.46	120.83	110.60
22	BA	1937	A	N1-C6-N6	-20.45	106.33	118.60
22	BA	783	A	N1-C6-N6	-20.44	106.34	118.60
55	D3	76	A	N1-C6-N6	-20.44	106.34	118.60
55	D3	31	A	C2-N3-C4	20.41	120.81	110.60
22	BA	10	A	N1-C6-N6	-20.40	106.36	118.60
22	BA	821	A	N1-C6-N6	-20.40	106.36	118.60
22	BA	1744	A	N1-C6-N6	-20.38	106.37	118.60
22	BA	2134	A	C2-N3-C4	20.36	120.78	110.60
22	BA	1815	A	N1-C6-N6	-20.36	106.39	118.60
22	BA	1936	A	C2-N3-C4	20.35	120.78	110.60
22	BA	861	A	N1-C6-N6	-20.35	106.39	118.60
55	D3	9	A	C2-N3-C4	20.34	120.77	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	219	A	C2-N3-C4	20.34	120.77	110.60
22	BA	1544	A	C2-N3-C4	20.34	120.77	110.60
22	BA	1048	A	C2-N3-C4	20.33	120.77	110.60
22	BA	1189	A	C2-N3-C4	20.33	120.77	110.60
22	BA	443	A	N1-C6-N6	-20.32	106.41	118.60
22	BA	1237	A	N1-C6-N6	-20.29	106.43	118.60
22	BA	2173	A	C2-N3-C4	20.29	120.74	110.60
22	BA	1142	A	C2-N3-C4	20.28	120.74	110.60
22	BA	2765	A	N1-C6-N6	-20.28	106.43	118.60
22	BA	1214	A	N1-C6-N6	-20.27	106.44	118.60
22	BA	1254	A	N1-C2-N3	-20.27	119.17	129.30
22	BA	1610	A	N1-C2-N3	-20.26	119.17	129.30
22	BA	1664	A	N1-C6-N6	-20.26	106.44	118.60
22	BA	2031	A	C2-N3-C4	20.25	120.72	110.60
22	BA	514	A	N1-C2-N3	-20.22	119.19	129.30
22	BA	1786	A	N1-C6-N6	-20.20	106.48	118.60
22	BA	800	A	N1-C2-N3	-20.20	119.20	129.30
55	D3	38	A	C2-N3-C4	20.19	120.69	110.60
22	BA	983	A	N1-C2-N3	-20.19	119.21	129.30
55	D3	26	A	C2-N3-C4	20.18	120.69	110.60
22	BA	2451	A	N1-C6-N6	-20.15	106.51	118.60
22	BA	1353	A	C2-N3-C4	20.14	120.67	110.60
22	BA	330	A	C2-N3-C4	20.13	120.67	110.60
22	BA	689	A	C2-N3-C4	20.13	120.66	110.60
22	BA	1321	A	C2-N3-C4	20.12	120.66	110.60
22	BA	2764	A	N1-C6-N6	-20.11	106.53	118.60
22	BA	2119	A	N1-C6-N6	-20.10	106.54	118.60
22	BA	764	A	N1-C2-N3	-20.10	119.25	129.30
22	BA	101	A	C2-N3-C4	20.09	120.65	110.60
22	BA	13	A	C2-N3-C4	20.09	120.65	110.60
22	BA	111	A	N1-C6-N6	-20.08	106.55	118.60
22	BA	2173	A	N1-C6-N6	-20.07	106.56	118.60
22	BA	1434	A	N1-C6-N6	-20.07	106.56	118.60
22	BA	1328	A	N1-C6-N6	-20.06	106.56	118.60
22	BA	2327	A	N1-C6-N6	-20.06	106.56	118.60
22	BA	845	A	C2-N3-C4	20.05	120.62	110.60
22	BA	979	A	N1-C6-N6	-20.04	106.58	118.60
22	BA	2114	A	C2-N3-C4	20.04	120.62	110.60
22	BA	2163	A	C2-N3-C4	20.04	120.62	110.60
22	BA	2809	A	C2-N3-C4	20.03	120.61	110.60
22	BA	2171	A	N1-C2-N3	-20.02	119.29	129.30
22	BA	783	A	N1-C2-N3	-20.00	119.30	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	126	A	N1-C6-N6	-19.98	106.61	118.60
22	BA	371	A	N1-C6-N6	-19.98	106.61	118.60
22	BA	608	A	C2-N3-C4	19.98	120.59	110.60
54	D2	76	A	N1-C2-N3	-19.98	119.31	129.30
22	BA	2266	A	N1-C6-N6	-19.97	106.62	118.60
22	BA	2614	A	N1-C6-N6	-19.97	106.62	118.60
22	BA	216	A	C2-N3-C4	19.96	120.58	110.60
22	BA	227	A	N1-C6-N6	-19.96	106.62	118.60
22	BA	1253	A	N1-C2-N3	-19.96	119.32	129.30
22	BA	1237	A	N1-C2-N3	-19.96	119.32	129.30
22	BA	1395	A	N1-C6-N6	-19.94	106.63	118.60
22	BA	603	A	N1-C6-N6	-19.94	106.64	118.60
22	BA	1285	A	N1-C6-N6	-19.94	106.64	118.60
22	BA	861	A	C2-N3-C4	19.93	120.57	110.60
22	BA	1977	A	N1-C2-N3	-19.93	119.34	129.30
22	BA	2566	A	N1-C6-N6	-19.93	106.64	118.60
22	BA	391	A	C2-N3-C4	19.92	120.56	110.60
22	BA	788	A	N1-C2-N3	-19.92	119.34	129.30
22	BA	223	A	N1-C6-N6	-19.91	106.66	118.60
22	BA	1858	A	N1-C6-N6	-19.91	106.66	118.60
22	BA	1253	A	N1-C6-N6	-19.90	106.66	118.60
22	BA	1632	A	C2-N3-C4	19.90	120.55	110.60
22	BA	685	A	N1-C6-N6	-19.90	106.66	118.60
22	BA	1226	A	N1-C2-N3	-19.88	119.36	129.30
22	BA	1000	A	N1-C2-N3	-19.87	119.36	129.30
22	BA	2766	A	C2-N3-C4	19.87	120.54	110.60
22	BA	13	A	N1-C6-N6	-19.87	106.68	118.60
22	BA	900	A	C2-N3-C4	19.87	120.53	110.60
22	BA	1129	A	N1-C6-N6	-19.87	106.68	118.60
22	BA	1262	A	C2-N3-C4	19.87	120.53	110.60
22	BA	479	A	N1-C2-N3	-19.86	119.37	129.30
22	BA	2542	A	N1-C6-N6	-19.86	106.68	118.60
22	BA	204	A	N1-C6-N6	-19.86	106.69	118.60
22	BA	2497	A	C2-N3-C4	19.84	120.52	110.60
23	BB	99	A	C2-N3-C4	19.84	120.52	110.60
22	BA	430	A	C2-N3-C4	19.84	120.52	110.60
22	BA	2738	A	N1-C2-N3	-19.84	119.38	129.30
22	BA	2823	A	C2-N3-C4	19.83	120.52	110.60
22	BA	219	A	N1-C6-N6	-19.83	106.70	118.60
55	D3	73	A	C2-N3-C4	19.83	120.51	110.60
22	BA	1021	A	N1-C6-N6	-19.82	106.70	118.60
22	BA	2273	A	N1-C6-N6	-19.82	106.71	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2267	A	C2-N3-C4	19.80	120.50	110.60
22	BA	10	A	C2-N3-C4	19.80	120.50	110.60
22	BA	119	A	N1-C6-N6	-19.79	106.73	118.60
22	BA	1603	A	C2-N3-C4	19.79	120.49	110.60
22	BA	1966	A	N1-C6-N6	-19.79	106.73	118.60
22	BA	2031	A	N1-C2-N3	-19.79	119.41	129.30
22	BA	53	A	N1-C6-N6	-19.78	106.73	118.60
22	BA	1978	A	N1-C6-N6	-19.78	106.73	118.60
22	BA	2287	A	C2-N3-C4	19.77	120.49	110.60
22	BA	2497	A	N1-C2-N3	-19.77	119.42	129.30
22	BA	972	A	C2-N3-C4	19.77	120.48	110.60
22	BA	241	A	N1-C6-N6	-19.76	106.74	118.60
22	BA	972	A	N1-C2-N3	-19.76	119.42	129.30
22	BA	126	A	C2-N3-C4	19.75	120.47	110.60
22	BA	910	A	C2-N3-C4	19.75	120.47	110.60
22	BA	820	A	N1-C2-N3	-19.74	119.43	129.30
22	BA	2518	A	N1-C2-N3	-19.74	119.43	129.30
22	BA	2461	A	C2-N3-C4	19.74	120.47	110.60
22	BA	2781	A	N1-C2-N3	-19.74	119.43	129.30
22	BA	1936	A	N1-C2-N3	-19.74	119.43	129.30
22	BA	2542	A	N1-C2-N3	-19.74	119.43	129.30
22	BA	528	A	C2-N3-C4	19.74	120.47	110.60
22	BA	2564	A	C2-N3-C4	19.73	120.47	110.60
22	BA	1069	A	N1-C6-N6	-19.73	106.76	118.60
22	BA	1126	A	N1-C6-N6	-19.73	106.76	118.60
22	BA	2101	A	N1-C2-N3	-19.72	119.44	129.30
22	BA	2134	A	N1-C6-N6	-19.72	106.77	118.60
22	BA	2054	A	C2-N3-C4	19.72	120.46	110.60
22	BA	10	A	N1-C2-N3	-19.71	119.45	129.30
22	BA	221	A	N1-C2-N3	-19.71	119.45	129.30
22	BA	2147	A	N1-C6-N6	-19.70	106.78	118.60
22	BA	262	A	C2-N3-C4	19.69	120.44	110.60
22	BA	1057	A	C2-N3-C4	19.68	120.44	110.60
55	D3	58	A	C2-N3-C4	19.68	120.44	110.60
22	BA	1469	A	N1-C6-N6	-19.68	106.79	118.60
22	BA	739	A	N1-C6-N6	-19.68	106.79	118.60
22	BA	1803	A	N1-C6-N6	-19.67	106.80	118.60
22	BA	1819	A	C2-N3-C4	19.66	120.43	110.60
22	BA	401	A	N1-C6-N6	-19.66	106.80	118.60
22	BA	299	A	C2-N3-C4	19.66	120.43	110.60
22	BA	1419	A	N1-C6-N6	-19.66	106.81	118.60
22	BA	2766	A	N1-C2-N3	-19.66	119.47	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2212	A	C2-N3-C4	19.65	120.43	110.60
22	BA	792	A	C2-N3-C4	19.65	120.43	110.60
22	BA	1755	A	N1-C6-N6	-19.65	106.81	118.60
22	BA	310	A	N1-C6-N6	-19.64	106.81	118.60
23	BB	57	A	C2-N3-C4	19.64	120.42	110.60
22	BA	896	A	N1-C6-N6	-19.64	106.82	118.60
22	BA	1254	A	N1-C6-N6	-19.64	106.82	118.60
22	BA	1392	A	N1-C2-N3	-19.64	119.48	129.30
23	BB	73	A	C2-N3-C4	19.63	120.42	110.60
22	BA	330	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	2031	A	N1-C6-N6	-19.62	106.83	118.60
22	BA	820	A	C2-N3-C4	19.62	120.41	110.60
22	BA	984	A	N1-C2-N3	-19.62	119.49	129.30
22	BA	278	A	N1-C6-N6	-19.61	106.83	118.60
22	BA	345	A	C2-N3-C4	19.61	120.41	110.60
55	D3	58	A	N1-C6-N6	-19.61	106.83	118.60
22	BA	160	A	N1-C6-N6	-19.61	106.83	118.60
22	BA	320	A	C2-N3-C4	19.61	120.41	110.60
22	BA	637	A	N1-C2-N3	-19.61	119.50	129.30
22	BA	675	A	N1-C2-N3	-19.61	119.50	129.30
22	BA	1701	A	C2-N3-C4	19.60	120.40	110.60
22	BA	753	A	C2-N3-C4	19.60	120.40	110.60
22	BA	1785	A	N1-C6-N6	-19.60	106.84	118.60
22	BA	432	A	C2-N3-C4	19.60	120.40	110.60
22	BA	1241	A	C2-N3-C4	19.59	120.39	110.60
55	D3	37	A	N1-C6-N6	-19.59	106.85	118.60
22	BA	528	A	N1-C6-N6	-19.58	106.85	118.60
22	BA	1286	A	N1-C6-N6	-19.58	106.85	118.60
22	BA	1302	A	N1-C2-N3	-19.58	119.51	129.30
22	BA	2298	A	N1-C6-N6	-19.58	106.85	118.60
22	BA	160	A	N1-C2-N3	-19.58	119.51	129.30
22	BA	1634	A	N1-C2-N3	-19.57	119.51	129.30
22	BA	959	A	N1-C2-N3	-19.57	119.52	129.30
22	BA	1535	A	C2-N3-C4	19.57	120.38	110.60
22	BA	749	A	N1-C6-N6	-19.57	106.86	118.60
22	BA	203	A	C2-N3-C4	19.57	120.38	110.60
22	BA	2014	A	N1-C6-N6	-19.56	106.86	118.60
22	BA	2740	A	C2-N3-C4	19.56	120.38	110.60
22	BA	1762	A	C2-N3-C4	19.56	120.38	110.60
22	BA	802	A	C2-N3-C4	19.55	120.37	110.60
22	BA	2639	A	N1-C6-N6	-19.55	106.87	118.60
22	BA	1871	A	N1-C2-N3	-19.55	119.53	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	627	A	N1-C2-N3	-19.55	119.53	129.30
22	BA	322	A	N1-C6-N6	-19.54	106.88	118.60
22	BA	764	A	C2-N3-C4	19.53	120.36	110.60
22	BA	1672	A	N1-C2-N3	-19.53	119.54	129.30
22	BA	479	A	C2-N3-C4	19.52	120.36	110.60
22	BA	1155	A	N1-C2-N3	-19.52	119.54	129.30
22	BA	1912	A	N1-C6-N6	-19.52	106.89	118.60
22	BA	2778	A	C2-N3-C4	19.52	120.36	110.60
22	BA	190	A	C2-N3-C4	19.51	120.36	110.60
22	BA	2602	A	N1-C6-N6	-19.51	106.89	118.60
22	BA	432	A	N1-C6-N6	-19.51	106.89	118.60
22	BA	917	A	C2-N3-C4	19.51	120.36	110.60
22	BA	2005	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	2134	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	118	A	N1-C2-N3	-19.50	119.55	129.30
22	BA	362	A	C2-N3-C4	19.50	120.35	110.60
22	BA	1383	A	N1-C6-N6	-19.50	106.90	118.60
22	BA	2117	A	N1-C6-N6	-19.50	106.90	118.60
22	BA	1960	A	C2-N3-C4	19.50	120.35	110.60
22	BA	2119	A	N1-C2-N3	-19.49	119.55	129.30
22	BA	2376	A	C2-N3-C4	19.49	120.34	110.60
22	BA	1226	A	C2-N3-C4	19.49	120.34	110.60
22	BA	320	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	1759	A	C2-N3-C4	19.48	120.34	110.60
22	BA	602	A	N1-C6-N6	-19.48	106.91	118.60
54	D2	58	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	71	A	N1-C6-N6	-19.48	106.91	118.60
22	BA	131	A	C2-N3-C4	19.48	120.34	110.60
22	BA	735	A	N1-C6-N6	-19.47	106.92	118.60
22	BA	310	A	C2-N3-C4	19.47	120.33	110.60
22	BA	103	A	N1-C6-N6	-19.47	106.92	118.60
22	BA	845	A	N1-C6-N6	-19.47	106.92	118.60
22	BA	1535	A	N1-C6-N6	-19.47	106.92	118.60
22	BA	2322	A	C2-N3-C4	19.46	120.33	110.60
22	BA	1927	A	N1-C2-N3	-19.46	119.57	129.30
22	BA	196	A	N1-C6-N6	-19.46	106.93	118.60
22	BA	1342	A	N1-C2-N3	-19.45	119.57	129.30
22	BA	1890	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	2776	A	N1-C6-N6	-19.45	106.93	118.60
22	BA	1321	A	N1-C6-N6	-19.45	106.93	118.60
23	BB	94	A	C2-N3-C4	19.45	120.33	110.60
22	BA	1307	A	C2-N3-C4	19.45	120.32	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	216	A	N1-C6-N6	-19.44	106.93	118.60
22	BA	1780	A	N1-C2-N3	-19.44	119.58	129.30
22	BA	2879	A	C2-N3-C4	19.44	120.32	110.60
22	BA	532	A	N1-C6-N6	-19.44	106.94	118.60
22	BA	980	A	C2-N3-C4	19.44	120.32	110.60
22	BA	1932	A	N1-C6-N6	-19.44	106.94	118.60
22	BA	1020	A	N1-C6-N6	-19.44	106.94	118.60
22	BA	2335	A	C2-N3-C4	19.44	120.32	110.60
22	BA	637	A	N1-C6-N6	-19.44	106.94	118.60
22	BA	1932	A	N1-C2-N3	-19.44	119.58	129.30
22	BA	422	A	N1-C2-N3	-19.43	119.58	129.30
22	BA	1640	A	N1-C6-N6	-19.43	106.94	118.60
22	BA	149	A	N1-C6-N6	-19.43	106.94	118.60
22	BA	197	A	C2-N3-C4	19.43	120.31	110.60
22	BA	2052	A	C2-N3-C4	19.43	120.31	110.60
22	BA	2062	A	N1-C2-N3	-19.43	119.59	129.30
22	BA	203	A	N1-C2-N3	-19.42	119.59	129.30
55	D3	21	A	C2-N3-C4	19.42	120.31	110.60
22	BA	74	A	C2-N3-C4	19.42	120.31	110.60
22	BA	118	A	N1-C6-N6	-19.42	106.95	118.60
22	BA	2014	A	C2-N3-C4	19.42	120.31	110.60
22	BA	1366	A	N1-C6-N6	-19.42	106.95	118.60
22	BA	2823	A	N1-C2-N3	-19.42	119.59	129.30
22	BA	423	A	N1-C2-N3	-19.41	119.59	129.30
22	BA	866	A	C2-N3-C4	19.41	120.31	110.60
22	BA	1268	A	C2-N3-C4	19.41	120.30	110.60
22	BA	1353	A	N1-C6-N6	-19.41	106.95	118.60
22	BA	2266	A	C2-N3-C4	19.40	120.30	110.60
22	BA	900	A	N1-C2-N3	-19.40	119.60	129.30
22	BA	1365	A	N1-C6-N6	-19.40	106.96	118.60
22	BA	1420	A	C2-N3-C4	19.39	120.30	110.60
22	BA	749	A	C2-N3-C4	19.39	120.29	110.60
22	BA	1829	A	C2-N3-C4	19.39	120.29	110.60
22	BA	449	A	C2-N3-C4	19.39	120.29	110.60
22	BA	2726	A	N1-C2-N3	-19.39	119.61	129.30
22	BA	165	A	N1-C2-N3	-19.38	119.61	129.30
22	BA	322	A	N1-C2-N3	-19.38	119.61	129.30
22	BA	739	A	N1-C2-N3	-19.38	119.61	129.30
22	BA	217	A	N1-C2-N3	-19.38	119.61	129.30
22	BA	2823	A	N1-C6-N6	-19.38	106.97	118.60
22	BA	226	A	C2-N3-C4	19.38	120.29	110.60
22	BA	460	A	N1-C6-N6	-19.38	106.97	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1286	A	N1-C2-N3	-19.38	119.61	129.30
22	BA	735	A	C2-N3-C4	19.37	120.29	110.60
22	BA	216	A	N1-C2-N3	-19.37	119.61	129.30
22	BA	2117	A	N1-C2-N3	-19.37	119.62	129.30
22	BA	975	A	C2-N3-C4	19.36	120.28	110.60
22	BA	1419	A	N1-C2-N3	-19.36	119.62	129.30
22	BA	1420	A	N1-C6-N6	-19.36	106.99	118.60
22	BA	959	A	C2-N3-C4	19.35	120.28	110.60
22	BA	1616	A	N1-C6-N6	-19.35	106.99	118.60
22	BA	2727	A	C2-N3-C4	19.35	120.28	110.60
22	BA	332	A	N1-C2-N3	-19.35	119.62	129.30
22	BA	402	A	N1-C6-N6	-19.35	106.99	118.60
22	BA	2589	A	N1-C2-N3	-19.35	119.63	129.30
22	BA	2602	A	N1-C2-N3	-19.35	119.63	129.30
22	BA	1322	A	N1-C6-N6	-19.34	106.99	118.60
22	BA	2183	A	C2-N3-C4	19.34	120.27	110.60
22	BA	204	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	1805	A	C2-N3-C4	19.34	120.27	110.60
22	BA	2721	A	C2-N3-C4	19.34	120.27	110.60
22	BA	404	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	1127	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	1490	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	310	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	422	A	C2-N3-C4	19.34	120.27	110.60
22	BA	71	A	N1-C2-N3	-19.34	119.63	129.30
22	BA	362	A	N1-C2-N3	-19.34	119.63	129.30
23	BB	78	A	N1-C6-N6	-19.34	107.00	118.60
22	BA	466	A	N1-C2-N3	-19.33	119.63	129.30
22	BA	2191	A	C2-N3-C4	19.33	120.27	110.60
22	BA	127	A	N1-C2-N3	-19.33	119.64	129.30
22	BA	918	A	C2-N3-C4	19.33	120.26	110.60
22	BA	2077	A	C2-N3-C4	19.33	120.27	110.60
22	BA	71	A	C2-N3-C4	19.33	120.26	110.60
22	BA	572	A	C2-N3-C4	19.33	120.26	110.60
22	BA	2726	A	C2-N3-C4	19.33	120.26	110.60
22	BA	1032	A	N1-C2-N3	-19.33	119.64	129.30
22	BA	1126	A	C2-N3-C4	19.32	120.26	110.60
22	BA	2358	A	N1-C2-N3	-19.32	119.64	129.30
55	D3	21	A	N1-C6-N6	-19.32	107.01	118.60
22	BA	412	A	N1-C6-N6	-19.31	107.01	118.60
22	BA	1785	A	N1-C2-N3	-19.31	119.64	129.30
22	BA	1805	A	N1-C6-N6	-19.31	107.01	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2451	A	C2-N3-C4	19.31	120.26	110.60
22	BA	825	A	C2-N3-C4	19.31	120.25	110.60
22	BA	1111	A	N1-C6-N6	-19.31	107.02	118.60
22	BA	217	A	C2-N3-C4	19.30	120.25	110.60
22	BA	2328	A	C2-N3-C4	19.30	120.25	110.60
22	BA	2565	A	N1-C6-N6	-19.30	107.02	118.60
22	BA	526	A	N1-C6-N6	-19.30	107.02	118.60
22	BA	300	A	N1-C6-N6	-19.30	107.02	118.60
22	BA	457	A	N1-C6-N6	-19.30	107.02	118.60
22	BA	2572	A	N1-C2-N3	-19.30	119.65	129.30
22	BA	2126	A	C2-N3-C4	19.30	120.25	110.60
22	BA	482	A	C2-N3-C4	19.30	120.25	110.60
22	BA	2736	A	C2-N3-C4	19.29	120.25	110.60
22	BA	1698	A	N1-C6-N6	-19.29	107.03	118.60
22	BA	2005	A	N1-C6-N6	-19.29	107.03	118.60
22	BA	2013	A	N1-C6-N6	-19.29	107.03	118.60
22	BA	1359	A	N1-C6-N6	-19.29	107.03	118.60
22	BA	2809	A	N1-C6-N6	-19.29	107.03	118.60
22	BA	483	A	C2-N3-C4	19.29	120.24	110.60
22	BA	1067	A	C2-N3-C4	19.28	120.24	110.60
22	BA	2887	A	C2-N3-C4	19.28	120.24	110.60
22	BA	917	A	N1-C6-N6	-19.28	107.03	118.60
55	D3	35	A	N1-C2-N3	-19.28	119.66	129.30
22	BA	1393	A	N1-C2-N3	-19.28	119.66	129.30
22	BA	299	A	N1-C2-N3	-19.27	119.66	129.30
22	BA	1268	A	N1-C2-N3	-19.27	119.66	129.30
22	BA	1762	A	N1-C6-N6	-19.27	107.03	118.60
22	BA	1819	A	N1-C2-N3	-19.27	119.66	129.30
22	BA	899	A	C2-N3-C4	19.27	120.24	110.60
22	BA	538	A	N1-C2-N3	-19.27	119.67	129.30
22	BA	1213	A	C2-N3-C4	19.27	120.23	110.60
22	BA	384	A	N1-C2-N3	-19.27	119.67	129.30
22	BA	1204	A	N1-C6-N6	-19.26	107.04	118.60
22	BA	2288	A	N1-C6-N6	-19.26	107.04	118.60
22	BA	529	A	N1-C2-N3	-19.26	119.67	129.30
22	BA	265	A	N1-C2-N3	-19.26	119.67	129.30
22	BA	1677	A	N1-C2-N3	-19.26	119.67	129.30
22	BA	2757	A	N1-C2-N3	-19.26	119.67	129.30
22	BA	793	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	1780	A	N1-C6-N6	-19.25	107.05	118.60
22	BA	1598	A	C2-N3-C4	19.25	120.23	110.60
22	BA	1098	A	C2-N3-C4	19.25	120.22	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D2	28	A	C2-N3-C4	19.25	120.22	110.60
22	BA	241	A	N1-C2-N3	-19.24	119.68	129.30
22	BA	529	A	C2-N3-C4	19.24	120.22	110.60
22	BA	933	A	C2-N3-C4	19.24	120.22	110.60
22	BA	2119	A	C2-N3-C4	19.24	120.22	110.60
22	BA	2287	A	N1-C6-N6	-19.24	107.06	118.60
22	BA	2266	A	N1-C2-N3	-19.24	119.68	129.30
22	BA	2478	A	C2-N3-C4	19.24	120.22	110.60
22	BA	2850	A	C2-N3-C4	19.24	120.22	110.60
22	BA	2758	A	N1-C2-N3	-19.23	119.68	129.30
22	BA	13	A	N1-C2-N3	-19.23	119.68	129.30
22	BA	1156	A	C2-N3-C4	19.23	120.22	110.60
22	BA	2560	A	C2-N3-C4	19.23	120.22	110.60
22	BA	182	A	N1-C6-N6	-19.23	107.06	118.60
22	BA	655	A	N1-C6-N6	-19.23	107.06	118.60
22	BA	1522	A	N1-C6-N6	-19.23	107.06	118.60
55	D3	37	A	C2-N3-C4	19.23	120.21	110.60
22	BA	324	A	N1-C2-N3	-19.22	119.69	129.30
22	BA	644	A	N1-C6-N6	-19.22	107.07	118.60
23	BB	45	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	654	A	C2-N3-C4	19.22	120.21	110.60
22	BA	1365	A	N1-C2-N3	-19.22	119.69	129.30
22	BA	2868	A	C2-N3-C4	19.22	120.21	110.60
22	BA	981	A	N1-C6-N6	-19.22	107.07	118.60
22	BA	1050	A	C2-N3-C4	19.22	120.21	110.60
22	BA	845	A	N1-C2-N3	-19.21	119.69	129.30
22	BA	49	A	N1-C2-N3	-19.21	119.69	129.30
22	BA	181	A	C2-N3-C4	19.21	120.20	110.60
22	BA	218	A	N1-C6-N6	-19.21	107.07	118.60
22	BA	346	A	N1-C6-N6	-19.21	107.08	118.60
22	BA	2406	A	N1-C2-N3	-19.21	119.70	129.30
23	BB	59	A	N1-C2-N3	-19.21	119.70	129.30
22	BA	1544	A	N1-C2-N3	-19.21	119.70	129.30
22	BA	2758	A	C2-N3-C4	19.21	120.20	110.60
22	BA	412	A	C2-N3-C4	19.20	120.20	110.60
22	BA	49	A	C2-N3-C4	19.20	120.20	110.60
22	BA	1665	A	C2-N3-C4	19.20	120.20	110.60
22	BA	2564	A	N1-C2-N3	-19.20	119.70	129.30
23	BB	57	A	N1-C2-N3	-19.20	119.70	129.30
22	BA	1928	A	N1-C6-N6	-19.20	107.08	118.60
22	BA	2634	A	C2-N3-C4	19.20	120.20	110.60
22	BA	391	A	N1-C2-N3	-19.19	119.70	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1744	A	N1-C2-N3	-19.19	119.70	129.30
22	BA	2333	A	N1-C6-N6	-19.19	107.08	118.60
22	BA	1028	A	N1-C6-N6	-19.19	107.09	118.60
22	BA	1268	A	N1-C6-N6	-19.19	107.09	118.60
22	BA	866	A	N1-C2-N3	-19.19	119.71	129.30
22	BA	947	A	C2-N3-C4	19.19	120.19	110.60
22	BA	734	A	N1-C6-N6	-19.18	107.09	118.60
55	D3	26	A	N1-C2-N3	-19.18	119.71	129.30
22	BA	1378	A	C2-N3-C4	19.18	120.19	110.60
55	D3	26	A	N1-C6-N6	-19.18	107.09	118.60
22	BA	454	A	N1-C6-N6	-19.18	107.09	118.60
22	BA	941	A	N1-C2-N3	-19.18	119.71	129.30
23	BB	78	A	N1-C2-N3	-19.18	119.71	129.30
22	BA	910	A	N1-C2-N3	-19.18	119.71	129.30
22	BA	2227	A	C2-N3-C4	19.18	120.19	110.60
22	BA	1384	A	N1-C2-N3	-19.18	119.71	129.30
54	D2	31	A	C2-N3-C4	19.18	120.19	110.60
22	BA	878	A	C2-N3-C4	19.18	120.19	110.60
22	BA	941	A	C2-N3-C4	19.18	120.19	110.60
22	BA	1853	A	N1-C2-N3	-19.18	119.71	129.30
54	D2	69	A	C2-N3-C4	19.18	120.19	110.60
22	BA	84	A	N1-C6-N6	-19.17	107.10	118.60
22	BA	2883	A	N1-C2-N3	-19.17	119.71	129.30
54	D2	38	A	N1-C2-N3	-19.17	119.72	129.30
22	BA	483	A	N1-C6-N6	-19.17	107.10	118.60
22	BA	1274	A	N1-C2-N3	-19.17	119.72	129.30
22	BA	643	A	N1-C2-N3	-19.17	119.72	129.30
22	BA	892	A	N1-C6-N6	-19.17	107.10	118.60
22	BA	2270	A	C2-N3-C4	19.17	120.18	110.60
22	BA	2288	A	N1-C2-N3	-19.17	119.72	129.30
22	BA	734	A	C2-N3-C4	19.16	120.18	110.60
22	BA	1008	A	N1-C6-N6	-19.16	107.10	118.60
22	BA	637	A	C2-N3-C4	19.16	120.18	110.60
22	BA	119	A	C2-N3-C4	19.16	120.18	110.60
22	BA	345	A	N1-C6-N6	-19.16	107.11	118.60
22	BA	1871	A	C2-N3-C4	19.16	120.18	110.60
54	D2	21	A	N1-C2-N3	-19.16	119.72	129.30
22	BA	1129	A	N1-C2-N3	-19.15	119.72	129.30
22	BA	896	A	N1-C2-N3	-19.15	119.72	129.30
22	BA	547	A	N1-C2-N3	-19.15	119.72	129.30
22	BA	829	A	N1-C6-N6	-19.15	107.11	118.60
55	D3	58	A	N1-C2-N3	-19.15	119.73	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	789	A	N1-C2-N3	-19.14	119.73	129.30
22	BA	1366	A	C2-N3-C4	19.14	120.17	110.60
22	BA	95	A	C2-N3-C4	19.14	120.17	110.60
23	BB	99	A	N1-C6-N6	-19.14	107.11	118.60
22	BA	144	A	C2-N3-C4	19.14	120.17	110.60
22	BA	685	A	C2-N3-C4	19.14	120.17	110.60
22	BA	1876	A	C2-N3-C4	19.14	120.17	110.60
22	BA	1952	A	C2-N3-C4	19.14	120.17	110.60
22	BA	2284	A	C2-N3-C4	19.14	120.17	110.60
22	BA	1545	A	N1-C2-N3	-19.14	119.73	129.30
22	BA	1713	A	N1-C2-N3	-19.13	119.73	129.30
55	D3	64	A	C2-N3-C4	19.13	120.17	110.60
22	BA	322	A	C2-N3-C4	19.13	120.17	110.60
22	BA	616	A	C2-N3-C4	19.13	120.17	110.60
55	D3	21	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	655	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	1912	A	N1-C2-N3	-19.13	119.73	129.30
22	BA	449	A	N1-C2-N3	-19.13	119.74	129.30
22	BA	1650	A	C2-N3-C4	19.13	120.16	110.60
22	BA	1548	A	C2-N3-C4	19.12	120.16	110.60
22	BA	255	A	C2-N3-C4	19.12	120.16	110.60
22	BA	654	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	1953	A	N1-C6-N6	-19.12	107.13	118.60
22	BA	2482	A	N1-C6-N6	-19.12	107.13	118.60
54	D2	59	A	C2-N3-C4	19.12	120.16	110.60
22	BA	1545	A	C2-N3-C4	19.12	120.16	110.60
22	BA	1189	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	2336	A	N1-C2-N3	-19.12	119.74	129.30
22	BA	181	A	N1-C6-N6	-19.11	107.13	118.60
22	BA	1970	A	N1-C2-N3	-19.11	119.75	129.30
22	BA	2657	A	N1-C2-N3	-19.11	119.75	129.30
22	BA	1598	A	N1-C6-N6	-19.11	107.14	118.60
22	BA	2451	A	N1-C2-N3	-19.11	119.75	129.30
22	BA	2273	A	C2-N3-C4	19.10	120.15	110.60
22	BA	1175	A	C2-N3-C4	19.10	120.15	110.60
22	BA	73	A	N1-C2-N3	-19.10	119.75	129.30
22	BA	756	A	C2-N3-C4	19.10	120.15	110.60
22	BA	602	A	C2-N3-C4	19.10	120.15	110.60
22	BA	2851	A	C2-N3-C4	19.10	120.15	110.60
22	BA	2799	A	C2-N3-C4	19.10	120.15	110.60
22	BA	28	A	C2-N3-C4	19.09	120.15	110.60
22	BA	167	A	C2-N3-C4	19.09	120.15	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	943	A	C2-N3-C4	19.09	120.15	110.60
22	BA	1919	A	N1-C6-N6	-19.09	107.14	118.60
22	BA	2800	A	N1-C6-N6	-19.09	107.14	118.60
22	BA	613	A	N1-C2-N3	-19.09	119.75	129.30
22	BA	1403	A	C2-N3-C4	19.09	120.15	110.60
22	BA	1966	A	C2-N3-C4	19.09	120.15	110.60
22	BA	1204	A	C2-N3-C4	19.09	120.15	110.60
22	BA	1301	A	C2-N3-C4	19.09	120.14	110.60
22	BA	2856	A	C2-N3-C4	19.09	120.14	110.60
22	BA	1307	A	N1-C6-N6	-19.09	107.15	118.60
22	BA	2070	A	C2-N3-C4	19.09	120.14	110.60
22	BA	311	A	N1-C6-N6	-19.09	107.15	118.60
22	BA	1583	A	N1-C2-N3	-19.09	119.76	129.30
22	BA	1570	A	N1-C6-N6	-19.08	107.15	118.60
22	BA	1677	A	C2-N3-C4	19.08	120.14	110.60
22	BA	1039	A	C2-N3-C4	19.08	120.14	110.60
22	BA	1253	A	C2-N3-C4	19.08	120.14	110.60
22	BA	1938	A	C2-N3-C4	19.08	120.14	110.60
22	BA	401	A	C2-N3-C4	19.08	120.14	110.60
22	BA	945	A	C2-N3-C4	19.08	120.14	110.60
22	BA	2432	A	N1-C2-N3	-19.08	119.76	129.30
22	BA	309	A	N1-C6-N6	-19.08	107.15	118.60
22	BA	1142	A	N1-C2-N3	-19.07	119.76	129.30
22	BA	1786	A	C2-N3-C4	19.07	120.14	110.60
22	BA	892	A	N1-C2-N3	-19.07	119.76	129.30
22	BA	1439	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	2199	A	N1-C2-N3	-19.07	119.76	129.30
22	BA	984	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	988	A	N1-C6-N6	-19.07	107.16	118.60
22	BA	2566	A	N1-C2-N3	-19.07	119.76	129.30
22	BA	223	A	N1-C2-N3	-19.07	119.77	129.30
22	BA	118	A	C2-N3-C4	19.07	120.13	110.60
22	BA	432	A	N1-C2-N3	-19.07	119.77	129.30
22	BA	1932	A	C2-N3-C4	19.07	120.13	110.60
22	BA	255	A	N1-C2-N3	-19.07	119.77	129.30
22	BA	483	A	N1-C2-N3	-19.07	119.77	129.30
22	BA	1214	A	N1-C2-N3	-19.07	119.77	129.30
54	D2	26	A	C2-N3-C4	19.07	120.13	110.60
22	BA	2184	A	C2-N3-C4	19.06	120.13	110.60
22	BA	2336	A	N1-C6-N6	-19.06	107.16	118.60
22	BA	470	A	C2-N3-C4	19.06	120.13	110.60
22	BA	1367	A	C2-N3-C4	19.06	120.13	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1784	A	C2-N3-C4	19.06	120.13	110.60
22	BA	1937	A	N1-C2-N3	-19.06	119.77	129.30
22	BA	2005	A	C2-N3-C4	19.06	120.13	110.60
22	BA	2169	A	C2-N3-C4	19.06	120.13	110.60
22	BA	311	A	N1-C2-N3	-19.06	119.77	129.30
22	BA	332	A	C2-N3-C4	19.06	120.13	110.60
22	BA	1469	A	C2-N3-C4	19.06	120.13	110.60
22	BA	222	A	N1-C2-N3	-19.05	119.77	129.30
22	BA	959	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	1981	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	2003	A	C2-N3-C4	19.05	120.13	110.60
22	BA	538	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	1566	A	N1-C2-N3	-19.05	119.78	129.30
22	BA	2014	A	N1-C2-N3	-19.05	119.78	129.30
22	BA	2358	A	C2-N3-C4	19.05	120.12	110.60
22	BA	526	A	N1-C2-N3	-19.05	119.78	129.30
22	BA	1000	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	1433	A	C2-N3-C4	19.05	120.12	110.60
22	BA	2738	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	2749	A	N1-C2-N3	-19.05	119.78	129.30
23	BB	45	A	C2-N3-C4	19.05	120.12	110.60
22	BA	788	A	N1-C6-N6	-19.05	107.17	118.60
22	BA	861	A	N1-C2-N3	-19.05	119.78	129.30
22	BA	878	A	N1-C2-N3	-19.05	119.78	129.30
22	BA	1977	A	C2-N3-C4	19.05	120.12	110.60
54	D2	31	A	N1-C2-N3	-19.05	119.78	129.30
22	BA	1189	A	N1-C6-N6	-19.04	107.17	118.60
22	BA	1522	A	N1-C2-N3	-19.04	119.78	129.30
22	BA	1427	A	N1-C6-N6	-19.04	107.17	118.60
22	BA	670	A	C2-N3-C4	19.04	120.12	110.60
22	BA	1070	A	N1-C6-N6	-19.04	107.18	118.60
22	BA	2212	A	N1-C2-N3	-19.04	119.78	129.30
22	BA	439	A	C2-N3-C4	19.04	120.12	110.60
22	BA	1762	A	N1-C2-N3	-19.04	119.78	129.30
54	D2	14	A	C2-N3-C4	19.04	120.12	110.60
22	BA	1553	A	C2-N3-C4	19.04	120.12	110.60
22	BA	161	A	N1-C6-N6	-19.03	107.18	118.60
22	BA	443	A	N1-C2-N3	-19.03	119.78	129.30
22	BA	1387	A	C2-N3-C4	19.03	120.12	110.60
22	BA	1918	A	C2-N3-C4	19.03	120.11	110.60
22	BA	2288	A	C2-N3-C4	19.03	120.11	110.60
22	BA	2572	A	N1-C6-N6	-19.03	107.18	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	149	A	C2-N3-C4	19.03	120.11	110.60
22	BA	1453	A	N1-C2-N3	-19.03	119.78	129.30
22	BA	574	A	N1-C6-N6	-19.03	107.18	118.60
22	BA	899	A	N1-C2-N3	-19.03	119.79	129.30
22	BA	1590	A	C2-N3-C4	19.03	120.11	110.60
22	BA	2761	A	C2-N3-C4	19.03	120.11	110.60
22	BA	1010	A	C2-N3-C4	19.02	120.11	110.60
22	BA	1204	A	N1-C2-N3	-19.02	119.79	129.30
23	BB	104	A	C2-N3-C4	19.02	120.11	110.60
22	BA	614	A	N1-C2-N3	-19.02	119.79	129.30
22	BA	28	A	N1-C2-N3	-19.02	119.79	129.30
22	BA	608	A	N1-C6-N6	-19.02	107.19	118.60
22	BA	2378	A	N1-C6-N6	-19.02	107.19	118.60
22	BA	1067	A	N1-C2-N3	-19.01	119.79	129.30
22	BA	1509	A	N1-C2-N3	-19.01	119.79	129.30
22	BA	2639	A	C2-N3-C4	19.01	120.11	110.60
22	BA	2660	A	N1-C6-N6	-19.01	107.19	118.60
22	BA	2741	A	C2-N3-C4	19.01	120.11	110.60
54	D2	76	A	N1-C6-N6	-19.01	107.19	118.60
22	BA	508	A	N1-C2-N3	-19.01	119.79	129.30
22	BA	734	A	N1-C2-N3	-19.01	119.79	129.30
22	BA	1039	A	N1-C2-N3	-19.01	119.80	129.30
22	BA	374	A	C2-N3-C4	19.01	120.10	110.60
22	BA	911	A	C2-N3-C4	19.01	120.11	110.60
22	BA	2327	A	C2-N3-C4	19.01	120.11	110.60
22	BA	563	A	C2-N3-C4	19.01	120.10	110.60
22	BA	1928	A	N1-C2-N3	-19.01	119.80	129.30
22	BA	1378	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	1746	A	C2-N3-C4	19.00	120.10	110.60
22	BA	2062	A	C2-N3-C4	19.00	120.10	110.60
22	BA	2733	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	609	A	C2-N3-C4	19.00	120.10	110.60
22	BA	2227	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	2614	A	C2-N3-C4	19.00	120.10	110.60
22	BA	1133	A	N1-C6-N6	-19.00	107.20	118.60
22	BA	1773	A	C2-N3-C4	19.00	120.10	110.60
22	BA	1978	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	2346	A	N1-C2-N3	-19.00	119.80	129.30
22	BA	2497	A	N1-C6-N6	-19.00	107.20	118.60
22	BA	1785	A	C2-N3-C4	19.00	120.10	110.60
22	BA	49	A	N1-C6-N6	-19.00	107.20	118.60
22	BA	789	A	C2-N3-C4	18.99	120.10	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1321	A	N1-C2-N3	-18.99	119.80	129.30
22	BA	2733	A	C2-N3-C4	18.99	120.10	110.60
22	BA	492	A	C2-N3-C4	18.99	120.10	110.60
22	BA	1918	A	N1-C6-N6	-18.99	107.20	118.60
22	BA	2740	A	N1-C2-N3	-18.99	119.80	129.30
22	BA	1301	A	N1-C6-N6	-18.99	107.21	118.60
22	BA	1077	A	C2-N3-C4	18.99	120.09	110.60
22	BA	1664	A	C2-N3-C4	18.99	120.09	110.60
22	BA	127	A	C2-N3-C4	18.98	120.09	110.60
22	BA	2725	A	C2-N3-C4	18.98	120.09	110.60
22	BA	1969	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	2749	A	C2-N3-C4	18.98	120.09	110.60
22	BA	161	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	911	A	N1-C2-N3	-18.98	119.81	129.30
22	BA	1847	A	C2-N3-C4	18.98	120.09	110.60
22	BA	21	A	C2-N3-C4	18.98	120.09	110.60
22	BA	504	A	C2-N3-C4	18.98	120.09	110.60
22	BA	572	A	N1-C2-N3	-18.97	119.81	129.30
22	BA	1096	A	C2-N3-C4	18.97	120.09	110.60
22	BA	927	A	C2-N3-C4	18.97	120.09	110.60
22	BA	1095	A	C2-N3-C4	18.97	120.09	110.60
22	BA	2654	A	N1-C2-N3	-18.97	119.81	129.30
22	BA	2734	A	C2-N3-C4	18.97	120.08	110.60
22	BA	693	A	C2-N3-C4	18.97	120.08	110.60
22	BA	1549	A	C2-N3-C4	18.97	120.08	110.60
22	BA	2211	A	N1-C6-N6	-18.97	107.22	118.60
22	BA	1069	A	C2-N3-C4	18.97	120.08	110.60
22	BA	1635	A	C2-N3-C4	18.97	120.08	110.60
23	BB	39	A	N1-C6-N6	-18.97	107.22	118.60
22	BA	582	A	C2-N3-C4	18.96	120.08	110.60
22	BA	2590	A	N1-C2-N3	-18.96	119.82	129.30
22	BA	270	A	N1-C6-N6	-18.96	107.22	118.60
22	BA	1509	A	N1-C6-N6	-18.96	107.22	118.60
22	BA	2199	A	C2-N3-C4	18.96	120.08	110.60
22	BA	1265	A	N1-C6-N6	-18.96	107.22	118.60
22	BA	300	A	C2-N3-C4	18.96	120.08	110.60
22	BA	1009	A	C2-N3-C4	18.96	120.08	110.60
22	BA	1815	A	N1-C2-N3	-18.96	119.82	129.30
22	BA	2887	A	N1-C2-N3	-18.96	119.82	129.30
22	BA	340	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	563	A	N1-C2-N3	-18.95	119.82	129.30
22	BA	1327	A	N1-C2-N3	-18.95	119.82	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	53	A	N1-C2-N3	-18.95	119.82	129.30
22	BA	218	A	N1-C2-N3	-18.95	119.82	129.30
22	BA	1367	A	N1-C2-N3	-18.95	119.82	129.30
22	BA	1508	A	C2-N3-C4	18.95	120.08	110.60
23	BB	99	A	N1-C2-N3	-18.95	119.82	129.30
22	BA	616	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	2176	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	502	A	C2-N3-C4	18.95	120.07	110.60
22	BA	1384	A	C2-N3-C4	18.95	120.07	110.60
22	BA	632	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	1544	A	N1-C6-N6	-18.95	107.23	118.60
22	BA	2821	A	N1-C2-N3	-18.95	119.83	129.30
22	BA	1927	A	C2-N3-C4	18.95	120.07	110.60
22	BA	1088	A	N1-C2-N3	-18.94	119.83	129.30
22	BA	311	A	C2-N3-C4	18.94	120.07	110.60
22	BA	2080	A	C2-N3-C4	18.94	120.07	110.60
22	BA	2101	A	C2-N3-C4	18.94	120.07	110.60
22	BA	173	A	C2-N3-C4	18.94	120.07	110.60
22	BA	1552	A	N1-C6-N6	-18.94	107.24	118.60
22	BA	547	A	C2-N3-C4	18.94	120.07	110.60
22	BA	1759	A	N1-C6-N6	-18.94	107.24	118.60
22	BA	616	A	N1-C2-N3	-18.93	119.83	129.30
22	BA	1086	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	792	A	N1-C2-N3	-18.93	119.83	129.30
22	BA	2042	A	C2-N3-C4	18.93	120.07	110.60
22	BA	1308	A	C2-N3-C4	18.93	120.06	110.60
23	BB	73	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	199	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	1505	A	C2-N3-C4	18.93	120.06	110.60
22	BA	14	A	N1-C6-N6	-18.93	107.24	118.60
22	BA	621	A	N1-C2-N3	-18.93	119.84	129.30
22	BA	149	A	N1-C2-N3	-18.93	119.84	129.30
22	BA	2270	A	N1-C2-N3	-18.93	119.84	129.30
22	BA	2776	A	N1-C2-N3	-18.93	119.84	129.30
22	BA	627	A	N1-C6-N6	-18.92	107.25	118.60
22	BA	2227	A	N1-C6-N6	-18.92	107.25	118.60
22	BA	1336	A	C2-N3-C4	18.92	120.06	110.60
55	D3	7	A	N1-C6-N6	-18.92	107.25	118.60
22	BA	2225	A	C2-N3-C4	18.92	120.06	110.60
22	BA	125	A	N1-C2-N3	-18.91	119.84	129.30
22	BA	371	A	C2-N3-C4	18.91	120.06	110.60
22	BA	820	A	N1-C6-N6	-18.91	107.25	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	196	A	C2-N3-C4	18.91	120.06	110.60
22	BA	1077	A	N1-C2-N3	-18.91	119.84	129.30
22	BA	563	A	N1-C6-N6	-18.91	107.25	118.60
22	BA	2411	A	N1-C6-N6	-18.91	107.25	118.60
22	BA	1701	A	N1-C2-N3	-18.91	119.85	129.30
23	BB	108	A	C2-N3-C4	18.91	120.06	110.60
22	BA	2097	A	C2-N3-C4	18.91	120.05	110.60
22	BA	2590	A	C2-N3-C4	18.91	120.05	110.60
55	D3	76	A	C2-N3-C4	18.91	120.05	110.60
22	BA	402	A	N1-C2-N3	-18.91	119.85	129.30
22	BA	2336	A	C2-N3-C4	18.91	120.05	110.60
22	BA	1713	A	C2-N3-C4	18.90	120.05	110.60
22	BA	1580	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	1757	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	1889	A	C2-N3-C4	18.90	120.05	110.60
22	BA	2434	A	N1-C6-N6	-18.90	107.26	118.60
23	BB	78	A	C2-N3-C4	18.90	120.05	110.60
22	BA	320	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	631	A	N1-C2-N3	-18.90	119.85	129.30
22	BA	1328	A	C2-N3-C4	18.90	120.05	110.60
22	BA	1265	A	C2-N3-C4	18.90	120.05	110.60
22	BA	2211	A	N1-C2-N3	-18.89	119.85	129.30
22	BA	38	A	C2-N3-C4	18.89	120.05	110.60
22	BA	621	A	C2-N3-C4	18.89	120.05	110.60
22	BA	972	A	N1-C6-N6	-18.89	107.26	118.60
22	BA	1046	A	N1-C2-N3	-18.89	119.85	129.30
22	BA	2378	A	C2-N3-C4	18.89	120.05	110.60
22	BA	1274	A	C2-N3-C4	18.89	120.05	110.60
55	D3	73	A	N1-C2-N3	-18.89	119.85	129.30
22	BA	199	A	C2-N3-C4	18.89	120.05	110.60
22	BA	1046	A	C2-N3-C4	18.89	120.05	110.60
22	BA	2176	A	C2-N3-C4	18.89	120.04	110.60
22	BA	2450	A	N1-C6-N6	-18.89	107.27	118.60
22	BA	2821	A	C2-N3-C4	18.89	120.04	110.60
22	BA	470	A	N1-C2-N3	-18.89	119.86	129.30
22	BA	575	A	C2-N3-C4	18.89	120.04	110.60
22	BA	2478	A	N1-C6-N6	-18.89	107.27	118.60
22	BA	1495	A	C2-N3-C4	18.89	120.04	110.60
22	BA	1877	A	C2-N3-C4	18.89	120.04	110.60
22	BA	279	A	C2-N3-C4	18.88	120.04	110.60
22	BA	900	A	N1-C6-N6	-18.88	107.27	118.60
22	BA	1342	A	N1-C6-N6	-18.88	107.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1952	A	N1-C6-N6	-18.88	107.27	118.60
22	BA	547	A	N1-C6-N6	-18.88	107.27	118.60
22	BA	1420	A	N1-C2-N3	-18.88	119.86	129.30
22	BA	2019	A	N1-C2-N3	-18.88	119.86	129.30
22	BA	1020	A	N1-C2-N3	-18.88	119.86	129.30
22	BA	2169	A	N1-C6-N6	-18.88	107.27	118.60
22	BA	2448	A	N1-C6-N6	-18.88	107.28	118.60
22	BA	2587	A	C2-N3-C4	18.88	120.04	110.60
22	BA	2741	A	N1-C6-N6	-18.88	107.27	118.60
22	BA	2564	A	N1-C6-N6	-18.88	107.28	118.60
22	BA	896	A	C2-N3-C4	18.87	120.04	110.60
22	BA	1522	A	C2-N3-C4	18.87	120.04	110.60
22	BA	2670	A	C2-N3-C4	18.87	120.04	110.60
22	BA	443	A	C2-N3-C4	18.87	120.03	110.60
22	BA	781	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	1913	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	2675	A	C2-N3-C4	18.87	120.03	110.60
22	BA	74	A	N1-C2-N3	-18.87	119.87	129.30
22	BA	528	A	N1-C2-N3	-18.87	119.87	129.30
22	BA	1655	A	C2-N3-C4	18.87	120.03	110.60
54	D2	5	A	C2-N3-C4	18.87	120.03	110.60
54	D2	9	A	N1-C2-N3	-18.87	119.87	129.30
22	BA	2886	A	N1-C6-N6	-18.87	107.28	118.60
22	BA	309	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	538	A	C2-N3-C4	18.86	120.03	110.60
22	BA	1050	A	N1-C6-N6	-18.86	107.28	118.60
22	BA	2352	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	2541	A	N1-C6-N6	-18.86	107.28	118.60
22	BA	2748	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	2778	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	1640	A	C2-N3-C4	18.86	120.03	110.60
22	BA	2376	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	608	A	N1-C2-N3	-18.86	119.87	129.30
55	D3	38	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	1970	A	C2-N3-C4	18.86	120.03	110.60
22	BA	2886	A	C2-N3-C4	18.86	120.03	110.60
22	BA	354	A	N1-C6-N6	-18.86	107.28	118.60
22	BA	1010	A	N1-C2-N3	-18.86	119.87	129.30
22	BA	1655	A	N1-C6-N6	-18.86	107.29	118.60
22	BA	1890	A	C2-N3-C4	18.86	120.03	110.60
23	BB	53	A	N1-C6-N6	-18.86	107.29	118.60
22	BA	457	A	N1-C2-N3	-18.85	119.87	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D3	37	A	N1-C2-N3	-18.85	119.87	129.30
22	BA	1913	A	C2-N3-C4	18.85	120.03	110.60
22	BA	2893	A	N1-C2-N3	-18.85	119.87	129.30
22	BA	592	A	C2-N3-C4	18.85	120.03	110.60
22	BA	1496	A	N1-C6-N6	-18.85	107.29	118.60
22	BA	1155	A	C2-N3-C4	18.85	120.03	110.60
54	D2	14	A	N1-C2-N3	-18.85	119.88	129.30
22	BA	819	A	C2-N3-C4	18.85	120.02	110.60
22	BA	1632	A	N1-C6-N6	-18.85	107.29	118.60
22	BA	2147	A	C2-N3-C4	18.85	120.02	110.60
23	BB	29	A	C2-N3-C4	18.85	120.02	110.60
23	BB	104	A	N1-C2-N3	-18.85	119.88	129.30
23	BB	108	A	N1-C6-N6	-18.85	107.29	118.60
54	D2	14	A	N1-C6-N6	-18.85	107.29	118.60
22	BA	479	A	N1-C6-N6	-18.85	107.29	118.60
22	BA	631	A	C2-N3-C4	18.85	120.02	110.60
54	D2	58	A	C2-N3-C4	18.85	120.02	110.60
22	BA	1194	A	C2-N3-C4	18.84	120.02	110.60
22	BA	2531	A	N1-C2-N3	-18.84	119.88	129.30
22	BA	1579	A	C2-N3-C4	18.84	120.02	110.60
22	BA	2654	A	N1-C6-N6	-18.84	107.30	118.60
22	BA	2835	A	N1-C2-N3	-18.84	119.88	129.30
22	BA	309	A	C2-N3-C4	18.83	120.02	110.60
22	BA	2542	A	C2-N3-C4	18.83	120.02	110.60
22	BA	505	A	C2-N3-C4	18.83	120.02	110.60
22	BA	586	A	N1-C2-N3	-18.83	119.88	129.30
22	BA	203	A	N1-C6-N6	-18.83	107.30	118.60
22	BA	508	A	C2-N3-C4	18.83	120.01	110.60
22	BA	1569	A	C2-N3-C4	18.83	120.02	110.60
22	BA	1759	A	N1-C2-N3	-18.83	119.89	129.30
22	BA	2469	A	N1-C2-N3	-18.83	119.89	129.30
22	BA	2757	A	C2-N3-C4	18.83	120.02	110.60
22	BA	324	A	C2-N3-C4	18.83	120.01	110.60
54	D2	35	A	N1-C6-N6	-18.83	107.30	118.60
55	D3	14	A	N1-C2-N3	-18.83	119.89	129.30
22	BA	503	A	C2-N3-C4	18.82	120.01	110.60
22	BA	2225	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	2418	A	C2-N3-C4	18.82	120.01	110.60
23	BB	108	A	N1-C2-N3	-18.82	119.89	129.30
23	BB	109	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	1393	A	N1-C6-N6	-18.82	107.31	118.60
22	BA	1641	A	N1-C2-N3	-18.82	119.89	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	429	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	1096	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	2590	A	N1-C6-N6	-18.82	107.31	118.60
22	BA	1890	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	2298	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	2665	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	676	A	N1-C6-N6	-18.82	107.31	118.60
22	BA	2051	A	N1-C6-N6	-18.82	107.31	118.60
22	BA	2241	A	C2-N3-C4	18.82	120.01	110.60
22	BA	2335	A	N1-C2-N3	-18.82	119.89	129.30
22	BA	933	A	N1-C6-N6	-18.81	107.31	118.60
22	BA	1054	A	C2-N3-C4	18.81	120.01	110.60
22	BA	1284	A	N1-C2-N3	-18.81	119.89	129.30
22	BA	2126	A	N1-C6-N6	-18.81	107.31	118.60
55	D3	31	A	N1-C2-N3	-18.81	119.89	129.30
22	BA	182	A	C2-N3-C4	18.81	120.00	110.60
22	BA	2386	A	C2-N3-C4	18.81	120.00	110.60
22	BA	241	A	C2-N3-C4	18.81	120.00	110.60
22	BA	482	A	N1-C2-N3	-18.81	119.90	129.30
22	BA	804	A	N1-C2-N3	-18.81	119.90	129.30
22	BA	2198	A	N1-C2-N3	-18.81	119.90	129.30
22	BA	507	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	910	A	N1-C6-N6	-18.80	107.32	118.60
22	BA	1579	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	1597	A	C2-N3-C4	18.80	120.00	110.60
22	BA	83	A	C2-N3-C4	18.80	120.00	110.60
22	BA	191	A	C2-N3-C4	18.80	120.00	110.60
22	BA	532	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	603	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	627	A	C2-N3-C4	18.80	120.00	110.60
22	BA	676	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	1698	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	294	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	742	A	C2-N3-C4	18.80	120.00	110.60
22	BA	1717	A	C2-N3-C4	18.80	120.00	110.60
22	BA	1937	A	C2-N3-C4	18.80	120.00	110.60
22	BA	195	A	N1-C2-N3	-18.80	119.90	129.30
22	BA	347	A	C2-N3-C4	18.80	120.00	110.60
22	BA	643	A	C2-N3-C4	18.80	120.00	110.60
22	BA	1532	A	C2-N3-C4	18.80	120.00	110.60
22	BA	1609	A	N1-C6-N6	-18.80	107.32	118.60
22	BA	256	A	C2-N3-C4	18.79	120.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	614	A	C2-N3-C4	18.79	120.00	110.60
22	BA	1755	A	C2-N3-C4	18.79	120.00	110.60
22	BA	190	A	N1-C6-N6	-18.79	107.33	118.60
22	BA	1504	A	C2-N3-C4	18.79	120.00	110.60
22	BA	2639	A	N1-C2-N3	-18.79	119.90	129.30
22	BA	454	A	N1-C2-N3	-18.79	119.91	129.30
23	BB	53	A	N1-C2-N3	-18.79	119.91	129.30
22	BA	233	A	N1-C2-N3	-18.79	119.91	129.30
22	BA	626	A	N1-C2-N3	-18.79	119.91	129.30
22	BA	556	A	C2-N3-C4	18.78	119.99	110.60
22	BA	1342	A	C2-N3-C4	18.78	119.99	110.60
55	D3	7	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	502	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	2809	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	64	A	C2-N3-C4	18.78	119.99	110.60
22	BA	1616	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	1147	A	C2-N3-C4	18.78	119.99	110.60
54	D2	38	A	N1-C6-N6	-18.78	107.33	118.60
54	D2	59	A	N1-C6-N6	-18.78	107.33	118.60
22	BA	609	A	N1-C2-N3	-18.78	119.91	129.30
22	BA	2037	A	C2-N3-C4	18.78	119.99	110.60
22	BA	2171	A	C2-N3-C4	18.78	119.99	110.60
22	BA	1272	A	N1-C2-N3	-18.77	119.91	129.30
22	BA	1508	A	N1-C2-N3	-18.77	119.91	129.30
22	BA	2366	A	C2-N3-C4	18.77	119.99	110.60
22	BA	453	A	N1-C6-N6	-18.77	107.34	118.60
22	BA	504	A	N1-C2-N3	-18.77	119.91	129.30
22	BA	2776	A	C2-N3-C4	18.77	119.99	110.60
23	BB	58	A	N1-C2-N3	-18.77	119.92	129.30
23	BB	46	A	C2-N3-C4	18.77	119.98	110.60
55	D3	9	A	N1-C6-N6	-18.77	107.34	118.60
22	BA	501	A	N1-C6-N6	-18.77	107.34	118.60
22	BA	1384	A	N1-C6-N6	-18.77	107.34	118.60
22	BA	1048	A	N1-C6-N6	-18.76	107.34	118.60
22	BA	2675	A	N1-C6-N6	-18.76	107.34	118.60
22	BA	522	A	C2-N3-C4	18.76	119.98	110.60
22	BA	980	A	N1-C2-N3	-18.76	119.92	129.30
22	BA	1395	A	C2-N3-C4	18.76	119.98	110.60
22	BA	2082	A	C2-N3-C4	18.76	119.98	110.60
22	BA	2705	A	N1-C2-N3	-18.76	119.92	129.30
22	BA	2706	A	C2-N3-C4	18.76	119.98	110.60
22	BA	1571	A	N1-C2-N3	-18.76	119.92	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2013	A	C2-N3-C4	18.76	119.98	110.60
22	BA	2734	A	N1-C6-N6	-18.76	107.35	118.60
22	BA	2753	A	C2-N3-C4	18.76	119.98	110.60
22	BA	1690	A	C2-N3-C4	18.76	119.98	110.60
22	BA	501	A	C2-N3-C4	18.75	119.98	110.60
22	BA	706	A	N1-C6-N6	-18.75	107.35	118.60
22	BA	1095	A	N1-C2-N3	-18.75	119.92	129.30
22	BA	2388	A	N1-C2-N3	-18.75	119.92	129.30
22	BA	2163	A	N1-C2-N3	-18.75	119.92	129.30
23	BB	53	A	C2-N3-C4	18.75	119.98	110.60
22	BA	866	A	N1-C6-N6	-18.75	107.35	118.60
22	BA	213	A	N1-C2-N3	-18.75	119.93	129.30
22	BA	1434	A	C2-N3-C4	18.75	119.97	110.60
22	BA	244	A	N1-C2-N3	-18.75	119.93	129.30
22	BA	899	A	N1-C6-N6	-18.75	107.35	118.60
22	BA	2090	A	C2-N3-C4	18.75	119.97	110.60
54	D2	73	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	655	A	C2-N3-C4	18.74	119.97	110.60
22	BA	2753	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	125	A	C2-N3-C4	18.74	119.97	110.60
22	BA	1028	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	1919	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	793	A	C2-N3-C4	18.74	119.97	110.60
22	BA	918	A	N1-C2-N3	-18.74	119.93	129.30
22	BA	1918	A	N1-C2-N3	-18.73	119.93	129.30
22	BA	2059	A	N1-C2-N3	-18.73	119.93	129.30
22	BA	716	A	C2-N3-C4	18.73	119.97	110.60
22	BA	2531	A	C2-N3-C4	18.73	119.97	110.60
22	BA	2750	A	N1-C2-N3	-18.73	119.94	129.30
22	BA	602	A	N1-C2-N3	-18.73	119.94	129.30
22	BA	2158	A	C2-N3-C4	18.73	119.96	110.60
22	BA	2388	A	N1-C6-N6	-18.73	107.36	118.60
55	D3	35	A	C2-N3-C4	18.73	119.97	110.60
22	BA	1966	A	N1-C2-N3	-18.73	119.94	129.30
22	BA	1515	A	C2-N3-C4	18.73	119.96	110.60
23	BB	58	A	N1-C6-N6	-18.73	107.36	118.60
22	BA	176	A	C2-N3-C4	18.72	119.96	110.60
22	BA	423	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	449	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	878	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	1553	A	N1-C6-N6	-18.72	107.37	118.60
54	D2	49	A	C2-N3-C4	18.72	119.96	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D2	51	A	C2-N3-C4	18.72	119.96	110.60
22	BA	1090	A	N1-C2-N3	-18.72	119.94	129.30
22	BA	1698	A	C2-N3-C4	18.72	119.96	110.60
22	BA	2749	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	222	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	761	A	N1-C6-N6	-18.72	107.37	118.60
22	BA	1213	A	N1-C2-N3	-18.72	119.94	129.30
22	BA	196	A	N1-C2-N3	-18.71	119.94	129.30
22	BA	1089	A	C2-N3-C4	18.71	119.96	110.60
22	BA	1569	A	N1-C2-N3	-18.71	119.94	129.30
22	BA	2163	A	N1-C6-N6	-18.71	107.37	118.60
23	BB	101	A	N1-C2-N3	-18.71	119.94	129.30
22	BA	73	A	C2-N3-C4	18.71	119.95	110.60
22	BA	1885	A	N1-C2-N3	-18.71	119.95	129.30
22	BA	2792	A	C2-N3-C4	18.71	119.95	110.60
22	BA	2377	A	N1-C2-N3	-18.70	119.95	129.30
22	BA	2482	A	C2-N3-C4	18.70	119.95	110.60
22	BA	190	A	N1-C2-N3	-18.70	119.95	129.30
22	BA	1151	A	C2-N3-C4	18.70	119.95	110.60
22	BA	2426	A	N1-C2-N3	-18.70	119.95	129.30
54	D2	58	A	N1-C2-N3	-18.70	119.95	129.30
22	BA	1913	A	N1-C2-N3	-18.70	119.95	129.30
22	BA	2513	A	C2-N3-C4	18.70	119.95	110.60
22	BA	2741	A	N1-C2-N3	-18.70	119.95	129.30
22	BA	2158	A	N1-C6-N6	-18.70	107.38	118.60
22	BA	2662	A	C2-N3-C4	18.70	119.95	110.60
22	BA	344	A	C2-N3-C4	18.70	119.95	110.60
22	BA	1367	A	N1-C6-N6	-18.70	107.38	118.60
22	BA	1494	A	C2-N3-C4	18.70	119.95	110.60
23	BB	59	A	C2-N3-C4	18.70	119.95	110.60
22	BA	1275	A	N1-C2-N3	-18.70	119.95	129.30
22	BA	2518	A	N1-C6-N6	-18.70	107.38	118.60
22	BA	1815	A	C2-N3-C4	18.69	119.95	110.60
54	D2	31	A	N1-C6-N6	-18.69	107.38	118.60
22	BA	743	A	C2-N3-C4	18.69	119.95	110.60
22	BA	936	A	C2-N3-C4	18.69	119.95	110.60
22	BA	2298	A	C2-N3-C4	18.69	119.94	110.60
22	BA	1580	A	C2-N3-C4	18.69	119.94	110.60
22	BA	631	A	N1-C6-N6	-18.69	107.39	118.60
22	BA	705	A	C2-N3-C4	18.69	119.94	110.60
22	BA	2309	A	C2-N3-C4	18.69	119.94	110.60
22	BA	172	A	C2-N3-C4	18.68	119.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	471	A	N1-C6-N6	-18.68	107.39	118.60
22	BA	633	A	C2-N3-C4	18.68	119.94	110.60
22	BA	1008	A	C2-N3-C4	18.68	119.94	110.60
22	BA	1032	A	N1-C6-N6	-18.68	107.39	118.60
22	BA	1635	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	2753	A	N1-C6-N6	-18.68	107.39	118.60
23	BB	52	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	344	A	N1-C2-N3	-18.68	119.96	129.30
55	D3	38	A	N1-C6-N6	-18.68	107.39	118.60
22	BA	2333	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	1745	A	C2-N3-C4	18.68	119.94	110.60
22	BA	1801	A	C2-N3-C4	18.68	119.94	110.60
22	BA	1916	A	C2-N3-C4	18.68	119.94	110.60
22	BA	2748	A	C2-N3-C4	18.68	119.94	110.60
22	BA	1241	A	N1-C2-N3	-18.68	119.96	129.30
22	BA	1579	A	N1-C6-N6	-18.68	107.39	118.60
22	BA	2433	A	N1-C6-N6	-18.68	107.39	118.60
22	BA	2764	A	C2-N3-C4	18.68	119.94	110.60
22	BA	2660	A	N1-C2-N3	-18.67	119.96	129.30
54	D2	73	A	C2-N3-C4	18.67	119.94	110.60
22	BA	2468	A	C2-N3-C4	18.67	119.94	110.60
22	BA	2851	A	N1-C6-N6	-18.67	107.40	118.60
22	BA	1040	A	C2-N3-C4	18.67	119.94	110.60
22	BA	146	A	C2-N3-C4	18.67	119.93	110.60
22	BA	705	A	N1-C2-N3	-18.67	119.97	129.30
22	BA	2837	A	C2-N3-C4	18.67	119.93	110.60
22	BA	1264	A	N1-C2-N3	-18.67	119.97	129.30
22	BA	1700	A	N1-C2-N3	-18.67	119.97	129.30
22	BA	2566	A	C2-N3-C4	18.66	119.93	110.60
22	BA	1593	A	C2-N3-C4	18.66	119.93	110.60
22	BA	126	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	207	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	614	A	N1-C6-N6	-18.66	107.40	118.60
22	BA	676	A	C2-N3-C4	18.66	119.93	110.60
22	BA	1070	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	2835	A	N1-C6-N6	-18.66	107.40	118.60
22	BA	1936	A	N1-C6-N6	-18.66	107.40	118.60
22	BA	1247	A	C2-N3-C4	18.66	119.93	110.60
22	BA	460	A	C2-N3-C4	18.66	119.93	110.60
22	BA	2169	A	N1-C2-N3	-18.66	119.97	129.30
22	BA	165	A	C2-N3-C4	18.65	119.93	110.60
22	BA	877	A	N1-C2-N3	-18.65	119.97	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	155	A	C2-N3-C4	18.65	119.93	110.60
22	BA	945	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	1494	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	1048	A	N1-C2-N3	-18.65	119.97	129.30
22	BA	1916	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	2826	A	N1-C2-N3	-18.65	119.97	129.30
22	BA	503	A	N1-C2-N3	-18.65	119.98	129.30
22	BA	761	A	C2-N3-C4	18.65	119.92	110.60
22	BA	1126	A	N1-C2-N3	-18.65	119.97	129.30
22	BA	1634	A	C2-N3-C4	18.65	119.92	110.60
22	BA	1819	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	2317	A	C2-N3-C4	18.65	119.92	110.60
22	BA	1569	A	N1-C6-N6	-18.65	107.41	118.60
22	BA	1276	A	C2-N3-C4	18.65	119.92	110.60
22	BA	920	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	299	A	N1-C6-N6	-18.64	107.41	118.60
22	BA	404	A	N1-C6-N6	-18.64	107.41	118.60
22	BA	447	A	C2-N3-C4	18.64	119.92	110.60
22	BA	825	A	N1-C6-N6	-18.64	107.41	118.60
22	BA	1477	A	C2-N3-C4	18.64	119.92	110.60
22	BA	2425	A	C2-N3-C4	18.64	119.92	110.60
22	BA	223	A	C2-N3-C4	18.64	119.92	110.60
22	BA	1383	A	C2-N3-C4	18.64	119.92	110.60
22	BA	1808	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	279	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	802	A	N1-C2-N3	-18.64	119.98	129.30
22	BA	2058	A	N1-C6-N6	-18.64	107.42	118.60
22	BA	94	A	C2-N3-C4	18.63	119.92	110.60
22	BA	1641	A	N1-C6-N6	-18.63	107.42	118.60
22	BA	2900	A	C2-N3-C4	18.63	119.92	110.60
22	BA	2810	A	C2-N3-C4	18.63	119.92	110.60
22	BA	497	A	N1-C2-N3	-18.63	119.99	129.30
22	BA	735	A	N1-C2-N3	-18.63	119.99	129.30
22	BA	1583	A	C2-N3-C4	18.63	119.91	110.60
22	BA	2679	A	C2-N3-C4	18.63	119.91	110.60
22	BA	1287	A	N1-C6-N6	-18.62	107.42	118.60
22	BA	1689	A	N1-C2-N3	-18.62	119.99	129.30
22	BA	2587	A	N1-C2-N3	-18.62	119.99	129.30
22	BA	925	A	C2-N3-C4	18.62	119.91	110.60
22	BA	1427	A	C2-N3-C4	18.62	119.91	110.60
22	BA	161	A	C2-N3-C4	18.62	119.91	110.60
22	BA	460	A	N1-C2-N3	-18.62	119.99	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1134	A	C2-N3-C4	18.62	119.91	110.60
22	BA	1254	A	C2-N3-C4	18.62	119.91	110.60
22	BA	2750	A	N1-C6-N6	-18.62	107.43	118.60
22	BA	2868	A	N1-C2-N3	-18.62	119.99	129.30
55	D3	76	A	N1-C2-N3	-18.61	119.99	129.30
22	BA	2346	A	N1-C6-N6	-18.61	107.43	118.60
22	BA	2358	A	N1-C6-N6	-18.61	107.43	118.60
22	BA	2482	A	N1-C2-N3	-18.61	119.99	129.30
22	BA	794	A	C2-N3-C4	18.61	119.90	110.60
22	BA	1495	A	N1-C2-N3	-18.61	120.00	129.30
22	BA	1885	A	C2-N3-C4	18.61	119.91	110.60
22	BA	2211	A	C2-N3-C4	18.61	119.91	110.60
22	BA	2439	A	N1-C2-N3	-18.61	120.00	129.30
22	BA	2750	A	C2-N3-C4	18.61	119.90	110.60
22	BA	199	A	N1-C2-N3	-18.61	120.00	129.30
22	BA	541	A	C2-N3-C4	18.61	119.90	110.60
22	BA	1354	A	C2-N3-C4	18.61	119.90	110.60
22	BA	265	A	C2-N3-C4	18.60	119.90	110.60
22	BA	73	A	N1-C6-N6	-18.60	107.44	118.60
22	BA	83	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	1853	A	C2-N3-C4	18.60	119.90	110.60
22	BA	2665	A	N1-C6-N6	-18.60	107.44	118.60
22	BA	1801	A	N1-C2-N3	-18.60	120.00	129.30
23	BB	57	A	N1-C6-N6	-18.60	107.44	118.60
22	BA	218	A	C2-N3-C4	18.60	119.90	110.60
22	BA	1089	A	N1-C2-N3	-18.60	120.00	129.30
22	BA	515	A	C2-N3-C4	18.59	119.90	110.60
22	BA	1413	A	C2-N3-C4	18.59	119.90	110.60
22	BA	1552	A	C2-N3-C4	18.59	119.90	110.60
22	BA	2311	A	N1-C2-N3	-18.59	120.00	129.30
22	BA	340	A	C2-N3-C4	18.59	119.90	110.60
22	BA	270	A	N1-C2-N3	-18.59	120.00	129.30
22	BA	599	A	C2-N3-C4	18.59	119.90	110.60
22	BA	677	A	C2-N3-C4	18.59	119.89	110.60
22	BA	1111	A	N1-C2-N3	-18.59	120.00	129.30
22	BA	1490	A	N1-C6-N6	-18.59	107.44	118.60
22	BA	1508	A	N1-C6-N6	-18.59	107.44	118.60
22	BA	1641	A	C2-N3-C4	18.59	119.89	110.60
22	BA	52	A	N1-C2-N3	-18.59	120.00	129.30
22	BA	1085	A	C2-N3-C4	18.59	119.89	110.60
22	BA	2088	A	C2-N3-C4	18.59	119.89	110.60
22	BA	2660	A	C2-N3-C4	18.59	119.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2835	A	C2-N3-C4	18.59	119.89	110.60
22	BA	94	A	N1-C6-N6	-18.59	107.45	118.60
22	BA	255	A	N1-C6-N6	-18.59	107.45	118.60
22	BA	661	A	C2-N3-C4	18.59	119.89	110.60
22	BA	1809	A	C2-N3-C4	18.58	119.89	110.60
22	BA	2019	A	C2-N3-C4	18.58	119.89	110.60
22	BA	2378	A	N1-C2-N3	-18.58	120.01	129.30
54	D2	23	A	C2-N3-C4	18.58	119.89	110.60
22	BA	2764	A	N1-C2-N3	-18.58	120.01	129.30
22	BA	502	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	613	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	2872	A	N1-C2-N3	-18.58	120.01	129.30
22	BA	2879	A	N1-C2-N3	-18.58	120.01	129.30
22	BA	1583	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	2297	A	N1-C6-N6	-18.58	107.45	118.60
22	BA	2893	A	C2-N3-C4	18.57	119.89	110.60
22	BA	1853	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	1877	A	N1-C2-N3	-18.57	120.01	129.30
22	BA	909	A	C2-N3-C4	18.57	119.89	110.60
22	BA	1772	A	C2-N3-C4	18.57	119.89	110.60
22	BA	2322	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	2665	A	C2-N3-C4	18.57	119.89	110.60
23	BB	58	A	C2-N3-C4	18.57	119.89	110.60
22	BA	1632	A	N1-C2-N3	-18.57	120.02	129.30
55	D3	7	A	C2-N3-C4	18.57	119.89	110.60
22	BA	1194	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	2468	A	N1-C2-N3	-18.57	120.02	129.30
22	BA	666	A	C2-N3-C4	18.57	119.88	110.60
22	BA	975	A	N1-C6-N6	-18.57	107.46	118.60
22	BA	1269	A	C2-N3-C4	18.57	119.88	110.60
22	BA	905	A	C2-N3-C4	18.56	119.88	110.60
22	BA	979	A	C2-N3-C4	18.56	119.88	110.60
22	BA	83	A	N1-C6-N6	-18.56	107.46	118.60
22	BA	1274	A	N1-C6-N6	-18.56	107.46	118.60
22	BA	2033	A	N1-C6-N6	-18.56	107.46	118.60
22	BA	2170	A	N1-C6-N6	-18.56	107.46	118.60
22	BA	101	A	N1-C6-N6	-18.56	107.46	118.60
22	BA	2015	A	N1-C2-N3	-18.56	120.02	129.30
22	BA	1690	A	N1-C2-N3	-18.56	120.02	129.30
54	D2	73	A	N1-C6-N6	-18.56	107.47	118.60
22	BA	1566	A	C2-N3-C4	18.55	119.88	110.60
22	BA	1749	A	C2-N3-C4	18.55	119.88	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2108	A	N1-C6-N6	-18.55	107.47	118.60
22	BA	2820	A	N1-C2-N3	-18.55	120.02	129.30
22	BA	1637	A	C2-N3-C4	18.55	119.88	110.60
22	BA	1679	A	N1-C6-N6	-18.55	107.47	118.60
23	BB	104	A	N1-C6-N6	-18.55	107.47	118.60
22	BA	2826	A	C2-N3-C4	18.55	119.88	110.60
22	BA	217	A	N1-C6-N6	-18.55	107.47	118.60
22	BA	1754	A	N1-C2-N3	-18.55	120.03	129.30
22	BA	2733	A	N1-C6-N6	-18.55	107.47	118.60
22	BA	526	A	C2-N3-C4	18.55	119.87	110.60
22	BA	1669	A	N1-C6-N6	-18.55	107.47	118.60
22	BA	2147	A	N1-C2-N3	-18.55	120.03	129.30
22	BA	2700	A	C2-N3-C4	18.55	119.87	110.60
22	BA	2530	A	N1-C6-N6	-18.54	107.47	118.60
22	BA	401	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	428	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1395	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	1553	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	718	A	C2-N3-C4	18.54	119.87	110.60
22	BA	833	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1111	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1307	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	1503	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1858	A	C2-N3-C4	18.54	119.87	110.60
22	BA	270	A	C2-N3-C4	18.54	119.87	110.60
22	BA	457	A	C2-N3-C4	18.54	119.87	110.60
22	BA	1098	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	1496	A	C2-N3-C4	18.54	119.87	110.60
22	BA	2042	A	N1-C6-N6	-18.54	107.48	118.60
22	BA	927	A	N1-C2-N3	-18.54	120.03	129.30
22	BA	2873	A	N1-C6-N6	-18.54	107.48	118.60
22	BA	207	A	C2-N3-C4	18.53	119.87	110.60
22	BA	670	A	N1-C2-N3	-18.53	120.03	129.30
22	BA	1773	A	N1-C6-N6	-18.53	107.48	118.60
22	BA	1373	A	C2-N3-C4	18.53	119.86	110.60
22	BA	1635	A	N1-C6-N6	-18.53	107.48	118.60
22	BA	1654	A	N1-C6-N6	-18.53	107.48	118.60
22	BA	2142	A	C2-N3-C4	18.53	119.86	110.60
22	BA	2212	A	N1-C6-N6	-18.53	107.48	118.60
22	BA	256	A	N1-C2-N3	-18.53	120.03	129.30
22	BA	792	A	N1-C6-N6	-18.53	107.48	118.60
22	BA	1784	A	N1-C2-N3	-18.53	120.04	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2274	A	N1-C6-N6	-18.53	107.48	118.60
54	D2	21	A	N1-C6-N6	-18.53	107.48	118.60
22	BA	362	A	N1-C6-N6	-18.52	107.48	118.60
22	BA	980	A	N1-C6-N6	-18.52	107.48	118.60
22	BA	761	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	1230	A	C2-N3-C4	18.52	119.86	110.60
22	BA	1322	A	N1-C2-N3	-18.52	120.04	129.30
22	BA	2198	A	C2-N3-C4	18.52	119.86	110.60
22	BA	2392	A	C2-N3-C4	18.52	119.86	110.60
22	BA	1901	A	N1-C6-N6	-18.52	107.49	118.60
54	D2	76	A	C2-N3-C4	18.52	119.86	110.60
22	BA	56	A	C2-N3-C4	18.52	119.86	110.60
22	BA	718	A	N1-C6-N6	-18.52	107.49	118.60
22	BA	1080	A	C2-N3-C4	18.52	119.86	110.60
22	BA	1634	A	N1-C6-N6	-18.52	107.49	118.60
22	BA	2516	A	C2-N3-C4	18.52	119.86	110.60
22	BA	38	A	N1-C6-N6	-18.52	107.49	118.60
22	BA	265	A	N1-C6-N6	-18.52	107.49	118.60
22	BA	2810	A	N1-C6-N6	-18.52	107.49	118.60
23	BB	46	A	N1-C6-N6	-18.52	107.49	118.60
22	BA	2126	A	N1-C2-N3	-18.51	120.04	129.30
22	BA	1285	A	C2-N3-C4	18.51	119.86	110.60
22	BA	53	A	C2-N3-C4	18.51	119.86	110.60
22	BA	384	A	N1-C6-N6	-18.51	107.50	118.60
22	BA	2094	A	C2-N3-C4	18.51	119.86	110.60
22	BA	752	A	C2-N3-C4	18.51	119.85	110.60
22	BA	1359	A	N1-C2-N3	-18.51	120.05	129.30
23	BB	109	A	C2-N3-C4	18.51	119.85	110.60
22	BA	1652	A	N1-C2-N3	-18.51	120.05	129.30
22	BA	800	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	1439	A	C2-N3-C4	18.50	119.85	110.60
23	BB	101	A	C2-N3-C4	18.50	119.85	110.60
22	BA	1088	A	N1-C6-N6	-18.50	107.50	118.60
22	BA	917	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	1953	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	2154	A	C2-N3-C4	18.50	119.85	110.60
22	BA	2377	A	C2-N3-C4	18.50	119.85	110.60
22	BA	2547	A	C2-N3-C4	18.50	119.85	110.60
22	BA	2407	A	C2-N3-C4	18.50	119.85	110.60
22	BA	2425	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	2721	A	N1-C2-N3	-18.50	120.05	129.30
22	BA	1711	A	C2-N3-C4	18.50	119.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	222	A	C2-N3-C4	18.49	119.85	110.60
22	BA	453	A	C2-N3-C4	18.49	119.85	110.60
22	BA	1366	A	N1-C2-N3	-18.49	120.05	129.30
22	BA	2432	A	N1-C6-N6	-18.49	107.50	118.60
22	BA	428	A	N1-C6-N6	-18.49	107.50	118.60
22	BA	478	A	C2-N3-C4	18.49	119.84	110.60
22	BA	2476	A	N1-C2-N3	-18.49	120.06	129.30
54	D2	41	A	C2-N3-C4	18.49	119.84	110.60
22	BA	1652	A	C2-N3-C4	18.49	119.84	110.60
22	BA	1899	A	N1-C6-N6	-18.49	107.51	118.60
22	BA	282	A	C2-N3-C4	18.49	119.84	110.60
22	BA	1046	A	N1-C6-N6	-18.49	107.51	118.60
22	BA	1308	A	N1-C6-N6	-18.49	107.51	118.60
22	BA	52	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	423	A	C2-N3-C4	18.48	119.84	110.60
22	BA	920	A	C2-N3-C4	18.48	119.84	110.60
22	BA	1070	A	C2-N3-C4	18.48	119.84	110.60
22	BA	1287	A	C2-N3-C4	18.48	119.84	110.60
22	BA	1308	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	1899	A	C2-N3-C4	18.48	119.84	110.60
22	BA	344	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	2734	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	782	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	2019	A	N1-C6-N6	-18.48	107.51	118.60
22	BA	2478	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	2765	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	2352	A	C2-N3-C4	18.48	119.84	110.60
22	BA	346	A	C2-N3-C4	18.48	119.84	110.60
22	BA	677	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	1237	A	C2-N3-C4	18.48	119.84	110.60
22	BA	2173	A	N1-C2-N3	-18.48	120.06	129.30
22	BA	2577	A	C2-N3-C4	18.48	119.84	110.60
22	BA	722	A	C2-N3-C4	18.48	119.84	110.60
22	BA	2377	A	N1-C6-N6	-18.48	107.52	118.60
55	D3	14	A	C2-N3-C4	18.47	119.84	110.60
22	BA	478	A	N1-C2-N3	-18.47	120.06	129.30
22	BA	197	A	N1-C2-N3	-18.47	120.06	129.30
22	BA	294	A	N1-C6-N6	-18.47	107.52	118.60
22	BA	973	A	N1-C2-N3	-18.47	120.06	129.30
22	BA	1175	A	N1-C6-N6	-18.47	107.52	118.60
22	BA	1889	A	N1-C2-N3	-18.47	120.07	129.30
22	BA	1912	A	C2-N3-C4	18.47	119.83	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	45	A	N1-C2-N3	-18.47	120.06	129.30
22	BA	156	A	C2-N3-C4	18.47	119.83	110.60
22	BA	2058	A	N1-C2-N3	-18.47	120.07	129.30
22	BA	572	A	N1-C6-N6	-18.47	107.52	118.60
22	BA	1571	A	C2-N3-C4	18.47	119.83	110.60
22	BA	1876	A	N1-C6-N6	-18.47	107.52	118.60
22	BA	2052	A	N1-C2-N3	-18.47	120.07	129.30
22	BA	2654	A	C2-N3-C4	18.47	119.83	110.60
22	BA	2740	A	N1-C6-N6	-18.47	107.52	118.60
22	BA	592	A	N1-C6-N6	-18.46	107.52	118.60
22	BA	2309	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	251	A	C2-N3-C4	18.46	119.83	110.60
22	BA	973	A	N1-C6-N6	-18.46	107.52	118.60
22	BA	1090	A	C2-N3-C4	18.46	119.83	110.60
22	BA	429	A	C2-N3-C4	18.46	119.83	110.60
22	BA	1419	A	C2-N3-C4	18.46	119.83	110.60
22	BA	1545	A	N1-C6-N6	-18.46	107.52	118.60
23	BB	34	A	C2-N3-C4	18.46	119.83	110.60
22	BA	1354	A	N1-C6-N6	-18.46	107.53	118.60
22	BA	1655	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	44	A	C2-N3-C4	18.46	119.83	110.60
22	BA	918	A	N1-C6-N6	-18.46	107.53	118.60
22	BA	127	A	N1-C6-N6	-18.46	107.53	118.60
22	BA	428	A	N1-C2-N3	-18.46	120.07	129.30
22	BA	181	A	N1-C2-N3	-18.45	120.07	129.30
22	BA	503	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	2469	A	C2-N3-C4	18.45	119.83	110.60
22	BA	91	A	N1-C2-N3	-18.45	120.07	129.30
22	BA	979	A	N1-C2-N3	-18.45	120.07	129.30
22	BA	877	A	C2-N3-C4	18.45	119.83	110.60
22	BA	1722	A	N1-C2-N3	-18.45	120.08	129.30
22	BA	2886	A	N1-C2-N3	-18.45	120.08	129.30
23	BB	109	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	1039	A	N1-C6-N6	-18.45	107.53	118.60
22	BA	829	A	N1-C2-N3	-18.45	120.08	129.30
22	BA	125	A	N1-C6-N6	-18.44	107.53	118.60
22	BA	1745	A	N1-C2-N3	-18.44	120.08	129.30
22	BA	2176	A	N1-C2-N3	-18.44	120.08	129.30
22	BA	2541	A	C2-N3-C4	18.44	119.82	110.60
54	D2	38	A	C2-N3-C4	18.44	119.82	110.60
22	BA	2682	A	N1-C2-N3	-18.44	120.08	129.30
22	BA	2887	A	N1-C6-N6	-18.44	107.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1347	A	N1-C6-N6	-18.43	107.54	118.60
22	BA	715	A	C2-N3-C4	18.43	119.82	110.60
22	BA	945	A	N1-C2-N3	-18.43	120.08	129.30
22	BA	300	A	N1-C2-N3	-18.43	120.08	129.30
55	D3	9	A	N1-C2-N3	-18.43	120.09	129.30
22	BA	74	A	N1-C6-N6	-18.43	107.54	118.60
22	BA	742	A	N1-C2-N3	-18.43	120.09	129.30
22	BA	1494	A	N1-C2-N3	-18.43	120.09	129.30
22	BA	6	A	C2-N3-C4	18.43	119.81	110.60
22	BA	1009	A	N1-C2-N3	-18.43	120.09	129.30
22	BA	2020	A	C2-N3-C4	18.43	119.81	110.60
22	BA	1246	A	C2-N3-C4	18.42	119.81	110.60
22	BA	2381	A	C2-N3-C4	18.42	119.81	110.60
22	BA	943	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	1129	A	C2-N3-C4	18.42	119.81	110.60
22	BA	1916	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	586	A	N1-C6-N6	-18.42	107.55	118.60
22	BA	1477	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	819	A	N1-C2-N3	-18.42	120.09	129.30
22	BA	2135	A	C2-N3-C4	18.42	119.81	110.60
22	BA	402	A	C2-N3-C4	18.41	119.81	110.60
22	BA	1050	A	N1-C2-N3	-18.41	120.09	129.30
22	BA	1133	A	C2-N3-C4	18.41	119.81	110.60
22	BA	2820	A	C2-N3-C4	18.41	119.81	110.60
22	BA	454	A	C2-N3-C4	18.41	119.81	110.60
22	BA	1040	A	N1-C6-N6	-18.41	107.55	118.60
22	BA	1496	A	N1-C2-N3	-18.41	120.10	129.30
22	BA	2340	A	C2-N3-C4	18.41	119.80	110.60
22	BA	404	A	C2-N3-C4	18.41	119.80	110.60
22	BA	167	A	N1-C2-N3	-18.41	120.10	129.30
22	BA	472	A	N1-C6-N6	-18.40	107.56	118.60
22	BA	633	A	N1-C2-N3	-18.40	120.10	129.30
22	BA	14	A	C2-N3-C4	18.40	119.80	110.60
22	BA	63	A	N1-C2-N3	-18.40	120.10	129.30
22	BA	1095	A	N1-C6-N6	-18.40	107.56	118.60
22	BA	751	A	N1-C6-N6	-18.40	107.56	118.60
22	BA	1809	A	N1-C2-N3	-18.40	120.10	129.30
22	BA	2406	A	C2-N3-C4	18.40	119.80	110.60
22	BA	221	A	N1-C6-N6	-18.39	107.56	118.60
22	BA	2042	A	N1-C2-N3	-18.39	120.11	129.30
22	BA	195	A	C2-N3-C4	18.39	119.79	110.60
22	BA	1089	A	N1-C6-N6	-18.39	107.57	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2205	A	C2-N3-C4	18.39	119.79	110.60
22	BA	226	A	N1-C2-N3	-18.39	120.11	129.30
22	BA	374	A	N1-C6-N6	-18.39	107.57	118.60
22	BA	2829	A	C2-N3-C4	18.39	119.79	110.60
22	BA	1566	A	N1-C6-N6	-18.38	107.57	118.60
22	BA	2311	A	N1-C6-N6	-18.38	107.57	118.60
22	BA	501	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	1156	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	1987	A	C2-N3-C4	18.38	119.79	110.60
22	BA	2635	A	C2-N3-C4	18.38	119.79	110.60
22	BA	2657	A	C2-N3-C4	18.38	119.79	110.60
22	BA	706	A	C2-N3-C4	18.38	119.79	110.60
22	BA	1571	A	N1-C6-N6	-18.38	107.57	118.60
22	BA	1757	A	N1-C6-N6	-18.38	107.57	118.60
22	BA	142	A	C2-N3-C4	18.38	119.79	110.60
22	BA	1630	A	N1-C6-N6	-18.38	107.57	118.60
22	BA	574	A	N1-C2-N3	-18.38	120.11	129.30
22	BA	1597	A	N1-C6-N6	-18.38	107.57	118.60
22	BA	1787	A	C2-N3-C4	18.38	119.79	110.60
22	BA	574	A	C2-N3-C4	18.37	119.79	110.60
22	BA	716	A	N1-C2-N3	-18.37	120.11	129.30
22	BA	42	A	C2-N3-C4	18.37	119.79	110.60
22	BA	103	A	C2-N3-C4	18.37	119.78	110.60
22	BA	219	A	N1-C2-N3	-18.37	120.11	129.30
22	BA	352	A	C2-N3-C4	18.37	119.79	110.60
22	BA	1067	A	N1-C6-N6	-18.37	107.58	118.60
22	BA	1689	A	C2-N3-C4	18.37	119.78	110.60
22	BA	1872	A	C2-N3-C4	18.37	119.78	110.60
22	BA	2225	A	N1-C6-N6	-18.37	107.58	118.60
22	BA	2267	A	N1-C2-N3	-18.37	120.12	129.30
22	BA	1783	A	N1-C6-N6	-18.37	107.58	118.60
22	BA	2117	A	C2-N3-C4	18.37	119.78	110.60
22	BA	1591	A	C2-N3-C4	18.37	119.78	110.60
22	BA	340	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	2598	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	2589	A	N1-C6-N6	-18.36	107.58	118.60
22	BA	2322	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	453	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	505	A	N1-C2-N3	-18.36	120.12	129.30
22	BA	1244	A	C2-N3-C4	18.36	119.78	110.60
22	BA	1610	A	N1-C6-N6	-18.36	107.59	118.60
22	BA	227	A	C2-N3-C4	18.35	119.78	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	233	A	C2-N3-C4	18.35	119.78	110.60
22	BA	1103	A	N1-C6-N6	-18.35	107.59	118.60
22	BA	1866	A	C2-N3-C4	18.35	119.78	110.60
23	BB	101	A	N1-C6-N6	-18.35	107.59	118.60
22	BA	471	A	C2-N3-C4	18.35	119.78	110.60
22	BA	2614	A	N1-C2-N3	-18.35	120.12	129.30
22	BA	2748	A	N1-C6-N6	-18.35	107.59	118.60
22	BA	1616	A	C2-N3-C4	18.35	119.77	110.60
22	BA	1757	A	C2-N3-C4	18.35	119.77	110.60
22	BA	2311	A	C2-N3-C4	18.35	119.77	110.60
22	BA	2851	A	N1-C2-N3	-18.34	120.13	129.30
22	BA	330	A	N1-C2-N3	-18.34	120.13	129.30
22	BA	1509	A	C2-N3-C4	18.34	119.77	110.60
22	BA	1630	A	C2-N3-C4	18.34	119.77	110.60
54	D2	9	A	N1-C6-N6	-18.34	107.60	118.60
22	BA	751	A	C2-N3-C4	18.34	119.77	110.60
22	BA	1528	A	C2-N3-C4	18.34	119.77	110.60
22	BA	1735	A	C2-N3-C4	18.33	119.77	110.60
22	BA	1086	A	N1-C2-N3	-18.33	120.13	129.30
22	BA	2411	A	N1-C2-N3	-18.33	120.13	129.30
22	BA	1802	A	N1-C2-N3	-18.33	120.14	129.30
22	BA	1808	A	C2-N3-C4	18.33	119.77	110.60
22	BA	1085	A	N1-C6-N6	-18.33	107.60	118.60
22	BA	1700	A	C2-N3-C4	18.32	119.76	110.60
23	BB	115	A	C2-N3-C4	18.32	119.76	110.60
22	BA	981	A	N1-C2-N3	-18.32	120.14	129.30
22	BA	1073	A	N1-C2-N3	-18.32	120.14	129.30
22	BA	1755	A	N1-C2-N3	-18.32	120.14	129.30
22	BA	2778	A	N1-C6-N6	-18.32	107.61	118.60
22	BA	1502	A	C2-N3-C4	18.32	119.76	110.60
22	BA	2433	A	C2-N3-C4	18.32	119.76	110.60
22	BA	2826	A	N1-C6-N6	-18.32	107.61	118.60
22	BA	272	A	C2-N3-C4	18.32	119.76	110.60
22	BA	603	A	C2-N3-C4	18.32	119.76	110.60
22	BA	332	A	N1-C6-N6	-18.32	107.61	118.60
22	BA	2411	A	C2-N3-C4	18.32	119.76	110.60
22	BA	2247	A	C2-N3-C4	18.31	119.76	110.60
55	D3	36	A	N1-C2-N3	-18.31	120.14	129.30
22	BA	2135	A	N1-C2-N3	-18.31	120.14	129.30
22	BA	447	A	N1-C2-N3	-18.31	120.14	129.30
22	BA	1672	A	C2-N3-C4	18.31	119.75	110.60
22	BA	1969	A	C2-N3-C4	18.31	119.75	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1609	A	N1-C2-N3	-18.31	120.15	129.30
22	BA	1780	A	C2-N3-C4	18.31	119.75	110.60
22	BA	2781	A	C2-N3-C4	18.31	119.75	110.60
22	BA	1570	A	C2-N3-C4	18.31	119.75	110.60
22	BA	1801	A	N1-C6-N6	-18.31	107.62	118.60
22	BA	1689	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	2376	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	1580	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	2530	A	C2-N3-C4	18.30	119.75	110.60
22	BA	342	A	C2-N3-C4	18.30	119.75	110.60
22	BA	1359	A	C2-N3-C4	18.30	119.75	110.60
22	BA	1784	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	213	A	C2-N3-C4	18.30	119.75	110.60
22	BA	556	A	N1-C2-N3	-18.30	120.15	129.30
22	BA	1284	A	C2-N3-C4	18.30	119.75	110.60
22	BA	1700	A	N1-C6-N6	-18.30	107.62	118.60
22	BA	1103	A	C2-N3-C4	18.29	119.75	110.60
22	BA	167	A	N1-C6-N6	-18.29	107.62	118.60
22	BA	1609	A	C2-N3-C4	18.29	119.75	110.60
22	BA	2781	A	N1-C6-N6	-18.29	107.63	118.60
22	BA	497	A	C2-N3-C4	18.29	119.74	110.60
22	BA	575	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	670	A	N1-C6-N6	-18.28	107.63	118.60
22	BA	1535	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	751	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	1431	A	C2-N3-C4	18.28	119.74	110.60
22	BA	19	A	C2-N3-C4	18.28	119.74	110.60
22	BA	626	A	C2-N3-C4	18.28	119.74	110.60
22	BA	1515	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	2598	A	C2-N3-C4	18.28	119.74	110.60
22	BA	821	A	N1-C2-N3	-18.28	120.16	129.30
22	BA	2459	A	C2-N3-C4	18.28	119.74	110.60
23	BB	52	A	C2-N3-C4	18.28	119.74	110.60
22	BA	368	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	960	A	C2-N3-C4	18.27	119.74	110.60
22	BA	2314	A	C2-N3-C4	18.27	119.74	110.60
22	BA	1713	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	1717	A	N1-C2-N3	-18.27	120.16	129.30
22	BA	2426	A	C2-N3-C4	18.27	119.74	110.60
22	BA	2813	A	C2-N3-C4	18.27	119.74	110.60
22	BA	2070	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	2471	A	C2-N3-C4	18.27	119.73	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	471	A	N1-C2-N3	-18.27	120.17	129.30
22	BA	1073	A	C2-N3-C4	18.27	119.73	110.60
22	BA	1156	A	N1-C6-N6	-18.27	107.64	118.60
22	BA	1786	A	N1-C2-N3	-18.26	120.17	129.30
22	BA	2872	A	C2-N3-C4	18.26	119.73	110.60
22	BA	391	A	N1-C6-N6	-18.26	107.64	118.60
22	BA	1433	A	N1-C2-N3	-18.26	120.17	129.30
22	BA	2268	A	N1-C6-N6	-18.26	107.65	118.60
22	BA	2705	A	N1-C6-N6	-18.26	107.65	118.60
22	BA	2309	A	N1-C6-N6	-18.26	107.65	118.60
22	BA	2893	A	N1-C6-N6	-18.26	107.65	118.60
55	D3	31	A	N1-C6-N6	-18.26	107.65	118.60
22	BA	1040	A	N1-C2-N3	-18.25	120.17	129.30
22	BA	1596	A	C2-N3-C4	18.25	119.73	110.60
22	BA	354	A	C2-N3-C4	18.25	119.72	110.60
22	BA	975	A	N1-C2-N3	-18.25	120.17	129.30
22	BA	863	A	C2-N3-C4	18.25	119.72	110.60
22	BA	1745	A	N1-C6-N6	-18.25	107.65	118.60
22	BA	1084	A	N1-C6-N6	-18.25	107.65	118.60
22	BA	706	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	718	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	788	A	C2-N3-C4	18.24	119.72	110.60
22	BA	104	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	415	A	C2-N3-C4	18.24	119.72	110.60
22	BA	2158	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	2860	A	N1-C2-N3	-18.24	120.18	129.30
22	BA	482	A	N1-C6-N6	-18.24	107.66	118.60
22	BA	1495	A	N1-C6-N6	-18.24	107.66	118.60
22	BA	2114	A	N1-C6-N6	-18.24	107.66	118.60
22	BA	2598	A	N1-C6-N6	-18.24	107.66	118.60
22	BA	244	A	C2-N3-C4	18.23	119.72	110.60
22	BA	244	A	N1-C6-N6	-18.23	107.66	118.60
22	BA	1705	A	C2-N3-C4	18.23	119.72	110.60
22	BA	2058	A	C2-N3-C4	18.23	119.72	110.60
23	BB	59	A	N1-C6-N6	-18.23	107.66	118.60
22	BA	1739	A	C2-N3-C4	18.23	119.71	110.60
22	BA	101	A	N1-C2-N3	-18.22	120.19	129.30
22	BA	104	A	C2-N3-C4	18.22	119.71	110.60
22	BA	1096	A	N1-C6-N6	-18.22	107.67	118.60
22	BA	1998	A	C2-N3-C4	18.22	119.71	110.60
22	BA	371	A	N1-C2-N3	-18.22	120.19	129.30
22	BA	2531	A	N1-C6-N6	-18.22	107.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1032	A	C2-N3-C4	18.22	119.71	110.60
22	BA	1008	A	N1-C2-N3	-18.22	120.19	129.30
22	BA	513	A	N1-C2-N3	-18.21	120.19	129.30
22	BA	1286	A	C2-N3-C4	18.21	119.71	110.60
22	BA	1854	A	C2-N3-C4	18.21	119.71	110.60
22	BA	1626	A	N1-C6-N6	-18.21	107.67	118.60
22	BA	1165	A	N1-C6-N6	-18.21	107.67	118.60
22	BA	632	A	C2-N3-C4	18.21	119.70	110.60
22	BA	1586	A	N1-C6-N6	-18.21	107.67	118.60
22	BA	2051	A	C2-N3-C4	18.21	119.70	110.60
22	BA	2114	A	N1-C2-N3	-18.21	120.20	129.30
22	BA	2799	A	N1-C2-N3	-18.21	120.20	129.30
22	BA	752	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	988	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	195	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	94	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	368	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	1175	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	497	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	1952	A	N1-C2-N3	-18.20	120.20	129.30
22	BA	1241	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	1453	A	N1-C6-N6	-18.20	107.68	118.60
22	BA	231	A	C2-N3-C4	18.19	119.70	110.60
23	BB	46	A	N1-C2-N3	-18.19	120.20	129.30
22	BA	715	A	N1-C2-N3	-18.19	120.20	129.30
22	BA	1551	A	C2-N3-C4	18.19	119.70	110.60
22	BA	996	A	C2-N3-C4	18.19	119.69	110.60
22	BA	2726	A	N1-C6-N6	-18.19	107.69	118.60
55	D3	73	A	N1-C6-N6	-18.19	107.69	118.60
22	BA	1143	A	C2-N3-C4	18.19	119.69	110.60
22	BA	1169	A	C2-N3-C4	18.19	119.69	110.60
22	BA	2071	A	C2-N3-C4	18.19	119.69	110.60
22	BA	2412	A	C2-N3-C4	18.19	119.69	110.60
22	BA	1260	A	C2-N3-C4	18.18	119.69	110.60
22	BA	1327	A	C2-N3-C4	18.18	119.69	110.60
22	BA	412	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	2577	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	1877	A	N1-C6-N6	-18.18	107.69	118.60
54	D2	59	A	N1-C2-N3	-18.18	120.21	129.30
22	BA	626	A	N1-C6-N6	-18.18	107.69	118.60
22	BA	721	A	C2-N3-C4	18.17	119.69	110.60
22	BA	1264	A	C2-N3-C4	18.17	119.69	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1552	A	N1-C2-N3	-18.17	120.21	129.30
22	BA	1470	A	C2-N3-C4	18.17	119.69	110.60
22	BA	1586	A	C2-N3-C4	18.17	119.68	110.60
22	BA	191	A	N1-C6-N6	-18.17	107.70	118.60
22	BA	2199	A	N1-C6-N6	-18.17	107.70	118.60
22	BA	52	A	C2-N3-C4	18.16	119.68	110.60
22	BA	1525	A	C2-N3-C4	18.16	119.68	110.60
22	BA	2534	A	C2-N3-C4	18.16	119.68	110.60
22	BA	2873	A	N1-C2-N3	-18.16	120.22	129.30
22	BA	730	A	C2-N3-C4	18.16	119.68	110.60
22	BA	804	A	C2-N3-C4	18.16	119.68	110.60
22	BA	2800	A	N1-C2-N3	-18.16	120.22	129.30
22	BA	1809	A	N1-C6-N6	-18.16	107.71	118.60
22	BA	384	A	C2-N3-C4	18.16	119.68	110.60
22	BA	928	A	C2-N3-C4	18.15	119.68	110.60
22	BA	1938	A	N1-C6-N6	-18.15	107.71	118.60
22	BA	1439	A	N1-C2-N3	-18.15	120.22	129.30
22	BA	1090	A	N1-C6-N6	-18.15	107.71	118.60
22	BA	1134	A	N1-C6-N6	-18.15	107.71	118.60
22	BA	1265	A	N1-C2-N3	-18.15	120.22	129.30
22	BA	1640	A	N1-C2-N3	-18.15	120.23	129.30
22	BA	2108	A	C2-N3-C4	18.15	119.67	110.60
22	BA	2873	A	C2-N3-C4	18.15	119.67	110.60
22	BA	204	A	C2-N3-C4	18.15	119.67	110.60
22	BA	1876	A	N1-C2-N3	-18.15	120.23	129.30
22	BA	2560	A	N1-C2-N3	-18.15	120.23	129.30
23	BB	29	A	N1-C6-N6	-18.15	107.71	118.60
22	BA	2270	A	N1-C6-N6	-18.14	107.71	118.60
22	BA	2278	A	C2-N3-C4	18.14	119.67	110.60
22	BA	103	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	727	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	990	A	C2-N3-C4	18.14	119.67	110.60
22	BA	743	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	1393	A	C2-N3-C4	18.14	119.67	110.60
22	BA	2432	A	C2-N3-C4	18.14	119.67	110.60
22	BA	5	A	C2-N3-C4	18.14	119.67	110.60
22	BA	1127	A	C2-N3-C4	18.14	119.67	110.60
22	BA	749	A	N1-C2-N3	-18.14	120.23	129.30
22	BA	2850	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	165	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	256	A	N1-C6-N6	-18.14	107.72	118.60
22	BA	794	A	N1-C2-N3	-18.14	120.23	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1810	A	C2-N3-C4	18.14	119.67	110.60
22	BA	2015	A	C2-N3-C4	18.14	119.67	110.60
22	BA	1069	A	N1-C2-N3	-18.13	120.23	129.30
23	BB	119	A	C2-N3-C4	18.13	119.67	110.60
22	BA	345	A	N1-C2-N3	-18.13	120.24	129.30
22	BA	988	A	C2-N3-C4	18.13	119.67	110.60
22	BA	1103	A	N1-C2-N3	-18.13	120.23	129.30
22	BA	1143	A	N1-C2-N3	-18.13	120.23	129.30
22	BA	2657	A	N1-C6-N6	-18.13	107.72	118.60
22	BA	2369	A	C2-N3-C4	18.13	119.66	110.60
22	BA	609	A	N1-C6-N6	-18.12	107.73	118.60
22	BA	943	A	N1-C6-N6	-18.12	107.73	118.60
22	BA	1919	A	C2-N3-C4	18.12	119.66	110.60
22	BA	2541	A	N1-C2-N3	-18.12	120.24	129.30
22	BA	294	A	C2-N3-C4	18.12	119.66	110.60
23	BB	15	A	C2-N3-C4	18.12	119.66	110.60
22	BA	14	A	N1-C2-N3	-18.11	120.24	129.30
22	BA	374	A	N1-C2-N3	-18.11	120.24	129.30
22	BA	2860	A	N1-C6-N6	-18.11	107.73	118.60
22	BA	191	A	N1-C2-N3	-18.11	120.25	129.30
22	BA	515	A	N1-C2-N3	-18.11	120.25	129.30
22	BA	1654	A	N1-C2-N3	-18.11	120.25	129.30
22	BA	262	A	N1-C6-N6	-18.10	107.74	118.60
22	BA	829	A	C2-N3-C4	18.10	119.65	110.60
22	BA	1084	A	C2-N3-C4	18.10	119.65	110.60
22	BA	1610	A	C2-N3-C4	18.10	119.65	110.60
22	BA	2534	A	N1-C2-N3	-18.10	120.25	129.30
22	BA	2868	A	N1-C6-N6	-18.10	107.74	118.60
22	BA	152	A	C2-N3-C4	18.10	119.65	110.60
22	BA	2425	A	N1-C6-N6	-18.10	107.74	118.60
22	BA	1789	A	C2-N3-C4	18.10	119.65	110.60
22	BA	2565	A	C2-N3-C4	18.10	119.65	110.60
22	BA	2675	A	N1-C2-N3	-18.10	120.25	129.30
22	BA	833	A	N1-C2-N3	-18.10	120.25	129.30
22	BA	2328	A	N1-C6-N6	-18.10	107.74	118.60
22	BA	226	A	N1-C6-N6	-18.09	107.75	118.60
22	BA	715	A	N1-C6-N6	-18.09	107.75	118.60
22	BA	2632	A	C2-N3-C4	18.09	119.64	110.60
22	BA	1453	A	C2-N3-C4	18.09	119.64	110.60
22	BA	2814	A	C2-N3-C4	18.09	119.64	110.60
22	BA	804	A	N1-C6-N6	-18.09	107.75	118.60
22	BA	2392	A	N1-C6-N6	-18.09	107.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	644	A	C2-N3-C4	18.08	119.64	110.60
22	BA	2062	A	N1-C6-N6	-18.08	107.75	118.60
22	BA	911	A	N1-C6-N6	-18.08	107.75	118.60
22	BA	909	A	N1-C6-N6	-18.08	107.75	118.60
22	BA	348	A	C2-N3-C4	18.08	119.64	110.60
22	BA	1304	A	C2-N3-C4	18.08	119.64	110.60
22	BA	1900	A	N1-C2-N3	-18.08	120.26	129.30
22	BA	477	A	N1-C2-N3	-18.07	120.26	129.30
22	BA	849	A	C2-N3-C4	18.07	119.64	110.60
22	BA	781	A	C2-N3-C4	18.07	119.64	110.60
22	BA	1871	A	N1-C6-N6	-18.07	107.76	118.60
22	BA	643	A	N1-C6-N6	-18.07	107.76	118.60
22	BA	1322	A	C2-N3-C4	18.07	119.64	110.60
22	BA	750	A	N1-C2-N3	-18.07	120.27	129.30
22	BA	111	A	N1-C2-N3	-18.07	120.27	129.30
22	BA	1009	A	N1-C6-N6	-18.07	107.76	118.60
22	BA	1073	A	N1-C6-N6	-18.07	107.76	118.60
23	BB	39	A	N1-C2-N3	-18.07	120.27	129.30
22	BA	941	A	N1-C6-N6	-18.06	107.76	118.60
54	D2	35	A	N1-C2-N3	-18.06	120.27	129.30
22	BA	2170	A	C2-N3-C4	18.06	119.63	110.60
22	BA	960	A	N1-C2-N3	-18.06	120.27	129.30
22	BA	1142	A	N1-C6-N6	-18.06	107.77	118.60
22	BA	2711	A	C2-N3-C4	18.06	119.63	110.60
22	BA	2883	A	N1-C6-N6	-18.06	107.77	118.60
54	D2	9	A	C2-N3-C4	18.06	119.63	110.60
22	BA	1551	A	N1-C6-N6	-18.05	107.77	118.60
22	BA	1010	A	N1-C6-N6	-18.05	107.77	118.60
22	BA	1133	A	N1-C2-N3	-18.05	120.27	129.30
22	BA	492	A	N1-C2-N3	-18.05	120.27	129.30
22	BA	668	A	C2-N3-C4	18.05	119.63	110.60
22	BA	844	A	C2-N3-C4	18.05	119.63	110.60
22	BA	1938	A	N1-C2-N3	-18.05	120.28	129.30
22	BA	2814	A	N1-C2-N3	-18.05	120.28	129.30
22	BA	2513	A	N1-C6-N6	-18.05	107.77	118.60
22	BA	2821	A	N1-C6-N6	-18.05	107.77	118.60
22	BA	699	A	N1-C6-N6	-18.04	107.77	118.60
22	BA	1014	A	C2-N3-C4	18.04	119.62	110.60
22	BA	1226	A	N1-C6-N6	-18.04	107.77	118.60
22	BA	1650	A	N1-C6-N6	-18.04	107.78	118.60
22	BA	2281	A	C2-N3-C4	18.04	119.62	110.60
22	BA	1608	A	N1-C2-N3	-18.04	120.28	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	207	A	N1-C6-N6	-18.04	107.78	118.60
22	BA	920	A	N1-C6-N6	-18.04	107.78	118.60
22	BA	1981	A	N1-C2-N3	-18.04	120.28	129.30
22	BA	1900	A	N1-C6-N6	-18.04	107.78	118.60
54	D2	51	A	N1-C2-N3	-18.04	120.28	129.30
22	BA	699	A	C2-N3-C4	18.03	119.62	110.60
22	BA	2009	A	C2-N3-C4	18.03	119.62	110.60
22	BA	2051	A	N1-C2-N3	-18.03	120.28	129.30
22	BA	430	A	N1-C2-N3	-18.03	120.28	129.30
22	BA	990	A	N1-C2-N3	-18.03	120.28	129.30
22	BA	947	A	N1-C2-N3	-18.03	120.28	129.30
22	BA	2476	A	C2-N3-C4	18.02	119.61	110.60
22	BA	2095	A	C2-N3-C4	18.02	119.61	110.60
22	BA	2439	A	C2-N3-C4	18.02	119.61	110.60
22	BA	2450	A	C2-N3-C4	18.02	119.61	110.60
22	BA	699	A	N1-C2-N3	-18.02	120.29	129.30
22	BA	1690	A	N1-C6-N6	-18.01	107.79	118.60
22	BA	1427	A	N1-C2-N3	-18.01	120.30	129.30
22	BA	1889	A	N1-C6-N6	-18.01	107.79	118.60
23	BB	115	A	N1-C6-N6	-18.01	107.79	118.60
22	BA	182	A	N1-C2-N3	-18.01	120.30	129.30
23	BB	73	A	N1-C2-N3	-18.01	120.30	129.30
22	BA	1678	A	N1-C6-N6	-18.00	107.80	118.60
22	BA	1901	A	N1-C2-N3	-18.00	120.30	129.30
22	BA	2534	A	N1-C6-N6	-18.00	107.80	118.60
22	BA	2813	A	N1-C6-N6	-18.00	107.80	118.60
23	BB	52	A	N1-C6-N6	-18.00	107.80	118.60
22	BA	430	A	N1-C6-N6	-17.99	107.80	118.60
22	BA	1978	A	C2-N3-C4	17.99	119.60	110.60
22	BA	1077	A	N1-C6-N6	-17.99	107.81	118.60
54	D2	35	A	C2-N3-C4	17.99	119.60	110.60
22	BA	1654	A	C2-N3-C4	17.99	119.59	110.60
22	BA	2705	A	C2-N3-C4	17.99	119.59	110.60
22	BA	2530	A	N1-C2-N3	-17.99	120.31	129.30
22	BA	84	A	C2-N3-C4	17.99	119.59	110.60
22	BA	750	A	C2-N3-C4	17.98	119.59	110.60
22	BA	1754	A	N1-C6-N6	-17.98	107.81	118.60
22	BA	1347	A	C2-N3-C4	17.98	119.59	110.60
55	D3	36	A	C2-N3-C4	17.98	119.59	110.60
22	BA	2468	A	N1-C6-N6	-17.97	107.82	118.60
22	BA	2589	A	C2-N3-C4	17.97	119.59	110.60
22	BA	927	A	N1-C6-N6	-17.97	107.82	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	507	A	N1-C6-N6	-17.97	107.82	118.60
22	BA	477	A	C2-N3-C4	17.97	119.58	110.60
22	BA	990	A	N1-C6-N6	-17.97	107.82	118.60
22	BA	2406	A	N1-C6-N6	-17.97	107.82	118.60
22	BA	877	A	N1-C6-N6	-17.97	107.82	118.60
23	BB	15	A	N1-C6-N6	-17.96	107.82	118.60
22	BA	111	A	C2-N3-C4	17.96	119.58	110.60
22	BA	515	A	N1-C6-N6	-17.96	107.82	118.60
22	BA	1847	A	N1-C6-N6	-17.96	107.82	118.60
22	BA	1614	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	1373	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	1127	A	N1-C6-N6	-17.96	107.83	118.60
22	BA	1679	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	2418	A	N1-C6-N6	-17.96	107.83	118.60
22	BA	2813	A	N1-C2-N3	-17.96	120.32	129.30
22	BA	1773	A	N1-C2-N3	-17.95	120.33	129.30
22	BA	213	A	N1-C6-N6	-17.95	107.83	118.60
22	BA	2340	A	N1-C2-N3	-17.95	120.33	129.30
22	BA	1029	A	C2-N3-C4	17.94	119.57	110.60
22	BA	513	A	C2-N3-C4	17.94	119.57	110.60
22	BA	1134	A	N1-C2-N3	-17.94	120.33	129.30
22	BA	2287	A	N1-C2-N3	-17.94	120.33	129.30
22	BA	478	A	N1-C6-N6	-17.94	107.84	118.60
22	BA	1165	A	C2-N3-C4	17.94	119.57	110.60
22	BA	1205	A	N1-C6-N6	-17.94	107.84	118.60
22	BA	716	A	N1-C6-N6	-17.93	107.84	118.60
22	BA	2635	A	N1-C6-N6	-17.93	107.84	118.60
22	BA	1866	A	N1-C2-N3	-17.93	120.33	129.30
22	BA	1885	A	N1-C6-N6	-17.93	107.84	118.60
22	BA	1247	A	N1-C6-N6	-17.93	107.84	118.60
22	BA	1608	A	C2-N3-C4	17.93	119.56	110.60
22	BA	91	A	C2-N3-C4	17.93	119.56	110.60
22	BA	1383	A	N1-C2-N3	-17.93	120.34	129.30
22	BA	1679	A	C2-N3-C4	17.92	119.56	110.60
22	BA	2476	A	N1-C6-N6	-17.92	107.85	118.60
22	BA	28	A	N1-C6-N6	-17.92	107.85	118.60
54	D2	26	A	N1-C6-N6	-17.92	107.85	118.60
22	BA	2433	A	N1-C2-N3	-17.92	120.34	129.30
22	BA	1676	A	N1-C2-N3	-17.90	120.35	129.30
22	BA	2882	A	C2-N3-C4	17.90	119.55	110.60
22	BA	2435	A	C2-N3-C4	17.90	119.55	110.60
22	BA	1854	A	N1-C2-N3	-17.90	120.35	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2381	A	N1-C6-N6	-17.90	107.86	118.60
22	BA	2725	A	N1-C2-N3	-17.90	120.35	129.30
22	BA	472	A	N1-C2-N3	-17.89	120.35	129.30
22	BA	2800	A	C2-N3-C4	17.89	119.55	110.60
22	BA	1678	A	C2-N3-C4	17.89	119.54	110.60
22	BA	89	A	N1-C6-N6	-17.89	107.87	118.60
22	BA	2366	A	N1-C2-N3	-17.89	120.36	129.30
22	BA	1717	A	N1-C6-N6	-17.87	107.88	118.60
22	BA	1385	A	N1-C6-N6	-17.87	107.88	118.60
22	BA	1285	A	N1-C2-N3	-17.87	120.37	129.30
22	BA	2547	A	N1-C6-N6	-17.86	107.88	118.60
22	BA	470	A	N1-C6-N6	-17.86	107.88	118.60
22	BA	2171	A	N1-C6-N6	-17.86	107.88	118.60
22	BA	1144	A	C2-N3-C4	17.86	119.53	110.60
22	BA	1469	A	N1-C2-N3	-17.86	120.37	129.30
22	BA	1147	A	N1-C6-N6	-17.86	107.89	118.60
22	BA	1477	A	N1-C6-N6	-17.86	107.89	118.60
22	BA	2183	A	N1-C2-N3	-17.85	120.38	129.30
54	D2	26	A	N1-C2-N3	-17.85	120.38	129.30
22	BA	727	A	N1-C6-N6	-17.84	107.89	118.60
22	BA	2426	A	N1-C6-N6	-17.84	107.90	118.60
22	BA	2727	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	1301	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	1276	A	N1-C6-N6	-17.84	107.90	118.60
23	BB	66	A	N1-C2-N3	-17.84	120.38	129.30
22	BA	2346	A	C2-N3-C4	17.84	119.52	110.60
22	BA	104	A	N1-C6-N6	-17.84	107.90	118.60
22	BA	1021	A	N1-C2-N3	-17.83	120.38	129.30
22	BA	1287	A	N1-C2-N3	-17.83	120.38	129.30
22	BA	1230	A	N1-C6-N6	-17.83	107.90	118.60
22	BA	2850	A	N1-C2-N3	-17.83	120.39	129.30
22	BA	504	A	N1-C6-N6	-17.83	107.90	118.60
22	BA	1808	A	N1-C6-N6	-17.83	107.90	118.60
22	BA	2003	A	N1-C2-N3	-17.83	120.39	129.30
22	BA	675	A	N1-C6-N6	-17.83	107.90	118.60
22	BA	1872	A	N1-C2-N3	-17.83	120.39	129.30
22	BA	346	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	1262	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	2335	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	2327	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	2600	A	C2-N3-C4	17.82	119.51	110.60
22	BA	2879	A	N1-C6-N6	-17.82	107.91	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1789	A	N1-C6-N6	-17.82	107.91	118.60
22	BA	1678	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	2274	A	N1-C2-N3	-17.82	120.39	129.30
22	BA	2565	A	N1-C2-N3	-17.81	120.39	129.30
22	BA	2060	A	C2-N3-C4	17.81	119.50	110.60
22	BA	1205	A	N1-C2-N3	-17.81	120.40	129.30
22	BA	1927	A	N1-C6-N6	-17.81	107.92	118.60
22	BA	472	A	C2-N3-C4	17.80	119.50	110.60
22	BA	1014	A	N1-C6-N6	-17.80	107.92	118.60
22	BA	2560	A	N1-C6-N6	-17.80	107.92	118.60
22	BA	2736	A	N1-C6-N6	-17.79	107.92	118.60
22	BA	685	A	N1-C2-N3	-17.79	120.40	129.30
22	BA	983	A	C2-N3-C4	17.79	119.50	110.60
22	BA	1928	A	C2-N3-C4	17.79	119.50	110.60
22	BA	1858	A	N1-C2-N3	-17.79	120.41	129.30
22	BA	1264	A	N1-C6-N6	-17.79	107.93	118.60
22	BA	1085	A	N1-C2-N3	-17.79	120.41	129.30
22	BA	1272	A	N1-C6-N6	-17.78	107.93	118.60
22	BA	1722	A	C2-N3-C4	17.78	119.49	110.60
22	BA	2366	A	N1-C6-N6	-17.78	107.93	118.60
23	BB	39	A	C2-N3-C4	17.78	119.49	110.60
22	BA	342	A	N1-C6-N6	-17.78	107.93	118.60
22	BA	2883	A	C2-N3-C4	17.78	119.49	110.60
22	BA	347	A	N1-C6-N6	-17.78	107.93	118.60
22	BA	2453	A	N1-C6-N6	-17.78	107.93	118.60
22	BA	368	A	C2-N3-C4	17.78	119.49	110.60
22	BA	2060	A	N1-C6-N6	-17.78	107.94	118.60
22	BA	1977	A	N1-C6-N6	-17.77	107.94	118.60
22	BA	1848	A	C2-N3-C4	17.77	119.49	110.60
22	BA	282	A	N1-C2-N3	-17.77	120.42	129.30
22	BA	793	A	N1-C2-N3	-17.77	120.42	129.30
22	BA	1275	A	N1-C6-N6	-17.77	107.94	118.60
22	BA	1570	A	N1-C2-N3	-17.76	120.42	129.30
22	BA	2572	A	C2-N3-C4	17.76	119.48	110.60
22	BA	492	A	N1-C6-N6	-17.76	107.95	118.60
22	BA	1001	A	C2-N3-C4	17.76	119.48	110.60
22	BA	2170	A	N1-C2-N3	-17.76	120.42	129.30
22	BA	447	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	1433	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	2333	A	C2-N3-C4	17.75	119.48	110.60
22	BA	1848	A	N1-C2-N3	-17.75	120.42	129.30
22	BA	590	A	C2-N3-C4	17.75	119.47	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2820	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	1847	A	N1-C2-N3	-17.75	120.43	129.30
22	BA	508	A	N1-C6-N6	-17.75	107.95	118.60
22	BA	1354	A	N1-C2-N3	-17.74	120.43	129.30
22	BA	2369	A	N1-C2-N3	-17.74	120.43	129.30
55	D3	23	A	C2-N3-C4	17.74	119.47	110.60
22	BA	973	A	C2-N3-C4	17.74	119.47	110.60
22	BA	2054	A	N1-C2-N3	-17.74	120.43	129.30
22	BA	2810	A	N1-C2-N3	-17.74	120.43	129.30
22	BA	2198	A	N1-C6-N6	-17.73	107.96	118.60
22	BA	2082	A	N1-C2-N3	-17.73	120.44	129.30
22	BA	756	A	N1-C6-N6	-17.73	107.96	118.60
22	BA	802	A	N1-C6-N6	-17.73	107.96	118.60
23	BB	66	A	C2-N3-C4	17.73	119.46	110.60
22	BA	63	A	C2-N3-C4	17.73	119.46	110.60
22	BA	1900	A	C2-N3-C4	17.73	119.46	110.60
54	D2	21	A	C2-N3-C4	17.73	119.46	110.60
22	BA	480	A	C2-N3-C4	17.72	119.46	110.60
22	BA	1327	A	N1-C6-N6	-17.72	107.97	118.60
22	BA	2682	A	C2-N3-C4	17.71	119.46	110.60
22	BA	1098	A	N1-C6-N6	-17.71	107.97	118.60
22	BA	1787	A	N1-C6-N6	-17.71	107.97	118.60
22	BA	2872	A	N1-C6-N6	-17.71	107.97	118.60
55	D3	14	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	1802	A	C2-N3-C4	17.70	119.45	110.60
54	D2	51	A	N1-C6-N6	-17.70	107.98	118.60
22	BA	632	A	N1-C2-N3	-17.70	120.45	129.30
22	BA	155	A	N1-C2-N3	-17.69	120.45	129.30
22	BA	227	A	N1-C2-N3	-17.69	120.45	129.30
22	BA	1953	A	C2-N3-C4	17.69	119.44	110.60
23	BB	15	A	N1-C2-N3	-17.69	120.46	129.30
22	BA	1304	A	N1-C6-N6	-17.69	107.99	118.60
22	BA	1586	A	N1-C2-N3	-17.69	120.46	129.30
22	BA	278	A	N1-C2-N3	-17.68	120.46	129.30
22	BA	1029	A	N1-C2-N3	-17.68	120.46	129.30
22	BA	2154	A	N1-C2-N3	-17.68	120.46	129.30
22	BA	1754	A	C2-N3-C4	17.68	119.44	110.60
22	BA	782	A	C2-N3-C4	17.68	119.44	110.60
22	BA	2632	A	N1-C6-N6	-17.67	108.00	118.60
23	BB	50	A	C2-N3-C4	17.67	119.43	110.60
22	BA	556	A	N1-C6-N6	-17.66	108.00	118.60
22	BA	2738	A	C2-N3-C4	17.66	119.43	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2191	A	N1-C2-N3	-17.66	120.47	129.30
22	BA	689	A	N1-C6-N6	-17.65	108.01	118.60
22	BA	722	A	N1-C2-N3	-17.65	120.47	129.30
22	BA	1434	A	N1-C2-N3	-17.65	120.48	129.30
22	BA	541	A	N1-C6-N6	-17.64	108.01	118.60
22	BA	1626	A	N1-C2-N3	-17.64	120.48	129.30
22	BA	2899	A	C2-N3-C4	17.64	119.42	110.60
22	BA	727	A	C2-N3-C4	17.64	119.42	110.60
22	BA	1505	A	N1-C2-N3	-17.64	120.48	129.30
22	BA	2059	A	C2-N3-C4	17.64	119.42	110.60
22	BA	1302	A	C2-N3-C4	17.63	119.42	110.60
22	BA	2080	A	N1-C2-N3	-17.63	120.48	129.30
22	BA	2856	A	N1-C2-N3	-17.63	120.48	129.30
22	BA	2082	A	N1-C6-N6	-17.63	108.02	118.60
22	BA	63	A	N1-C6-N6	-17.63	108.02	118.60
22	BA	1626	A	C2-N3-C4	17.63	119.41	110.60
22	BA	925	A	N1-C2-N3	-17.63	120.49	129.30
22	BA	89	A	C2-N3-C4	17.62	119.41	110.60
22	BA	1373	A	N1-C6-N6	-17.62	108.03	118.60
22	BA	2037	A	N1-C6-N6	-17.62	108.03	118.60
22	BA	172	A	N1-C2-N3	-17.61	120.50	129.30
22	BA	633	A	N1-C6-N6	-17.61	108.03	118.60
22	BA	661	A	N1-C6-N6	-17.61	108.04	118.60
22	BA	1151	A	N1-C2-N3	-17.61	120.50	129.30
22	BA	2882	A	N1-C6-N6	-17.60	108.04	118.60
22	BA	2761	A	N1-C6-N6	-17.60	108.04	118.60
22	BA	480	A	N1-C2-N3	-17.59	120.50	129.30
22	BA	756	A	N1-C2-N3	-17.59	120.50	129.30
22	BA	1783	A	C2-N3-C4	17.59	119.40	110.60
22	BA	2369	A	N1-C6-N6	-17.59	108.04	118.60
22	BA	1572	A	C2-N3-C4	17.59	119.40	110.60
22	BA	2439	A	N1-C6-N6	-17.59	108.05	118.60
22	BA	844	A	N1-C6-N6	-17.58	108.05	118.60
22	BA	1981	A	C2-N3-C4	17.58	119.39	110.60
22	BA	782	A	N1-C2-N3	-17.57	120.51	129.30
22	BA	1749	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	1783	A	N1-C2-N3	-17.57	120.51	129.30
22	BA	2412	A	N1-C2-N3	-17.57	120.52	129.30
22	BA	382	A	N1-C6-N6	-17.57	108.06	118.60
22	BA	1275	A	C2-N3-C4	17.57	119.39	110.60
22	BA	2059	A	N1-C6-N6	-17.56	108.06	118.60
22	BA	1821	A	N1-C6-N6	-17.56	108.06	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	781	A	N1-C2-N3	-17.56	120.52	129.30
22	BA	382	A	C2-N3-C4	17.56	119.38	110.60
22	BA	1598	A	N1-C2-N3	-17.55	120.52	129.30
22	BA	2392	A	N1-C2-N3	-17.55	120.52	129.30
22	BA	2721	A	N1-C6-N6	-17.55	108.07	118.60
22	BA	466	A	C2-N3-C4	17.55	119.38	110.60
22	BA	221	A	C2-N3-C4	17.55	119.37	110.60
55	D3	64	A	N1-C2-N3	-17.55	120.53	129.30
22	BA	819	A	N1-C6-N6	-17.54	108.08	118.60
22	BA	983	A	N1-C6-N6	-17.53	108.08	118.60
22	BA	1054	A	N1-C2-N3	-17.53	120.53	129.30
22	BA	144	A	N1-C2-N3	-17.53	120.53	129.30
22	BA	1664	A	N1-C2-N3	-17.53	120.53	129.30
22	BA	2434	A	C2-N3-C4	17.53	119.36	110.60
22	BA	2471	A	N1-C2-N3	-17.53	120.54	129.30
22	BA	1572	A	N1-C2-N3	-17.52	120.54	129.30
22	BA	1470	A	N1-C2-N3	-17.52	120.54	129.30
22	BA	2278	A	N1-C2-N3	-17.52	120.54	129.30
22	BA	2814	A	N1-C6-N6	-17.52	108.09	118.60
22	BA	1739	A	N1-C2-N3	-17.52	120.54	129.30
22	BA	91	A	N1-C6-N6	-17.51	108.09	118.60
22	BA	477	A	N1-C6-N6	-17.51	108.09	118.60
22	BA	522	A	N1-C2-N3	-17.51	120.54	129.30
22	BA	197	A	N1-C6-N6	-17.51	108.09	118.60
22	BA	1147	A	N1-C2-N3	-17.50	120.55	129.30
22	BA	2453	A	C2-N3-C4	17.50	119.35	110.60
22	BA	2757	A	N1-C6-N6	-17.50	108.10	118.60
22	BA	2469	A	N1-C6-N6	-17.50	108.10	118.60
22	BA	2860	A	C2-N3-C4	17.50	119.35	110.60
22	BA	1260	A	N1-C6-N6	-17.49	108.11	118.60
54	D2	5	A	N1-C2-N3	-17.49	120.56	129.30
22	BA	505	A	N1-C6-N6	-17.49	108.11	118.60
22	BA	1672	A	N1-C6-N6	-17.49	108.11	118.60
22	BA	1084	A	N1-C2-N3	-17.48	120.56	129.30
22	BA	666	A	N1-C2-N3	-17.48	120.56	129.30
22	BA	251	A	N1-C6-N6	-17.48	108.11	118.60
22	BA	480	A	N1-C6-N6	-17.47	108.12	118.60
22	BA	1650	A	N1-C2-N3	-17.47	120.56	129.30
22	BA	1794	A	N1-C6-N6	-17.47	108.12	118.60
22	BA	1665	A	N1-C2-N3	-17.47	120.57	129.30
22	BA	1772	A	N1-C6-N6	-17.47	108.12	118.60
22	BA	2268	A	C2-N3-C4	17.47	119.33	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2792	A	N1-C6-N6	-17.47	108.12	118.60
22	BA	2009	A	N1-C2-N3	-17.46	120.57	129.30
22	BA	1848	A	N1-C6-N6	-17.46	108.12	118.60
22	BA	1676	A	C2-N3-C4	17.46	119.33	110.60
22	BA	905	A	N1-C6-N6	-17.46	108.12	118.60
22	BA	21	A	N1-C2-N3	-17.46	120.57	129.30
22	BA	1503	A	N1-C2-N3	-17.45	120.58	129.30
22	BA	928	A	N1-C6-N6	-17.45	108.13	118.60
22	BA	1665	A	N1-C6-N6	-17.44	108.14	118.60
22	BA	947	A	N1-C6-N6	-17.44	108.14	118.60
22	BA	1803	A	C2-N3-C4	17.43	119.32	110.60
22	BA	2587	A	N1-C6-N6	-17.43	108.14	118.60
22	BA	42	A	N1-C2-N3	-17.43	120.58	129.30
22	BA	2471	A	N1-C6-N6	-17.43	108.14	118.60
22	BA	172	A	N1-C6-N6	-17.43	108.14	118.60
22	BA	1677	A	N1-C6-N6	-17.42	108.15	118.60
22	BA	2013	A	N1-C2-N3	-17.42	120.59	129.30
22	BA	2015	A	N1-C6-N6	-17.42	108.15	118.60
22	BA	429	A	N1-C6-N6	-17.41	108.16	118.60
22	BA	1244	A	N1-C2-N3	-17.41	120.60	129.30
22	BA	2600	A	N1-C2-N3	-17.41	120.60	129.30
22	BA	821	A	C2-N3-C4	17.40	119.30	110.60
22	BA	279	A	N1-C6-N6	-17.40	108.16	118.60
22	BA	1525	A	N1-C2-N3	-17.39	120.60	129.30
22	BA	1676	A	N1-C6-N6	-17.39	108.17	118.60
22	BA	2547	A	N1-C2-N3	-17.38	120.61	129.30
22	BA	2662	A	N1-C2-N3	-17.38	120.61	129.30
22	BA	2711	A	N1-C6-N6	-17.38	108.17	118.60
22	BA	2101	A	N1-C6-N6	-17.37	108.18	118.60
22	BA	661	A	N1-C2-N3	-17.37	120.61	129.30
22	BA	1246	A	N1-C6-N6	-17.37	108.18	118.60
22	BA	1385	A	C2-N3-C4	17.37	119.28	110.60
22	BA	2241	A	N1-C6-N6	-17.37	108.18	118.60
22	BA	1637	A	N1-C2-N3	-17.36	120.62	129.30
22	BA	1205	A	C2-N3-C4	17.36	119.28	110.60
22	BA	2268	A	N1-C2-N3	-17.36	120.62	129.30
54	D2	28	A	N1-C2-N3	-17.36	120.62	129.30
22	BA	352	A	N1-C2-N3	-17.36	120.62	129.30
22	BA	415	A	N1-C2-N3	-17.36	120.62	129.30
23	BB	94	A	N1-C2-N3	-17.34	120.63	129.30
22	BA	1789	A	N1-C2-N3	-17.34	120.63	129.30
22	BA	21	A	N1-C6-N6	-17.33	108.20	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	439	A	N1-C2-N3	-17.33	120.64	129.30
22	BA	155	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	1403	A	N1-C6-N6	-17.32	108.21	118.60
22	BA	95	A	N1-C2-N3	-17.31	120.64	129.30
22	BA	1502	A	N1-C6-N6	-17.31	108.21	118.60
22	BA	1969	A	N1-C6-N6	-17.31	108.22	118.60
22	BA	2090	A	N1-C2-N3	-17.30	120.65	129.30
22	BA	2352	A	N1-C6-N6	-17.30	108.22	118.60
22	BA	2052	A	N1-C6-N6	-17.30	108.22	118.60
22	BA	2829	A	N1-C6-N6	-17.30	108.22	118.60
22	BA	507	A	C2-N3-C4	17.29	119.25	110.60
22	BA	2009	A	N1-C6-N6	-17.29	108.23	118.60
22	BA	1810	A	N1-C2-N3	-17.29	120.66	129.30
22	BA	1230	A	N1-C2-N3	-17.29	120.66	129.30
22	BA	1899	A	N1-C2-N3	-17.29	120.66	129.30
22	BA	1504	A	N1-C2-N3	-17.28	120.66	129.30
22	BA	2670	A	N1-C2-N3	-17.28	120.66	129.30
22	BA	909	A	N1-C2-N3	-17.28	120.66	129.30
54	D2	49	A	N1-C6-N6	-17.27	108.23	118.60
22	BA	849	A	N1-C6-N6	-17.27	108.24	118.60
22	BA	2725	A	N1-C6-N6	-17.27	108.24	118.60
22	BA	1336	A	N1-C2-N3	-17.27	120.67	129.30
22	BA	2900	A	N1-C2-N3	-17.26	120.67	129.30
22	BA	668	A	N1-C2-N3	-17.26	120.67	129.30
22	BA	156	A	N1-C2-N3	-17.25	120.67	129.30
22	BA	1794	A	C2-N3-C4	17.25	119.22	110.60
22	BA	1549	A	N1-C6-N6	-17.25	108.25	118.60
22	BA	1829	A	N1-C2-N3	-17.25	120.67	129.30
22	BA	1262	A	N1-C2-N3	-17.25	120.68	129.30
22	BA	131	A	N1-C2-N3	-17.24	120.68	129.30
22	BA	1302	A	N1-C6-N6	-17.24	108.25	118.60
22	BA	689	A	N1-C2-N3	-17.23	120.68	129.30
22	BA	2682	A	N1-C6-N6	-17.23	108.26	118.60
22	BA	1431	A	N1-C6-N6	-17.23	108.27	118.60
22	BA	2727	A	N1-C6-N6	-17.23	108.26	118.60
22	BA	2837	A	N1-C2-N3	-17.22	120.69	129.30
54	D2	41	A	N1-C6-N6	-17.22	108.27	118.60
22	BA	2679	A	N1-C2-N3	-17.21	120.69	129.30
22	BA	2600	A	N1-C6-N6	-17.21	108.28	118.60
22	BA	582	A	N1-C2-N3	-17.20	120.70	129.30
22	BA	2706	A	N1-C2-N3	-17.20	120.70	129.30
22	BA	693	A	N1-C2-N3	-17.20	120.70	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1803	A	N1-C2-N3	-17.19	120.70	129.30
22	BA	1608	A	N1-C6-N6	-17.19	108.28	118.60
22	BA	1705	A	N1-C2-N3	-17.19	120.70	129.30
54	D2	69	A	N1-C6-N6	-17.19	108.29	118.60
22	BA	2388	A	C2-N3-C4	17.18	119.19	110.60
22	BA	1027	A	C2-N3-C4	17.18	119.19	110.60
22	BA	1151	A	N1-C6-N6	-17.18	108.29	118.60
22	BA	1596	A	N1-C2-N3	-17.17	120.72	129.30
22	BA	2314	A	N1-C6-N6	-17.17	108.30	118.60
22	BA	2274	A	C2-N3-C4	17.17	119.18	110.60
22	BA	599	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	2314	A	N1-C2-N3	-17.16	120.72	129.30
23	BB	50	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	1987	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	575	A	N1-C6-N6	-17.16	108.31	118.60
22	BA	2097	A	N1-C2-N3	-17.16	120.72	129.30
22	BA	2097	A	N1-C6-N6	-17.16	108.31	118.60
22	BA	2700	A	N1-C2-N3	-17.15	120.72	129.30
22	BA	654	A	N1-C6-N6	-17.15	108.31	118.60
22	BA	1593	A	N1-C6-N6	-17.15	108.31	118.60
54	D2	49	A	N1-C2-N3	-17.15	120.72	129.30
22	BA	142	A	N1-C6-N6	-17.15	108.31	118.60
22	BA	2634	A	N1-C2-N3	-17.15	120.73	129.30
22	BA	2407	A	N1-C2-N3	-17.14	120.73	129.30
22	BA	800	A	C2-N3-C4	17.14	119.17	110.60
22	BA	1711	A	N1-C2-N3	-17.14	120.73	129.30
22	BA	753	A	N1-C6-N6	-17.13	108.32	118.60
22	BA	1057	A	N1-C6-N6	-17.13	108.32	118.60
22	BA	1387	A	N1-C2-N3	-17.13	120.74	129.30
22	BA	1746	A	N1-C2-N3	-17.12	120.74	129.30
22	BA	2273	A	N1-C2-N3	-17.12	120.74	129.30
22	BA	2448	A	C2-N3-C4	17.12	119.16	110.60
22	BA	2448	A	N1-C2-N3	-17.12	120.74	129.30
22	BA	1821	A	C2-N3-C4	17.11	119.15	110.60
22	BA	1029	A	N1-C6-N6	-17.11	108.33	118.60
22	BA	1746	A	N1-C6-N6	-17.11	108.33	118.60
22	BA	1169	A	N1-C2-N3	-17.10	120.75	129.30
22	BA	1591	A	N1-C2-N3	-17.10	120.75	129.30
54	D2	28	A	N1-C6-N6	-17.10	108.34	118.60
23	BB	94	A	N1-C6-N6	-17.09	108.34	118.60
22	BA	1080	A	N1-C2-N3	-17.09	120.75	129.30
22	BA	2071	A	N1-C6-N6	-17.09	108.34	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1603	A	N1-C6-N6	-17.09	108.35	118.60
22	BA	1027	A	N1-C6-N6	-17.09	108.35	118.60
22	BA	1272	A	C2-N3-C4	17.09	119.14	110.60
22	BA	1866	A	N1-C6-N6	-17.09	108.35	118.60
55	D3	23	A	N1-C6-N6	-17.08	108.35	118.60
22	BA	1525	A	N1-C6-N6	-17.08	108.35	118.60
22	BA	1403	A	N1-C2-N3	-17.08	120.76	129.30
22	BA	586	A	C2-N3-C4	17.08	119.14	110.60
22	BA	2856	A	N1-C6-N6	-17.08	108.35	118.60
22	BA	2516	A	N1-C2-N3	-17.08	120.76	129.30
22	BA	2191	A	N1-C6-N6	-17.07	108.36	118.60
22	BA	173	A	N1-C2-N3	-17.07	120.76	129.30
22	BA	789	A	N1-C6-N6	-17.07	108.36	118.60
22	BA	2297	A	C2-N3-C4	17.07	119.13	110.60
22	BA	590	A	N1-C2-N3	-17.07	120.77	129.30
22	BA	2386	A	N1-C2-N3	-17.07	120.77	129.30
54	D2	23	A	N1-C6-N6	-17.07	108.36	118.60
22	BA	354	A	N1-C2-N3	-17.06	120.77	129.30
22	BA	2142	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	2247	A	N1-C2-N3	-17.05	120.78	129.30
22	BA	1080	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	1987	A	N1-C6-N6	-17.05	108.37	118.60
22	BA	439	A	N1-C6-N6	-17.05	108.37	118.60
54	D2	41	A	N1-C2-N3	-17.05	120.78	129.30
22	BA	1470	A	N1-C6-N6	-17.04	108.38	118.60
22	BA	1532	A	N1-C2-N3	-17.04	120.78	129.30
22	BA	1596	A	N1-C6-N6	-17.04	108.38	118.60
22	BA	1669	A	N1-C2-N3	-17.03	120.78	129.30
22	BA	2205	A	N1-C6-N6	-17.03	108.38	118.60
54	D2	69	A	N1-C2-N3	-17.03	120.78	129.30
22	BA	1960	A	N1-C2-N3	-17.03	120.78	129.30
22	BA	936	A	N1-C6-N6	-17.03	108.38	118.60
22	BA	1284	A	N1-C6-N6	-17.02	108.39	118.60
22	BA	1722	A	N1-C6-N6	-17.02	108.39	118.60
22	BA	863	A	N1-C2-N3	-17.02	120.79	129.30
23	BB	119	A	N1-C6-N6	-17.02	108.39	118.60
22	BA	1020	A	C2-N3-C4	17.02	119.11	110.60
22	BA	1027	A	N1-C2-N3	-17.02	120.79	129.30
22	BA	2317	A	N1-C6-N6	-17.01	108.39	118.60
22	BA	1328	A	N1-C2-N3	-17.00	120.80	129.30
22	BA	2761	A	N1-C2-N3	-17.00	120.80	129.30
23	BB	119	A	N1-C2-N3	-17.00	120.80	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	981	A	C2-N3-C4	17.00	119.10	110.60
22	BA	2020	A	N1-C6-N6	-17.00	108.40	118.60
22	BA	352	A	N1-C6-N6	-17.00	108.40	118.60
55	D3	36	A	N1-C6-N6	-17.00	108.40	118.60
22	BA	2281	A	N1-C2-N3	-16.99	120.80	129.30
22	BA	146	A	N1-C2-N3	-16.99	120.81	129.30
22	BA	1711	A	N1-C6-N6	-16.99	108.41	118.60
22	BA	42	A	N1-C6-N6	-16.98	108.41	118.60
22	BA	1998	A	N1-C2-N3	-16.98	120.81	129.30
22	BA	2142	A	N1-C2-N3	-16.97	120.81	129.30
22	BA	2278	A	N1-C6-N6	-16.97	108.42	118.60
22	BA	233	A	N1-C6-N6	-16.97	108.42	118.60
22	BA	2706	A	N1-C6-N6	-16.97	108.42	118.60
22	BA	2003	A	N1-C6-N6	-16.97	108.42	118.60
22	BA	996	A	N1-C2-N3	-16.96	120.82	129.30
22	BA	1269	A	N1-C6-N6	-16.96	108.42	118.60
22	BA	44	A	N1-C6-N6	-16.96	108.42	118.60
22	BA	1549	A	N1-C2-N3	-16.96	120.82	129.30
22	BA	2700	A	N1-C6-N6	-16.96	108.42	118.60
22	BA	1387	A	N1-C6-N6	-16.95	108.43	118.60
22	BA	2135	A	N1-C6-N6	-16.95	108.43	118.60
22	BA	1590	A	N1-C2-N3	-16.95	120.82	129.30
22	BA	95	A	N1-C6-N6	-16.95	108.43	118.60
22	BA	2281	A	N1-C6-N6	-16.94	108.43	118.60
22	BA	1572	A	N1-C6-N6	-16.94	108.44	118.60
22	BA	905	A	N1-C2-N3	-16.94	120.83	129.30
22	BA	2095	A	N1-C6-N6	-16.94	108.44	118.60
22	BA	1614	A	C2-N3-C4	16.94	119.07	110.60
22	BA	176	A	N1-C2-N3	-16.93	120.83	129.30
22	BA	2241	A	N1-C2-N3	-16.93	120.83	129.30
22	BA	1503	A	N1-C6-N6	-16.93	108.44	118.60
22	BA	1505	A	N1-C6-N6	-16.92	108.45	118.60
22	BA	2736	A	N1-C2-N3	-16.91	120.84	129.30
22	BA	64	A	N1-C2-N3	-16.91	120.84	129.30
22	BA	1269	A	N1-C2-N3	-16.91	120.84	129.30
22	BA	142	A	N1-C2-N3	-16.91	120.85	129.30
22	BA	251	A	N1-C2-N3	-16.91	120.85	129.30
22	BA	928	A	N1-C2-N3	-16.90	120.85	129.30
22	BA	1735	A	N1-C2-N3	-16.90	120.85	129.30
22	BA	2088	A	N1-C2-N3	-16.89	120.85	129.30
22	BA	849	A	N1-C2-N3	-16.89	120.86	129.30
22	BA	1143	A	N1-C6-N6	-16.89	108.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2054	A	N1-C6-N6	-16.89	108.47	118.60
22	BA	1593	A	N1-C2-N3	-16.89	120.86	129.30
22	BA	2284	A	N1-C2-N3	-16.89	120.86	129.30
22	BA	422	A	N1-C6-N6	-16.88	108.47	118.60
22	BA	1854	A	N1-C6-N6	-16.88	108.47	118.60
22	BA	1001	A	N1-C2-N3	-16.88	120.86	129.30
22	BA	231	A	N1-C2-N3	-16.88	120.86	129.30
22	BA	19	A	N1-C2-N3	-16.87	120.86	129.30
22	BA	131	A	N1-C6-N6	-16.87	108.48	118.60
22	BA	272	A	N1-C2-N3	-16.87	120.87	129.30
22	BA	6	A	N1-C2-N3	-16.86	120.87	129.30
22	BA	2418	A	N1-C2-N3	-16.86	120.87	129.30
22	BA	2577	A	N1-C6-N6	-16.86	108.48	118.60
22	BA	2461	A	N1-C2-N3	-16.86	120.87	129.30
22	BA	1247	A	N1-C2-N3	-16.85	120.87	129.30
22	BA	64	A	N1-C6-N6	-16.85	108.49	118.60
22	BA	2088	A	N1-C6-N6	-16.85	108.49	118.60
22	BA	89	A	N1-C2-N3	-16.85	120.88	129.30
22	BA	342	A	N1-C2-N3	-16.84	120.88	129.30
22	BA	1244	A	N1-C6-N6	-16.84	108.50	118.60
22	BA	173	A	N1-C6-N6	-16.83	108.50	118.60
22	BA	348	A	N1-C2-N3	-16.83	120.88	129.30
22	BA	56	A	N1-C2-N3	-16.83	120.88	129.30
22	BA	1528	A	N1-C2-N3	-16.82	120.89	129.30
22	BA	152	A	N1-C2-N3	-16.82	120.89	129.30
22	BA	693	A	N1-C6-N6	-16.81	108.51	118.60
22	BA	146	A	N1-C6-N6	-16.81	108.51	118.60
22	BA	1194	A	N1-C2-N3	-16.81	120.89	129.30
22	BA	721	A	N1-C2-N3	-16.80	120.90	129.30
22	BA	1970	A	N1-C6-N6	-16.80	108.52	118.60
23	BB	34	A	N1-C6-N6	-16.80	108.52	118.60
23	BB	29	A	N1-C2-N3	-16.80	120.90	129.30
22	BA	1548	A	N1-C2-N3	-16.80	120.90	129.30
22	BA	1502	A	N1-C2-N3	-16.79	120.90	129.30
22	BA	844	A	N1-C2-N3	-16.79	120.91	129.30
22	BA	936	A	N1-C2-N3	-16.78	120.91	129.30
22	BA	2317	A	N1-C2-N3	-16.78	120.91	129.30
22	BA	1385	A	N1-C2-N3	-16.78	120.91	129.30
22	BA	2435	A	N1-C6-N6	-16.78	108.53	118.60
22	BA	2837	A	N1-C6-N6	-16.78	108.53	118.60
22	BA	2516	A	N1-C6-N6	-16.77	108.53	118.60
22	BA	2412	A	N1-C6-N6	-16.77	108.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	5	A	N1-C6-N6	-16.75	108.55	118.60
22	BA	2247	A	N1-C6-N6	-16.74	108.55	118.60
22	BA	2094	A	N1-C2-N3	-16.74	120.93	129.30
22	BA	2095	A	N1-C2-N3	-16.73	120.93	129.30
22	BA	1336	A	N1-C6-N6	-16.73	108.56	118.60
22	BA	677	A	N1-C6-N6	-16.73	108.56	118.60
22	BA	1213	A	N1-C6-N6	-16.72	108.56	118.60
22	BA	2792	A	N1-C2-N3	-16.72	120.94	129.30
22	BA	599	A	N1-C6-N6	-16.72	108.57	118.60
22	BA	541	A	N1-C2-N3	-16.71	120.94	129.30
22	BA	1413	A	N1-C2-N3	-16.70	120.95	129.30
22	BA	1548	A	N1-C6-N6	-16.70	108.58	118.60
23	BB	66	A	N1-C6-N6	-16.68	108.59	118.60
54	D2	5	A	N1-C6-N6	-16.68	108.59	118.60
22	BA	668	A	N1-C6-N6	-16.68	108.59	118.60
22	BA	176	A	N1-C6-N6	-16.67	108.60	118.60
22	BA	1772	A	N1-C2-N3	-16.67	120.97	129.30
22	BA	2632	A	N1-C2-N3	-16.67	120.97	129.30
22	BA	1791	A	N1-C6-N6	-16.67	108.60	118.60
22	BA	1603	A	N1-C2-N3	-16.66	120.97	129.30
22	BA	2900	A	N1-C6-N6	-16.65	108.61	118.60
22	BA	2020	A	N1-C2-N3	-16.65	120.97	129.30
22	BA	1431	A	N1-C2-N3	-16.65	120.98	129.30
22	BA	1749	A	N1-C2-N3	-16.63	120.99	129.30
22	BA	2459	A	N1-C2-N3	-16.62	120.99	129.30
22	BA	44	A	N1-C2-N3	-16.62	120.99	129.30
22	BA	2711	A	N1-C2-N3	-16.62	120.99	129.30
22	BA	2080	A	N1-C6-N6	-16.61	108.63	118.60
22	BA	996	A	N1-C6-N6	-16.60	108.64	118.60
22	BA	825	A	N1-C2-N3	-16.59	121.00	129.30
22	BA	1960	A	N1-C6-N6	-16.59	108.65	118.60
22	BA	2829	A	N1-C2-N3	-16.58	121.01	129.30
22	BA	5	A	N1-C2-N3	-16.57	121.01	129.30
22	BA	1169	A	N1-C6-N6	-16.57	108.66	118.60
22	BA	730	A	N1-C2-N3	-16.57	121.01	129.30
22	BA	1590	A	N1-C6-N6	-16.57	108.66	118.60
22	BA	2634	A	N1-C6-N6	-16.56	108.67	118.60
55	D3	23	A	N1-C2-N3	-16.55	121.02	129.30
22	BA	2407	A	N1-C6-N6	-16.55	108.67	118.60
22	BA	1246	A	N1-C2-N3	-16.54	121.03	129.30
22	BA	1014	A	N1-C2-N3	-16.54	121.03	129.30
22	BA	1791	A	N1-C2-N3	-16.53	121.03	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	38	A	N1-C2-N3	-16.53	121.04	129.30
22	BA	56	A	N1-C6-N6	-16.52	108.69	118.60
22	BA	753	A	N1-C2-N3	-16.52	121.04	129.30
22	BA	863	A	N1-C6-N6	-16.52	108.69	118.60
22	BA	2435	A	N1-C2-N3	-16.52	121.04	129.30
22	BA	2635	A	N1-C2-N3	-16.52	121.04	129.30
22	BA	2882	A	N1-C2-N3	-16.51	121.04	129.30
22	BA	730	A	N1-C6-N6	-16.50	108.70	118.60
22	BA	1057	A	N1-C2-N3	-16.50	121.05	129.30
22	BA	2205	A	N1-C2-N3	-16.50	121.05	129.30
23	BB	34	A	N1-C2-N3	-16.50	121.05	129.30
22	BA	1630	A	N1-C2-N3	-16.49	121.05	129.30
22	BA	1637	A	N1-C6-N6	-16.49	108.70	118.60
22	BA	2184	A	N1-C6-N6	-16.49	108.71	118.60
22	BA	2461	A	N1-C6-N6	-16.48	108.71	118.60
22	BA	1504	A	N1-C6-N6	-16.48	108.71	118.60
22	BA	752	A	N1-C2-N3	-16.48	121.06	129.30
22	BA	2090	A	N1-C6-N6	-16.48	108.71	118.60
22	BA	2670	A	N1-C6-N6	-16.47	108.72	118.60
22	BA	1304	A	N1-C2-N3	-16.47	121.07	129.30
22	BA	324	A	N1-C6-N6	-16.45	108.73	118.60
22	BA	2434	A	N1-C2-N3	-16.45	121.07	129.30
22	BA	1821	A	N1-C2-N3	-16.44	121.08	129.30
22	BA	1787	A	N1-C2-N3	-16.43	121.08	129.30
22	BA	348	A	N1-C6-N6	-16.41	108.75	118.60
22	BA	2033	A	C2-N3-C4	16.41	118.80	110.60
22	BA	721	A	N1-C6-N6	-16.39	108.77	118.60
22	BA	262	A	N1-C2-N3	-16.38	121.11	129.30
22	BA	1276	A	N1-C2-N3	-16.38	121.11	129.30
22	BA	1144	A	N1-C2-N3	-16.38	121.11	129.30
22	BA	1805	A	N1-C2-N3	-16.37	121.11	129.30
22	BA	1528	A	N1-C6-N6	-16.37	108.78	118.60
55	D3	35	A	N1-C6-N6	-16.37	108.78	118.60
22	BA	2071	A	N1-C2-N3	-16.36	121.12	129.30
22	BA	2899	A	N1-C2-N3	-16.36	121.12	129.30
23	BB	50	A	N1-C6-N6	-16.36	108.78	118.60
54	D2	23	A	N1-C2-N3	-16.36	121.12	129.30
22	BA	1705	A	N1-C6-N6	-16.36	108.79	118.60
22	BA	960	A	N1-C6-N6	-16.36	108.79	118.60
22	BA	6	A	N1-C6-N6	-16.35	108.79	118.60
22	BA	1165	A	N1-C2-N3	-16.34	121.13	129.30
23	BB	115	A	N1-C2-N3	-16.34	121.13	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1532	A	N1-C6-N6	-16.34	108.80	118.60
22	BA	1353	A	N1-C2-N3	-16.33	121.13	129.30
22	BA	1597	A	N1-C2-N3	-16.33	121.14	129.30
22	BA	2037	A	N1-C2-N3	-16.30	121.15	129.30
22	BA	272	A	N1-C6-N6	-16.29	108.83	118.60
22	BA	644	A	N1-C2-N3	-16.28	121.16	129.30
22	BA	2453	A	N1-C2-N3	-16.26	121.17	129.30
22	BA	2381	A	N1-C2-N3	-16.25	121.18	129.30
22	BA	833	A	N1-C6-N6	-16.24	108.86	118.60
22	BA	1614	A	N1-C6-N6	-16.24	108.86	118.60
22	BA	1998	A	N1-C6-N6	-16.24	108.86	118.60
22	BA	1591	A	N1-C6-N6	-16.22	108.87	118.60
22	BA	2077	A	N1-C6-N6	-16.22	108.87	118.60
22	BA	2513	A	N1-C2-N3	-16.22	121.19	129.30
22	BA	1791	A	C2-N3-C4	16.21	118.70	110.60
22	BA	582	A	N1-C6-N6	-16.20	108.88	118.60
22	BA	522	A	N1-C6-N6	-16.18	108.89	118.60
22	BA	2070	A	N1-C2-N3	-16.17	121.22	129.30
22	BA	1735	A	N1-C6-N6	-16.16	108.90	118.60
22	BA	1829	A	N1-C6-N6	-16.15	108.91	118.60
22	BA	1551	A	N1-C2-N3	-16.15	121.23	129.30
22	BA	347	A	N1-C2-N3	-16.14	121.23	129.30
22	BA	1144	A	N1-C6-N6	-16.14	108.91	118.60
22	BA	1802	A	N1-C6-N6	-16.14	108.92	118.60
22	BA	933	A	N1-C2-N3	-16.14	121.23	129.30
22	BA	466	A	N1-C6-N6	-16.12	108.93	118.60
22	BA	666	A	N1-C6-N6	-16.12	108.93	118.60
22	BA	742	A	N1-C6-N6	-16.12	108.93	118.60
22	BA	2184	A	N1-C2-N3	-16.10	121.25	129.30
22	BA	750	A	N1-C6-N6	-16.05	108.97	118.60
22	BA	156	A	N1-C6-N6	-16.05	108.97	118.60
22	BA	152	A	N1-C6-N6	-16.04	108.97	118.60
22	BA	2679	A	N1-C6-N6	-16.03	108.98	118.60
22	BA	1872	A	N1-C6-N6	-16.03	108.98	118.60
22	BA	2094	A	N1-C6-N6	-16.01	109.00	118.60
22	BA	1739	A	N1-C6-N6	-15.99	109.00	118.60
22	BA	2899	A	N1-C6-N6	-15.99	109.01	118.60
22	BA	2154	A	N1-C6-N6	-15.98	109.01	118.60
22	BA	415	A	N1-C6-N6	-15.97	109.02	118.60
22	BA	231	A	N1-C6-N6	-15.96	109.03	118.60
22	BA	2430	A	N1-C6-N6	-15.94	109.04	118.60
22	BA	1260	A	N1-C2-N3	-15.92	121.34	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	144	A	N1-C6-N6	-15.90	109.06	118.60
22	BA	2662	A	N1-C6-N6	-15.89	109.06	118.60
22	BA	743	A	N1-C6-N6	-15.89	109.07	118.60
22	BA	2284	A	N1-C6-N6	-15.87	109.08	118.60
22	BA	382	A	N1-C2-N3	-15.86	121.37	129.30
22	BA	722	A	N1-C6-N6	-15.86	109.08	118.60
22	BA	1413	A	N1-C6-N6	-15.84	109.10	118.60
22	BA	1794	A	N1-C2-N3	-15.83	121.38	129.30
22	BA	19	A	N1-C6-N6	-15.81	109.11	118.60
22	BA	925	A	N1-C6-N6	-15.78	109.13	118.60
22	BA	590	A	N1-C6-N6	-15.77	109.14	118.60
22	BA	794	A	N1-C6-N6	-15.76	109.14	118.60
22	BA	2766	A	N1-C6-N6	-15.75	109.15	118.60
22	BA	705	A	N1-C6-N6	-15.74	109.16	118.60
22	BA	2077	A	N1-C2-N3	-15.69	121.46	129.30
22	BA	2108	A	N1-C2-N3	-15.69	121.46	129.30
22	BA	2386	A	N1-C6-N6	-15.63	109.22	118.60
22	BA	592	A	N1-C2-N3	-15.63	121.48	129.30
22	BA	2340	A	N1-C6-N6	-15.59	109.25	118.60
22	BA	2799	A	N1-C6-N6	-15.56	109.26	118.60
22	BA	2033	A	N1-C2-N3	-15.50	121.55	129.30
22	BA	1054	A	N1-C6-N6	-15.44	109.34	118.60
22	BA	1347	A	N1-C2-N3	-15.44	121.58	129.30
22	BA	2328	A	N1-C2-N3	-15.39	121.61	129.30
55	D3	64	A	N1-C6-N6	-15.29	109.42	118.60
22	BA	1810	A	N1-C6-N6	-15.19	109.48	118.60
22	BA	2459	A	N1-C6-N6	-15.11	109.54	118.60
22	BA	513	A	N1-C6-N6	-15.08	109.55	118.60
22	BA	282	A	N1-C6-N6	-15.04	109.58	118.60
22	BA	2183	A	N1-C6-N6	-14.27	110.04	118.60
22	BA	2297	A	N1-C2-N3	-14.20	122.20	129.30
22	BA	2430	A	C2-N3-C4	13.87	117.53	110.60
22	BA	1385	A	N7-C8-N9	-13.62	106.99	113.80
22	BA	1021	A	N3-C4-C5	-13.36	117.45	126.80
22	BA	84	A	N7-C8-N9	-13.31	107.14	113.80
22	BA	204	A	N7-C8-N9	-13.21	107.19	113.80
22	BA	1515	A	C5-C6-N6	13.20	134.26	123.70
22	BA	479	A	N7-C8-N9	-13.20	107.20	113.80
22	BA	2776	A	N7-C8-N9	-13.12	107.24	113.80
22	BA	1912	A	N7-C8-N9	-13.03	107.29	113.80
22	BA	2117	A	N7-C8-N9	-12.82	107.39	113.80
22	BA	2009	A	N7-C8-N9	-12.81	107.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2430	A	N1-C2-N3	-12.78	122.91	129.30
22	BA	2572	A	N7-C8-N9	-12.74	107.43	113.80
22	BA	213	A	N7-C8-N9	-12.72	107.44	113.80
22	BA	2388	A	N7-C8-N9	-12.72	107.44	113.80
22	BA	783	A	N3-C4-C5	-12.65	117.94	126.80
22	BA	764	A	C5-C6-N6	12.62	133.79	123.70
22	BA	2033	A	N7-C8-N9	-12.60	107.50	113.80
22	BA	1247	A	N7-C8-N9	-12.58	107.51	113.80
22	BA	371	A	N7-C8-N9	-12.56	107.52	113.80
22	BA	2060	A	N7-C8-N9	-12.56	107.52	113.80
22	BA	1630	A	N7-C8-N9	-12.55	107.53	113.80
22	BA	1652	A	N7-C8-N9	-12.54	107.53	113.80
22	BA	1147	A	N7-C8-N9	-12.54	107.53	113.80
22	BA	1272	A	N7-C8-N9	-12.53	107.54	113.80
22	BA	1655	A	N7-C8-N9	-12.49	107.55	113.80
22	BA	310	A	N7-C8-N9	-12.49	107.55	113.80
22	BA	1566	A	N7-C8-N9	-12.49	107.55	113.80
22	BA	905	A	N7-C8-N9	-12.47	107.56	113.80
55	D3	7	A	N7-C8-N9	-12.47	107.56	113.80
22	BA	614	A	N7-C8-N9	-12.47	107.57	113.80
22	BA	1937	A	N7-C8-N9	-12.46	107.57	113.80
22	BA	621	A	C5-C6-N6	12.46	133.67	123.70
22	BA	1274	A	N7-C8-N9	-12.45	107.58	113.80
22	BA	1936	A	N3-C4-C5	-12.45	118.09	126.80
22	BA	2589	A	N7-C8-N9	-12.44	107.58	113.80
22	BA	1419	A	N7-C8-N9	-12.43	107.59	113.80
22	BA	613	A	N3-C4-C5	-12.42	118.11	126.80
22	BA	1515	A	N7-C8-N9	-12.39	107.60	113.80
22	BA	2542	A	N7-C8-N9	-12.39	107.61	113.80
22	BA	2765	A	N3-C4-C5	-12.38	118.14	126.80
22	BA	756	A	N7-C8-N9	-12.38	107.61	113.80
54	D2	58	A	N7-C8-N9	-12.38	107.61	113.80
22	BA	1001	A	C5-C6-N6	12.37	133.60	123.70
22	BA	1634	A	N7-C8-N9	-12.37	107.61	113.80
22	BA	1669	A	N3-C4-C5	-12.37	118.14	126.80
22	BA	2792	A	N7-C8-N9	-12.37	107.62	113.80
22	BA	821	A	C5-C6-N6	12.36	133.59	123.70
22	BA	2369	A	N7-C8-N9	-12.36	107.62	113.80
22	BA	125	A	N7-C8-N9	-12.36	107.62	113.80
22	BA	1088	A	N3-C4-C5	-12.34	118.16	126.80
22	BA	2758	A	C5-C6-N6	12.32	133.56	123.70
22	BA	161	A	N7-C8-N9	-12.31	107.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	829	A	N7-C8-N9	-12.31	107.64	113.80
22	BA	1378	A	C5-C6-N6	12.30	133.54	123.70
22	BA	1652	A	C5-C6-N6	12.26	133.51	123.70
22	BA	278	A	N3-C4-C5	-12.25	118.23	126.80
22	BA	332	A	N7-C8-N9	-12.24	107.68	113.80
22	BA	1275	A	N7-C8-N9	-12.24	107.68	113.80
22	BA	322	A	N7-C8-N9	-12.24	107.68	113.80
22	BA	1853	A	N7-C8-N9	-12.23	107.68	113.80
22	BA	1937	A	C5-C6-N6	12.23	133.49	123.70
22	BA	457	A	N7-C8-N9	-12.23	107.69	113.80
22	BA	655	A	N7-C8-N9	-12.23	107.69	113.80
22	BA	354	A	N7-C8-N9	-12.22	107.69	113.80
22	BA	454	A	N7-C8-N9	-12.22	107.69	113.80
22	BA	1583	A	N7-C8-N9	-12.21	107.69	113.80
22	BA	1155	A	C5-C6-N6	12.21	133.47	123.70
23	BB	119	A	N7-C8-N9	-12.20	107.70	113.80
54	D2	9	A	N7-C8-N9	-12.20	107.70	113.80
22	BA	627	A	N7-C8-N9	-12.20	107.70	113.80
22	BA	1509	A	N7-C8-N9	-12.19	107.71	113.80
22	BA	199	A	N7-C8-N9	-12.18	107.71	113.80
22	BA	2381	A	N7-C8-N9	-12.17	107.72	113.80
22	BA	637	A	N7-C8-N9	-12.16	107.72	113.80
22	BA	2388	A	C5-C6-N6	12.15	133.42	123.70
22	BA	1453	A	N7-C8-N9	-12.15	107.72	113.80
22	BA	1237	A	C5-C6-N6	12.14	133.41	123.70
22	BA	1504	A	N7-C8-N9	-12.14	107.73	113.80
22	BA	222	A	N7-C8-N9	-12.14	107.73	113.80
22	BA	1111	A	N7-C8-N9	-12.14	107.73	113.80
22	BA	2119	A	N7-C8-N9	-12.14	107.73	113.80
22	BA	1020	A	C5-C6-N6	12.13	133.40	123.70
22	BA	1032	A	N7-C8-N9	-12.13	107.74	113.80
22	BA	1784	A	N7-C8-N9	-12.12	107.74	113.80
22	BA	1722	A	N7-C8-N9	-12.11	107.74	113.80
22	BA	2883	A	N7-C8-N9	-12.11	107.74	113.80
22	BA	111	A	C5-C6-N6	12.10	133.38	123.70
22	BA	981	A	C5-C6-N6	12.09	133.38	123.70
22	BA	1819	A	N7-C8-N9	-12.09	107.75	113.80
22	BA	2062	A	N7-C8-N9	-12.08	107.76	113.80
22	BA	1133	A	N7-C8-N9	-12.08	107.76	113.80
22	BA	661	A	N7-C8-N9	-12.07	107.76	113.80
22	BA	2439	A	N7-C8-N9	-12.07	107.77	113.80
22	BA	529	A	C5-C6-N6	12.07	133.35	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2450	A	C5-C6-N6	12.07	133.35	123.70
54	D2	73	A	N7-C8-N9	-12.06	107.77	113.80
22	BA	443	A	C5-C6-N6	12.04	133.33	123.70
22	BA	1427	A	N7-C8-N9	-12.04	107.78	113.80
22	BA	1522	A	N7-C8-N9	-12.04	107.78	113.80
22	BA	2135	A	N7-C8-N9	-12.03	107.78	113.80
22	BA	84	A	C5-C6-N6	12.02	133.32	123.70
22	BA	2003	A	N7-C8-N9	-12.02	107.79	113.80
22	BA	821	A	N7-C8-N9	-12.02	107.79	113.80
22	BA	1668	A	N7-C8-N9	-12.01	107.80	113.80
54	D2	35	A	N7-C8-N9	-12.00	107.80	113.80
22	BA	2154	A	N7-C8-N9	-12.00	107.80	113.80
22	BA	1803	A	C5-C6-N6	12.00	133.30	123.70
22	BA	1913	A	N7-C8-N9	-11.99	107.80	113.80
22	BA	2738	A	C5-C6-N6	11.99	133.29	123.70
22	BA	1302	A	N7-C8-N9	-11.98	107.81	113.80
22	BA	1919	A	C5-C6-N6	11.98	133.28	123.70
22	BA	668	A	N7-C8-N9	-11.97	107.81	113.80
22	BA	2471	A	N7-C8-N9	-11.97	107.81	113.80
22	BA	1046	A	N7-C8-N9	-11.97	107.82	113.80
22	BA	1815	A	N7-C8-N9	-11.97	107.82	113.80
22	BA	2566	A	C5-C6-N6	11.97	133.28	123.70
22	BA	1129	A	C5-C6-N6	11.97	133.27	123.70
22	BA	2340	A	N7-C8-N9	-11.96	107.82	113.80
22	BA	2761	A	N7-C8-N9	-11.96	107.82	113.80
55	D3	76	A	C5-C6-N6	11.96	133.26	123.70
22	BA	1786	A	C5-C6-N6	11.95	133.26	123.70
22	BA	1204	A	N7-C8-N9	-11.94	107.83	113.80
22	BA	119	A	N7-C8-N9	-11.94	107.83	113.80
22	BA	1616	A	N7-C8-N9	-11.93	107.83	113.80
22	BA	1698	A	N7-C8-N9	-11.93	107.84	113.80
22	BA	1342	A	N7-C8-N9	-11.92	107.84	113.80
22	BA	2117	A	C5-C6-N6	11.92	133.23	123.70
22	BA	1205	A	N7-C8-N9	-11.91	107.84	113.80
23	BB	108	A	N7-C8-N9	-11.91	107.84	113.80
22	BA	538	A	N7-C8-N9	-11.91	107.84	113.80
22	BA	844	A	N7-C8-N9	-11.91	107.84	113.80
22	BA	2014	A	N7-C8-N9	-11.91	107.84	113.80
22	BA	10	A	N7-C8-N9	-11.91	107.85	113.80
22	BA	1829	A	N3-C4-C5	-11.91	118.46	126.80
22	BA	1502	A	N7-C8-N9	-11.91	107.85	113.80
22	BA	1165	A	N7-C8-N9	-11.90	107.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1978	A	C5-C6-N6	11.90	133.22	123.70
22	BA	1805	A	N7-C8-N9	-11.90	107.85	113.80
22	BA	2829	A	N7-C8-N9	-11.89	107.85	113.80
22	BA	111	A	N7-C8-N9	-11.89	107.85	113.80
22	BA	1040	A	N7-C8-N9	-11.89	107.85	113.80
22	BA	2287	A	N7-C8-N9	-11.89	107.86	113.80
22	BA	1057	A	N3-C4-C5	-11.89	118.48	126.80
22	BA	155	A	N7-C8-N9	-11.88	107.86	113.80
22	BA	196	A	C5-C6-N6	11.88	133.20	123.70
22	BA	925	A	N7-C8-N9	-11.88	107.86	113.80
22	BA	352	A	N7-C8-N9	-11.87	107.86	113.80
22	BA	603	A	C5-C6-N6	11.87	133.19	123.70
22	BA	1434	A	C5-C6-N6	11.87	133.19	123.70
22	BA	1701	A	C5-C6-N6	11.87	133.19	123.70
22	BA	734	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	2211	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	1322	A	C5-C6-N6	11.86	133.19	123.70
22	BA	2670	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	453	A	N7-C8-N9	-11.86	107.87	113.80
22	BA	101	A	N3-C4-C5	-11.85	118.50	126.80
22	BA	1780	A	C5-C6-N6	11.85	133.18	123.70
22	BA	223	A	C5-C6-N6	11.85	133.18	123.70
22	BA	1490	A	N3-C4-C5	-11.85	118.50	126.80
22	BA	2119	A	C5-C6-N6	11.82	133.16	123.70
22	BA	126	A	C5-C6-N6	11.82	133.15	123.70
22	BA	471	A	N7-C8-N9	-11.82	107.89	113.80
22	BA	340	A	N7-C8-N9	-11.81	107.89	113.80
22	BA	265	A	N7-C8-N9	-11.81	107.89	113.80
22	BA	1070	A	N7-C8-N9	-11.81	107.89	113.80
22	BA	2298	A	N7-C8-N9	-11.81	107.90	113.80
22	BA	1569	A	N7-C8-N9	-11.80	107.90	113.80
22	BA	861	A	C5-C6-N6	11.80	133.14	123.70
22	BA	1144	A	N7-C8-N9	-11.80	107.90	113.80
22	BA	804	A	N7-C8-N9	-11.80	107.90	113.80
22	BA	1134	A	N7-C8-N9	-11.79	107.91	113.80
22	BA	1858	A	N7-C8-N9	-11.79	107.91	113.80
22	BA	197	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	909	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	532	A	N3-C4-C5	-11.78	118.55	126.80
22	BA	2654	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	2879	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	2572	A	C5-C6-N6	11.78	133.12	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2750	A	N7-C8-N9	-11.78	107.91	113.80
22	BA	896	A	N7-C8-N9	-11.77	107.92	113.80
22	BA	1384	A	N7-C8-N9	-11.77	107.92	113.80
22	BA	1597	A	N7-C8-N9	-11.77	107.92	113.80
22	BA	1928	A	C5-C6-N6	11.77	133.11	123.70
55	D3	37	A	C5-C6-N6	11.77	133.11	123.70
22	BA	979	A	N7-C8-N9	-11.76	107.92	113.80
22	BA	443	A	N7-C8-N9	-11.76	107.92	113.80
22	BA	1579	A	N7-C8-N9	-11.76	107.92	113.80
22	BA	2882	A	N7-C8-N9	-11.76	107.92	113.80
22	BA	896	A	C5-C6-N6	11.75	133.10	123.70
22	BA	2435	A	N7-C8-N9	-11.75	107.92	113.80
22	BA	1503	A	N7-C8-N9	-11.75	107.92	113.80
23	BB	78	A	N7-C8-N9	-11.75	107.92	113.80
54	D2	23	A	N7-C8-N9	-11.75	107.92	113.80
22	BA	53	A	C5-C6-N6	11.75	133.10	123.70
22	BA	2764	A	C5-C6-N6	11.75	133.10	123.70
22	BA	2837	A	N7-C8-N9	-11.74	107.93	113.80
22	BA	241	A	N7-C8-N9	-11.74	107.93	113.80
22	BA	783	A	C5-C6-N6	11.74	133.09	123.70
22	BA	2346	A	N7-C8-N9	-11.74	107.93	113.80
22	BA	861	A	N7-C8-N9	-11.73	107.93	113.80
22	BA	1069	A	C5-C6-N6	11.73	133.09	123.70
22	BA	2660	A	N7-C8-N9	-11.73	107.94	113.80
22	BA	1395	A	N7-C8-N9	-11.73	107.94	113.80
22	BA	2134	A	N7-C8-N9	-11.73	107.94	113.80
22	BA	749	A	C5-C6-N6	11.72	133.08	123.70
54	D2	58	A	C5-C6-N6	11.72	133.07	123.70
54	D2	28	A	N7-C8-N9	-11.72	107.94	113.80
22	BA	1286	A	N7-C8-N9	-11.71	107.94	113.80
54	D2	38	A	N7-C8-N9	-11.71	107.94	113.80
22	BA	144	A	N7-C8-N9	-11.71	107.95	113.80
22	BA	1155	A	N7-C8-N9	-11.71	107.95	113.80
22	BA	2020	A	N7-C8-N9	-11.71	107.95	113.80
22	BA	1912	A	C5-C6-N6	11.71	133.06	123.70
22	BA	428	A	N7-C8-N9	-11.70	107.95	113.80
22	BA	1073	A	N7-C8-N9	-11.70	107.95	113.80
22	BA	1129	A	N7-C8-N9	-11.70	107.95	113.80
22	BA	2333	A	N7-C8-N9	-11.70	107.95	113.80
22	BA	2835	A	N7-C8-N9	-11.69	107.95	113.80
22	BA	599	A	N7-C8-N9	-11.69	107.95	113.80
22	BA	547	A	N7-C8-N9	-11.69	107.96	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	563	A	N7-C8-N9	-11.69	107.96	113.80
23	BB	59	A	N7-C8-N9	-11.69	107.96	113.80
22	BA	2764	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	574	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	2171	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	2266	A	N7-C8-N9	-11.68	107.96	113.80
22	BA	2461	A	N3-C4-C5	-11.68	118.63	126.80
22	BA	227	A	C5-C6-N6	11.67	133.03	123.70
22	BA	800	A	N7-C8-N9	-11.65	107.97	113.80
55	D3	14	A	N7-C8-N9	-11.65	107.97	113.80
22	BA	1570	A	C5-C6-N6	11.65	133.02	123.70
22	BA	586	A	C5-C6-N6	11.65	133.02	123.70
22	BA	1378	A	N7-C8-N9	-11.65	107.98	113.80
22	BA	1953	A	C5-C6-N6	11.65	133.02	123.70
22	BA	1668	A	C5-C6-N6	11.64	133.02	123.70
22	BA	1080	A	N7-C8-N9	-11.64	107.98	113.80
22	BA	2565	A	C5-C6-N6	11.64	133.01	123.70
22	BA	1395	A	C5-C6-N6	11.64	133.01	123.70
22	BA	2077	A	N3-C4-C5	-11.64	118.65	126.80
22	BA	2665	A	N7-C8-N9	-11.64	107.98	113.80
22	BA	508	A	N7-C8-N9	-11.64	107.98	113.80
22	BA	788	A	C5-C6-N6	11.64	133.01	123.70
22	BA	1755	A	C5-C6-N6	11.64	133.01	123.70
22	BA	1580	A	N7-C8-N9	-11.63	107.98	113.80
22	BA	1876	A	N7-C8-N9	-11.63	107.98	113.80
22	BA	2542	A	C5-C6-N6	11.63	133.01	123.70
22	BA	227	A	N7-C8-N9	-11.63	107.98	113.80
22	BA	1050	A	N7-C8-N9	-11.63	107.98	113.80
22	BA	460	A	C5-C6-N6	11.62	133.00	123.70
22	BA	863	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	1328	A	C5-C6-N6	11.62	133.00	123.70
22	BA	2298	A	C5-C6-N6	11.62	133.00	123.70
22	BA	2800	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	1000	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	2241	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	529	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	2090	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	2469	A	N7-C8-N9	-11.62	107.99	113.80
22	BA	196	A	N7-C8-N9	-11.61	107.99	113.80
22	BA	2095	A	N7-C8-N9	-11.61	107.99	113.80
22	BA	1089	A	N7-C8-N9	-11.61	108.00	113.80
22	BA	1664	A	C5-C6-N6	11.61	132.99	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D2	5	A	N7-C8-N9	-11.61	108.00	113.80
22	BA	2288	A	N7-C8-N9	-11.61	108.00	113.80
22	BA	979	A	C5-C6-N6	11.60	132.98	123.70
22	BA	1020	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	56	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	482	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	689	A	N7-C8-N9	-11.60	108.00	113.80
55	D3	37	A	N7-C8-N9	-11.60	108.00	113.80
22	BA	401	A	C5-C6-N6	11.59	132.98	123.70
55	D3	58	A	C5-C6-N6	11.59	132.97	123.70
22	BA	1635	A	N7-C8-N9	-11.59	108.01	113.80
22	BA	1744	A	C5-C6-N6	11.59	132.97	123.70
22	BA	877	A	N7-C8-N9	-11.58	108.01	113.80
22	BA	753	A	N3-C4-C5	-11.58	118.69	126.80
22	BA	2267	A	C5-C6-N6	11.58	132.97	123.70
22	BA	632	A	N7-C8-N9	-11.58	108.01	113.80
22	BA	1786	A	N7-C8-N9	-11.58	108.01	113.80
22	BA	1815	A	C5-C6-N6	11.58	132.96	123.70
22	BA	983	A	N7-C8-N9	-11.57	108.01	113.80
22	BA	2566	A	N7-C8-N9	-11.57	108.02	113.80
54	D2	49	A	N7-C8-N9	-11.57	108.02	113.80
22	BA	829	A	C5-C6-N6	11.56	132.95	123.70
22	BA	2225	A	N7-C8-N9	-11.56	108.02	113.80
22	BA	342	A	N7-C8-N9	-11.56	108.02	113.80
22	BA	2590	A	N7-C8-N9	-11.56	108.02	113.80
22	BA	324	A	N7-C8-N9	-11.56	108.02	113.80
22	BA	103	A	C5-C6-N6	11.55	132.94	123.70
22	BA	742	A	N7-C8-N9	-11.55	108.02	113.80
22	BA	402	A	C5-C6-N6	11.55	132.94	123.70
22	BA	2534	A	N7-C8-N9	-11.55	108.02	113.80
22	BA	2711	A	N7-C8-N9	-11.55	108.02	113.80
22	BA	2273	A	C5-C6-N6	11.55	132.94	123.70
22	BA	371	A	C5-C6-N6	11.55	132.94	123.70
22	BA	693	A	N7-C8-N9	-11.55	108.03	113.80
22	BA	1392	A	C5-C6-N6	11.54	132.94	123.70
54	D2	76	A	N7-C8-N9	-11.55	108.03	113.80
22	BA	1938	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	2602	A	N3-C4-C5	-11.54	118.72	126.80
23	BB	109	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	2005	A	N7-C8-N9	-11.54	108.03	113.80
22	BA	2448	A	C5-C6-N6	11.54	132.93	123.70
22	BA	218	A	C5-C6-N6	11.53	132.93	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2632	A	N7-C8-N9	-11.53	108.03	113.80
22	BA	792	A	N7-C8-N9	-11.53	108.03	113.80
22	BA	2736	A	N7-C8-N9	-11.53	108.03	113.80
22	BA	13	A	C5-C6-N6	11.53	132.92	123.70
22	BA	984	A	N3-C4-C5	-11.53	118.73	126.80
22	BA	1469	A	C5-C6-N6	11.53	132.92	123.70
22	BA	2114	A	N3-C4-C5	-11.53	118.73	126.80
23	BB	94	A	N3-C4-C5	-11.53	118.73	126.80
22	BA	718	A	N7-C8-N9	-11.52	108.04	113.80
22	BA	1393	A	C5-C6-N6	11.52	132.92	123.70
22	BA	71	A	C5-C6-N6	11.52	132.91	123.70
22	BA	800	A	C5-C6-N6	11.52	132.91	123.70
22	BA	2418	A	N7-C8-N9	-11.51	108.05	113.80
22	BA	2451	A	C5-C6-N6	11.51	132.91	123.70
22	BA	2725	A	N7-C8-N9	-11.51	108.05	113.80
23	BB	52	A	N7-C8-N9	-11.51	108.05	113.80
22	BA	221	A	C5-C6-N6	11.51	132.91	123.70
22	BA	1111	A	C5-C6-N6	11.51	132.91	123.70
22	BA	1749	A	N7-C8-N9	-11.51	108.05	113.80
22	BA	2614	A	C5-C6-N6	11.51	132.91	123.70
22	BA	2758	A	N7-C8-N9	-11.51	108.05	113.80
22	BA	1705	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	1785	A	C5-C6-N6	11.50	132.90	123.70
22	BA	309	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	382	A	N7-C8-N9	-11.50	108.05	113.80
22	BA	241	A	C5-C6-N6	11.50	132.90	123.70
22	BA	1901	A	N3-C4-C5	-11.50	118.75	126.80
22	BA	1214	A	C5-C6-N6	11.49	132.90	123.70
54	D2	41	A	N7-C8-N9	-11.49	108.05	113.80
22	BA	2314	A	N7-C8-N9	-11.49	108.06	113.80
22	BA	1286	A	C5-C6-N6	11.49	132.89	123.70
22	BA	2336	A	N7-C8-N9	-11.49	108.06	113.80
22	BA	344	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	2173	A	C5-C6-N6	11.48	132.89	123.70
22	BA	676	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	28	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	1509	A	C5-C6-N6	11.48	132.88	123.70
22	BA	2327	A	C5-C6-N6	11.48	132.88	123.70
22	BA	167	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	526	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	1966	A	N7-C8-N9	-11.48	108.06	113.80
22	BA	384	A	C5-C6-N6	11.47	132.88	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2478	A	N7-C8-N9	-11.47	108.06	113.80
55	D3	21	A	N7-C8-N9	-11.47	108.06	113.80
22	BA	592	A	N3-C4-C5	-11.47	118.77	126.80
22	BA	866	A	N7-C8-N9	-11.47	108.06	113.80
22	BA	933	A	N3-C4-C5	-11.47	118.77	126.80
22	BA	2013	A	N7-C8-N9	-11.47	108.06	113.80
22	BA	2288	A	C5-C6-N6	11.47	132.88	123.70
22	BA	1285	A	C5-C6-N6	11.47	132.87	123.70
22	BA	1535	A	N7-C8-N9	-11.47	108.07	113.80
22	BA	2169	A	N7-C8-N9	-11.47	108.07	113.80
22	BA	2482	A	C5-C6-N6	11.47	132.88	123.70
22	BA	2635	A	N7-C8-N9	-11.47	108.07	113.80
22	BA	2560	A	N7-C8-N9	-11.47	108.07	113.80
22	BA	1392	A	N3-C4-C5	-11.46	118.78	126.80
22	BA	2158	A	N7-C8-N9	-11.46	108.07	113.80
54	D2	59	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	270	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	502	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	272	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	670	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	947	A	N7-C8-N9	-11.46	108.07	113.80
22	BA	1966	A	C5-C6-N6	11.46	132.86	123.70
22	BA	118	A	C5-C6-N6	11.45	132.86	123.70
22	BA	1596	A	N7-C8-N9	-11.45	108.07	113.80
22	BA	2336	A	C5-C6-N6	11.45	132.86	123.70
23	BB	73	A	N3-C4-C5	-11.45	118.78	126.80
22	BA	2281	A	N7-C8-N9	-11.45	108.08	113.80
22	BA	1308	A	N7-C8-N9	-11.45	108.08	113.80
22	BA	391	A	N7-C8-N9	-11.45	108.08	113.80
22	BA	449	A	N7-C8-N9	-11.45	108.08	113.80
22	BA	1981	A	C5-C6-N6	11.45	132.86	123.70
22	BA	1189	A	N3-C4-C5	-11.45	118.79	126.80
22	BA	1230	A	N7-C8-N9	-11.45	108.08	113.80
22	BA	2565	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	191	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	1889	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	2176	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	2639	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	2776	A	C5-C6-N6	11.44	132.85	123.70
22	BA	103	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	1367	A	N7-C8-N9	-11.44	108.08	113.80
22	BA	374	A	N7-C8-N9	-11.43	108.08	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2893	A	N7-C8-N9	-11.43	108.08	113.80
23	BB	53	A	N7-C8-N9	-11.43	108.08	113.80
22	BA	412	A	C5-C6-N6	11.43	132.84	123.70
22	BA	454	A	C5-C6-N6	11.43	132.84	123.70
22	BA	483	A	N7-C8-N9	-11.43	108.08	113.80
22	BA	1383	A	C5-C6-N6	11.43	132.84	123.70
22	BA	2266	A	C5-C6-N6	11.43	132.84	123.70
23	BB	39	A	C5-C6-N6	11.43	132.84	123.70
23	BB	45	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	1439	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	1700	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	2198	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	52	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	959	A	C5-C6-N6	11.42	132.84	123.70
22	BA	1214	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	1327	A	N7-C8-N9	-11.42	108.09	113.80
22	BA	1603	A	N3-C4-C5	-11.42	118.81	126.80
54	D2	76	A	C5-C6-N6	11.41	132.83	123.70
22	BA	1773	A	N7-C8-N9	-11.41	108.09	113.80
22	BA	2328	A	N3-C4-C5	-11.41	118.81	126.80
22	BA	528	A	C5-C6-N6	11.41	132.83	123.70
22	BA	1086	A	N3-C4-C5	-11.41	118.81	126.80
22	BA	1960	A	N7-C8-N9	-11.41	108.10	113.80
22	BA	149	A	C5-C6-N6	11.41	132.83	123.70
22	BA	1987	A	N7-C8-N9	-11.41	108.10	113.80
22	BA	899	A	N7-C8-N9	-11.41	108.10	113.80
22	BA	2054	A	N7-C8-N9	-11.40	108.10	113.80
22	BA	83	A	N7-C8-N9	-11.40	108.10	113.80
22	BA	1420	A	N7-C8-N9	-11.40	108.10	113.80
22	BA	346	A	C5-C6-N6	11.40	132.82	123.70
22	BA	1969	A	N7-C8-N9	-11.40	108.10	113.80
23	BB	57	A	N7-C8-N9	-11.40	108.10	113.80
22	BA	497	A	N7-C8-N9	-11.39	108.10	113.80
22	BA	2850	A	N3-C4-C5	-11.39	118.83	126.80
22	BA	1890	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	621	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	2358	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	2634	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	2705	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	2873	A	N7-C8-N9	-11.39	108.11	113.80
22	BA	10	A	C5-C6-N6	11.38	132.81	123.70
22	BA	322	A	C5-C6-N6	11.38	132.81	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1069	A	N7-C8-N9	-11.38	108.11	113.80
22	BA	504	A	N7-C8-N9	-11.38	108.11	113.80
22	BA	781	A	C5-C6-N6	11.38	132.80	123.70
22	BA	1254	A	C5-C6-N6	11.37	132.80	123.70
22	BA	1783	A	C5-C6-N6	11.38	132.80	123.70
22	BA	1070	A	C5-C6-N6	11.37	132.80	123.70
22	BA	2147	A	C5-C6-N6	11.37	132.80	123.70
22	BA	2700	A	N7-C8-N9	-11.37	108.11	113.80
22	BA	1505	A	N7-C8-N9	-11.37	108.12	113.80
22	BA	1610	A	C5-C6-N6	11.37	132.80	123.70
22	BA	1981	A	N7-C8-N9	-11.37	108.11	113.80
22	BA	2778	A	N7-C8-N9	-11.37	108.12	113.80
55	D3	9	A	N3-C4-C5	-11.37	118.84	126.80
22	BA	685	A	C5-C6-N6	11.37	132.79	123.70
22	BA	1420	A	C5-C6-N6	11.37	132.79	123.70
22	BA	2227	A	C5-C6-N6	11.37	132.79	123.70
22	BA	1048	A	N3-C4-C5	-11.36	118.85	126.80
22	BA	2800	A	C5-C6-N6	11.36	132.79	123.70
22	BA	2821	A	N7-C8-N9	-11.36	108.12	113.80
22	BA	278	A	C5-C6-N6	11.35	132.78	123.70
22	BA	845	A	N7-C8-N9	-11.35	108.12	113.80
22	BA	2448	A	N7-C8-N9	-11.35	108.12	113.80
22	BA	74	A	N7-C8-N9	-11.35	108.12	113.80
55	D3	31	A	N3-C4-C5	-11.35	118.85	126.80
22	BA	1169	A	N7-C8-N9	-11.35	108.12	113.80
22	BA	2600	A	N7-C8-N9	-11.35	108.12	113.80
22	BA	262	A	N3-C4-C5	-11.35	118.86	126.80
22	BA	644	A	N7-C8-N9	-11.35	108.13	113.80
22	BA	2274	A	C5-C6-N6	11.35	132.78	123.70
22	BA	2530	A	N7-C8-N9	-11.35	108.13	113.80
23	BB	34	A	N7-C8-N9	-11.35	108.13	113.80
22	BA	910	A	N7-C8-N9	-11.34	108.13	113.80
22	BA	1871	A	N7-C8-N9	-11.34	108.13	113.80
22	BA	2033	A	C5-C6-N6	11.34	132.77	123.70
22	BA	637	A	C5-C6-N6	11.34	132.77	123.70
22	BA	1253	A	N7-C8-N9	-11.34	108.13	113.80
22	BA	1133	A	C5-C6-N6	11.34	132.77	123.70
54	D2	35	A	C5-C6-N6	11.34	132.77	123.70
22	BA	63	A	N7-C8-N9	-11.33	108.13	113.80
22	BA	255	A	N7-C8-N9	-11.33	108.14	113.80
22	BA	501	A	N7-C8-N9	-11.33	108.13	113.80
22	BA	532	A	C5-C6-N6	11.33	132.76	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	735	A	N7-C8-N9	-11.33	108.14	113.80
22	BA	750	A	N7-C8-N9	-11.33	108.14	113.80
22	BA	2052	A	N7-C8-N9	-11.33	108.14	113.80
22	BA	14	A	C5-C6-N6	11.32	132.76	123.70
22	BA	749	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	1365	A	N3-C4-C5	-11.32	118.87	126.80
22	BA	1780	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	2662	A	N3-C4-C5	-11.32	118.87	126.80
22	BA	655	A	C5-C6-N6	11.32	132.76	123.70
22	BA	1126	A	C5-C6-N6	11.32	132.76	123.70
22	BA	1260	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	1151	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	2733	A	N7-C8-N9	-11.32	108.14	113.80
22	BA	892	A	N3-C4-C5	-11.31	118.88	126.80
22	BA	2173	A	N3-C4-C5	-11.31	118.88	126.80
22	BA	2386	A	N7-C8-N9	-11.31	108.14	113.80
22	BA	507	A	C5-C6-N6	11.31	132.75	123.70
22	BA	983	A	C5-C6-N6	11.31	132.75	123.70
54	D2	69	A	N7-C8-N9	-11.31	108.14	113.80
22	BA	631	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	1028	A	N3-C4-C5	-11.30	118.89	126.80
22	BA	2284	A	N3-C4-C5	-11.30	118.89	126.80
22	BA	699	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	789	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	402	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	1090	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	330	A	N3-C4-C5	-11.30	118.89	126.80
23	BB	29	A	N7-C8-N9	-11.30	108.15	113.80
22	BA	1528	A	N3-C4-C5	-11.29	118.89	126.80
22	BA	1039	A	N7-C8-N9	-11.29	108.15	113.80
22	BA	878	A	N7-C8-N9	-11.29	108.16	113.80
22	BA	820	A	N7-C8-N9	-11.29	108.16	113.80
22	BA	251	A	N3-C4-C5	-11.29	118.90	126.80
22	BA	825	A	N7-C8-N9	-11.29	108.16	113.80
22	BA	575	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	603	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	1640	A	C5-C6-N6	11.29	132.73	123.70
54	D2	21	A	C5-C6-N6	11.28	132.73	123.70
22	BA	204	A	C5-C6-N6	11.28	132.72	123.70
22	BA	627	A	C5-C6-N6	11.28	132.72	123.70
22	BA	1253	A	C5-C6-N6	11.28	132.73	123.70
22	BA	2297	A	N7-C8-N9	-11.28	108.16	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1783	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	2518	A	N3-C4-C5	-11.28	118.90	126.80
22	BA	1641	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	2170	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	2406	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	91	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	1532	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	1548	A	N7-C8-N9	-11.28	108.16	113.80
22	BA	2468	A	N7-C8-N9	-11.27	108.16	113.80
22	BA	1794	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	2826	A	N7-C8-N9	-11.27	108.16	113.80
22	BA	119	A	C5-C6-N6	11.27	132.72	123.70
22	BA	1254	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	996	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	2682	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	752	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	71	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	348	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	602	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	1762	A	C5-C6-N6	11.27	132.71	123.70
22	BA	2183	A	N3-C4-C5	-11.27	118.91	126.80
54	D2	14	A	N7-C8-N9	-11.27	108.17	113.80
22	BA	2322	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	142	A	N7-C8-N9	-11.26	108.17	113.80
22	BA	2541	A	C5-C6-N6	11.26	132.71	123.70
22	BA	172	A	N7-C8-N9	-11.25	108.17	113.80
22	BA	1269	A	N7-C8-N9	-11.25	108.17	113.80
22	BA	1359	A	N7-C8-N9	-11.25	108.17	113.80
22	BA	1672	A	N7-C8-N9	-11.25	108.17	113.80
22	BA	900	A	N7-C8-N9	-11.25	108.17	113.80
22	BA	2541	A	N7-C8-N9	-11.25	108.17	113.80
22	BA	219	A	C5-C6-N6	11.25	132.70	123.70
22	BA	602	A	C5-C6-N6	11.25	132.70	123.70
22	BA	945	A	N7-C8-N9	-11.25	108.18	113.80
22	BA	1711	A	N7-C8-N9	-11.25	108.18	113.80
22	BA	2094	A	N7-C8-N9	-11.25	108.18	113.80
22	BA	2886	A	N7-C8-N9	-11.25	108.18	113.80
22	BA	49	A	C5-C6-N6	11.24	132.69	123.70
22	BA	346	A	N7-C8-N9	-11.24	108.18	113.80
22	BA	2411	A	C5-C6-N6	11.24	132.70	123.70
22	BA	1265	A	C5-C6-N6	11.24	132.69	123.70
22	BA	1522	A	C5-C6-N6	11.24	132.69	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2781	A	C5-C6-N6	11.24	132.69	123.70
22	BA	244	A	N7-C8-N9	-11.23	108.18	113.80
22	BA	918	A	N7-C8-N9	-11.23	108.18	113.80
54	D2	38	A	C5-C6-N6	11.23	132.69	123.70
22	BA	1890	A	C5-C6-N6	11.23	132.68	123.70
22	BA	2126	A	N7-C8-N9	-11.23	108.19	113.80
22	BA	2211	A	C5-C6-N6	11.23	132.68	123.70
22	BA	73	A	C5-C6-N6	11.23	132.68	123.70
22	BA	299	A	C5-C6-N6	11.23	132.68	123.70
22	BA	2014	A	C5-C6-N6	11.23	132.68	123.70
22	BA	330	A	C5-C6-N6	11.22	132.68	123.70
22	BA	2432	A	C5-C6-N6	11.22	132.68	123.70
22	BA	64	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	190	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	735	A	C5-C6-N6	11.22	132.68	123.70
54	D2	21	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	309	A	C5-C6-N6	11.22	132.68	123.70
22	BA	2088	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	526	A	C5-C6-N6	11.22	132.67	123.70
23	BB	15	A	N7-C8-N9	-11.22	108.19	113.80
22	BA	310	A	C5-C6-N6	11.21	132.67	123.70
22	BA	471	A	C5-C6-N6	11.21	132.67	123.70
22	BA	2823	A	C5-C6-N6	11.21	132.67	123.70
22	BA	470	A	N7-C8-N9	-11.21	108.19	113.80
22	BA	2333	A	C5-C6-N6	11.21	132.67	123.70
22	BA	2734	A	N7-C8-N9	-11.21	108.20	113.80
22	BA	320	A	C5-C6-N6	11.21	132.66	123.70
22	BA	1304	A	N7-C8-N9	-11.21	108.20	113.80
22	BA	2433	A	C5-C6-N6	11.21	132.66	123.70
22	BA	2660	A	C5-C6-N6	11.21	132.66	123.70
54	D2	31	A	C5-C6-N6	11.20	132.66	123.70
22	BA	219	A	N3-C4-C5	-11.20	118.96	126.80
22	BA	1366	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	2060	A	C5-C6-N6	11.20	132.66	123.70
22	BA	2482	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	1439	A	C5-C6-N6	11.20	132.66	123.70
22	BA	42	A	N7-C8-N9	-11.20	108.20	113.80
22	BA	2378	A	C5-C6-N6	11.19	132.65	123.70
22	BA	1142	A	N7-C8-N9	-11.19	108.20	113.80
22	BA	1545	A	N7-C8-N9	-11.19	108.20	113.80
22	BA	973	A	N7-C8-N9	-11.19	108.21	113.80
22	BA	1598	A	C5-C6-N6	11.19	132.65	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1678	A	N7-C8-N9	-11.19	108.21	113.80
22	BA	988	A	C5-C6-N6	11.19	132.65	123.70
22	BA	1427	A	C5-C6-N6	11.19	132.65	123.70
22	BA	1640	A	N7-C8-N9	-11.19	108.21	113.80
22	BA	1679	A	C5-C6-N6	11.19	132.65	123.70
22	BA	2205	A	N7-C8-N9	-11.19	108.21	113.80
22	BA	2873	A	C5-C6-N6	11.19	132.65	123.70
55	D3	21	A	C5-C6-N6	11.19	132.65	123.70
23	BB	53	A	C5-C6-N6	11.18	132.65	123.70
22	BA	666	A	N7-C8-N9	-11.18	108.21	113.80
22	BA	1808	A	N7-C8-N9	-11.18	108.21	113.80
22	BA	231	A	N7-C8-N9	-11.18	108.21	113.80
22	BA	574	A	C5-C6-N6	11.18	132.64	123.70
22	BA	2268	A	N7-C8-N9	-11.18	108.21	113.80
22	BA	270	A	C5-C6-N6	11.17	132.64	123.70
22	BA	1610	A	N7-C8-N9	-11.17	108.21	113.80
22	BA	2284	A	N7-C8-N9	-11.17	108.21	113.80
22	BA	1757	A	C5-C6-N6	11.17	132.64	123.70
22	BA	1367	A	C5-C6-N6	11.17	132.63	123.70
22	BA	1419	A	C5-C6-N6	11.17	132.63	123.70
22	BA	1977	A	N7-C8-N9	-11.17	108.22	113.80
22	BA	2654	A	C5-C6-N6	11.17	132.63	123.70
22	BA	477	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	917	A	C5-C6-N6	11.16	132.63	123.70
22	BA	1336	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	2031	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	2412	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	1274	A	C5-C6-N6	11.16	132.63	123.70
22	BA	706	A	N7-C8-N9	-11.16	108.22	113.80
22	BA	1194	A	N7-C8-N9	-11.15	108.22	113.80
22	BA	1535	A	C5-C6-N6	11.15	132.62	123.70
22	BA	2058	A	N7-C8-N9	-11.15	108.22	113.80
22	BA	311	A	C5-C6-N6	11.15	132.62	123.70
22	BA	447	A	N7-C8-N9	-11.15	108.22	113.80
22	BA	2270	A	N7-C8-N9	-11.15	108.22	113.80
22	BA	675	A	N7-C8-N9	-11.15	108.22	113.80
22	BA	1654	A	C5-C6-N6	11.15	132.62	123.70
22	BA	538	A	C5-C6-N6	11.15	132.62	123.70
22	BA	1801	A	N7-C8-N9	-11.15	108.23	113.80
22	BA	2309	A	N7-C8-N9	-11.15	108.23	113.80
22	BA	2766	A	N3-C4-C5	-11.15	119.00	126.80
22	BA	89	A	N7-C8-N9	-11.15	108.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	160	A	C5-C6-N6	11.15	132.62	123.70
22	BA	181	A	C5-C6-N6	11.15	132.62	123.70
22	BA	739	A	C5-C6-N6	11.15	132.62	123.70
22	BA	1347	A	N7-C8-N9	-11.15	108.23	113.80
22	BA	2170	A	C5-C6-N6	11.15	132.62	123.70
22	BA	311	A	N7-C8-N9	-11.14	108.23	113.80
22	BA	892	A	N7-C8-N9	-11.14	108.23	113.80
22	BA	1387	A	N3-C4-C5	-11.14	119.00	126.80
22	BA	1572	A	N7-C8-N9	-11.14	108.23	113.80
22	BA	734	A	C5-C6-N6	11.14	132.61	123.70
22	BA	216	A	C5-C6-N6	11.14	132.61	123.70
22	BA	1787	A	N3-C4-C5	-11.14	119.00	126.80
22	BA	1885	A	N7-C8-N9	-11.14	108.23	113.80
22	BA	1237	A	N7-C8-N9	-11.14	108.23	113.80
22	BA	2080	A	N3-C4-C5	-11.13	119.01	126.80
22	BA	2531	A	N7-C8-N9	-11.13	108.23	113.80
22	BA	1321	A	C5-C6-N6	11.13	132.60	123.70
22	BA	541	A	N7-C8-N9	-11.13	108.24	113.80
22	BA	1403	A	N7-C8-N9	-11.13	108.24	113.80
22	BA	2602	A	C5-C6-N6	11.13	132.60	123.70
22	BA	2856	A	N7-C8-N9	-11.13	108.24	113.80
22	BA	582	A	N3-C4-C5	-11.13	119.01	126.80
22	BA	2134	A	C5-C6-N6	11.13	132.60	123.70
22	BA	1590	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	2199	A	C5-C6-N6	11.12	132.60	123.70
22	BA	294	A	N7-C8-N9	-11.12	108.24	113.80
22	BA	2031	A	C5-C6-N6	11.12	132.59	123.70
22	BA	2741	A	N7-C8-N9	-11.11	108.24	113.80
22	BA	1027	A	N7-C8-N9	-11.11	108.24	113.80
22	BA	1098	A	N7-C8-N9	-11.11	108.24	113.80
22	BA	216	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	1754	A	C5-C6-N6	11.11	132.59	123.70
22	BA	1970	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	182	A	C5-C6-N6	11.11	132.59	123.70
22	BA	928	A	N7-C8-N9	-11.11	108.25	113.80
22	BA	1008	A	C5-C6-N6	11.11	132.59	123.70
23	BB	45	A	C5-C6-N6	11.11	132.58	123.70
23	BB	39	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	233	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	675	A	N3-C4-C5	-11.10	119.03	126.80
22	BA	689	A	N3-C4-C5	-11.10	119.03	126.80
22	BA	1359	A	C5-C6-N6	11.10	132.58	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1932	A	C5-C6-N6	11.10	132.58	123.70
22	BA	2287	A	N3-C4-C5	-11.10	119.03	126.80
22	BA	2602	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	626	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	1307	A	C5-C6-N6	11.10	132.58	123.70
54	D2	28	A	N3-C4-C5	-11.10	119.03	126.80
22	BA	256	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	1551	A	N7-C8-N9	-11.10	108.25	113.80
22	BA	221	A	N7-C8-N9	-11.09	108.25	113.80
23	BB	115	A	N7-C8-N9	-11.09	108.25	113.80
22	BA	1268	A	N7-C8-N9	-11.09	108.25	113.80
22	BA	2614	A	N7-C8-N9	-11.09	108.25	113.80
55	D3	26	A	N7-C8-N9	-11.09	108.25	113.80
22	BA	1244	A	N7-C8-N9	-11.09	108.25	113.80
22	BA	1609	A	N7-C8-N9	-11.09	108.25	113.80
22	BA	294	A	C5-C6-N6	11.09	132.57	123.70
22	BA	1616	A	C5-C6-N6	11.09	132.57	123.70
22	BA	2042	A	N7-C8-N9	-11.09	108.26	113.80
1	AA	961	U	N3-C2-O2	-11.09	114.44	122.20
22	BA	2058	A	C5-C6-N6	11.09	132.57	123.70
22	BA	460	A	N7-C8-N9	-11.09	108.26	113.80
22	BA	1321	A	N3-C4-C5	-11.09	119.04	126.80
22	BA	1913	A	C5-C6-N6	11.09	132.57	123.70
22	BA	2005	A	C5-C6-N6	11.09	132.57	123.70
22	BA	2765	A	C5-C6-N6	11.08	132.57	123.70
22	BA	2860	A	C5-C6-N6	11.08	132.56	123.70
22	BA	2665	A	C5-C6-N6	11.08	132.56	123.70
22	BA	1287	A	N7-C8-N9	-11.08	108.26	113.80
22	BA	1858	A	C5-C6-N6	11.08	132.56	123.70
22	BA	94	A	C5-C6-N6	11.07	132.56	123.70
22	BA	404	A	N7-C8-N9	-11.07	108.26	113.80
22	BA	1698	A	C5-C6-N6	11.07	132.56	123.70
22	BA	300	A	C5-C6-N6	11.07	132.56	123.70
22	BA	547	A	C5-C6-N6	11.07	132.56	123.70
22	BA	1773	A	C5-C6-N6	11.07	132.56	123.70
22	BA	131	A	N7-C8-N9	-11.07	108.27	113.80
22	BA	1746	A	N7-C8-N9	-11.07	108.27	113.80
23	BB	58	A	C5-C6-N6	11.07	132.56	123.70
54	D2	14	A	C5-C6-N6	11.07	132.56	123.70
22	BA	1204	A	C5-C6-N6	11.07	132.55	123.70
22	BA	1701	A	N7-C8-N9	-11.07	108.27	113.80
22	BA	466	A	N7-C8-N9	-11.06	108.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	718	A	C5-C6-N6	11.06	132.55	123.70
22	BA	1383	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	1916	A	C5-C6-N6	11.06	132.55	123.70
22	BA	21	A	N7-C8-N9	-11.06	108.27	113.80
22	BA	782	A	C5-C6-N6	11.05	132.54	123.70
22	BA	1571	A	C5-C6-N6	11.05	132.54	123.70
55	D3	23	A	N7-C8-N9	-11.05	108.27	113.80
22	BA	432	A	N7-C8-N9	-11.05	108.28	113.80
22	BA	2142	A	N7-C8-N9	-11.05	108.27	113.80
22	BA	2478	A	C5-C6-N6	11.05	132.54	123.70
22	BA	614	A	C5-C6-N6	11.05	132.54	123.70
22	BA	2037	A	N3-C4-C5	-11.05	119.06	126.80
22	BA	2176	A	C5-C6-N6	11.05	132.54	123.70
23	BB	104	A	N7-C8-N9	-11.05	108.28	113.80
22	BA	1048	A	C5-C6-N6	11.05	132.54	123.70
22	BA	1366	A	C5-C6-N6	11.05	132.54	123.70
22	BA	1810	A	N3-C4-C5	-11.04	119.07	126.80
22	BA	1103	A	C5-C6-N6	11.04	132.53	123.70
22	BA	1570	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	2311	A	C5-C6-N6	11.04	132.53	123.70
55	D3	73	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	1246	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	1353	A	N3-C4-C5	-11.04	119.07	126.80
22	BA	1552	A	N7-C8-N9	-11.04	108.28	113.80
22	BA	892	A	C5-C6-N6	11.04	132.53	123.70
22	BA	432	A	C5-C6-N6	11.04	132.53	123.70
22	BA	423	A	N7-C8-N9	-11.03	108.28	113.80
22	BA	1393	A	N7-C8-N9	-11.03	108.29	113.80
22	BA	945	A	C5-C6-N6	11.03	132.52	123.70
22	BA	1960	A	N3-C4-C5	-11.03	119.08	126.80
23	BB	99	A	C5-C6-N6	11.03	132.52	123.70
22	BA	608	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	2054	A	N3-C4-C5	-11.02	119.08	126.80
22	BA	2411	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	190	A	N3-C4-C5	-11.02	119.08	126.80
22	BA	1353	A	N7-C8-N9	-11.02	108.29	113.80
22	BA	2809	A	N3-C4-C5	-11.02	119.09	126.80
22	BA	2042	A	C5-C6-N6	11.02	132.51	123.70
22	BA	972	A	N7-C8-N9	-11.01	108.29	113.80
22	BA	1918	A	C5-C6-N6	11.01	132.51	123.70
22	BA	2227	A	N7-C8-N9	-11.01	108.29	113.80
22	BA	2287	A	C5-C6-N6	11.01	132.51	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1744	A	N3-C4-C5	-11.01	119.09	126.80
22	BA	19	A	N7-C8-N9	-11.01	108.30	113.80
22	BA	1548	A	N3-C4-C5	-11.01	119.10	126.80
22	BA	1285	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	2887	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	165	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	2184	A	N3-C4-C5	-11.00	119.10	126.80
22	BA	2497	A	C5-C6-N6	11.00	132.50	123.70
22	BA	2753	A	C5-C6-N6	11.00	132.50	123.70
22	BA	505	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	457	A	C5-C6-N6	11.00	132.50	123.70
22	BA	507	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	616	A	N7-C8-N9	-11.00	108.30	113.80
22	BA	825	A	N3-C4-C5	-11.00	119.10	126.80
22	BA	1287	A	C5-C6-N6	11.00	132.50	123.70
22	BA	483	A	C5-C6-N6	10.99	132.50	123.70
22	BA	2657	A	N7-C8-N9	-10.99	108.30	113.80
22	BA	676	A	C5-C6-N6	10.99	132.49	123.70
22	BA	1508	A	N7-C8-N9	-10.99	108.30	113.80
22	BA	1717	A	N7-C8-N9	-10.99	108.30	113.80
22	BA	1847	A	N3-C4-C5	-10.99	119.11	126.80
22	BA	644	A	C5-C6-N6	10.99	132.49	123.70
22	BA	631	A	C5-C6-N6	10.99	132.49	123.70
22	BA	1048	A	N7-C8-N9	-10.99	108.31	113.80
22	BA	2163	A	N3-C4-C5	-10.99	119.11	126.80
22	BA	226	A	N3-C4-C5	-10.98	119.11	126.80
22	BA	2740	A	C5-C6-N6	10.98	132.49	123.70
22	BA	2851	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	2015	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	1553	A	C5-C6-N6	10.98	132.48	123.70
22	BA	2820	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	1549	A	N7-C8-N9	-10.98	108.31	113.80
22	BA	244	A	C5-C6-N6	10.98	132.48	123.70
22	BA	2706	A	N3-C4-C5	-10.98	119.11	126.80
22	BA	616	A	C5-C6-N6	10.97	132.48	123.70
22	BA	1953	A	N7-C8-N9	-10.97	108.31	113.80
22	BA	1126	A	N7-C8-N9	-10.97	108.31	113.80
22	BA	1614	A	N7-C8-N9	-10.97	108.31	113.80
22	BA	2051	A	C5-C6-N6	10.97	132.48	123.70
22	BA	2019	A	N7-C8-N9	-10.97	108.32	113.80
22	BA	2126	A	C5-C6-N6	10.97	132.47	123.70
22	BA	936	A	N7-C8-N9	-10.96	108.32	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	980	A	C5-C6-N6	10.96	132.47	123.70
22	BA	345	A	N3-C4-C5	-10.96	119.13	126.80
22	BA	1143	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	1773	A	N3-C4-C5	-10.96	119.13	126.80
22	BA	1001	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	126	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	501	A	C5-C6-N6	10.96	132.47	123.70
22	BA	1095	A	C5-C6-N6	10.96	132.47	123.70
22	BA	2434	A	C5-C6-N6	10.96	132.47	123.70
22	BA	2850	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	161	A	C5-C6-N6	10.96	132.47	123.70
22	BA	320	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	354	A	C5-C6-N6	10.96	132.47	123.70
22	BA	2297	A	C5-C6-N6	10.96	132.47	123.70
22	BA	1032	A	C5-C6-N6	10.96	132.47	123.70
22	BA	362	A	N7-C8-N9	-10.96	108.32	113.80
22	BA	927	A	N7-C8-N9	-10.95	108.32	113.80
22	BA	1175	A	C5-C6-N6	10.95	132.46	123.70
22	BA	1000	A	C5-C6-N6	10.95	132.46	123.70
22	BA	1054	A	N7-C8-N9	-10.95	108.32	113.80
22	BA	1609	A	C5-C6-N6	10.95	132.46	123.70
22	BA	1665	A	N7-C8-N9	-10.95	108.32	113.80
22	BA	2191	A	N7-C8-N9	-10.95	108.32	113.80
22	BA	165	A	C5-C6-N6	10.95	132.46	123.70
22	BA	819	A	N7-C8-N9	-10.95	108.33	113.80
22	BA	975	A	C5-C6-N6	10.95	132.46	123.70
22	BA	1189	A	C5-C6-N6	10.95	132.46	123.70
22	BA	917	A	N7-C8-N9	-10.95	108.33	113.80
22	BA	1175	A	N7-C8-N9	-10.95	108.33	113.80
22	BA	1328	A	N3-C4-C5	-10.95	119.14	126.80
22	BA	1077	A	N7-C8-N9	-10.94	108.33	113.80
22	BA	2158	A	C5-C6-N6	10.94	132.45	123.70
55	D3	7	A	C5-C6-N6	10.94	132.46	123.70
22	BA	2163	A	C5-C6-N6	10.94	132.45	123.70
22	BA	608	A	C5-C6-N6	10.94	132.45	123.70
22	BA	917	A	N3-C4-C5	-10.94	119.14	126.80
22	BA	1384	A	C5-C6-N6	10.94	132.45	123.70
22	BA	1735	A	N7-C8-N9	-10.94	108.33	113.80
22	BA	2169	A	C5-C6-N6	10.94	132.45	123.70
22	BA	2705	A	C5-C6-N6	10.94	132.45	123.70
22	BA	368	A	C5-C6-N6	10.93	132.45	123.70
22	BA	374	A	N3-C4-C5	-10.93	119.15	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2311	A	N7-C8-N9	-10.93	108.33	113.80
22	BA	2799	A	N3-C4-C5	-10.93	119.15	126.80
22	BA	1057	A	N7-C8-N9	-10.93	108.33	113.80
22	BA	1494	A	N7-C8-N9	-10.93	108.33	113.80
22	BA	2377	A	C5-C6-N6	10.93	132.44	123.70
23	BB	99	A	N7-C8-N9	-10.93	108.34	113.80
55	D3	76	A	N7-C8-N9	-10.93	108.34	113.80
22	BA	1269	A	N3-C4-C5	-10.93	119.15	126.80
22	BA	1496	A	C5-C6-N6	10.93	132.44	123.70
22	BA	1268	A	C5-C6-N6	10.92	132.44	123.70
22	BA	1495	A	C5-C6-N6	10.92	132.44	123.70
22	BA	2823	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	706	A	C5-C6-N6	10.92	132.43	123.70
22	BA	1265	A	N7-C8-N9	-10.92	108.34	113.80
22	BA	716	A	N7-C8-N9	-10.91	108.34	113.80
22	BA	1413	A	N7-C8-N9	-10.91	108.34	113.80
54	D2	73	A	C5-C6-N6	10.91	132.43	123.70
23	BB	50	A	N7-C8-N9	-10.91	108.34	113.80
22	BA	502	A	C5-C6-N6	10.91	132.43	123.70
22	BA	1632	A	N7-C8-N9	-10.91	108.35	113.80
22	BA	1365	A	C5-C6-N6	10.90	132.42	123.70
22	BA	265	A	C5-C6-N6	10.90	132.42	123.70
22	BA	453	A	C5-C6-N6	10.90	132.42	123.70
22	BA	83	A	C5-C6-N6	10.90	132.42	123.70
22	BA	1090	A	C5-C6-N6	10.90	132.42	123.70
22	BA	282	A	N7-C8-N9	-10.90	108.35	113.80
22	BA	2809	A	C5-C6-N6	10.90	132.42	123.70
55	D3	38	A	N3-C4-C5	-10.90	119.17	126.80
22	BA	345	A	N7-C8-N9	-10.90	108.35	113.80
22	BA	1050	A	C5-C6-N6	10.90	132.42	123.70
22	BA	2639	A	C5-C6-N6	10.90	132.42	123.70
22	BA	751	A	C5-C6-N6	10.89	132.41	123.70
22	BA	1525	A	N7-C8-N9	-10.89	108.35	113.80
22	BA	1549	A	N3-C4-C5	-10.89	119.17	126.80
22	BA	2407	A	N7-C8-N9	-10.89	108.35	113.80
22	BA	764	A	N7-C8-N9	-10.89	108.35	113.80
22	BA	1713	A	N7-C8-N9	-10.89	108.35	113.80
22	BA	1900	A	C5-C6-N6	10.89	132.41	123.70
22	BA	677	A	N7-C8-N9	-10.89	108.35	113.80
22	BA	794	A	N7-C8-N9	-10.89	108.35	113.80
22	BA	1759	A	C5-C6-N6	10.89	132.41	123.70
22	BA	347	A	N3-C4-C5	-10.89	119.18	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1387	A	N7-C8-N9	-10.89	108.36	113.80
22	BA	2634	A	N3-C4-C5	-10.89	119.18	126.80
23	BB	108	A	C5-C6-N6	10.89	132.41	123.70
55	D3	9	A	C5-C6-N6	10.89	132.41	123.70
22	BA	1014	A	N7-C8-N9	-10.89	108.36	113.80
22	BA	2657	A	C5-C6-N6	10.89	132.41	123.70
22	BA	632	A	C5-C6-N6	10.88	132.41	123.70
22	BA	1678	A	C5-C6-N6	10.88	132.41	123.70
22	BA	1746	A	N3-C4-C5	-10.88	119.18	126.80
22	BA	2835	A	C5-C6-N6	10.88	132.41	123.70
22	BA	131	A	N3-C4-C5	-10.88	119.18	126.80
22	BA	654	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	1916	A	N7-C8-N9	-10.88	108.36	113.80
23	BB	58	A	N7-C8-N9	-10.88	108.36	113.80
23	BB	101	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	608	A	N3-C4-C5	-10.88	119.18	126.80
22	BA	2268	A	C5-C6-N6	10.88	132.41	123.70
22	BA	2675	A	C5-C6-N6	10.88	132.40	123.70
22	BA	14	A	N7-C8-N9	-10.88	108.36	113.80
22	BA	340	A	C5-C6-N6	10.87	132.40	123.70
22	BA	347	A	N7-C8-N9	-10.87	108.36	113.80
22	BA	522	A	N3-C4-C5	-10.87	119.19	126.80
22	BA	685	A	N3-C4-C5	-10.87	119.19	126.80
22	BA	1553	A	N7-C8-N9	-10.87	108.36	113.80
22	BA	793	A	C5-C6-N6	10.87	132.39	123.70
22	BA	820	A	C5-C6-N6	10.87	132.40	123.70
22	BA	1046	A	C5-C6-N6	10.87	132.39	123.70
22	BA	2070	A	N7-C8-N9	-10.87	108.37	113.80
55	D3	64	A	N3-C4-C5	-10.87	119.19	126.80
22	BA	1096	A	C5-C6-N6	10.86	132.39	123.70
22	BA	1952	A	C5-C6-N6	10.86	132.39	123.70
54	D2	9	A	C5-C6-N6	10.86	132.39	123.70
22	BA	181	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	1241	A	N3-C4-C5	-10.86	119.20	126.80
22	BA	1453	A	C5-C6-N6	10.86	132.39	123.70
22	BA	362	A	C5-C6-N6	10.86	132.38	123.70
22	BA	699	A	C5-C6-N6	10.86	132.39	123.70
22	BA	1431	A	N7-C8-N9	-10.86	108.37	113.80
22	BA	910	A	C5-C6-N6	10.85	132.38	123.70
22	BA	514	A	C5-C6-N6	10.85	132.38	123.70
22	BA	118	A	N7-C8-N9	-10.85	108.38	113.80
22	BA	2748	A	N7-C8-N9	-10.85	108.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1508	A	C5-C6-N6	10.85	132.38	123.70
22	BA	2821	A	C5-C6-N6	10.85	132.38	123.70
22	BA	1373	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	1067	A	C5-C6-N6	10.84	132.37	123.70
22	BA	1998	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	2346	A	C5-C6-N6	10.84	132.37	123.70
22	BA	2513	A	N3-C4-C5	-10.84	119.21	126.80
22	BA	1494	A	C5-C6-N6	10.84	132.37	123.70
22	BA	2753	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	1583	A	C5-C6-N6	10.84	132.37	123.70
22	BA	2900	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	721	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	2097	A	N7-C8-N9	-10.84	108.38	113.80
22	BA	2530	A	C5-C6-N6	10.84	132.37	123.70
23	BB	99	A	N3-C4-C5	-10.84	119.22	126.80
22	BA	1127	A	C5-C6-N6	10.83	132.37	123.70
22	BA	1262	A	N3-C4-C5	-10.83	119.22	126.80
22	BA	2173	A	N7-C8-N9	-10.83	108.39	113.80
23	BB	46	A	C5-C6-N6	10.83	132.36	123.70
22	BA	127	A	C5-C6-N6	10.83	132.36	123.70
22	BA	556	A	N7-C8-N9	-10.83	108.39	113.80
22	BA	1802	A	N7-C8-N9	-10.83	108.39	113.80
22	BA	866	A	C5-C6-N6	10.82	132.36	123.70
22	BA	2212	A	C5-C6-N6	10.82	132.36	123.70
22	BA	2589	A	C5-C6-N6	10.82	132.36	123.70
22	BA	2727	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	1665	A	N3-C4-C5	-10.82	119.22	126.80
54	D2	26	A	N3-C4-C5	-10.82	119.22	126.80
22	BA	900	A	C5-C6-N6	10.82	132.35	123.70
22	BA	1566	A	C5-C6-N6	10.82	132.35	123.70
22	BA	2748	A	C5-C6-N6	10.82	132.36	123.70
22	BA	1634	A	C5-C6-N6	10.82	132.35	123.70
22	BA	2309	A	C5-C6-N6	10.82	132.35	123.70
22	BA	2366	A	N3-C4-C5	-10.82	119.23	126.80
55	D3	9	A	N7-C8-N9	-10.82	108.39	113.80
22	BA	2886	A	C5-C6-N6	10.81	132.35	123.70
22	BA	127	A	N7-C8-N9	-10.81	108.39	113.80
22	BA	988	A	N7-C8-N9	-10.81	108.39	113.80
22	BA	1085	A	N7-C8-N9	-10.81	108.39	113.80
22	BA	1089	A	C5-C6-N6	10.81	132.35	123.70
22	BA	1632	A	N3-C4-C5	-10.81	119.23	126.80
22	BA	160	A	N7-C8-N9	-10.81	108.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	57	A	C5-C6-N6	10.81	132.35	123.70
22	BA	404	A	C5-C6-N6	10.81	132.35	123.70
22	BA	412	A	N7-C8-N9	-10.81	108.39	113.80
22	BA	802	A	N3-C4-C5	-10.81	119.23	126.80
22	BA	715	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	1008	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	1477	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	1579	A	C5-C6-N6	10.81	132.34	123.70
22	BA	1626	A	C5-C6-N6	10.81	132.34	123.70
22	BA	973	A	C5-C6-N6	10.80	132.34	123.70
22	BA	2459	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	1096	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	2810	A	C5-C6-N6	10.80	132.34	123.70
22	BA	1598	A	N3-C4-C5	-10.80	119.24	126.80
22	BA	1641	A	C5-C6-N6	10.80	132.34	123.70
22	BA	2101	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	38	A	N7-C8-N9	-10.79	108.40	113.80
22	BA	1689	A	N7-C8-N9	-10.79	108.40	113.80
22	BA	2077	A	N7-C8-N9	-10.80	108.40	113.80
22	BA	344	A	C5-C6-N6	10.79	132.33	123.70
22	BA	101	A	C5-C6-N6	10.79	132.33	123.70
22	BA	176	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	2564	A	C5-C6-N6	10.79	132.33	123.70
22	BA	223	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	515	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	1580	A	C5-C6-N6	10.79	132.33	123.70
22	BA	941	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	2518	A	N7-C8-N9	-10.79	108.41	113.80
22	BA	2813	A	C5-C6-N6	10.79	132.33	123.70
22	BA	1272	A	C5-C6-N6	10.78	132.33	123.70
22	BA	2851	A	C5-C6-N6	10.79	132.33	123.70
23	BB	78	A	C5-C6-N6	10.79	132.33	123.70
22	BA	633	A	N7-C8-N9	-10.78	108.41	113.80
22	BA	878	A	C5-C6-N6	10.78	132.32	123.70
22	BA	980	A	N7-C8-N9	-10.78	108.41	113.80
22	BA	1142	A	N3-C4-C5	-10.78	119.25	126.80
22	BA	2407	A	N3-C4-C5	-10.78	119.26	126.80
22	BA	52	A	C5-C6-N6	10.78	132.32	123.70
22	BA	2883	A	C5-C6-N6	10.78	132.32	123.70
22	BA	2726	A	N7-C8-N9	-10.78	108.41	113.80
22	BA	1342	A	C5-C6-N6	10.77	132.32	123.70
22	BA	1365	A	N7-C8-N9	-10.77	108.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1213	A	N3-C4-C5	-10.77	119.26	126.80
22	BA	2335	A	N7-C8-N9	-10.77	108.41	113.80
22	BA	217	A	C5-C6-N6	10.77	132.31	123.70
22	BA	959	A	N7-C8-N9	-10.77	108.42	113.80
22	BA	1301	A	N3-C4-C5	-10.77	119.26	126.80
22	BA	199	A	C5-C6-N6	10.77	132.31	123.70
22	BA	1095	A	N7-C8-N9	-10.77	108.42	113.80
22	BA	2733	A	C5-C6-N6	10.77	132.31	123.70
22	BA	849	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	2317	A	N7-C8-N9	-10.76	108.42	113.80
54	D2	59	A	C5-C6-N6	10.76	132.31	123.70
55	D3	38	A	C5-C6-N6	10.76	132.31	123.70
22	BA	94	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	1084	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	345	A	C5-C6-N6	10.76	132.30	123.70
22	BA	430	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	528	A	N7-C8-N9	-10.76	108.42	113.80
22	BA	761	A	N7-C8-N9	-10.76	108.42	113.80
55	D3	73	A	N3-C4-C5	-10.76	119.27	126.80
22	BA	563	A	C5-C6-N6	10.75	132.30	123.70
22	BA	439	A	N7-C8-N9	-10.75	108.42	113.80
22	BA	1214	A	N3-C4-C5	-10.75	119.27	126.80
22	BA	1205	A	C5-C6-N6	10.75	132.30	123.70
22	BA	412	A	N3-C4-C5	-10.75	119.28	126.80
22	BA	899	A	C5-C6-N6	10.75	132.30	123.70
22	BA	1276	A	N7-C8-N9	-10.75	108.43	113.80
22	BA	933	A	C5-C6-N6	10.75	132.30	123.70
22	BA	1284	A	N7-C8-N9	-10.75	108.43	113.80
22	BA	2598	A	C5-C6-N6	10.75	132.30	123.70
22	BA	173	A	N3-C4-C5	-10.74	119.28	126.80
22	BA	2750	A	C5-C6-N6	10.74	132.29	123.70
22	BA	6	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	1586	A	C5-C6-N6	10.74	132.29	123.70
22	BA	984	A	C5-C6-N6	10.74	132.29	123.70
22	BA	1745	A	C5-C6-N6	10.74	132.29	123.70
22	BA	2267	A	N7-C8-N9	-10.74	108.43	113.80
22	BA	1403	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	1226	A	N7-C8-N9	-10.73	108.44	113.80
22	BA	1544	A	C5-C6-N6	10.73	132.29	123.70
22	BA	2322	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	2392	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	2406	A	C5-C6-N6	10.73	132.29	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	693	A	N3-C4-C5	-10.73	119.29	126.80
22	BA	1593	A	N7-C8-N9	-10.73	108.44	113.80
22	BA	2476	A	C5-C6-N6	10.73	132.28	123.70
22	BA	2590	A	C5-C6-N6	10.73	132.28	123.70
23	BB	73	A	C5-C6-N6	10.73	132.28	123.70
1	AA	95	C	C2-N1-C1'	10.73	130.60	118.80
22	BA	49	A	N7-C8-N9	-10.73	108.44	113.80
22	BA	1552	A	C5-C6-N6	10.73	132.28	123.70
22	BA	1759	A	N7-C8-N9	-10.73	108.44	113.80
22	BA	2108	A	N7-C8-N9	-10.73	108.44	113.80
22	BA	423	A	C5-C6-N6	10.72	132.28	123.70
22	BA	685	A	N7-C8-N9	-10.72	108.44	113.80
22	BA	2070	A	N3-C4-C5	-10.72	119.29	126.80
22	BA	2386	A	N3-C4-C5	-10.72	119.29	126.80
22	BA	197	A	N3-C4-C5	-10.72	119.30	126.80
22	BA	1899	A	N3-C4-C5	-10.72	119.30	126.80
22	BA	2749	A	C5-C6-N6	10.72	132.28	123.70
22	BA	1054	A	N3-C4-C5	-10.72	119.30	126.80
22	BA	1301	A	N7-C8-N9	-10.72	108.44	113.80
22	BA	2108	A	C5-C6-N6	10.72	132.28	123.70
22	BA	2738	A	N7-C8-N9	-10.72	108.44	113.80
22	BA	2887	A	C5-C6-N6	10.72	132.28	123.70
22	BA	2741	A	C5-C6-N6	10.72	132.27	123.70
22	BA	1127	A	N7-C8-N9	-10.71	108.44	113.80
22	BA	182	A	N7-C8-N9	-10.71	108.44	113.80
22	BA	190	A	C5-C6-N6	10.71	132.27	123.70
22	BA	497	A	C5-C6-N6	10.71	132.27	123.70
22	BA	2826	A	C5-C6-N6	10.71	132.27	123.70
22	BA	401	A	N7-C8-N9	-10.71	108.44	113.80
22	BA	1084	A	C5-C6-N6	10.71	132.27	123.70
22	BA	1744	A	N7-C8-N9	-10.71	108.44	113.80
22	BA	472	A	C5-C6-N6	10.71	132.27	123.70
22	BA	503	A	N7-C8-N9	-10.71	108.45	113.80
22	BA	960	A	N7-C8-N9	-10.71	108.45	113.80
22	BA	1785	A	N7-C8-N9	-10.71	108.45	113.80
23	BB	52	A	C5-C6-N6	10.71	132.27	123.70
22	BA	95	A	N3-C4-C5	-10.71	119.31	126.80
22	BA	415	A	N3-C4-C5	-10.71	119.31	126.80
22	BA	156	A	N3-C4-C5	-10.70	119.31	126.80
22	BA	2273	A	N3-C4-C5	-10.71	119.31	126.80
22	BA	2461	A	N7-C8-N9	-10.71	108.45	113.80
22	BA	2019	A	C5-C6-N6	10.70	132.26	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	109	A	C5-C6-N6	10.70	132.26	123.70
22	BA	332	A	C5-C6-N6	10.70	132.26	123.70
22	BA	1608	A	N7-C8-N9	-10.70	108.45	113.80
22	BA	44	A	N7-C8-N9	-10.70	108.45	113.80
22	BA	845	A	C5-C6-N6	10.70	132.26	123.70
22	BA	1927	A	N7-C8-N9	-10.70	108.45	113.80
22	BA	2727	A	N3-C4-C5	-10.70	119.31	126.80
22	BA	2740	A	N3-C4-C5	-10.70	119.31	126.80
22	BA	125	A	C5-C6-N6	10.69	132.25	123.70
22	BA	1009	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	1791	A	N7-C8-N9	-10.69	108.45	113.80
55	D3	38	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	788	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	1073	A	C5-C6-N6	10.69	132.25	123.70
22	BA	1689	A	C5-C6-N6	10.69	132.25	123.70
22	BA	2212	A	N7-C8-N9	-10.69	108.45	113.80
22	BA	2893	A	C5-C6-N6	10.69	132.25	123.70
22	BA	38	A	N3-C4-C5	-10.69	119.32	126.80
22	BA	1655	A	C5-C6-N6	10.69	132.25	123.70
22	BA	2376	A	N7-C8-N9	-10.69	108.46	113.80
22	BA	13	A	N3-C4-C5	-10.68	119.32	126.80
22	BA	833	A	N7-C8-N9	-10.68	108.46	113.80
22	BA	1000	A	N3-C4-C5	-10.68	119.32	126.80
22	BA	1632	A	C5-C6-N6	10.68	132.25	123.70
22	BA	2451	A	N7-C8-N9	-10.68	108.46	113.80
22	BA	2547	A	N7-C8-N9	-10.68	108.46	113.80
22	BA	44	A	N3-C4-C5	-10.68	119.33	126.80
22	BA	472	A	N7-C8-N9	-10.68	108.46	113.80
22	BA	1275	A	C5-C6-N6	10.67	132.24	123.70
22	BA	391	A	N3-C4-C5	-10.67	119.33	126.80
22	BA	384	A	N7-C8-N9	-10.67	108.47	113.80
22	BA	176	A	N3-C4-C5	-10.67	119.33	126.80
22	BA	1469	A	N3-C4-C5	-10.67	119.33	126.80
22	BA	330	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	1650	A	N7-C8-N9	-10.66	108.47	113.80
22	BA	1952	A	N7-C8-N9	-10.66	108.47	113.80
55	D3	26	A	N3-C4-C5	-10.66	119.33	126.80
22	BA	752	A	N3-C4-C5	-10.66	119.34	126.80
22	BA	1876	A	N3-C4-C5	-10.66	119.34	126.80
22	BA	2267	A	N3-C4-C5	-10.66	119.34	126.80
22	BA	626	A	C5-C6-N6	10.66	132.22	123.70
22	BA	1998	A	N3-C4-C5	-10.66	119.34	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1590	A	N3-C4-C5	-10.65	119.34	126.80
22	BA	1085	A	C5-C6-N6	10.65	132.22	123.70
22	BA	1302	A	C5-C6-N6	10.65	132.22	123.70
22	BA	2392	A	C5-C6-N6	10.65	132.22	123.70
22	BA	975	A	N3-C4-C5	-10.65	119.35	126.80
22	BA	1772	A	N7-C8-N9	-10.65	108.48	113.80
22	BA	1544	A	N3-C4-C5	-10.65	119.35	126.80
22	BA	1900	A	N7-C8-N9	-10.65	108.48	113.80
22	BA	2097	A	N3-C4-C5	-10.65	119.35	126.80
22	BA	2450	A	N7-C8-N9	-10.65	108.48	113.80
22	BA	2734	A	C5-C6-N6	10.64	132.22	123.70
22	BA	727	A	N7-C8-N9	-10.64	108.48	113.80
22	BA	2082	A	N3-C4-C5	-10.64	119.35	126.80
22	BA	1307	A	N7-C8-N9	-10.64	108.48	113.80
22	BA	1354	A	C5-C6-N6	10.64	132.21	123.70
22	BA	1654	A	N7-C8-N9	-10.64	108.48	113.80
22	BA	2327	A	N3-C4-C5	-10.64	119.35	126.80
22	BA	1635	A	C5-C6-N6	10.64	132.21	123.70
22	BA	203	A	C5-C6-N6	10.63	132.21	123.70
22	BA	1877	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	104	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	1301	A	C5-C6-N6	10.63	132.21	123.70
22	BA	1262	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	1307	A	N3-C4-C5	-10.63	119.36	126.80
22	BA	1757	A	N7-C8-N9	-10.63	108.48	113.80
22	BA	1978	A	N7-C8-N9	-10.63	108.49	113.80
22	BA	216	A	N3-C4-C5	-10.62	119.36	126.80
22	BA	1098	A	N3-C4-C5	-10.62	119.36	126.80
22	BA	2052	A	N3-C4-C5	-10.62	119.36	126.80
22	BA	739	A	N3-C4-C5	-10.62	119.36	126.80
22	BA	2171	A	C5-C6-N6	10.62	132.20	123.70
22	BA	2513	A	N7-C8-N9	-10.62	108.49	113.80
22	BA	2679	A	N3-C4-C5	-10.62	119.37	126.80
22	BA	1789	A	N7-C8-N9	-10.61	108.49	113.80
22	BA	514	A	N7-C8-N9	-10.61	108.49	113.80
22	BA	1586	A	N7-C8-N9	-10.61	108.49	113.80
22	BA	1876	A	C5-C6-N6	10.61	132.19	123.70
22	BA	972	A	C5-C6-N6	10.61	132.19	123.70
22	BA	2757	A	C5-C6-N6	10.61	132.19	123.70
22	BA	2850	A	C5-C6-N6	10.61	132.19	123.70
23	BB	34	A	N3-C4-C5	-10.61	119.37	126.80
22	BA	730	A	N3-C4-C5	-10.61	119.38	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1872	A	N3-C4-C5	-10.61	119.38	126.80
22	BA	2059	A	N7-C8-N9	-10.61	108.50	113.80
22	BA	2459	A	N3-C4-C5	-10.61	119.38	126.80
22	BA	256	A	C5-C6-N6	10.60	132.18	123.70
22	BA	2518	A	C5-C6-N6	10.60	132.18	123.70
22	BA	793	A	N3-C4-C5	-10.60	119.38	126.80
22	BA	1009	A	C5-C6-N6	10.60	132.18	123.70
22	BA	2013	A	C5-C6-N6	10.60	132.18	123.70
22	BA	2191	A	N3-C4-C5	-10.60	119.38	126.80
55	D3	26	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1431	A	N3-C4-C5	-10.60	119.38	126.80
22	BA	262	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	920	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	1871	A	C5-C6-N6	10.60	132.18	123.70
22	BA	936	A	N3-C4-C5	-10.60	119.38	126.80
22	BA	1637	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	64	A	N3-C4-C5	-10.60	119.38	126.80
22	BA	368	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	613	A	C5-C6-N6	10.60	132.18	123.70
22	BA	1745	A	N7-C8-N9	-10.60	108.50	113.80
22	BA	1853	A	C5-C6-N6	10.60	132.18	123.70
22	BA	532	A	N7-C8-N9	-10.59	108.50	113.80
22	BA	503	A	C5-C6-N6	10.59	132.17	123.70
22	BA	1739	A	N3-C4-C5	-10.59	119.39	126.80
22	BA	2679	A	N7-C8-N9	-10.59	108.50	113.80
23	BB	15	A	C5-C6-N6	10.59	132.17	123.70
22	BA	2879	A	N3-C4-C5	-10.59	119.39	126.80
22	BA	1759	A	N3-C4-C5	-10.59	119.39	126.80
22	BA	2799	A	N7-C8-N9	-10.59	108.51	113.80
22	BA	918	A	C5-C6-N6	10.58	132.16	123.70
22	BA	2531	A	C5-C6-N6	10.58	132.16	123.70
22	BA	2358	A	C5-C6-N6	10.58	132.16	123.70
22	BA	2851	A	N3-C4-C5	-10.58	119.39	126.80
22	BA	1809	A	C5-C6-N6	10.58	132.16	123.70
22	BA	739	A	N7-C8-N9	-10.57	108.51	113.80
22	BA	2856	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	2721	A	N7-C8-N9	-10.57	108.51	113.80
22	BA	428	A	C5-C6-N6	10.57	132.16	123.70
22	BA	1848	A	C5-C6-N6	10.57	132.16	123.70
22	BA	217	A	N7-C8-N9	-10.57	108.52	113.80
22	BA	981	A	N7-C8-N9	-10.57	108.52	113.80
22	BA	1545	A	C5-C6-N6	10.57	132.16	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2352	A	N7-C8-N9	-10.57	108.52	113.80
22	BA	160	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	439	A	N3-C4-C5	-10.57	119.40	126.80
22	BA	716	A	C5-C6-N6	10.56	132.15	123.70
22	BA	2872	A	C5-C6-N6	10.56	132.15	123.70
22	BA	1544	A	N7-C8-N9	-10.56	108.52	113.80
22	BA	2090	A	N3-C4-C5	-10.56	119.41	126.80
22	BA	2247	A	N3-C4-C5	-10.56	119.41	126.80
22	BA	609	A	N7-C8-N9	-10.55	108.52	113.80
22	BA	990	A	C5-C6-N6	10.55	132.14	123.70
22	BA	1700	A	C5-C6-N6	10.56	132.15	123.70
22	BA	1535	A	N3-C4-C5	-10.55	119.41	126.80
22	BA	1690	A	N7-C8-N9	-10.55	108.52	113.80
22	BA	5	A	N3-C4-C5	-10.55	119.42	126.80
22	BA	2736	A	N3-C4-C5	-10.55	119.41	126.80
22	BA	2327	A	N7-C8-N9	-10.55	108.53	113.80
22	BA	705	A	N7-C8-N9	-10.54	108.53	113.80
22	BA	1156	A	C5-C6-N6	10.55	132.14	123.70
22	BA	1805	A	N3-C4-C5	-10.54	119.42	126.80
22	BA	1932	A	N7-C8-N9	-10.54	108.53	113.80
22	BA	735	A	N3-C4-C5	-10.54	119.42	126.80
22	BA	1077	A	C5-C6-N6	10.54	132.13	123.70
22	BA	1354	A	N3-C4-C5	-10.54	119.42	126.80
22	BA	1553	A	N3-C4-C5	-10.54	119.42	126.80
22	BA	1690	A	C5-C6-N6	10.54	132.13	123.70
22	BA	2433	A	N7-C8-N9	-10.54	108.53	113.80
22	BA	2434	A	N7-C8-N9	-10.54	108.53	113.80
22	BA	1591	A	N3-C4-C5	-10.54	119.42	126.80
23	BB	59	A	C5-C6-N6	10.54	132.13	123.70
22	BA	2376	A	C5-C6-N6	10.54	132.13	123.70
22	BA	761	A	C5-C6-N6	10.54	132.13	123.70
22	BA	1626	A	N7-C8-N9	-10.53	108.54	113.80
22	BA	2278	A	N7-C8-N9	-10.53	108.53	113.80
22	BA	2378	A	N7-C8-N9	-10.53	108.54	113.80
22	BA	2814	A	N7-C8-N9	-10.53	108.54	113.80
22	BA	104	A	C5-C6-N6	10.52	132.12	123.70
22	BA	74	A	N3-C4-C5	-10.52	119.44	126.80
22	BA	514	A	N3-C4-C5	-10.52	119.43	126.80
22	BA	1067	A	N7-C8-N9	-10.52	108.54	113.80
55	D3	64	A	N7-C8-N9	-10.52	108.54	113.80
22	BA	792	A	C5-C6-N6	10.52	132.12	123.70
22	BA	1936	A	C5-C6-N6	10.52	132.12	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	804	A	C5-C6-N6	10.52	132.11	123.70
22	BA	126	A	N3-C4-C5	-10.51	119.44	126.80
22	BA	167	A	C5-C6-N6	10.51	132.11	123.70
22	BA	279	A	N7-C8-N9	-10.51	108.54	113.80
22	BA	643	A	N7-C8-N9	-10.51	108.54	113.80
22	BA	910	A	N3-C4-C5	-10.51	119.44	126.80
22	BA	1353	A	C5-C6-N6	10.51	132.11	123.70
22	BA	2317	A	N3-C4-C5	-10.51	119.44	126.80
22	BA	2516	A	N3-C4-C5	-10.51	119.44	126.80
22	BA	2810	A	N7-C8-N9	-10.51	108.54	113.80
55	D3	73	A	C5-C6-N6	10.51	132.11	123.70
22	BA	478	A	N7-C8-N9	-10.51	108.55	113.80
22	BA	152	A	N3-C4-C5	-10.51	119.44	126.80
22	BA	522	A	N7-C8-N9	-10.51	108.55	113.80
22	BA	1434	A	N3-C4-C5	-10.51	119.45	126.80
22	BA	191	A	N3-C4-C5	-10.50	119.45	126.80
22	BA	1086	A	C5-C6-N6	10.50	132.10	123.70
22	BA	1821	A	N7-C8-N9	-10.50	108.55	113.80
22	BA	213	A	C5-C6-N6	10.50	132.10	123.70
22	BA	1276	A	N3-C4-C5	-10.50	119.45	126.80
22	BA	1469	A	N7-C8-N9	-10.50	108.55	113.80
22	BA	1496	A	N7-C8-N9	-10.50	108.55	113.80
22	BA	191	A	C5-C6-N6	10.50	132.10	123.70
22	BA	1010	A	C5-C6-N6	10.50	132.10	123.70
22	BA	53	A	N7-C8-N9	-10.50	108.55	113.80
22	BA	1175	A	N3-C4-C5	-10.50	119.45	126.80
22	BA	1805	A	C5-C6-N6	10.50	132.10	123.70
22	BA	2432	A	N7-C8-N9	-10.50	108.55	113.80
22	BA	643	A	C5-C6-N6	10.49	132.09	123.70
22	BA	877	A	C5-C6-N6	10.49	132.10	123.70
22	BA	1028	A	N7-C8-N9	-10.49	108.55	113.80
22	BA	2163	A	N7-C8-N9	-10.49	108.55	113.80
22	BA	2335	A	N3-C4-C5	-10.49	119.45	126.80
23	BB	94	A	N7-C8-N9	-10.49	108.55	113.80
22	BA	146	A	N7-C8-N9	-10.49	108.56	113.80
22	BA	1226	A	C5-C6-N6	10.49	132.09	123.70
22	BA	1490	A	C5-C6-N6	10.49	132.09	123.70
22	BA	1789	A	C5-C6-N6	10.49	132.09	123.70
22	BA	2675	A	N3-C4-C5	-10.49	119.46	126.80
54	D2	69	A	N3-C4-C5	-10.49	119.46	126.80
22	BA	743	A	N7-C8-N9	-10.49	108.56	113.80
22	BA	1039	A	C5-C6-N6	10.49	132.09	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D2	23	A	N3-C4-C5	-10.49	119.46	126.80
22	BA	2199	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	2425	A	C5-C6-N6	10.48	132.09	123.70
54	D2	26	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	722	A	N7-C8-N9	-10.48	108.56	113.80
22	BA	911	A	C5-C6-N6	10.48	132.09	123.70
22	BA	478	A	C5-C6-N6	10.48	132.08	123.70
22	BA	845	A	N3-C4-C5	-10.48	119.46	126.80
22	BA	1877	A	C5-C6-N6	10.48	132.09	123.70
22	BA	900	A	N3-C4-C5	-10.48	119.47	126.80
22	BA	1336	A	N3-C4-C5	-10.48	119.47	126.80
22	BA	56	A	N3-C4-C5	-10.47	119.47	126.80
22	BA	1156	A	N3-C4-C5	-10.47	119.47	126.80
22	BA	1938	A	N3-C4-C5	-10.47	119.47	126.80
22	BA	2453	A	C5-C6-N6	10.47	132.08	123.70
22	BA	721	A	N3-C4-C5	-10.47	119.47	126.80
22	BA	226	A	C5-C6-N6	10.47	132.07	123.70
22	BA	2721	A	N3-C4-C5	-10.47	119.47	126.80
22	BA	1762	A	N3-C4-C5	-10.47	119.47	126.80
22	BA	644	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	782	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	945	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	149	A	N7-C8-N9	-10.46	108.57	113.80
22	BA	1265	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	1029	A	C5-C6-N6	10.46	132.07	123.70
55	D3	36	A	C5-C6-N6	10.46	132.07	123.70
22	BA	299	A	N3-C4-C5	-10.46	119.48	126.80
22	BA	609	A	N3-C4-C5	-10.45	119.48	126.80
22	BA	1433	A	N3-C4-C5	-10.45	119.48	126.80
22	BA	1847	A	C5-C6-N6	10.45	132.06	123.70
22	BA	1854	A	N7-C8-N9	-10.45	108.57	113.80
22	BA	447	A	N3-C4-C5	-10.45	119.48	126.80
22	BA	572	A	N3-C4-C5	-10.45	119.48	126.80
22	BA	1126	A	N3-C4-C5	-10.45	119.49	126.80
22	BA	2534	A	C5-C6-N6	10.45	132.06	123.70
22	BA	2749	A	N7-C8-N9	-10.45	108.58	113.80
23	BB	101	A	C5-C6-N6	10.45	132.06	123.70
22	BA	666	A	N3-C4-C5	-10.44	119.49	126.80
22	BA	1009	A	N3-C4-C5	-10.44	119.49	126.80
22	BA	975	A	N7-C8-N9	-10.44	108.58	113.80
22	BA	1569	A	C5-C6-N6	10.44	132.05	123.70
22	BA	1470	A	N3-C4-C5	-10.44	119.49	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1735	A	N3-C4-C5	-10.44	119.49	126.80
54	D2	51	A	C5-C6-N6	10.44	132.05	123.70
54	D2	51	A	N7-C8-N9	-10.44	108.58	113.80
22	BA	63	A	C5-C6-N6	10.44	132.05	123.70
22	BA	933	A	N7-C8-N9	-10.44	108.58	113.80
22	BA	1532	A	N3-C4-C5	-10.44	119.50	126.80
22	BA	2082	A	N7-C8-N9	-10.44	108.58	113.80
22	BA	207	A	C5-C6-N6	10.43	132.05	123.70
22	BA	528	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	1010	A	N7-C8-N9	-10.43	108.58	113.80
22	BA	715	A	C5-C6-N6	10.43	132.04	123.70
22	BA	1593	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	819	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	1260	A	N3-C4-C5	-10.43	119.50	126.80
22	BA	255	A	C5-C6-N6	10.43	132.04	123.70
22	BA	1308	A	C5-C6-N6	10.42	132.04	123.70
22	BA	1321	A	N7-C8-N9	-10.42	108.59	113.80
23	BB	57	A	N3-C4-C5	-10.42	119.51	126.80
22	BA	1264	A	C5-C6-N6	10.42	132.03	123.70
22	BA	1373	A	N3-C4-C5	-10.42	119.51	126.80
22	BA	19	A	N3-C4-C5	-10.41	119.51	126.80
22	BA	492	A	N3-C4-C5	-10.41	119.51	126.80
22	BA	1241	A	N7-C8-N9	-10.41	108.59	113.80
22	BA	1713	A	C5-C6-N6	10.41	132.03	123.70
22	BA	2184	A	N7-C8-N9	-10.41	108.59	113.80
22	BA	2225	A	C5-C6-N6	10.41	132.03	123.70
16	AP	48	GLU	CB-CA-C	-10.41	89.59	110.40
22	BA	947	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	1970	A	N3-C4-C5	-10.40	119.52	126.80
54	D2	31	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	74	A	C5-C6-N6	10.40	132.02	123.70
22	BA	592	A	N7-C8-N9	-10.40	108.60	113.80
22	BA	670	A	C5-C6-N6	10.40	132.02	123.70
22	BA	1029	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	1598	A	N7-C8-N9	-10.40	108.60	113.80
22	BA	2433	A	N3-C4-C5	-10.40	119.52	126.80
22	BA	2765	A	N7-C8-N9	-10.40	108.60	113.80
22	BA	2037	A	N7-C8-N9	-10.40	108.60	113.80
22	BA	2868	A	N3-C4-C5	-10.39	119.52	126.80
22	BA	470	A	C5-C6-N6	10.39	132.01	123.70
22	BA	480	A	N7-C8-N9	-10.39	108.60	113.80
22	BA	2101	A	C5-C6-N6	10.39	132.01	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	492	A	N7-C8-N9	-10.39	108.61	113.80
22	BA	2587	A	N3-C4-C5	-10.39	119.53	126.80
22	BA	2809	A	N7-C8-N9	-10.39	108.60	113.80
23	BB	29	A	N3-C4-C5	-10.39	119.53	126.80
22	BA	1801	A	C5-C6-N6	10.39	132.01	123.70
22	BA	2071	A	N3-C4-C5	-10.39	119.53	126.80
55	D3	31	A	N7-C8-N9	-10.39	108.61	113.80
22	BA	144	A	N3-C4-C5	-10.38	119.53	126.80
22	BA	2322	A	C5-C6-N6	10.38	132.01	123.70
22	BA	2015	A	C5-C6-N6	10.38	132.01	123.70
22	BA	2814	A	C5-C6-N6	10.38	132.00	123.70
22	BA	449	A	C5-C6-N6	10.38	132.00	123.70
22	BA	480	A	C5-C6-N6	10.38	132.00	123.70
22	BA	1787	A	N7-C8-N9	-10.38	108.61	113.80
22	BA	2088	A	N3-C4-C5	-10.38	119.53	126.80
22	BA	222	A	C5-C6-N6	10.38	132.00	123.70
22	BA	1327	A	C5-C6-N6	10.38	132.00	123.70
22	BA	2412	A	N3-C4-C5	-10.38	119.54	126.80
22	BA	1755	A	N7-C8-N9	-10.37	108.61	113.80
22	BA	2013	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	21	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	320	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	2059	A	C5-C6-N6	10.37	132.00	123.70
22	BA	2670	A	N3-C4-C5	-10.37	119.54	126.80
22	BA	504	A	C5-C6-N6	10.37	131.99	123.70
22	BA	819	A	C5-C6-N6	10.37	131.99	123.70
22	BA	391	A	C5-C6-N6	10.36	131.99	123.70
22	BA	513	A	N3-C4-C5	-10.36	119.55	126.80
22	BA	2273	A	N7-C8-N9	-10.36	108.62	113.80
22	BA	2366	A	C5-C6-N6	10.36	131.99	123.70
22	BA	2761	A	N3-C4-C5	-10.36	119.55	126.80
22	BA	1677	A	N7-C8-N9	-10.36	108.62	113.80
22	BA	572	A	C5-C6-N6	10.36	131.99	123.70
22	BA	1637	A	N3-C4-C5	-10.36	119.55	126.80
22	BA	508	A	C5-C6-N6	10.36	131.99	123.70
22	BA	943	A	N3-C4-C5	-10.36	119.55	126.80
22	BA	477	A	C5-C6-N6	10.35	131.98	123.70
22	BA	1088	A	N7-C8-N9	-10.35	108.62	113.80
22	BA	1664	A	N3-C4-C5	-10.35	119.55	126.80
22	BA	2541	A	N3-C4-C5	-10.35	119.55	126.80
22	BA	374	A	C5-C6-N6	10.35	131.98	123.70
22	BA	1591	A	N7-C8-N9	-10.35	108.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1477	A	C5-C6-N6	10.35	131.98	123.70
22	BA	1754	A	N7-C8-N9	-10.35	108.62	113.80
22	BA	1241	A	C5-C6-N6	10.35	131.98	123.70
22	BA	1571	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	429	A	C5-C6-N6	10.34	131.97	123.70
22	BA	990	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	1134	A	C5-C6-N6	10.34	131.97	123.70
22	BA	1819	A	N3-C4-C5	-10.34	119.56	126.80
22	BA	2476	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	2425	A	N7-C8-N9	-10.34	108.63	113.80
22	BA	2820	A	C5-C6-N6	10.34	131.97	123.70
22	BA	2212	A	N3-C4-C5	-10.33	119.57	126.80
22	BA	633	A	C5-C6-N6	10.33	131.97	123.70
22	BA	1040	A	C5-C6-N6	10.33	131.97	123.70
55	D3	58	A	N7-C8-N9	-10.33	108.64	113.80
22	BA	722	A	N3-C4-C5	-10.32	119.57	126.80
22	BA	849	A	N3-C4-C5	-10.32	119.57	126.80
22	BA	960	A	N3-C4-C5	-10.32	119.57	126.80
22	BA	1413	A	N3-C4-C5	-10.32	119.57	126.80
22	BA	1103	A	N7-C8-N9	-10.32	108.64	113.80
22	BA	2700	A	N3-C4-C5	-10.32	119.57	126.80
22	BA	196	A	N3-C4-C5	-10.32	119.57	126.80
22	BA	609	A	C5-C6-N6	10.32	131.96	123.70
22	BA	793	A	N7-C8-N9	-10.32	108.64	113.80
22	BA	1028	A	C5-C6-N6	10.32	131.96	123.70
22	BA	2778	A	C5-C6-N6	10.32	131.96	123.70
22	BA	861	A	N3-C4-C5	-10.32	119.58	126.80
22	BA	2418	A	N3-C4-C5	-10.32	119.58	126.80
22	BA	2439	A	C5-C6-N6	10.32	131.95	123.70
22	BA	6	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	91	A	C5-C6-N6	10.31	131.95	123.70
22	BA	430	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	996	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	590	A	N7-C8-N9	-10.31	108.65	113.80
22	BA	1927	A	C5-C6-N6	10.31	131.95	123.70
22	BA	2241	A	N3-C4-C5	-10.31	119.58	126.80
22	BA	705	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	541	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	1786	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	2126	A	N3-C4-C5	-10.30	119.59	126.80
22	BA	1928	A	N7-C8-N9	-10.30	108.65	113.80
22	BA	1373	A	C5-C6-N6	10.30	131.94	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	482	A	C5-C6-N6	10.30	131.94	123.70
22	BA	2726	A	C5-C6-N6	10.30	131.94	123.70
22	BA	479	A	C5-C6-N6	10.29	131.93	123.70
22	BA	920	A	C5-C6-N6	10.29	131.93	123.70
22	BA	1050	A	N3-C4-C5	-10.29	119.60	126.80
22	BA	2577	A	N3-C4-C5	-10.29	119.60	126.80
22	BA	2577	A	N7-C8-N9	-10.29	108.66	113.80
22	BA	866	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	1014	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	1977	A	C5-C6-N6	10.28	131.93	123.70
22	BA	89	A	C5-C6-N6	10.28	131.92	123.70
22	BA	582	A	N7-C8-N9	-10.28	108.66	113.80
22	BA	670	A	N3-C4-C5	-10.28	119.61	126.80
22	BA	980	A	N3-C4-C5	-10.28	119.60	126.80
22	BA	1603	A	N7-C8-N9	-10.28	108.66	113.80
22	BA	1899	A	C5-C6-N6	10.28	131.92	123.70
22	BA	447	A	C5-C6-N6	10.28	131.92	123.70
22	BA	1952	A	N3-C4-C5	-10.28	119.61	126.80
22	BA	2031	A	N3-C4-C5	-10.28	119.61	126.80
22	BA	2198	A	C5-C6-N6	10.28	131.92	123.70
22	BA	1213	A	N7-C8-N9	-10.27	108.66	113.80
22	BA	2134	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	752	A	C5-C6-N6	10.27	131.91	123.70
22	BA	1650	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	2468	A	C5-C6-N6	10.27	131.91	123.70
22	BA	2635	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	2426	A	C5-C6-N6	10.27	131.91	123.70
22	BA	899	A	N3-C4-C5	-10.27	119.61	126.80
22	BA	2868	A	C5-C6-N6	10.27	131.91	123.70
22	BA	49	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	927	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	2094	A	N3-C4-C5	-10.26	119.61	126.80
22	BA	1189	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	2335	A	C5-C6-N6	10.26	131.91	123.70
55	D3	36	A	N7-C8-N9	-10.26	108.67	113.80
22	BA	256	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	1597	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	1889	A	C5-C6-N6	10.26	131.91	123.70
22	BA	2227	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	182	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	505	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	2014	A	N3-C4-C5	-10.26	119.62	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	146	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	167	A	N3-C4-C5	-10.26	119.62	126.80
22	BA	195	A	C5-C6-N6	10.26	131.90	123.70
23	BB	46	A	N3-C4-C5	-10.25	119.62	126.80
22	BA	556	A	N3-C4-C5	-10.25	119.62	126.80
22	BA	181	A	N3-C4-C5	-10.25	119.62	126.80
22	BA	1308	A	N3-C4-C5	-10.25	119.62	126.80
54	D2	26	A	C5-C6-N6	10.25	131.90	123.70
22	BA	1551	A	N3-C4-C5	-10.25	119.63	126.80
22	BA	2082	A	C5-C6-N6	10.25	131.90	123.70
22	BA	2778	A	N3-C4-C5	-10.25	119.63	126.80
22	BA	2810	A	N3-C4-C5	-10.25	119.63	126.80
55	D3	14	A	C5-C6-N6	10.25	131.90	123.70
22	BA	2376	A	N3-C4-C5	-10.24	119.63	126.80
22	BA	943	A	C5-C6-N6	10.24	131.89	123.70
22	BA	1080	A	N3-C4-C5	-10.24	119.63	126.80
23	BB	104	A	C5-C6-N6	10.24	131.89	123.70
22	BA	2205	A	N3-C4-C5	-10.24	119.63	126.80
22	BA	2377	A	N7-C8-N9	-10.24	108.68	113.80
22	BA	2497	A	N7-C8-N9	-10.24	108.68	113.80
22	BA	1640	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	1134	A	N3-C4-C5	-10.23	119.64	126.80
23	BB	66	A	N7-C8-N9	-10.23	108.68	113.80
22	BA	1085	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	2478	A	N3-C4-C5	-10.23	119.64	126.80
22	BA	272	A	N3-C4-C5	-10.22	119.64	126.80
22	BA	730	A	N7-C8-N9	-10.22	108.69	113.80
22	BA	2108	A	N3-C4-C5	-10.22	119.64	126.80
22	BA	470	A	N3-C4-C5	-10.22	119.65	126.80
22	BA	1495	A	N7-C8-N9	-10.22	108.69	113.80
22	BA	1730	C	N1-C2-O2	10.22	125.03	118.90
22	BA	1027	A	C5-C6-N6	10.22	131.88	123.70
22	BA	152	A	N7-C8-N9	-10.22	108.69	113.80
22	BA	1676	A	C5-C6-N6	10.22	131.88	123.70
22	BA	1717	A	N3-C4-C5	-10.22	119.65	126.80
22	BA	1705	A	N3-C4-C5	-10.22	119.65	126.80
22	BA	207	A	N7-C8-N9	-10.21	108.69	113.80
22	BA	1287	A	N3-C4-C5	-10.21	119.65	126.80
54	D2	51	A	N3-C4-C5	-10.21	119.65	126.80
55	D3	31	A	C5-C6-N6	10.21	131.87	123.70
22	BA	1328	A	N7-C8-N9	-10.21	108.70	113.80
22	BA	2886	A	N3-C4-C5	-10.21	119.66	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1669	A	C5-C6-N6	10.20	131.86	123.70
22	BA	1392	A	N7-C8-N9	-10.20	108.70	113.80
22	BA	1151	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	1789	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	2837	A	N3-C4-C5	-10.20	119.66	126.80
22	BA	1677	A	N3-C4-C5	-10.19	119.67	126.80
22	BA	753	A	N7-C8-N9	-10.19	108.70	113.80
22	BA	925	A	N3-C4-C5	-10.19	119.67	126.80
22	BA	1829	A	N7-C8-N9	-10.19	108.70	113.80
22	BA	142	A	N3-C4-C5	-10.19	119.67	126.80
22	BA	941	A	C5-C6-N6	10.19	131.85	123.70
22	BA	1069	A	N3-C4-C5	-10.19	119.67	126.80
22	BA	1655	A	N3-C4-C5	-10.19	119.67	126.80
54	D2	5	A	N3-C4-C5	-10.19	119.67	126.80
54	D2	49	A	N3-C4-C5	-10.19	119.67	126.80
22	BA	1144	A	N3-C4-C5	-10.19	119.67	126.80
23	BB	45	A	N3-C4-C5	-10.19	119.67	126.80
22	BA	432	A	N3-C4-C5	-10.18	119.67	126.80
22	BA	592	A	C5-C6-N6	10.18	131.85	123.70
22	BA	792	A	N3-C4-C5	-10.18	119.67	126.80
22	BA	1808	A	C5-C6-N6	10.18	131.84	123.70
22	BA	1433	A	N7-C8-N9	-10.18	108.71	113.80
22	BA	1528	A	N7-C8-N9	-10.18	108.71	113.80
22	BA	1821	A	C5-C6-N6	10.18	131.84	123.70
22	BA	716	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	1354	A	N7-C8-N9	-10.17	108.71	113.80
22	BA	1679	A	N3-C4-C5	-10.17	119.68	126.80
22	BA	2453	A	N7-C8-N9	-10.17	108.72	113.80
22	BA	156	A	N7-C8-N9	-10.16	108.72	113.80
22	BA	483	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	2270	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	2614	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	633	A	N3-C4-C5	-10.16	119.69	126.80
22	BA	959	A	N3-C4-C5	-10.15	119.69	126.80
22	BA	1677	A	C5-C6-N6	10.15	131.82	123.70
22	BA	1772	A	N3-C4-C5	-10.15	119.69	126.80
22	BA	2352	A	C5-C6-N6	10.15	131.82	123.70
22	BA	1866	A	N3-C4-C5	-10.15	119.69	126.80
22	BA	1889	A	N3-C4-C5	-10.15	119.69	126.80
22	BA	422	A	N7-C8-N9	-10.15	108.73	113.80
22	BA	616	A	N3-C4-C5	-10.15	119.70	126.80
22	BA	1969	A	C5-C6-N6	10.15	131.82	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2823	A	N3-C4-C5	-10.15	119.70	126.80
22	BA	346	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	362	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	789	A	N3-C4-C5	-10.14	119.70	126.80
54	D2	41	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	1877	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	1098	A	C5-C6-N6	10.14	131.81	123.70
22	BA	1787	A	C5-C6-N6	10.14	131.81	123.70
22	BA	2813	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	231	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	1010	A	N3-C4-C5	-10.14	119.70	126.80
22	BA	1347	A	C5-C6-N6	10.14	131.81	123.70
22	BA	927	A	C5-C6-N6	10.13	131.81	123.70
22	BA	1784	A	C5-C6-N6	10.13	131.81	123.70
22	BA	2071	A	N7-C8-N9	-10.13	108.73	113.80
22	BA	2899	A	N7-C8-N9	-10.13	108.73	113.80
22	BA	466	A	C5-C6-N6	10.13	131.81	123.70
22	BA	1635	A	N3-C4-C5	-10.13	119.71	126.80
22	BA	2497	A	N3-C4-C5	-10.13	119.71	126.80
22	BA	2114	A	N7-C8-N9	-10.13	108.74	113.80
23	BB	46	A	N7-C8-N9	-10.13	108.74	113.80
22	BA	572	A	N7-C8-N9	-10.12	108.74	113.80
22	BA	1385	A	C5-C6-N6	10.12	131.80	123.70
22	BA	1477	A	N3-C4-C5	-10.12	119.71	126.80
22	BA	2199	A	N3-C4-C5	-10.13	119.71	126.80
22	BA	2266	A	N3-C4-C5	-10.12	119.71	126.80
22	BA	2547	A	C5-C6-N6	10.12	131.80	123.70
22	BA	2564	A	N3-C4-C5	-10.12	119.72	126.80
22	BA	2080	A	N7-C8-N9	-10.12	108.74	113.80
22	BA	255	A	N3-C4-C5	-10.12	119.72	126.80
22	BA	1505	A	N3-C4-C5	-10.12	119.72	126.80
22	BA	1672	A	C5-C6-N6	10.12	131.79	123.70
22	BA	1156	A	N7-C8-N9	-10.12	108.74	113.80
22	BA	2426	A	N7-C8-N9	-10.12	108.74	113.80
23	BB	115	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	2020	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	1366	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	2598	A	N7-C8-N9	-10.11	108.74	113.80
22	BA	2757	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	1194	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	42	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	1084	A	N3-C4-C5	-10.11	119.72	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	863	A	N3-C4-C5	-10.11	119.72	126.80
22	BA	13	A	N7-C8-N9	-10.11	108.75	113.80
22	BA	460	A	N3-C4-C5	-10.11	119.73	126.80
22	BA	1690	A	N3-C4-C5	-10.11	119.73	126.80
22	BA	918	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	1918	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	675	A	C5-C6-N6	10.10	131.78	123.70
22	BA	2482	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	1014	A	C5-C6-N6	10.10	131.78	123.70
22	BA	1095	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	1439	A	N3-C4-C5	-10.10	119.73	126.80
22	BA	749	A	N3-C4-C5	-10.09	119.73	126.80
22	BA	750	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	2135	A	N3-C4-C5	-10.09	119.73	126.80
22	BA	2247	A	N7-C8-N9	-10.09	108.75	113.80
22	BA	1586	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	2425	A	N3-C4-C5	-10.09	119.74	126.80
22	BA	251	A	C5-C6-N6	10.09	131.77	123.70
22	BA	218	A	N7-C8-N9	-10.09	108.76	113.80
22	BA	1717	A	C5-C6-N6	10.09	131.77	123.70
22	BA	300	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	654	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	1067	A	N3-C4-C5	-10.08	119.74	126.80
22	BA	1919	A	N7-C8-N9	-10.08	108.76	113.80
22	BA	2412	A	C5-C6-N6	10.08	131.77	123.70
22	BA	2757	A	N7-C8-N9	-10.08	108.76	113.80
22	BA	1086	A	N7-C8-N9	-10.08	108.76	113.80
22	BA	1194	A	C5-C6-N6	10.08	131.76	123.70
22	BA	2900	A	N3-C4-C5	-10.08	119.75	126.80
55	D3	58	A	N3-C4-C5	-10.08	119.75	126.80
55	D3	23	A	C5-C6-N6	10.07	131.76	123.70
22	BA	172	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	2781	A	N7-C8-N9	-10.07	108.76	113.80
22	BA	2513	A	C5-C6-N6	10.07	131.75	123.70
22	BA	2565	A	N3-C4-C5	-10.07	119.75	126.80
22	BA	1749	A	N3-C4-C5	-10.06	119.76	126.80
54	D2	59	A	N3-C4-C5	-10.06	119.75	126.80
22	BA	207	A	N3-C4-C5	-10.06	119.76	126.80
22	BA	2706	A	N7-C8-N9	-10.06	108.77	113.80
22	BA	781	A	N7-C8-N9	-10.06	108.77	113.80
22	BA	1784	A	N3-C4-C5	-10.06	119.76	126.80
22	BA	2453	A	N3-C4-C5	-10.05	119.76	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	371	A	N3-C4-C5	-10.05	119.77	126.80
22	BA	1885	A	C5-C6-N6	10.05	131.74	123.70
22	BA	1966	A	N3-C4-C5	-10.05	119.77	126.80
22	BA	1021	A	C5-C6-N6	10.05	131.74	123.70
22	BA	2270	A	C5-C6-N6	10.05	131.74	123.70
22	BA	1246	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	2147	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	1268	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	2169	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	2392	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	743	A	N3-C4-C5	-10.04	119.77	126.80
22	BA	1322	A	N7-C8-N9	-10.04	108.78	113.80
22	BA	1722	A	C5-C6-N6	10.04	131.73	123.70
22	BA	2003	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	1571	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	2381	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	2899	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	1133	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	1029	A	N7-C8-N9	-10.03	108.79	113.80
22	BA	2530	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	2792	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	2879	A	C5-C6-N6	10.03	131.72	123.70
22	BA	1579	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	2309	A	N3-C4-C5	-10.03	119.78	126.80
22	BA	1848	A	N3-C4-C5	-10.02	119.78	126.80
23	BB	29	A	C5-C6-N6	10.02	131.72	123.70
22	BA	677	A	N3-C4-C5	-10.02	119.79	126.80
22	BA	1383	A	N3-C4-C5	-10.02	119.79	126.80
22	BA	1495	A	N3-C4-C5	-10.02	119.79	126.80
22	BA	556	A	C5-C6-N6	10.02	131.71	123.70
22	BA	911	A	N3-C4-C5	-10.01	119.79	126.80
22	BA	1165	A	C5-C6-N6	10.01	131.71	123.70
22	BA	1701	A	N3-C4-C5	-10.01	119.79	126.80
22	BA	1916	A	N3-C4-C5	-10.01	119.80	126.80
22	BA	602	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	820	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	1264	A	N7-C8-N9	-10.00	108.80	113.80
22	BA	1664	A	N7-C8-N9	-10.00	108.80	113.80
22	BA	14	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	1551	A	C5-C6-N6	10.00	131.70	123.70
22	BA	1597	A	C5-C6-N6	10.00	131.70	123.70
22	BA	1803	A	N7-C8-N9	-10.00	108.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1858	A	N3-C4-C5	-10.00	119.80	126.80
22	BA	449	A	N3-C4-C5	-9.99	119.80	126.80
22	BA	471	A	N3-C4-C5	-9.99	119.80	126.80
22	BA	478	A	N3-C4-C5	-9.99	119.81	126.80
23	BB	73	A	N7-C8-N9	-9.99	108.80	113.80
22	BA	1938	A	C5-C6-N6	9.99	131.69	123.70
22	BA	643	A	N3-C4-C5	-9.99	119.81	126.80
22	BA	802	A	C5-C6-N6	9.99	131.69	123.70
22	BA	1230	A	N3-C4-C5	-9.99	119.81	126.80
22	BA	1570	A	N3-C4-C5	-9.99	119.81	126.80
22	BA	219	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	1169	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	1490	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	1630	A	C5-C6-N6	9.98	131.69	123.70
22	BA	1918	A	N7-C8-N9	-9.98	108.81	113.80
22	BA	149	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	1420	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	1508	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	1096	A	N3-C4-C5	-9.98	119.82	126.80
22	BA	2142	A	N3-C4-C5	-9.98	119.81	126.80
22	BA	1427	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	28	A	C5-C6-N6	9.97	131.68	123.70
22	BA	279	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	502	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	504	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	1809	A	N7-C8-N9	-9.97	108.81	113.80
22	BA	2114	A	C5-C6-N6	9.97	131.68	123.70
22	BA	632	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	5	A	N7-C8-N9	-9.97	108.82	113.80
22	BA	401	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	718	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	1654	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	2434	A	N3-C4-C5	-9.97	119.82	126.80
22	BA	515	A	N3-C4-C5	-9.96	119.82	126.80
23	BB	115	A	C5-C6-N6	9.96	131.67	123.70
23	BB	58	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	101	A	N7-C8-N9	-9.96	108.82	113.80
22	BA	217	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	943	A	N7-C8-N9	-9.96	108.82	113.80
22	BA	1755	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	422	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	1819	A	C5-C6-N6	9.96	131.67	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2225	A	N3-C4-C5	-9.96	119.83	126.80
22	BA	715	A	N3-C4-C5	-9.95	119.83	126.80
22	BA	1608	A	C5-C6-N6	9.95	131.66	123.70
22	BA	1504	A	N3-C4-C5	-9.95	119.84	126.80
22	BA	1143	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	928	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	2682	A	C5-C6-N6	9.94	131.65	123.70
22	BA	515	A	C5-C6-N6	9.94	131.65	123.70
22	BA	429	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	1378	A	N3-C4-C5	-9.94	119.84	126.80
22	BA	482	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	2826	A	N3-C4-C5	-9.93	119.85	126.80
23	BB	15	A	N3-C4-C5	-9.93	119.85	126.80
23	BB	66	A	N3-C4-C5	-9.93	119.85	126.80
22	BA	28	A	N3-C4-C5	-9.92	119.85	126.80
22	BA	1433	A	C5-C6-N6	9.92	131.64	123.70
22	BA	2590	A	N3-C4-C5	-9.92	119.85	126.80
22	BA	825	A	C5-C6-N6	9.92	131.64	123.70
22	BA	979	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	1572	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	2531	A	N3-C4-C5	-9.92	119.86	126.80
22	BA	1276	A	C5-C6-N6	9.92	131.63	123.70
22	BA	1367	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	2158	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	2741	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	38	A	C5-C6-N6	9.91	131.63	123.70
22	BA	661	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	1304	A	C5-C6-N6	9.91	131.63	123.70
22	BA	2051	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	2814	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	203	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	1854	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	2547	A	N3-C4-C5	-9.91	119.86	126.80
22	BA	279	A	C5-C6-N6	9.90	131.62	123.70
22	BA	453	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	1809	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	300	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	1347	A	N3-C4-C5	-9.90	119.87	126.80
55	D3	37	A	N3-C4-C5	-9.90	119.87	126.80
22	BA	802	A	N7-C8-N9	-9.90	108.85	113.80
22	BA	2378	A	N3-C4-C5	-9.89	119.88	126.80
55	D3	35	A	N3-C4-C5	-9.89	119.88	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2516	A	N7-C8-N9	-9.89	108.86	113.80
22	BA	118	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	203	A	N7-C8-N9	-9.88	108.86	113.80
22	BA	2176	A	N3-C4-C5	-9.89	119.88	126.80
22	BA	756	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	2377	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	727	A	C5-C6-N6	9.88	131.61	123.70
22	BA	1494	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	2587	A	N7-C8-N9	-9.88	108.86	113.80
22	BA	794	A	N3-C4-C5	-9.88	119.88	126.80
22	BA	1866	A	C5-C6-N6	9.88	131.60	123.70
22	BA	226	A	N7-C8-N9	-9.88	108.86	113.80
22	BA	501	A	N3-C4-C5	-9.88	119.89	126.80
22	BA	878	A	N3-C4-C5	-9.88	119.89	126.80
22	BA	2753	A	N3-C4-C5	-9.88	119.89	126.80
22	BA	599	A	N3-C4-C5	-9.88	119.89	126.80
22	BA	2336	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	2632	A	C5-C6-N6	9.87	131.60	123.70
22	BA	2639	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	1502	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	2675	A	N7-C8-N9	-9.87	108.87	113.80
22	BA	751	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	2042	A	N3-C4-C5	-9.87	119.89	126.80
22	BA	631	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	1077	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	1226	A	N3-C4-C5	-9.86	119.90	126.80
22	BA	1791	A	C5-C6-N6	9.85	131.58	123.70
22	BA	1801	A	N3-C4-C5	-9.85	119.90	126.80
22	BA	2297	A	N3-C4-C5	-9.85	119.91	126.80
22	BA	348	A	N3-C4-C5	-9.85	119.91	126.80
23	BB	101	A	N3-C4-C5	-9.85	119.91	126.80
22	BA	342	A	N3-C4-C5	-9.84	119.91	126.80
22	BA	2821	A	N3-C4-C5	-9.84	119.91	126.80
55	D3	21	A	N3-C4-C5	-9.84	119.91	126.80
22	BA	95	A	N7-C8-N9	-9.84	108.88	113.80
22	BA	1614	A	C5-C6-N6	9.84	131.57	123.70
22	BA	94	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	173	A	N7-C8-N9	-9.83	108.88	113.80
22	BA	340	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	492	A	C5-C6-N6	9.83	131.56	123.70
22	BA	505	A	C5-C6-N6	9.83	131.57	123.70
22	BA	1689	A	N3-C4-C5	-9.83	119.92	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2887	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	1039	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	2278	A	N3-C4-C5	-9.83	119.92	126.80
22	BA	1274	A	N3-C4-C5	-9.82	119.92	126.80
22	BA	2435	A	N3-C4-C5	-9.82	119.92	126.80
22	BA	2749	A	N3-C4-C5	-9.82	119.92	126.80
22	BA	613	A	N7-C8-N9	-9.82	108.89	113.80
22	BA	1545	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	2062	A	C5-C6-N6	9.82	131.56	123.70
22	BA	2268	A	N3-C4-C5	-9.82	119.93	126.80
22	BA	911	A	N7-C8-N9	-9.82	108.89	113.80
22	BA	2587	A	C5-C6-N6	9.82	131.55	123.70
54	D2	14	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	428	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	477	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	1711	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	2632	A	N3-C4-C5	-9.81	119.94	126.80
22	BA	2829	A	N3-C4-C5	-9.81	119.93	126.80
22	BA	1470	A	N7-C8-N9	-9.81	108.90	113.80
22	BA	71	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	103	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	1496	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	2721	A	C5-C6-N6	9.80	131.54	123.70
54	D2	31	A	N7-C8-N9	-9.80	108.90	113.80
22	BA	2451	A	N3-C4-C5	-9.80	119.94	126.80
22	BA	590	A	N3-C4-C5	-9.79	119.94	126.80
22	BA	1866	A	N7-C8-N9	-9.79	108.91	113.80
22	BA	575	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	2564	A	N7-C8-N9	-9.79	108.91	113.80
22	BA	1008	A	N3-C4-C5	-9.79	119.95	126.80
22	BA	344	A	N3-C4-C5	-9.78	119.95	126.80
22	BA	2734	A	N3-C4-C5	-9.78	119.95	126.80
22	BA	781	A	N3-C4-C5	-9.78	119.95	126.80
22	BA	1580	A	N3-C4-C5	-9.78	119.96	126.80
23	BB	53	A	N3-C4-C5	-9.78	119.96	126.80
22	BA	1284	A	C5-C6-N6	9.78	131.52	123.70
22	BA	1285	A	N3-C4-C5	-9.78	119.96	126.80
22	BA	782	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	1596	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	2860	A	N7-C8-N9	-9.77	108.92	113.80
22	BA	751	A	N7-C8-N9	-9.77	108.92	113.80
22	BA	2726	A	N3-C4-C5	-9.77	119.96	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1919	A	N3-C4-C5	-9.77	119.96	126.80
22	BA	513	A	N7-C8-N9	-9.77	108.92	113.80
55	D3	35	A	N7-C8-N9	-9.77	108.92	113.80
55	D3	35	A	C5-C6-N6	9.76	131.51	123.70
22	BA	761	A	N3-C4-C5	-9.76	119.97	126.80
22	BA	734	A	N3-C4-C5	-9.76	119.97	126.80
22	BA	382	A	N3-C4-C5	-9.76	119.97	126.80
22	BA	104	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	197	A	C5-C6-N6	9.75	131.50	123.70
22	BA	1103	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	1503	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	1713	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	742	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	1470	A	C5-C6-N6	9.75	131.50	123.70
22	BA	1552	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	1762	A	N7-C8-N9	-9.75	108.93	113.80
22	BA	1890	A	N3-C4-C5	-9.75	119.97	126.80
22	BA	1970	A	C5-C6-N6	9.75	131.50	123.70
22	BA	2665	A	N3-C4-C5	-9.75	119.98	126.80
22	BA	83	A	N3-C4-C5	-9.75	119.98	126.80
22	BA	2740	A	N7-C8-N9	-9.75	108.93	113.80
22	BA	73	A	N7-C8-N9	-9.74	108.93	113.80
22	BA	972	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	2733	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	480	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	227	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	1608	A	N3-C4-C5	-9.74	119.98	126.80
22	BA	1650	A	C5-C6-N6	9.74	131.49	123.70
22	BA	262	A	C5-C6-N6	9.73	131.49	123.70
22	BA	429	A	N7-C8-N9	-9.73	108.93	113.80
22	BA	2711	A	N3-C4-C5	-9.73	119.99	126.80
22	BA	2820	A	N3-C4-C5	-9.73	119.99	126.80
22	BA	2015	A	N3-C4-C5	-9.73	119.99	126.80
23	BB	104	A	N3-C4-C5	-9.73	119.99	126.80
22	BA	2534	A	N3-C4-C5	-9.73	119.99	126.80
22	BA	849	A	C5-C6-N6	9.73	131.48	123.70
22	BA	172	A	C5-C6-N6	9.72	131.48	123.70
22	BA	430	A	C5-C6-N6	9.72	131.48	123.70
23	BB	66	A	C5-C6-N6	9.72	131.48	123.70
22	BA	1772	A	C5-C6-N6	9.72	131.48	123.70
22	BA	1794	A	C5-C6-N6	9.72	131.47	123.70
22	BA	2095	A	N3-C4-C5	-9.72	120.00	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2147	A	N3-C4-C5	-9.72	120.00	126.80
22	BA	541	A	C5-C6-N6	9.71	131.47	123.70
22	BA	2198	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	155	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	2281	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	2381	A	C5-C6-N6	9.71	131.47	123.70
22	BA	668	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	311	A	N3-C4-C5	-9.71	120.00	126.80
22	BA	909	A	N3-C4-C5	-9.71	120.01	126.80
22	BA	1088	A	C5-C6-N6	9.71	131.47	123.70
22	BA	1745	A	N3-C4-C5	-9.71	120.01	126.80
22	BA	1676	A	N7-C8-N9	-9.70	108.95	113.80
22	BA	352	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	920	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	905	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	1572	A	C5-C6-N6	9.70	131.46	123.70
22	BA	1143	A	C5-C6-N6	9.70	131.46	123.70
22	BA	2154	A	N3-C4-C5	-9.70	120.01	126.80
22	BA	676	A	N3-C4-C5	-9.69	120.01	126.80
22	BA	1040	A	N3-C4-C5	-9.69	120.02	126.80
22	BA	1641	A	N3-C4-C5	-9.69	120.02	126.80
55	D3	17	C	N1-C2-O2	9.69	124.72	118.90
22	BA	1900	A	N3-C4-C5	-9.69	120.02	126.80
22	BA	2468	A	N3-C4-C5	-9.69	120.02	126.80
55	D3	76	A	N3-C4-C5	-9.69	120.02	126.80
22	BA	53	A	N3-C4-C5	-9.69	120.02	126.80
22	BA	1913	A	N3-C4-C5	-9.69	120.02	126.80
22	BA	2183	A	N7-C8-N9	-9.69	108.96	113.80
22	BA	2430	A	C5-C6-N6	9.69	131.45	123.70
22	BA	1089	A	N3-C4-C5	-9.68	120.02	126.80
22	BA	699	A	N3-C4-C5	-9.68	120.02	126.80
22	BA	941	A	N3-C4-C5	-9.68	120.02	126.80
54	D2	58	A	N3-C4-C5	-9.68	120.02	126.80
22	BA	1522	A	N3-C4-C5	-9.68	120.02	126.80
22	BA	52	A	N3-C4-C5	-9.68	120.03	126.80
22	BA	2062	A	N3-C4-C5	-9.68	120.03	126.80
22	BA	1147	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	2418	A	C5-C6-N6	9.67	131.44	123.70
22	BA	2560	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	310	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	332	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	2288	A	N3-C4-C5	-9.67	120.03	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1027	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	1901	A	C5-C6-N6	9.67	131.44	123.70
55	D3	23	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	586	A	N7-C8-N9	-9.67	108.97	113.80
22	BA	1073	A	N3-C4-C5	-9.67	120.03	126.80
22	BA	497	A	N3-C4-C5	-9.66	120.03	126.80
22	BA	2873	A	N3-C4-C5	-9.66	120.03	126.80
22	BA	503	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	574	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	2882	A	C5-C6-N6	9.66	131.43	123.70
22	BA	10	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	1927	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	1987	A	N3-C4-C5	-9.66	120.04	126.80
22	BA	2070	A	C5-C6-N6	9.65	131.42	123.70
22	BA	2600	A	C5-C6-N6	9.65	131.42	123.70
22	BA	2019	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	2835	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	508	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	990	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	2358	A	N3-C4-C5	-9.64	120.05	126.80
22	BA	342	A	C5-C6-N6	9.64	131.41	123.70
22	BA	1802	A	C5-C6-N6	9.64	131.41	123.70
22	BA	1569	A	N3-C4-C5	-9.64	120.06	126.80
22	BA	1609	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	2598	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	1001	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	1260	A	C5-C6-N6	9.63	131.41	123.70
22	BA	1872	A	C5-C6-N6	9.63	131.41	123.70
22	BA	1384	A	N3-C4-C5	-9.63	120.06	126.80
22	BA	984	A	N7-C8-N9	-9.62	108.99	113.80
22	BA	2352	A	N3-C4-C5	-9.62	120.07	126.80
22	BA	1885	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	2135	A	C5-C6-N6	9.61	131.39	123.70
22	BA	127	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	199	A	N3-C4-C5	-9.61	120.07	126.80
22	BA	2328	A	C5-C6-N6	9.61	131.39	123.70
22	BA	563	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	233	A	C5-C6-N6	9.60	131.38	123.70
22	BA	1678	A	N3-C4-C5	-9.60	120.08	126.80
55	D3	14	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	1525	A	N3-C4-C5	-9.60	120.08	126.80
22	BA	789	A	C5-C6-N6	9.59	131.37	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1304	A	N3-C4-C5	-9.59	120.09	126.80
23	BB	108	A	N3-C4-C5	-9.59	120.08	126.80
55	D3	36	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	1899	A	N7-C8-N9	-9.59	109.01	113.80
22	BA	73	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	2893	A	N3-C4-C5	-9.59	120.09	126.80
22	BA	270	A	N3-C4-C5	-9.58	120.09	126.80
22	BA	2635	A	C5-C6-N6	9.58	131.37	123.70
22	BA	2660	A	N3-C4-C5	-9.58	120.09	126.80
22	BA	1090	A	N3-C4-C5	-9.57	120.10	126.80
22	BA	244	A	N3-C4-C5	-9.57	120.10	126.80
22	BA	928	A	C5-C6-N6	9.57	131.35	123.70
22	BA	155	A	C5-C6-N6	9.55	131.34	123.70
22	BA	1284	A	N3-C4-C5	-9.55	120.11	126.80
22	BA	322	A	N3-C4-C5	-9.55	120.11	126.80
22	BA	1147	A	C5-C6-N6	9.55	131.34	123.70
22	BA	2872	A	N3-C4-C5	-9.55	120.12	126.80
22	BA	2868	A	N7-C8-N9	-9.54	109.03	113.80
22	BA	1204	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	1871	A	N3-C4-C5	-9.54	120.12	126.80
22	BA	1803	A	N3-C4-C5	-9.53	120.13	126.80
23	BB	109	A	N3-C4-C5	-9.53	120.13	126.80
22	BA	347	A	C5-C6-N6	9.53	131.32	123.70
22	BA	1528	A	C5-C6-N6	9.53	131.32	123.70
22	BA	382	A	C5-C6-N6	9.53	131.32	123.70
22	BA	354	A	N3-C4-C5	-9.52	120.13	126.80
22	BA	2037	A	C5-C6-N6	9.52	131.32	123.70
22	BA	1802	A	N3-C4-C5	-9.52	120.13	126.80
22	BA	2051	A	N7-C8-N9	-9.52	109.04	113.80
54	D2	73	A	N3-C4-C5	-9.52	120.13	126.80
22	BA	2340	A	N3-C4-C5	-9.52	120.14	126.80
54	D2	35	A	N3-C4-C5	-9.52	120.14	126.80
22	BA	1783	A	N3-C4-C5	-9.52	120.14	126.80
22	BA	1901	A	N7-C8-N9	-9.52	109.04	113.80
22	BA	324	A	N3-C4-C5	-9.51	120.14	126.80
22	BA	1749	A	C5-C6-N6	9.51	131.31	123.70
22	BA	2328	A	N7-C8-N9	-9.51	109.04	113.80
22	BA	1815	A	N3-C4-C5	-9.51	120.14	126.80
22	BA	2298	A	N3-C4-C5	-9.51	120.14	126.80
23	BB	78	A	N3-C4-C5	-9.50	120.15	126.80
23	BB	59	A	N3-C4-C5	-9.50	120.15	126.80
22	BA	1046	A	N3-C4-C5	-9.50	120.15	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1854	A	C5-C6-N6	9.50	131.30	123.70
22	BA	764	A	N3-C4-C5	-9.49	120.15	126.80
22	BA	1434	A	N7-C8-N9	-9.49	109.05	113.80
22	BA	1794	A	N3-C4-C5	-9.49	120.15	126.80
22	BA	2170	A	N3-C4-C5	-9.49	120.16	126.80
54	D2	49	A	C5-C6-N6	9.49	131.29	123.70
22	BA	2560	A	C5-C6-N6	9.49	131.29	123.70
22	BA	1932	A	N3-C4-C5	-9.49	120.16	126.80
22	BA	384	A	N3-C4-C5	-9.49	120.16	126.80
22	BA	2776	A	N3-C4-C5	-9.49	120.16	126.80
23	BB	119	A	N3-C4-C5	-9.49	120.16	126.80
22	BA	1213	A	C5-C6-N6	9.48	131.29	123.70
22	BA	661	A	C5-C6-N6	9.48	131.28	123.70
22	BA	1322	A	N3-C4-C5	-9.48	120.17	126.80
22	BA	2058	A	N3-C4-C5	-9.48	120.17	126.80
22	BA	2411	A	N3-C4-C5	-9.48	120.17	126.80
22	BA	2750	A	N3-C4-C5	-9.48	120.17	126.80
22	BA	960	A	C5-C6-N6	9.47	131.28	123.70
22	BA	1359	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	1525	A	C5-C6-N6	9.47	131.28	123.70
22	BA	233	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	1596	A	C5-C6-N6	9.47	131.28	123.70
22	BA	1630	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	1698	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	877	A	N3-C4-C5	-9.47	120.17	126.80
22	BA	547	A	N3-C4-C5	-9.46	120.17	126.80
22	BA	1700	A	N3-C4-C5	-9.46	120.17	126.80
22	BA	1244	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	706	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	2366	A	N7-C8-N9	-9.46	109.07	113.80
22	BA	2469	A	N3-C4-C5	-9.46	120.18	126.80
22	BA	2748	A	N3-C4-C5	-9.45	120.18	126.80
22	BA	2657	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	909	A	C5-C6-N6	9.45	131.26	123.70
22	BA	1142	A	C5-C6-N6	9.45	131.26	123.70
22	BA	142	A	C5-C6-N6	9.45	131.26	123.70
22	BA	1676	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	1808	A	N3-C4-C5	-9.45	120.19	126.80
23	BB	50	A	N3-C4-C5	-9.45	120.19	126.80
22	BA	472	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	1395	A	N3-C4-C5	-9.44	120.19	126.80
22	BA	1247	A	C5-C6-N6	9.44	131.25	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	422	A	C5-C6-N6	9.43	131.25	123.70
22	BA	2314	A	C5-C6-N6	9.43	131.25	123.70
22	BA	1969	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	905	A	C5-C6-N6	9.43	131.24	123.70
22	BA	1230	A	C5-C6-N6	9.43	131.24	123.70
22	BA	2311	A	N3-C4-C5	-9.43	120.20	126.80
23	BB	52	A	N3-C4-C5	-9.43	120.20	126.80
22	BA	829	A	N3-C4-C5	-9.42	120.20	126.80
22	BA	2071	A	C5-C6-N6	9.42	131.24	123.70
22	BA	223	A	N3-C4-C5	-9.42	120.21	126.80
22	BA	309	A	N3-C4-C5	-9.42	120.20	126.80
22	BA	1616	A	N3-C4-C5	-9.42	120.21	126.80
22	BA	1936	A	N3-C4-N9	9.41	134.93	127.40
22	BA	1431	A	C5-C6-N6	9.41	131.23	123.70
22	BA	165	A	N3-C4-C5	-9.41	120.22	126.80
22	BA	294	A	N3-C4-C5	-9.41	120.22	126.80
22	BA	2711	A	C5-C6-N6	9.41	131.22	123.70
22	BA	1515	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	2142	A	C5-C6-N6	9.40	131.22	123.70
22	BA	2426	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	2860	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	479	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	1977	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	443	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	614	A	N3-C4-C5	-9.40	120.22	126.80
22	BA	1593	A	C5-C6-N6	9.40	131.22	123.70
22	BA	2577	A	C5-C6-N6	9.40	131.22	123.70
22	BA	603	A	N3-C4-C5	-9.39	120.22	126.80
22	BA	1057	A	C5-C6-N6	9.39	131.22	123.70
22	BA	2476	A	N3-C4-C5	-9.39	120.22	126.80
22	BA	1393	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	402	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	2758	A	N3-C4-C5	-9.39	120.23	126.80
22	BA	1021	A	N7-C8-N9	-9.38	109.11	113.80
22	BA	1668	A	N3-C4-C5	-9.38	120.23	126.80
55	D3	7	A	N3-C4-C5	-9.38	120.23	126.80
22	BA	42	A	C5-C6-N6	9.38	131.20	123.70
22	BA	654	A	C5-C6-N6	9.38	131.20	123.70
22	BA	282	A	N3-C4-C5	-9.38	120.24	126.80
22	BA	947	A	C5-C6-N6	9.37	131.20	123.70
22	BA	2005	A	N3-C4-C5	-9.37	120.24	126.80
22	BA	575	A	C5-C6-N6	9.37	131.20	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	756	A	C5-C6-N6	9.37	131.20	123.70
22	BA	2766	A	N7-C8-N9	-9.37	109.11	113.80
22	BA	1669	A	N7-C8-N9	-9.37	109.11	113.80
22	BA	2274	A	N7-C8-N9	-9.37	109.11	113.80
22	BA	278	A	N7-C8-N9	-9.37	109.11	113.80
22	BA	1757	A	N3-C4-C5	-9.37	120.24	126.80
23	BB	119	A	C5-C6-N6	9.37	131.19	123.70
22	BA	125	A	N3-C4-C5	-9.37	120.24	126.80
22	BA	1111	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	2278	A	C5-C6-N6	9.36	131.19	123.70
22	BA	1810	A	N7-C8-N9	-9.36	109.12	113.80
22	BA	2369	A	C5-C6-N6	9.36	131.19	123.70
1	AA	87	C	N3-C2-O2	-9.36	115.35	121.90
22	BA	1722	A	N3-C4-C5	-9.36	120.25	126.80
22	BA	161	A	N3-C4-C5	-9.35	120.26	126.80
22	BA	2792	A	C5-C6-N6	9.35	131.18	123.70
22	BA	1165	A	N3-C4-C5	-9.35	120.26	126.80
22	BA	368	A	N3-C4-C5	-9.35	120.26	126.80
22	BA	844	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	2314	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	91	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	1665	A	C5-C6-N6	9.34	131.17	123.70
22	BA	1785	A	N3-C4-C5	-9.34	120.26	126.80
22	BA	804	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	1912	A	N3-C4-C5	-9.33	120.27	126.80
22	BA	1872	A	N7-C8-N9	-9.33	109.14	113.80
22	BA	538	A	N3-C4-C5	-9.32	120.27	126.80
22	BA	655	A	N3-C4-C5	-9.32	120.27	126.80
22	BA	1502	A	C5-C6-N6	9.32	131.16	123.70
22	BA	2471	A	C5-C6-N6	9.32	131.15	123.70
22	BA	1936	A	N7-C8-N9	-9.31	109.14	113.80
22	BA	2682	A	N3-C4-C5	-9.31	120.28	126.80
22	BA	241	A	N3-C4-C5	-9.31	120.28	126.80
22	BA	95	A	C5-C6-N6	9.31	131.15	123.70
22	BA	2211	A	N3-C4-C5	-9.31	120.28	126.80
22	BA	626	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	2101	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	896	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	1626	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	727	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	2764	A	N3-C4-C5	-9.30	120.29	126.80
22	BA	1070	A	N3-C4-C5	-9.29	120.29	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	637	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	1080	A	C5-C6-N6	9.29	131.13	123.70
22	BA	1509	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	1342	A	N3-C4-C5	-9.29	120.30	126.80
22	BA	2119	A	N3-C4-C5	-9.28	120.30	126.80
22	BA	454	A	N3-C4-C5	-9.28	120.31	126.80
22	BA	2406	A	N3-C4-C5	-9.28	120.31	126.80
22	BA	2274	A	N3-C4-C5	-9.28	120.31	126.80
22	BA	5	A	C5-C6-N6	9.27	131.12	123.70
22	BA	2829	A	C5-C6-N6	9.27	131.12	123.70
22	BA	2009	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	1247	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	2654	A	N3-C4-C5	-9.27	120.31	126.80
22	BA	677	A	C5-C6-N6	9.26	131.11	123.70
22	BA	1385	A	C5-N7-C8	9.26	108.53	103.90
22	BA	1953	A	N3-C4-C5	-9.26	120.32	126.80
22	BA	668	A	C5-C6-N6	9.26	131.11	123.70
22	BA	621	A	N3-C4-C5	-9.26	120.32	126.80
22	BA	2205	A	C5-C6-N6	9.25	131.10	123.70
22	BA	2241	A	C5-C6-N6	9.25	131.10	123.70
22	BA	627	A	N3-C4-C5	-9.24	120.33	126.80
55	D3	62	C	N3-C2-O2	-9.24	115.43	121.90
22	BA	1652	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	1739	A	N7-C8-N9	-9.24	109.18	113.80
22	BA	2469	A	C5-C6-N6	9.24	131.09	123.70
22	BA	1566	A	N3-C4-C5	-9.24	120.33	126.80
22	BA	1773	A	C5-N7-C8	9.24	108.52	103.90
22	BA	44	A	C5-C6-N6	9.23	131.09	123.70
22	BA	1711	A	C5-C6-N6	9.23	131.09	123.70
22	BA	1264	A	N3-C4-C5	-9.23	120.34	126.80
22	BA	2095	A	C5-C6-N6	9.23	131.08	123.70
22	BA	299	A	N7-C8-N9	-9.23	109.19	113.80
22	BA	21	A	C5-C6-N6	9.22	131.08	123.70
22	BA	218	A	N3-C4-C5	-9.22	120.34	126.80
54	D2	41	A	C5-C6-N6	9.22	131.08	123.70
22	BA	2009	A	C5-C6-N6	9.22	131.07	123.70
22	BA	2882	A	N3-C4-C5	-9.22	120.35	126.80
22	BA	844	A	C5-C6-N6	9.21	131.07	123.70
22	BA	1583	A	N3-C4-C5	-9.21	120.35	126.80
22	BA	1634	A	N3-C4-C5	-9.20	120.36	126.80
22	BA	352	A	C5-C6-N6	9.20	131.06	123.70
22	BA	2761	A	C5-C6-N6	9.20	131.06	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	371	A	C5-N7-C8	9.19	108.50	103.90
22	BA	2727	A	C5-C6-N6	9.19	131.05	123.70
22	BA	1262	A	C5-C6-N6	9.18	131.04	123.70
22	BA	195	A	N3-C4-C5	-9.18	120.38	126.80
22	BA	1937	A	N3-C4-C5	-9.18	120.37	126.80
22	BA	2725	A	N3-C4-C5	-9.18	120.37	126.80
22	BA	996	A	C5-C6-N6	9.18	131.04	123.70
22	BA	529	A	N3-C4-C5	-9.18	120.38	126.80
22	BA	2800	A	N3-C4-C5	-9.18	120.38	126.80
22	BA	1327	A	N3-C4-C5	-9.17	120.38	126.80
22	BA	1403	A	C5-C6-N6	9.16	131.03	123.70
22	BA	1129	A	N3-C4-C5	-9.16	120.39	126.80
22	BA	1853	A	N3-C4-C5	-9.15	120.39	126.80
22	BA	2706	A	C5-C6-N6	9.15	131.02	123.70
22	BA	251	A	N7-C8-N9	-9.14	109.23	113.80
22	BA	1237	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	265	A	N3-C4-C5	-9.14	120.40	126.80
22	BA	2813	A	N7-C8-N9	-9.13	109.23	113.80
22	BA	1672	A	N3-C4-C5	-9.13	120.41	126.80
22	BA	2781	A	N3-C4-C5	-9.13	120.41	126.80
22	BA	2430	A	N3-C4-C5	-9.12	120.42	126.80
23	BB	50	A	C5-C6-N6	9.11	130.99	123.70
22	BA	2117	A	C5-N7-C8	9.11	108.45	103.90
22	BA	2439	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	1503	A	C5-C6-N6	9.10	130.98	123.70
22	BA	2471	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	1780	A	N3-C4-C5	-9.10	120.43	126.80
22	BA	2097	A	C5-C6-N6	9.10	130.98	123.70
23	BB	39	A	N3-C4-C5	-9.09	120.43	126.80
22	BA	213	A	N3-C4-C5	-9.09	120.44	126.80
22	BA	1754	A	N3-C4-C5	-9.09	120.44	126.80
22	BA	2247	A	C5-C6-N6	9.09	130.97	123.70
23	BB	34	A	C5-C6-N6	9.09	130.97	123.70
22	BA	222	A	N3-C4-C5	-9.09	120.44	126.80
22	BA	2388	A	N3-C4-C5	-9.09	120.44	126.80
22	BA	2281	A	C5-C6-N6	9.08	130.97	123.70
22	BA	415	A	N7-C8-N9	-9.08	109.26	113.80
22	BA	2448	A	N3-C4-C5	-9.08	120.44	126.80
22	BA	2736	A	C5-C6-N6	9.08	130.96	123.70
22	BA	973	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	1679	A	N7-C8-N9	-9.07	109.26	113.80
22	BA	1810	A	C4-C5-C6	9.07	121.54	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	457	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	988	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	1155	A	N3-C4-C5	-9.07	120.45	126.80
22	BA	64	A	C5-C6-N6	9.06	130.95	123.70
22	BA	111	A	N3-C4-C5	-9.06	120.46	126.80
22	BA	2600	A	N3-C4-C5	-9.06	120.46	126.80
22	BA	2662	A	C5-C6-N6	9.06	130.95	123.70
22	BA	2191	A	C5-C6-N6	9.05	130.94	123.70
22	BA	2776	A	C5-N7-C8	9.05	108.43	103.90
22	BA	2432	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	2516	A	C5-C6-N6	9.04	130.94	123.70
22	BA	526	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	1928	A	N3-C4-C5	-9.04	120.47	126.80
22	BA	936	A	C5-C6-N6	9.03	130.93	123.70
22	BA	2725	A	C5-C6-N6	9.03	130.92	123.70
22	BA	63	A	N3-C4-C5	-9.03	120.48	126.80
22	BA	586	A	N3-C4-C5	-9.02	120.48	126.80
22	BA	1246	A	C5-C6-N6	9.02	130.91	123.70
22	BA	1739	A	C5-C6-N6	9.02	130.91	123.70
22	BA	1791	A	N3-C4-C5	-9.02	120.49	126.80
22	BA	1127	A	N3-C4-C5	-9.01	120.49	126.80
22	BA	1549	A	C5-C6-N6	9.01	130.91	123.70
22	BA	146	A	C5-C6-N6	9.01	130.90	123.70
23	BB	94	A	C5-C6-N6	9.01	130.91	123.70
22	BA	423	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	1987	A	C5-C6-N6	9.00	130.90	123.70
22	BA	2542	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	829	A	C5-N7-C8	9.00	108.40	103.90
22	BA	1269	A	C5-C6-N6	9.00	130.90	123.70
22	BA	1978	A	N3-C4-C5	-9.00	120.50	126.80
22	BA	1821	A	N3-C4-C5	-8.99	120.50	126.80
22	BA	2705	A	N3-C4-C5	-8.99	120.51	126.80
54	D2	23	A	C5-C6-N6	8.99	130.89	123.70
22	BA	2317	A	C5-C6-N6	8.99	130.89	123.70
22	BA	173	A	C5-C6-N6	8.98	130.89	123.70
54	D2	38	A	N3-C4-C5	-8.98	120.51	126.80
22	BA	2435	A	C5-C6-N6	8.98	130.88	123.70
22	BA	2856	A	C5-C6-N6	8.97	130.88	123.70
54	D2	69	A	C5-C6-N6	8.97	130.88	123.70
22	BA	1057	A	C5-N7-C8	8.96	108.38	103.90
22	BA	1735	A	C5-C6-N6	8.96	130.87	123.70
22	BA	1810	A	C5-C6-N6	8.96	130.87	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	730	A	C5-C6-N6	8.96	130.87	123.70
22	BA	89	A	N3-C4-C5	-8.96	120.53	126.80
22	BA	2171	A	N3-C4-C5	-8.96	120.53	126.80
22	BA	1453	A	N3-C4-C5	-8.95	120.53	126.80
22	BA	1614	A	N3-C4-C5	-8.95	120.54	126.80
54	D2	76	A	N3-C4-C5	-8.94	120.55	126.80
1	AA	961	U	N1-C2-N3	8.93	120.26	114.90
54	D2	9	A	N3-C4-C5	-8.92	120.55	126.80
22	BA	833	A	N3-C4-C5	-8.91	120.56	126.80
22	BA	2080	A	C5-C6-N6	8.91	130.83	123.70
54	D2	28	A	C5-C6-N6	8.91	130.83	123.70
22	BA	689	A	C5-C6-N6	8.91	130.83	123.70
22	BA	2369	A	N3-C4-C5	-8.91	120.56	126.80
22	BA	2117	A	N3-C4-C5	-8.91	120.56	126.80
22	BA	2346	A	N3-C4-C5	-8.90	120.57	126.80
22	BA	1912	A	C5-N7-C8	8.90	108.35	103.90
22	BA	721	A	C5-C6-N6	8.90	130.82	123.70
22	BA	2700	A	C5-C6-N6	8.89	130.81	123.70
22	BA	2900	A	C5-C6-N6	8.89	130.81	123.70
22	BA	2059	A	N3-C4-C5	-8.89	120.58	126.80
22	BA	1205	A	N3-C4-C5	-8.88	120.58	126.80
22	BA	693	A	C5-C6-N6	8.88	130.81	123.70
22	BA	1591	A	C5-C6-N6	8.88	130.80	123.70
22	BA	1937	A	C5-N7-C8	8.87	108.34	103.90
22	BA	1746	A	C5-C6-N6	8.87	130.79	123.70
22	BA	2899	A	C5-C6-N6	8.87	130.79	123.70
22	BA	1151	A	C5-C6-N6	8.85	130.78	123.70
22	BA	2003	A	C5-C6-N6	8.85	130.78	123.70
22	BA	1981	A	N3-C4-C5	-8.85	120.61	126.80
22	BA	1275	A	N3-C4-C5	-8.84	120.61	126.80
22	BA	2566	A	N3-C4-C5	-8.84	120.61	126.80
22	BA	1630	A	C5-N7-C8	8.83	108.31	103.90
22	BA	152	A	C5-C6-N6	8.83	130.76	123.70
22	BA	1244	A	C5-C6-N6	8.83	130.76	123.70
22	BA	513	A	C5-C6-N6	8.82	130.76	123.70
22	BA	1144	A	C5-C6-N6	8.82	130.75	123.70
22	BA	1936	A	C4-C5-C6	8.82	121.41	117.00
22	BA	2872	A	N7-C8-N9	-8.81	109.39	113.80
22	BA	471	A	C5-N7-C8	8.81	108.30	103.90
22	BA	507	A	N3-C4-C5	-8.81	120.64	126.80
22	BA	1169	A	C5-C6-N6	8.81	130.75	123.70
22	BA	2407	A	C5-C6-N6	8.81	130.75	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	981	A	N3-C4-C5	-8.80	120.64	126.80
22	BA	415	A	C5-C6-N6	8.79	130.73	123.70
22	BA	2837	A	C5-C6-N6	8.79	130.73	123.70
22	BA	1088	A	N3-C4-N9	8.79	134.43	127.40
22	BA	404	A	N3-C4-C5	-8.78	120.65	126.80
22	BA	1603	A	C5-C6-N6	8.78	130.72	123.70
22	BA	2333	A	N3-C4-C5	-8.78	120.66	126.80
22	BA	1504	A	C5-C6-N6	8.78	130.72	123.70
22	BA	1032	A	N3-C4-C5	-8.77	120.66	126.80
22	BA	156	A	C5-C6-N6	8.77	130.71	123.70
22	BA	750	A	C5-C6-N6	8.76	130.71	123.70
22	BA	1532	A	C5-C6-N6	8.76	130.71	123.70
22	BA	176	A	C5-C6-N6	8.75	130.70	123.70
22	BA	613	A	N3-C4-N9	8.75	134.40	127.40
22	BA	1528	A	C4-C5-C6	8.75	121.38	117.00
22	BA	1021	A	N3-C4-N9	8.73	134.38	127.40
54	D2	58	A	C5-N7-C8	8.73	108.26	103.90
22	BA	788	A	N3-C4-C5	-8.72	120.69	126.80
22	BA	2033	A	C5-N7-C8	8.72	108.26	103.90
22	BA	646	U	O4'-C1'-N1	8.71	115.17	108.20
22	BA	1133	A	C5-N7-C8	8.71	108.26	103.90
22	BA	354	A	C5-N7-C8	8.71	108.25	103.90
22	BA	1505	A	C5-C6-N6	8.71	130.67	123.70
22	BA	2883	A	N3-C4-C5	-8.71	120.70	126.80
22	BA	599	A	C5-C6-N6	8.71	130.66	123.70
22	BA	2020	A	C5-C6-N6	8.70	130.66	123.70
22	BA	644	A	C5-N7-C8	8.70	108.25	103.90
1	AA	439	U	C2-N1-C1'	8.70	128.14	117.70
22	BA	466	A	N3-C4-C5	-8.69	120.72	126.80
22	BA	783	A	N7-C8-N9	-8.68	109.46	113.80
22	BA	1147	A	C5-N7-C8	8.68	108.24	103.90
55	D3	9	A	C5-N7-C8	8.68	108.24	103.90
22	BA	2766	A	N3-C4-N9	8.67	134.34	127.40
22	BA	825	A	C5-N7-C8	8.66	108.23	103.90
22	BA	439	A	C5-C6-N6	8.66	130.63	123.70
22	BA	861	A	C5-N7-C8	8.66	108.23	103.90
22	BA	614	A	C5-N7-C8	8.65	108.23	103.90
54	D2	5	A	C5-C6-N6	8.65	130.62	123.70
22	BA	131	A	C5-C6-N6	8.64	130.61	123.70
22	BA	2388	A	C5-N7-C8	8.64	108.22	103.90
22	BA	454	A	C5-N7-C8	8.64	108.22	103.90
22	BA	1829	A	N3-C4-N9	8.64	134.31	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2154	A	C5-C6-N6	8.63	130.61	123.70
22	BA	1515	A	C5-N7-C8	8.63	108.22	103.90
22	BA	833	A	C5-C6-N6	8.62	130.60	123.70
22	BA	983	A	N3-C4-C5	-8.62	120.77	126.80
22	BA	2287	A	C5-N7-C8	8.62	108.21	103.90
22	BA	2090	A	C5-C6-N6	8.61	130.59	123.70
22	BA	348	A	C5-C6-N6	8.61	130.59	123.70
22	BA	2792	A	C5-N7-C8	8.61	108.20	103.90
22	BA	1419	A	N3-C4-C5	-8.61	120.78	126.80
22	BA	1876	A	C5-N7-C8	8.60	108.20	103.90
22	BA	1353	A	C5-N7-C8	8.60	108.20	103.90
22	BA	2088	A	C5-C6-N6	8.60	130.58	123.70
22	BA	1336	A	C5-C6-N6	8.60	130.58	123.70
22	BA	1610	A	N3-C4-C5	-8.59	120.79	126.80
22	BA	1590	A	C5-C6-N6	8.59	130.57	123.70
22	BA	2033	A	N3-C4-C5	-8.58	120.79	126.80
54	D2	28	A	C5-N7-C8	8.58	108.19	103.90
22	BA	2052	A	C5-C6-N6	8.58	130.56	123.70
22	BA	6	A	C5-C6-N6	8.57	130.56	123.70
55	D3	37	A	C5-N7-C8	8.57	108.19	103.90
22	BA	272	A	C5-C6-N6	8.56	130.55	123.70
22	BA	689	A	C5-N7-C8	8.56	108.18	103.90
22	BA	1998	A	C5-C6-N6	8.56	130.55	123.70
22	BA	1302	A	N3-C4-C5	-8.56	120.81	126.80
22	BA	2850	A	C5-N7-C8	8.55	108.17	103.90
55	D3	7	A	C5-N7-C8	8.55	108.17	103.90
22	BA	204	A	N3-C4-C5	-8.54	120.82	126.80
22	BA	892	A	C5-N7-C8	8.54	108.17	103.90
22	BA	1069	A	C5-N7-C8	8.54	108.17	103.90
22	BA	1286	A	N3-C4-C5	-8.53	120.83	126.80
22	BA	753	A	C5-C6-N6	8.53	130.53	123.70
22	BA	1254	A	N3-C4-C5	-8.53	120.83	126.80
22	BA	56	A	C5-C6-N6	8.52	130.52	123.70
54	D2	35	A	C5-N7-C8	8.52	108.16	103.90
22	BA	1214	A	C5-N7-C8	8.52	108.16	103.90
22	BA	1387	A	C5-C6-N6	8.52	130.51	123.70
22	BA	945	A	C5-N7-C8	8.51	108.16	103.90
22	BA	199	A	C5-N7-C8	8.51	108.16	103.90
22	BA	2430	A	C4-C5-C6	8.51	121.25	117.00
22	BA	2602	A	C5-N7-C8	8.51	108.15	103.90
54	D2	21	A	N3-C4-C5	-8.50	120.85	126.80
22	BA	1548	A	C5-C6-N6	8.50	130.50	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2297	A	C5-N7-C8	8.49	108.14	103.90
22	BA	1247	A	C5-N7-C8	8.48	108.14	103.90
22	BA	1253	A	N3-C4-C5	-8.48	120.86	126.80
22	BA	756	A	C5-N7-C8	8.48	108.14	103.90
22	BA	2134	A	C5-N7-C8	8.48	108.14	103.90
22	BA	2589	A	N3-C4-C5	-8.48	120.86	126.80
22	BA	1655	A	C5-N7-C8	8.48	108.14	103.90
1	AA	961	U	C2-N3-C4	-8.46	121.92	127.00
22	BA	905	A	C5-N7-C8	8.46	108.13	103.90
22	BA	1805	A	C5-N7-C8	8.46	108.13	103.90
22	BA	2738	A	N3-C4-C5	-8.45	120.88	126.80
22	BA	479	A	C5-N7-C8	8.45	108.12	103.90
22	BA	1847	A	N7-C8-N9	-8.44	109.58	113.80
22	BA	1272	A	N3-C4-C5	-8.44	120.89	126.80
22	BA	322	A	C5-N7-C8	8.44	108.12	103.90
22	BA	1385	A	N3-C4-C5	-8.44	120.89	126.80
22	BA	1048	A	C5-N7-C8	8.44	108.12	103.90
22	BA	821	A	N3-C4-C5	-8.43	120.90	126.80
22	BA	2135	A	C5-N7-C8	8.43	108.12	103.90
22	BA	2572	A	N3-C4-C5	-8.43	120.90	126.80
22	BA	1597	A	C5-N7-C8	8.42	108.11	103.90
22	BA	197	A	C5-N7-C8	8.42	108.11	103.90
22	BA	2381	A	C5-N7-C8	8.42	108.11	103.90
22	BA	310	A	C5-N7-C8	8.41	108.11	103.90
22	BA	783	A	N3-C4-N9	8.41	134.13	127.40
22	BA	119	A	N3-C4-C5	-8.41	120.92	126.80
23	BB	57	A	C5-N7-C8	8.41	108.10	103.90
22	BA	1073	A	C5-N7-C8	8.40	108.10	103.90
22	BA	1580	A	C5-N7-C8	8.40	108.10	103.90
22	BA	195	A	N7-C8-N9	-8.40	109.60	113.80
22	BA	231	A	C5-C6-N6	8.40	130.42	123.70
22	BA	896	A	C5-N7-C8	8.40	108.10	103.90
22	BA	590	A	C5-C6-N6	8.39	130.41	123.70
22	BA	2119	A	C5-N7-C8	8.39	108.10	103.90
54	D2	23	A	C5-N7-C8	8.39	108.09	103.90
22	BA	2670	A	C5-C6-N6	8.39	130.41	123.70
22	BA	204	A	C5-N7-C8	8.38	108.09	103.90
22	BA	1427	A	C5-N7-C8	8.38	108.09	103.90
22	BA	1730	C	N3-C2-O2	-8.38	116.03	121.90
22	BA	1274	A	C5-N7-C8	8.38	108.09	103.90
22	BA	2765	A	N3-C4-N9	8.38	134.10	127.40
22	BA	2662	A	C4-C5-C6	8.37	121.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	666	A	C5-C6-N6	8.36	130.39	123.70
22	BA	734	A	C5-N7-C8	8.36	108.08	103.90
23	BB	29	A	C5-N7-C8	8.36	108.08	103.90
22	BA	2014	A	C5-N7-C8	8.36	108.08	103.90
22	BA	2077	A	C5-C6-N6	8.36	130.38	123.70
22	BA	1566	A	C5-N7-C8	8.35	108.08	103.90
22	BA	1535	A	C5-N7-C8	8.35	108.07	103.90
22	BA	2297	A	N9-C4-C5	8.35	109.14	105.80
22	BA	705	A	C5-C6-N6	8.34	130.38	123.70
22	BA	2169	A	C5-N7-C8	8.34	108.07	103.90
22	BA	2184	A	C5-C6-N6	8.34	130.37	123.70
22	BA	1637	A	C5-C6-N6	8.33	130.37	123.70
22	BA	1829	A	C5-C6-N6	8.33	130.37	123.70
22	BA	2241	A	C5-N7-C8	8.33	108.06	103.90
22	BA	863	A	C5-C6-N6	8.33	130.36	123.70
22	BA	909	A	C5-N7-C8	8.33	108.06	103.90
22	BA	1165	A	C5-N7-C8	8.33	108.06	103.90
22	BA	1705	A	C5-C6-N6	8.33	130.36	123.70
22	BA	221	A	N3-C4-C5	-8.32	120.97	126.80
22	BA	2565	A	C5-N7-C8	8.32	108.06	103.90
22	BA	324	A	C5-C6-N6	8.32	130.36	123.70
22	BA	2183	A	N3-C4-N9	8.32	134.06	127.40
22	BA	1652	A	C5-N7-C8	8.32	108.06	103.90
22	BA	2176	A	C5-N7-C8	8.31	108.06	103.90
22	BA	251	A	C4-C5-C6	8.30	121.15	117.00
22	BA	1509	A	C5-N7-C8	8.30	108.05	103.90
22	BA	513	A	C4-C5-C6	8.30	121.15	117.00
22	BA	1960	A	C5-C6-N6	8.30	130.34	123.70
22	BA	1522	A	C5-N7-C8	8.30	108.05	103.90
22	BA	1787	A	C4-C5-C6	8.29	121.15	117.00
22	BA	1730	C	C2-N1-C1'	8.29	127.92	118.80
22	BA	538	A	C5-N7-C8	8.29	108.04	103.90
22	BA	2340	A	C5-C6-N6	8.29	130.33	123.70
22	BA	2288	A	C5-N7-C8	8.28	108.04	103.90
22	BA	1722	A	C5-N7-C8	8.28	108.04	103.90
22	BA	1913	A	C5-N7-C8	8.28	108.04	103.90
22	BA	125	A	C5-N7-C8	8.28	108.04	103.90
22	BA	522	A	C5-C6-N6	8.28	130.32	123.70
22	BA	794	A	C5-C6-N6	8.27	130.32	123.70
22	BA	1020	A	N3-C4-C5	-8.27	121.01	126.80
22	BA	2126	A	C5-N7-C8	8.27	108.04	103.90
22	BA	1786	A	C5-N7-C8	8.27	108.03	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1080	A	C5-N7-C8	8.26	108.03	103.90
22	BA	2634	A	C5-C6-N6	8.26	130.31	123.70
22	BA	2077	A	C4-C5-C6	8.26	121.13	117.00
22	BA	191	A	C5-N7-C8	8.25	108.03	103.90
22	BA	608	A	C5-N7-C8	8.25	108.03	103.90
22	BA	213	A	C5-N7-C8	8.25	108.02	103.90
22	BA	900	A	C5-N7-C8	8.25	108.03	103.90
22	BA	1098	A	C5-N7-C8	8.25	108.03	103.90
1	AA	1008	U	O4'-C1'-N1	8.24	114.80	108.20
22	BA	2879	A	C5-N7-C8	8.24	108.02	103.90
22	BA	1265	A	C5-N7-C8	8.24	108.02	103.90
22	BA	2009	A	C5-N7-C8	8.24	108.02	103.90
22	BA	742	A	C5-C6-N6	8.24	130.29	123.70
22	BA	1490	A	N3-C4-N9	8.24	133.99	127.40
54	D2	69	A	C5-N7-C8	8.24	108.02	103.90
54	D2	73	A	C5-N7-C8	8.24	108.02	103.90
22	BA	111	A	C5-N7-C8	8.23	108.02	103.90
22	BA	460	A	C5-N7-C8	8.23	108.02	103.90
22	BA	1204	A	C5-N7-C8	8.23	108.02	103.90
22	BA	1353	A	N9-C4-C5	8.22	109.09	105.80
22	BA	979	A	C5-N7-C8	8.22	108.01	103.90
22	BA	1313	U	C2-N1-C1'	8.22	127.57	117.70
55	D3	17	C	C2-N1-C1'	8.22	127.85	118.80
22	BA	2572	A	C5-N7-C8	8.22	108.01	103.90
22	BA	2761	A	C5-N7-C8	8.22	108.01	103.90
23	BB	119	A	C5-N7-C8	8.22	108.01	103.90
22	BA	1111	A	C5-N7-C8	8.21	108.01	103.90
22	BA	1504	A	C5-N7-C8	8.21	108.01	103.90
22	BA	2108	A	C5-N7-C8	8.21	108.00	103.90
22	BA	718	A	C5-N7-C8	8.20	108.00	103.90
22	BA	1070	A	C5-N7-C8	8.20	108.00	103.90
22	BA	1829	A	C4-C5-C6	8.20	121.10	117.00
22	BA	2450	A	N3-C4-C5	-8.20	121.06	126.80
22	BA	1384	A	C5-N7-C8	8.20	108.00	103.90
22	BA	2060	A	N3-C4-C5	-8.20	121.06	126.80
22	BA	743	A	C5-C6-N6	8.19	130.26	123.70
22	BA	2054	A	C5-C6-N6	8.20	130.26	123.70
22	BA	933	A	C5-N7-C8	8.19	108.00	103.90
54	D2	49	A	C5-N7-C8	8.19	108.00	103.90
22	BA	2386	A	C5-C6-N6	8.19	130.25	123.70
22	BA	592	A	C5-N7-C8	8.19	107.99	103.90
22	BA	1089	A	C5-N7-C8	8.19	108.00	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	722	A	C5-C6-N6	8.18	130.24	123.70
22	BA	1276	A	C5-N7-C8	8.18	107.99	103.90
22	BA	947	A	C5-N7-C8	8.18	107.99	103.90
22	BA	655	A	C5-N7-C8	8.17	107.98	103.90
22	BA	1057	A	C4-C5-C6	8.17	121.08	117.00
1	AA	87	C	C6-N1-C2	-8.16	117.03	120.30
22	BA	2736	A	C5-N7-C8	8.16	107.98	103.90
22	BA	661	A	C5-N7-C8	8.16	107.98	103.90
22	BA	752	A	C5-N7-C8	8.16	107.98	103.90
22	BA	1551	A	C5-N7-C8	8.16	107.98	103.90
22	BA	2461	A	C5-C6-N6	8.16	130.23	123.70
22	BA	196	A	C5-N7-C8	8.16	107.98	103.90
1	AA	95	C	C6-N1-C1'	-8.15	111.02	120.80
22	BA	19	A	C5-C6-N6	8.15	130.22	123.70
22	BA	1378	A	C5-N7-C8	8.15	107.97	103.90
22	BA	374	A	C5-N7-C8	8.15	107.97	103.90
22	BA	2482	A	C5-N7-C8	8.15	107.97	103.90
22	BA	2679	A	C5-C6-N6	8.14	130.22	123.70
22	BA	1583	A	C5-N7-C8	8.14	107.97	103.90
22	BA	2211	A	C5-N7-C8	8.14	107.97	103.90
22	BA	2850	A	C4-C5-C6	8.14	121.07	117.00
22	BA	1502	A	C5-N7-C8	8.14	107.97	103.90
22	BA	332	A	C5-N7-C8	8.13	107.97	103.90
22	BA	2829	A	C5-N7-C8	8.13	107.97	103.90
22	BA	1000	A	C5-N7-C8	8.13	107.97	103.90
22	BA	1314	C	C2-N1-C1'	8.13	127.74	118.80
22	BA	1413	A	C5-C6-N6	8.13	130.20	123.70
22	BA	340	A	C5-N7-C8	8.12	107.96	103.90
22	BA	1090	A	C5-N7-C8	8.12	107.96	103.90
22	BA	346	A	C5-N7-C8	8.12	107.96	103.90
22	BA	532	A	C5-N7-C8	8.11	107.96	103.90
22	BA	1050	A	C5-N7-C8	8.11	107.96	103.90
22	BA	412	A	C5-N7-C8	8.11	107.95	103.90
22	BA	2665	A	C5-N7-C8	8.11	107.95	103.90
22	BA	167	A	C5-N7-C8	8.10	107.95	103.90
22	BA	1054	A	C5-C6-N6	8.10	130.18	123.70
22	BA	428	A	C5-N7-C8	8.10	107.95	103.90
22	BA	1175	A	C5-N7-C8	8.10	107.95	103.90
22	BA	1634	A	C5-N7-C8	8.10	107.95	103.90
22	BA	1579	A	C5-N7-C8	8.09	107.95	103.90
22	BA	532	A	N3-C4-N9	8.09	133.87	127.40
22	BA	2077	A	C5-N7-C8	8.09	107.95	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1260	A	C5-N7-C8	8.09	107.94	103.90
22	BA	1749	A	C5-N7-C8	8.09	107.94	103.90
22	BA	2158	A	C5-N7-C8	8.09	107.94	103.90
22	BA	155	A	C5-N7-C8	8.09	107.94	103.90
22	BA	161	A	C5-N7-C8	8.09	107.94	103.90
22	BA	632	A	C5-N7-C8	8.08	107.94	103.90
54	D2	5	A	C5-N7-C8	8.08	107.94	103.90
22	BA	821	A	C5-N7-C8	8.08	107.94	103.90
22	BA	1420	A	C5-N7-C8	8.08	107.94	103.90
22	BA	1532	A	C5-N7-C8	8.08	107.94	103.90
22	BA	2070	A	C5-N7-C8	8.07	107.94	103.90
22	BA	2799	A	C5-C6-N6	8.07	130.16	123.70
22	BA	2142	A	C5-N7-C8	8.07	107.93	103.90
22	BA	2154	A	C5-N7-C8	8.07	107.93	103.90
22	BA	1635	A	C5-N7-C8	8.06	107.93	103.90
55	D3	21	A	C5-N7-C8	8.06	107.93	103.90
22	BA	1144	A	C5-N7-C8	8.05	107.93	103.90
22	BA	2632	A	C5-N7-C8	8.05	107.93	103.90
22	BA	910	A	C5-N7-C8	8.05	107.92	103.90
22	BA	227	A	C5-N7-C8	8.05	107.92	103.90
22	BA	1548	A	C5-N7-C8	8.05	107.92	103.90
22	BA	1616	A	C5-N7-C8	8.05	107.92	103.90
22	BA	56	A	C5-N7-C8	8.05	107.92	103.90
22	BA	443	A	C5-N7-C8	8.05	107.92	103.90
22	BA	84	A	C5-N7-C8	8.05	107.92	103.90
22	BA	899	A	C5-N7-C8	8.04	107.92	103.90
22	BA	101	A	N3-C4-N9	8.04	133.83	127.40
22	BA	1046	A	C5-N7-C8	8.04	107.92	103.90
22	BA	1194	A	C5-N7-C8	8.04	107.92	103.90
22	BA	2298	A	C5-N7-C8	8.04	107.92	103.90
22	BA	2660	A	C5-N7-C8	8.04	107.92	103.90
22	BA	2266	A	C5-N7-C8	8.04	107.92	103.90
22	BA	1439	A	C5-N7-C8	8.04	107.92	103.90
22	BA	2163	A	C5-N7-C8	8.03	107.92	103.90
22	BA	547	A	C5-N7-C8	8.03	107.92	103.90
22	BA	1453	A	C5-N7-C8	8.03	107.91	103.90
22	BA	14	A	C5-N7-C8	8.03	107.91	103.90
22	BA	1403	A	C5-N7-C8	8.03	107.91	103.90
23	BB	34	A	C5-N7-C8	8.03	107.91	103.90
22	BA	1872	A	C4-C5-C6	8.02	121.01	117.00
22	BA	2170	A	C5-N7-C8	8.02	107.91	103.90
22	BA	637	A	C5-N7-C8	8.02	107.91	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D2	59	A	C5-N7-C8	8.02	107.91	103.90
22	BA	508	A	C5-N7-C8	8.02	107.91	103.90
22	BA	1347	A	C5-N7-C8	8.02	107.91	103.90
22	BA	262	A	C5-N7-C8	8.02	107.91	103.90
22	BA	1287	A	C5-N7-C8	8.02	107.91	103.90
22	BA	1966	A	C5-N7-C8	8.02	107.91	103.90
22	BA	2851	A	C5-N7-C8	8.02	107.91	103.90
22	BA	1040	A	C5-N7-C8	8.01	107.90	103.90
22	BA	2322	A	C5-N7-C8	8.01	107.91	103.90
22	BA	670	A	C5-N7-C8	8.01	107.90	103.90
22	BA	1698	A	C5-N7-C8	8.01	107.90	103.90
22	BA	820	A	C5-N7-C8	8.00	107.90	103.90
22	BA	347	A	C5-N7-C8	8.00	107.90	103.90
22	BA	2094	A	C5-C6-N6	8.00	130.10	123.70
22	BA	1155	A	C5-N7-C8	7.99	107.89	103.90
22	BA	2173	A	C5-N7-C8	7.99	107.89	103.90
22	BA	925	A	C5-C6-N6	7.99	130.09	123.70
22	BA	64	A	C5-N7-C8	7.99	107.89	103.90
22	BA	2412	A	C4-C5-C6	7.98	120.99	117.00
22	BA	2478	A	C5-N7-C8	7.98	107.89	103.90
22	BA	453	A	C5-N7-C8	7.98	107.89	103.90
22	BA	1029	A	C4-C5-C6	7.98	120.99	117.00
22	BA	716	A	C5-N7-C8	7.98	107.89	103.90
22	BA	1815	A	C5-N7-C8	7.97	107.89	103.90
23	BB	53	A	C5-N7-C8	7.97	107.89	103.90
22	BA	1669	A	C4-C5-C6	7.97	120.98	117.00
22	BA	352	A	C5-N7-C8	7.97	107.89	103.90
22	BA	1783	A	C5-N7-C8	7.97	107.88	103.90
22	BA	2412	A	C5-N7-C8	7.97	107.88	103.90
55	D3	73	A	C5-N7-C8	7.97	107.88	103.90
22	BA	2541	A	C5-N7-C8	7.96	107.88	103.90
22	BA	2766	A	C5-C6-N6	7.96	130.07	123.70
22	BA	1570	A	C5-N7-C8	7.96	107.88	103.90
22	BA	255	A	C5-N7-C8	7.96	107.88	103.90
22	BA	342	A	C5-N7-C8	7.96	107.88	103.90
54	D2	14	A	C5-N7-C8	7.96	107.88	103.90
22	BA	1669	A	N3-C4-N9	7.96	133.76	127.40
22	BA	320	A	C5-N7-C8	7.95	107.88	103.90
22	BA	2062	A	C5-N7-C8	7.95	107.88	103.90
22	BA	504	A	C5-N7-C8	7.95	107.88	103.90
22	BA	71	A	C5-N7-C8	7.95	107.88	103.90
22	BA	693	A	C5-N7-C8	7.95	107.88	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	345	A	C5-N7-C8	7.95	107.88	103.90
22	BA	2114	A	N3-C4-N9	7.95	133.76	127.40
22	BA	1503	A	C5-N7-C8	7.95	107.87	103.90
22	BA	101	A	C4-C5-C6	7.94	120.97	117.00
22	BA	144	A	C5-C6-N6	7.94	130.05	123.70
22	BA	470	A	C5-N7-C8	7.94	107.87	103.90
22	BA	1392	A	C5-N7-C8	7.94	107.87	103.90
22	BA	2589	A	C5-N7-C8	7.94	107.87	103.90
22	BA	2225	A	C5-N7-C8	7.94	107.87	103.90
22	BA	2821	A	C5-N7-C8	7.94	107.87	103.90
22	BA	2542	A	C5-N7-C8	7.93	107.87	103.90
55	D3	14	A	C5-N7-C8	7.93	107.87	103.90
22	BA	2418	A	C5-N7-C8	7.93	107.87	103.90
22	BA	845	A	C5-N7-C8	7.93	107.87	103.90
22	BA	1981	A	C5-N7-C8	7.93	107.86	103.90
22	BA	1085	A	C5-N7-C8	7.93	107.86	103.90
22	BA	1640	A	C5-N7-C8	7.93	107.86	103.90
23	BB	108	A	C5-N7-C8	7.93	107.86	103.90
54	D2	9	A	C5-N7-C8	7.92	107.86	103.90
22	BA	126	A	C5-N7-C8	7.92	107.86	103.90
22	BA	2614	A	C5-N7-C8	7.92	107.86	103.90
22	BA	10	A	C5-N7-C8	7.92	107.86	103.90
22	BA	103	A	C5-N7-C8	7.92	107.86	103.90
22	BA	735	A	C5-N7-C8	7.92	107.86	103.90
22	BA	2635	A	C5-N7-C8	7.92	107.86	103.90
22	BA	330	A	C5-N7-C8	7.92	107.86	103.90
22	BA	2448	A	C5-N7-C8	7.92	107.86	103.90
22	BA	2530	A	C5-N7-C8	7.92	107.86	103.90
55	D3	23	A	C5-N7-C8	7.92	107.86	103.90
22	BA	1307	A	C5-N7-C8	7.92	107.86	103.90
22	BA	749	A	C5-N7-C8	7.91	107.86	103.90
22	BA	2733	A	C5-N7-C8	7.91	107.86	103.90
22	BA	917	A	C5-N7-C8	7.91	107.86	103.90
22	BA	1269	A	C5-N7-C8	7.91	107.86	103.90
22	BA	2835	A	C5-N7-C8	7.91	107.86	103.90
22	BA	457	A	C5-N7-C8	7.91	107.85	103.90
22	BA	2461	A	N3-C4-N9	7.91	133.73	127.40
22	BA	204	A	C8-N9-C4	7.91	108.96	105.80
22	BA	2778	A	C5-N7-C8	7.91	107.85	103.90
22	BA	1387	A	C5-N7-C8	7.90	107.85	103.90
22	BA	2183	A	C4-C5-C6	7.90	120.95	117.00
22	BA	2284	A	N3-C4-N9	7.90	133.72	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1096	A	C5-N7-C8	7.90	107.85	103.90
22	BA	483	A	C5-N7-C8	7.90	107.85	103.90
22	BA	574	A	C5-N7-C8	7.90	107.85	103.90
22	BA	602	A	C5-N7-C8	7.90	107.85	103.90
22	BA	613	A	C5-N7-C8	7.90	107.85	103.90
55	D3	26	A	C5-N7-C8	7.90	107.85	103.90
22	BA	344	A	C5-N7-C8	7.89	107.84	103.90
22	BA	866	A	C5-N7-C8	7.89	107.84	103.90
22	BA	2799	A	N3-C4-N9	7.89	133.71	127.40
22	BA	44	A	C5-N7-C8	7.88	107.84	103.90
22	BA	1889	A	C5-N7-C8	7.88	107.84	103.90
22	BA	582	A	C5-C6-N6	7.88	130.00	123.70
22	BA	1871	A	C5-N7-C8	7.88	107.84	103.90
22	BA	2750	A	C5-N7-C8	7.88	107.84	103.90
23	BB	45	A	C5-N7-C8	7.88	107.84	103.90
22	BA	2227	A	C5-N7-C8	7.88	107.84	103.90
22	BA	2003	A	C5-N7-C8	7.88	107.84	103.90
22	BA	256	A	C5-N7-C8	7.87	107.84	103.90
22	BA	627	A	C5-N7-C8	7.87	107.84	103.90
22	BA	1014	A	C5-N7-C8	7.87	107.84	103.90
22	BA	2314	A	C5-N7-C8	7.87	107.84	103.90
22	BA	1272	A	C5-N7-C8	7.87	107.84	103.90
22	BA	541	A	C5-N7-C8	7.87	107.83	103.90
22	BA	1126	A	C5-N7-C8	7.87	107.83	103.90
22	BA	2095	A	C5-N7-C8	7.87	107.83	103.90
22	BA	668	A	C5-N7-C8	7.86	107.83	103.90
22	BA	144	A	C5-N7-C8	7.86	107.83	103.90
22	BA	190	A	C5-N7-C8	7.86	107.83	103.90
22	BA	1383	A	C5-N7-C8	7.86	107.83	103.90
22	BA	2430	A	N7-C8-N9	-7.86	109.87	113.80
22	BA	877	A	C5-N7-C8	7.86	107.83	103.90
22	BA	2386	A	C5-N7-C8	7.86	107.83	103.90
22	BA	676	A	C5-N7-C8	7.86	107.83	103.90
22	BA	1848	A	N7-C8-N9	-7.86	109.87	113.80
22	BA	502	A	C5-N7-C8	7.86	107.83	103.90
22	BA	1668	A	C5-N7-C8	7.86	107.83	103.90
22	BA	1009	A	C5-N7-C8	7.85	107.83	103.90
22	BA	1272	A	C8-N9-C4	7.85	108.94	105.80
22	BA	2042	A	C5-N7-C8	7.85	107.83	103.90
22	BA	2534	A	C5-N7-C8	7.85	107.83	103.90
22	BA	2654	A	C5-N7-C8	7.85	107.82	103.90
22	BA	278	A	N3-C4-N9	7.85	133.68	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	878	A	C5-N7-C8	7.84	107.82	103.90
22	BA	1590	A	C5-N7-C8	7.84	107.82	103.90
22	BA	2461	A	C4-C5-C6	7.84	120.92	117.00
22	BA	101	A	C5-N7-C8	7.84	107.82	103.90
22	BA	1134	A	C5-N7-C8	7.84	107.82	103.90
22	BA	2191	A	C5-N7-C8	7.84	107.82	103.90
22	BA	2837	A	C5-N7-C8	7.84	107.82	103.90
22	BA	2080	A	C4-C5-C6	7.83	120.92	117.00
22	BA	447	A	C5-N7-C8	7.83	107.82	103.90
23	BB	94	A	C5-N7-C8	7.83	107.82	103.90
23	BB	59	A	C5-N7-C8	7.83	107.81	103.90
23	BB	109	A	C5-N7-C8	7.83	107.81	103.90
22	BA	415	A	C4-C5-C6	7.82	120.91	117.00
22	BA	2005	A	C5-N7-C8	7.82	107.81	103.90
23	BB	115	A	C5-N7-C8	7.82	107.81	103.90
22	BA	362	A	C5-N7-C8	7.82	107.81	103.90
22	BA	1129	A	C5-N7-C8	7.82	107.81	103.90
22	BA	2670	A	C5-N7-C8	7.82	107.81	103.90
55	D3	31	A	C5-N7-C8	7.82	107.81	103.90
22	BA	1858	A	C5-N7-C8	7.82	107.81	103.90
22	BA	2205	A	C5-N7-C8	7.82	107.81	103.90
22	BA	382	A	C5-N7-C8	7.81	107.81	103.90
23	BB	52	A	C5-N7-C8	7.81	107.81	103.90
22	BA	2309	A	C5-N7-C8	7.81	107.81	103.90
22	BA	2386	A	C4-C5-C6	7.81	120.91	117.00
22	BA	2461	A	C5-N7-C8	7.81	107.80	103.90
22	BA	1392	A	N9-C4-C5	7.80	108.92	105.80
22	BA	1773	A	C4-C5-C6	7.80	120.90	117.00
22	BA	1735	A	C5-N7-C8	7.80	107.80	103.90
23	BB	94	A	C4-C5-C6	7.80	120.90	117.00
22	BA	83	A	C5-N7-C8	7.80	107.80	103.90
22	BA	84	A	C8-N9-C4	7.80	108.92	105.80
22	BA	925	A	C5-N7-C8	7.80	107.80	103.90
22	BA	1054	A	C5-N7-C8	7.80	107.80	103.90
22	BA	311	A	C5-N7-C8	7.79	107.80	103.90
22	BA	74	A	C5-N7-C8	7.79	107.80	103.90
22	BA	1088	A	C5-N7-C8	7.79	107.80	103.90
22	BA	2765	A	C5-N7-C8	7.79	107.79	103.90
22	BA	270	A	C5-N7-C8	7.79	107.79	103.90
22	BA	1819	A	C5-N7-C8	7.79	107.79	103.90
22	BA	216	A	C5-N7-C8	7.78	107.79	103.90
22	BA	1342	A	C5-N7-C8	7.78	107.79	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2031	A	C5-N7-C8	7.78	107.79	103.90
55	D3	17	C	C6-N1-C2	-7.78	117.19	120.30
22	BA	2082	A	C5-N7-C8	7.78	107.79	103.90
22	BA	2826	A	C5-N7-C8	7.78	107.79	103.90
22	BA	89	A	C5-N7-C8	7.78	107.79	103.90
22	BA	1890	A	C5-N7-C8	7.78	107.79	103.90
22	BA	928	A	C5-N7-C8	7.77	107.79	103.90
22	BA	1665	A	C5-N7-C8	7.77	107.79	103.90
22	BA	2764	A	C5-N7-C8	7.77	107.79	103.90
22	BA	1367	A	C5-N7-C8	7.77	107.79	103.90
22	BA	1395	A	C5-N7-C8	7.77	107.79	103.90
22	BA	1508	A	C5-N7-C8	7.77	107.79	103.90
22	BA	2171	A	C5-N7-C8	7.77	107.78	103.90
22	BA	685	A	C5-N7-C8	7.77	107.78	103.90
22	BA	792	A	C5-N7-C8	7.77	107.78	103.90
22	BA	592	A	C4-C5-C6	7.76	120.88	117.00
22	BA	172	A	C5-N7-C8	7.76	107.78	103.90
22	BA	960	A	C5-N7-C8	7.76	107.78	103.90
22	BA	2054	A	C5-N7-C8	7.76	107.78	103.90
22	BA	1701	A	C5-N7-C8	7.76	107.78	103.90
22	BA	2725	A	C5-N7-C8	7.76	107.78	103.90
22	BA	2800	A	C5-N7-C8	7.76	107.78	103.90
22	BA	2407	A	C4-C5-C6	7.76	120.88	117.00
54	D2	41	A	C5-N7-C8	7.75	107.78	103.90
22	BA	1086	A	C5-N7-C8	7.75	107.78	103.90
22	BA	1787	A	C5-N7-C8	7.75	107.78	103.90
22	BA	1784	A	C5-N7-C8	7.75	107.78	103.90
22	BA	1095	A	C5-N7-C8	7.75	107.78	103.90
22	BA	2711	A	C5-N7-C8	7.75	107.78	103.90
22	BA	1077	A	C5-N7-C8	7.75	107.77	103.90
22	BA	1780	A	C5-N7-C8	7.75	107.77	103.90
22	BA	2366	A	C4-C5-C6	7.75	120.87	117.00
22	BA	2590	A	C5-N7-C8	7.75	107.77	103.90
23	BB	73	A	N3-C4-N9	7.75	133.60	127.40
22	BA	501	A	C5-N7-C8	7.74	107.77	103.90
22	BA	1269	A	C4-C5-C6	7.74	120.87	117.00
22	BA	1759	A	C5-N7-C8	7.74	107.77	103.90
22	BA	2856	A	C5-N7-C8	7.74	107.77	103.90
22	BA	241	A	C5-N7-C8	7.74	107.77	103.90
22	BA	819	A	C5-N7-C8	7.74	107.77	103.90
22	BA	2471	A	C5-N7-C8	7.74	107.77	103.90
22	BA	984	A	N3-C4-N9	7.74	133.59	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2015	A	C5-N7-C8	7.74	107.77	103.90
22	BA	699	A	C5-N7-C8	7.73	107.77	103.90
22	BA	1960	A	C5-N7-C8	7.73	107.77	103.90
22	BA	2327	A	C5-N7-C8	7.73	107.77	103.90
55	D3	31	A	N3-C4-N9	7.73	133.59	127.40
22	BA	2267	A	C5-N7-C8	7.73	107.77	103.90
22	BA	2284	A	C5-N7-C8	7.73	107.77	103.90
22	BA	391	A	C5-N7-C8	7.73	107.76	103.90
22	BA	529	A	C5-N7-C8	7.73	107.76	103.90
22	BA	2020	A	C5-N7-C8	7.73	107.76	103.90
22	BA	2560	A	C5-N7-C8	7.73	107.76	103.90
55	D3	64	A	N3-C4-N9	7.73	133.58	127.40
22	BA	181	A	C5-N7-C8	7.72	107.76	103.90
22	BA	844	A	C5-N7-C8	7.72	107.76	103.90
22	BA	2639	A	C5-N7-C8	7.72	107.76	103.90
22	BA	1596	A	C5-N7-C8	7.72	107.76	103.90
22	BA	2886	A	C5-N7-C8	7.72	107.76	103.90
22	BA	432	A	C5-N7-C8	7.72	107.76	103.90
22	BA	1336	A	C5-N7-C8	7.72	107.76	103.90
22	BA	118	A	C5-N7-C8	7.72	107.76	103.90
22	BA	2097	A	C5-N7-C8	7.72	107.76	103.90
22	BA	1039	A	C5-N7-C8	7.72	107.76	103.90
22	BA	1598	A	C5-N7-C8	7.72	107.76	103.90
22	BA	1669	A	C5-N7-C8	7.72	107.76	103.90
22	BA	278	A	C5-N7-C8	7.71	107.76	103.90
22	BA	1021	A	C5-C6-N1	7.71	121.56	117.70
55	D3	58	A	C5-N7-C8	7.71	107.76	103.90
22	BA	563	A	C5-N7-C8	7.71	107.76	103.90
22	BA	272	A	C5-N7-C8	7.71	107.75	103.90
1	AA	489	C	N3-C2-O2	-7.71	116.50	121.90
55	D3	17	C	N3-C2-O2	-7.71	116.50	121.90
22	BA	1528	A	C5-N7-C8	7.71	107.75	103.90
22	BA	1998	A	C4-C5-C6	7.70	120.85	117.00
22	BA	131	A	C5-N7-C8	7.70	107.75	103.90
22	BA	52	A	C5-N7-C8	7.70	107.75	103.90
22	BA	38	A	C5-N7-C8	7.70	107.75	103.90
55	D3	76	A	C5-N7-C8	7.70	107.75	103.90
22	BA	2882	A	C5-N7-C8	7.70	107.75	103.90
22	BA	1327	A	C5-N7-C8	7.69	107.75	103.90
22	BA	2758	A	C5-N7-C8	7.69	107.75	103.90
22	BA	5	A	C4-C5-C6	7.69	120.84	117.00
22	BA	1970	A	N3-C4-N9	7.69	133.55	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2433	A	C5-N7-C8	7.69	107.75	103.90
22	BA	1744	A	C5-N7-C8	7.69	107.74	103.90
22	BA	1032	A	C5-N7-C8	7.69	107.74	103.90
22	BA	1469	A	C5-N7-C8	7.69	107.74	103.90
22	BA	142	A	C5-N7-C8	7.68	107.74	103.90
22	BA	1549	A	C5-N7-C8	7.68	107.74	103.90
22	BA	2270	A	C5-N7-C8	7.68	107.74	103.90
22	BA	156	A	C4-C5-C6	7.68	120.84	117.00
22	BA	1304	A	C5-N7-C8	7.68	107.74	103.90
22	BA	2634	A	C5-N7-C8	7.68	107.74	103.90
22	BA	960	A	C4-C5-C6	7.68	120.84	117.00
22	BA	2336	A	C5-N7-C8	7.68	107.74	103.90
22	BA	2346	A	C5-N7-C8	7.68	107.74	103.90
22	BA	1067	A	C5-N7-C8	7.68	107.74	103.90
22	BA	1717	A	C5-N7-C8	7.68	107.74	103.90
22	BA	528	A	C5-N7-C8	7.67	107.74	103.90
22	BA	1205	A	C5-N7-C8	7.67	107.73	103.90
22	BA	2088	A	C5-N7-C8	7.67	107.73	103.90
22	BA	2435	A	C5-N7-C8	7.67	107.73	103.90
23	BB	15	A	C5-N7-C8	7.67	107.73	103.90
22	BA	2369	A	C5-N7-C8	7.67	107.73	103.90
22	BA	2706	A	C4-C5-C6	7.67	120.83	117.00
22	BA	631	A	C5-N7-C8	7.66	107.73	103.90
22	BA	2273	A	C5-N7-C8	7.66	107.73	103.90
22	BA	616	A	C5-N7-C8	7.66	107.73	103.90
22	BA	2459	A	C5-C6-N6	7.66	129.83	123.70
22	BA	2184	A	C5-N7-C8	7.66	107.73	103.90
55	D3	38	A	C5-N7-C8	7.66	107.73	103.90
22	BA	482	A	C5-N7-C8	7.65	107.73	103.90
22	BA	2284	A	C5-C6-N6	7.65	129.82	123.70
22	BA	1308	A	C5-N7-C8	7.65	107.72	103.90
22	BA	1739	A	C4-C5-C6	7.65	120.83	117.00
22	BA	2547	A	C5-N7-C8	7.64	107.72	103.90
22	BA	28	A	C5-N7-C8	7.64	107.72	103.90
22	BA	675	A	C5-N7-C8	7.64	107.72	103.90
22	BA	2392	A	C4-C5-C6	7.64	120.82	117.00
22	BA	1057	A	N3-C4-N9	7.64	133.51	127.40
22	BA	1794	A	C5-N7-C8	7.64	107.72	103.90
22	BA	2518	A	N3-C4-N9	7.64	133.51	127.40
22	BA	282	A	C5-C6-N6	7.63	129.81	123.70
22	BA	1494	A	C5-N7-C8	7.63	107.72	103.90
22	BA	1632	A	C5-N7-C8	7.63	107.72	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D2	26	A	C5-N7-C8	7.63	107.72	103.90
22	BA	2602	A	N3-C4-N9	7.63	133.51	127.40
22	BA	2439	A	C5-N7-C8	7.63	107.72	103.90
22	BA	1593	A	C5-N7-C8	7.63	107.71	103.90
22	BA	633	A	C5-N7-C8	7.63	107.71	103.90
22	BA	1268	A	C5-N7-C8	7.63	107.71	103.90
22	BA	1569	A	C5-N7-C8	7.63	107.71	103.90
22	BA	1641	A	C5-N7-C8	7.63	107.71	103.90
22	BA	1678	A	C5-N7-C8	7.63	107.71	103.90
22	BA	1690	A	C5-N7-C8	7.63	107.71	103.90
22	BA	2090	A	C5-N7-C8	7.63	107.71	103.90
22	BA	1142	A	C5-N7-C8	7.62	107.71	103.90
22	BA	1021	A	C4-C5-C6	7.62	120.81	117.00
54	D2	38	A	C5-N7-C8	7.62	107.71	103.90
55	D3	64	A	C5-C6-N6	7.62	129.80	123.70
22	BA	182	A	C5-N7-C8	7.62	107.71	103.90
22	BA	1916	A	C5-N7-C8	7.61	107.71	103.90
22	BA	2013	A	C5-N7-C8	7.61	107.71	103.90
22	BA	1772	A	C5-N7-C8	7.61	107.71	103.90
23	BB	99	A	C5-N7-C8	7.61	107.70	103.90
22	BA	1746	A	C5-N7-C8	7.61	107.70	103.90
22	BA	892	A	N3-C4-N9	7.61	133.49	127.40
22	BA	1189	A	C5-N7-C8	7.60	107.70	103.90
22	BA	1048	A	N3-C4-N9	7.60	133.48	127.40
22	BA	2376	A	C5-N7-C8	7.60	107.70	103.90
22	BA	996	A	C5-N7-C8	7.60	107.70	103.90
22	BA	800	A	N3-C4-C5	-7.60	121.48	126.80
22	BA	804	A	C5-N7-C8	7.60	107.70	103.90
22	BA	1853	A	C5-N7-C8	7.59	107.70	103.90
22	BA	2518	A	C5-N7-C8	7.59	107.70	103.90
22	BA	1366	A	C5-N7-C8	7.59	107.70	103.90
22	BA	152	A	C4-C5-C6	7.59	120.80	117.00
22	BA	1505	A	C5-N7-C8	7.59	107.70	103.90
22	BA	1545	A	C5-N7-C8	7.59	107.70	103.90
22	BA	2060	A	C8-N9-C4	7.59	108.84	105.80
22	BA	1431	A	C5-N7-C8	7.59	107.69	103.90
22	BA	2080	A	N3-C4-N9	7.59	133.47	127.40
22	BA	94	A	C5-N7-C8	7.58	107.69	103.90
22	BA	119	A	C5-N7-C8	7.58	107.69	103.90
22	BA	2094	A	C5-N7-C8	7.58	107.69	103.90
22	BA	1365	A	C5-N7-C8	7.58	107.69	103.90
22	BA	2700	A	C5-N7-C8	7.58	107.69	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2572	A	C8-N9-C4	7.58	108.83	105.80
22	BA	1021	A	C5-N7-C8	7.58	107.69	103.90
22	BA	1419	A	C5-N7-C8	7.58	107.69	103.90
23	BB	94	A	N3-C4-N9	7.58	133.46	127.40
22	BA	1553	A	C5-N7-C8	7.58	107.69	103.90
22	BA	2328	A	N9-C4-C5	7.58	108.83	105.80
22	BA	936	A	C5-N7-C8	7.58	107.69	103.90
22	BA	1213	A	C4-C5-C6	7.57	120.79	117.00
22	BA	1321	A	C5-N7-C8	7.57	107.69	103.90
22	BA	582	A	C5-N7-C8	7.57	107.68	103.90
22	BA	231	A	C5-N7-C8	7.56	107.68	103.90
22	BA	532	A	C4-C5-C6	7.56	120.78	117.00
22	BA	750	A	N3-C4-N9	7.56	133.45	127.40
22	BA	1001	A	C5-N7-C8	7.56	107.68	103.90
22	BA	1226	A	C5-N7-C8	7.56	107.68	103.90
22	BA	1301	A	C5-N7-C8	7.56	107.68	103.90
22	BA	42	A	C5-N7-C8	7.56	107.68	103.90
22	BA	1801	A	C5-N7-C8	7.56	107.68	103.90
22	BA	2037	A	C5-N7-C8	7.56	107.68	103.90
22	BA	522	A	C4-C5-C6	7.55	120.78	117.00
22	BA	753	A	N3-C4-N9	7.55	133.44	127.40
22	BA	730	A	C4-C5-C6	7.55	120.77	117.00
22	BA	800	A	C8-N9-C4	7.55	108.82	105.80
22	BA	721	A	C5-N7-C8	7.55	107.67	103.90
22	BA	1365	A	N3-C4-N9	7.55	133.44	127.40
22	BA	2799	A	C4-C5-C6	7.54	120.77	117.00
22	BA	2198	A	C5-N7-C8	7.54	107.67	103.90
22	BA	2513	A	C5-N7-C8	7.54	107.67	103.90
22	BA	603	A	C5-N7-C8	7.54	107.67	103.90
22	BA	849	A	C5-N7-C8	7.54	107.67	103.90
22	BA	918	A	C5-N7-C8	7.54	107.67	103.90
22	BA	309	A	C5-N7-C8	7.53	107.67	103.90
22	BA	1528	A	N3-C4-N9	7.53	133.43	127.40
22	BA	1285	A	C5-N7-C8	7.53	107.67	103.90
22	BA	402	A	C5-N7-C8	7.53	107.67	103.90
22	BA	675	A	N3-C4-N9	7.53	133.42	127.40
22	BA	933	A	C4-C5-C6	7.53	120.77	117.00
22	BA	2340	A	C5-N7-C8	7.53	107.67	103.90
22	BA	2060	A	C5-N7-C8	7.53	107.67	103.90
22	BA	2173	A	N3-C4-N9	7.53	133.42	127.40
22	BA	1347	A	N9-C4-C5	7.53	108.81	105.80
22	BA	265	A	C5-N7-C8	7.53	107.66	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	439	A	C5-N7-C8	7.53	107.66	103.90
22	BA	1246	A	C5-N7-C8	7.53	107.66	103.90
22	BA	1847	A	C4-C5-C6	7.53	120.76	117.00
22	BA	1938	A	C5-N7-C8	7.53	107.66	103.90
23	BB	46	A	C5-N7-C8	7.53	107.66	103.90
22	BA	1028	A	C5-N7-C8	7.52	107.66	103.90
22	BA	626	A	C5-N7-C8	7.52	107.66	103.90
22	BA	1609	A	C5-N7-C8	7.52	107.66	103.90
22	BA	1987	A	C5-N7-C8	7.52	107.66	103.90
22	BA	2406	A	C5-N7-C8	7.52	107.66	103.90
22	BA	1169	A	C5-N7-C8	7.52	107.66	103.90
22	BA	1490	A	C5-N7-C8	7.52	107.66	103.90
22	BA	294	A	C5-N7-C8	7.52	107.66	103.90
22	BA	522	A	N3-C4-N9	7.51	133.41	127.40
22	BA	666	A	C5-N7-C8	7.51	107.66	103.90
22	BA	1544	A	C5-N7-C8	7.51	107.66	103.90
22	BA	1413	A	C5-N7-C8	7.50	107.65	103.90
22	BA	2893	A	C5-N7-C8	7.50	107.65	103.90
22	BA	176	A	C5-N7-C8	7.50	107.65	103.90
22	BA	706	A	C5-N7-C8	7.50	107.65	103.90
22	BA	2284	A	C4-C5-C6	7.50	120.75	117.00
22	BA	330	A	N3-C4-N9	7.50	133.40	127.40
22	BA	1275	A	C5-N7-C8	7.50	107.65	103.90
22	BA	84	A	N3-C4-C5	-7.50	121.55	126.80
22	BA	1848	A	C4-C5-C6	7.50	120.75	117.00
22	BA	2513	A	C4-C5-C6	7.50	120.75	117.00
22	BA	2459	A	C4-C5-C6	7.49	120.75	117.00
22	BA	621	A	C5-N7-C8	7.49	107.65	103.90
22	BA	1230	A	C5-N7-C8	7.49	107.65	103.90
22	BA	1385	A	C8-N9-C4	7.49	108.80	105.80
23	BB	78	A	C5-N7-C8	7.49	107.65	103.90
22	BA	1373	A	C5-N7-C8	7.49	107.64	103.90
22	BA	1241	A	C5-N7-C8	7.49	107.64	103.90
23	BB	58	A	C5-N7-C8	7.48	107.64	103.90
22	BA	599	A	C5-N7-C8	7.48	107.64	103.90
22	BA	2077	A	N3-C4-N9	7.48	133.39	127.40
22	BA	582	A	C4-C5-C6	7.48	120.74	117.00
22	BA	1953	A	C5-N7-C8	7.48	107.64	103.90
22	BA	479	A	C8-N9-C4	7.48	108.79	105.80
22	BA	863	A	C5-N7-C8	7.48	107.64	103.90
22	BA	1711	A	C5-N7-C8	7.48	107.64	103.90
22	BA	2679	A	N3-C4-N9	7.48	133.38	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2114	A	C5-N7-C8	7.48	107.64	103.90
22	BA	222	A	C5-N7-C8	7.47	107.64	103.90
22	BA	2883	A	C5-N7-C8	7.47	107.64	103.90
22	BA	244	A	C5-N7-C8	7.47	107.64	103.90
22	BA	449	A	C5-N7-C8	7.47	107.64	103.90
22	BA	149	A	C5-N7-C8	7.47	107.64	103.90
22	BA	1020	A	C5-N7-C8	7.47	107.63	103.90
22	BA	2600	A	C5-N7-C8	7.47	107.63	103.90
22	BA	497	A	C5-N7-C8	7.47	107.63	103.90
22	BA	1877	A	C5-N7-C8	7.46	107.63	103.90
22	BA	1912	A	C8-N9-C4	7.46	108.78	105.80
22	BA	401	A	C5-N7-C8	7.46	107.63	103.90
22	BA	1084	A	C5-N7-C8	7.46	107.63	103.90
22	BA	2101	A	C5-N7-C8	7.46	107.63	103.90
22	BA	2873	A	C5-N7-C8	7.46	107.63	103.90
22	BA	2887	A	C5-N7-C8	7.46	107.63	103.90
22	BA	348	A	C5-N7-C8	7.46	107.63	103.90
22	BA	753	A	C4-C5-C6	7.46	120.73	117.00
22	BA	980	A	C5-N7-C8	7.46	107.63	103.90
22	BA	2037	A	C4-C5-C6	7.45	120.72	117.00
22	BA	2317	A	C5-N7-C8	7.45	107.62	103.90
22	BA	793	A	C5-N7-C8	7.45	107.62	103.90
22	BA	613	A	C4-C5-C6	7.45	120.72	117.00
22	BA	2589	A	C8-N9-C4	7.44	108.78	105.80
22	BA	959	A	C5-N7-C8	7.44	107.62	103.90
22	BA	1552	A	C5-N7-C8	7.44	107.62	103.90
22	BA	21	A	C5-N7-C8	7.44	107.62	103.90
22	BA	2850	A	N3-C4-N9	7.44	133.35	127.40
55	D3	53	G	C5-C6-O6	7.44	133.06	128.60
22	BA	526	A	C5-N7-C8	7.43	107.62	103.90
22	BA	2268	A	C5-N7-C8	7.43	107.62	103.90
22	BA	146	A	C5-N7-C8	7.43	107.61	103.90
22	BA	278	A	C4-C5-C6	7.42	120.71	117.00
22	BA	1470	A	C4-C5-C6	7.42	120.71	117.00
22	BA	2328	A	C5-N7-C8	7.42	107.61	103.90
22	BA	2657	A	C5-N7-C8	7.42	107.61	103.90
22	BA	1269	A	N3-C4-N9	7.42	133.34	127.40
22	BA	2281	A	C5-N7-C8	7.42	107.61	103.90
22	BA	2058	A	C5-N7-C8	7.42	107.61	103.90
22	BA	1302	A	C5-N7-C8	7.41	107.61	103.90
22	BA	1387	A	C4-C5-C6	7.41	120.70	117.00
22	BA	2566	A	C5-N7-C8	7.41	107.61	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1010	A	C5-N7-C8	7.41	107.60	103.90
22	BA	1970	A	C5-N7-C8	7.40	107.60	103.90
22	BA	2468	A	C5-N7-C8	7.40	107.60	103.90
22	BA	1571	A	C5-N7-C8	7.40	107.60	103.90
22	BA	789	A	C5-N7-C8	7.40	107.60	103.90
22	BA	63	A	C5-N7-C8	7.40	107.60	103.90
22	BA	1127	A	C5-N7-C8	7.40	107.60	103.90
22	BA	2033	A	N9-C4-C5	7.39	108.76	105.80
22	BA	160	A	C5-N7-C8	7.39	107.60	103.90
22	BA	1787	A	N3-C4-N9	7.39	133.31	127.40
22	BA	2052	A	N3-C4-N9	7.39	133.31	127.40
22	BA	1730	C	C6-N1-C2	-7.39	117.34	120.30
54	D2	28	A	N3-C4-N9	7.39	133.31	127.40
22	BA	6	A	C5-N7-C8	7.39	107.59	103.90
22	BA	374	A	C4-C5-C6	7.39	120.69	117.00
22	BA	430	A	C5-N7-C8	7.39	107.59	103.90
22	BA	1286	A	C5-N7-C8	7.39	107.59	103.90
22	BA	2247	A	C4-C5-C6	7.38	120.69	117.00
22	BA	2662	A	N3-C4-N9	7.38	133.31	127.40
22	BA	1805	A	N9-C4-C5	7.38	108.75	105.80
22	BA	374	A	N3-C4-N9	7.38	133.30	127.40
22	BA	975	A	C5-N7-C8	7.38	107.59	103.90
22	BA	1008	A	C5-N7-C8	7.38	107.59	103.90
22	BA	2407	A	N3-C4-N9	7.38	133.30	127.40
22	BA	739	A	C5-N7-C8	7.38	107.59	103.90
22	BA	492	A	C5-N7-C8	7.37	107.59	103.90
22	BA	2809	A	C5-N7-C8	7.37	107.59	103.90
22	BA	1548	A	C4-C5-C6	7.37	120.69	117.00
22	BA	2411	A	C5-N7-C8	7.37	107.58	103.90
22	BA	44	A	C4-C5-C6	7.37	120.68	117.00
22	BA	13	A	C5-N7-C8	7.37	107.58	103.90
22	BA	1328	A	C5-N7-C8	7.37	107.58	103.90
22	BA	505	A	C5-N7-C8	7.37	107.58	103.90
22	BA	582	A	N3-C4-N9	7.37	133.29	127.40
22	BA	2899	A	C4-C5-C6	7.37	120.68	117.00
56	D4	1	U	C2-N1-C1'	7.36	126.54	117.70
22	BA	2776	A	C8-N9-C4	7.36	108.75	105.80
1	AA	960	U	C2-N1-C1'	7.36	126.53	117.70
22	BA	2071	A	C5-N7-C8	7.36	107.58	103.90
22	BA	391	A	N3-C4-N9	7.36	133.29	127.40
22	BA	575	A	C5-N7-C8	7.36	107.58	103.90
22	BA	705	A	N3-C4-N9	7.36	133.29	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1745	A	C5-N7-C8	7.36	107.58	103.90
22	BA	2019	A	C5-N7-C8	7.36	107.58	103.90
22	BA	1431	A	C4-C5-C6	7.35	120.68	117.00
22	BA	2820	A	C5-N7-C8	7.35	107.58	103.90
22	BA	2823	A	C5-N7-C8	7.35	107.58	103.90
22	BA	1029	A	C5-N7-C8	7.35	107.58	103.90
22	BA	730	A	C5-N7-C8	7.35	107.57	103.90
22	BA	2439	A	C8-N9-C4	7.35	108.74	105.80
22	BA	2749	A	C5-N7-C8	7.35	107.57	103.90
22	BA	1434	A	C5-N7-C8	7.34	107.57	103.90
54	D2	51	A	C5-N7-C8	7.34	107.57	103.90
22	BA	1739	A	N3-C4-N9	7.34	133.27	127.40
22	BA	1373	A	C4-C5-C6	7.34	120.67	117.00
55	D3	74	C	N1-C2-O2	7.34	123.31	118.90
22	BA	721	A	C4-C5-C6	7.34	120.67	117.00
22	BA	1262	A	C5-N7-C8	7.34	107.57	103.90
22	BA	1477	A	C5-N7-C8	7.34	107.57	103.90
23	BB	34	A	C4-C5-C6	7.34	120.67	117.00
22	BA	2212	A	C5-N7-C8	7.33	107.57	103.90
22	BA	996	A	C4-C5-C6	7.33	120.67	117.00
22	BA	1808	A	C5-N7-C8	7.33	107.56	103.90
54	D2	28	A	C4-C5-C6	7.33	120.67	117.00
22	BA	1054	A	C4-C5-C6	7.33	120.67	117.00
22	BA	1151	A	C5-N7-C8	7.33	107.56	103.90
22	BA	1810	A	N3-C4-N9	7.33	133.26	127.40
22	BA	19	A	C4-C5-C6	7.33	120.66	117.00
22	BA	262	A	C4-C5-C6	7.33	120.66	117.00
22	BA	614	A	C8-N9-C4	7.32	108.73	105.80
22	BA	1348	C	N1-C2-O2	7.32	123.29	118.90
22	BA	1700	A	C5-N7-C8	7.32	107.56	103.90
23	BB	73	A	C4-C5-C6	7.32	120.66	117.00
22	BA	1978	A	C5-N7-C8	7.32	107.56	103.90
22	BA	2727	A	C5-N7-C8	7.32	107.56	103.90
22	BA	1572	A	C4-C5-C6	7.31	120.66	117.00
22	BA	1821	A	C5-N7-C8	7.31	107.56	103.90
22	BA	2407	A	C5-N7-C8	7.31	107.56	103.90
22	BA	1591	A	C4-C5-C6	7.31	120.66	117.00
22	BA	1650	A	C5-N7-C8	7.31	107.55	103.90
22	BA	226	A	C4-C5-C6	7.31	120.65	117.00
22	BA	1713	A	C5-N7-C8	7.31	107.55	103.90
22	BA	1735	A	C4-C5-C6	7.31	120.65	117.00
22	BA	849	A	C4-C5-C6	7.30	120.65	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2900	A	C5-N7-C8	7.30	107.55	103.90
22	BA	1998	A	N3-C4-N9	7.30	133.24	127.40
22	BA	2287	A	N3-C4-N9	7.30	133.24	127.40
22	BA	1586	A	C5-N7-C8	7.30	107.55	103.90
22	BA	1654	A	C5-N7-C8	7.30	107.55	103.90
22	BA	654	A	C5-N7-C8	7.29	107.55	103.90
22	BA	983	A	C5-N7-C8	7.29	107.55	103.90
22	BA	2753	A	C5-N7-C8	7.29	107.55	103.90
22	BA	1495	A	C5-N7-C8	7.29	107.54	103.90
22	BA	1755	A	C5-N7-C8	7.29	107.54	103.90
22	BA	2392	A	C5-N7-C8	7.29	107.54	103.90
23	BB	73	A	C5-N7-C8	7.29	107.55	103.90
22	BA	1705	A	C5-N7-C8	7.29	107.54	103.90
22	BA	2378	A	C5-N7-C8	7.29	107.54	103.90
23	BB	39	A	C5-N7-C8	7.29	107.54	103.90
22	BA	1433	A	C5-N7-C8	7.28	107.54	103.90
22	BA	750	A	C4-C5-C6	7.28	120.64	117.00
22	BA	742	A	C5-N7-C8	7.28	107.54	103.90
22	BA	1630	A	N9-C4-C5	7.28	108.71	105.80
22	BA	609	A	C5-N7-C8	7.28	107.54	103.90
22	BA	2451	A	C5-N7-C8	7.28	107.54	103.90
22	BA	1548	A	N3-C4-N9	7.27	133.22	127.40
22	BA	1525	A	C5-N7-C8	7.27	107.54	103.90
29	BH	122	LEU	CA-CB-CG	7.27	132.03	115.30
22	BA	715	A	C5-N7-C8	7.27	107.53	103.90
22	BA	2721	A	C5-N7-C8	7.27	107.53	103.90
23	BB	104	A	C5-N7-C8	7.27	107.53	103.90
22	BA	1354	A	C5-N7-C8	7.27	107.53	103.90
22	BA	1603	A	N3-C4-N9	7.27	133.21	127.40
22	BA	1899	A	C5-N7-C8	7.27	107.53	103.90
23	BB	101	A	C5-N7-C8	7.27	107.53	103.90
22	BA	1789	A	C5-N7-C8	7.26	107.53	103.90
22	BA	2311	A	C5-N7-C8	7.26	107.53	103.90
22	BA	2705	A	C5-N7-C8	7.26	107.53	103.90
22	BA	2054	A	N3-C4-N9	7.26	133.21	127.40
22	BA	782	A	C5-N7-C8	7.26	107.53	103.90
22	BA	1572	A	C5-N7-C8	7.26	107.53	103.90
22	BA	705	A	C4-C5-C6	7.26	120.63	117.00
22	BA	1689	A	C5-N7-C8	7.26	107.53	103.90
22	BA	1496	A	C5-N7-C8	7.25	107.53	103.90
22	BA	2434	A	C5-N7-C8	7.25	107.53	103.90
22	BA	95	A	C4-C5-C6	7.25	120.63	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	477	A	C5-N7-C8	7.25	107.53	103.90
22	BA	2453	A	C5-N7-C8	7.25	107.53	103.90
22	BA	1819	A	N3-C4-N9	7.25	133.20	127.40
22	BA	2268	A	C4-C5-C6	7.25	120.63	117.00
22	BA	1603	A	C5-N7-C8	7.25	107.53	103.90
1	AA	489	C	C6-N1-C2	-7.25	117.40	120.30
22	BA	1284	A	C5-N7-C8	7.25	107.52	103.90
22	BA	2333	A	C5-N7-C8	7.25	107.52	103.90
22	BA	2497	A	C5-N7-C8	7.25	107.52	103.90
22	BA	2814	A	C5-N7-C8	7.25	107.52	103.90
22	BA	693	A	C4-C5-C6	7.24	120.62	117.00
22	BA	2459	A	C5-N7-C8	7.24	107.52	103.90
22	BA	480	A	C5-N7-C8	7.24	107.52	103.90
22	BA	1679	A	C4-C5-C6	7.24	120.62	117.00
22	BA	2453	A	C4-C5-C6	7.24	120.62	117.00
22	BA	1142	A	N3-C4-N9	7.24	133.19	127.40
22	BA	2199	A	C5-N7-C8	7.24	107.52	103.90
22	BA	802	A	N3-C4-N9	7.23	133.18	127.40
22	BA	2740	A	C4-C5-C6	7.23	120.61	117.00
22	BA	2433	A	C4-C5-C6	7.23	120.61	117.00
22	BA	1321	A	N3-C4-N9	7.23	133.18	127.40
22	BA	513	A	N3-C4-N9	7.23	133.18	127.40
22	BA	1387	A	N3-C4-N9	7.23	133.18	127.40
22	BA	2706	A	N3-C4-N9	7.23	133.18	127.40
22	BA	223	A	C5-N7-C8	7.22	107.51	103.90
22	BA	1927	A	C5-N7-C8	7.22	107.51	103.90
22	BA	2516	A	C4-C5-C6	7.22	120.61	117.00
1	AA	95	C	N1-C2-O2	7.22	123.23	118.90
22	BA	2727	A	N3-C4-N9	7.22	133.18	127.40
22	BA	2734	A	C5-N7-C8	7.22	107.51	103.90
54	D2	31	A	C5-N7-C8	7.22	107.51	103.90
22	BA	1260	A	C4-C5-C6	7.21	120.61	117.00
22	BA	1774	C	C6-N1-C2	-7.21	117.42	120.30
22	BA	1952	A	C5-N7-C8	7.21	107.50	103.90
22	BA	2117	A	C8-N9-C4	7.21	108.68	105.80
22	BA	2741	A	C5-N7-C8	7.21	107.51	103.90
22	BA	2082	A	C4-C5-C6	7.21	120.61	117.00
22	BA	156	A	N3-C4-N9	7.21	133.17	127.40
22	BA	251	A	N3-C4-N9	7.21	133.17	127.40
22	BA	644	A	C4-C5-C6	7.21	120.60	117.00
22	BA	2388	A	C8-N9-C4	7.21	108.68	105.80
23	BB	50	A	C5-N7-C8	7.21	107.50	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	190	A	N3-C4-N9	7.20	133.16	127.40
22	BA	213	A	C8-N9-C4	7.20	108.68	105.80
22	BA	1144	A	C4-C5-C6	7.20	120.60	117.00
22	BA	1970	A	C4-C5-C6	7.20	120.60	117.00
22	BA	2358	A	C5-N7-C8	7.20	107.50	103.90
22	BA	1553	A	N3-C4-N9	7.20	133.16	127.40
22	BA	1156	A	C5-N7-C8	7.20	107.50	103.90
22	BA	1802	A	C5-N7-C8	7.20	107.50	103.90
22	BA	1275	A	C8-N9-C4	7.20	108.68	105.80
22	BA	2163	A	N3-C4-N9	7.19	133.16	127.40
22	BA	2247	A	C5-N7-C8	7.19	107.50	103.90
22	BA	131	A	N3-C4-N9	7.19	133.15	127.40
22	BA	251	A	C5-N7-C8	7.19	107.49	103.90
22	BA	514	A	C5-C6-N1	7.19	121.29	117.70
22	BA	104	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1551	A	N9-C4-C5	7.18	108.67	105.80
22	BA	1960	A	C4-C5-C6	7.18	120.59	117.00
22	BA	1591	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1969	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1237	A	C5-N7-C8	7.18	107.49	103.90
22	BA	1872	A	N3-C4-N9	7.18	133.14	127.40
22	BA	1189	A	C4-C5-C6	7.18	120.59	117.00
22	BA	2726	A	C5-N7-C8	7.18	107.49	103.90
22	BA	156	A	C5-N7-C8	7.17	107.49	103.90
22	BA	173	A	C5-N7-C8	7.17	107.49	103.90
22	BA	447	A	C4-C5-C6	7.17	120.59	117.00
22	BA	1789	A	C4-C5-C6	7.17	120.58	117.00
23	BB	66	A	C4-C5-C6	7.17	120.59	117.00
54	D2	26	A	N3-C4-N9	7.17	133.14	127.40
22	BA	219	A	C5-N7-C8	7.17	107.48	103.90
22	BA	1746	A	C4-C5-C6	7.17	120.58	117.00
22	BA	752	A	C4-C5-C6	7.17	120.58	117.00
54	D2	26	A	C4-C5-C6	7.17	120.58	117.00
55	D3	53	G	N1-C6-O6	-7.17	115.60	119.90
22	BA	1664	A	C5-N7-C8	7.16	107.48	103.90
22	BA	2147	A	C5-N7-C8	7.16	107.48	103.90
22	BA	2184	A	C4-C5-C6	7.16	120.58	117.00
22	BA	191	A	C4-C5-C6	7.16	120.58	117.00
22	BA	819	A	C4-C5-C6	7.16	120.58	117.00
22	BA	1048	A	C4-C5-C6	7.16	120.58	117.00
22	BA	2662	A	N7-C8-N9	-7.16	110.22	113.80
55	D3	38	A	N3-C4-N9	7.16	133.13	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2054	A	C5-C6-N1	7.16	121.28	117.70
22	BA	2071	A	C4-C5-C6	7.15	120.58	117.00
22	BA	279	A	C5-N7-C8	7.15	107.48	103.90
22	BA	2297	A	C4-C5-N7	-7.15	107.12	110.70
22	BA	2335	A	N3-C4-N9	7.15	133.12	127.40
22	BA	2872	A	N9-C4-C5	7.15	108.66	105.80
55	D3	9	A	C4-C5-C6	7.15	120.58	117.00
22	BA	190	A	C4-C5-C6	7.15	120.58	117.00
22	BA	1103	A	C5-N7-C8	7.15	107.48	103.90
22	BA	1829	A	C5-N7-C8	7.15	107.47	103.90
22	BA	1785	A	C5-N7-C8	7.15	107.47	103.90
22	BA	1998	A	C5-N7-C8	7.14	107.47	103.90
54	D2	76	A	C5-N7-C8	7.14	107.47	103.90
22	BA	89	A	N9-C4-C5	7.14	108.66	105.80
22	BA	936	A	C4-C5-C6	7.14	120.57	117.00
22	BA	2335	A	C5-N7-C8	7.14	107.47	103.90
22	BA	2706	A	C5-N7-C8	7.14	107.47	103.90
22	BA	423	A	C5-N7-C8	7.14	107.47	103.90
22	BA	666	A	C4-C5-C6	7.14	120.57	117.00
22	BA	1014	A	C4-C5-C6	7.14	120.57	117.00
22	BA	1328	A	C4-C5-C6	7.14	120.57	117.00
50	B2	1	MET	CG-SD-CE	7.13	111.61	100.20
12	AL	102	LEU	CB-CA-C	7.13	123.75	110.20
22	BA	1393	A	C5-N7-C8	7.13	107.47	103.90
22	BA	2634	A	N3-C4-N9	7.13	133.10	127.40
22	BA	1307	A	C4-C5-C6	7.13	120.56	117.00
22	BA	507	A	C5-N7-C8	7.13	107.46	103.90
22	BA	2679	A	C4-C5-C6	7.13	120.56	117.00
22	BA	973	A	C5-N7-C8	7.12	107.46	103.90
22	BA	1614	A	C5-N7-C8	7.12	107.46	103.90
22	BA	2531	A	C5-N7-C8	7.12	107.46	103.90
55	D3	64	A	C4-C5-C6	7.12	120.56	117.00
22	BA	1213	A	N3-C4-N9	7.12	133.09	127.40
22	BA	1241	A	N3-C4-N9	7.12	133.09	127.40
22	BA	2080	A	C5-N7-C8	7.12	107.46	103.90
22	BA	2757	A	C5-N7-C8	7.12	107.46	103.90
22	BA	2810	A	C5-N7-C8	7.12	107.46	103.90
55	D3	36	A	C5-N7-C8	7.12	107.46	103.90
22	BA	19	A	C5-N7-C8	7.11	107.46	103.90
22	BA	1353	A	C4-C5-N7	-7.11	107.14	110.70
22	BA	49	A	C5-N7-C8	7.11	107.46	103.90
22	BA	95	A	C5-N7-C8	7.11	107.46	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	165	A	C5-N7-C8	7.11	107.46	103.90
22	BA	176	A	C4-C5-C6	7.11	120.56	117.00
22	BA	972	A	C5-N7-C8	7.11	107.45	103.90
22	BA	1054	A	N3-C4-N9	7.11	133.09	127.40
22	BA	1515	A	N9-C4-C5	7.11	108.64	105.80
22	BA	1854	A	C5-N7-C8	7.11	107.45	103.90
22	BA	217	A	C5-N7-C8	7.11	107.45	103.90
22	BA	221	A	C5-N7-C8	7.11	107.45	103.90
1	AA	1132	C	N1-C2-O2	7.10	123.16	118.90
22	BA	347	A	C4-C5-C6	7.10	120.55	117.00
22	BA	783	A	C4-C5-C6	7.10	120.55	117.00
22	BA	2009	A	C8-N9-C4	7.10	108.64	105.80
55	D3	64	A	C5-N7-C8	7.10	107.45	103.90
22	BA	2748	A	C5-N7-C8	7.10	107.45	103.90
22	BA	1028	A	N3-C4-N9	7.10	133.08	127.40
22	BA	300	A	C5-N7-C8	7.09	107.45	103.90
55	D3	73	A	N3-C4-N9	7.09	133.07	127.40
22	BA	941	A	C5-N7-C8	7.09	107.45	103.90
22	BA	984	A	C5-N7-C8	7.09	107.45	103.90
22	BA	1932	A	C5-N7-C8	7.09	107.45	103.90
22	BA	152	A	C5-N7-C8	7.09	107.44	103.90
22	BA	2328	A	C4-C5-C6	7.09	120.55	117.00
22	BA	722	A	N3-C4-N9	7.09	133.07	127.40
22	BA	927	A	C5-N7-C8	7.09	107.44	103.90
22	BA	1791	A	C4-C5-C6	7.09	120.54	117.00
22	BA	1027	A	C5-N7-C8	7.08	107.44	103.90
22	BA	1088	A	C4-C5-C6	7.08	120.54	117.00
22	BA	1213	A	C5-N7-C8	7.08	107.44	103.90
22	BA	1265	A	C4-C5-C6	7.08	120.54	117.00
22	BA	981	A	C5-N7-C8	7.08	107.44	103.90
22	BA	1189	A	N3-C4-N9	7.08	133.07	127.40
22	BA	1301	A	N3-C4-N9	7.08	133.06	127.40
22	BA	1354	A	C4-C5-C6	7.08	120.54	117.00
22	BA	1359	A	C5-N7-C8	7.08	107.44	103.90
22	BA	2297	A	C4-C5-C6	7.08	120.54	117.00
22	BA	1086	A	N3-C4-N9	7.08	133.06	127.40
22	BA	1570	A	C4-C5-C6	7.07	120.54	117.00
22	BA	226	A	N3-C4-N9	7.07	133.06	127.40
22	BA	368	A	C5-N7-C8	7.07	107.44	103.90
22	BA	2675	A	C5-N7-C8	7.07	107.44	103.90
22	BA	1009	A	C4-C5-C6	7.07	120.53	117.00
22	BA	2587	A	C5-N7-C8	7.07	107.43	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1276	A	C4-C5-C6	7.07	120.53	117.00
22	BA	556	A	C5-N7-C8	7.06	107.43	103.90
22	BA	1549	A	C4-C5-C6	7.06	120.53	117.00
22	BA	1677	A	C5-N7-C8	7.06	107.43	103.90
22	BA	2879	A	N3-C4-N9	7.06	133.05	127.40
22	BA	91	A	C5-N7-C8	7.05	107.43	103.90
22	BA	53	A	C5-N7-C8	7.05	107.43	103.90
22	BA	262	A	N9-C4-C5	7.05	108.62	105.80
22	BA	1665	A	C4-C5-C6	7.05	120.53	117.00
22	BA	1977	A	C5-N7-C8	7.05	107.42	103.90
22	BA	1919	A	C5-N7-C8	7.05	107.42	103.90
22	BA	2766	A	C4-C5-C6	7.05	120.52	117.00
22	BA	1027	A	C4-C5-C6	7.05	120.52	117.00
22	BA	2459	A	N3-C4-N9	7.05	133.04	127.40
22	BA	2634	A	C4-C5-C6	7.05	120.52	117.00
22	BA	2679	A	C5-N7-C8	7.05	107.42	103.90
22	BA	1254	A	C5-N7-C8	7.04	107.42	103.90
22	BA	1654	A	C4-C5-C6	7.04	120.52	117.00
22	BA	2352	A	C5-N7-C8	7.04	107.42	103.90
12	AL	103	ASP	N-CA-CB	-7.03	97.94	110.60
22	BA	2425	A	C5-N7-C8	7.03	107.42	103.90
22	BA	2799	A	C5-N7-C8	7.03	107.42	103.90
22	BA	2052	A	C5-C6-N1	7.03	121.22	117.70
22	BA	412	A	C4-C5-C6	7.03	120.52	117.00
22	BA	819	A	N3-C4-N9	7.03	133.02	127.40
22	BA	1746	A	N3-C4-N9	7.03	133.02	127.40
22	BA	2366	A	C5-N7-C8	7.03	107.41	103.90
22	BA	1322	A	C5-N7-C8	7.02	107.41	103.90
54	D2	21	A	C5-N7-C8	7.02	107.41	103.90
22	BA	226	A	C5-N7-C8	7.02	107.41	103.90
22	BA	415	A	N3-C4-N9	7.02	133.02	127.40
22	BA	1701	A	N9-C4-C5	7.01	108.61	105.80
22	BA	1783	A	C4-C5-C6	7.01	120.51	117.00
22	BA	2278	A	C5-N7-C8	7.01	107.41	103.90
22	BA	1866	A	C4-C5-C6	7.00	120.50	117.00
22	BA	515	A	C5-N7-C8	7.00	107.40	103.90
22	BA	2183	A	C5-C6-N6	7.00	129.30	123.70
22	BA	675	A	C4-C5-C6	6.99	120.50	117.00
22	BA	2090	A	C4-C5-C6	6.99	120.50	117.00
22	BA	1960	A	N3-C4-N9	6.99	132.99	127.40
22	BA	1885	A	C5-N7-C8	6.99	107.39	103.90
22	BA	2430	A	N9-C4-C5	6.99	108.59	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2598	A	C5-N7-C8	6.99	107.39	103.90
22	BA	127	A	C5-N7-C8	6.99	107.39	103.90
23	BB	31	C	C2-N1-C1'	6.99	126.48	118.80
22	BA	685	A	C4-C5-C6	6.98	120.49	117.00
22	BA	1302	A	C8-N9-C4	6.98	108.59	105.80
22	BA	2577	A	C4-C5-C6	6.98	120.49	117.00
22	BA	764	A	C5-N7-C8	6.98	107.39	103.90
22	BA	1938	A	N3-C4-N9	6.98	132.98	127.40
22	BA	2287	A	C4-C5-C6	6.98	120.49	117.00
22	BA	2851	A	C4-C5-C6	6.98	120.49	117.00
22	BA	173	A	C4-C5-C6	6.97	120.49	117.00
22	BA	1143	A	C5-N7-C8	6.97	107.39	103.90
22	BA	2388	A	C4-C5-C6	6.97	120.49	117.00
22	BA	1762	A	C5-N7-C8	6.97	107.38	103.90
22	BA	5	A	C5-N7-C8	6.97	107.38	103.90
22	BA	1274	A	C8-N9-C4	6.97	108.59	105.80
22	BA	2114	A	C4-C5-C6	6.97	120.48	117.00
22	BA	2267	A	C5-C6-N1	6.97	121.18	117.70
22	BA	750	A	C8-N9-C4	6.96	108.58	105.80
22	BA	1549	A	N3-C4-N9	6.96	132.97	127.40
22	BA	2740	A	C5-N7-C8	6.96	107.38	103.90
22	BA	677	A	N3-C4-N9	6.96	132.97	127.40
22	BA	917	A	N3-C4-N9	6.96	132.97	127.40
22	BA	1553	A	C4-C5-C6	6.96	120.48	117.00
22	BA	1593	A	C4-C5-C6	6.96	120.48	117.00
22	BA	1872	A	C5-N7-C8	6.96	107.38	103.90
22	BA	2377	A	C5-N7-C8	6.96	107.38	103.90
22	BA	218	A	C5-N7-C8	6.96	107.38	103.90
22	BA	49	A	N3-C4-N9	6.95	132.96	127.40
22	BA	541	A	C4-C5-C6	6.95	120.47	117.00
22	BA	1655	A	C8-N9-C4	6.95	108.58	105.80
22	BA	2135	A	C4-C5-C6	6.95	120.48	117.00
22	BA	753	A	C5-N7-C8	6.95	107.37	103.90
22	BA	522	A	C5-N7-C8	6.95	107.37	103.90
22	BA	693	A	N3-C4-N9	6.95	132.96	127.40
22	BA	272	A	C4-C5-C6	6.94	120.47	117.00
22	BA	2565	A	C4-C5-C6	6.94	120.47	117.00
22	BA	2813	A	C4-C5-C6	6.94	120.47	117.00
22	BA	927	A	N3-C4-N9	6.93	132.95	127.40
22	BA	1802	A	C4-C5-C6	6.93	120.47	117.00
22	BA	1247	A	N9-C4-C5	6.93	108.57	105.80
22	BA	1981	A	N9-C4-C5	6.93	108.57	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	42	A	C4-C5-C6	6.93	120.47	117.00
22	BA	197	A	C4-C5-C6	6.93	120.47	117.00
22	BA	2469	A	C5-N7-C8	6.93	107.36	103.90
22	BA	1722	A	C8-N9-C4	6.93	108.57	105.80
22	BA	689	A	C5-C6-N1	6.93	121.16	117.70
22	BA	945	A	C4-C5-C6	6.93	120.46	117.00
22	BA	2033	A	C4-C5-N7	-6.93	107.24	110.70
1	AA	439	U	C5-C4-O4	-6.92	121.75	125.90
23	BB	99	A	N3-C4-N9	6.92	132.94	127.40
22	BA	6	A	C4-C5-C6	6.92	120.46	117.00
22	BA	514	A	C5-N7-C8	6.92	107.36	103.90
22	BA	1143	A	C4-C5-C6	6.92	120.46	117.00
22	BA	1571	A	C4-C5-C6	6.92	120.46	117.00
22	BA	1598	A	C4-C5-C6	6.92	120.46	117.00
22	BA	176	A	N3-C4-N9	6.92	132.93	127.40
22	BA	975	A	C4-C5-C6	6.92	120.46	117.00
22	BA	1133	A	C4-C5-C6	6.92	120.46	117.00
22	BA	2015	A	C4-C5-C6	6.92	120.46	117.00
22	BA	2856	A	C4-C5-C6	6.92	120.46	117.00
22	BA	1899	A	C4-C5-C6	6.92	120.46	117.00
22	BA	300	A	N9-C4-C5	6.91	108.56	105.80
22	BA	64	A	C4-C5-C6	6.91	120.45	117.00
22	BA	925	A	N3-C4-N9	6.91	132.93	127.40
22	BA	1876	A	N3-C4-N9	6.91	132.93	127.40
22	BA	2052	A	C5-N7-C8	6.91	107.36	103.90
22	BA	668	A	C4-C5-C6	6.91	120.45	117.00
22	BA	753	A	C5-C6-N1	6.91	121.15	117.70
22	BA	1469	A	C4-C5-C6	6.91	120.45	117.00
22	BA	197	A	N3-C4-N9	6.91	132.93	127.40
22	BA	19	A	N3-C4-N9	6.91	132.92	127.40
22	BA	783	A	C5-N7-C8	6.91	107.35	103.90
22	BA	866	A	N3-C4-N9	6.91	132.93	127.40
22	BA	2814	A	C4-C5-C6	6.91	120.45	117.00
23	BB	115	A	N9-C4-C5	6.91	108.56	105.80
22	BA	1490	A	C4-C5-C6	6.90	120.45	117.00
22	BA	722	A	C4-C5-C6	6.90	120.45	117.00
22	BA	1637	A	N3-C4-N9	6.90	132.92	127.40
22	BA	2587	A	C4-C5-C6	6.90	120.45	117.00
22	BA	633	A	C4-C5-C6	6.90	120.45	117.00
22	BA	2577	A	N3-C4-N9	6.90	132.92	127.40
55	D3	62	C	C6-N1-C2	-6.90	117.54	120.30
22	BA	1772	A	C4-C5-C6	6.90	120.45	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2518	A	C4-C5-C6	6.90	120.45	117.00
22	BA	802	A	C4-C5-C6	6.89	120.45	117.00
22	BA	1328	A	N3-C4-N9	6.89	132.91	127.40
22	BA	685	A	N3-C4-N9	6.89	132.91	127.40
22	BA	1551	A	C4-C5-C6	6.89	120.44	117.00
22	BA	2738	A	C5-N7-C8	6.89	107.35	103.90
22	BA	1810	A	C5-N7-C8	6.89	107.34	103.90
22	BA	1603	A	C4-C5-C6	6.89	120.44	117.00
22	BA	1819	A	C8-N9-C4	6.89	108.56	105.80
22	BA	231	A	C4-C5-C6	6.88	120.44	117.00
22	BA	1532	A	C4-C5-C6	6.88	120.44	117.00
55	D3	9	A	N3-C4-N9	6.88	132.91	127.40
22	BA	191	A	N3-C4-N9	6.88	132.91	127.40
22	BA	1705	A	N3-C4-N9	6.88	132.91	127.40
55	D3	7	A	C8-N9-C4	6.88	108.55	105.80
22	BA	960	A	N3-C4-N9	6.88	132.90	127.40
22	BA	1900	A	C5-N7-C8	6.88	107.34	103.90
22	BA	1214	A	N9-C4-C5	6.88	108.55	105.80
22	BA	1901	A	N3-C4-N9	6.88	132.90	127.40
22	BA	1918	A	C5-N7-C8	6.88	107.34	103.90
22	BA	2883	A	C8-N9-C4	6.88	108.55	105.80
23	BB	29	A	N9-C4-C5	6.88	108.55	105.80
22	BA	2322	A	N3-C4-N9	6.88	132.90	127.40
22	BA	477	A	C4-C5-C6	6.88	120.44	117.00
22	BA	666	A	N3-C4-N9	6.87	132.90	127.40
22	BA	196	A	C4-C5-C6	6.87	120.43	117.00
22	BA	282	A	C5-N7-C8	6.87	107.33	103.90
22	BA	471	A	C4-C5-C6	6.87	120.43	117.00
22	BA	2541	A	C4-C5-C6	6.87	120.43	117.00
55	D3	26	A	N3-C4-N9	6.87	132.89	127.40
22	BA	910	A	N3-C4-N9	6.86	132.89	127.40
22	BA	917	A	C4-C5-C6	6.86	120.43	117.00
22	BA	1098	A	N3-C4-N9	6.86	132.89	127.40
22	BA	480	A	C4-C5-C6	6.86	120.43	117.00
22	BA	1477	A	C4-C5-C6	6.86	120.43	117.00
22	BA	1784	A	C8-N9-C4	6.86	108.55	105.80
22	BA	2899	A	C5-N7-C8	6.86	107.33	103.90
22	BA	716	A	C4-C5-C6	6.86	120.43	117.00
22	BA	2037	A	N3-C4-N9	6.86	132.88	127.40
22	BA	144	A	N3-C4-N9	6.85	132.88	127.40
22	BA	781	A	C5-N7-C8	6.85	107.33	103.90
22	BA	1244	A	C5-N7-C8	6.85	107.33	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2682	A	C5-N7-C8	6.85	107.33	103.90
22	BA	384	A	C5-N7-C8	6.85	107.33	103.90
55	D3	59	U	N1-C2-O2	6.85	127.59	122.80
55	D3	74	C	C2-N1-C1'	6.85	126.33	118.80
22	BA	782	A	C4-C5-C6	6.85	120.42	117.00
22	BA	988	A	C5-N7-C8	6.85	107.32	103.90
22	BA	1591	A	N3-C4-N9	6.85	132.88	127.40
22	BA	466	A	C5-N7-C8	6.85	107.32	103.90
22	BA	1385	A	C4-C5-N7	-6.85	107.28	110.70
22	BA	609	A	C4-C5-C6	6.84	120.42	117.00
22	BA	721	A	N3-C4-N9	6.84	132.87	127.40
22	BA	751	A	C5-N7-C8	6.84	107.32	103.90
22	BA	1419	A	C8-N9-C4	6.84	108.54	105.80
22	BA	1690	A	C4-C5-C6	6.84	120.42	117.00
22	BA	2700	A	C4-C5-C6	6.84	120.42	117.00
22	BA	677	A	C5-N7-C8	6.84	107.32	103.90
22	BA	990	A	C5-N7-C8	6.84	107.32	103.90
22	BA	1586	A	C4-C5-C6	6.84	120.42	117.00
22	BA	1876	A	C4-C5-C6	6.83	120.42	117.00
22	BA	1098	A	C4-C5-C6	6.83	120.42	117.00
22	BA	1403	A	C4-C5-C6	6.83	120.42	117.00
22	BA	1470	A	C5-N7-C8	6.83	107.31	103.90
22	BA	1597	A	N9-C4-C5	6.83	108.53	105.80
22	BA	2070	A	N9-C4-C5	6.83	108.53	105.80
22	BA	222	A	C8-N9-C4	6.83	108.53	105.80
22	BA	2736	A	C5-C6-N1	6.83	121.11	117.70
22	BA	582	A	C5-C6-N1	6.82	121.11	117.70
22	BA	1287	A	C4-C5-C6	6.82	120.41	117.00
22	BA	1803	A	C5-N7-C8	6.82	107.31	103.90
22	BA	2476	A	C5-N7-C8	6.82	107.31	103.90
22	BA	2675	A	C4-C5-C6	6.82	120.41	117.00
54	D2	51	A	C4-C5-C6	6.82	120.41	117.00
22	BA	1590	A	C4-C5-C6	6.82	120.41	117.00
22	BA	627	A	C8-N9-C4	6.82	108.53	105.80
22	BA	1762	A	N9-C4-C5	6.82	108.53	105.80
22	BA	1901	A	C5-N7-C8	6.82	107.31	103.90
22	BA	2097	A	C4-C5-C6	6.82	120.41	117.00
22	BA	2435	A	C4-C5-C6	6.82	120.41	117.00
22	BA	2757	A	C4-C5-C6	6.82	120.41	117.00
22	BA	2765	A	C4-C5-C6	6.82	120.41	117.00
54	D2	23	A	C4-C5-C6	6.82	120.41	117.00
22	BA	2333	A	C8-N9-C4	6.81	108.53	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1285	A	N9-C4-C5	6.81	108.52	105.80
22	BA	1672	A	C5-N7-C8	6.81	107.30	103.90
22	BA	2284	A	C5-C6-N1	6.81	121.10	117.70
22	BA	2530	A	C4-C5-C6	6.81	120.40	117.00
55	D3	58	A	N9-C4-C5	6.81	108.52	105.80
22	BA	324	A	C5-N7-C8	6.81	107.30	103.90
22	BA	608	A	C4-C5-C6	6.81	120.40	117.00
22	BA	1614	A	C4-C5-C6	6.81	120.40	117.00
22	BA	216	A	N3-C4-N9	6.80	132.84	127.40
22	BA	1744	A	N3-C4-N9	6.80	132.84	127.40
22	BA	2054	A	C4-C5-C6	6.80	120.40	117.00
22	BA	722	A	C5-N7-C8	6.80	107.30	103.90
22	BA	310	A	C8-N9-C4	6.80	108.52	105.80
22	BA	1866	A	C5-N7-C8	6.80	107.30	103.90
22	BA	1937	A	N9-C4-C5	6.80	108.52	105.80
22	BA	472	A	C5-N7-C8	6.80	107.30	103.90
22	BA	1637	A	C5-N7-C8	6.79	107.30	103.90
22	BA	592	A	N3-C4-N9	6.79	132.83	127.40
55	D3	31	A	C4-C5-C6	6.79	120.40	117.00
22	BA	207	A	C5-N7-C8	6.79	107.30	103.90
22	BA	233	A	C5-N7-C8	6.79	107.30	103.90
22	BA	825	A	C4-C5-C6	6.79	120.40	117.00
22	BA	1413	A	C4-C5-C6	6.79	120.40	117.00
22	BA	354	A	N9-C4-C5	6.79	108.52	105.80
22	BA	933	A	N3-C4-N9	6.79	132.83	127.40
22	BA	643	A	C5-N7-C8	6.79	107.29	103.90
22	BA	1241	A	C4-C5-C6	6.79	120.39	117.00
22	BA	2135	A	N3-C4-N9	6.79	132.83	127.40
22	BA	447	A	N3-C4-N9	6.78	132.83	127.40
22	BA	590	A	C5-N7-C8	6.78	107.29	103.90
22	BA	1470	A	N3-C4-N9	6.78	132.82	127.40
22	BA	503	A	C5-N7-C8	6.78	107.29	103.90
22	BA	2721	A	C4-C5-C6	6.78	120.39	117.00
22	BA	256	A	C4-C5-C6	6.78	120.39	117.00
22	BA	689	A	N9-C4-C5	6.78	108.51	105.80
55	D3	44	G	C4-N9-C1'	6.78	135.31	126.50
22	BA	56	A	C4-C5-C6	6.78	120.39	117.00
22	BA	1608	A	C4-C5-C6	6.78	120.39	117.00
22	BA	1630	A	C4-C5-N7	-6.78	107.31	110.70
55	D3	76	A	N9-C4-C5	6.77	108.51	105.80
22	BA	802	A	C5-N7-C8	6.77	107.29	103.90
22	BA	2090	A	N3-C4-N9	6.77	132.81	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	478	A	C4-C5-C6	6.77	120.38	117.00
22	BA	590	A	C4-C5-C6	6.77	120.38	117.00
22	BA	943	A	C5-N7-C8	6.77	107.28	103.90
22	BA	2856	A	N3-C4-N9	6.77	132.81	127.40
22	BA	2386	A	N3-C4-N9	6.76	132.81	127.40
1	AA	489	C	C2-N1-C1'	6.76	126.24	118.80
22	BA	1336	A	C4-C5-C6	6.76	120.38	117.00
22	BA	2809	A	C4-C5-C6	6.76	120.38	117.00
22	BA	2810	A	C4-C5-C6	6.76	120.38	117.00
22	BA	1433	A	C4-C5-C6	6.76	120.38	117.00
22	BA	1610	A	C5-N7-C8	6.76	107.28	103.90
22	BA	2247	A	N3-C4-N9	6.76	132.81	127.40
22	BA	794	A	N3-C4-N9	6.76	132.81	127.40
55	D3	74	C	C6-N1-C2	-6.76	117.60	120.30
22	BA	1901	A	C5-C6-N1	6.75	121.08	117.70
22	BA	2097	A	N3-C4-N9	6.75	132.80	127.40
54	D2	9	A	C8-N9-C4	6.75	108.50	105.80
22	BA	793	A	C4-C5-C6	6.75	120.38	117.00
22	BA	1626	A	C5-N7-C8	6.75	107.28	103.90
22	BA	1821	A	N9-C4-C5	6.75	108.50	105.80
22	BA	2873	A	C4-C5-C6	6.75	120.37	117.00
22	BA	556	A	C4-C5-C6	6.75	120.37	117.00
22	BA	2366	A	N3-C4-N9	6.74	132.79	127.40
55	D3	36	A	C4-C5-C6	6.74	120.37	117.00
22	BA	1032	A	C8-N9-C4	6.74	108.50	105.80
22	BA	1678	A	C4-C5-C6	6.74	120.37	117.00
22	BA	2088	A	N3-C4-N9	6.74	132.79	127.40
22	BA	2317	A	C4-C5-C6	6.74	120.37	117.00
22	BA	12	U	N3-C2-O2	-6.74	117.48	122.20
22	BA	2205	A	C4-C5-C6	6.74	120.37	117.00
22	BA	299	A	N9-C4-C5	6.74	108.49	105.80
22	BA	1027	A	N3-C4-N9	6.74	132.79	127.40
22	BA	1165	A	N9-C4-C5	6.74	108.50	105.80
22	BA	1634	A	C8-N9-C4	6.74	108.49	105.80
22	BA	1754	A	C5-N7-C8	6.74	107.27	103.90
22	BA	789	A	N3-C4-N9	6.73	132.79	127.40
22	BA	975	A	N3-C4-N9	6.73	132.79	127.40
22	BA	863	A	N3-C4-N9	6.73	132.78	127.40
22	BA	1677	A	C4-C5-C6	6.73	120.36	117.00
22	BA	1717	A	C4-C5-C6	6.73	120.37	117.00
22	BA	705	A	C5-N7-C8	6.73	107.26	103.90
22	BA	1276	A	N9-C4-C5	6.73	108.49	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1301	A	C4-C5-C6	6.73	120.36	117.00
22	BA	1665	A	N3-C4-N9	6.73	132.78	127.40
22	BA	920	A	C5-N7-C8	6.73	107.26	103.90
22	BA	528	A	N9-C4-C5	6.72	108.49	105.80
22	BA	2163	A	C4-C5-C6	6.72	120.36	117.00
22	BA	2758	A	N9-C4-C5	6.72	108.49	105.80
22	BA	142	A	C4-C5-C6	6.72	120.36	117.00
22	BA	2369	A	C8-N9-C4	6.72	108.49	105.80
23	BB	15	A	C4-C5-C6	6.72	120.36	117.00
22	BA	699	A	C4-C5-C6	6.72	120.36	117.00
22	BA	1387	A	C5-C6-N1	6.72	121.06	117.70
22	BA	2335	A	C4-C5-C6	6.72	120.36	117.00
1	AA	464	U	C5-C6-N1	6.71	126.06	122.70
22	BA	404	A	C5-N7-C8	6.71	107.26	103.90
22	BA	556	A	N3-C4-N9	6.71	132.77	127.40
22	BA	936	A	N3-C4-N9	6.71	132.77	127.40
22	BA	1583	A	C8-N9-C4	6.71	108.49	105.80
22	BA	330	A	C4-C5-C6	6.71	120.36	117.00
55	D3	35	A	N3-C4-N9	6.71	132.77	127.40
22	BA	2461	A	C5-C6-N1	6.71	121.06	117.70
22	BA	1084	A	C4-C5-C6	6.71	120.36	117.00
22	BA	324	A	C8-N9-C4	6.71	108.48	105.80
22	BA	925	A	C8-N9-C4	6.71	108.48	105.80
22	BA	1080	A	C4-C5-C6	6.71	120.35	117.00
22	BA	1144	A	N3-C4-N9	6.71	132.76	127.40
34	BM	12	MET	CG-SD-CE	6.71	110.93	100.20
22	BA	1134	A	N3-C4-N9	6.70	132.76	127.40
22	BA	219	A	N3-C4-N9	6.70	132.76	127.40
22	BA	735	A	N3-C4-N9	6.70	132.76	127.40
22	BA	996	A	N3-C4-N9	6.70	132.76	127.40
22	BA	2094	A	C4-C5-C6	6.70	120.35	117.00
1	AA	1388	C	C6-N1-C2	-6.70	117.62	120.30
22	BA	74	A	N3-C4-N9	6.70	132.76	127.40
22	BA	2412	A	N3-C4-N9	6.70	132.76	127.40
23	BB	66	A	C5-N7-C8	6.70	107.25	103.90
22	BA	572	A	C5-N7-C8	6.70	107.25	103.90
22	BA	470	A	N3-C4-N9	6.70	132.76	127.40
22	BA	609	A	N3-C4-N9	6.70	132.76	127.40
22	BA	654	A	N3-C4-N9	6.70	132.76	127.40
22	BA	1262	A	C5-C6-N1	6.70	121.05	117.70
22	BA	1608	A	C5-N7-C8	6.69	107.25	103.90
23	BB	46	A	C4-C5-C6	6.69	120.35	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	943	A	C4-C5-C6	6.69	120.35	117.00
22	BA	1143	A	N3-C4-N9	6.69	132.75	127.40
22	BA	1900	A	C4-C5-C6	6.69	120.34	117.00
22	BA	2700	A	N3-C4-N9	6.69	132.75	127.40
22	BA	131	A	C4-C5-C6	6.69	120.34	117.00
22	BA	677	A	C4-C5-C6	6.69	120.34	117.00
22	BA	1431	A	N3-C4-N9	6.69	132.75	127.40
22	BA	429	A	C4-C5-C6	6.69	120.34	117.00
22	BA	2108	A	N9-C4-C5	6.68	108.47	105.80
22	BA	2184	A	N3-C4-N9	6.68	132.75	127.40
22	BA	152	A	N3-C4-N9	6.68	132.74	127.40
22	BA	1134	A	C4-C5-C6	6.68	120.34	117.00
22	BA	1759	A	N3-C4-N9	6.68	132.74	127.40
22	BA	478	A	C5-N7-C8	6.67	107.24	103.90
22	BA	750	A	C5-N7-C8	6.67	107.24	103.90
22	BA	1088	A	C5-C6-N1	6.67	121.04	117.70
22	BA	1205	A	C8-N9-C4	6.67	108.47	105.80
23	BB	99	A	C4-C5-C6	6.67	120.34	117.00
22	BA	2823	A	N3-C4-N9	6.67	132.74	127.40
22	BA	644	A	N9-C4-C5	6.67	108.47	105.80
22	BA	689	A	C4-C5-C6	6.67	120.34	117.00
22	BA	2013	A	C4-C5-C6	6.67	120.33	117.00
55	D3	59	U	C2-N1-C1'	6.67	125.70	117.70
22	BA	64	A	N3-C4-N9	6.67	132.74	127.40
22	BA	1757	A	C5-N7-C8	6.67	107.23	103.90
22	BA	56	A	N3-C4-N9	6.67	132.73	127.40
22	BA	505	A	C4-C5-C6	6.67	120.33	117.00
22	BA	1373	A	N3-C4-N9	6.67	132.73	127.40
55	D3	74	C	N3-C2-O2	-6.67	117.23	121.90
22	BA	74	A	C4-C5-C6	6.67	120.33	117.00
22	BA	911	A	C5-N7-C8	6.67	107.23	103.90
22	BA	1928	A	C5-N7-C8	6.67	107.23	103.90
22	BA	1028	A	C4-C5-C6	6.66	120.33	117.00
22	BA	1175	A	C4-C5-C6	6.66	120.33	117.00
22	BA	1439	A	C4-C5-C6	6.66	120.33	117.00
22	BA	2516	A	C5-N7-C8	6.66	107.23	103.90
22	BA	2727	A	C4-C5-C6	6.66	120.33	117.00
22	BA	1705	A	C4-C5-C6	6.66	120.33	117.00
22	BA	925	A	C4-C5-C6	6.66	120.33	117.00
22	BA	1365	A	C4-C5-C6	6.66	120.33	117.00
22	BA	2513	A	N3-C4-N9	6.66	132.73	127.40
22	BA	2860	A	C4-C5-C6	6.66	120.33	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	430	A	N9-C4-C5	6.66	108.46	105.80
22	BA	781	A	C4-C5-C6	6.66	120.33	117.00
22	BA	1784	A	N3-C4-N9	6.66	132.73	127.40
22	BA	1809	A	C5-N7-C8	6.66	107.23	103.90
22	BA	2051	A	C5-N7-C8	6.66	107.23	103.90
22	BA	2564	A	C5-N7-C8	6.66	107.23	103.90
54	D2	31	A	C4-C5-C6	6.66	120.33	117.00
22	BA	1084	A	N3-C4-N9	6.66	132.73	127.40
22	BA	173	A	N3-C4-N9	6.66	132.72	127.40
55	D3	23	A	C4-C5-C6	6.66	120.33	117.00
22	BA	38	A	C4-C5-C6	6.65	120.33	117.00
22	BA	1772	A	N9-C4-C5	6.65	108.46	105.80
22	BA	345	A	N3-C4-N9	6.65	132.72	127.40
22	BA	2634	A	C5-C6-N1	6.65	121.03	117.70
23	BB	29	A	C4-C5-C6	6.65	120.33	117.00
22	BA	1689	A	C4-C5-C6	6.65	120.33	117.00
22	BA	2273	A	C4-C5-C6	6.65	120.32	117.00
22	BA	608	A	N3-C4-N9	6.65	132.72	127.40
23	BB	57	A	N3-C4-N9	6.65	132.72	127.40
22	BA	1156	A	C4-C5-C6	6.65	120.32	117.00
55	D3	35	A	C4-C5-C6	6.65	120.32	117.00
22	BA	845	A	N3-C4-N9	6.64	132.72	127.40
22	BA	2088	A	C4-C5-C6	6.64	120.32	117.00
22	BA	2199	A	C4-C5-C6	6.64	120.32	117.00
22	BA	1156	A	N3-C4-N9	6.64	132.71	127.40
22	BA	2434	A	C4-C5-C6	6.64	120.32	117.00
22	BA	2682	A	C8-N9-C4	6.64	108.46	105.80
22	BA	14	A	C4-C5-C6	6.64	120.32	117.00
22	BA	345	A	C4-C5-C6	6.64	120.32	117.00
22	BA	505	A	N3-C4-N9	6.64	132.71	127.40
22	BA	2322	A	C4-C5-C6	6.64	120.32	117.00
22	BA	849	A	N3-C4-N9	6.63	132.71	127.40
22	BA	1175	A	N3-C4-N9	6.63	132.71	127.40
22	BA	2340	A	C8-N9-C4	6.63	108.45	105.80
22	BA	1086	A	C4-C5-C6	6.63	120.32	117.00
22	BA	2082	A	N3-C4-N9	6.63	132.71	127.40
22	BA	2020	A	C4-C5-C6	6.63	120.31	117.00
22	BA	2531	A	N3-C4-N9	6.63	132.70	127.40
22	BA	793	A	N3-C4-N9	6.63	132.70	127.40
22	BA	1854	A	C4-C5-C6	6.63	120.31	117.00
22	BA	324	A	N3-C4-N9	6.63	132.70	127.40
22	BA	492	A	C4-C5-C6	6.63	120.31	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2191	A	C4-C5-C6	6.63	120.31	117.00
22	BA	1632	A	N3-C4-N9	6.62	132.70	127.40
22	BA	2425	A	C4-C5-C6	6.62	120.31	117.00
22	BA	299	A	C5-N7-C8	6.62	107.21	103.90
22	BA	572	A	N3-C4-N9	6.62	132.70	127.40
22	BA	1960	A	C5-C6-N1	6.62	121.01	117.70
22	BA	2882	A	N9-C4-C5	6.62	108.45	105.80
22	BA	219	A	C4-C5-C6	6.62	120.31	117.00
22	BA	2317	A	N3-C4-N9	6.62	132.70	127.40
22	BA	460	A	C4-C5-C6	6.62	120.31	117.00
22	BA	1847	A	N3-C4-N9	6.62	132.70	127.40
22	BA	1637	A	C4-C5-C6	6.62	120.31	117.00
22	BA	643	A	N3-C4-N9	6.61	132.69	127.40
22	BA	984	A	C4-C5-C6	6.61	120.31	117.00
22	BA	730	A	N3-C4-N9	6.61	132.69	127.40
22	BA	1010	A	C4-C5-C6	6.61	120.31	117.00
22	BA	1735	A	N3-C4-N9	6.61	132.69	127.40
22	BA	735	A	C4-C5-C6	6.61	120.31	117.00
22	BA	2635	A	C4-C5-C6	6.61	120.31	117.00
22	BA	2227	A	C4-C5-C6	6.61	120.31	117.00
22	BA	1970	A	C8-N9-C4	6.61	108.44	105.80
22	BA	2670	A	N3-C4-N9	6.61	132.69	127.40
23	BB	115	A	C4-C5-C6	6.61	120.30	117.00
22	BA	1085	A	C4-C5-C6	6.60	120.30	117.00
22	BA	1304	A	N9-C4-C5	6.60	108.44	105.80
22	BA	1632	A	C4-C5-C6	6.60	120.30	117.00
22	BA	1853	A	C8-N9-C4	6.60	108.44	105.80
22	BA	2837	A	C4-C5-C6	6.60	120.30	117.00
22	BA	2740	A	N3-C4-N9	6.60	132.68	127.40
22	BA	299	A	C4-C5-C6	6.60	120.30	117.00
22	BA	2765	A	C5-C6-N1	6.60	121.00	117.70
54	D2	31	A	N3-C4-N9	6.60	132.68	127.40
22	BA	1655	A	N3-C4-N9	6.60	132.68	127.40
22	BA	2453	A	N9-C4-C5	6.60	108.44	105.80
54	D2	41	A	C4-C5-C6	6.60	120.30	117.00
22	BA	439	A	C5-C6-N1	6.59	121.00	117.70
22	BA	1791	A	C5-N7-C8	6.59	107.20	103.90
22	BA	863	A	C4-C5-C6	6.59	120.30	117.00
22	BA	1759	A	C4-C5-C6	6.59	120.30	117.00
22	BA	144	A	C4-C5-C6	6.59	120.30	117.00
22	BA	513	A	C5-N7-C8	6.59	107.20	103.90
22	BA	2013	A	N3-C4-N9	6.59	132.67	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	794	A	C4-C5-C6	6.59	120.30	117.00
22	BA	1046	A	C8-N9-C4	6.59	108.44	105.80
22	BA	2809	A	N3-C4-N9	6.59	132.67	127.40
22	BA	1354	A	N3-C4-N9	6.59	132.67	127.40
22	BA	1572	A	N3-C4-N9	6.59	132.67	127.40
22	BA	2670	A	C4-C5-C6	6.59	120.29	117.00
56	D4	1	U	N1-C2-O2	6.59	127.41	122.80
22	BA	1889	A	C4-C5-C6	6.58	120.29	117.00
1	AA	998	C	N3-C2-O2	-6.58	117.30	121.90
22	BA	161	A	C8-N9-C4	6.58	108.43	105.80
22	BA	346	A	C4-C5-C6	6.58	120.29	117.00
22	BA	739	A	N9-C4-C5	6.58	108.43	105.80
22	BA	1919	A	C4-C5-C6	6.58	120.29	117.00
22	BA	2482	A	C4-C5-C6	6.58	120.29	117.00
22	BA	905	A	C8-N9-C4	6.58	108.43	105.80
22	BA	2542	A	C8-N9-C4	6.58	108.43	105.80
22	BA	167	A	C4-C5-C6	6.57	120.29	117.00
22	BA	1194	A	N9-C4-C5	6.57	108.43	105.80
22	BA	1308	A	C4-C5-C6	6.57	120.29	117.00
22	BA	1936	A	C5-N7-C8	6.57	107.19	103.90
22	BA	2851	A	N3-C4-N9	6.57	132.66	127.40
22	BA	2886	A	N3-C4-N9	6.57	132.66	127.40
55	D3	38	A	C4-C5-C6	6.57	120.29	117.00
22	BA	909	A	C5-C6-N1	6.57	120.99	117.70
1	AA	87	C	N1-C2-O2	6.57	122.84	118.90
22	BA	1000	A	N3-C4-N9	6.57	132.66	127.40
22	BA	1938	A	C4-C5-C6	6.57	120.28	117.00
22	BA	892	A	C4-C5-C6	6.57	120.28	117.00
22	BA	743	A	C5-N7-C8	6.56	107.18	103.90
22	BA	2381	A	C4-C5-C6	6.56	120.28	117.00
22	BA	2448	A	N9-C4-C5	6.56	108.42	105.80
22	BA	1151	A	N3-C4-N9	6.56	132.65	127.40
22	BA	2070	A	C4-C5-C6	6.56	120.28	117.00
22	BA	172	A	C4-C5-C6	6.55	120.28	117.00
22	BA	825	A	N3-C4-N9	6.55	132.64	127.40
22	BA	1433	A	N3-C4-N9	6.55	132.64	127.40
22	BA	1495	A	C4-C5-C6	6.55	120.28	117.00
23	BB	66	A	N3-C4-N9	6.55	132.64	127.40
1	AA	470	C	N3-C2-O2	-6.55	117.32	121.90
22	BA	470	A	C4-C5-C6	6.55	120.28	117.00
22	BA	2191	A	N3-C4-N9	6.55	132.64	127.40
22	BA	5	A	N3-C4-N9	6.55	132.64	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1142	A	C5-C6-N1	6.55	120.97	117.70
22	BA	28	A	N3-C4-N9	6.55	132.64	127.40
22	BA	412	A	N3-C4-N9	6.55	132.64	127.40
22	BA	1809	A	C4-C5-C6	6.55	120.27	117.00
22	BA	2577	A	C5-N7-C8	6.55	107.17	103.90
22	BA	2241	A	C4-C5-C6	6.54	120.27	117.00
22	BA	2183	A	C5-N7-C8	6.54	107.17	103.90
22	BA	2267	A	N9-C4-C5	6.54	108.42	105.80
22	BA	126	A	N9-C4-C5	6.54	108.42	105.80
22	BA	1029	A	N3-C4-N9	6.54	132.63	127.40
22	BA	1509	A	C8-N9-C4	6.54	108.42	105.80
22	BA	2646	C	C5-C6-N1	6.54	124.27	121.00
22	BA	2541	A	N3-C4-N9	6.54	132.63	127.40
22	BA	927	A	C4-C5-C6	6.54	120.27	117.00
22	BA	1321	A	C4-C5-C6	6.54	120.27	117.00
22	BA	1952	A	N3-C4-N9	6.54	132.63	127.40
22	BA	794	A	C5-N7-C8	6.53	107.17	103.90
22	BA	1937	A	C4-C5-N7	-6.53	107.43	110.70
22	BA	2598	A	C4-C5-C6	6.53	120.27	117.00
22	BA	2675	A	N3-C4-N9	6.53	132.63	127.40
22	BA	2879	A	C4-C5-C6	6.53	120.27	117.00
22	BA	2432	A	C5-N7-C8	6.53	107.17	103.90
22	BA	1134	A	C8-N9-C4	6.53	108.41	105.80
22	BA	2094	A	N3-C4-N9	6.53	132.62	127.40
22	BA	1698	A	C8-N9-C4	6.52	108.41	105.80
22	BA	1773	A	N3-C4-N9	6.52	132.62	127.40
22	BA	2418	A	C4-C5-C6	6.52	120.26	117.00
22	BA	203	A	C5-N7-C8	6.52	107.16	103.90
22	BA	1378	A	N9-C4-C5	6.52	108.41	105.80
1	AA	1132	C	C2-N1-C1'	6.52	125.97	118.80
22	BA	231	A	N3-C4-N9	6.52	132.62	127.40
22	BA	477	A	N3-C4-N9	6.52	132.61	127.40
22	BA	1677	A	N3-C4-N9	6.52	132.61	127.40
22	BA	526	A	N9-C4-C5	6.51	108.41	105.80
22	BA	2821	A	C4-C5-C6	6.51	120.26	117.00
55	D3	35	A	C5-N7-C8	6.51	107.16	103.90
22	BA	2108	A	C4-C5-C6	6.51	120.26	117.00
22	BA	2497	A	N9-C4-C5	6.51	108.41	105.80
22	BA	718	A	C4-C5-C6	6.51	120.26	117.00
22	BA	2392	A	N3-C4-N9	6.51	132.61	127.40
22	BA	1028	A	C5-C6-N1	6.51	120.95	117.70
22	BA	1403	A	N3-C4-N9	6.51	132.61	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1286	A	C8-N9-C4	6.51	108.40	105.80
22	BA	13	A	N9-C4-C5	6.51	108.40	105.80
22	BA	104	A	C4-C5-C6	6.51	120.25	117.00
22	BA	789	A	C4-C5-C6	6.51	120.25	117.00
22	BA	2872	A	C4-C5-C6	6.51	120.25	117.00
22	BA	2273	A	N9-C4-C5	6.50	108.40	105.80
22	BA	44	A	N3-C4-N9	6.50	132.60	127.40
22	BA	49	A	C4-C5-C6	6.50	120.25	117.00
22	BA	429	A	C5-N7-C8	6.50	107.15	103.90
22	BA	1001	A	N9-C4-C5	6.50	108.40	105.80
22	BA	1515	A	C4-C5-N7	-6.50	107.45	110.70
22	BA	2135	A	C8-N9-C4	6.50	108.40	105.80
23	BB	34	A	N3-C4-N9	6.50	132.60	127.40
22	BA	743	A	N3-C4-N9	6.50	132.60	127.40
22	BA	751	A	C4-C5-C6	6.50	120.25	117.00
22	BA	1169	A	C4-C5-C6	6.50	120.25	117.00
22	BA	825	A	C5-C6-N1	6.50	120.95	117.70
22	BA	1916	A	C4-C5-C6	6.50	120.25	117.00
22	BA	2377	A	C4-C5-C6	6.50	120.25	117.00
22	BA	354	A	C4-C5-N7	-6.50	107.45	110.70
22	BA	980	A	C4-C5-C6	6.50	120.25	117.00
22	BA	1385	A	N9-C4-C5	6.50	108.40	105.80
22	BA	2274	A	C4-C5-C6	6.50	120.25	117.00
22	BA	2468	A	N3-C4-N9	6.50	132.60	127.40
54	D2	5	A	N3-C4-N9	6.50	132.60	127.40
54	D2	49	A	C4-C5-C6	6.50	120.25	117.00
22	BA	125	A	C8-N9-C4	6.49	108.40	105.80
22	BA	863	A	C5-C6-N1	6.49	120.95	117.70
22	BA	2721	A	N3-C4-N9	6.49	132.59	127.40
23	BB	58	A	C4-C5-C6	6.49	120.25	117.00
22	BA	21	A	N3-C4-N9	6.49	132.59	127.40
22	BA	146	A	C4-C5-C6	6.49	120.25	117.00
22	BA	933	A	N9-C4-C5	6.49	108.40	105.80
22	BA	2781	A	C5-N7-C8	6.49	107.15	103.90
22	BA	742	A	C8-N9-C4	6.49	108.39	105.80
22	BA	844	A	N9-C4-C5	6.49	108.40	105.80
22	BA	1102	C	C5-C6-N1	6.49	124.24	121.00
22	BA	1847	A	C5-N7-C8	6.49	107.14	103.90
22	BA	592	A	N9-C4-C5	6.49	108.39	105.80
22	BA	2059	A	C5-N7-C8	6.48	107.14	103.90
55	D3	17	C	C5-C6-N1	6.48	124.24	121.00
17	AQ	75	LEU	CB-CG-CD1	-6.48	99.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	362	A	N3-C4-N9	6.48	132.58	127.40
22	BA	900	A	N3-C4-N9	6.48	132.58	127.40
22	BA	983	A	C8-N9-C4	6.48	108.39	105.80
22	BA	1722	A	C4-C5-C6	6.48	120.24	117.00
22	BA	2309	A	C4-C5-C6	6.48	120.24	117.00
22	BA	38	A	N9-C4-C5	6.48	108.39	105.80
22	BA	2070	A	C5-C6-N1	6.48	120.94	117.70
22	BA	2900	A	C4-C5-C6	6.48	120.24	117.00
22	BA	586	A	C4-C5-C6	6.48	120.24	117.00
22	BA	182	A	C4-C5-C6	6.47	120.24	117.00
22	BA	391	A	C4-C5-C6	6.47	120.24	117.00
22	BA	439	A	C4-C5-C6	6.47	120.24	117.00
22	BA	2020	A	C5-C6-N1	6.47	120.94	117.70
22	BA	466	A	C4-C5-C6	6.47	120.24	117.00
22	BA	727	A	N3-C4-N9	6.47	132.58	127.40
22	BA	899	A	N3-C4-N9	6.47	132.58	127.40
22	BA	1353	A	C5-C6-N1	6.47	120.94	117.70
22	BA	2003	A	C8-N9-C4	6.47	108.39	105.80
22	BA	332	A	C8-N9-C4	6.47	108.39	105.80
22	BA	1308	A	N3-C4-N9	6.47	132.57	127.40
22	BA	1794	A	C4-C5-C6	6.47	120.23	117.00
22	BA	73	A	C5-N7-C8	6.47	107.13	103.90
22	BA	2547	A	N9-C4-C5	6.47	108.39	105.80
22	BA	207	A	C4-C5-C6	6.46	120.23	117.00
22	BA	804	A	C8-N9-C4	6.46	108.39	105.80
22	BA	947	A	N3-C4-N9	6.46	132.57	127.40
22	BA	1253	A	C5-N7-C8	6.46	107.13	103.90
22	BA	2764	A	N9-C4-C5	6.46	108.38	105.80
22	BA	867	C	N1-C2-O2	6.46	122.78	118.90
22	BA	990	A	C4-C5-C6	6.46	120.23	117.00
22	BA	2868	A	N3-C4-N9	6.46	132.57	127.40
22	BA	2088	A	C5-C6-N1	6.46	120.93	117.70
22	BA	959	A	C4-C5-C6	6.46	120.23	117.00
22	BA	1566	A	C8-N9-C4	6.46	108.38	105.80
22	BA	1603	A	C5-C6-N1	6.46	120.93	117.70
22	BA	1637	A	C5-C6-N1	6.46	120.93	117.70
22	BA	196	A	N3-C4-N9	6.46	132.56	127.40
22	BA	497	A	C8-N9-C4	6.45	108.38	105.80
22	BA	1009	A	N3-C4-N9	6.45	132.56	127.40
22	BA	1027	A	C8-N9-C4	6.45	108.38	105.80
22	BA	1336	A	N3-C4-N9	6.45	132.56	127.40
22	BA	2327	A	C4-C5-C6	6.45	120.23	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	512	G	O4'-C1'-N9	6.45	113.36	108.20
22	BA	910	A	C4-C5-C6	6.45	120.22	117.00
22	BA	1151	A	C5-C6-N1	6.45	120.93	117.70
22	BA	1668	A	N9-C4-C5	6.45	108.38	105.80
22	BA	255	A	N3-C4-N9	6.45	132.56	127.40
22	BA	1635	A	N3-C4-N9	6.45	132.56	127.40
22	BA	2278	A	C4-C5-C6	6.45	120.22	117.00
22	BA	821	A	N9-C4-C5	6.45	108.38	105.80
22	BA	1652	A	N9-C4-C5	6.45	108.38	105.80
22	BA	2602	A	C4-C5-C6	6.45	120.22	117.00
22	BA	2665	A	C4-C5-C6	6.45	120.22	117.00
22	BA	91	A	C8-N9-C4	6.44	108.38	105.80
55	D3	73	A	C4-C5-C6	6.44	120.22	117.00
22	BA	1313	U	N1-C2-O2	6.44	127.31	122.80
22	BA	1786	A	C4-C5-C6	6.44	120.22	117.00
22	BA	1819	A	C5-C6-N1	6.44	120.92	117.70
22	BA	788	A	C5-N7-C8	6.44	107.12	103.90
22	BA	2184	A	C5-C6-N1	6.44	120.92	117.70
22	BA	1590	A	N3-C4-N9	6.44	132.55	127.40
22	BA	2534	A	C4-C5-C6	6.44	120.22	117.00
22	BA	621	A	N9-C4-C5	6.44	108.38	105.80
22	BA	1427	A	C4-C5-C6	6.44	120.22	117.00
22	BA	1548	A	C5-C6-N1	6.44	120.92	117.70
22	BA	1900	A	N3-C4-N9	6.44	132.55	127.40
22	BA	272	A	N3-C4-N9	6.43	132.55	127.40
22	BA	1783	A	N9-C4-C5	6.43	108.37	105.80
22	BA	2860	A	C5-N7-C8	6.43	107.12	103.90
22	BA	2052	A	C4-C5-C6	6.43	120.22	117.00
22	BA	324	A	C5-C6-N1	6.43	120.91	117.70
22	BA	1434	A	C4-C5-C6	6.43	120.21	117.00
22	BA	1969	A	C8-N9-C4	6.43	108.37	105.80
1	AA	1173	U	C2-N1-C1'	6.43	125.41	117.70
22	BA	1392	A	C5-C6-N1	6.43	120.91	117.70
22	BA	279	A	N3-C4-N9	6.42	132.54	127.40
22	BA	2750	A	C8-N9-C4	6.42	108.37	105.80
22	BA	497	A	C4-C5-C6	6.42	120.21	117.00
22	BA	2212	A	C4-C5-C6	6.42	120.21	117.00
22	BA	1532	A	N3-C4-N9	6.42	132.54	127.40
22	BA	1144	A	C8-N9-C4	6.42	108.37	105.80
1	AA	1173	U	C5-C6-N1	6.42	125.91	122.70
22	BA	670	A	C4-C5-C6	6.42	120.21	117.00
22	BA	1749	A	N9-C4-C5	6.42	108.37	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	131	A	C5-C6-N1	6.42	120.91	117.70
22	BA	142	A	N3-C4-N9	6.42	132.53	127.40
22	BA	1579	A	C4-C5-C6	6.42	120.21	117.00
56	D4	1	U	N3-C2-O2	-6.42	117.71	122.20
22	BA	928	A	C4-C5-C6	6.42	120.21	117.00
22	BA	1246	A	C5-C6-N1	6.42	120.91	117.70
22	BA	1655	A	C4-C5-C6	6.42	120.21	117.00
22	BA	715	A	C4-C5-C6	6.41	120.21	117.00
22	BA	1262	A	N3-C4-N9	6.41	132.53	127.40
22	BA	2094	A	C5-C6-N1	6.41	120.91	117.70
54	D2	35	A	C4-C5-C6	6.41	120.21	117.00
22	BA	1247	A	C5-C6-N1	6.41	120.91	117.70
40	BS	1	MET	CG-SD-CE	6.41	110.46	100.20
22	BA	439	A	N3-C4-N9	6.41	132.53	127.40
22	BA	1469	A	N9-C4-C5	6.41	108.36	105.80
22	BA	2352	A	C4-C5-C6	6.41	120.20	117.00
12	AL	103	ASP	N-CA-C	6.41	128.30	111.00
22	BA	347	A	N3-C4-N9	6.41	132.53	127.40
22	BA	572	A	C4-C5-C6	6.41	120.20	117.00
22	BA	2868	A	C5-N7-C8	6.41	107.10	103.90
22	BA	2826	A	C4-C5-C6	6.41	120.20	117.00
22	BA	800	A	C5-N7-C8	6.41	107.10	103.90
22	BA	1050	A	C4-C5-C6	6.41	120.20	117.00
22	BA	2761	A	C5-C6-N1	6.41	120.90	117.70
22	BA	1597	A	C4-C5-N7	-6.40	107.50	110.70
22	BA	348	A	C4-C5-C6	6.40	120.20	117.00
22	BA	2425	A	N3-C4-N9	6.40	132.52	127.40
22	BA	1014	A	N9-C4-C5	6.40	108.36	105.80
22	BA	1151	A	C4-C5-C6	6.40	120.20	117.00
22	BA	453	A	C4-C5-C6	6.40	120.20	117.00
22	BA	1640	A	C4-C5-C6	6.40	120.20	117.00
22	BA	262	A	N3-C4-N9	6.39	132.51	127.40
22	BA	632	A	C4-C5-C6	6.39	120.20	117.00
22	BA	833	A	C5-N7-C8	6.39	107.10	103.90
22	BA	918	A	N3-C4-N9	6.39	132.52	127.40
22	BA	1535	A	N3-C4-N9	6.39	132.51	127.40
22	BA	2547	A	C4-C5-C6	6.39	120.20	117.00
22	BA	2564	A	N9-C4-C5	6.39	108.36	105.80
22	BA	644	A	C4-C5-N7	-6.39	107.50	110.70
22	BA	1274	A	C4-C5-C6	6.39	120.20	117.00
22	BA	1598	A	N3-C4-N9	6.39	132.51	127.40
22	BA	1676	A	C4-C5-C6	6.39	120.19	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2062	A	C8-N9-C4	6.39	108.36	105.80
22	BA	1652	A	C8-N9-C4	6.39	108.36	105.80
22	BA	752	A	N3-C4-N9	6.39	132.51	127.40
22	BA	599	A	C4-C5-C6	6.38	120.19	117.00
22	BA	742	A	N3-C4-N9	6.38	132.51	127.40
22	BA	1008	A	N9-C4-C5	6.38	108.35	105.80
22	BA	1570	A	N9-C4-C5	6.38	108.35	105.80
22	BA	167	A	N3-C4-N9	6.38	132.51	127.40
22	BA	1805	A	C5-C6-N1	6.38	120.89	117.70
22	BA	2426	A	C5-N7-C8	6.38	107.09	103.90
22	BA	382	A	C4-C5-C6	6.38	120.19	117.00
22	BA	2761	A	C4-C5-C6	6.38	120.19	117.00
22	BA	21	A	C4-C5-C6	6.38	120.19	117.00
22	BA	1608	A	N3-C4-N9	6.38	132.50	127.40
23	BB	57	A	C4-C5-C6	6.38	120.19	117.00
22	BA	144	A	C5-C6-N1	6.37	120.89	117.70
22	BA	1103	A	C4-C5-C6	6.37	120.19	117.00
22	BA	1214	A	C4-C5-N7	-6.37	107.51	110.70
22	BA	1342	A	C8-N9-C4	6.37	108.35	105.80
22	BA	2757	A	N3-C4-N9	6.37	132.50	127.40
22	BA	504	A	N3-C4-N9	6.37	132.50	127.40
22	BA	497	A	N3-C4-N9	6.37	132.50	127.40
22	BA	1505	A	C5-C6-N1	6.37	120.89	117.70
22	BA	2051	A	C4-C5-C6	6.37	120.19	117.00
22	BA	203	A	N9-C4-C5	6.37	108.35	105.80
22	BA	1789	A	N3-C4-N9	6.37	132.49	127.40
22	BA	1801	A	N3-C4-N9	6.37	132.49	127.40
22	BA	1805	A	C4-C5-N7	-6.37	107.52	110.70
12	AL	101	ALA	CB-CA-C	-6.37	100.55	110.10
22	BA	502	A	C4-C5-C6	6.37	120.18	117.00
22	BA	1762	A	C4-C5-C6	6.37	120.18	117.00
22	BA	727	A	C8-N9-C4	6.36	108.35	105.80
22	BA	1111	A	C8-N9-C4	6.36	108.34	105.80
22	BA	1650	A	N9-C4-C5	6.36	108.34	105.80
22	BA	1901	A	N9-C4-C5	6.36	108.34	105.80
22	BA	38	A	C5-C6-N1	6.36	120.88	117.70
22	BA	1866	A	N3-C4-N9	6.36	132.49	127.40
22	BA	52	A	N3-C4-N9	6.36	132.49	127.40
22	BA	844	A	C5-C6-N1	6.36	120.88	117.70
22	BA	866	A	C8-N9-C4	6.36	108.34	105.80
22	BA	2886	A	C4-C5-C6	6.36	120.18	117.00
22	BA	279	A	C4-C5-C6	6.35	120.18	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	670	A	N3-C4-N9	6.35	132.48	127.40
22	BA	743	A	C4-C5-C6	6.35	120.18	117.00
22	BA	1952	A	C4-C5-C6	6.35	120.18	117.00
22	BA	2682	A	N3-C4-N9	6.35	132.48	127.40
22	BA	1020	A	C8-N9-C4	6.35	108.34	105.80
22	BA	1717	A	N3-C4-N9	6.35	132.48	127.40
1	AA	813	U	N3-C2-O2	-6.35	117.75	122.20
22	BA	1095	A	C4-C5-C6	6.35	120.17	117.00
22	BA	1785	A	N9-C4-C5	6.35	108.34	105.80
22	BA	959	A	N3-C4-N9	6.35	132.48	127.40
22	BA	1284	A	C4-C5-C6	6.35	120.17	117.00
22	BA	1313	U	N3-C2-O2	-6.35	117.76	122.20
22	BA	2820	A	N3-C4-N9	6.35	132.48	127.40
12	AL	101	ALA	N-CA-C	6.34	128.13	111.00
22	BA	2670	A	C5-C6-N1	6.34	120.87	117.70
54	D2	6	C	C2-N1-C1'	6.34	125.78	118.80
54	D2	69	A	C4-C5-C6	6.34	120.17	117.00
22	BA	2565	A	N9-C4-C5	6.34	108.34	105.80
22	BA	2868	A	C4-C5-C6	6.34	120.17	117.00
22	BA	422	A	C5-N7-C8	6.34	107.07	103.90
22	BA	1746	A	C5-C6-N1	6.34	120.87	117.70
22	BA	2328	A	C5-C6-N1	6.34	120.87	117.70
22	BA	2451	A	N9-C4-C5	6.34	108.34	105.80
22	BA	401	A	N9-C4-C5	6.34	108.33	105.80
22	BA	715	A	N3-C4-N9	6.34	132.47	127.40
22	BA	2826	A	N3-C4-N9	6.34	132.47	127.40
22	BA	2346	A	C8-N9-C4	6.33	108.33	105.80
22	BA	2778	A	C4-C5-C6	6.33	120.17	117.00
22	BA	515	A	N3-C4-N9	6.33	132.47	127.40
22	BA	529	A	N9-C4-C5	6.33	108.33	105.80
22	BA	1956	U	N1-C2-O2	6.33	127.23	122.80
22	BA	1969	A	C4-C5-C6	6.33	120.17	117.00
22	BA	181	A	C4-C5-C6	6.33	120.17	117.00
22	BA	1858	A	N3-C4-N9	6.33	132.46	127.40
22	BA	689	A	N3-C4-N9	6.33	132.46	127.40
22	BA	457	A	C8-N9-C4	6.33	108.33	105.80
22	BA	863	A	C8-N9-C4	6.33	108.33	105.80
22	BA	1672	A	C8-N9-C4	6.33	108.33	105.80
22	BA	2198	A	C4-C5-C6	6.32	120.16	117.00
22	BA	384	A	C4-C5-C6	6.32	120.16	117.00
22	BA	1679	A	C5-N7-C8	6.32	107.06	103.90
22	BA	2376	A	C4-C5-C6	6.32	120.16	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	501	A	C4-C5-C6	6.32	120.16	117.00
22	BA	2792	A	N9-C4-C5	6.32	108.33	105.80
22	BA	1899	A	N3-C4-N9	6.32	132.45	127.40
22	BA	1336	A	C5-C6-N1	6.32	120.86	117.70
22	BA	1749	A	C4-C5-C6	6.32	120.16	117.00
22	BA	2336	A	C4-C5-C6	6.32	120.16	117.00
22	BA	2468	A	C4-C5-C6	6.32	120.16	117.00
22	BA	2327	A	N9-C4-C5	6.31	108.33	105.80
22	BA	633	A	N3-C4-N9	6.31	132.45	127.40
22	BA	861	A	N9-C4-C5	6.31	108.33	105.80
22	BA	1096	A	C4-C5-C6	6.31	120.16	117.00
22	BA	748	G	O4'-C1'-N9	6.31	113.25	108.20
22	BA	2147	A	N9-C4-C5	6.31	108.32	105.80
22	BA	6	A	N3-C4-N9	6.31	132.45	127.40
22	BA	2433	A	N3-C4-N9	6.31	132.45	127.40
22	BA	2778	A	N3-C4-N9	6.31	132.45	127.40
22	BA	1080	A	N3-C4-N9	6.31	132.44	127.40
22	BA	1230	A	C5-C6-N1	6.31	120.85	117.70
22	BA	2042	A	C4-C5-C6	6.31	120.15	117.00
22	BA	2469	A	C8-N9-C4	6.31	108.32	105.80
22	BA	241	A	N9-C4-C5	6.30	108.32	105.80
22	BA	947	A	C4-C5-C6	6.30	120.15	117.00
22	BA	1347	A	C4-C5-N7	-6.30	107.55	110.70
22	BA	1551	A	C4-C5-N7	-6.30	107.55	110.70
22	BA	1664	A	N9-C4-C5	6.30	108.32	105.80
22	BA	1705	A	C5-C6-N1	6.30	120.85	117.70
22	BA	1413	A	N3-C4-N9	6.30	132.44	127.40
22	BA	1705	A	C8-N9-C4	6.30	108.32	105.80
22	BA	1126	A	C4-C5-C6	6.30	120.15	117.00
22	BA	1522	A	C8-N9-C4	6.30	108.32	105.80
22	BA	492	A	N3-C4-N9	6.30	132.44	127.40
23	BB	50	A	C4-C5-C6	6.30	120.15	117.00
22	BA	103	A	C4-C5-C6	6.29	120.15	117.00
22	BA	1274	A	N3-C4-N9	6.29	132.44	127.40
22	BA	1977	A	C8-N9-C4	6.29	108.32	105.80
22	BA	2682	A	C4-C5-C6	6.29	120.15	117.00
22	BA	453	A	C8-N9-C4	6.29	108.32	105.80
22	BA	575	A	N3-C4-N9	6.29	132.43	127.40
22	BA	943	A	N3-C4-N9	6.29	132.43	127.40
22	BA	1367	A	C4-C5-C6	6.29	120.15	117.00
22	BA	1544	A	N3-C4-N9	6.29	132.43	127.40
22	BA	1597	A	C4-C5-C6	6.29	120.14	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2199	A	N3-C4-N9	6.29	132.43	127.40
22	BA	2225	A	N3-C4-N9	6.29	132.43	127.40
22	BA	2761	A	N3-C4-N9	6.29	132.43	127.40
1	AA	993	G	C4-N9-C1'	6.29	134.67	126.50
22	BA	1287	A	N3-C4-N9	6.29	132.43	127.40
22	BA	911	A	C4-C5-C6	6.29	120.14	117.00
22	BA	255	A	C4-C5-C6	6.29	120.14	117.00
22	BA	1579	A	N3-C4-N9	6.29	132.43	127.40
22	BA	1877	A	C4-C5-C6	6.29	120.14	117.00
22	BA	2205	A	N3-C4-N9	6.29	132.43	127.40
22	BA	1596	A	C4-C5-C6	6.28	120.14	117.00
22	BA	2212	A	N3-C4-N9	6.28	132.43	127.40
22	BA	2837	A	N3-C4-N9	6.28	132.43	127.40
22	BA	95	A	N3-C4-N9	6.28	132.43	127.40
22	BA	371	A	C4-C5-N7	-6.28	107.56	110.70
22	BA	391	A	C8-N9-C4	6.28	108.31	105.80
22	BA	980	A	N3-C4-N9	6.28	132.42	127.40
22	BA	1803	A	N9-C4-C5	6.28	108.31	105.80
54	D2	49	A	N3-C4-N9	6.28	132.42	127.40
22	BA	1549	A	C5-C6-N1	6.28	120.84	117.70
22	BA	2478	A	C4-C5-C6	6.28	120.14	117.00
22	BA	538	A	C8-N9-C4	6.28	108.31	105.80
22	BA	2725	A	C5-C6-N1	6.28	120.84	117.70
22	BA	756	A	C5-C6-N1	6.28	120.84	117.70
22	BA	1453	A	C8-N9-C4	6.28	108.31	105.80
22	BA	655	A	C8-N9-C4	6.27	108.31	105.80
22	BA	1754	A	C4-C5-C6	6.27	120.14	117.00
22	BA	2516	A	N3-C4-N9	6.27	132.42	127.40
22	BA	2632	A	C4-C5-C6	6.27	120.14	117.00
22	BA	1755	A	N9-C4-C5	6.27	108.31	105.80
22	BA	1000	A	C4-C5-C6	6.27	120.14	117.00
22	BA	1434	A	N9-C4-C5	6.27	108.31	105.80
22	BA	2095	A	C4-C5-C6	6.27	120.14	117.00
22	BA	2587	A	N3-C4-N9	6.27	132.41	127.40
22	BA	514	A	N9-C4-C5	6.27	108.31	105.80
22	BA	1392	A	C4-C5-N7	-6.27	107.57	110.70
22	BA	1654	A	N3-C4-N9	6.27	132.41	127.40
22	BA	256	A	N3-C4-N9	6.27	132.41	127.40
22	BA	1626	A	C4-C5-C6	6.27	120.13	117.00
22	BA	2448	A	C4-C5-C6	6.27	120.13	117.00
22	BA	716	A	N3-C4-N9	6.26	132.41	127.40
22	BA	1226	A	N9-C4-C5	6.26	108.31	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D2	69	A	C5-C6-N1	6.26	120.83	117.70
22	BA	52	A	C4-C5-C6	6.26	120.13	117.00
22	BA	422	A	N3-C4-N9	6.26	132.41	127.40
23	BB	29	A	C4-C5-N7	-6.26	107.57	110.70
22	BA	1938	A	C8-N9-C4	6.26	108.30	105.80
54	D2	28	A	C5-C6-N1	6.26	120.83	117.70
22	BA	1858	A	C8-N9-C4	6.26	108.30	105.80
22	BA	507	A	C8-N9-C4	6.26	108.30	105.80
22	BA	1095	A	N3-C4-N9	6.26	132.41	127.40
22	BA	1169	A	N3-C4-N9	6.26	132.41	127.40
22	BA	2893	A	C8-N9-C4	6.26	108.30	105.80
22	BA	2614	A	N9-C4-C5	6.25	108.30	105.80
22	BA	2879	A	C8-N9-C4	6.25	108.30	105.80
22	BA	371	A	C8-N9-C4	6.25	108.30	105.80
22	BA	1073	A	C4-C5-C6	6.25	120.12	117.00
22	BA	2314	A	N9-C4-C5	6.25	108.30	105.80
54	D2	23	A	N3-C4-N9	6.25	132.40	127.40
22	BA	10	A	C5-C6-N1	6.25	120.83	117.70
22	BA	616	A	N3-C4-N9	6.25	132.40	127.40
22	BA	661	A	C4-C5-C6	6.25	120.12	117.00
22	BA	1307	A	N3-C4-N9	6.25	132.40	127.40
23	BB	52	A	C4-C5-C6	6.25	120.12	117.00
22	BA	1650	A	C4-C5-C6	6.25	120.12	117.00
22	BA	599	A	C8-N9-C4	6.24	108.30	105.80
22	BA	2173	A	C4-C5-C6	6.24	120.12	117.00
55	D3	62	C	C6-N1-C1'	6.24	128.29	120.80
22	BA	454	A	N9-C4-C5	6.24	108.30	105.80
22	BA	920	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1722	A	N3-C4-N9	6.24	132.39	127.40
22	BA	845	A	C5-C6-N1	6.24	120.82	117.70
22	BA	2560	A	N9-C4-C5	6.24	108.30	105.80
23	BB	119	A	C8-N9-C4	6.24	108.30	105.80
22	BA	144	A	C8-N9-C4	6.24	108.30	105.80
22	BA	347	A	N9-C4-C5	6.24	108.30	105.80
22	BA	478	A	N3-C4-N9	6.24	132.39	127.40
22	BA	1966	A	N9-C4-C5	6.24	108.30	105.80
22	BA	2309	A	N3-C4-N9	6.24	132.39	127.40
22	BA	2566	A	N9-C4-C5	6.24	108.30	105.80
22	BA	94	A	C4-C5-C6	6.24	120.12	117.00
22	BA	1050	A	N3-C4-N9	6.24	132.39	127.40
22	BA	2031	A	N3-C4-N9	6.24	132.39	127.40
22	BA	2450	A	C5-N7-C8	6.24	107.02	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	59	A	C8-N9-C4	6.24	108.30	105.80
22	BA	483	A	N3-C4-N9	6.24	132.39	127.40
22	BA	1877	A	N3-C4-N9	6.24	132.39	127.40
22	BA	528	A	C4-C5-C6	6.23	120.12	117.00
22	BA	28	A	C8-N9-C4	6.23	108.29	105.80
22	BA	1803	A	C4-C5-C6	6.23	120.12	117.00
23	BB	52	A	C8-N9-C4	6.23	108.29	105.80
22	BA	2478	A	N3-C4-N9	6.23	132.38	127.40
22	BA	1505	A	N3-C4-N9	6.23	132.38	127.40
22	BA	1679	A	N3-C4-N9	6.23	132.38	127.40
22	BA	2043	C	C2-N1-C1'	6.23	125.65	118.80
22	BA	160	A	N3-C4-N9	6.23	132.38	127.40
22	BA	792	A	N3-C4-N9	6.23	132.38	127.40
22	BA	1502	A	C4-C5-C6	6.22	120.11	117.00
40	BS	86	MET	CG-SD-CE	6.22	110.16	100.20
54	D2	35	A	C8-N9-C4	6.22	108.29	105.80
22	BA	119	A	N9-C4-C5	6.22	108.29	105.80
22	BA	1246	A	N9-C4-C5	6.22	108.29	105.80
22	BA	1383	A	N9-C4-C5	6.22	108.29	105.80
22	BA	2126	A	N3-C4-N9	6.22	132.38	127.40
35	BN	1	MET	CG-SD-CE	6.22	110.16	100.20
22	BA	1126	A	N9-C4-C5	6.22	108.29	105.80
22	BA	515	A	C4-C5-C6	6.22	120.11	117.00
22	BA	1096	A	N3-C4-N9	6.22	132.38	127.40
22	BA	2736	A	N9-C4-C5	6.22	108.29	105.80
22	BA	693	A	C8-N9-C4	6.22	108.29	105.80
22	BA	866	A	C4-C5-C6	6.22	120.11	117.00
22	BA	2471	A	C8-N9-C4	6.22	108.29	105.80
22	BA	541	A	N9-C4-C5	6.22	108.29	105.80
22	BA	1496	A	N9-C4-C5	6.22	108.29	105.80
22	BA	1504	A	C4-C5-C6	6.22	120.11	117.00
22	BA	1635	A	C4-C5-C6	6.22	120.11	117.00
22	BA	1969	A	N3-C4-N9	6.22	132.37	127.40
22	BA	2266	A	N3-C4-N9	6.21	132.37	127.40
22	BA	91	A	C4-C5-C6	6.21	120.11	117.00
22	BA	1155	A	N9-C4-C5	6.21	108.28	105.80
22	BA	2469	A	C5-C6-N1	6.21	120.81	117.70
22	BA	2900	A	N3-C4-N9	6.21	132.37	127.40
22	BA	2679	A	C5-C6-N1	6.21	120.81	117.70
22	BA	1956	U	N3-C2-O2	-6.21	117.86	122.20
22	BA	2003	A	C5-C6-N1	6.21	120.80	117.70
22	BA	918	A	C4-C5-C6	6.20	120.10	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1966	A	C4-C5-C6	6.20	120.10	117.00
54	D2	69	A	N3-C4-N9	6.20	132.36	127.40
22	BA	1265	A	N3-C4-N9	6.20	132.36	127.40
22	BA	2058	A	C4-C5-C6	6.20	120.10	117.00
22	BA	2753	A	C4-C5-C6	6.20	120.10	117.00
22	BA	1711	A	C4-C5-C6	6.20	120.10	117.00
22	BA	91	A	N3-C4-N9	6.20	132.36	127.40
22	BA	244	A	C4-C5-C6	6.20	120.10	117.00
22	BA	1262	A	C4-C5-C6	6.20	120.10	117.00
22	BA	1264	A	C5-N7-C8	6.20	107.00	103.90
22	BA	1580	A	C4-C5-C6	6.20	120.10	117.00
22	BA	1977	A	N3-C4-N9	6.20	132.36	127.40
22	BA	2590	A	N3-C4-N9	6.20	132.36	127.40
23	BB	15	A	N3-C4-N9	6.20	132.36	127.40
23	BB	45	A	N3-C4-N9	6.20	132.36	127.40
22	BA	1304	A	C4-C5-C6	6.20	120.10	117.00
22	BA	2340	A	C4-C5-C6	6.20	120.10	117.00
22	BA	2813	A	C5-N7-C8	6.20	107.00	103.90
22	BA	504	A	C4-C5-C6	6.20	120.10	117.00
22	BA	1147	A	N9-C4-C5	6.20	108.28	105.80
22	BA	1569	A	C8-N9-C4	6.20	108.28	105.80
22	BA	1739	A	C5-N7-C8	6.20	107.00	103.90
22	BA	1805	A	C4-C5-C6	6.20	120.10	117.00
22	BA	219	A	N9-C4-C5	6.19	108.28	105.80
54	D2	51	A	N3-C4-N9	6.19	132.35	127.40
55	D3	23	A	N9-C4-C5	6.19	108.28	105.80
22	BA	262	A	C4-C5-N7	-6.19	107.60	110.70
22	BA	631	A	C4-C5-C6	6.19	120.10	117.00
22	BA	2736	A	C4-C5-C6	6.19	120.10	117.00
22	BA	2820	A	C4-C5-C6	6.19	120.10	117.00
22	BA	56	A	C5-C6-N1	6.19	120.80	117.70
22	BA	756	A	C8-N9-C4	6.19	108.28	105.80
22	BA	2328	A	N3-C4-N9	6.19	132.35	127.40
22	BA	2590	A	C8-N9-C4	6.19	108.28	105.80
22	BA	2670	A	C8-N9-C4	6.19	108.28	105.80
54	D2	5	A	C4-C5-C6	6.19	120.09	117.00
22	BA	223	A	N9-C4-C5	6.19	108.28	105.80
22	BA	2171	A	C8-N9-C4	6.19	108.28	105.80
22	BA	2899	A	N3-C4-N9	6.19	132.35	127.40
22	BA	2381	A	N9-C4-C5	6.18	108.27	105.80
22	BA	2635	A	C5-C6-N1	6.18	120.79	117.70
22	BA	2635	A	N3-C4-N9	6.18	132.35	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2792	A	C4-C5-C6	6.18	120.09	117.00
1	AA	1158	C	C2-N1-C1'	6.18	125.60	118.80
22	BA	42	A	N3-C4-N9	6.18	132.35	127.40
22	BA	471	A	N3-C4-N9	6.18	132.34	127.40
22	BA	1077	A	N3-C4-N9	6.18	132.35	127.40
22	BA	1593	A	N3-C4-N9	6.18	132.34	127.40
54	D2	58	A	C8-N9-C4	6.18	108.27	105.80
22	BA	833	A	N9-C4-C5	6.18	108.27	105.80
22	BA	1953	A	C4-C5-C6	6.18	120.09	117.00
22	BA	522	A	C5-C6-N1	6.18	120.79	117.70
22	BA	2014	A	C4-C5-C6	6.18	120.09	117.00
22	BA	2560	A	C5-C6-N1	6.18	120.79	117.70
22	BA	1353	A	C4-C5-C6	6.17	120.09	117.00
22	BA	1889	A	N3-C4-N9	6.17	132.34	127.40
22	BA	2013	A	C5-C6-N1	6.17	120.79	117.70
22	BA	2726	A	N3-C4-N9	6.17	132.34	127.40
23	BB	45	A	C4-C5-C6	6.17	120.09	117.00
22	BA	829	A	C8-N9-C4	6.17	108.27	105.80
22	BA	73	A	N9-C4-C5	6.17	108.27	105.80
22	BA	2531	A	C4-C5-C6	6.17	120.09	117.00
22	BA	13	A	C4-C5-C6	6.17	120.08	117.00
22	BA	1586	A	N3-C4-N9	6.17	132.34	127.40
22	BA	2711	A	C4-C5-C6	6.17	120.08	117.00
22	BA	342	A	C4-C5-C6	6.17	120.08	117.00
22	BA	742	A	C5-C6-N1	6.17	120.78	117.70
22	BA	1383	A	C4-C5-C6	6.17	120.08	117.00
22	BA	1786	A	N3-C4-N9	6.17	132.33	127.40
22	BA	2281	A	C4-C5-C6	6.17	120.08	117.00
22	BA	2814	A	N3-C4-N9	6.17	132.33	127.40
54	D2	73	A	C8-N9-C4	6.17	108.27	105.80
22	BA	643	A	C4-C5-C6	6.16	120.08	117.00
22	BA	1194	A	C4-C5-C6	6.16	120.08	117.00
22	BA	2340	A	N3-C4-N9	6.16	132.33	127.40
22	BA	2792	A	C4-C5-N7	-6.16	107.62	110.70
22	BA	217	A	N3-C4-N9	6.16	132.33	127.40
22	BA	1067	A	C4-C5-C6	6.16	120.08	117.00
22	BA	95	A	N9-C4-C5	6.16	108.26	105.80
22	BA	346	A	N3-C4-N9	6.16	132.33	127.40
22	BA	1525	A	C4-C5-C6	6.16	120.08	117.00
22	BA	1858	A	C5-C6-N1	6.16	120.78	117.70
22	BA	2376	A	N3-C4-N9	6.16	132.33	127.40
54	D2	5	A	C5-C6-N1	6.16	120.78	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	10	A	N9-C4-C5	6.16	108.26	105.80
22	BA	1348	C	N3-C2-O2	-6.16	117.59	121.90
26	BE	188	MET	CG-SD-CE	6.16	110.05	100.20
22	BA	320	A	N9-C4-C5	6.16	108.26	105.80
22	BA	973	A	C8-N9-C4	6.16	108.26	105.80
22	BA	2134	A	N3-C4-N9	6.16	132.32	127.40
22	BA	2766	A	C5-C6-N1	6.16	120.78	117.70
22	BA	925	A	C5-C6-N1	6.16	120.78	117.70
22	BA	1194	A	C5-C6-N1	6.16	120.78	117.70
22	BA	1757	A	C4-C5-C6	6.16	120.08	117.00
22	BA	1802	A	N3-C4-N9	6.16	132.32	127.40
22	BA	2468	A	C8-N9-C4	6.16	108.26	105.80
22	BA	479	A	C5-C6-N1	6.15	120.78	117.70
22	BA	1165	A	C4-C5-N7	-6.15	107.62	110.70
22	BA	2195	U	C2-N1-C1'	6.15	125.08	117.70
55	D3	64	A	C5-C6-N1	6.15	120.78	117.70
22	BA	432	A	N3-C4-N9	6.15	132.32	127.40
22	BA	507	A	C4-C5-C6	6.15	120.08	117.00
22	BA	216	A	C4-C5-C6	6.15	120.08	117.00
22	BA	262	A	C5-C6-N1	6.15	120.78	117.70
22	BA	265	A	C8-N9-C4	6.15	108.26	105.80
22	BA	794	A	C8-N9-C4	6.15	108.26	105.80
22	BA	1590	A	C5-C6-N1	6.15	120.77	117.70
22	BA	1664	A	C4-C5-C6	6.15	120.07	117.00
22	BA	2142	A	C4-C5-C6	6.15	120.07	117.00
22	BA	2270	A	C4-C5-C6	6.15	120.07	117.00
54	D2	41	A	N3-C4-N9	6.15	132.32	127.40
22	BA	322	A	N9-C4-C5	6.15	108.26	105.80
22	BA	637	A	C8-N9-C4	6.14	108.26	105.80
22	BA	899	A	C4-C5-C6	6.14	120.07	117.00
22	BA	1848	A	N3-C4-N9	6.14	132.32	127.40
23	BB	119	A	C4-C5-C6	6.14	120.07	117.00
22	BA	616	A	C4-C5-C6	6.14	120.07	117.00
22	BA	2327	A	N3-C4-N9	6.14	132.31	127.40
22	BA	2476	A	C4-C5-C6	6.14	120.07	117.00
23	BB	101	A	C4-C5-C6	6.14	120.07	117.00
22	BA	1544	A	C4-C5-C6	6.14	120.07	117.00
22	BA	126	A	C4-C5-C6	6.14	120.07	117.00
22	BA	599	A	C5-C6-N1	6.14	120.77	117.70
22	BA	718	A	N3-C4-N9	6.14	132.31	127.40
22	BA	1147	A	C5-C6-N1	6.14	120.77	117.70
22	BA	563	A	C8-N9-C4	6.14	108.25	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1085	A	N3-C4-N9	6.14	132.31	127.40
22	BA	1773	A	N9-C4-C5	6.14	108.25	105.80
22	BA	449	A	N3-C4-N9	6.13	132.31	127.40
22	BA	825	A	N9-C4-C5	6.13	108.25	105.80
22	BA	1477	A	N3-C4-N9	6.13	132.31	127.40
22	BA	2169	A	N3-C4-N9	6.13	132.31	127.40
22	BA	2856	A	C5-C6-N1	6.13	120.77	117.70
22	BA	1913	A	C8-N9-C4	6.13	108.25	105.80
22	BA	2003	A	N3-C4-N9	6.13	132.31	127.40
1	AA	439	U	C6-N1-C1'	-6.13	112.62	121.20
22	BA	590	A	N3-C4-N9	6.13	132.30	127.40
22	BA	668	A	C8-N9-C4	6.13	108.25	105.80
22	BA	2336	A	N3-C4-N9	6.13	132.30	127.40
22	BA	1253	A	C8-N9-C4	6.13	108.25	105.80
22	BA	1262	A	N9-C4-C5	6.13	108.25	105.80
22	BA	218	A	N9-C4-C5	6.12	108.25	105.80
22	BA	362	A	C4-C5-C6	6.12	120.06	117.00
22	BA	1469	A	N3-C4-N9	6.12	132.30	127.40
22	BA	1508	A	C4-C5-C6	6.12	120.06	117.00
22	BA	1899	A	N9-C4-C5	6.12	108.25	105.80
22	BA	2014	A	N3-C4-N9	6.12	132.30	127.40
55	D3	9	A	N9-C4-C5	6.12	108.25	105.80
22	BA	2666	C	N1-C2-O2	6.12	122.57	118.90
22	BA	2736	A	N3-C4-N9	6.12	132.30	127.40
22	BA	1226	A	C4-C5-C6	6.12	120.06	117.00
22	BA	415	A	C5-N7-C8	6.12	106.96	103.90
22	BA	2070	A	C4-C5-N7	-6.12	107.64	110.70
22	BA	1774	C	N3-C2-O2	-6.12	117.62	121.90
22	BA	2033	A	C8-N9-C4	6.12	108.25	105.80
22	BA	2126	A	C4-C5-C6	6.12	120.06	117.00
22	BA	2369	A	C5-C6-N1	6.12	120.76	117.70
22	BA	1147	A	C8-N9-C4	6.11	108.25	105.80
22	BA	1392	A	N3-C4-N9	6.11	132.29	127.40
22	BA	1403	A	C5-C6-N1	6.11	120.76	117.70
22	BA	38	A	N3-C4-N9	6.11	132.29	127.40
22	BA	1598	A	N9-C4-C5	6.11	108.25	105.80
22	BA	2700	A	C5-C6-N1	6.11	120.76	117.70
22	BA	428	A	N3-C4-N9	6.11	132.29	127.40
22	BA	1504	A	C8-N9-C4	6.11	108.24	105.80
23	BB	46	A	N3-C4-N9	6.11	132.29	127.40
23	BB	101	A	N3-C4-N9	6.11	132.29	127.40
1	AA	83	C	C2-N1-C1'	-6.11	112.08	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	181	A	N9-C4-C5	6.11	108.24	105.80
22	BA	320	A	C4-C5-C6	6.11	120.05	117.00
22	BA	945	A	N3-C4-N9	6.11	132.29	127.40
22	BA	1260	A	N3-C4-N9	6.11	132.29	127.40
22	BA	1264	A	C4-C5-C6	6.11	120.05	117.00
22	BA	2005	A	N9-C4-C5	6.11	108.24	105.80
22	BA	2071	A	N3-C4-N9	6.11	132.29	127.40
22	BA	111	A	N9-C4-C5	6.11	108.24	105.80
22	BA	340	A	C8-N9-C4	6.11	108.24	105.80
22	BA	825	A	C4-C5-N7	-6.11	107.65	110.70
22	BA	1230	A	N3-C4-N9	6.11	132.28	127.40
22	BA	1268	A	N3-C4-N9	6.11	132.28	127.40
22	BA	1307	A	N9-C4-C5	6.11	108.24	105.80
22	BA	1496	A	C4-C5-C6	6.11	120.05	117.00
22	BA	1784	A	C4-C5-C6	6.11	120.05	117.00
22	BA	2632	A	N9-C4-C5	6.11	108.24	105.80
55	D3	14	A	C8-N9-C4	6.11	108.24	105.80
22	BA	764	A	N9-C4-C5	6.10	108.24	105.80
22	BA	340	A	C4-C5-C6	6.10	120.05	117.00
22	BA	676	A	C4-C5-C6	6.10	120.05	117.00
22	BA	900	A	C4-C5-C6	6.10	120.05	117.00
22	BA	2273	A	N3-C4-N9	6.10	132.28	127.40
22	BA	2809	A	N9-C4-C5	6.10	108.24	105.80
23	BB	94	A	C5-C6-N1	6.10	120.75	117.70
22	BA	1502	A	C8-N9-C4	6.10	108.24	105.80
22	BA	2077	A	C5-C6-N1	6.10	120.75	117.70
22	BA	2469	A	N3-C4-N9	6.10	132.28	127.40
22	BA	2531	A	C8-N9-C4	6.10	108.24	105.80
54	D2	21	A	C8-N9-C4	6.10	108.24	105.80
22	BA	207	A	N3-C4-N9	6.10	132.28	127.40
22	BA	371	A	C4-C5-C6	6.10	120.05	117.00
22	BA	1067	A	N3-C4-N9	6.10	132.28	127.40
22	BA	2268	A	N3-C4-N9	6.10	132.28	127.40
22	BA	1572	A	C8-N9-C4	6.09	108.24	105.80
22	BA	2108	A	C4-C5-N7	-6.09	107.65	110.70
22	BA	2158	A	N3-C4-N9	6.09	132.28	127.40
22	BA	2211	A	C8-N9-C4	6.09	108.24	105.80
22	BA	1314	C	C5-C6-N1	6.09	124.05	121.00
54	D2	23	A	C5-C6-N1	6.09	120.75	117.70
22	BA	1284	A	N3-C4-N9	6.09	132.27	127.40
22	BA	127	A	N9-C4-C5	6.09	108.24	105.80
22	BA	792	A	C4-C5-C6	6.09	120.05	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	981	A	C4-C5-C6	6.09	120.05	117.00
22	BA	2020	A	N3-C4-N9	6.09	132.27	127.40
22	BA	347	A	C5-C6-N1	6.09	120.74	117.70
22	BA	782	A	N3-C4-N9	6.09	132.27	127.40
22	BA	945	A	N9-C4-C5	6.09	108.23	105.80
22	BA	1503	A	C4-C5-C6	6.09	120.04	117.00
22	BA	2241	A	N3-C4-N9	6.09	132.27	127.40
54	D2	76	A	C8-N9-C4	6.09	108.23	105.80
22	BA	13	A	N3-C4-N9	6.08	132.27	127.40
22	BA	508	A	N3-C4-N9	6.08	132.27	127.40
22	BA	1247	A	C4-C5-N7	-6.08	107.66	110.70
22	BA	1690	A	N3-C4-N9	6.08	132.27	127.40
22	BA	2154	A	C8-N9-C4	6.08	108.23	105.80
22	BA	2837	A	C8-N9-C4	6.08	108.23	105.80
22	BA	1347	A	C4-C5-C6	6.08	120.04	117.00
22	BA	1668	A	C5-C6-N1	6.08	120.74	117.70
22	BA	384	A	N3-C4-N9	6.08	132.26	127.40
22	BA	1641	A	C4-C5-C6	6.08	120.04	117.00
22	BA	1918	A	C4-C5-C6	6.08	120.04	117.00
22	BA	2003	A	C4-C5-C6	6.08	120.04	117.00
22	BA	2062	A	N3-C4-N9	6.08	132.26	127.40
22	BA	2169	A	C4-C5-C6	6.08	120.04	117.00
22	BA	2813	A	N3-C4-N9	6.08	132.26	127.40
22	BA	1069	A	N3-C4-N9	6.08	132.26	127.40
22	BA	1652	A	C4-C5-N7	-6.08	107.66	110.70
22	BA	2792	A	C8-N9-C4	6.08	108.23	105.80
22	BA	599	A	N3-C4-N9	6.08	132.26	127.40
22	BA	1366	A	N3-C4-N9	6.08	132.26	127.40
22	BA	1630	A	C5-C6-N1	6.08	120.74	117.70
22	BA	2835	A	C4-C5-C6	6.08	120.04	117.00
22	BA	514	A	N3-C4-N9	6.07	132.26	127.40
22	BA	602	A	N3-C4-N9	6.07	132.26	127.40
22	BA	1102	C	C6-N1-C2	-6.07	117.87	120.30
22	BA	2660	A	C8-N9-C4	6.07	108.23	105.80
22	BA	2837	A	C5-C6-N1	6.07	120.74	117.70
22	BA	460	A	N9-C4-C5	6.07	108.23	105.80
22	BA	2052	A	C8-N9-C4	6.07	108.23	105.80
22	BA	575	A	C8-N9-C4	6.07	108.23	105.80
22	BA	1495	A	N9-C4-C5	6.07	108.23	105.80
22	BA	1640	A	N3-C4-N9	6.07	132.26	127.40
22	BA	1755	A	C4-C5-C6	6.07	120.03	117.00
22	BA	2418	A	C5-C6-N1	6.07	120.74	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BX	56	MET	CG-SD-CE	6.07	109.91	100.20
22	BA	477	A	C8-N9-C4	6.07	108.23	105.80
22	BA	1713	A	N3-C4-N9	6.07	132.25	127.40
22	BA	300	A	C4-C5-C6	6.07	120.03	117.00
22	BA	1650	A	C5-C6-N1	6.07	120.73	117.70
1	AA	1317	C	C6-N1-C2	-6.07	117.87	120.30
22	BA	1494	A	C4-C5-C6	6.07	120.03	117.00
22	BA	1815	A	C8-N9-C4	6.07	108.23	105.80
22	BA	2835	A	C8-N9-C4	6.07	108.23	105.80
22	BA	2119	A	C8-N9-C4	6.06	108.23	105.80
22	BA	233	A	N3-C4-N9	6.06	132.25	127.40
55	D3	9	A	C4-C5-N7	-6.06	107.67	110.70
22	BA	2893	A	N3-C4-N9	6.06	132.25	127.40
22	BA	344	A	C4-C5-C6	6.06	120.03	117.00
22	BA	1194	A	C4-C5-N7	-6.06	107.67	110.70
22	BA	1508	A	N3-C4-N9	6.06	132.25	127.40
22	BA	2418	A	N3-C4-N9	6.06	132.25	127.40
22	BA	2439	A	N3-C4-N9	6.06	132.25	127.40
22	BA	2810	A	N3-C4-N9	6.06	132.25	127.40
22	BA	1597	A	C5-C6-N1	6.06	120.73	117.70
22	BA	1821	A	C4-C5-C6	6.06	120.03	117.00
22	BA	2829	A	C4-C5-C6	6.06	120.03	117.00
22	BA	1535	A	C4-C5-C6	6.06	120.03	117.00
22	BA	352	A	C8-N9-C4	6.05	108.22	105.80
22	BA	428	A	C8-N9-C4	6.05	108.22	105.80
55	D3	26	A	C5-C6-N1	6.05	120.73	117.70
22	BA	829	A	C4-C5-C6	6.05	120.03	117.00
22	BA	1987	A	C5-C6-N1	6.05	120.73	117.70
22	BA	1254	A	C8-N9-C4	6.05	108.22	105.80
22	BA	2090	A	C8-N9-C4	6.05	108.22	105.80
22	BA	2227	A	N3-C4-N9	6.05	132.24	127.40
22	BA	2267	A	N3-C4-N9	6.05	132.24	127.40
22	BA	118	A	N3-C4-N9	6.05	132.24	127.40
22	BA	1932	A	N9-C4-C5	6.05	108.22	105.80
23	BB	52	A	N3-C4-N9	6.05	132.24	127.40
22	BA	233	A	C8-N9-C4	6.05	108.22	105.80
22	BA	1434	A	N3-C4-N9	6.05	132.24	127.40
22	BA	2700	A	C8-N9-C4	6.05	108.22	105.80
22	BA	592	A	C4-C5-N7	-6.04	107.68	110.70
54	D2	58	A	C4-C5-N7	-6.04	107.68	110.70
22	BA	654	A	C4-C5-C6	6.04	120.02	117.00
22	BA	1008	A	C4-C5-C6	6.04	120.02	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2241	A	C5-C6-N1	6.04	120.72	117.70
55	D3	14	A	C4-C5-C6	6.04	120.02	117.00
22	BA	749	A	N9-C4-C5	6.04	108.22	105.80
22	BA	1829	A	C5-C6-N1	6.04	120.72	117.70
22	BA	2358	A	N3-C4-N9	6.04	132.23	127.40
55	D3	33	U	C2-N1-C1'	6.04	124.95	117.70
22	BA	21	A	C5-C6-N1	6.04	120.72	117.70
22	BA	453	A	N3-C4-N9	6.04	132.23	127.40
22	BA	454	A	C4-C5-N7	-6.04	107.68	110.70
20	AT	86	LEU	CA-CB-CG	6.04	129.19	115.30
22	BA	348	A	N3-C4-N9	6.04	132.23	127.40
22	BA	472	A	C4-C5-C6	6.04	120.02	117.00
22	BA	1392	A	C4-C5-C6	6.04	120.02	117.00
22	BA	2358	A	C8-N9-C4	6.04	108.22	105.80
22	BA	233	A	C4-C5-C6	6.04	120.02	117.00
22	BA	689	A	C4-C5-N7	-6.04	107.68	110.70
22	BA	430	A	C5-C6-N1	6.04	120.72	117.70
22	BA	2381	A	C8-N9-C4	6.04	108.21	105.80
22	BA	2482	A	N3-C4-N9	6.04	132.23	127.40
22	BA	160	A	N9-C4-C5	6.03	108.21	105.80
22	BA	574	A	C8-N9-C4	6.03	108.21	105.80
22	BA	1244	A	C5-C6-N1	6.03	120.72	117.70
22	BA	2381	A	C4-C5-N7	-6.03	107.68	110.70
22	BA	2530	A	N3-C4-N9	6.03	132.23	127.40
22	BA	820	A	N3-C4-N9	6.03	132.23	127.40
22	BA	1077	A	C4-C5-C6	6.03	120.02	117.00
22	BA	1126	A	N3-C4-N9	6.03	132.23	127.40
22	BA	2097	A	C5-C6-N1	6.03	120.72	117.70
22	BA	2317	A	C5-C6-N1	6.03	120.72	117.70
22	BA	1260	A	N9-C4-C5	6.03	108.21	105.80
22	BA	1322	A	C4-C5-C6	6.03	120.02	117.00
22	BA	1635	A	C8-N9-C4	6.03	108.21	105.80
22	BA	2117	A	C4-C5-N7	-6.03	107.69	110.70
22	BA	155	A	C4-C5-C6	6.03	120.02	117.00
22	BA	1090	A	C4-C5-C6	6.03	120.02	117.00
22	BA	1395	A	N9-C4-C5	6.03	108.21	105.80
55	D3	59	U	N3-C2-O2	-6.03	117.98	122.20
22	BA	574	A	C4-C5-C6	6.03	120.01	117.00
22	BA	1393	A	C4-C5-C6	6.03	120.01	117.00
22	BA	1544	A	N9-C4-C5	6.03	108.21	105.80
22	BA	1089	A	C8-N9-C4	6.03	108.21	105.80
22	BA	2298	A	C8-N9-C4	6.03	108.21	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	661	A	C8-N9-C4	6.02	108.21	105.80
22	BA	1204	A	C8-N9-C4	6.02	108.21	105.80
22	BA	1246	A	C4-C5-C6	6.02	120.01	117.00
22	BA	1439	A	N3-C4-N9	6.02	132.22	127.40
22	BA	182	A	N9-C4-C5	6.02	108.21	105.80
22	BA	294	A	C4-C5-C6	6.02	120.01	117.00
22	BA	368	A	C4-C5-C6	6.02	120.01	117.00
22	BA	1427	A	N3-C4-N9	6.02	132.22	127.40
22	BA	2225	A	C4-C5-C6	6.02	120.01	117.00
22	BA	2639	A	C5-C6-N1	6.02	120.71	117.70
22	BA	429	A	N3-C4-N9	6.02	132.22	127.40
22	BA	756	A	N9-C4-C5	6.02	108.21	105.80
22	BA	2019	A	N3-C4-N9	6.02	132.22	127.40
22	BA	2738	A	N9-C4-C5	6.02	108.21	105.80
22	BA	146	A	N3-C4-N9	6.02	132.22	127.40
22	BA	920	A	N3-C4-N9	6.02	132.22	127.40
22	BA	1773	A	C4-C5-N7	-6.02	107.69	110.70
22	BA	2019	A	C4-C5-C6	6.02	120.01	117.00
22	BA	861	A	C4-C5-N7	-6.02	107.69	110.70
22	BA	1069	A	C4-C5-C6	6.01	120.01	117.00
22	BA	1885	A	N3-C4-N9	6.01	132.21	127.40
22	BA	727	A	C5-N7-C8	6.01	106.91	103.90
22	BA	2270	A	N3-C4-N9	6.01	132.21	127.40
22	BA	2435	A	C8-N9-C4	6.01	108.20	105.80
55	D3	14	A	N3-C4-N9	6.01	132.21	127.40
22	BA	89	A	C4-C5-N7	-6.01	107.69	110.70
22	BA	422	A	C4-C5-C6	6.01	120.00	117.00
22	BA	460	A	C4-C5-N7	-6.01	107.69	110.70
22	BA	1378	A	C4-C5-N7	-6.01	107.69	110.70
22	BA	1901	A	C4-C5-C6	6.01	120.00	117.00
22	BA	2154	A	C4-C5-C6	6.01	120.00	117.00
22	BA	2725	A	N9-C4-C5	6.01	108.20	105.80
22	BA	2733	A	N3-C4-N9	6.01	132.21	127.40
22	BA	172	A	N3-C4-N9	6.01	132.21	127.40
22	BA	586	A	C5-N7-C8	6.01	106.90	103.90
22	BA	404	A	C8-N9-C4	6.01	108.20	105.80
22	BA	804	A	C4-C5-C6	6.01	120.00	117.00
22	BA	2471	A	C5-C6-N1	6.01	120.70	117.70
54	D2	38	A	C8-N9-C4	6.01	108.20	105.80
22	BA	482	A	C4-C5-C6	6.00	120.00	117.00
22	BA	1987	A	C4-C5-C6	6.00	120.00	117.00
22	BA	149	A	C4-C5-C6	6.00	120.00	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1129	A	N9-C4-C5	6.00	108.20	105.80
22	BA	1505	A	C4-C5-C6	6.00	120.00	117.00
22	BA	2009	A	C5-C6-N1	6.00	120.70	117.70
22	BA	2191	A	C5-C6-N1	6.00	120.70	117.70
23	BB	108	A	C8-N9-C4	6.00	108.20	105.80
22	BA	176	A	C5-C6-N1	6.00	120.70	117.70
22	BA	428	A	C4-C5-C6	6.00	120.00	117.00
22	BA	1264	A	N9-C4-C5	6.00	108.20	105.80
22	BA	1981	A	C4-C5-N7	-6.00	107.70	110.70
22	BA	2761	A	C8-N9-C4	6.00	108.20	105.80
22	BA	2792	A	C5-C6-N1	6.00	120.70	117.70
22	BA	243	U	N1-C2-O2	6.00	127.00	122.80
22	BA	430	A	C4-C5-C6	6.00	120.00	117.00
22	BA	482	A	N3-C4-N9	6.00	132.20	127.40
22	BA	739	A	N3-C4-N9	6.00	132.20	127.40
22	BA	2872	A	C5-N7-C8	6.00	106.90	103.90
55	D3	37	A	C4-C5-N7	-6.00	107.70	110.70
22	BA	1413	A	C5-C6-N1	6.00	120.70	117.70
22	BA	2170	A	C4-C5-C6	6.00	120.00	117.00
22	BA	2287	A	C8-N9-C4	6.00	108.20	105.80
22	BA	2887	A	C4-C5-C6	6.00	120.00	117.00
22	BA	508	A	C8-N9-C4	6.00	108.20	105.80
22	BA	2142	A	N9-C4-C5	6.00	108.20	105.80
22	BA	104	A	N3-C4-N9	5.99	132.19	127.40
22	BA	320	A	N3-C4-N9	5.99	132.19	127.40
22	BA	905	A	C4-C5-N7	-5.99	107.70	110.70
22	BA	2090	A	C5-C6-N1	5.99	120.70	117.70
23	BB	53	A	C4-C5-C6	5.99	120.00	117.00
22	BA	483	A	C4-C5-C6	5.99	120.00	117.00
1	AA	307	C	C2-N1-C1'	5.99	125.39	118.80
22	BA	2154	A	N3-C4-N9	5.99	132.19	127.40
22	BA	621	A	C5-C6-N1	5.99	120.69	117.70
22	BA	1427	A	C8-N9-C4	5.99	108.20	105.80
22	BA	1665	A	C5-C6-N1	5.99	120.69	117.70
22	BA	2062	A	C5-C6-N1	5.99	120.69	117.70
22	BA	2711	A	C8-N9-C4	5.99	108.20	105.80
22	BA	111	A	C4-C5-N7	-5.99	107.71	110.70
22	BA	1147	A	C4-C5-N7	-5.99	107.71	110.70
22	BA	1314	C	C6-N1-C2	-5.99	117.91	120.30
22	BA	2378	A	C4-C5-C6	5.99	119.99	117.00
1	AA	542	G	N7-C8-N9	5.99	116.09	113.10
22	BA	340	A	N3-C4-N9	5.99	132.19	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2411	A	C4-C5-C6	5.99	119.99	117.00
22	BA	2614	A	C4-C5-C6	5.99	119.99	117.00
22	BA	270	A	C4-C5-C6	5.98	119.99	117.00
22	BA	53	A	C4-C5-C6	5.98	119.99	117.00
22	BA	1010	A	N3-C4-N9	5.98	132.19	127.40
22	BA	1276	A	C4-C5-N7	-5.98	107.71	110.70
36	BO	1	MET	CG-SD-CE	5.98	109.77	100.20
22	BA	503	A	N3-C4-N9	5.98	132.19	127.40
22	BA	909	A	N9-C4-C5	5.98	108.19	105.80
22	BA	936	A	C5-C6-N1	5.98	120.69	117.70
22	BA	1127	A	C4-C5-C6	5.98	119.99	117.00
22	BA	1689	A	N3-C4-N9	5.98	132.18	127.40
22	BA	1847	A	N9-C4-C5	5.98	108.19	105.80
22	BA	2657	A	C4-C5-C6	5.98	119.99	117.00
22	BA	501	A	N3-C4-N9	5.98	132.18	127.40
22	BA	1502	A	N3-C4-N9	5.98	132.18	127.40
22	BA	1745	A	C4-C5-C6	5.98	119.99	117.00
22	BA	2590	A	C4-C5-C6	5.98	119.99	117.00
22	BA	1676	A	C5-N7-C8	5.98	106.89	103.90
22	BA	1700	A	C4-C5-C6	5.98	119.99	117.00
22	BA	401	A	C4-C5-C6	5.98	119.99	117.00
22	BA	734	A	C8-N9-C4	5.98	108.19	105.80
22	BA	1552	A	N9-C4-C5	5.97	108.19	105.80
22	BA	2051	A	N3-C4-N9	5.97	132.18	127.40
22	BA	2565	A	C4-C5-N7	-5.97	107.71	110.70
23	BB	59	A	N3-C4-N9	5.97	132.18	127.40
22	BA	1359	A	C8-N9-C4	5.97	108.19	105.80
22	BA	1918	A	N3-C4-N9	5.97	132.18	127.40
22	BA	2434	A	N9-C4-C5	5.97	108.19	105.80
22	BA	1366	A	C4-C5-C6	5.97	119.98	117.00
22	BA	1571	A	N9-C4-C5	5.97	108.19	105.80
22	BA	1730	C	C5-C6-N1	5.97	123.98	121.00
54	D2	59	A	C4-C5-C6	5.97	119.99	117.00
22	BA	165	A	C4-C5-C6	5.97	119.98	117.00
22	BA	1801	A	C4-C5-C6	5.97	119.98	117.00
54	D2	59	A	N3-C4-N9	5.97	132.18	127.40
22	BA	666	A	C5-C6-N1	5.97	120.68	117.70
22	BA	1214	A	N3-C4-N9	5.97	132.17	127.40
22	BA	2070	A	N3-C4-N9	5.97	132.18	127.40
22	BA	2727	A	C5-C6-N1	5.97	120.68	117.70
22	BA	821	A	C4-C5-N7	-5.97	107.72	110.70
22	BA	1641	A	N3-C4-N9	5.97	132.17	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	693	A	C5-C6-N1	5.96	120.68	117.70
22	BA	2311	A	C4-C5-C6	5.96	119.98	117.00
22	BA	2198	A	N3-C4-N9	5.96	132.17	127.40
22	BA	661	A	C5-C6-N1	5.96	120.68	117.70
22	BA	182	A	N3-C4-N9	5.96	132.17	127.40
22	BA	2119	A	N9-C4-C5	5.96	108.18	105.80
22	BA	1927	A	C4-C5-C6	5.96	119.98	117.00
22	BA	2288	A	N9-C4-C5	5.96	108.18	105.80
23	BB	78	A	C8-N9-C4	5.96	108.18	105.80
22	BA	508	A	C4-C5-C6	5.96	119.98	117.00
22	BA	1269	A	C5-C6-N1	5.96	120.68	117.70
22	BA	2278	A	N9-C4-C5	5.96	108.18	105.80
22	BA	2281	A	N3-C4-N9	5.96	132.17	127.40
54	D2	58	A	C4-C5-C6	5.96	119.98	117.00
22	BA	2741	A	N3-C4-N9	5.96	132.16	127.40
22	BA	2753	A	N3-C4-N9	5.96	132.16	127.40
22	BA	743	A	C5-C6-N1	5.95	120.68	117.70
22	BA	988	A	N9-C4-C5	5.95	108.18	105.80
22	BA	1609	A	N3-C4-N9	5.95	132.16	127.40
22	BA	2033	A	C4-C5-C6	5.95	119.98	117.00
22	BA	2776	A	C4-C5-N7	-5.95	107.72	110.70
1	AA	1087	G	C6-C5-N7	-5.95	126.83	130.40
22	BA	28	A	C4-C5-C6	5.95	119.97	117.00
22	BA	1040	A	C4-C5-C6	5.95	119.97	117.00
22	BA	1744	A	C4-C5-C6	5.95	119.97	117.00
22	BA	2321	U	N3-C2-O2	-5.95	118.03	122.20
22	BA	111	A	C8-N9-C4	5.95	108.18	105.80
22	BA	722	A	C5-C6-N1	5.95	120.67	117.70
22	BA	2734	A	N3-C4-N9	5.95	132.16	127.40
54	D2	69	A	N9-C4-C5	5.95	108.18	105.80
22	BA	155	A	N9-C4-C5	5.95	108.18	105.80
22	BA	2497	A	C4-C5-C6	5.95	119.97	117.00
22	BA	2829	A	N9-C4-C5	5.95	108.18	105.80
1	AA	542	G	C5-N7-C8	-5.94	101.33	104.30
22	BA	83	A	C4-C5-C6	5.94	119.97	117.00
22	BA	227	A	C4-C5-C6	5.94	119.97	117.00
22	BA	2893	A	C4-C5-C6	5.94	119.97	117.00
22	BA	761	A	C5-N7-C8	5.94	106.87	103.90
54	D2	28	A	C8-N9-C4	5.94	108.18	105.80
22	BA	742	A	C4-C5-C6	5.94	119.97	117.00
22	BA	1143	A	C8-N9-C4	5.94	108.17	105.80
22	BA	1494	A	N3-C4-N9	5.94	132.15	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	78	A	C5-C6-N1	5.94	120.67	117.70
22	BA	1214	A	C5-C6-N1	5.94	120.67	117.70
22	BA	574	A	N3-C4-N9	5.93	132.15	127.40
22	BA	761	A	N3-C4-N9	5.93	132.15	127.40
22	BA	896	A	C4-C5-N7	-5.93	107.73	110.70
22	BA	990	A	N9-C4-C5	5.93	108.17	105.80
22	BA	1237	A	C8-N9-C4	5.93	108.17	105.80
22	BA	1616	A	C8-N9-C4	5.93	108.17	105.80
22	BA	2274	A	C5-N7-C8	5.93	106.87	103.90
22	BA	2328	A	C4-C5-N7	-5.93	107.73	110.70
22	BA	2381	A	C5-C6-N1	5.93	120.67	117.70
22	BA	2406	A	C4-C5-C6	5.93	119.97	117.00
54	D2	58	A	N9-C4-C5	5.93	108.17	105.80
22	BA	756	A	C4-C5-C6	5.93	119.97	117.00
22	BA	821	A	C8-N9-C4	5.93	108.17	105.80
22	BA	2114	A	C5-C6-N1	5.93	120.67	117.70
23	BB	58	A	N3-C4-N9	5.93	132.15	127.40
22	BA	2749	A	C4-C5-C6	5.93	119.97	117.00
22	BA	1142	A	C4-C5-C6	5.93	119.97	117.00
22	BA	2418	A	N9-C4-C5	5.93	108.17	105.80
22	BA	668	A	N3-C4-N9	5.93	132.14	127.40
22	BA	344	A	N3-C4-N9	5.93	132.14	127.40
22	BA	905	A	N9-C4-C5	5.93	108.17	105.80
22	BA	1021	A	N9-C4-C5	5.93	108.17	105.80
22	BA	1669	A	C5-C6-N1	5.93	120.66	117.70
22	BA	2158	A	C4-C5-C6	5.93	119.96	117.00
22	BA	19	A	C5-C6-N1	5.92	120.66	117.70
22	BA	1089	A	N3-C4-N9	5.92	132.14	127.40
22	BA	2665	A	N3-C4-N9	5.92	132.14	127.40
22	BA	217	A	C4-C5-C6	5.92	119.96	117.00
22	BA	631	A	N3-C4-N9	5.92	132.14	127.40
22	BA	947	A	C5-C6-N1	5.92	120.66	117.70
22	BA	1808	A	N3-C4-N9	5.92	132.14	127.40
33	BL	55	MET	CG-SD-CE	5.92	109.67	100.20
22	BA	2183	A	C5-C6-N1	5.92	120.66	117.70
22	BA	2656	U	N1-C2-O2	5.92	126.94	122.80
1	AA	307	C	C6-N1-C2	-5.92	117.93	120.30
22	BA	348	A	C5-C6-N1	5.92	120.66	117.70
22	BA	1103	A	N3-C4-N9	5.92	132.14	127.40
22	BA	1322	A	N9-C4-C5	5.92	108.17	105.80
22	BA	1885	A	C4-C5-C6	5.92	119.96	117.00
22	BA	2474	U	C2-N1-C1'	5.92	124.80	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2705	A	C8-N9-C4	5.92	108.17	105.80
22	BA	119	A	C8-N9-C4	5.92	108.17	105.80
22	BA	1809	A	N3-C4-N9	5.92	132.13	127.40
22	BA	2352	A	N3-C4-N9	5.92	132.13	127.40
22	BA	2377	A	N3-C4-N9	5.92	132.13	127.40
22	BA	2829	A	C5-C6-N1	5.92	120.66	117.70
22	BA	52	A	C8-N9-C4	5.92	108.17	105.80
22	BA	342	A	C5-C6-N1	5.92	120.66	117.70
22	BA	1744	A	C5-C6-N1	5.92	120.66	117.70
22	BA	181	A	N3-C4-N9	5.91	132.13	127.40
22	BA	221	A	C8-N9-C4	5.91	108.17	105.80
22	BA	739	A	C4-C5-C6	5.91	119.96	117.00
22	BA	1086	A	C5-C6-N1	5.91	120.66	117.70
22	BA	2071	A	N9-C4-C5	5.91	108.17	105.80
22	BA	126	A	N3-C4-N9	5.91	132.13	127.40
22	BA	199	A	N9-C4-C5	5.91	108.16	105.80
22	BA	877	A	N3-C4-N9	5.91	132.13	127.40
22	BA	1916	A	N3-C4-N9	5.91	132.13	127.40
55	D3	21	A	N9-C4-C5	5.91	108.17	105.80
22	BA	14	A	N3-C4-N9	5.91	132.13	127.40
22	BA	146	A	N9-C4-C5	5.91	108.16	105.80
22	BA	896	A	N9-C4-C5	5.91	108.16	105.80
22	BA	2435	A	N3-C4-N9	5.91	132.13	127.40
22	BA	2887	A	N9-C4-C5	5.91	108.16	105.80
52	B4	1	MET	CG-SD-CE	5.91	109.66	100.20
22	BA	332	A	C4-C5-C6	5.91	119.95	117.00
22	BA	354	A	C4-C5-C6	5.91	119.95	117.00
22	BA	6	A	C5-C6-N1	5.91	120.65	117.70
22	BA	73	A	C4-C5-C6	5.91	119.95	117.00
22	BA	374	A	C8-N9-C4	5.91	108.16	105.80
22	BA	541	A	N3-C4-N9	5.91	132.12	127.40
22	BA	2037	A	C5-C6-N1	5.91	120.65	117.70
54	D2	41	A	C5-C6-N1	5.91	120.65	117.70
22	BA	1522	A	C4-C5-C6	5.90	119.95	117.00
22	BA	1700	A	N3-C4-N9	5.90	132.12	127.40
22	BA	1701	A	C5-C6-N1	5.90	120.65	117.70
22	BA	482	A	C8-N9-C4	5.90	108.16	105.80
22	BA	1230	A	C4-C5-C6	5.90	119.95	117.00
22	BA	1327	A	C8-N9-C4	5.90	108.16	105.80
22	BA	1609	A	C4-C5-C6	5.90	119.95	117.00
22	BA	1794	A	C8-N9-C4	5.90	108.16	105.80
22	BA	1819	A	C4-C5-C6	5.90	119.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1854	A	N3-C4-N9	5.90	132.12	127.40
22	BA	2042	A	N9-C4-C5	5.90	108.16	105.80
22	BA	2750	A	N3-C4-N9	5.90	132.12	127.40
22	BA	2800	A	C8-N9-C4	5.90	108.16	105.80
22	BA	877	A	C8-N9-C4	5.90	108.16	105.80
22	BA	2654	A	C8-N9-C4	5.90	108.16	105.80
22	BA	2829	A	C8-N9-C4	5.90	108.16	105.80
39	BR	1	MET	CG-SD-CE	5.90	109.64	100.20
22	BA	1151	A	C8-N9-C4	5.90	108.16	105.80
22	BA	1701	A	C4-C5-N7	-5.90	107.75	110.70
22	BA	547	A	C8-N9-C4	5.90	108.16	105.80
22	BA	1260	A	C4-C5-N7	-5.90	107.75	110.70
22	BA	1347	A	C5-C6-N1	5.90	120.65	117.70
22	BA	1815	A	C5-C6-N1	5.90	120.65	117.70
22	BA	127	A	C4-C5-C6	5.89	119.95	117.00
22	BA	829	A	C4-C5-N7	-5.89	107.75	110.70
22	BA	1040	A	C8-N9-C4	5.89	108.16	105.80
22	BA	1580	A	N3-C4-N9	5.89	132.12	127.40
22	BA	2534	A	N3-C4-N9	5.89	132.12	127.40
22	BA	2439	A	C4-C5-C6	5.89	119.95	117.00
22	BA	1039	A	N3-C4-N9	5.89	132.11	127.40
22	BA	1593	A	N9-C4-C5	5.89	108.16	105.80
22	BA	1664	A	N3-C4-N9	5.89	132.11	127.40
22	BA	2741	A	C4-C5-C6	5.89	119.94	117.00
22	BA	1420	A	N9-C4-C5	5.89	108.16	105.80
22	BA	2119	A	C4-C5-N7	-5.89	107.76	110.70
22	BA	2821	A	N3-C4-N9	5.89	132.11	127.40
22	BA	149	A	N3-C4-N9	5.89	132.11	127.40
22	BA	323	C	C2-N1-C1'	5.89	125.27	118.80
22	BA	371	A	N3-C4-N9	5.89	132.11	127.40
23	BB	104	A	N3-C4-N9	5.89	132.11	127.40
23	BB	115	A	C4-C5-N7	-5.89	107.76	110.70
22	BA	345	A	N9-C4-C5	5.88	108.15	105.80
22	BA	1367	A	N3-C4-N9	5.88	132.11	127.40
1	AA	1087	G	N7-C8-N9	5.88	116.04	113.10
22	BA	322	A	C8-N9-C4	5.88	108.15	105.80
22	BA	2598	A	N9-C4-C5	5.88	108.15	105.80
26	BE	153	LEU	CA-CB-CG	5.88	128.83	115.30
22	BA	878	A	N3-C4-N9	5.88	132.10	127.40
22	BA	2176	A	C4-C5-C6	5.88	119.94	117.00
22	BA	877	A	C4-C5-C6	5.88	119.94	117.00
22	BA	1745	A	N9-C4-C5	5.88	108.15	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	83	C	C6-N1-C1'	5.88	127.85	120.80
22	BA	614	A	C4-C5-N7	-5.88	107.76	110.70
22	BA	752	A	N9-C4-C5	5.88	108.15	105.80
22	BA	756	A	C4-C5-N7	-5.88	107.76	110.70
22	BA	2184	A	N9-C4-C5	5.88	108.15	105.80
22	BA	2225	A	C8-N9-C4	5.88	108.15	105.80
22	BA	443	A	C8-N9-C4	5.87	108.15	105.80
22	BA	1265	A	N9-C4-C5	5.87	108.15	105.80
23	BB	104	A	C5-C6-N1	5.87	120.64	117.70
55	D3	26	A	C4-C5-C6	5.87	119.94	117.00
22	BA	861	A	N3-C4-N9	5.87	132.10	127.40
22	BA	1275	A	C4-C5-C6	5.87	119.94	117.00
22	BA	1504	A	N3-C4-N9	5.87	132.10	127.40
22	BA	1713	A	C4-C5-C6	5.87	119.94	117.00
22	BA	2564	A	C4-C5-C6	5.87	119.94	117.00
22	BA	310	A	C4-C5-N7	-5.87	107.77	110.70
22	BA	457	A	N9-C4-C5	5.87	108.15	105.80
22	BA	979	A	C4-C5-C6	5.87	119.94	117.00
22	BA	1749	A	C5-C6-N1	5.87	120.64	117.70
22	BA	2459	A	C5-C6-N1	5.87	120.63	117.70
22	BA	2015	A	N3-C4-N9	5.87	132.09	127.40
22	BA	911	A	N3-C4-N9	5.87	132.09	127.40
1	AA	1132	C	C5-C6-N1	5.86	123.93	121.00
22	BA	592	A	C5-C6-N1	5.86	120.63	117.70
22	BA	905	A	C5-C6-N1	5.86	120.63	117.70
22	BA	1545	A	N3-C4-N9	5.86	132.09	127.40
22	BA	1749	A	C4-C5-N7	-5.86	107.77	110.70
22	BA	2639	A	N3-C4-N9	5.86	132.09	127.40
22	BA	2646	C	C6-N1-C2	-5.86	117.95	120.30
55	D3	37	A	N9-C4-C5	5.86	108.14	105.80
22	BA	878	A	C4-C5-C6	5.86	119.93	117.00
22	BA	1700	A	C8-N9-C4	5.86	108.14	105.80
22	BA	222	A	C5-C6-N1	5.86	120.63	117.70
22	BA	677	A	C8-N9-C4	5.86	108.14	105.80
22	BA	927	A	C8-N9-C4	5.86	108.14	105.80
22	BA	1189	A	N9-C4-C5	5.86	108.14	105.80
22	BA	1502	A	C5-C6-N1	5.86	120.63	117.70
22	BA	2134	A	C5-C6-N1	5.86	120.63	117.70
22	BA	2241	A	N9-C4-C5	5.86	108.14	105.80
22	BA	804	A	N3-C4-N9	5.86	132.09	127.40
22	BA	1133	A	N9-C4-C5	5.86	108.14	105.80
22	BA	1928	A	C4-C5-C6	5.86	119.93	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2281	A	C8-N9-C4	5.86	108.14	105.80
22	BA	449	A	C5-C6-N1	5.86	120.63	117.70
22	BA	1001	A	C4-C5-C6	5.86	119.93	117.00
22	BA	2170	A	N9-C4-C5	5.85	108.14	105.80
54	D2	14	A	N3-C4-N9	5.85	132.08	127.40
22	BA	928	A	N3-C4-N9	5.85	132.08	127.40
41	BT	1	MET	CG-SD-CE	5.85	109.56	100.20
22	BA	1308	A	C8-N9-C4	5.85	108.14	105.80
22	BA	1610	A	C8-N9-C4	5.85	108.14	105.80
22	BA	1937	A	C8-N9-C4	5.85	108.14	105.80
55	D3	7	A	N3-C4-N9	5.85	132.08	127.40
22	BA	352	A	C4-C5-C6	5.85	119.92	117.00
22	BA	352	A	N3-C4-N9	5.85	132.08	127.40
22	BA	1579	A	C8-N9-C4	5.85	108.14	105.80
22	BA	2227	A	N9-C4-C5	5.85	108.14	105.80
54	D2	23	A	N9-C4-C5	5.85	108.14	105.80
22	BA	126	A	C4-C5-N7	-5.84	107.78	110.70
22	BA	342	A	N9-C4-C5	5.84	108.14	105.80
22	BA	502	A	N3-C4-N9	5.84	132.07	127.40
22	BA	632	A	N3-C4-N9	5.84	132.08	127.40
22	BA	1040	A	N3-C4-N9	5.84	132.08	127.40
22	BA	1569	A	N3-C4-N9	5.84	132.07	127.40
22	BA	272	A	C5-C6-N1	5.84	120.62	117.70
22	BA	727	A	C4-C5-C6	5.84	119.92	117.00
22	BA	1630	A	C8-N9-C4	5.84	108.14	105.80
22	BA	382	A	C5-C6-N1	5.84	120.62	117.70
22	BA	1133	A	C4-C5-N7	-5.84	107.78	110.70
22	BA	2336	A	C8-N9-C4	5.84	108.14	105.80
22	BA	1214	A	C4-C5-C6	5.84	119.92	117.00
22	BA	2660	A	C4-C5-C6	5.84	119.92	117.00
22	BA	1133	A	N3-C4-N9	5.84	132.07	127.40
22	BA	1545	A	C4-C5-C6	5.84	119.92	117.00
22	BA	322	A	C4-C5-N7	-5.83	107.78	110.70
22	BA	979	A	N3-C4-N9	5.83	132.07	127.40
22	BA	1253	A	C5-C6-N1	5.83	120.62	117.70
26	BE	1	MET	CG-SD-CE	5.83	109.53	100.20
54	D2	5	A	C8-N9-C4	5.83	108.13	105.80
22	BA	661	A	N3-C4-N9	5.83	132.06	127.40
22	BA	751	A	N3-C4-N9	5.83	132.06	127.40
22	BA	1268	A	C4-C5-C6	5.83	119.92	117.00
22	BA	2448	A	C4-C5-N7	-5.83	107.78	110.70
22	BA	614	A	N3-C4-N9	5.83	132.06	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	909	A	C4-C5-N7	-5.83	107.78	110.70
22	BA	1070	A	C8-N9-C4	5.83	108.13	105.80
22	BA	1165	A	C5-C6-N1	5.83	120.61	117.70
22	BA	1566	A	C4-C5-C6	5.83	119.92	117.00
22	BA	1772	A	C4-C5-N7	-5.83	107.79	110.70
22	BA	282	A	N3-C4-N9	5.83	132.06	127.40
22	BA	63	A	C4-C5-C6	5.83	119.91	117.00
22	BA	227	A	N9-C4-C5	5.83	108.13	105.80
22	BA	575	A	C4-C5-C6	5.83	119.91	117.00
22	BA	789	A	C8-N9-C4	5.83	108.13	105.80
22	BA	973	A	N3-C4-N9	5.83	132.06	127.40
22	BA	1069	A	C4-C5-N7	-5.83	107.79	110.70
22	BA	1276	A	N3-C4-N9	5.83	132.06	127.40
22	BA	1913	A	C4-C5-C6	5.83	119.91	117.00
22	BA	173	A	C5-C6-N1	5.82	120.61	117.70
22	BA	1244	A	C4-C5-C6	5.82	119.91	117.00
22	BA	2660	A	N3-C4-N9	5.82	132.06	127.40
54	D2	23	A	C4-C5-N7	-5.82	107.79	110.70
22	BA	504	A	C8-N9-C4	5.82	108.13	105.80
22	BA	1365	A	C5-C6-N1	5.82	120.61	117.70
22	BA	199	A	C8-N9-C4	5.82	108.13	105.80
22	BA	933	A	C4-C5-N7	-5.82	107.79	110.70
22	BA	2137	U	C2-N1-C1'	5.82	124.68	117.70
22	BA	2176	A	N9-C4-C5	5.82	108.13	105.80
22	BA	1676	A	N3-C4-N9	5.82	132.06	127.40
22	BA	368	A	N3-C4-N9	5.82	132.05	127.40
22	BA	644	A	N3-C4-N9	5.82	132.05	127.40
22	BA	706	A	C4-C5-C6	5.82	119.91	117.00
22	BA	905	A	C4-C5-C6	5.82	119.91	117.00
22	BA	1086	A	N9-C4-C5	5.82	108.13	105.80
22	BA	1801	A	C8-N9-C4	5.82	108.13	105.80
22	BA	2516	A	N9-C4-C5	5.82	108.13	105.80
22	BA	1080	A	C8-N9-C4	5.82	108.13	105.80
22	BA	1205	A	C4-C5-C6	5.82	119.91	117.00
22	BA	1919	A	N3-C4-N9	5.82	132.05	127.40
55	D3	62	C	N1-C2-N3	5.81	123.27	119.20
22	BA	103	A	N3-C4-N9	5.81	132.05	127.40
22	BA	432	A	C4-C5-C6	5.81	119.91	117.00
22	BA	1711	A	N9-C4-C5	5.81	108.12	105.80
22	BA	2810	A	N9-C4-C5	5.81	108.12	105.80
23	BB	15	A	C8-N9-C4	5.81	108.12	105.80
54	D2	73	A	C4-C5-C6	5.81	119.91	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	371	A	N9-C4-C5	5.81	108.12	105.80
22	BA	749	A	N3-C4-N9	5.81	132.05	127.40
22	BA	1230	A	C8-N9-C4	5.81	108.12	105.80
23	BB	109	A	C4-C5-C6	5.81	119.91	117.00
1	AA	618	C	C6-N1-C2	-5.81	117.98	120.30
22	BA	2600	A	C4-C5-C6	5.81	119.90	117.00
23	BB	53	A	N3-C4-N9	5.81	132.04	127.40
22	BA	332	A	N3-C4-N9	5.81	132.04	127.40
22	BA	282	A	C5-C6-N1	5.80	120.60	117.70
22	BA	563	A	N3-C4-N9	5.80	132.04	127.40
40	BS	82	MET	CG-SD-CE	5.80	109.49	100.20
22	BA	945	A	C4-C5-N7	-5.80	107.80	110.70
22	BA	2781	A	N9-C4-C5	5.80	108.12	105.80
22	BA	460	A	N3-C4-N9	5.80	132.04	127.40
22	BA	1039	A	C4-C5-C6	5.80	119.90	117.00
22	BA	1650	A	N3-C4-N9	5.80	132.04	127.40
22	BA	2281	A	C5-C6-N1	5.80	120.60	117.70
22	BA	2378	A	N9-C4-C5	5.80	108.12	105.80
22	BA	219	A	C5-C6-N1	5.80	120.60	117.70
22	BA	1155	A	C4-C5-N7	-5.80	107.80	110.70
22	BA	1169	A	C5-C6-N1	5.80	120.60	117.70
22	BA	1596	A	N3-C4-N9	5.80	132.04	127.40
22	BA	2749	A	N9-C4-C5	5.80	108.12	105.80
22	BA	2873	A	N3-C4-N9	5.80	132.04	127.40
23	BB	39	A	N9-C4-C5	5.80	108.12	105.80
23	BB	109	A	C8-N9-C4	5.80	108.12	105.80
22	BA	56	A	C8-N9-C4	5.80	108.12	105.80
22	BA	309	A	C8-N9-C4	5.80	108.12	105.80
22	BA	449	A	C8-N9-C4	5.80	108.12	105.80
22	BA	1014	A	N3-C4-N9	5.80	132.04	127.40
22	BA	2711	A	C5-C6-N1	5.79	120.60	117.70
23	BB	109	A	N3-C4-N9	5.79	132.04	127.40
22	BA	480	A	N3-C4-N9	5.79	132.03	127.40
22	BA	911	A	N9-C4-C5	5.79	108.12	105.80
22	BA	1938	A	C5-C6-N1	5.79	120.60	117.70
22	BA	53	A	N9-C4-C5	5.79	108.12	105.80
22	BA	2733	A	C4-C5-C6	5.79	119.90	117.00
22	BA	781	A	N3-C4-N9	5.79	132.03	127.40
22	BA	1046	A	N3-C4-N9	5.79	132.03	127.40
22	BA	1571	A	N3-C4-N9	5.79	132.03	127.40
22	BA	2600	A	N9-C4-C5	5.79	108.12	105.80
23	BB	119	A	N9-C4-C5	5.79	108.12	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	382	A	N9-C4-C5	5.79	108.12	105.80
22	BA	614	A	C4-C5-C6	5.79	119.89	117.00
22	BA	1420	A	N3-C4-N9	5.79	132.03	127.40
22	BA	1890	A	N3-C4-N9	5.79	132.03	127.40
22	BA	1165	A	C4-C5-C6	5.79	119.89	117.00
22	BA	94	A	N9-C4-C5	5.79	108.11	105.80
22	BA	142	A	C8-N9-C4	5.79	108.11	105.80
22	BA	637	A	N9-C4-C5	5.79	108.11	105.80
22	BA	1247	A	C8-N9-C4	5.79	108.11	105.80
22	BA	1998	A	C5-C6-N1	5.79	120.59	117.70
22	BA	2063	C	C6-N1-C2	-5.78	117.99	120.30
22	BA	2734	A	C8-N9-C4	5.78	108.11	105.80
22	BA	1327	A	C4-C5-C6	5.78	119.89	117.00
22	BA	2835	A	N3-C4-N9	5.78	132.02	127.40
55	D3	37	A	C4-C5-C6	5.78	119.89	117.00
22	BA	345	A	C5-C6-N1	5.78	120.59	117.70
22	BA	626	A	C4-C5-C6	5.78	119.89	117.00
22	BA	1050	A	C8-N9-C4	5.78	108.11	105.80
22	BA	1858	A	C4-C5-C6	5.78	119.89	117.00
22	BA	752	A	C4-C5-N7	-5.78	107.81	110.70
22	BA	1073	A	N3-C4-N9	5.78	132.02	127.40
55	D3	23	A	C4-C5-N7	-5.78	107.81	110.70
22	BA	118	A	C4-C5-C6	5.78	119.89	117.00
22	BA	699	A	N3-C4-N9	5.78	132.02	127.40
22	BA	739	A	C5-C6-N1	5.78	120.59	117.70
22	BA	2013	A	C8-N9-C4	5.78	108.11	105.80
22	BA	204	A	C5-C6-N1	5.77	120.59	117.70
22	BA	299	A	N3-C4-N9	5.77	132.02	127.40
22	BA	734	A	N3-C4-N9	5.77	132.02	127.40
22	BA	1010	A	N9-C4-C5	5.77	108.11	105.80
22	BA	1301	A	C5-C6-N1	5.77	120.59	117.70
22	BA	2266	A	C8-N9-C4	5.77	108.11	105.80
22	BA	503	A	C4-C5-C6	5.77	119.89	117.00
22	BA	761	A	C4-C5-C6	5.77	119.89	117.00
22	BA	983	A	C4-C5-C6	5.77	119.89	117.00
22	BA	1672	A	N3-C4-N9	5.77	132.02	127.40
22	BA	602	A	C4-C5-C6	5.77	119.88	117.00
22	BA	1640	A	N9-C4-C5	5.77	108.11	105.80
22	BA	2314	A	C4-C5-C6	5.77	119.88	117.00
22	BA	1590	A	N9-C4-C5	5.77	108.11	105.80
22	BA	2335	A	C8-N9-C4	5.77	108.11	105.80
22	BA	502	A	N9-C4-C5	5.76	108.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	528	A	N3-C4-N9	5.76	132.01	127.40
22	BA	1403	A	N9-C4-C5	5.76	108.11	105.80
22	BA	2288	A	C4-C5-N7	-5.76	107.82	110.70
22	BA	2407	A	C5-C6-N1	5.76	120.58	117.70
22	BA	146	A	C5-C6-N1	5.76	120.58	117.70
22	BA	2435	A	C5-C6-N1	5.76	120.58	117.70
22	BA	2451	A	C5-C6-N1	5.76	120.58	117.70
22	BA	2733	A	C8-N9-C4	5.76	108.11	105.80
22	BA	1698	A	N3-C4-N9	5.76	132.01	127.40
22	BA	2031	A	C5-C6-N1	5.76	120.58	117.70
22	BA	2614	A	N3-C4-N9	5.76	132.01	127.40
31	BJ	108	MET	CG-SD-CE	5.76	109.42	100.20
22	BA	165	A	N3-C4-N9	5.76	132.01	127.40
22	BA	861	A	C4-C5-C6	5.76	119.88	117.00
22	BA	2734	A	C4-C5-C6	5.76	119.88	117.00
54	D2	14	A	C4-C5-C6	5.76	119.88	117.00
22	BA	143	C	C2-N1-C1'	5.76	125.13	118.80
22	BA	918	A	C8-N9-C4	5.76	108.10	105.80
22	BA	1089	A	C4-C5-C6	5.76	119.88	117.00
22	BA	1269	A	C8-N9-C4	5.76	108.10	105.80
22	BA	454	A	C8-N9-C4	5.76	108.10	105.80
22	BA	718	A	C8-N9-C4	5.76	108.10	105.80
22	BA	2266	A	C4-C5-C6	5.76	119.88	117.00
22	BA	2270	A	N9-C4-C5	5.76	108.10	105.80
23	BB	37	C	C6-N1-C2	-5.76	118.00	120.30
1	AA	564	C	C2-N1-C1'	5.75	125.13	118.80
22	BA	71	A	N9-C4-C5	5.75	108.10	105.80
22	BA	402	A	C4-C5-C6	5.75	119.88	117.00
22	BA	603	A	N9-C4-C5	5.75	108.10	105.80
22	BA	2378	A	N3-C4-N9	5.75	132.00	127.40
22	BA	2748	A	N3-C4-N9	5.75	132.00	127.40
22	BA	2900	A	C5-C6-N1	5.75	120.58	117.70
22	BA	1668	A	C8-N9-C4	5.75	108.10	105.80
22	BA	1757	A	N3-C4-N9	5.75	132.00	127.40
22	BA	2392	A	N9-C4-C5	5.75	108.10	105.80
22	BA	1762	A	N3-C4-N9	5.75	132.00	127.40
22	BA	1808	A	C8-N9-C4	5.75	108.10	105.80
22	BA	2534	A	C8-N9-C4	5.75	108.10	105.80
1	AA	993	G	C8-N9-C1'	-5.75	119.53	127.00
22	BA	432	A	C5-C6-N1	5.75	120.57	117.70
22	BA	632	A	N9-C4-C5	5.75	108.10	105.80
22	BA	783	A	C5-C6-N1	5.75	120.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	972	A	N3-C4-N9	5.75	132.00	127.40
22	BA	1503	A	C5-C6-N1	5.75	120.57	117.70
22	BA	1808	A	C4-C5-C6	5.75	119.87	117.00
22	BA	2432	A	C4-C5-C6	5.75	119.87	117.00
37	BP	13	MET	CG-SD-CE	5.75	109.39	100.20
22	BA	1359	A	N3-C4-N9	5.75	132.00	127.40
22	BA	608	A	N9-C4-C5	5.74	108.10	105.80
22	BA	2142	A	C4-C5-N7	-5.74	107.83	110.70
22	BA	2781	A	C4-C5-C6	5.74	119.87	117.00
22	BA	1359	A	C4-C5-C6	5.74	119.87	117.00
22	BA	1784	A	C5-C6-N1	5.74	120.57	117.70
22	BA	2799	A	C5-C6-N1	5.74	120.57	117.70
23	BB	29	A	C5-C6-N1	5.74	120.57	117.70
1	AA	438	U	O4'-C1'-N1	5.74	112.79	108.20
22	BA	676	A	N3-C4-N9	5.74	131.99	127.40
22	BA	1384	A	C4-C5-C6	5.74	119.87	117.00
22	BA	1570	A	C4-C5-N7	-5.74	107.83	110.70
22	BA	1890	A	C8-N9-C4	5.74	108.10	105.80
22	BA	1931	U	N1-C2-O2	5.74	126.82	122.80
22	BA	2176	A	N3-C4-N9	5.74	131.99	127.40
22	BA	1664	A	C5-C6-N1	5.74	120.57	117.70
22	BA	1912	A	C4-C5-N7	-5.74	107.83	110.70
22	BA	2358	A	C4-C5-C6	5.74	119.87	117.00
23	BB	31	C	C6-N1-C2	-5.74	118.00	120.30
22	BA	1393	A	N3-C4-N9	5.74	131.99	127.40
22	BA	1918	A	N9-C4-C5	5.74	108.09	105.80
22	BA	2267	A	C4-C5-C6	5.74	119.87	117.00
22	BA	2726	A	C4-C5-C6	5.74	119.87	117.00
22	BA	1504	A	C5-C6-N1	5.74	120.57	117.70
22	BA	1899	A	C5-C6-N1	5.74	120.57	117.70
22	BA	311	A	C4-C5-C6	5.73	119.87	117.00
22	BA	272	A	C8-N9-C4	5.73	108.09	105.80
22	BA	845	A	C4-C5-C6	5.73	119.87	117.00
22	BA	1304	A	C4-C5-N7	-5.73	107.83	110.70
22	BA	2134	A	C4-C5-N7	-5.73	107.83	110.70
22	BA	278	A	N9-C4-C5	5.73	108.09	105.80
22	BA	294	A	N3-C4-N9	5.73	131.98	127.40
22	BA	1669	A	N9-C4-C5	5.73	108.09	105.80
22	BA	2142	A	N3-C4-N9	5.73	131.99	127.40
55	D3	61	C	N1-C2-O2	5.73	122.34	118.90
22	BA	2434	A	N3-C4-N9	5.73	131.98	127.40
55	D3	37	A	N3-C4-N9	5.73	131.98	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	103	U	N3-C2-O2	-5.73	118.19	122.20
22	BA	2009	A	C4-C5-C6	5.73	119.86	117.00
22	BA	2450	A	C8-N9-C4	5.73	108.09	105.80
22	BA	2471	A	N9-C4-C5	5.73	108.09	105.80
41	BT	24	MET	CG-SD-CE	5.73	109.36	100.20
22	BA	1014	A	C4-C5-N7	-5.73	107.84	110.70
22	BA	1169	A	C8-N9-C4	5.73	108.09	105.80
22	BA	1495	A	N3-C4-N9	5.73	131.98	127.40
22	BA	1912	A	N3-C4-N9	5.73	131.98	127.40
22	BA	896	A	C8-N9-C4	5.72	108.09	105.80
22	BA	1503	A	N3-C4-N9	5.72	131.98	127.40
43	BV	1	MET	CG-SD-CE	5.72	109.36	100.20
22	BA	83	A	N3-C4-N9	5.72	131.98	127.40
22	BA	199	A	C4-C5-N7	-5.72	107.84	110.70
22	BA	354	A	C8-N9-C4	5.72	108.09	105.80
22	BA	1419	A	C5-C6-N1	5.72	120.56	117.70
22	BA	1885	A	C8-N9-C4	5.72	108.09	105.80
22	BA	1978	A	N9-C4-C5	5.72	108.09	105.80
22	BA	2412	A	C8-N9-C4	5.72	108.09	105.80
22	BA	2711	A	N3-C4-N9	5.72	131.98	127.40
23	BB	46	A	N9-C4-C5	5.72	108.09	105.80
22	BA	1060	U	C5-C4-O4	-5.72	122.47	125.90
22	BA	2095	A	N3-C4-N9	5.72	131.98	127.40
22	BA	1522	A	N3-C4-N9	5.72	131.98	127.40
22	BA	1678	A	N3-C4-N9	5.72	131.98	127.40
54	D2	35	A	C4-C5-N7	-5.72	107.84	110.70
22	BA	64	A	C5-C6-N1	5.72	120.56	117.70
48	B0	15	MET	CG-SD-CE	5.72	109.35	100.20
22	BA	10	A	C8-N9-C4	5.72	108.09	105.80
22	BA	103	A	C8-N9-C4	5.72	108.09	105.80
22	BA	311	A	N3-C4-N9	5.72	131.97	127.40
22	BA	793	A	C5-C6-N1	5.72	120.56	117.70
22	BA	1515	A	C8-N9-C4	5.72	108.09	105.80
22	BA	2706	A	C5-C6-N1	5.72	120.56	117.70
22	BA	2776	A	N3-C4-N9	5.72	131.97	127.40
22	BA	63	A	C8-N9-C4	5.71	108.09	105.80
22	BA	1267	U	N3-C2-O2	-5.71	118.20	122.20
22	BA	1987	A	C8-N9-C4	5.71	108.09	105.80
22	BA	2679	A	C8-N9-C4	5.71	108.09	105.80
22	BA	1920	C	C5-C6-N1	5.71	123.86	121.00
22	BA	231	A	C5-C6-N1	5.71	120.56	117.70
22	BA	820	A	C4-C5-C6	5.71	119.86	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2173	A	C5-C6-N1	5.71	120.56	117.70
22	BA	2268	A	C8-N9-C4	5.71	108.08	105.80
22	BA	2829	A	C4-C5-N7	-5.71	107.84	110.70
22	BA	167	A	C8-N9-C4	5.71	108.08	105.80
22	BA	627	A	N3-C4-N9	5.71	131.97	127.40
22	BA	1147	A	C4-C5-C6	5.71	119.86	117.00
22	BA	2755	C	N1-C2-O2	5.71	122.33	118.90
22	BA	412	A	N9-C4-C5	5.71	108.08	105.80
22	BA	899	A	C8-N9-C4	5.71	108.08	105.80
22	BA	1057	A	C4-C5-N7	-5.71	107.85	110.70
22	BA	1384	A	N3-C4-N9	5.71	131.97	127.40
22	BA	2826	A	C8-N9-C4	5.71	108.08	105.80
22	BA	94	A	N3-C4-N9	5.71	131.96	127.40
22	BA	119	A	C5-C6-N1	5.71	120.55	117.70
23	BB	108	A	C4-C5-C6	5.71	119.85	117.00
22	BA	2327	A	C5-C6-N1	5.70	120.55	117.70
22	BA	2886	A	C8-N9-C4	5.70	108.08	105.80
22	BA	244	A	N3-C4-N9	5.70	131.96	127.40
22	BA	734	A	C4-C5-N7	-5.70	107.85	110.70
22	BA	1285	A	C4-C5-C6	5.70	119.85	117.00
22	BA	2809	A	C5-C6-N1	5.70	120.55	117.70
1	AA	528	C	C2-N1-C1'	5.70	125.07	118.80
22	BA	71	A	N3-C4-N9	5.70	131.96	127.40
22	BA	309	A	C4-C5-C6	5.70	119.85	117.00
22	BA	749	A	C4-C5-C6	5.70	119.85	117.00
22	BA	984	A	C5-C6-N1	5.70	120.55	117.70
22	BA	1060	U	N3-C4-O4	5.70	123.39	119.40
22	BA	1420	A	C4-C5-C6	5.70	119.85	117.00
22	BA	1913	A	C4-C5-N7	-5.70	107.85	110.70
31	BJ	1	MET	CG-SD-CE	5.70	109.32	100.20
22	BA	844	A	C8-N9-C4	5.70	108.08	105.80
22	BA	2270	A	C5-C6-N1	5.70	120.55	117.70
22	BA	2426	A	N3-C4-N9	5.70	131.96	127.40
22	BA	203	A	C4-C5-C6	5.70	119.85	117.00
22	BA	2749	A	N3-C4-N9	5.70	131.96	127.40
22	BA	160	A	C5-C6-N1	5.70	120.55	117.70
22	BA	449	A	C4-C5-C6	5.70	119.85	117.00
22	BA	972	A	C5-C6-N1	5.70	120.55	117.70
22	BA	1927	A	N9-C4-C5	5.70	108.08	105.80
23	BB	39	A	C4-C5-C6	5.70	119.85	117.00
22	BA	430	A	N3-C4-N9	5.69	131.96	127.40
22	BA	685	A	C5-C6-N1	5.69	120.55	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1522	A	C4-C5-N7	-5.69	107.85	110.70
22	BA	149	A	N9-C4-C5	5.69	108.08	105.80
22	BA	160	A	C4-C5-C6	5.69	119.85	117.00
22	BA	231	A	C8-N9-C4	5.69	108.08	105.80
22	BA	2882	A	C4-C5-N7	-5.69	107.85	110.70
54	D2	35	A	N3-C4-N9	5.69	131.96	127.40
22	BA	342	A	N3-C4-N9	5.69	131.95	127.40
22	BA	529	A	C5-C6-N1	5.69	120.55	117.70
22	BA	1916	A	N9-C4-C5	5.69	108.08	105.80
22	BA	270	A	N3-C4-N9	5.69	131.95	127.40
22	BA	941	A	N3-C4-N9	5.69	131.95	127.40
22	BA	706	A	C8-N9-C4	5.69	108.08	105.80
22	BA	979	A	N9-C4-C5	5.69	108.08	105.80
22	BA	2158	A	C8-N9-C4	5.69	108.08	105.80
46	BY	30	MET	CG-SD-CE	5.69	109.30	100.20
22	BA	352	A	C5-C6-N1	5.69	120.54	117.70
22	BA	833	A	C5-C6-N1	5.69	120.54	117.70
22	BA	2748	A	C4-C5-C6	5.69	119.84	117.00
22	BA	19	A	C8-N9-C4	5.68	108.07	105.80
22	BA	928	A	N9-C4-C5	5.68	108.07	105.80
22	BA	1155	A	C8-N9-C4	5.68	108.07	105.80
22	BA	1503	A	C8-N9-C4	5.68	108.07	105.80
22	BA	1871	A	N3-C4-N9	5.68	131.95	127.40
22	BA	2381	A	N3-C4-N9	5.68	131.95	127.40
55	D3	44	G	C8-N9-C1'	-5.68	119.61	127.00
1	AA	1349	A	O5'-P-OP1	-5.68	100.58	105.70
22	BA	1786	A	N9-C4-C5	5.68	108.07	105.80
22	BA	2042	A	N3-C4-N9	5.68	131.95	127.40
22	BA	479	A	N3-C4-N9	5.68	131.94	127.40
22	BA	661	A	N9-C4-C5	5.68	108.07	105.80
22	BA	2014	A	N9-C4-C5	5.68	108.07	105.80
22	BA	1395	A	C8-N9-C4	5.68	108.07	105.80
22	BA	2266	A	C5-C6-N1	5.68	120.54	117.70
24	BC	225	MET	CG-SD-CE	5.68	109.29	100.20
22	BA	1384	A	C8-N9-C4	5.68	108.07	105.80
22	BA	1535	A	N9-C4-C5	5.68	108.07	105.80
22	BA	1711	A	N3-C4-N9	5.68	131.94	127.40
22	BA	2284	A	C8-N9-C4	5.68	108.07	105.80
23	BB	50	A	N9-C4-C5	5.68	108.07	105.80
31	BJ	92	MET	CG-SD-CE	5.68	109.28	100.20
22	BA	14	A	N9-C4-C5	5.68	108.07	105.80
22	BA	443	A	N9-C4-C5	5.68	108.07	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1070	A	N9-C4-C5	5.68	108.07	105.80
22	BA	2873	A	C8-N9-C4	5.68	108.07	105.80
22	BA	44	A	N9-C4-C5	5.67	108.07	105.80
22	BA	794	A	C5-C6-N1	5.67	120.54	117.70
22	BA	1246	A	N3-C4-N9	5.67	131.94	127.40
22	BA	2176	A	C4-C5-N7	-5.67	107.86	110.70
22	BA	819	A	C8-N9-C4	5.67	108.07	105.80
22	BA	2478	A	C8-N9-C4	5.67	108.07	105.80
54	D2	59	A	N9-C4-C5	5.67	108.07	105.80
22	BA	196	A	C8-N9-C4	5.67	108.07	105.80
22	BA	1069	A	N9-C4-C5	5.67	108.07	105.80
22	BA	1912	A	C4-C5-C6	5.67	119.84	117.00
22	BA	2080	A	C5-C6-N1	5.67	120.53	117.70
22	BA	2241	A	C4-C5-N7	-5.67	107.86	110.70
22	BA	655	A	N9-C4-C5	5.67	108.07	105.80
22	BA	1608	A	C8-N9-C4	5.67	108.07	105.80
22	BA	1987	A	N3-C4-N9	5.67	131.94	127.40
22	BA	2298	A	N9-C4-C5	5.67	108.07	105.80
1	AA	1158	C	N3-C2-O2	-5.67	117.93	121.90
22	BA	439	A	N9-C4-C5	5.67	108.07	105.80
22	BA	1551	A	C5-C6-N1	5.67	120.53	117.70
22	BA	1569	A	C5-C6-N1	5.67	120.53	117.70
22	BA	1672	A	C4-C5-C6	5.67	119.83	117.00
22	BA	2198	A	C8-N9-C4	5.67	108.07	105.80
22	BA	2764	A	C4-C5-N7	-5.67	107.86	110.70
23	BB	108	A	N3-C4-N9	5.67	131.94	127.40
27	BF	17	MET	CG-SD-CE	5.67	109.27	100.20
22	BA	402	A	N9-C4-C5	5.67	108.07	105.80
22	BA	1504	A	N9-C4-C5	5.67	108.07	105.80
22	BA	2170	A	C4-C5-N7	-5.67	107.87	110.70
22	BA	2322	A	C5-C6-N1	5.67	120.53	117.70
22	BA	2602	A	C4-C5-N7	-5.67	107.87	110.70
22	BA	2820	A	C8-N9-C4	5.67	108.07	105.80
23	BB	115	A	C5-C6-N1	5.67	120.53	117.70
55	D3	36	A	N3-C4-N9	5.67	131.93	127.40
55	D3	58	A	C4-C5-C6	5.67	119.83	117.00
27	BF	130	MET	CG-SD-CE	5.67	109.27	100.20
22	BA	996	A	C8-N9-C4	5.66	108.07	105.80
22	BA	1535	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	1966	A	N3-C4-N9	5.66	131.93	127.40
22	BA	2134	A	N9-C4-C5	5.66	108.06	105.80
22	BA	2566	A	C8-N9-C4	5.66	108.06	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2882	A	C5-C6-N1	5.66	120.53	117.70
22	BA	2705	A	C4-C5-C6	5.66	119.83	117.00
22	BA	344	A	C8-N9-C4	5.66	108.06	105.80
22	BA	602	A	C8-N9-C4	5.66	108.06	105.80
22	BA	1267	U	N1-C2-O2	5.66	126.76	122.80
22	BA	1913	A	N3-C4-N9	5.66	131.93	127.40
22	BA	2058	A	N9-C4-C5	5.66	108.06	105.80
22	BA	675	A	C8-N9-C4	5.66	108.06	105.80
22	BA	1744	A	N9-C4-C5	5.66	108.06	105.80
22	BA	2386	A	C5-C6-N1	5.66	120.53	117.70
22	BA	1668	A	C4-C5-N7	-5.66	107.87	110.70
22	BA	2516	A	C5-C6-N1	5.66	120.53	117.70
54	D2	69	A	C4-C5-N7	-5.66	107.87	110.70
55	D3	21	A	N3-C4-N9	5.66	131.93	127.40
22	BA	2009	A	N3-C4-N9	5.65	131.92	127.40
22	BA	2860	A	N9-C4-C5	5.65	108.06	105.80
22	BA	197	A	C8-N9-C4	5.65	108.06	105.80
22	BA	1307	A	C4-C5-N7	-5.65	107.87	110.70
22	BA	1378	A	C4-C5-C6	5.65	119.83	117.00
22	BA	1871	A	C4-C5-C6	5.65	119.83	117.00
22	BA	2882	A	C4-C5-C6	5.65	119.83	117.00
22	BA	310	A	N3-C4-N9	5.65	131.92	127.40
22	BA	699	A	C8-N9-C4	5.65	108.06	105.80
22	BA	2632	A	C4-C5-N7	-5.65	107.88	110.70
23	BB	29	A	N3-C4-N9	5.65	131.92	127.40
22	BA	454	A	C4-C5-C6	5.65	119.83	117.00
22	BA	515	A	C5-C6-N1	5.65	120.53	117.70
22	BA	2014	A	C8-N9-C4	5.65	108.06	105.80
22	BA	2887	A	N3-C4-N9	5.65	131.92	127.40
1	AA	1109	C	C6-N1-C2	-5.65	118.04	120.30
22	BA	347	A	C4-C5-N7	-5.65	107.88	110.70
22	BA	2513	A	N9-C4-C5	5.65	108.06	105.80
22	BA	1244	A	N3-C4-N9	5.65	131.92	127.40
22	BA	1525	A	N9-C4-C5	5.65	108.06	105.80
22	BA	1632	A	N9-C4-C5	5.65	108.06	105.80
22	BA	155	A	C8-N9-C4	5.64	108.06	105.80
22	BA	282	A	C8-N9-C4	5.64	108.06	105.80
22	BA	1265	A	C4-C5-N7	-5.64	107.88	110.70
22	BA	1794	A	N3-C4-N9	5.64	131.91	127.40
22	BA	2587	A	N9-C4-C5	5.64	108.06	105.80
23	BB	119	A	C4-C5-N7	-5.64	107.88	110.70
22	BA	1001	A	C4-C5-N7	-5.64	107.88	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1890	A	C4-C5-C6	5.64	119.82	117.00
22	BA	2564	A	N3-C4-N9	5.64	131.91	127.40
22	BA	382	A	N3-C4-N9	5.64	131.91	127.40
22	BA	2311	A	N3-C4-N9	5.64	131.91	127.40
22	BA	2565	A	N3-C4-N9	5.64	131.91	127.40
22	BA	1780	A	C4-C5-C6	5.64	119.82	117.00
1	AA	92	U	C2-N1-C1'	5.64	124.47	117.70
22	BA	244	A	C8-N9-C4	5.64	108.06	105.80
22	BA	348	A	C8-N9-C4	5.64	108.06	105.80
22	BA	756	A	N3-C4-N9	5.64	131.91	127.40
22	BA	2205	A	C5-C6-N1	5.64	120.52	117.70
22	BA	2654	A	C4-C5-C6	5.64	119.82	117.00
22	BA	538	A	C4-C5-N7	-5.63	107.88	110.70
22	BA	706	A	N3-C4-N9	5.63	131.91	127.40
22	BA	1453	A	C4-C5-C6	5.63	119.82	117.00
22	BA	1853	A	N3-C4-N9	5.63	131.91	127.40
22	BA	1953	A	N9-C4-C5	5.63	108.05	105.80
22	BA	1383	A	N3-C4-N9	5.63	131.91	127.40
22	BA	1913	A	N9-C4-C5	5.63	108.05	105.80
22	BA	2411	A	N3-C4-N9	5.63	131.90	127.40
22	BA	1998	A	C8-N9-C4	5.63	108.05	105.80
22	BA	2406	A	C8-N9-C4	5.63	108.05	105.80
54	D2	23	A	C8-N9-C4	5.63	108.05	105.80
22	BA	282	A	C4-C5-C6	5.63	119.81	117.00
22	BA	310	A	C5-C6-N1	5.63	120.51	117.70
22	BA	401	A	C4-C5-N7	-5.63	107.89	110.70
22	BA	928	A	C5-C6-N1	5.63	120.51	117.70
22	BA	1420	A	C4-C5-N7	-5.63	107.89	110.70
23	BB	59	A	C4-C5-C6	5.63	119.81	117.00
22	BA	1583	A	N3-C4-N9	5.62	131.90	127.40
22	BA	492	A	N9-C4-C5	5.62	108.05	105.80
22	BA	541	A	C5-C6-N1	5.62	120.51	117.70
22	BA	1439	A	N9-C4-C5	5.62	108.05	105.80
22	BA	1553	A	C8-N9-C4	5.62	108.05	105.80
22	BA	255	A	C5-C6-N1	5.62	120.51	117.70
22	BA	1366	A	C5-C6-N1	5.62	120.51	117.70
22	BA	2750	A	C4-C5-C6	5.62	119.81	117.00
22	BA	310	A	N9-C4-C5	5.62	108.05	105.80
22	BA	547	A	N3-C4-N9	5.62	131.89	127.40
22	BA	1503	A	N9-C4-C5	5.62	108.05	105.80
22	BA	1509	A	C4-C5-C6	5.62	119.81	117.00
22	BA	1981	A	C4-C5-C6	5.62	119.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2020	A	C8-N9-C4	5.62	108.05	105.80
23	BB	34	A	C5-C6-N1	5.62	120.51	117.70
22	BA	749	A	C4-C5-N7	-5.62	107.89	110.70
22	BA	788	A	C8-N9-C4	5.62	108.05	105.80
22	BA	2037	A	N9-C4-C5	5.62	108.05	105.80
22	BA	2792	A	N3-C4-N9	5.62	131.89	127.40
22	BA	1085	A	N9-C4-C5	5.61	108.05	105.80
22	BA	1876	A	C8-N9-C4	5.61	108.05	105.80
22	BA	2278	A	N3-C4-N9	5.61	131.89	127.40
22	BA	2736	A	C4-C5-N7	-5.61	107.89	110.70
22	BA	909	A	C8-N9-C4	5.61	108.05	105.80
22	BA	125	A	N3-C4-N9	5.61	131.89	127.40
22	BA	172	A	N9-C4-C5	5.61	108.04	105.80
22	BA	941	A	C4-C5-C6	5.61	119.81	117.00
22	BA	979	A	C8-N9-C4	5.61	108.04	105.80
22	BA	2602	A	C5-C6-N1	5.61	120.50	117.70
22	BA	2829	A	N3-C4-N9	5.61	131.89	127.40
54	D2	73	A	N3-C4-N9	5.61	131.89	127.40
22	BA	563	A	C4-C5-C6	5.61	119.80	117.00
22	BA	981	A	N9-C4-C5	5.61	108.04	105.80
22	BA	1090	A	N3-C4-N9	5.61	131.89	127.40
22	BA	1431	A	C5-C6-N1	5.61	120.50	117.70
22	BA	1711	A	C5-C6-N1	5.61	120.50	117.70
22	BA	2406	A	N3-C4-N9	5.61	131.88	127.40
22	BA	198	C	C5-C6-N1	5.61	123.80	121.00
22	BA	227	A	N3-C4-N9	5.61	131.88	127.40
22	BA	2273	A	C4-C5-N7	-5.61	107.90	110.70
22	BA	191	A	C8-N9-C4	5.60	108.04	105.80
22	BA	631	A	C8-N9-C4	5.60	108.04	105.80
22	BA	947	A	C8-N9-C4	5.60	108.04	105.80
22	BA	2426	A	C4-C5-C6	5.60	119.80	117.00
22	BA	2547	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	83	A	N9-C4-C5	5.60	108.04	105.80
22	BA	529	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	761	A	C5-C6-N1	5.60	120.50	117.70
22	BA	792	A	C8-N9-C4	5.60	108.04	105.80
22	BA	1383	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	2482	A	N9-C4-C5	5.60	108.04	105.80
22	BA	2298	A	C4-C5-C6	5.60	119.80	117.00
22	BA	2665	A	C8-N9-C4	5.60	108.04	105.80
22	BA	342	A	C8-N9-C4	5.60	108.04	105.80
22	BA	727	A	C5-C6-N1	5.60	120.50	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1204	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	1204	A	N9-C4-C5	5.60	108.04	105.80
22	BA	1552	A	C4-C5-C6	5.60	119.80	117.00
22	BA	2126	A	C4-C5-N7	-5.60	107.90	110.70
1	AA	81	A	O4'-C1'-N9	5.60	112.68	108.20
22	BA	241	A	C8-N9-C4	5.60	108.04	105.80
22	BA	1070	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	1927	A	N3-C4-N9	5.60	131.88	127.40
22	BA	2108	A	N3-C4-N9	5.60	131.88	127.40
22	BA	2169	A	C8-N9-C4	5.60	108.04	105.80
55	D3	44	G	N3-C4-C5	-5.60	125.80	128.60
22	BA	74	A	C8-N9-C4	5.60	108.04	105.80
22	BA	626	A	N3-C4-N9	5.60	131.88	127.40
22	BA	1272	A	C4-C5-C6	5.60	119.80	117.00
22	BA	2169	A	C4-C5-N7	-5.60	107.90	110.70
22	BA	2476	A	N9-C4-C5	5.60	108.04	105.80
22	BA	2314	A	C4-C5-N7	-5.59	107.90	110.70
22	BA	2657	A	N3-C4-N9	5.59	131.88	127.40
22	BA	2758	A	C4-C5-N7	-5.59	107.90	110.70
22	BA	829	A	N3-C4-N9	5.59	131.87	127.40
22	BA	1532	A	C5-C6-N1	5.59	120.50	117.70
22	BA	1749	A	N3-C4-N9	5.59	131.87	127.40
22	BA	49	A	C8-N9-C4	5.59	108.04	105.80
22	BA	1080	A	C5-C6-N1	5.59	120.50	117.70
22	BA	2005	A	C4-C5-N7	-5.59	107.90	110.70
22	BA	2497	A	N3-C4-N9	5.59	131.87	127.40
22	BA	1569	A	C4-C5-C6	5.59	119.80	117.00
22	BA	1900	A	C8-N9-C4	5.59	108.04	105.80
22	BA	2298	A	C4-C5-N7	-5.59	107.91	110.70
22	BA	2635	A	N9-C4-C5	5.59	108.04	105.80
22	BA	1993	U	N3-C2-O2	-5.59	118.29	122.20
22	BA	2711	A	N9-C4-C5	5.59	108.03	105.80
22	BA	309	A	N9-C4-C5	5.59	108.03	105.80
22	BA	330	A	C5-C6-N1	5.59	120.49	117.70
22	BA	572	A	C5-C6-N1	5.59	120.49	117.70
22	BA	751	A	N9-C4-C5	5.59	108.03	105.80
22	BA	1343	G	C4-N9-C1'	5.59	133.76	126.50
22	BA	1630	A	C4-C5-C6	5.59	119.79	117.00
22	BA	2059	A	C4-C5-C6	5.59	119.79	117.00
22	BA	2376	A	N9-C4-C5	5.59	108.03	105.80
22	BA	575	A	C5-C6-N1	5.58	120.49	117.70
22	BA	1285	A	C4-C5-N7	-5.58	107.91	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	227	A	C8-N9-C4	5.58	108.03	105.80
22	BA	471	A	C8-N9-C4	5.58	108.03	105.80
22	BA	1028	A	N9-C4-C5	5.58	108.03	105.80
22	BA	1046	A	C4-C5-C6	5.58	119.79	117.00
22	BA	1367	A	N9-C4-C5	5.58	108.03	105.80
22	BA	2274	A	N9-C4-C5	5.58	108.03	105.80
55	D3	76	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	515	A	C8-N9-C4	5.58	108.03	105.80
22	BA	1260	A	C5-C6-N1	5.58	120.49	117.70
22	BA	38	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	53	A	N3-C4-N9	5.58	131.86	127.40
22	BA	161	A	C4-C5-C6	5.58	119.79	117.00
22	BA	471	A	C4-C5-N7	-5.58	107.91	110.70
22	BA	1815	A	N3-C4-N9	5.58	131.86	127.40
22	BA	2054	A	C8-N9-C4	5.58	108.03	105.80
22	BA	2062	A	C4-C5-C6	5.58	119.79	117.00
22	BA	2433	A	N9-C4-C5	5.58	108.03	105.80
22	BA	2813	A	N9-C4-C5	5.58	108.03	105.80
23	BB	78	A	N3-C4-N9	5.58	131.86	127.40
22	BA	203	A	C5-C6-N1	5.58	120.49	117.70
22	BA	1285	A	C5-C6-N1	5.58	120.49	117.70
22	BA	1755	A	N3-C4-N9	5.58	131.86	127.40
22	BA	2126	A	N9-C4-C5	5.58	108.03	105.80
22	BA	2542	A	N9-C4-C5	5.58	108.03	105.80
22	BA	270	A	C8-N9-C4	5.58	108.03	105.80
22	BA	492	A	C5-C6-N1	5.58	120.49	117.70
22	BA	654	A	C5-C6-N1	5.58	120.49	117.70
22	BA	44	A	C5-C6-N1	5.58	120.49	117.70
22	BA	1596	A	C8-N9-C4	5.58	108.03	105.80
22	BA	2883	A	C4-C5-C6	5.58	119.79	117.00
22	BA	472	A	N3-C4-N9	5.57	131.86	127.40
22	BA	1525	A	N3-C4-N9	5.57	131.86	127.40
22	BA	2657	A	C8-N9-C4	5.57	108.03	105.80
22	BA	2776	A	C4-C5-C6	5.57	119.79	117.00
22	BA	71	A	C4-C5-C6	5.57	119.79	117.00
55	D3	31	A	C5-C6-N1	5.57	120.49	117.70
22	BA	1977	A	C4-C5-C6	5.57	119.78	117.00
22	BA	1889	A	C8-N9-C4	5.57	108.03	105.80
23	BB	58	A	N9-C4-C5	5.57	108.03	105.80
22	BA	423	A	N9-C4-C5	5.57	108.03	105.80
22	BA	910	A	C8-N9-C4	5.57	108.03	105.80
55	D3	58	A	P-O3'-C3'	5.57	126.38	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	764	A	C5-C6-N1	5.57	120.48	117.70
22	BA	844	A	C4-C5-N7	-5.57	107.92	110.70
22	BA	2766	A	C5-N7-C8	5.57	106.68	103.90
22	BA	2799	A	C8-N9-C4	5.57	108.03	105.80
22	BA	2882	A	C8-N9-C4	5.57	108.03	105.80
54	D2	49	A	C8-N9-C4	5.57	108.03	105.80
22	BA	1469	A	C4-C5-N7	-5.56	107.92	110.70
22	BA	1544	A	C5-C6-N1	5.56	120.48	117.70
22	BA	1552	A	C5-C6-N1	5.56	120.48	117.70
22	BA	2095	A	N9-C4-C5	5.56	108.03	105.80
22	BA	457	A	C5-C6-N1	5.56	120.48	117.70
22	BA	541	A	C4-C5-N7	-5.56	107.92	110.70
22	BA	1126	A	C5-C6-N1	5.56	120.48	117.70
22	BA	1393	A	C8-N9-C4	5.56	108.03	105.80
22	BA	1932	A	C5-C6-N1	5.56	120.48	117.70
22	BA	2778	A	C8-N9-C4	5.56	108.03	105.80
22	BA	2800	A	C4-C5-C6	5.56	119.78	117.00
1	AA	496	A	O4'-C1'-N9	5.56	112.65	108.20
22	BA	941	A	N9-C4-C5	5.56	108.02	105.80
22	BA	2635	A	C8-N9-C4	5.56	108.02	105.80
22	BA	627	A	C4-C5-C6	5.56	119.78	117.00
22	BA	734	A	C4-C5-C6	5.56	119.78	117.00
22	BA	972	A	N9-C4-C5	5.56	108.02	105.80
22	BA	1772	A	N3-C4-N9	5.56	131.85	127.40
22	BA	2014	A	C4-C5-N7	-5.56	107.92	110.70
23	BB	104	A	C4-C5-C6	5.56	119.78	117.00
55	D3	58	A	C4-C5-N7	-5.56	107.92	110.70
22	BA	213	A	C4-C5-C6	5.56	119.78	117.00
22	BA	470	A	C8-N9-C4	5.56	108.02	105.80
22	BA	1133	A	C8-N9-C4	5.56	108.02	105.80
22	BA	1194	A	N3-C4-N9	5.56	131.85	127.40
22	BA	1597	A	N3-C4-N9	5.56	131.85	127.40
22	BA	1987	A	N9-C4-C5	5.56	108.02	105.80
22	BA	2095	A	C5-C6-N1	5.56	120.48	117.70
22	BA	2388	A	N3-C4-N9	5.56	131.84	127.40
22	BA	2823	A	C4-C5-C6	5.56	119.78	117.00
24	BC	181	MET	CG-SD-CE	5.56	109.09	100.20
22	BA	1936	A	C5-C6-N1	5.56	120.48	117.70
22	BA	241	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	311	A	N9-C4-C5	5.55	108.02	105.80
22	BA	735	A	C8-N9-C4	5.55	108.02	105.80
22	BA	1129	A	C8-N9-C4	5.55	108.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1509	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	1745	A	N3-C4-N9	5.55	131.84	127.40
22	BA	2614	A	C5-C6-N1	5.55	120.48	117.70
22	BA	342	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	401	A	N3-C4-N9	5.55	131.84	127.40
22	BA	1111	A	C4-C5-C6	5.55	119.78	117.00
22	BA	2134	A	C8-N9-C4	5.55	108.02	105.80
22	BA	2761	A	N9-C4-C5	5.55	108.02	105.80
22	BA	608	A	C4-C5-N7	-5.55	107.92	110.70
22	BA	1204	A	N3-C4-N9	5.55	131.84	127.40
22	BA	1268	A	C5-C6-N1	5.55	120.47	117.70
22	BA	2247	A	C5-C6-N1	5.55	120.47	117.70
23	BB	34	A	N9-C4-C5	5.55	108.02	105.80
22	BA	1780	A	N9-C4-C5	5.55	108.02	105.80
23	BB	53	A	C8-N9-C4	5.55	108.02	105.80
23	BB	73	A	C5-C6-N1	5.55	120.47	117.70
22	BA	227	A	C4-C5-N7	-5.55	107.93	110.70
55	D3	21	A	C4-C5-N7	-5.55	107.93	110.70
22	BA	2101	A	N3-C4-N9	5.54	131.84	127.40
22	BA	28	A	C5-C6-N1	5.54	120.47	117.70
22	BA	507	A	N3-C4-N9	5.54	131.83	127.40
22	BA	1366	A	N9-C4-C5	5.54	108.02	105.80
22	BA	2513	A	C5-C6-N1	5.54	120.47	117.70
22	BA	2639	A	N9-C4-C5	5.54	108.02	105.80
22	BA	165	A	C8-N9-C4	5.54	108.02	105.80
22	BA	603	A	C4-C5-C6	5.54	119.77	117.00
22	BA	1353	A	N3-C4-N9	5.54	131.83	127.40
22	BA	1552	A	N3-C4-N9	5.54	131.83	127.40
22	BA	1593	A	C5-C6-N1	5.54	120.47	117.70
22	BA	1276	A	C5-C6-N1	5.54	120.47	117.70
22	BA	1634	A	N3-C4-N9	5.54	131.83	127.40
22	BA	2614	A	C4-C5-N7	-5.54	107.93	110.70
30	BI	22	MET	CG-SD-CE	5.54	109.06	100.20
54	D2	49	A	C5-C6-N1	5.54	120.47	117.70
55	D3	21	A	C4-C5-C6	5.54	119.77	117.00
1	AA	439	U	N3-C4-O4	5.54	123.28	119.40
22	BA	1040	A	C5-C6-N1	5.54	120.47	117.70
22	BA	1054	A	C5-C6-N1	5.54	120.47	117.70
22	BA	1570	A	N3-C4-N9	5.54	131.83	127.40
22	BA	1854	A	N9-C4-C5	5.54	108.02	105.80
22	BA	443	A	C4-C5-N7	-5.54	107.93	110.70
22	BA	1050	A	C4-C5-N7	-5.54	107.93	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2095	A	C8-N9-C4	5.54	108.02	105.80
22	BA	1783	A	C4-C5-N7	-5.54	107.93	110.70
22	BA	1805	A	N3-C4-N9	5.54	131.83	127.40
22	BA	2639	A	C4-C5-C6	5.54	119.77	117.00
56	D4	7	U	N1-C2-O2	5.54	126.68	122.80
22	BA	103	A	N9-C4-C5	5.53	108.01	105.80
22	BA	501	A	C8-N9-C4	5.53	108.01	105.80
22	BA	666	A	C8-N9-C4	5.53	108.01	105.80
22	BA	943	A	N9-C4-C5	5.53	108.01	105.80
22	BA	1000	A	N9-C4-C5	5.53	108.01	105.80
22	BA	1275	A	N3-C4-N9	5.53	131.83	127.40
22	BA	1321	A	C5-C6-N1	5.53	120.47	117.70
22	BA	1616	A	N3-C4-N9	5.53	131.83	127.40
22	BA	2031	A	C4-C5-C6	5.53	119.77	117.00
1	AA	316	C	C6-N1-C2	-5.53	118.09	120.30
1	AA	406	G	C4-N9-C1'	5.53	133.69	126.50
22	BA	1090	A	N9-C4-C5	5.53	108.01	105.80
22	BA	1367	A	C8-N9-C4	5.53	108.01	105.80
22	BA	1757	A	C8-N9-C4	5.53	108.01	105.80
22	BA	1848	A	C5-N7-C8	5.53	106.67	103.90
22	BA	2094	A	C8-N9-C4	5.53	108.01	105.80
22	BA	892	A	C8-N9-C4	5.53	108.01	105.80
22	BA	1655	A	C5-C6-N1	5.53	120.46	117.70
22	BA	2632	A	N3-C4-N9	5.53	131.82	127.40
22	BA	1000	A	C8-N9-C4	5.53	108.01	105.80
22	BA	1490	A	C5-C6-N1	5.53	120.46	117.70
22	BA	2267	A	C4-C5-N7	-5.53	107.94	110.70
22	BA	2634	A	C8-N9-C4	5.53	108.01	105.80
22	BA	155	A	N3-C4-N9	5.53	131.82	127.40
22	BA	529	A	C8-N9-C4	5.53	108.01	105.80
22	BA	549	G	O4'-C1'-N9	5.53	112.62	108.20
22	BA	705	A	C5-C6-N1	5.53	120.46	117.70
22	BA	734	A	N9-C4-C5	5.53	108.01	105.80
22	BA	909	A	C4-C5-C6	5.53	119.76	117.00
22	BA	1050	A	N9-C4-C5	5.53	108.01	105.80
22	BA	1057	A	C5-C6-N1	5.53	120.46	117.70
22	BA	2005	A	C8-N9-C4	5.53	108.01	105.80
22	BA	2309	A	C8-N9-C4	5.53	108.01	105.80
22	BA	861	A	C5-C6-N1	5.52	120.46	117.70
22	BA	878	A	N9-C4-C5	5.52	108.01	105.80
22	BA	905	A	N3-C4-N9	5.52	131.82	127.40
22	BA	1632	A	C5-C6-N1	5.52	120.46	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1821	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	10	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	2654	A	N9-C4-C5	5.52	108.01	105.80
23	BB	45	A	C8-N9-C4	5.52	108.01	105.80
22	BA	14	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	114	U	C2-N1-C1'	5.52	124.32	117.70
22	BA	705	A	C8-N9-C4	5.52	108.01	105.80
22	BA	1057	A	N9-C4-C5	5.52	108.01	105.80
22	BA	1080	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	1641	A	C8-N9-C4	5.52	108.01	105.80
22	BA	2388	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	2755	C	C2-N1-C1'	5.52	124.87	118.80
22	BA	432	A	N9-C4-C5	5.52	108.01	105.80
22	BA	1111	A	N3-C4-N9	5.52	131.81	127.40
22	BA	1928	A	N9-C4-C5	5.52	108.01	105.80
22	BA	1640	A	C4-C5-N7	-5.52	107.94	110.70
22	BA	2212	A	N9-C4-C5	5.52	108.01	105.80
22	BA	781	A	N9-C4-C5	5.51	108.01	105.80
22	BA	2314	A	C5-C6-N1	5.51	120.46	117.70
22	BA	2600	A	C8-N9-C4	5.51	108.01	105.80
23	BB	42	C	N1-C2-O2	5.51	122.21	118.90
56	D4	7	U	N3-C2-O2	-5.51	118.34	122.20
1	AA	582	C	C6-N1-C2	-5.51	118.09	120.30
22	BA	538	A	N3-C4-N9	5.51	131.81	127.40
1	AA	503	C	C5-C6-N1	5.51	123.75	121.00
22	BA	556	A	C8-N9-C4	5.51	108.00	105.80
22	BA	979	A	C4-C5-N7	-5.51	107.94	110.70
22	BA	1434	A	C4-C5-N7	-5.51	107.94	110.70
22	BA	1535	A	C5-C6-N1	5.51	120.46	117.70
22	BA	2031	A	N9-C4-C5	5.51	108.00	105.80
1	AA	979	C	N3-C2-O2	-5.51	118.04	121.90
22	BA	216	A	C5-C6-N1	5.51	120.45	117.70
22	BA	721	A	C8-N9-C4	5.51	108.00	105.80
22	BA	2014	A	C5-C6-N1	5.51	120.45	117.70
22	BA	2823	A	C8-N9-C4	5.51	108.00	105.80
22	BA	125	A	C4-C5-C6	5.51	119.75	117.00
22	BA	1327	A	N3-C4-N9	5.51	131.81	127.40
22	BA	1690	A	N9-C4-C5	5.51	108.00	105.80
22	BA	1966	A	C4-C5-N7	-5.51	107.95	110.70
22	BA	255	A	C8-N9-C4	5.51	108.00	105.80
22	BA	2432	A	N3-C4-N9	5.51	131.81	127.40
22	BA	2740	A	N9-C4-C5	5.51	108.00	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2741	A	C5-C6-N1	5.51	120.45	117.70
22	BA	2761	A	C4-C5-N7	-5.51	107.95	110.70
22	BA	2764	A	C8-N9-C4	5.51	108.00	105.80
22	BA	1084	A	C8-N9-C4	5.50	108.00	105.80
54	D2	58	A	N3-C4-N9	5.50	131.80	127.40
22	BA	374	A	C5-C6-N1	5.50	120.45	117.70
22	BA	483	A	C8-N9-C4	5.50	108.00	105.80
22	BA	655	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	670	A	C8-N9-C4	5.50	108.00	105.80
22	BA	1267	U	C2-N1-C1'	5.50	124.30	117.70
22	BA	1308	A	C5-C6-N1	5.50	120.45	117.70
22	BA	1509	A	N3-C4-N9	5.50	131.80	127.40
22	BA	2725	A	C8-N9-C4	5.50	108.00	105.80
1	AA	998	C	N1-C2-O2	5.50	122.20	118.90
22	BA	371	A	C5-C6-N1	5.50	120.45	117.70
22	BA	909	A	N3-C4-N9	5.50	131.80	127.40
54	D2	41	A	C8-N9-C4	5.50	108.00	105.80
22	BA	83	A	C8-N9-C4	5.50	108.00	105.80
22	BA	973	A	C4-C5-C6	5.50	119.75	117.00
22	BA	1419	A	N9-C4-C5	5.50	108.00	105.80
22	BA	1504	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	1522	A	N9-C4-C5	5.50	108.00	105.80
22	BA	2020	A	N9-C4-C5	5.50	108.00	105.80
22	BA	89	A	C4-C5-C6	5.50	119.75	117.00
22	BA	346	A	C4-C5-N7	-5.50	107.95	110.70
22	BA	447	A	C8-N9-C4	5.50	108.00	105.80
22	BA	1342	A	N3-C4-N9	5.50	131.80	127.40
22	BA	2101	A	C4-C5-C6	5.50	119.75	117.00
23	BB	53	A	N9-C4-C5	5.50	108.00	105.80
22	BA	655	A	C4-C5-C6	5.50	119.75	117.00
22	BA	155	A	C5-C6-N1	5.49	120.45	117.70
22	BA	1226	A	N3-C4-N9	5.49	131.79	127.40
22	BA	2741	A	C8-N9-C4	5.49	108.00	105.80
22	BA	1314	C	N1-C2-O2	5.49	122.19	118.90
22	BA	590	A	C5-C6-N1	5.49	120.44	117.70
22	BA	1678	A	C8-N9-C4	5.49	108.00	105.80
22	BA	199	A	C5-C6-N1	5.49	120.44	117.70
22	BA	526	A	C4-C5-N7	-5.49	107.96	110.70
22	BA	632	A	C4-C5-N7	-5.49	107.96	110.70
22	BA	1253	A	N9-C4-C5	5.49	108.00	105.80
22	BA	2453	A	N3-C4-N9	5.49	131.79	127.40
54	D2	59	A	C4-C5-N7	-5.49	107.95	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D2	59	A	C8-N9-C4	5.49	108.00	105.80
22	BA	84	A	N9-C4-C5	5.49	108.00	105.80
22	BA	1626	A	N3-C4-N9	5.49	131.79	127.40
22	BA	2598	A	N3-C4-N9	5.49	131.79	127.40
22	BA	563	A	C5-C6-N1	5.49	120.44	117.70
22	BA	892	A	C4-C5-N7	-5.49	107.96	110.70
22	BA	1246	A	C4-C5-N7	-5.49	107.96	110.70
22	BA	2298	A	N3-C4-N9	5.49	131.79	127.40
1	AA	611	C	C6-N1-C2	-5.48	118.11	120.30
22	BA	173	A	N9-C4-C5	5.48	107.99	105.80
22	BA	216	A	C8-N9-C4	5.48	107.99	105.80
22	BA	1616	A	C4-C5-C6	5.48	119.74	117.00
22	BA	103	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	979	A	C5-C6-N1	5.48	120.44	117.70
22	BA	1328	A	C5-C6-N1	5.48	120.44	117.70
22	BA	203	A	N3-C4-N9	5.48	131.78	127.40
22	BA	218	A	C4-C5-C6	5.48	119.74	117.00
22	BA	503	A	C8-N9-C4	5.48	107.99	105.80
22	BA	644	A	C5-C6-N1	5.48	120.44	117.70
22	BA	1089	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	1616	A	C5-C6-N1	5.48	120.44	117.70
22	BA	1755	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	2288	A	C4-C5-C6	5.48	119.74	117.00
22	BA	2288	A	N3-C4-N9	5.48	131.78	127.40
22	BA	2418	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	2530	A	N9-C4-C5	5.48	107.99	105.80
22	BA	676	A	N9-C4-C5	5.48	107.99	105.80
22	BA	1596	A	N9-C4-C5	5.48	107.99	105.80
22	BA	1815	A	N9-C4-C5	5.48	107.99	105.80
22	BA	2042	A	C4-C5-N7	-5.48	107.96	110.70
22	BA	2727	A	C8-N9-C4	5.48	107.99	105.80
54	D2	51	A	N9-C4-C5	5.48	107.99	105.80
1	AA	1317	C	C5-C6-N1	5.48	123.74	121.00
22	BA	161	A	N3-C4-N9	5.48	131.78	127.40
22	BA	190	A	C8-N9-C4	5.48	107.99	105.80
22	BA	222	A	N3-C4-N9	5.48	131.78	127.40
22	BA	74	A	C5-C6-N1	5.47	120.44	117.70
22	BA	155	A	C4-C5-N7	-5.47	107.96	110.70
22	BA	213	A	N3-C4-N9	5.47	131.78	127.40
22	BA	1427	A	C4-C5-N7	-5.47	107.96	110.70
22	BA	1515	A	C5-C6-N1	5.47	120.44	117.70
22	BA	2333	A	N3-C4-N9	5.47	131.78	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2734	A	C5-C6-N1	5.47	120.44	117.70
55	D3	73	A	C8-N9-C4	5.47	107.99	105.80
22	BA	320	A	C4-C5-N7	-5.47	107.96	110.70
22	BA	1001	A	C5-C6-N1	5.47	120.44	117.70
22	BA	1439	A	C4-C5-N7	-5.47	107.96	110.70
22	BA	1786	A	C4-C5-N7	-5.47	107.96	110.70
22	BA	2227	A	C4-C5-N7	-5.47	107.96	110.70
22	BA	1413	A	N9-C4-C5	5.47	107.99	105.80
22	BA	2778	A	C5-C6-N1	5.47	120.44	117.70
22	BA	547	A	C4-C5-C6	5.47	119.73	117.00
22	BA	1127	A	N9-C4-C5	5.47	107.99	105.80
54	D2	14	A	N9-C4-C5	5.47	107.99	105.80
54	D2	73	A	C4-C5-N7	-5.47	107.97	110.70
22	BA	1665	A	N9-C4-C5	5.47	107.99	105.80
22	BA	1890	A	N9-C4-C5	5.47	107.99	105.80
22	BA	1073	A	C8-N9-C4	5.46	107.99	105.80
22	BA	1496	A	N3-C4-N9	5.46	131.77	127.40
22	BA	1809	A	N9-C4-C5	5.46	107.99	105.80
22	BA	2518	A	C5-C6-N1	5.46	120.43	117.70
23	BB	78	A	N9-C4-C5	5.46	107.99	105.80
54	D2	38	A	N9-C4-C5	5.46	107.98	105.80
22	BA	142	A	C5-C6-N1	5.46	120.43	117.70
22	BA	1126	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	2211	A	N3-C4-N9	5.46	131.77	127.40
1	AA	409	U	N3-C2-O2	-5.46	118.38	122.20
22	BA	845	A	C8-N9-C4	5.46	107.98	105.80
22	BA	1314	C	C6-N1-C1'	-5.46	114.25	120.80
22	BA	1634	A	C4-C5-C6	5.46	119.73	117.00
22	BA	2058	A	N3-C4-N9	5.46	131.77	127.40
22	BA	2377	A	N9-C4-C5	5.46	107.98	105.80
22	BA	2711	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	480	A	N9-C4-C5	5.46	107.98	105.80
22	BA	730	A	C5-C6-N1	5.46	120.43	117.70
22	BA	990	A	N3-C4-N9	5.46	131.77	127.40
22	BA	2287	A	C5-C6-N1	5.46	120.43	117.70
22	BA	661	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	739	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	1919	A	N9-C4-C5	5.46	107.98	105.80
22	BA	2725	A	C4-C5-N7	-5.46	107.97	110.70
22	BA	632	A	C8-N9-C4	5.46	107.98	105.80
22	BA	1070	A	C4-C5-C6	5.46	119.73	117.00
22	BA	1698	A	C4-C5-C6	5.46	119.73	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	199	A	N3-C4-N9	5.46	131.76	127.40
22	BA	1545	A	N9-C4-C5	5.46	107.98	105.80
22	BA	2191	A	N9-C4-C5	5.46	107.98	105.80
1	AA	979	C	N1-C2-O2	5.45	122.17	118.90
22	BA	13	A	C4-C5-N7	-5.45	107.97	110.70
22	BA	432	A	C4-C5-N7	-5.45	107.97	110.70
22	BA	1580	A	C8-N9-C4	5.45	107.98	105.80
55	D3	36	A	N9-C4-C5	5.45	107.98	105.80
22	BA	320	A	C5-C6-N1	5.45	120.43	117.70
22	BA	432	A	C8-N9-C4	5.45	107.98	105.80
22	BA	1067	A	N9-C4-C5	5.45	107.98	105.80
22	BA	1477	A	N9-C4-C5	5.45	107.98	105.80
54	D2	14	A	C8-N9-C4	5.45	107.98	105.80
22	BA	309	A	N3-C4-N9	5.45	131.76	127.40
22	BA	602	A	C4-C5-N7	-5.45	107.97	110.70
22	BA	1342	A	C4-C5-C6	5.45	119.72	117.00
22	BA	1348	C	C6-N1-C2	-5.45	118.12	120.30
22	BA	1603	A	N9-C4-C5	5.45	107.98	105.80
22	BA	2147	A	C5-C6-N1	5.45	120.43	117.70
22	BA	466	A	C8-N9-C4	5.45	107.98	105.80
22	BA	1802	A	C8-N9-C4	5.45	107.98	105.80
22	BA	2469	A	C4-C5-C6	5.45	119.72	117.00
22	BA	223	A	C4-C5-C6	5.45	119.72	117.00
22	BA	2572	A	C4-C5-N7	-5.45	107.98	110.70
22	BA	2821	A	N9-C4-C5	5.45	107.98	105.80
23	BB	37	C	N3-C2-O2	-5.45	118.09	121.90
22	BA	300	A	C5-C6-N1	5.45	120.42	117.70
22	BA	621	A	C4-C5-N7	-5.45	107.98	110.70
22	BA	1111	A	C4-C5-N7	-5.45	107.98	110.70
22	BA	2340	A	C5-C6-N1	5.45	120.42	117.70
22	BA	1439	A	C8-N9-C4	5.44	107.98	105.80
54	D2	41	A	N9-C4-C5	5.44	107.98	105.80
54	D2	73	A	N9-C4-C5	5.44	107.98	105.80
22	BA	95	A	C5-C6-N1	5.44	120.42	117.70
22	BA	2211	A	C4-C5-N7	-5.44	107.98	110.70
22	BA	412	A	C4-C5-N7	-5.44	107.98	110.70
22	BA	1609	A	C8-N9-C4	5.44	107.98	105.80
22	BA	2366	A	N9-C4-C5	5.44	107.98	105.80
22	BA	2482	A	C4-C5-N7	-5.44	107.98	110.70
22	BA	2705	A	N9-C4-C5	5.44	107.98	105.80
22	BA	2741	A	N9-C4-C5	5.44	107.98	105.80
54	D2	9	A	C4-C5-C6	5.44	119.72	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	457	A	C4-C5-N7	-5.44	107.98	110.70
22	BA	820	A	N9-C4-C5	5.44	107.97	105.80
22	BA	1885	A	C5-C6-N1	5.44	120.42	117.70
22	BA	2478	A	N9-C4-C5	5.44	107.97	105.80
22	BA	181	A	C4-C5-N7	-5.44	107.98	110.70
22	BA	635	C	C6-N1-C2	-5.44	118.12	120.30
22	BA	1060	U	O4'-C1'-N1	-5.44	103.85	108.20
22	BA	2071	A	C5-C6-N1	5.43	120.42	117.70
22	BA	2211	A	C4-C5-C6	5.43	119.72	117.00
54	D2	76	A	N3-C4-N9	5.43	131.75	127.40
22	BA	505	A	C8-N9-C4	5.43	107.97	105.80
22	BA	1378	A	N3-C4-N9	5.43	131.75	127.40
22	BA	1505	A	C8-N9-C4	5.43	107.97	105.80
22	BA	1566	A	N3-C4-N9	5.43	131.75	127.40
23	BB	119	A	C5-C6-N1	5.43	120.42	117.70
22	BA	6	A	N9-C4-C5	5.43	107.97	105.80
22	BA	195	A	C5-C6-N1	5.43	120.42	117.70
22	BA	346	A	N9-C4-C5	5.43	107.97	105.80
22	BA	1384	A	N9-C4-C5	5.43	107.97	105.80
22	BA	1433	A	C5-C6-N1	5.43	120.42	117.70
22	BA	1698	A	C5-C6-N1	5.43	120.42	117.70
22	BA	2547	A	N3-C4-N9	5.43	131.74	127.40
54	D2	38	A	C4-C5-C6	5.43	119.72	117.00
54	D2	14	A	C4-C5-N7	-5.43	107.99	110.70
23	BB	50	A	N3-C4-N9	5.43	131.74	127.40
22	BA	345	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	402	A	C8-N9-C4	5.42	107.97	105.80
22	BA	676	A	C8-N9-C4	5.42	107.97	105.80
22	BA	715	A	C8-N9-C4	5.42	107.97	105.80
22	BA	1165	A	C8-N9-C4	5.42	107.97	105.80
22	BA	2748	A	C8-N9-C4	5.42	107.97	105.80
25	BD	165	MET	CG-SD-CE	5.42	108.88	100.20
22	BA	1336	A	N9-C4-C5	5.42	107.97	105.80
22	BA	2129	C	C5-C6-N1	5.42	123.71	121.00
22	BA	947	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	2043	C	C6-N1-C2	-5.42	118.13	120.30
22	BA	1342	A	C5-C6-N1	5.42	120.41	117.70
22	BA	1395	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	2476	A	N3-C4-N9	5.42	131.74	127.40
22	BA	2590	A	C5-C6-N1	5.42	120.41	117.70
22	BA	384	A	C8-N9-C4	5.42	107.97	105.80
22	BA	718	A	C4-C5-N7	-5.42	107.99	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1532	A	N9-C4-C5	5.42	107.97	105.80
55	D3	62	C	C5-C4-N4	5.42	123.99	120.20
22	BA	1129	A	C4-C5-C6	5.42	119.71	117.00
22	BA	1794	A	C5-C6-N1	5.42	120.41	117.70
22	BA	2019	A	C8-N9-C4	5.42	107.97	105.80
22	BA	2205	A	C8-N9-C4	5.42	107.97	105.80
22	BA	1395	A	C4-C5-C6	5.42	119.71	117.00
22	BA	1403	A	C4-C5-N7	-5.42	107.99	110.70
22	BA	1637	A	C8-N9-C4	5.42	107.97	105.80
22	BA	1780	A	C8-N9-C4	5.42	107.97	105.80
22	BA	1966	A	C5-C6-N1	5.42	120.41	117.70
22	BA	2147	A	C4-C5-C6	5.42	119.71	117.00
1	AA	754	C	C2-N1-C1'	5.41	124.75	118.80
22	BA	735	A	C5-C6-N1	5.41	120.41	117.70
22	BA	752	A	C5-C6-N1	5.41	120.41	117.70
22	BA	1039	A	N9-C4-C5	5.41	107.97	105.80
22	BA	1494	A	N9-C4-C5	5.41	107.97	105.80
22	BA	2142	A	C5-C6-N1	5.41	120.41	117.70
22	BA	1286	A	N9-C4-C5	5.41	107.97	105.80
22	BA	1313	U	C6-N1-C1'	-5.41	113.62	121.20
22	BA	1652	A	C5-C6-N1	5.41	120.41	117.70
22	BA	1889	A	N9-C4-C5	5.41	107.97	105.80
22	BA	2407	A	C8-N9-C4	5.41	107.97	105.80
55	D3	58	A	N3-C4-N9	5.41	131.73	127.40
56	D4	7	U	C2-N1-C1'	5.41	124.19	117.70
22	BA	190	A	C5-C6-N1	5.41	120.41	117.70
22	BA	197	A	C5-C6-N1	5.41	120.41	117.70
22	BA	265	A	N9-C4-C5	5.41	107.96	105.80
22	BA	483	A	C5-C6-N1	5.41	120.41	117.70
22	BA	1090	A	C4-C5-N7	-5.41	108.00	110.70
22	BA	1616	A	N9-C4-C5	5.41	107.96	105.80
22	BA	1713	A	C8-N9-C4	5.41	107.96	105.80
22	BA	2088	A	C8-N9-C4	5.41	107.96	105.80
22	BA	161	A	N9-C4-C5	5.41	107.96	105.80
22	BA	207	A	N9-C4-C5	5.41	107.96	105.80
22	BA	256	A	N9-C4-C5	5.41	107.96	105.80
22	BA	482	A	C5-C6-N1	5.41	120.40	117.70
22	BA	980	A	N9-C4-C5	5.41	107.96	105.80
22	BA	2311	A	C8-N9-C4	5.41	107.96	105.80
22	BA	2632	A	C5-C6-N1	5.41	120.41	117.70
34	BM	136	MET	CG-SD-CE	5.41	108.85	100.20
22	BA	2005	A	C5-C6-N1	5.41	120.40	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	108	A	N9-C4-C5	5.41	107.96	105.80
1	AA	307	C	N3-C2-O2	-5.41	118.12	121.90
22	BA	528	A	C4-C5-N7	-5.41	108.00	110.70
22	BA	844	A	C4-C5-C6	5.41	119.70	117.00
22	BA	1204	A	C5-C6-N1	5.41	120.40	117.70
23	BB	119	A	N3-C4-N9	5.41	131.72	127.40
22	BA	322	A	C4-C5-C6	5.40	119.70	117.00
22	BA	368	A	C8-N9-C4	5.40	107.96	105.80
22	BA	1244	A	C8-N9-C4	5.40	107.96	105.80
22	BA	1772	A	C5-C6-N1	5.40	120.40	117.70
22	BA	526	A	C8-N9-C4	5.40	107.96	105.80
22	BA	2451	A	N3-C4-N9	5.40	131.72	127.40
22	BA	160	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	637	A	C4-C5-N7	-5.40	108.00	110.70
22	BA	792	A	C5-C6-N1	5.40	120.40	117.70
22	BA	1427	A	N9-C4-C5	5.40	107.96	105.80
22	BA	2860	A	N3-C4-N9	5.40	131.72	127.40
22	BA	1853	A	C4-C5-C6	5.40	119.70	117.00
22	BA	2288	A	C8-N9-C4	5.40	107.96	105.80
22	BA	721	A	C5-C6-N1	5.40	120.40	117.70
22	BA	2478	A	C4-C5-N7	-5.40	108.00	110.70
23	BB	115	A	N3-C4-N9	5.40	131.72	127.40
22	BA	13	A	C5-C6-N1	5.39	120.40	117.70
22	BA	199	A	C4-C5-C6	5.39	119.70	117.00
22	BA	340	A	C4-C5-N7	-5.39	108.00	110.70
22	BA	654	A	C8-N9-C4	5.39	107.96	105.80
22	BA	699	A	N9-C4-C5	5.39	107.96	105.80
22	BA	1272	A	N3-C4-N9	5.39	131.72	127.40
55	D3	37	A	C8-N9-C4	5.39	107.96	105.80
22	BA	586	A	N9-C4-C5	5.39	107.96	105.80
22	BA	1237	A	N9-C4-C5	5.39	107.96	105.80
22	BA	2358	A	C5-C6-N1	5.39	120.40	117.70
55	D3	76	A	C5-C6-N1	5.39	120.40	117.70
22	BA	63	A	N3-C4-N9	5.39	131.71	127.40
22	BA	270	A	N9-C4-C5	5.39	107.96	105.80
22	BA	1268	A	C8-N9-C4	5.39	107.96	105.80
22	BA	1580	A	C4-C5-N7	-5.39	108.00	110.70
22	BA	2077	A	N9-C4-C5	5.39	107.96	105.80
22	BA	631	A	N9-C4-C5	5.39	107.96	105.80
22	BA	2051	A	N9-C4-C5	5.39	107.96	105.80
22	BA	2287	A	C4-C5-N7	-5.39	108.01	110.70
22	BA	2635	A	C4-C5-N7	-5.39	108.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2800	A	N3-C4-N9	5.39	131.71	127.40
22	BA	2617	U	N3-C2-O2	-5.39	118.43	122.20
23	BB	45	A	N9-C4-C5	5.39	107.95	105.80
22	BA	2278	A	C5-C6-N1	5.39	120.39	117.70
22	BA	2564	A	C5-C6-N1	5.39	120.39	117.70
22	BA	603	A	C8-N9-C4	5.38	107.95	105.80
22	BA	1791	A	N3-C4-N9	5.38	131.71	127.40
22	BA	2418	A	C8-N9-C4	5.38	107.95	105.80
47	BZ	47	MET	CG-SD-CE	5.38	108.82	100.20
22	BA	443	A	N3-C4-N9	5.38	131.71	127.40
22	BA	2225	A	C5-C6-N1	5.38	120.39	117.70
22	BA	402	A	N3-C4-N9	5.38	131.71	127.40
22	BA	1000	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	2497	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	2758	A	C5-C6-N1	5.38	120.39	117.70
22	BA	933	A	C5-C6-N1	5.38	120.39	117.70
22	BA	2071	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	2170	A	N3-C4-N9	5.38	131.70	127.40
22	BA	602	A	C5-C6-N1	5.38	120.39	117.70
22	BA	1046	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	2602	A	C8-N9-C4	5.38	107.95	105.80
22	BA	2721	A	C5-C6-N1	5.38	120.39	117.70
29	BH	1	MET	CG-SD-CE	5.38	108.81	100.20
1	AA	457	G	N1-C6-O6	-5.38	116.67	119.90
22	BA	472	A	N9-C4-C5	5.38	107.95	105.80
22	BA	1359	A	C5-C6-N1	5.38	120.39	117.70
23	BB	53	A	C4-C5-N7	-5.38	108.01	110.70
22	BA	42	A	C5-C6-N1	5.37	120.39	117.70
22	BA	453	A	C4-C5-N7	-5.37	108.01	110.70
22	BA	941	A	C5-C6-N1	5.37	120.39	117.70
22	BA	1551	A	N3-C4-N9	5.37	131.70	127.40
22	BA	1890	A	C5-C6-N1	5.37	120.39	117.70
22	BA	2753	A	N9-C4-C5	5.37	107.95	105.80
1	AA	1087	G	C5-N7-C8	-5.37	101.61	104.30
22	BA	12	U	N1-C2-O2	5.37	126.56	122.80
22	BA	482	A	N9-C4-C5	5.37	107.95	105.80
22	BA	2456	C	C6-N1-C2	-5.37	118.15	120.30
22	BA	362	A	C8-N9-C4	5.37	107.95	105.80
22	BA	900	A	N9-C4-C5	5.37	107.95	105.80
22	BA	1254	A	C5-C6-N1	5.37	120.39	117.70
1	AA	536	C	C2-N1-C1'	5.37	124.70	118.80
22	BA	278	A	C5-C6-N1	5.37	120.38	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1073	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	1754	A	N3-C4-N9	5.37	131.69	127.40
22	BA	1890	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	2411	A	C8-N9-C4	5.37	107.95	105.80
22	BA	10	A	N3-C4-N9	5.37	131.69	127.40
22	BA	195	A	N3-C4-N9	5.37	131.69	127.40
22	BA	300	A	N3-C4-N9	5.37	131.69	127.40
22	BA	792	A	N9-C4-C5	5.37	107.95	105.80
22	BA	1129	A	C4-C5-N7	-5.37	108.02	110.70
22	BA	1260	A	C8-N9-C4	5.37	107.95	105.80
22	BA	1378	A	C5-C6-N1	5.37	120.38	117.70
22	BA	1378	A	C8-N9-C4	5.37	107.95	105.80
22	BA	2850	A	C4-C5-N7	-5.37	108.02	110.70
1	AA	498	A	N3-C4-N9	5.36	131.69	127.40
22	BA	5	A	N9-C4-C5	5.36	107.95	105.80
22	BA	84	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	161	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	1147	A	N3-C4-N9	5.36	131.69	127.40
22	BA	1268	A	N9-C4-C5	5.36	107.94	105.80
22	BA	1302	A	C4-C5-C6	5.36	119.68	117.00
22	BA	1304	A	C5-C6-N1	5.36	120.38	117.70
22	BA	1794	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	2451	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	1502	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	2211	A	N9-C4-C5	5.36	107.94	105.80
22	BA	2435	A	N9-C4-C5	5.36	107.94	105.80
22	BA	1073	A	N9-C4-C5	5.36	107.94	105.80
22	BA	1678	A	N9-C4-C5	5.36	107.94	105.80
22	BA	2566	A	C4-C5-N7	-5.36	108.02	110.70
55	D3	23	A	N3-C4-N9	5.36	131.69	127.40
22	BA	127	A	N3-C4-N9	5.36	131.69	127.40
22	BA	382	A	C8-N9-C4	5.36	107.94	105.80
55	D3	7	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	602	A	N9-C4-C5	5.36	107.94	105.80
22	BA	1039	A	C5-C6-N1	5.36	120.38	117.70
22	BA	2082	A	N9-C4-C5	5.36	107.94	105.80
22	BA	2154	A	C5-C6-N1	5.36	120.38	117.70
22	BA	943	A	C5-C6-N1	5.36	120.38	117.70
22	BA	1008	A	N3-C4-N9	5.36	131.69	127.40
22	BA	1085	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	1532	A	C4-C5-N7	-5.36	108.02	110.70
22	BA	2322	A	C8-N9-C4	5.35	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2327	A	C4-C5-N7	-5.35	108.02	110.70
1	AA	1097	C	N3-C4-C5	5.35	124.04	121.90
22	BA	119	A	C4-C5-N7	-5.35	108.02	110.70
22	BA	172	A	C5-C6-N1	5.35	120.38	117.70
22	BA	1548	A	C8-N9-C4	5.35	107.94	105.80
22	BA	1830	C	C6-N1-C2	-5.35	118.16	120.30
22	BA	2726	A	C5-C6-N1	5.35	120.38	117.70
22	BA	927	A	C5-C6-N1	5.35	120.38	117.70
22	BA	2657	A	N9-C4-C5	5.35	107.94	105.80
22	BA	2851	A	N9-C4-C5	5.35	107.94	105.80
22	BA	340	A	C5-C6-N1	5.35	120.38	117.70
22	BA	346	A	C8-N9-C4	5.35	107.94	105.80
22	BA	626	A	C8-N9-C4	5.35	107.94	105.80
22	BA	900	A	C5-C6-N1	5.35	120.38	117.70
22	BA	1039	A	C8-N9-C4	5.35	107.94	105.80
51	B3	49	MET	CG-SD-CE	5.35	108.76	100.20
22	BA	404	A	N3-C4-N9	5.35	131.68	127.40
22	BA	1009	A	N9-C4-C5	5.35	107.94	105.80
22	BA	1111	A	N9-C4-C5	5.35	107.94	105.80
22	BA	1801	A	C5-C6-N1	5.35	120.37	117.70
22	BA	1871	A	C8-N9-C4	5.35	107.94	105.80
22	BA	2147	A	N3-C4-N9	5.35	131.68	127.40
22	BA	2205	A	N9-C4-C5	5.35	107.94	105.80
34	BM	1	MET	CG-SD-CE	5.35	108.75	100.20
1	AA	307	C	N1-C2-O2	5.35	122.11	118.90
22	BA	1086	A	C4-C5-N7	-5.35	108.03	110.70
22	BA	21	A	C8-N9-C4	5.34	107.94	105.80
22	BA	603	A	N3-C4-N9	5.34	131.68	127.40
22	BA	613	A	C5-C6-N1	5.34	120.37	117.70
22	BA	1597	A	C8-N9-C4	5.34	107.94	105.80
22	BA	2058	A	C8-N9-C4	5.34	107.94	105.80
22	BA	2654	A	N3-C4-N9	5.34	131.68	127.40
22	BA	538	A	C4-C5-C6	5.34	119.67	117.00
22	BA	900	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	2726	A	C8-N9-C4	5.34	107.94	105.80
1	AA	498	A	C5-C6-N1	5.34	120.37	117.70
1	AA	1173	U	C5-C4-O4	-5.34	122.69	125.90
22	BA	892	A	C5-C6-N1	5.34	120.37	117.70
22	BA	1598	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	244	A	N9-C4-C5	5.34	107.94	105.80
22	BA	960	A	C8-N9-C4	5.34	107.94	105.80
22	BA	1508	A	N9-C4-C5	5.34	107.94	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1525	A	C5-C6-N1	5.34	120.37	117.70
22	BA	2346	A	C4-C5-C6	5.34	119.67	117.00
22	BA	167	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	730	A	N9-C4-C5	5.34	107.94	105.80
22	BA	1328	A	N9-C4-C5	5.34	107.94	105.80
22	BA	1593	A	C4-C5-N7	-5.34	108.03	110.70
22	BA	2560	A	N3-C4-N9	5.34	131.67	127.40
22	BA	2764	A	C5-C6-N1	5.34	120.37	117.70
22	BA	2879	A	C5-C6-N1	5.34	120.37	117.70
22	BA	1853	A	C5-C6-N1	5.33	120.37	117.70
22	BA	2241	A	C8-N9-C4	5.33	107.93	105.80
22	BA	2886	A	C5-C6-N1	5.33	120.37	117.70
22	BA	847	U	N3-C2-O2	-5.33	118.47	122.20
22	BA	1000	A	C5-C6-N1	5.33	120.37	117.70
22	BA	1698	A	C4-C5-N7	-5.33	108.03	110.70
22	BA	2171	A	N3-C4-N9	5.33	131.67	127.40
22	BA	2666	C	N3-C2-O2	-5.33	118.17	121.90
22	BA	391	A	C5-C6-N1	5.33	120.36	117.70
22	BA	1322	A	N3-C4-N9	5.33	131.67	127.40
22	BA	2835	A	C4-C5-N7	-5.33	108.03	110.70
22	BA	2851	A	C4-C5-N7	-5.33	108.03	110.70
22	BA	2369	A	N9-C4-C5	5.33	107.93	105.80
54	D2	28	A	C4-C5-N7	-5.33	108.03	110.70
1	AA	618	C	N1-C2-O2	5.33	122.10	118.90
22	BA	251	A	N9-C4-C5	5.33	107.93	105.80
22	BA	332	A	C4-C5-N7	-5.33	108.04	110.70
22	BA	429	A	N9-C4-C5	5.33	107.93	105.80
22	BA	547	A	N9-C4-C5	5.33	107.93	105.80
22	BA	1679	A	N9-C4-C5	5.33	107.93	105.80
22	BA	1876	A	C4-C5-N7	-5.33	108.04	110.70
22	BA	2189	U	P-O3'-C3'	5.33	126.09	119.70
23	BB	99	A	C5-C6-N1	5.33	120.36	117.70
22	BA	195	A	N9-C4-C5	5.33	107.93	105.80
22	BA	221	A	N9-C4-C5	5.33	107.93	105.80
22	BA	265	A	C4-C5-C6	5.33	119.66	117.00
22	BA	2738	A	C4-C5-C6	5.33	119.66	117.00
1	AA	924	C	C6-N1-C2	-5.32	118.17	120.30
22	BA	42	A	N9-C4-C5	5.32	107.93	105.80
22	BA	1384	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	2560	A	C4-C5-C6	5.32	119.66	117.00
22	BA	2721	A	N9-C4-C5	5.32	107.93	105.80
55	D3	7	A	C4-C5-C6	5.32	119.66	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	131	A	C8-N9-C4	5.32	107.93	105.80
22	BA	547	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	655	A	N3-C4-N9	5.32	131.66	127.40
22	BA	1189	A	C5-C6-N1	5.32	120.36	117.70
22	BA	2471	A	C4-C5-N7	-5.32	108.04	110.70
22	BA	501	A	N9-C4-C5	5.32	107.93	105.80
22	BA	988	A	C4-C5-C6	5.32	119.66	117.00
22	BA	1580	A	N9-C4-C5	5.32	107.93	105.80
22	BA	1871	A	N9-C4-C5	5.32	107.93	105.80
22	BA	2274	A	N3-C4-N9	5.32	131.66	127.40
22	BA	2411	A	N9-C4-C5	5.32	107.93	105.80
54	D2	59	A	C5-C6-N1	5.32	120.36	117.70
22	BA	483	A	N9-C4-C5	5.32	107.93	105.80
22	BA	783	A	N9-C4-C5	5.32	107.93	105.80
22	BA	1586	A	N9-C4-C5	5.32	107.93	105.80
24	BC	132	MET	CA-CB-CG	-5.32	104.26	113.30
22	BA	241	A	C5-C6-N1	5.32	120.36	117.70
22	BA	2117	A	N3-C4-N9	5.32	131.65	127.40
22	BA	632	A	C5-C6-N1	5.31	120.36	117.70
22	BA	294	A	C8-N9-C4	5.31	107.92	105.80
22	BA	479	A	C4-C5-N7	-5.31	108.04	110.70
22	BA	608	A	C5-C6-N1	5.31	120.36	117.70
22	BA	2778	A	N9-C4-C5	5.31	107.92	105.80
1	AA	440	C	C2-N1-C1'	5.31	124.64	118.80
22	BA	936	A	C8-N9-C4	5.31	107.92	105.80
22	BA	1080	A	N9-C4-C5	5.31	107.92	105.80
22	BA	1711	A	C8-N9-C4	5.31	107.92	105.80
22	BA	1785	A	C4-C5-N7	-5.31	108.05	110.70
22	BA	94	A	C4-C5-N7	-5.31	108.05	110.70
22	BA	111	A	C4-C5-C6	5.31	119.65	117.00
22	BA	161	A	C5-C6-N1	5.31	120.35	117.70
22	BA	423	A	C5-C6-N1	5.31	120.35	117.70
22	BA	1717	A	C5-C6-N1	5.31	120.35	117.70
22	BA	2273	A	C5-C6-N1	5.31	120.35	117.70
22	BA	2823	A	C5-C6-N1	5.31	120.35	117.70
22	BA	2835	A	N9-C4-C5	5.31	107.92	105.80
55	D3	76	A	C4-C5-C6	5.31	119.65	117.00
22	BA	182	A	C5-C6-N1	5.31	120.35	117.70
22	BA	820	A	C5-C6-N1	5.31	120.35	117.70
22	BA	1502	A	N9-C4-C5	5.31	107.92	105.80
22	BA	1794	A	N9-C4-C5	5.31	107.92	105.80
22	BA	1960	A	N9-C4-C5	5.31	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2077	A	C4-C5-N7	-5.31	108.05	110.70
1	AA	1262	C	N3-C2-O2	-5.30	118.19	121.90
22	BA	1395	A	C5-C6-N1	5.30	120.35	117.70
22	BA	1803	A	C4-C5-N7	-5.30	108.05	110.70
22	BA	2169	A	N9-C4-C5	5.30	107.92	105.80
22	BA	2749	A	C5-C6-N1	5.30	120.35	117.70
22	BA	2873	A	N9-C4-C5	5.30	107.92	105.80
23	BB	101	A	C5-C6-N1	5.30	120.35	117.70
55	D3	64	A	C8-N9-C4	5.30	107.92	105.80
22	BA	2632	A	C8-N9-C4	5.30	107.92	105.80
22	BA	73	A	N3-C4-N9	5.30	131.64	127.40
22	BA	878	A	C8-N9-C4	5.30	107.92	105.80
22	BA	1237	A	N3-C4-N9	5.30	131.64	127.40
22	BA	1614	A	N3-C4-N9	5.30	131.64	127.40
22	BA	2158	A	C4-C5-N7	-5.30	108.05	110.70
22	BA	829	A	N9-C4-C5	5.30	107.92	105.80
22	BA	899	A	C5-C6-N1	5.30	120.35	117.70
22	BA	1175	A	C4-C5-N7	-5.30	108.05	110.70
22	BA	1535	A	C8-N9-C4	5.30	107.92	105.80
22	BA	2868	A	C5-C6-N1	5.30	120.35	117.70
25	BD	11	MET	CG-SD-CE	5.30	108.68	100.20
23	BB	45	A	C5-C6-N1	5.30	120.35	117.70
26	BE	141	MET	CG-SD-CE	5.30	108.68	100.20
22	BA	243	U	C2-N1-C1'	5.30	124.06	117.70
22	BA	793	A	N9-C4-C5	5.30	107.92	105.80
22	BA	2170	A	C8-N9-C4	5.30	107.92	105.80
22	BA	670	A	C5-C6-N1	5.29	120.35	117.70
22	BA	1566	A	N9-C4-C5	5.29	107.92	105.80
22	BA	1759	A	C5-C6-N1	5.29	120.35	117.70
23	BB	104	A	C8-N9-C4	5.29	107.92	105.80
54	D2	49	A	C4-C5-N7	-5.29	108.05	110.70
22	BA	83	A	C4-C5-N7	-5.29	108.05	110.70
22	BA	1070	A	N3-C4-N9	5.29	131.63	127.40
22	BA	1420	A	C8-N9-C4	5.29	107.92	105.80
22	BA	2003	A	N9-C4-C5	5.29	107.92	105.80
22	BA	2560	A	C4-C5-N7	-5.29	108.05	110.70
22	BA	538	A	N9-C4-C5	5.29	107.92	105.80
22	BA	802	A	C5-C6-N1	5.29	120.35	117.70
1	AA	409	U	C2-N1-C1'	5.29	124.05	117.70
22	BA	265	A	N3-C4-N9	5.29	131.63	127.40
22	BA	1544	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	1626	A	N9-C4-C5	5.29	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	722	A	C8-N9-C4	5.29	107.92	105.80
22	BA	788	A	N3-C4-N9	5.29	131.63	127.40
22	BA	1786	A	C8-N9-C4	5.29	107.92	105.80
22	BA	2675	A	N9-C4-C5	5.29	107.92	105.80
34	BM	105	MET	CG-SD-CE	5.29	108.66	100.20
55	D3	21	A	C8-N9-C4	5.29	107.92	105.80
22	BA	1596	A	C5-C6-N1	5.29	120.34	117.70
22	BA	1953	A	N3-C4-N9	5.29	131.63	127.40
1	AA	1158	C	N1-C2-O2	5.29	122.07	118.90
22	BA	1664	A	C4-C5-N7	-5.29	108.06	110.70
54	D2	9	A	C4-C5-N7	-5.29	108.06	110.70
22	BA	227	A	C5-C6-N1	5.28	120.34	117.70
22	BA	332	A	N9-C4-C5	5.28	107.91	105.80
22	BA	352	A	N9-C4-C5	5.28	107.91	105.80
55	D3	21	A	C5-C6-N1	5.28	120.34	117.70
22	BA	322	A	N3-C4-N9	5.28	131.62	127.40
22	BA	693	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	706	A	N9-C4-C5	5.28	107.91	105.80
22	BA	2015	A	N9-C4-C5	5.28	107.91	105.80
22	BA	2063	C	N3-C2-O2	-5.28	118.20	121.90
22	BA	2572	A	C4-C5-C6	5.28	119.64	117.00
22	BA	670	A	N9-C4-C5	5.28	107.91	105.80
22	BA	1204	A	C4-C5-C6	5.28	119.64	117.00
23	BB	39	A	C8-N9-C4	5.28	107.91	105.80
22	BA	1652	A	C4-C5-C6	5.28	119.64	117.00
22	BA	1932	A	N3-C4-N9	5.28	131.62	127.40
23	BB	34	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	428	A	C5-C6-N1	5.28	120.34	117.70
22	BA	1241	A	C5-C6-N1	5.28	120.34	117.70
22	BA	1287	A	N9-C4-C5	5.28	107.91	105.80
22	BA	1373	A	C8-N9-C4	5.28	107.91	105.80
22	BA	2660	A	C4-C5-N7	-5.28	108.06	110.70
23	BB	46	A	C4-C5-N7	-5.28	108.06	110.70
22	BA	172	A	C8-N9-C4	5.28	107.91	105.80
22	BA	1005	C	C6-N1-C2	-5.28	118.19	120.30
22	BA	1354	A	N9-C4-C5	5.28	107.91	105.80
22	BA	1877	A	N9-C4-C5	5.28	107.91	105.80
22	BA	1952	A	C5-C6-N1	5.28	120.34	117.70
22	BA	1978	A	C4-C5-C6	5.28	119.64	117.00
22	BA	2800	A	N9-C4-C5	5.28	107.91	105.80
1	AA	409	U	N1-C2-O2	5.27	126.49	122.80
22	BA	947	A	N9-C4-C5	5.27	107.91	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2837	A	N9-C4-C5	5.27	107.91	105.80
22	BA	1040	A	N9-C4-C5	5.27	107.91	105.80
22	BA	1532	A	C8-N9-C4	5.27	107.91	105.80
22	BA	2184	A	C4-C5-N7	-5.27	108.06	110.70
22	BA	2266	A	N9-C4-C5	5.27	107.91	105.80
22	BA	2542	A	C4-C5-N7	-5.27	108.06	110.70
23	BB	57	A	C8-N9-C4	5.27	107.91	105.80
35	BN	110	MET	CG-SD-CE	5.27	108.64	100.20
22	BA	1713	A	C5-C6-N1	5.27	120.34	117.70
22	BA	5	A	C5-C6-N1	5.27	120.33	117.70
22	BA	699	A	C4-C5-N7	-5.27	108.06	110.70
22	BA	1791	A	C8-N9-C4	5.27	107.91	105.80
54	D2	35	A	N9-C4-C5	5.27	107.91	105.80
54	D2	49	A	N9-C4-C5	5.27	107.91	105.80
22	BA	44	A	C4-C5-N7	-5.27	108.07	110.70
22	BA	300	A	C4-C5-N7	-5.27	108.07	110.70
22	BA	716	A	N9-C4-C5	5.27	107.91	105.80
22	BA	833	A	C8-N9-C4	5.27	107.91	105.80
22	BA	917	A	C5-C6-N1	5.27	120.33	117.70
22	BA	324	A	C4-C5-C6	5.27	119.63	117.00
22	BA	344	A	N9-C4-C5	5.27	107.91	105.80
22	BA	1230	A	N9-C4-C5	5.27	107.91	105.80
22	BA	2003	A	C4-C5-N7	-5.27	108.07	110.70
22	BA	2541	A	C8-N9-C4	5.27	107.91	105.80
22	BA	2639	A	C8-N9-C4	5.27	107.91	105.80
22	BA	42	A	C8-N9-C4	5.26	107.91	105.80
22	BA	182	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	1244	A	N9-C4-C5	5.26	107.91	105.80
22	BA	1302	A	N3-C4-N9	5.26	131.61	127.40
22	BA	1735	A	C8-N9-C4	5.26	107.91	105.80
22	BA	2314	A	C8-N9-C4	5.26	107.91	105.80
22	BA	2868	A	N9-C4-C5	5.26	107.91	105.80
22	BA	195	A	C4-C5-C6	5.26	119.63	117.00
22	BA	1566	A	C4-C5-N7	-5.26	108.07	110.70
55	D3	26	A	C8-N9-C4	5.26	107.91	105.80
22	BA	213	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	983	A	N3-C4-N9	5.26	131.61	127.40
22	BA	1008	A	C4-C5-N7	-5.26	108.07	110.70
22	BA	1144	A	C5-C6-N1	5.26	120.33	117.70
22	BA	1342	A	N9-C4-C5	5.26	107.91	105.80
22	BA	1640	A	C5-C6-N1	5.26	120.33	117.70
22	BA	972	A	C8-N9-C4	5.26	107.90	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1348	C	C2-N1-C1'	5.26	124.59	118.80
22	BA	2430	A	C5-N7-C8	5.26	106.53	103.90
22	BA	278	A	C4-C5-N7	-5.26	108.07	110.70
23	BB	104	A	N9-C4-C5	5.26	107.90	105.80
1	AA	1124	G	N3-C4-C5	-5.26	125.97	128.60
22	BA	1591	A	C5-C6-N1	5.26	120.33	117.70
22	BA	2530	A	C8-N9-C4	5.25	107.90	105.80
22	BA	125	A	C4-C5-N7	-5.25	108.07	110.70
22	BA	505	A	C5-C6-N1	5.25	120.33	117.70
22	BA	1509	A	N9-C4-C5	5.25	107.90	105.80
22	BA	2270	A	C4-C5-N7	-5.25	108.07	110.70
22	BA	764	A	N3-C4-N9	5.25	131.60	127.40
22	BA	972	A	C4-C5-C6	5.25	119.63	117.00
22	BA	1590	A	C4-C5-N7	-5.25	108.07	110.70
22	BA	1701	A	N3-C4-N9	5.25	131.60	127.40
22	BA	1815	A	C4-C5-N7	-5.25	108.07	110.70
22	BA	2163	A	C4-C5-N7	-5.25	108.07	110.70
22	BA	2766	A	C8-N9-C4	5.25	107.90	105.80
22	BA	443	A	C4-C5-C6	5.25	119.62	117.00
22	BA	1505	A	N9-C4-C5	5.25	107.90	105.80
22	BA	1916	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	2060	A	C6-N1-C2	5.25	121.75	118.60
23	BB	38	C	C2-N1-C1'	5.25	124.57	118.80
22	BA	64	A	C8-N9-C4	5.25	107.90	105.80
22	BA	616	A	N9-C4-C5	5.25	107.90	105.80
22	BA	677	A	C5-C6-N1	5.25	120.32	117.70
22	BA	985	C	C2-N1-C1'	5.25	124.57	118.80
22	BA	1655	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	1848	A	N9-C4-C5	5.25	107.90	105.80
22	BA	2205	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	2266	A	C4-C5-N7	-5.25	108.08	110.70
22	BA	453	A	N9-C4-C5	5.25	107.90	105.80
22	BA	2753	A	C8-N9-C4	5.25	107.90	105.80
1	AA	960	U	N3-C2-O2	-5.24	118.53	122.20
22	BA	528	A	C5-C6-N1	5.24	120.32	117.70
22	BA	749	A	C8-N9-C4	5.24	107.90	105.80
22	BA	750	A	C5-C6-N1	5.24	120.32	117.70
22	BA	1142	A	C8-N9-C4	5.24	107.90	105.80
22	BA	1395	A	N3-C4-N9	5.24	131.59	127.40
22	BA	2346	A	N3-C4-N9	5.24	131.59	127.40
22	BA	685	A	N9-C4-C5	5.24	107.90	105.80
22	BA	1583	A	C4-C5-C6	5.24	119.62	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1689	A	N9-C4-C5	5.24	107.90	105.80
22	BA	234	U	N3-C2-O2	-5.24	118.53	122.20
22	BA	1385	A	C5-C6-N1	5.24	120.32	117.70
22	BA	1545	A	C5-C6-N1	5.24	120.32	117.70
22	BA	2386	A	C8-N9-C4	5.24	107.90	105.80
55	D3	44	G	N3-C4-N9	5.24	129.14	126.00
22	BA	340	A	N9-C4-C5	5.24	107.89	105.80
22	BA	637	A	N3-C4-N9	5.24	131.59	127.40
22	BA	1328	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	2534	A	N9-C4-C5	5.24	107.89	105.80
22	BA	2778	A	C4-C5-N7	-5.24	108.08	110.70
26	BE	199	MET	CG-SD-CE	5.24	108.58	100.20
22	BA	1503	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	382	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	609	A	C5-C6-N1	5.24	120.32	117.70
22	BA	621	A	C8-N9-C4	5.24	107.89	105.80
22	BA	996	A	C5-C6-N1	5.24	120.32	117.70
22	BA	1134	A	C5-C6-N1	5.24	120.32	117.70
22	BA	2082	A	C4-C5-N7	-5.24	108.08	110.70
22	BA	2386	A	N9-C4-C5	5.24	107.89	105.80
22	BA	2547	A	C5-C6-N1	5.24	120.32	117.70
32	BK	113	MET	CG-SD-CE	5.24	108.58	100.20
22	BA	279	A	C8-N9-C4	5.23	107.89	105.80
32	BK	20	MET	CG-SD-CE	5.23	108.57	100.20
1	AA	489	C	N1-C2-O2	5.23	122.04	118.90
22	BA	218	A	C4-C5-N7	-5.23	108.08	110.70
22	BA	322	A	C5-C6-N1	5.23	120.32	117.70
22	BA	1205	A	N3-C4-N9	5.23	131.59	127.40
22	BA	1889	A	C4-C5-N7	-5.23	108.08	110.70
22	BA	2432	A	C8-N9-C4	5.23	107.89	105.80
22	BA	675	A	C5-C6-N1	5.23	120.31	117.70
22	BA	1367	A	C4-C5-N7	-5.23	108.08	110.70
22	BA	156	A	C5-C6-N1	5.23	120.31	117.70
22	BA	2733	A	C4-C5-N7	-5.23	108.09	110.70
22	BA	1008	A	C5-C6-N1	5.23	120.31	117.70
22	BA	1284	A	C8-N9-C4	5.23	107.89	105.80
22	BA	1453	A	N9-C4-C5	5.23	107.89	105.80
22	BA	1746	A	C8-N9-C4	5.23	107.89	105.80
22	BA	2171	A	C4-C5-C6	5.23	119.61	117.00
22	BA	2734	A	N9-C4-C5	5.23	107.89	105.80
22	BA	1571	A	C4-C5-N7	-5.23	108.09	110.70
22	BA	2104	C	N1-C2-O2	5.23	122.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	71	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	820	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	1103	A	N9-C4-C5	5.22	107.89	105.80
22	BA	1366	A	C8-N9-C4	5.22	107.89	105.80
22	BA	1744	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	2059	A	N9-C4-C5	5.22	107.89	105.80
22	BA	2311	A	N9-C4-C5	5.22	107.89	105.80
22	BA	2883	A	N3-C4-N9	5.22	131.58	127.40
55	D3	61	C	N3-C2-O2	-5.22	118.24	121.90
22	BA	172	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	2147	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	899	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	917	A	N9-C4-C5	5.22	107.89	105.80
22	BA	449	A	N9-C4-C5	5.22	107.89	105.80
22	BA	1096	A	C4-C5-N7	-5.22	108.09	110.70
22	BA	1453	A	N3-C4-N9	5.22	131.57	127.40
22	BA	1635	A	C5-C6-N1	5.22	120.31	117.70
22	BA	2589	A	N3-C4-N9	5.22	131.58	127.40
33	BL	1	MET	CG-SD-CE	5.22	108.55	100.20
22	BA	918	A	C5-C6-N1	5.22	120.31	117.70
22	BA	2369	A	C4-C5-C6	5.22	119.61	117.00
22	BA	522	A	C8-N9-C4	5.22	107.89	105.80
22	BA	1701	A	C4-C5-C6	5.22	119.61	117.00
22	BA	428	A	C4-C5-N7	-5.21	108.09	110.70
22	BA	878	A	C4-C5-N7	-5.21	108.09	110.70
22	BA	2654	A	C4-C5-N7	-5.21	108.09	110.70
22	BA	2814	A	C8-N9-C4	5.21	107.89	105.80
22	BA	526	A	C5-C6-N1	5.21	120.31	117.70
22	BA	1665	A	C4-C5-N7	-5.21	108.09	110.70
22	BA	1960	A	C8-N9-C4	5.21	107.88	105.80
22	BA	1014	A	C5-C6-N1	5.21	120.30	117.70
22	BA	1155	A	C5-C6-N1	5.21	120.30	117.70
22	BA	1286	A	C4-C5-N7	-5.21	108.10	110.70
22	BA	1937	A	C4-C5-C6	5.21	119.60	117.00
22	BA	2513	A	C4-C5-N7	-5.21	108.10	110.70
22	BA	196	A	C4-C5-N7	-5.21	108.10	110.70
22	BA	1090	A	C8-N9-C4	5.21	107.88	105.80
22	BA	2542	A	C5-C6-N1	5.21	120.30	117.70
22	BA	2587	A	C5-C6-N1	5.21	120.30	117.70
54	D2	9	A	N3-C4-N9	5.21	131.57	127.40
22	BA	241	A	C4-C5-C6	5.21	119.60	117.00
22	BA	2119	A	C5-C6-N1	5.21	120.30	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BD	1	MET	CG-SD-CE	5.21	108.53	100.20
22	BA	643	A	C8-N9-C4	5.20	107.88	105.80
22	BA	2600	A	C5-C6-N1	5.20	120.30	117.70
22	BA	503	A	C5-C6-N1	5.20	120.30	117.70
22	BA	532	A	C5-C6-N1	5.20	120.30	117.70
22	BA	1610	A	N9-C4-C5	5.20	107.88	105.80
22	BA	1616	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	2333	A	C4-C5-C6	5.20	119.60	117.00
23	BB	45	A	C4-C5-N7	-5.20	108.10	110.70
55	D3	38	A	C5-C6-N1	5.20	120.30	117.70
1	AA	1087	G	C4-N9-C1'	5.20	133.26	126.50
22	BA	204	A	N3-C4-N9	5.20	131.56	127.40
22	BA	311	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	1050	A	C5-C6-N1	5.20	120.30	117.70
54	D2	9	A	N9-C4-C5	5.20	107.88	105.80
54	D2	76	A	C4-C5-C6	5.20	119.60	117.00
22	BA	761	A	N9-C4-C5	5.20	107.88	105.80
22	BA	878	A	C5-C6-N1	5.20	120.30	117.70
22	BA	910	A	C5-C6-N1	5.20	120.30	117.70
22	BA	1020	A	C4-C5-C6	5.20	119.60	117.00
22	BA	1803	A	N3-C4-N9	5.20	131.56	127.40
22	BA	2577	A	C5-C6-N1	5.20	120.30	117.70
22	BA	2662	A	C5-N7-C8	5.20	106.50	103.90
22	BA	2665	A	N9-C4-C5	5.20	107.88	105.80
22	BA	563	A	N9-C4-C5	5.20	107.88	105.80
22	BA	118	A	N9-C4-C5	5.20	107.88	105.80
22	BA	586	A	N3-C4-N9	5.20	131.56	127.40
22	BA	820	A	C8-N9-C4	5.20	107.88	105.80
22	BA	928	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	1274	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	1780	A	C4-C5-N7	-5.20	108.10	110.70
22	BA	1789	A	C8-N9-C4	5.20	107.88	105.80
22	BA	2900	A	N9-C4-C5	5.20	107.88	105.80
22	BA	734	A	C5-C6-N1	5.19	120.30	117.70
22	BA	1889	A	C5-C6-N1	5.19	120.30	117.70
22	BA	64	A	N9-C4-C5	5.19	107.88	105.80
22	BA	1583	A	C4-C5-N7	-5.19	108.10	110.70
22	BA	2497	A	C5-C6-N1	5.19	120.30	117.70
23	BB	78	A	C4-C5-C6	5.19	119.60	117.00
55	D3	7	A	C5-C6-N1	5.19	120.30	117.70
22	BA	668	A	C5-C6-N1	5.19	120.30	117.70
22	BA	752	A	C8-N9-C4	5.19	107.88	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2412	A	C4-C5-N7	-5.19	108.11	110.70
23	BB	108	A	C5-C6-N1	5.19	120.30	117.70
22	BA	104	A	C8-N9-C4	5.19	107.88	105.80
22	BA	670	A	C4-C5-N7	-5.19	108.11	110.70
22	BA	1342	A	C4-C5-N7	-5.19	108.11	110.70
22	BA	1690	A	C4-C5-N7	-5.19	108.11	110.70
22	BA	1952	A	C8-N9-C4	5.19	107.88	105.80
22	BA	2615	U	C2-N1-C1'	5.19	123.93	117.70
22	BA	1610	A	C4-C5-C6	5.19	119.59	117.00
22	BA	1785	A	C4-C5-C6	5.19	119.59	117.00
22	BA	896	A	N3-C4-N9	5.18	131.55	127.40
22	BA	1352	U	N3-C2-O2	-5.18	118.57	122.20
22	BA	1780	A	N3-C4-N9	5.18	131.55	127.40
22	BA	2837	A	C4-C5-N7	-5.18	108.11	110.70
23	BB	101	A	C8-N9-C4	5.18	107.87	105.80
22	BA	716	A	C4-C5-N7	-5.18	108.11	110.70
23	BB	34	A	C8-N9-C4	5.18	107.87	105.80
22	BA	167	A	N9-C4-C5	5.18	107.87	105.80
22	BA	1098	A	C8-N9-C4	5.18	107.87	105.80
22	BA	2453	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	2459	A	C8-N9-C4	5.18	107.87	105.80
22	BA	256	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	423	A	C8-N9-C4	5.18	107.87	105.80
22	BA	616	A	C5-C6-N1	5.18	120.29	117.70
22	BA	616	A	C8-N9-C4	5.18	107.87	105.80
22	BA	637	A	C5-C6-N1	5.18	120.29	117.70
22	BA	788	A	C4-C5-C6	5.18	119.59	117.00
22	BA	1287	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	1717	A	N9-C4-C5	5.18	107.87	105.80
22	BA	1749	A	C8-N9-C4	5.18	107.87	105.80
22	BA	1876	A	C5-C6-N1	5.18	120.29	117.70
22	BA	2101	A	N9-C4-C5	5.18	107.87	105.80
23	BB	57	A	C4-C5-N7	-5.18	108.11	110.70
1	AA	95	C	C5-C6-N1	5.18	123.59	121.00
22	BA	1098	A	C4-C5-N7	-5.18	108.11	110.70
22	BA	1433	A	N9-C4-C5	5.18	107.87	105.80
22	BA	1640	A	C8-N9-C4	5.18	107.87	105.80
22	BA	2176	A	C8-N9-C4	5.18	107.87	105.80
22	BA	849	A	C8-N9-C4	5.17	107.87	105.80
22	BA	1469	A	C5-C6-N1	5.17	120.29	117.70
22	BA	1569	A	N9-C4-C5	5.17	107.87	105.80
22	BA	1635	A	C4-C5-N7	-5.17	108.11	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2600	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	352	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	430	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	866	A	C5-C6-N1	5.17	120.29	117.70
1	AA	1124	G	C5-C6-N1	5.17	114.08	111.50
22	BA	631	A	C4-C5-N7	-5.17	108.11	110.70
22	BA	1001	A	N3-C4-N9	5.17	131.54	127.40
22	BA	1830	C	C5-C6-N1	5.17	123.59	121.00
22	BA	2899	A	N9-C4-C5	5.17	107.87	105.80
55	D3	1	G	P-O3'-C3'	5.17	125.91	119.70
22	BA	920	A	C5-C6-N1	5.17	120.28	117.70
22	BA	2900	A	C8-N9-C4	5.17	107.87	105.80
1	AA	1215	G	C4-C5-N7	5.17	112.87	110.80
22	BA	920	A	C8-N9-C4	5.17	107.87	105.80
22	BA	1069	A	C8-N9-C4	5.17	107.87	105.80
22	BA	1918	A	C5-C6-N1	5.17	120.28	117.70
22	BA	2451	A	C4-C5-C6	5.17	119.58	117.00
22	BA	2474	U	N3-C2-O2	-5.17	118.58	122.20
22	BA	125	A	N9-C4-C5	5.17	107.87	105.80
22	BA	422	A	C5-C6-N1	5.17	120.28	117.70
22	BA	2657	A	C4-C5-N7	-5.17	108.12	110.70
22	BA	2776	A	N9-C4-C5	5.17	107.87	105.80
50	B2	22	MET	CG-SD-CE	5.17	108.46	100.20
22	BA	21	A	N9-C4-C5	5.16	107.86	105.80
22	BA	603	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	919	U	N3-C2-O2	-5.16	118.58	122.20
22	BA	975	A	N9-C4-C5	5.16	107.86	105.80
22	BA	1020	A	N9-C4-C5	5.16	107.87	105.80
22	BA	1268	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	1754	A	N9-C4-C5	5.16	107.86	105.80
22	BA	2059	A	N3-C4-N9	5.16	131.53	127.40
1	AA	570	G	C4-N9-C1'	5.16	133.21	126.50
22	BA	556	A	C5-C6-N1	5.16	120.28	117.70
22	BA	849	A	C5-C6-N1	5.16	120.28	117.70
22	BA	2060	A	C4-C5-C6	5.16	119.58	117.00
22	BA	2821	A	C8-N9-C4	5.16	107.86	105.80
22	BA	718	A	N9-C4-C5	5.16	107.86	105.80
22	BA	1205	A	C4-C5-N7	-5.16	108.12	110.70
22	BA	2158	A	N9-C4-C5	5.16	107.86	105.80
22	BA	2530	A	C4-C5-N7	-5.16	108.12	110.70
1	AA	1172	C	C2-N1-C1'	5.16	124.47	118.80
22	BA	753	A	N9-C4-C5	5.16	107.86	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2764	A	C4-C5-C6	5.16	119.58	117.00
22	BA	1431	A	N9-C4-C5	5.15	107.86	105.80
22	BA	2656	U	C2-N1-C1'	5.15	123.88	117.70
22	BA	2750	A	C5-C6-N1	5.15	120.28	117.70
35	BN	24	MET	CG-SD-CE	5.15	108.44	100.20
54	D2	21	A	N9-C4-C5	5.15	107.86	105.80
22	BA	348	A	N9-C4-C5	5.15	107.86	105.80
22	BA	1285	A	N3-C4-N9	5.15	131.52	127.40
22	BA	1289	C	C2-N1-C1'	5.15	124.47	118.80
22	BA	2169	A	C5-C6-N1	5.15	120.28	117.70
22	BA	2851	A	C5-C6-N1	5.15	120.28	117.70
23	BB	108	A	C4-C5-N7	-5.15	108.12	110.70
24	BC	201	MET	CG-SD-CE	5.15	108.44	100.20
22	BA	344	A	C4-C5-N7	-5.15	108.12	110.70
22	BA	1009	A	C4-C5-N7	-5.15	108.13	110.70
22	BA	2856	A	C8-N9-C4	5.15	107.86	105.80
1	AA	311	C	C6-N1-C2	-5.15	118.24	120.30
22	BA	223	A	N3-C4-N9	5.15	131.52	127.40
22	BA	633	A	N9-C4-C5	5.15	107.86	105.80
22	BA	1095	A	N9-C4-C5	5.15	107.86	105.80
22	BA	1307	A	C5-C6-N1	5.15	120.27	117.70
22	BA	1759	A	N9-C4-C5	5.15	107.86	105.80
22	BA	2005	A	N3-C4-N9	5.15	131.52	127.40
22	BA	2317	A	N9-C4-C5	5.15	107.86	105.80
22	BA	2434	A	C5-C6-N1	5.15	120.27	117.70
22	BA	1127	A	N3-C4-N9	5.15	131.52	127.40
22	BA	2309	A	C4-C5-N7	-5.15	108.13	110.70
22	BA	2705	A	N3-C4-N9	5.15	131.52	127.40
22	BA	309	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	502	A	C8-N9-C4	5.14	107.86	105.80
22	BA	1928	A	N3-C4-N9	5.14	131.52	127.40
22	BA	1596	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	2270	A	C8-N9-C4	5.14	107.86	105.80
22	BA	1496	A	C5-C6-N1	5.14	120.27	117.70
22	BA	2119	A	N3-C4-N9	5.14	131.51	127.40
22	BA	1189	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	1549	A	N9-C4-C5	5.14	107.86	105.80
22	BA	1634	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	204	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	478	A	C8-N9-C4	5.14	107.86	105.80
22	BA	1711	A	C4-C5-N7	-5.14	108.13	110.70
22	BA	2095	A	C4-C5-N7	-5.14	108.13	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2199	A	N9-C4-C5	5.13	107.85	105.80
22	BA	2468	A	C5-C6-N1	5.13	120.27	117.70
22	BA	466	A	N3-C4-N9	5.13	131.51	127.40
22	BA	789	A	C5-C6-N1	5.13	120.27	117.70
22	BA	1048	A	C4-C5-N7	-5.13	108.13	110.70
47	BZ	54	MET	CG-SD-CE	5.13	108.41	100.20
22	BA	311	A	C8-N9-C4	5.13	107.85	105.80
22	BA	483	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	743	A	C8-N9-C4	5.13	107.85	105.80
22	BA	1322	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	1495	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	1987	A	C4-C5-N7	-5.13	108.13	110.70
22	BA	599	A	N9-C4-C5	5.13	107.85	105.80
54	D2	38	A	N3-C4-N9	5.13	131.50	127.40
22	BA	167	A	C5-C6-N1	5.13	120.26	117.70
22	BA	1354	A	C5-C6-N1	5.13	120.26	117.70
22	BA	2191	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	2369	A	N3-C4-N9	5.13	131.50	127.40
22	BA	196	A	N9-C4-C5	5.13	107.85	105.80
22	BA	502	A	C4-C5-N7	-5.13	108.14	110.70
22	BA	457	A	C4-C5-C6	5.12	119.56	117.00
22	BA	1871	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	64	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	152	A	C5-C6-N1	5.12	120.26	117.70
22	BA	668	A	N9-C4-C5	5.12	107.85	105.80
22	BA	685	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	706	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	1978	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	2656	U	N3-C2-O2	-5.12	118.61	122.20
22	BA	2809	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	471	A	N9-C4-C5	5.12	107.85	105.80
22	BA	501	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	1096	A	C8-N9-C4	5.12	107.85	105.80
22	BA	1294	U	N3-C2-O2	-5.12	118.61	122.20
22	BA	1579	A	C5-C6-N1	5.12	120.26	117.70
22	BA	1678	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	2097	A	N9-C4-C5	5.12	107.85	105.80
22	BA	2317	A	C8-N9-C4	5.12	107.85	105.80
22	BA	443	A	C5-C6-N1	5.12	120.26	117.70
22	BA	761	A	C8-N9-C4	5.12	107.85	105.80
22	BA	1032	A	N9-C4-C5	5.12	107.85	105.80
22	BA	1286	A	C5-C6-N1	5.12	120.26	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1936	A	C8-N9-C1'	-5.12	118.49	127.70
22	BA	1336	A	C8-N9-C4	5.12	107.85	105.80
22	BA	197	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	1785	A	C5-C6-N1	5.12	120.26	117.70
22	BA	2037	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	2126	A	C8-N9-C4	5.12	107.85	105.80
22	BA	2378	A	C4-C5-N7	-5.12	108.14	110.70
22	BA	2590	A	C4-C5-N7	-5.12	108.14	110.70
1	AA	854	U	N3-C2-O2	-5.11	118.62	122.20
22	BA	310	A	C4-C5-C6	5.11	119.56	117.00
22	BA	896	A	C4-C5-C6	5.11	119.56	117.00
22	BA	1032	A	N3-C4-N9	5.11	131.49	127.40
22	BA	1786	A	C5-C6-N1	5.11	120.26	117.70
22	BA	2108	A	C5-C6-N1	5.11	120.26	117.70
22	BA	2392	A	C4-C5-N7	-5.11	108.14	110.70
22	BA	2660	A	N9-C4-C5	5.11	107.84	105.80
22	BA	2665	A	C4-C5-N7	-5.11	108.14	110.70
23	BB	99	A	N9-C4-C5	5.11	107.84	105.80
28	BG	75	MET	CG-SD-CE	5.11	108.38	100.20
22	BA	1029	A	N9-C4-C5	5.11	107.84	105.80
22	BA	2887	A	C4-C5-N7	-5.11	108.14	110.70
22	BA	2471	A	C4-C5-C6	5.11	119.56	117.00
22	BA	2063	C	N1-C2-O2	5.11	121.97	118.90
22	BA	146	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	1237	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	1383	A	C5-C6-N1	5.11	120.25	117.70
22	BA	1735	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	2474	U	N1-C2-O2	5.11	126.38	122.80
22	BA	2675	A	C5-C6-N1	5.11	120.25	117.70
22	BA	402	A	C4-C5-N7	-5.11	108.15	110.70
22	BA	149	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	1762	A	C5-C6-N1	5.10	120.25	117.70
22	BA	217	A	N9-C4-C5	5.10	107.84	105.80
22	BA	270	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	1808	A	C5-C6-N1	5.10	120.25	117.70
22	BA	2376	A	C5-C6-N1	5.10	120.25	117.70
22	BA	2562	U	N3-C2-O2	-5.10	118.63	122.20
54	D2	26	A	C5-C6-N1	5.10	120.25	117.70
1	AA	932	C	C2-N1-C1'	5.10	124.41	118.80
1	AA	1348	U	C2-N1-C1'	5.10	123.82	117.70
22	BA	217	A	C8-N9-C4	5.10	107.84	105.80
22	BA	415	A	C5-C6-N1	5.10	120.25	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	563	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	936	A	N9-C4-C5	5.10	107.84	105.80
22	BA	988	A	C8-N9-C4	5.10	107.84	105.80
22	BA	1089	A	N9-C4-C5	5.10	107.84	105.80
22	BA	1549	A	C8-N9-C4	5.10	107.84	105.80
22	BA	1932	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	2471	A	N3-C4-N9	5.10	131.48	127.40
22	BA	439	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	676	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	1175	A	N9-C4-C5	5.10	107.84	105.80
22	BA	1262	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	1434	A	C5-C6-N1	5.10	120.25	117.70
23	BB	15	A	C4-C5-N7	-5.10	108.15	110.70
22	BA	2333	A	C5-C6-N1	5.10	120.25	117.70
30	BI	1	MET	CG-SD-CE	5.10	108.35	100.20
55	D3	9	A	C5-C6-N1	5.10	120.25	117.70
22	BA	181	A	C5-C6-N1	5.09	120.25	117.70
22	BA	354	A	C5-C6-N1	5.09	120.25	117.70
22	BA	1783	A	N3-C4-N9	5.09	131.47	127.40
22	BA	2060	A	N3-C4-N9	5.09	131.47	127.40
22	BA	2376	A	C4-C5-N7	-5.09	108.15	110.70
23	BB	109	A	N9-C4-C5	5.09	107.84	105.80
22	BA	56	A	C4-C5-N7	-5.09	108.15	110.70
22	BA	423	A	N3-C4-N9	5.09	131.47	127.40
22	BA	1522	A	C5-C6-N1	5.09	120.25	117.70
22	BA	2243	U	N3-C2-O2	-5.09	118.64	122.20
1	AA	86	G	N3-C4-N9	-5.09	122.95	126.00
1	AA	570	G	C8-N9-C1'	-5.09	120.38	127.00
22	BA	626	A	N9-C4-C5	5.09	107.84	105.80
22	BA	1304	A	N3-C4-N9	5.09	131.47	127.40
22	BA	2781	A	N3-C4-N9	5.09	131.47	127.40
55	D3	76	A	N3-C4-N9	5.09	131.47	127.40
22	BA	1776	G	C4-N9-C1'	5.09	133.11	126.50
22	BA	479	A	N9-C4-C5	5.09	107.83	105.80
22	BA	735	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	1159	U	N3-C2-O2	-5.09	118.64	122.20
22	BA	1175	A	C8-N9-C4	5.09	107.83	105.80
22	BA	1359	A	N9-C4-C5	5.09	107.83	105.80
22	BA	2346	A	N9-C4-C5	5.09	107.83	105.80
22	BA	2534	A	C4-C5-N7	-5.09	108.16	110.70
22	BA	2542	A	N3-C4-N9	5.09	131.47	127.40
22	BA	2800	A	C4-C5-N7	-5.08	108.16	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	503	C	C6-N1-C2	-5.08	118.27	120.30
22	BA	1020	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	1650	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	1789	A	N9-C4-C5	5.08	107.83	105.80
54	D2	38	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	574	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	1453	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	1477	A	C8-N9-C4	5.08	107.83	105.80
22	BA	1641	A	C5-C6-N1	5.08	120.24	117.70
22	BA	2346	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	176	A	C8-N9-C4	5.08	107.83	105.80
22	BA	482	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	1745	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	104	A	N9-C4-C5	5.08	107.83	105.80
22	BA	118	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	404	A	C5-C6-N1	5.08	120.24	117.70
22	BA	453	A	C5-C6-N1	5.08	120.24	117.70
22	BA	1205	A	N9-C4-C5	5.08	107.83	105.80
22	BA	1385	A	C4-C5-C6	5.08	119.54	117.00
1	AA	810	C	C6-N1-C2	-5.08	118.27	120.30
22	BA	1264	A	N3-C4-N9	5.08	131.46	127.40
56	D4	1	U	C6-N1-C1'	-5.08	114.09	121.20
22	BA	256	A	C8-N9-C4	5.08	107.83	105.80
22	BA	423	A	C4-C5-C6	5.08	119.54	117.00
22	BA	867	C	N3-C2-O2	-5.08	118.35	121.90
22	BA	2058	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	2173	A	C8-N9-C4	5.08	107.83	105.80
22	BA	2182	U	N1-C2-O2	5.08	126.35	122.80
22	BA	2198	A	N9-C4-C5	5.08	107.83	105.80
22	BA	2750	A	C4-C5-N7	-5.08	108.16	110.70
22	BA	126	A	C5-C6-N1	5.07	120.24	117.70
22	BA	1077	A	C8-N9-C4	5.07	107.83	105.80
22	BA	1095	A	C4-C5-N7	-5.07	108.16	110.70
22	BA	2189	U	N1-C2-O2	5.07	126.35	122.80
22	BA	2433	A	C4-C5-N7	-5.07	108.16	110.70
54	D2	31	A	C4-C5-N7	-5.07	108.16	110.70
22	BA	221	A	C4-C5-C6	5.07	119.53	117.00
22	BA	959	A	N9-C4-C5	5.07	107.83	105.80
22	BA	2281	A	N9-C4-C5	5.07	107.83	105.80
22	BA	1067	A	C4-C5-N7	-5.07	108.17	110.70
22	BA	2821	A	C4-C5-N7	-5.07	108.17	110.70
1	AA	1132	C	C6-N1-C2	-5.07	118.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	917	A	C4-C5-N7	-5.07	108.17	110.70
1	AA	792	A	O4'-C1'-N9	5.07	112.25	108.20
22	BA	1632	A	C4-C5-N7	-5.07	108.17	110.70
22	BA	1700	A	C5-C6-N1	5.07	120.23	117.70
23	BB	50	A	C8-N9-C4	5.07	107.83	105.80
22	BA	1730	C	C6-N1-C1'	-5.06	114.72	120.80
1	AA	208	U	N1-C2-O2	5.06	126.34	122.80
22	BA	149	A	C5-C6-N1	5.06	120.23	117.70
22	BA	1254	A	N3-C4-N9	5.06	131.45	127.40
22	BA	2450	A	N9-C4-C5	5.06	107.83	105.80
22	BA	222	A	C4-C5-C6	5.06	119.53	117.00
22	BA	118	A	C8-N9-C4	5.06	107.82	105.80
22	BA	311	A	C5-C6-N1	5.06	120.23	117.70
22	BA	2031	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	2176	A	C5-C6-N1	5.06	120.23	117.70
22	BA	2309	A	N9-C4-C5	5.06	107.82	105.80
22	BA	2426	A	N9-C4-C5	5.06	107.82	105.80
22	BA	2850	A	N9-C4-C5	5.06	107.82	105.80
1	AA	1087	G	C4-C5-N7	5.06	112.82	110.80
22	BA	142	A	C4-C5-N7	-5.06	108.17	110.70
22	BA	226	A	N9-C4-C5	5.06	107.82	105.80
22	BA	900	A	C8-N9-C4	5.06	107.82	105.80
22	BA	1854	A	C5-C6-N1	5.06	120.23	117.70
22	BA	2019	A	C5-C6-N1	5.06	120.23	117.70
22	BA	1754	A	C8-N9-C4	5.06	107.82	105.80
23	BB	39	A	N3-C4-N9	5.06	131.44	127.40
22	BA	1054	A	C8-N9-C4	5.05	107.82	105.80
22	BA	1103	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	1508	A	C4-C5-N7	-5.05	108.17	110.70
23	BB	39	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	1387	A	N9-C4-C5	5.05	107.82	105.80
23	BB	50	A	C5-C6-N1	5.05	120.23	117.70
22	BA	216	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	845	A	N9-C4-C5	5.05	107.82	105.80
22	BA	1040	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	1614	A	N9-C4-C5	5.05	107.82	105.80
22	BA	1654	A	C8-N9-C4	5.05	107.82	105.80
22	BA	2322	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	2450	A	C6-N1-C2	5.05	121.63	118.60
1	AA	252	U	C2-N1-C1'	5.05	123.76	117.70
22	BA	1762	A	C4-C5-N7	-5.05	108.17	110.70
22	BA	1815	A	C4-C5-C6	5.05	119.52	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2171	A	C4-C5-N7	-5.05	108.18	110.70
22	BA	2314	A	N3-C4-N9	5.05	131.44	127.40
22	BA	735	A	N9-C4-C5	5.05	107.82	105.80
22	BA	1032	A	C4-C5-N7	-5.05	108.18	110.70
22	BA	1103	A	C8-N9-C4	5.05	107.82	105.80
22	BA	1866	A	N9-C4-C5	5.05	107.82	105.80
22	BA	2009	A	C4-C5-N7	-5.05	108.18	110.70
22	BA	2662	A	N9-C4-C5	5.05	107.82	105.80
22	BA	1698	A	N9-C4-C5	5.04	107.82	105.80
22	BA	1735	A	C5-C6-N1	5.04	120.22	117.70
1	AA	618	C	N3-C2-O2	-5.04	118.37	121.90
22	BA	401	A	C5-C6-N1	5.04	120.22	117.70
22	BA	1156	A	C5-C6-N1	5.04	120.22	117.70
54	D2	41	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	861	A	C8-N9-C4	5.04	107.82	105.80
22	BA	1046	A	N9-C4-C5	5.04	107.82	105.80
23	BB	58	A	C4-C5-N7	-5.04	108.18	110.70
22	BA	1420	A	C5-C6-N1	5.04	120.22	117.70
22	BA	2134	A	C4-C5-C6	5.04	119.52	117.00
22	BA	2758	A	C8-N9-C4	5.04	107.82	105.80
22	BA	2776	A	C5-C6-N1	5.04	120.22	117.70
1	AA	1201	A	C5-C6-N6	-5.04	119.67	123.70
22	BA	1431	A	C8-N9-C4	5.04	107.81	105.80
22	BA	2031	A	C8-N9-C4	5.04	107.81	105.80
24	BC	146	MET	CG-SD-CE	5.04	108.26	100.20
22	BA	706	A	C5-C6-N1	5.04	120.22	117.70
22	BA	1494	A	C5-C6-N1	5.04	120.22	117.70
22	BA	2560	A	C8-N9-C4	5.04	107.81	105.80
1	AA	1228	C	N1-C2-O2	5.04	121.92	118.90
22	BA	574	A	N9-C4-C5	5.04	107.81	105.80
22	BA	2541	A	N9-C4-C5	5.04	107.81	105.80
22	BA	1039	A	C4-C5-N7	-5.03	108.18	110.70
22	BA	1156	A	N9-C4-C5	5.03	107.81	105.80
22	BA	1735	A	N9-C4-C5	5.03	107.81	105.80
22	BA	1877	A	C5-C6-N1	5.03	120.22	117.70
22	BA	2435	A	C4-C5-N7	-5.03	108.18	110.70
22	BA	2600	A	N3-C4-N9	5.03	131.43	127.40
22	BA	244	A	C4-C5-N7	-5.03	108.18	110.70
22	BA	362	A	C4-C5-N7	-5.03	108.18	110.70
22	BA	1226	A	C4-C5-N7	-5.03	108.18	110.70
23	BB	70	C	C6-N1-C2	-5.03	118.29	120.30
22	BA	1609	A	C5-C6-N1	5.03	120.22	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2733	A	C5-C6-N1	5.03	120.22	117.70
22	BA	1327	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	1419	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	1552	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	1586	A	C8-N9-C4	5.03	107.81	105.80
22	BA	2748	A	N9-C4-C5	5.03	107.81	105.80
1	AA	1068	G	C4-N9-C1'	5.03	133.04	126.50
22	BA	217	A	C5-C6-N1	5.03	120.21	117.70
22	BA	1098	A	C5-C6-N1	5.03	120.21	117.70
22	BA	1327	A	N9-C4-C5	5.03	107.81	105.80
22	BA	1354	A	C4-C5-N7	-5.03	108.19	110.70
22	BA	1598	A	C5-C6-N1	5.03	120.21	117.70
22	BA	2725	A	N3-C4-N9	5.03	131.42	127.40
22	BA	2733	A	N9-C4-C5	5.03	107.81	105.80
22	BA	125	A	C5-C6-N1	5.03	120.21	117.70
22	BA	279	A	C5-C6-N1	5.03	120.21	117.70
22	BA	1641	A	N9-C4-C5	5.03	107.81	105.80
22	BA	1787	A	C5-C6-N1	5.03	120.21	117.70
22	BA	1829	A	C8-N9-C4	5.03	107.81	105.80
22	BA	2126	A	C5-C6-N1	5.03	120.21	117.70
22	BA	2129	C	C6-N1-C2	-5.03	118.29	120.30
22	BA	2322	A	N9-C4-C5	5.03	107.81	105.80
1	AA	87	C	C5-C6-N1	5.02	123.51	121.00
22	BA	2051	A	C5-C6-N1	5.02	120.21	117.70
22	BA	2565	A	C8-N9-C4	5.02	107.81	105.80
22	BA	2406	A	N9-C4-C5	5.02	107.81	105.80
32	BK	7	MET	CG-SD-CE	5.02	108.24	100.20
22	BA	272	A	N9-C4-C5	5.02	107.81	105.80
22	BA	538	A	C5-C6-N1	5.02	120.21	117.70
22	BA	715	A	C5-C6-N1	5.02	120.21	117.70
1	AA	1168	U	N1-C2-O2	5.02	126.31	122.80
22	BA	152	A	N9-C4-C5	5.02	107.81	105.80
22	BA	221	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	899	A	N9-C4-C5	5.02	107.81	105.80
22	BA	2005	A	C4-C5-C6	5.02	119.51	117.00
22	BA	2059	A	C8-N9-C4	5.02	107.81	105.80
23	BB	57	A	C5-C6-N1	5.02	120.21	117.70
22	BA	792	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	833	A	C4-C5-C6	5.02	119.51	117.00
22	BA	2354	C	C6-N1-C2	-5.02	118.29	120.30
23	BB	94	A	N9-C4-C5	5.02	107.81	105.80
23	BB	109	A	C5-C6-N1	5.02	120.21	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	616	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	1496	A	C4-C5-N7	-5.02	108.19	110.70
22	BA	74	A	N9-C4-C5	5.01	107.81	105.80
22	BA	526	A	C4-C5-C6	5.01	119.51	117.00
22	BA	821	A	C4-C5-C6	5.01	119.51	117.00
22	BA	981	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	981	A	C8-N9-C4	5.01	107.81	105.80
22	BA	1384	A	C5-C6-N1	5.01	120.21	117.70
22	BA	1665	A	C8-N9-C4	5.01	107.81	105.80
22	BA	1932	A	C4-C5-C6	5.01	119.51	117.00
22	BA	2336	A	N9-C4-C5	5.01	107.81	105.80
22	BA	2810	A	C4-C5-N7	-5.01	108.19	110.70
54	D2	5	A	C4-C5-N7	-5.01	108.19	110.70
1	AA	1262	C	C6-N1-C2	-5.01	118.30	120.30
22	BA	89	A	C5-C6-N1	5.01	120.21	117.70
1	AA	58	C	C6-N1-C2	-5.01	118.30	120.30
1	AA	660	C	C5-C6-N1	5.01	123.51	121.00
22	BA	101	A	C5-C6-N1	5.01	120.21	117.70
22	BA	1129	A	N3-C4-N9	5.01	131.41	127.40
22	BA	1634	A	N9-C4-C5	5.01	107.81	105.80
22	BA	2173	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	2461	A	C8-N9-C4	5.01	107.80	105.80
22	BA	63	A	N9-C4-C5	5.01	107.80	105.80
22	BA	1366	A	C4-C5-N7	-5.01	108.19	110.70
22	BA	1791	A	N9-C4-C5	5.01	107.80	105.80
22	BA	1978	A	N3-C4-N9	5.01	131.41	127.40
23	BB	59	A	C5-C6-N1	5.01	120.20	117.70
22	BA	2448	A	C8-N9-C4	5.01	107.80	105.80
55	D3	73	A	C4-C5-N7	-5.01	108.20	110.70
55	D3	73	A	C5-C6-N1	5.01	120.20	117.70
22	BA	12	U	C2-N1-C1'	5.01	123.71	117.70
22	BA	1246	A	C8-N9-C4	5.01	107.80	105.80
22	BA	2171	A	N9-C4-C5	5.00	107.80	105.80
54	D2	31	A	N9-C4-C5	5.00	107.80	105.80
1	AA	95	C	C6-N1-C2	-5.00	118.30	120.30
22	BA	218	A	N3-C4-N9	5.00	131.40	127.40
22	BA	233	A	C5-C6-N1	5.00	120.20	117.70
22	BA	1096	A	N9-C4-C5	5.00	107.80	105.80
22	BA	1545	A	C8-N9-C4	5.00	107.80	105.80
22	BA	2577	A	C8-N9-C4	5.00	107.80	105.80
22	BA	2814	A	N9-C4-C5	5.00	107.80	105.80
23	BB	101	A	N9-C4-C5	5.00	107.80	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	109	A	C4-C5-N7	-5.00	108.20	110.70
22	BA	191	A	C5-C6-N1	5.00	120.20	117.70
22	BA	460	A	C8-N9-C4	5.00	107.80	105.80
22	BA	1508	A	C8-N9-C4	5.00	107.80	105.80
22	BA	1728	C	C6-N1-C2	-5.00	118.30	120.30
22	BA	2482	A	C8-N9-C4	5.00	107.80	105.80
22	BA	2736	A	C8-N9-C4	5.00	107.80	105.80
22	BA	2899	A	C5-C6-N1	5.00	120.20	117.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AC	60	PRO	Peptide
5	AE	89	HIS	Peptide
51	B3	31	HIS	Peptide
29	BH	41	LYS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16591	184	0
2	AB	1753	0	1780	19	0
3	AC	1624	0	1696	37	0
4	AD	1643	0	1707	19	0
5	AE	1144	0	1184	13	0
6	AF	862	0	864	13	0
7	AG	1181	0	1238	25	0
8	AH	979	0	1031	11	0
9	AI	1022	0	1070	24	0
10	AJ	795	0	836	21	0
11	AK	877	0	887	12	0
12	AL	957	0	1017	8	0
13	AM	883	0	941	66	0
14	AN	799	0	841	18	0
15	AO	714	0	734	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	AP	649	0	666	11	0
17	AQ	648	0	691	11	0
18	AR	455	0	478	11	0
19	AS	656	0	679	21	0
20	AT	670	0	719	4	0
21	AU	465	0	491	4	0
22	BA	62209	0	31307	228	0
23	BB	2569	0	1301	7	0
24	BC	2082	0	2154	13	0
25	BD	1566	0	1618	10	0
26	BE	1552	0	1619	13	0
27	BF	1410	0	1444	37	0
28	BG	1323	0	1371	12	0
29	BH	1110	0	1148	9	0
30	BI	522	0	522	15	0
31	BJ	1129	0	1162	4	0
32	BK	946	0	1023	4	0
33	BL	1053	0	1129	8	0
34	BM	1075	0	1155	9	0
35	BN	945	0	989	5	0
36	BO	900	0	935	1	0
37	BP	917	0	962	6	0
38	BQ	947	0	1019	4	0
39	BR	816	0	839	4	0
40	BS	857	0	922	6	0
41	BT	738	0	807	7	0
42	BU	779	0	831	4	0
43	BV	753	0	780	2	0
44	BW	580	0	594	0	0
45	BX	625	0	652	4	0
46	BY	501	0	531	8	0
47	BZ	449	0	488	3	0
48	B0	444	0	458	3	0
49	B1	414	0	442	2	0
50	B2	377	0	418	1	0
51	B3	504	0	572	8	0
52	B4	302	0	343	5	0
53	D1	57	0	59	7	0
54	D2	1634	0	842	18	0
55	D3	1604	0	817	29	0
56	D4	189	0	96	13	0
57	AA	35	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	BA	134	0	0	1	0
57	BC	1	0	0	0	0
57	BD	1	0	0	0	0
57	D2	1	0	0	0	0
58	BA	51	0	67	4	0
59	AA	166	0	0	4	0
59	AK	2	0	0	0	0
59	AM	1	0	0	0	0
59	AN	2	0	0	0	0
59	AQ	1	0	0	0	0
59	BA	614	0	0	4	0
59	BC	6	0	0	0	0
59	BD	3	0	0	0	0
59	BE	1	0	0	0	0
59	BJ	1	0	0	0	0
59	BL	1	0	0	0	0
59	BN	2	0	0	0	0
All	All	146607	0	97557	882	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (882) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:7:ILE:HD12	27:BF:112:ARG:CD	1.04	1.50
13:AM:7:ILE:CD1	27:BF:112:ARG:HD2	1.36	1.48
13:AM:7:ILE:CD1	27:BF:112:ARG:CD	1.89	1.44
13:AM:7:ILE:HD12	27:BF:112:ARG:CG	1.51	1.40
13:AM:43:VAL:CG1	13:AM:48:LEU:HD11	1.54	1.37
13:AM:7:ILE:CD1	27:BF:112:ARG:CG	2.08	1.30
13:AM:7:ILE:HD11	27:BF:112:ARG:HD2	1.24	1.19
13:AM:43:VAL:HG13	13:AM:48:LEU:HD11	1.28	1.14
13:AM:7:ILE:HD12	27:BF:112:ARG:HD3	1.29	1.14
13:AM:43:VAL:HG11	13:AM:48:LEU:HD11	1.30	1.13
1:AA:1493:A:H1'	56:D4:7:U:H5	1.13	1.12
19:AS:5:LEU:HD12	19:AS:7:LYS:H	1.05	1.07
13:AM:7:ILE:CD1	27:BF:112:ARG:HG2	1.80	1.07
13:AM:71:ARG:NH1	27:BF:115:ARG:HH22	1.54	1.04
1:AA:1493:A:H1'	56:D4:7:U:C5	1.93	1.04
1:AA:1076:U:OP1	2:AB:174:LYS:NZ	1.93	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:7:ILE:HD13	27:BF:112:ARG:CG	1.93	0.98
22:BA:2099:U:H3	22:BA:2190:G:H1	1.10	0.98
13:AM:43:VAL:CG1	13:AM:48:LEU:CD1	2.43	0.97
54:D2:15:G:H22	54:D2:48:C:H42	1.01	0.96
22:BA:881:G:H1	22:BA:895:U:H3	0.95	0.95
1:AA:458:U:O2	1:AA:474:G:N1	2.00	0.94
55:D3:35:A:N6	56:D4:2:U:O4	2.03	0.92
18:AR:34:THR:HG22	18:AR:35:GLU:H	1.35	0.90
16:AP:6:LEU:HD23	16:AP:19:VAL:HG12	1.50	0.90
1:AA:823:C:HO2'	8:AH:2:SER:N	1.67	0.90
19:AS:5:LEU:CD1	19:AS:7:LYS:H	1.84	0.90
13:AM:43:VAL:HG13	13:AM:48:LEU:CD1	2.00	0.90
1:AA:1009:U:H3	1:AA:1020:G:H1	1.18	0.87
19:AS:5:LEU:HD12	19:AS:7:LYS:N	1.89	0.86
15:AO:89:ARG:NH2	22:BA:712:G:O5'	2.08	0.86
54:D2:15:G:H22	54:D2:48:C:N4	1.74	0.86
54:D2:15:G:N2	54:D2:48:C:H42	1.74	0.85
13:AM:57:ARG:NH2	30:BI:35:ASP:OD1	2.10	0.83
13:AM:43:VAL:HG11	13:AM:48:LEU:CD1	2.07	0.83
1:AA:694:A:HO2'	55:D3:38:A:HO2'	1.06	0.82
58:BA:3001:ERY:O6	53:D1:3:LEU:O	1.97	0.81
13:AM:71:ARG:HH11	27:BF:115:ARG:HH22	1.27	0.80
19:AS:5:LEU:CD1	19:AS:7:LYS:HB2	2.12	0.79
22:BA:2099:U:O2	22:BA:2190:G:N2	2.14	0.79
13:AM:7:ILE:HD12	27:BF:112:ARG:HG2	1.50	0.77
1:AA:458:U:O2	1:AA:474:G:N2	2.17	0.76
13:AM:7:ILE:HD13	27:BF:112:ARG:HG2	1.54	0.76
1:AA:458:U:O2	1:AA:474:G:C2	2.39	0.75
13:AM:79:ARG:NH1	30:BI:56:ARG:HH21	1.84	0.75
1:AA:1305:G:H21	1:AA:1332:A:H2	1.35	0.74
3:AC:57:ILE:HG22	3:AC:66:VAL:HG23	1.69	0.74
55:D3:36:A:N1	56:D4:1:U:O4	2.21	0.74
13:AM:43:VAL:HG11	13:AM:48:LEU:HD21	1.68	0.74
13:AM:7:ILE:HD13	27:BF:112:ARG:CB	2.17	0.73
13:AM:79:ARG:CZ	30:BI:56:ARG:NH2	2.52	0.73
13:AM:71:ARG:NH1	27:BF:115:ARG:NH2	2.36	0.73
18:AR:34:THR:HG22	18:AR:35:GLU:N	2.02	0.73
13:AM:79:ARG:NH1	30:BI:56:ARG:NH2	2.38	0.72
22:BA:475:C:O2	22:BA:479:A:N6	2.24	0.70
1:AA:1073:U:O2'	2:AB:103:ASN:OD1	2.03	0.70
25:BD:13:ARG:HH12	37:BP:56:HIS:HA	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:33:THR:HG22	15:AO:63:ARG:HH11	1.57	0.70
55:D3:36:A:C2	56:D4:1:U:H5	2.09	0.70
16:AP:6:LEU:CD2	16:AP:19:VAL:HG12	2.21	0.70
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.56	0.69
19:AS:5:LEU:HD13	19:AS:7:LYS:HB2	1.74	0.69
1:AA:1076:U:P	2:AB:174:LYS:HZ1	2.13	0.69
1:AA:1078:U:H4'	5:AE:138:ARG:CZ	2.23	0.69
13:AM:43:VAL:HG21	13:AM:48:LEU:CD2	2.23	0.68
9:AI:130:ARG:NH2	54:D2:33:U:H5	1.91	0.68
1:AA:352:C:OP2	59:AA:1704:HOH:O	2.11	0.68
54:D2:37:T6A:H8	54:D2:37:T6A:H5''	1.58	0.68
55:D3:15:G:H3'	55:D3:16:H2U:H2'	1.76	0.68
1:AA:1055:A:O2'	3:AC:156:ARG:NH1	2.26	0.67
13:AM:8:ASN:HD22	13:AM:22:ILE:HA	1.60	0.67
4:AD:105:MET:HG2	4:AD:171:LEU:HD13	1.77	0.67
9:AI:130:ARG:NH2	54:D2:33:U:C5	2.63	0.67
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.75	0.67
13:AM:7:ILE:CD1	27:BF:112:ARG:CB	2.73	0.66
55:D3:15:G:H5'	55:D3:16:H2U:H62	1.78	0.65
6:AF:29:ILE:HD13	6:AF:64:VAL:HG11	1.79	0.65
22:BA:2821:A:OP2	57:BA:3109:MG:MG	1.40	0.65
22:BA:2134:A:OP2	22:BA:2157:G:N2	2.30	0.65
6:AF:90:MET:SD	18:AR:61:ARG:NH1	2.71	0.64
1:AA:1009:U:O2	1:AA:1020:G:N2	2.27	0.64
1:AA:1229:A:OP2	13:AM:113:ARG:NH1	2.30	0.64
33:BL:109:LYS:HG2	33:BL:126:ARG:HB2	1.79	0.64
7:AG:148:ASN:O	7:AG:148:ASN:ND2	2.30	0.64
1:AA:1086:U:H2'	1:AA:1087:G:H8	1.63	0.64
1:AA:212:G:H2'	1:AA:213:G:H8	1.63	0.63
5:AE:55:GLU:HG3	5:AE:57:PRO:HD2	1.80	0.63
22:BA:2114:A:H61	22:BA:2119:A:H62	1.46	0.63
55:D3:55:PSU:HN1	55:D3:57:G:H5''	1.62	0.63
1:AA:352:C:OP2	57:AA:1608:MG:MG	1.41	0.63
1:AA:429:U:H5'	4:AD:9:LEU:HD11	1.81	0.63
16:AP:6:LEU:HD23	16:AP:19:VAL:CG1	2.27	0.63
22:BA:2760:C:H1'	28:BG:139:GLN:HE22	1.61	0.63
9:AI:123:ARG:NH1	9:AI:124:ARG:O	2.32	0.63
29:BH:84:ALA:HB2	29:BH:90:LEU:HD23	1.81	0.62
1:AA:1086:U:H2'	1:AA:1087:G:C8	2.34	0.62
22:BA:585:G:N7	38:BQ:6:ARG:NH1	2.47	0.62
13:AM:57:ARG:NH2	30:BI:35:ASP:CG	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:89:ARG:NH2	22:BA:712:G:P	2.73	0.62
55:D3:34:G:O6	56:D4:3:C:N3	2.32	0.62
1:AA:1103:C:OP1	2:AB:95:ARG:NH2	2.32	0.62
4:AD:129:VAL:HG21	4:AD:146:ARG:HH21	1.65	0.62
13:AM:9:ILE:HG21	27:BF:143:TYR:HE2	1.64	0.62
22:BA:652:U:OP1	22:BA:654:A:N6	2.31	0.62
1:AA:110:C:O2'	16:AP:25:ARG:O	2.18	0.62
4:AD:100:ASN:OD1	4:AD:111:ARG:NH1	2.33	0.62
6:AF:86:ARG:NH1	18:AR:64:TYR:O	2.33	0.62
55:D3:51:U:O4	55:D3:63:G:O6	2.18	0.62
1:AA:1012:A:OP2	19:AS:17:LYS:NZ	2.33	0.61
13:AM:79:ARG:NH2	30:BI:56:ARG:NH2	2.48	0.61
1:AA:208:U:N3	1:AA:211:G:N1	2.47	0.61
7:AG:151:PHE:CZ	11:AK:56:ARG:HG2	2.36	0.61
7:AG:79:ARG:CG	7:AG:79:ARG:HH21	2.13	0.61
1:AA:1363:A:O2'	1:AA:1365:G:N7	2.29	0.61
17:AQ:68:SER:OG	17:AQ:69:LYS:N	2.32	0.61
19:AS:5:LEU:HD13	19:AS:7:LYS:HE2	1.82	0.61
1:AA:694:A:O2'	55:D3:38:A:O2'	1.92	0.61
3:AC:83:ASP:O	3:AC:87:LEU:N	2.33	0.61
4:AD:102:VAL:HG23	4:AD:114:ALA:HB1	1.83	0.61
13:AM:43:VAL:CG2	13:AM:48:LEU:HG	2.30	0.61
8:AH:43:GLU:HG3	8:AH:101:ILE:HD13	1.83	0.60
22:BA:2365:G:N7	51:B3:39:LYS:NZ	2.45	0.60
41:BT:11:LEU:O	46:BY:29:ARG:NH2	2.34	0.60
13:AM:4:ILE:HG22	13:AM:60:VAL:HG11	1.83	0.60
22:BA:2107:G:H1	22:BA:2182:U:H3	1.48	0.60
24:BC:262:ARG:O	24:BC:265:LYS:NZ	2.33	0.60
22:BA:2469:A:N6	22:BA:2481:G:O2'	2.34	0.60
55:D3:62:C:H2'	55:D3:63:G:H8	1.67	0.60
1:AA:958:A:OP1	19:AS:55:ARG:NH2	2.32	0.60
34:BM:50:ARG:HG3	34:BM:65:ILE:HD11	1.83	0.60
1:AA:411:A:H4'	1:AA:412:A:H5'	1.83	0.60
1:AA:1144:G:H21	1:AA:1146:A:H62	1.49	0.60
6:AF:30:THR:HA	6:AF:34:GLY:H	1.67	0.60
9:AI:17:ALA:HB2	9:AI:67:VAL:HG12	1.82	0.60
5:AE:105:ILE:O	5:AE:112:ARG:NH2	2.34	0.59
10:AJ:28:THR:O	10:AJ:32:THR:OG1	2.16	0.59
13:AM:43:VAL:HG22	13:AM:48:LEU:HG	1.84	0.59
22:BA:1174:U:O2	22:BA:1177:G:N1	2.33	0.59
2:AB:43:LEU:HA	2:AB:46:THR:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:84:THR:HG21	9:AI:103:PHE:HB3	1.85	0.59
23:BB:43:C:O2	27:BF:92:ARG:NH2	2.36	0.59
1:AA:1073:U:O2	2:AB:103:ASN:ND2	2.35	0.59
13:AM:71:ARG:HH12	27:BF:115:ARG:HH22	1.45	0.59
13:AM:43:VAL:HG11	13:AM:48:LEU:CD2	2.33	0.59
22:BA:2848:G:O2'	22:BA:2867:G:N2	2.32	0.59
13:AM:43:VAL:HG21	13:AM:48:LEU:HD21	1.83	0.59
52:B4:2:LYS:NZ	52:B4:32:LYS:O	2.36	0.59
1:AA:1005:A:N7	1:AA:1024:G:O2'	2.36	0.59
9:AI:18:ARG:NH1	9:AI:18:ARG:HG3	2.16	0.59
22:BA:2523:G:HO2'	22:BA:2764:A:HO2'	1.51	0.59
9:AI:128:SER:OG	9:AI:130:ARG:O	2.20	0.58
22:BA:1779:U:OP2	22:BA:1784:A:N6	2.35	0.58
55:D3:6:G:N2	55:D3:68:C:O2	2.36	0.58
22:BA:877:A:O2'	22:BA:900:A:N6	2.36	0.58
25:BD:181:ASP:HB3	25:BD:186:LEU:HB2	1.85	0.58
28:BG:27:LYS:HG2	28:BG:32:GLU:HG3	1.84	0.58
6:AF:37:HIS:HB3	6:AF:97:THR:HG22	1.85	0.58
14:AN:19:TYR:O	14:AN:23:ARG:N	2.31	0.58
53:D1:4:ILE:HG13	53:D1:4:ILE:O	2.03	0.58
1:AA:1081:A:OP1	5:AE:23:LYS:HB2	2.03	0.58
22:BA:1007:C:OP1	31:BJ:37:ARG:NH2	2.36	0.58
22:BA:2511:U:O4	22:BA:2575:C:N3	2.36	0.58
1:AA:202:G:O2'	1:AA:467:U:O4	2.21	0.58
3:AC:57:ILE:CG2	3:AC:66:VAL:HG23	2.32	0.58
10:AJ:83:THR:O	10:AJ:87:LEU:N	2.37	0.58
14:AN:47:LYS:O	14:AN:50:THR:OG1	2.19	0.58
1:AA:210:C:O2	1:AA:211:G:N1	2.36	0.57
1:AA:264:C:O3'	17:AQ:65:ARG:NH1	2.37	0.57
13:AM:67:GLY:HA3	27:BF:113:ASP:OD2	2.04	0.57
7:AG:129:GLU:O	7:AG:131:LYS:NZ	2.36	0.57
8:AH:74:SER:HB3	8:AH:130:ALA:HB3	1.86	0.57
9:AI:14:SER:O	9:AI:14:SER:OG	2.22	0.57
28:BG:22:GLN:NE2	28:BG:38:ASN:O	2.37	0.57
1:AA:683:G:N2	11:AK:39:GLY:O	2.37	0.57
1:AA:445:G:H1	1:AA:489:C:H5	1.53	0.57
7:AG:68:ASN:O	7:AG:138:ARG:NH1	2.38	0.57
9:AI:18:ARG:HG3	9:AI:18:ARG:HH11	1.70	0.57
9:AI:130:ARG:HD3	54:D2:35:A:OP1	2.05	0.57
3:AC:7:PRO:O	3:AC:11:ARG:NH1	2.38	0.57
20:AT:81:ALA:O	20:AT:85:LYS:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2796:U:H2'	22:BA:2797:U:H2'	1.87	0.56
21:AU:31:GLU:HG3	21:AU:35:ARG:HE	1.70	0.56
22:BA:568:U:H1'	22:BA:2030:6MZ:H9C1	1.86	0.56
22:BA:2467:C:O2	34:BM:123:LYS:NZ	2.36	0.56
1:AA:718:A:O2'	21:AU:35:ARG:NH2	2.39	0.56
13:AM:9:ILE:HG12	27:BF:143:TYR:CE2	2.40	0.56
32:BK:88:ASN:ND2	32:BK:90:ASN:OD1	2.38	0.56
8:AH:77:ARG:NH1	8:AH:79:SER:O	2.39	0.56
10:AJ:45:ARG:NH2	10:AJ:47:GLU:OE1	2.38	0.56
22:BA:1392:A:N6	41:BT:18:GLU:OE1	2.38	0.56
26:BE:189:THR:HG22	26:BE:191:ASP:H	1.70	0.56
55:D3:51:U:H3	55:D3:63:G:H1	0.86	0.56
55:D3:16:H2U:HN3	55:D3:60:U:H1'	1.71	0.56
22:BA:882:G:N2	22:BA:883:G:N7	2.54	0.56
1:AA:500:G:H5''	12:AL:121:ARG:HH12	1.70	0.56
22:BA:2478:A:H5'	52:B4:32:LYS:HE2	1.88	0.56
22:BA:2131:U:H5'	22:BA:2132:U:H5''	1.88	0.56
22:BA:881:G:O6	22:BA:895:U:O4	2.24	0.56
22:BA:627:A:OP1	33:BL:78:ARG:NH1	2.39	0.55
1:AA:352:C:OP2	59:AA:1706:HOH:O	2.18	0.55
1:AA:929:G:C2	1:AA:1389:C:O2	2.60	0.55
5:AE:13:GLU:OE2	5:AE:68:ARG:NH2	2.39	0.55
22:BA:1607:C:N4	22:BA:1622:G:OP2	2.38	0.55
46:BY:49:ASP:OD1	46:BY:52:ARG:NH2	2.38	0.55
1:AA:1308:U:H2'	1:AA:1309:G:H8	1.71	0.55
15:AO:64:ARG:HH12	15:AO:88:ARG:HD3	1.70	0.55
22:BA:2821:A:OP2	35:BN:3:HIS:NE2	2.40	0.55
3:AC:34:ASP:OD2	14:AN:65:ARG:NH1	2.39	0.55
22:BA:281:C:H2'	22:BA:282:A:H8	1.71	0.55
1:AA:1391:U:H2'	1:AA:1392:G:H8	1.71	0.55
1:AA:976:G:OP2	1:AA:1358:U:O2'	2.24	0.55
1:AA:1291:U:H2'	1:AA:1292:G:H8	1.72	0.55
22:BA:404:A:N6	22:BA:421:C:O2'	2.40	0.55
22:BA:2109:U:OP1	22:BA:2149:U:O2'	2.24	0.55
25:BD:46:ARG:NH2	25:BD:88:GLU:O	2.39	0.55
13:AM:79:ARG:CZ	30:BI:56:ARG:HH21	2.16	0.55
27:BF:102:ARG:HG2	30:BI:24:ILE:HD12	1.88	0.55
54:D2:15:G:O6	54:D2:48:C:O2	2.25	0.55
55:D3:36:A:C2	56:D4:1:U:C5	2.94	0.55
22:BA:994:C:O2	39:BR:10:LYS:NZ	2.38	0.54
22:BA:2515:C:H2'	22:BA:2516:A:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BD:39:ASP:N	25:BD:39:ASP:OD1	2.41	0.54
9:AI:12:ARG:HG3	9:AI:13:LYS:H	1.72	0.54
14:AN:83:LYS:NZ	14:AN:86:GLU:OE1	2.39	0.54
28:BG:104:ASN:ND2	28:BG:114:ASP:OD1	2.41	0.54
40:BS:73:LYS:HB2	40:BS:106:VAL:HB	1.88	0.54
14:AN:26:LEU:HD23	14:AN:48:LEU:HD13	1.87	0.54
54:D2:51:A:H61	54:D2:63:C:H42	1.54	0.54
18:AR:34:THR:CG2	18:AR:35:GLU:H	2.14	0.54
22:BA:2278:A:OP1	34:BM:10:ARG:NH2	2.40	0.54
7:AG:151:PHE:CE1	11:AK:56:ARG:HG2	2.43	0.54
1:AA:464:U:N3	1:AA:466:A:OP2	2.41	0.54
7:AG:84:THR:HG21	55:D3:32:PSU:O2'	2.07	0.54
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.89	0.54
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.89	0.54
17:AQ:47:HIS:NE2	17:AQ:49:GLU:OE1	2.40	0.54
36:BO:31:THR:O	36:BO:102:ARG:NH1	2.33	0.54
3:AC:66:VAL:CG1	3:AC:101:ILE:HD13	2.38	0.54
5:AE:157:ARG:NH2	8:AH:99:LEU:O	2.41	0.54
7:AG:57:SER:O	7:AG:61:ALA:N	2.33	0.54
22:BA:880:G:H2'	22:BA:881:G:H8	1.72	0.54
1:AA:87:C:H2'	1:AA:88:U:H4'	1.90	0.54
22:BA:2267:A:H5''	22:BA:2268:A:H5'	1.89	0.54
1:AA:85:U:OP2	1:AA:86:G:N2	2.38	0.53
1:AA:1027:C:N3	1:AA:1028:C:N4	2.56	0.53
27:BF:105:THR:HA	30:BI:38:SER:HB2	1.90	0.53
10:AJ:63:ASP:OD2	14:AN:85:ARG:NH1	2.42	0.53
28:BG:107:LEU:O	28:BG:152:ARG:NH2	2.36	0.53
4:AD:54:GLN:HG2	4:AD:199:LEU:HD22	1.91	0.53
13:AM:54:ASP:HA	13:AM:57:ARG:HD2	1.89	0.53
22:BA:2608:G:C6	53:D1:1:FME:HCN	2.43	0.53
1:AA:147:G:H2'	1:AA:148:G:C8	2.44	0.53
22:BA:275:C:H2'	22:BA:276:U:H4'	1.91	0.53
22:BA:2106:U:H2'	22:BA:2107:G:H8	1.74	0.53
22:BA:2756:U:OP2	52:B4:19:ARG:NE	2.39	0.53
55:D3:15:G:H5'	55:D3:16:H2U:H2'	1.90	0.53
3:AC:177:THR:O	3:AC:177:THR:OG1	2.26	0.53
16:AP:44:SER:O	16:AP:44:SER:OG	2.27	0.53
22:BA:1:G:H2'	22:BA:2:G:H8	1.74	0.53
1:AA:426:U:OP1	4:AD:36:GLN:NE2	2.42	0.52
10:AJ:35:GLN:N	10:AJ:78:GLU:OE1	2.41	0.52
19:AS:5:LEU:CD1	19:AS:7:LYS:N	2.61	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:17:U:O4'	1:AA:1080:A:H1'	2.09	0.52
1:AA:673:A:H2'	1:AA:674:G:C8	2.45	0.52
1:AA:1074:G:H4'	2:AB:102:THR:O	2.09	0.52
11:AK:23:ILE:HD11	11:AK:86:VAL:HG22	1.91	0.52
19:AS:12:ASP:OD1	19:AS:38:SER:OG	2.26	0.52
24:BC:260:ASN:ND2	24:BC:263:THR:OG1	2.37	0.52
1:AA:157:U:O2	1:AA:164:G:O6	2.28	0.52
22:BA:2608:G:O6	53:D1:1:FME:HCN	2.09	0.52
42:BU:4:LYS:O	42:BU:94:ARG:NH2	2.43	0.52
1:AA:486:U:H2'	1:AA:487:A:H8	1.75	0.52
27:BF:140:GLU:HA	30:BI:28:VAL:HG12	1.90	0.52
1:AA:108:G:H5'	1:AA:109:A:H5''	1.92	0.52
7:AG:63:GLU:OE2	7:AG:70:ARG:NH2	2.34	0.52
13:AM:9:ILE:HD13	27:BF:143:TYR:OH	2.10	0.52
23:BB:1:U:H2'	23:BB:2:G:H8	1.73	0.52
37:BP:88:ARG:NH2	37:BP:110:ILE:O	2.39	0.52
3:AC:114:LYS:NZ	3:AC:187:SER:OG	2.43	0.52
22:BA:864:G:O2'	22:BA:914:G:O6	2.26	0.52
18:AR:34:THR:CG2	18:AR:35:GLU:N	2.73	0.52
22:BA:2532:G:N2	22:BA:2663:G:O2'	2.43	0.52
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.45	0.52
2:AB:214:LEU:HA	2:AB:217:VAL:HG12	1.92	0.52
28:BG:17:VAL:HG11	28:BG:50:LEU:HD21	1.92	0.52
1:AA:1297:G:O2'	7:AG:114:LYS:NZ	2.43	0.51
6:AF:14:GLN:HG3	6:AF:17:GLN:HG3	1.91	0.51
16:AP:50:THR:HG23	16:AP:50:THR:O	2.09	0.51
22:BA:619:G:OP2	22:BA:620:G:N2	2.43	0.51
22:BA:1365:A:OP1	45:BX:3:ARG:NH2	2.37	0.51
24:BC:162:VAL:HG11	24:BC:174:LEU:HD13	1.91	0.51
1:AA:1071:C:H2'	1:AA:1072:G:H8	1.76	0.51
3:AC:148:GLY:HA3	3:AC:172:ARG:H	1.75	0.51
9:AI:18:ARG:HH11	9:AI:18:ARG:CG	2.24	0.51
1:AA:858:G:O6	59:AA:1705:HOH:O	2.18	0.51
22:BA:1801:A:OP2	24:BC:150:LYS:NZ	2.41	0.51
22:BA:1469:A:H2'	22:BA:1470:A:C8	2.45	0.51
22:BA:444:C:OP1	26:BE:40:ARG:NH2	2.44	0.51
1:AA:108:G:C6	20:AT:10:ARG:HG2	2.45	0.51
22:BA:589:U:H2'	22:BA:590:A:H8	1.75	0.51
31:BJ:32:LEU:HD22	31:BJ:54:ILE:HG21	1.92	0.51
1:AA:494:G:H2'	1:AA:496:A:H8	1.76	0.51
1:AA:1390:U:H6	1:AA:1390:U:O5'	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:70:THR:HG22	3:AC:72:ARG:H	1.75	0.51
13:AM:106:ALA:HB3	13:AM:110:LYS:HD3	1.93	0.51
55:D3:36:A:N1	56:D4:1:U:C4	2.78	0.51
13:AM:7:ILE:HG21	27:BF:112:ARG:HG2	1.92	0.51
59:BA:3213:HOH:O	53:D1:1:FME:CE	2.58	0.51
1:AA:208:U:O4	1:AA:211:G:N2	2.44	0.51
14:AN:15:LEU:HD23	14:AN:54:ASP:HB2	1.94	0.50
27:BF:8:TYR:HA	27:BF:12:VAL:HB	1.93	0.50
46:BY:16:THR:O	46:BY:20:ASN:ND2	2.44	0.50
12:AL:68:GLY:O	12:AL:99:ARG:NH1	2.42	0.50
22:BA:24:G:O2'	40:BS:78:GLU:O	2.29	0.50
23:BB:1:U:H2'	23:BB:2:G:C8	2.46	0.50
26:BE:111:GLU:OE1	26:BE:114:ARG:NH1	2.44	0.50
54:D2:21:A:N6	54:D2:46:G7M:O2'	2.41	0.50
3:AC:156:ARG:H	3:AC:163:ALA:HA	1.76	0.50
1:AA:1078:U:O4'	5:AE:89:HIS:HE1	1.94	0.50
22:BA:196:A:OP2	33:BL:47:ARG:NH1	2.43	0.50
22:BA:617:G:OP1	26:BE:102:ARG:NH2	2.40	0.50
22:BA:1068:G:N2	22:BA:1095:A:O3'	2.40	0.50
14:AN:24:ALA:O	14:AN:28:ALA:N	2.45	0.50
26:BE:148:ILE:HB	26:BE:169:VAL:HG22	1.94	0.50
22:BA:1799:G:OP1	24:BC:258:ARG:NH1	2.35	0.50
42:BU:47:LYS:HD3	42:BU:48:PRO:HD2	1.94	0.50
12:AL:109:ASP:OD1	12:AL:109:ASP:N	2.40	0.50
26:BE:51:GLU:OE2	26:BE:88:ARG:NH1	2.45	0.50
45:BX:72:ARG:NH1	45:BX:78:TYR:OH	2.43	0.50
1:AA:626:G:O2'	16:AP:51:ARG:NH2	2.41	0.50
5:AE:115:LEU:HD13	5:AE:123:VAL:HG21	1.93	0.50
19:AS:25:SER:HB2	19:AS:28:LYS:HZ1	1.77	0.50
46:BY:3:ALA:HB2	46:BY:52:ARG:HD3	1.93	0.50
5:AE:13:GLU:HG2	5:AE:39:VAL:HG12	1.92	0.49
7:AG:76:LYS:HD2	7:AG:77:SER:H	1.77	0.49
11:AK:87:LYS:HE3	11:AK:113:VAL:HG13	1.95	0.49
19:AS:5:LEU:HD12	19:AS:5:LEU:C	2.32	0.49
22:BA:2720:U:OP1	37:BP:53:ARG:NH2	2.45	0.49
1:AA:1144:G:N2	1:AA:1146:A:H62	2.10	0.49
3:AC:57:ILE:HG22	3:AC:66:VAL:CG2	2.40	0.49
55:D3:36:A:N1	56:D4:1:U:C5	2.80	0.49
1:AA:713:G:H2'	1:AA:714:G:C8	2.47	0.49
1:AA:1526:G:OP1	21:AU:45:ARG:NH2	2.45	0.49
9:AI:80:ARG:O	9:AI:84:THR:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:83:ASP:HA	3:AC:86:LYS:HB3	1.94	0.49
22:BA:1432:G:H2'	22:BA:1433:A:C8	2.47	0.49
24:BC:66:ASP:OD2	24:BC:102:ARG:NH1	2.46	0.49
40:BS:33:LEU:O	40:BS:37:THR:OG1	2.29	0.49
1:AA:1037:C:H2'	1:AA:1038:C:H6	1.78	0.49
8:AH:54:ASP:OD1	8:AH:54:ASP:N	2.36	0.49
10:AJ:81:GLU:O	10:AJ:84:VAL:N	2.44	0.49
13:AM:43:VAL:CG1	13:AM:48:LEU:CG	2.90	0.49
41:BT:13:ALA:HB3	41:BT:33:LYS:HE3	1.95	0.49
4:AD:172:GLU:HB2	4:AD:181:THR:HB	1.95	0.49
10:AJ:45:ARG:HB3	10:AJ:69:THR:HG23	1.94	0.49
22:BA:1028:A:H2'	22:BA:1029:A:C8	2.48	0.49
22:BA:1434:A:H2'	22:BA:1435:G:C8	2.47	0.49
22:BA:1568:G:H4'	24:BC:59:LYS:HB3	1.95	0.49
1:AA:618:C:H1'	16:AP:14:ARG:HH12	1.77	0.49
22:BA:281:C:H2'	22:BA:282:A:C8	2.48	0.49
58:BA:3001:ERY:O10	58:BA:3001:ERY:H11	2.13	0.49
34:BM:42:THR:HG22	34:BM:93:VAL:HG12	1.93	0.49
52:B4:16:ILE:HG12	52:B4:25:VAL:HG22	1.95	0.49
2:AB:32:PHE:HE2	2:AB:35:ARG:HH12	1.60	0.49
11:AK:23:ILE:HG13	11:AK:86:VAL:HA	1.95	0.49
14:AN:39:GLU:O	14:AN:43:ASN:HB2	2.12	0.49
22:BA:195:A:H61	22:BA:198:C:H3'	1.77	0.49
22:BA:631:A:OP2	51:B3:23:LYS:NZ	2.45	0.49
22:BA:2502:G:H5''	22:BA:2503:2MA:H5''	1.95	0.49
1:AA:208:U:C4	1:AA:211:G:N1	2.81	0.49
1:AA:532:A:C6	3:AC:193:TYR:HE1	2.30	0.49
13:AM:107:ARG:NH1	13:AM:111:GLY:O	2.46	0.49
22:BA:856:G:H2'	22:BA:857:G:C8	2.47	0.49
22:BA:2306:C:N4	27:BF:39:GLY:O	2.41	0.49
13:AM:43:VAL:HG11	13:AM:48:LEU:CG	2.43	0.49
19:AS:6:LYS:HD2	19:AS:6:LYS:HA	1.59	0.49
1:AA:1097:C:O3'	2:AB:139:ARG:NH2	2.45	0.48
12:AL:53:CYS:HB2	12:AL:67:ILE:HD11	1.94	0.48
22:BA:280:U:O4	22:BA:361:G:N2	2.46	0.48
22:BA:1636:U:H2'	22:BA:1637:A:C8	2.49	0.48
1:AA:1060:U:OP1	14:AN:85:ARG:NH2	2.46	0.48
22:BA:151:C:H2'	22:BA:152:A:H8	1.78	0.48
22:BA:1316:U:H2'	22:BA:1317:G:H8	1.78	0.48
22:BA:2134:A:O2'	22:BA:2159:G:N3	2.44	0.48
1:AA:208:U:N3	1:AA:211:G:C6	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:208:U:C2	1:AA:211:G:O6	2.65	0.48
15:AO:89:ARG:NH1	22:BA:713:G:N7	2.61	0.48
20:AT:44:LYS:HB3	20:AT:87:ALA:HB3	1.94	0.48
19:AS:12:ASP:OD1	19:AS:12:ASP:N	2.44	0.48
22:BA:1173:U:O2'	22:BA:1174:U:O4'	2.30	0.48
1:AA:1175:G:H2'	1:AA:1176:A:H8	1.77	0.48
22:BA:2172:U:H4'	22:BA:2173:A:H5'	1.96	0.48
32:BK:23:LYS:HB3	32:BK:40:LYS:HB3	1.95	0.48
25:BD:25:THR:OG1	25:BD:191:GLY:O	2.30	0.48
1:AA:946:A:H2'	1:AA:947:G:C8	2.49	0.48
3:AC:14:ILE:HG22	3:AC:15:VAL:HG23	1.94	0.48
24:BC:155:ALA:HB2	24:BC:162:VAL:HG23	1.95	0.48
1:AA:490:C:H2'	1:AA:491:G:H8	1.79	0.48
13:AM:66:GLU:HG3	13:AM:67:GLY:H	1.79	0.48
25:BD:49:GLN:HE21	25:BD:79:LEU:HB3	1.77	0.48
1:AA:259:G:OP1	20:AT:36:TYR:OH	2.25	0.48
3:AC:132:ARG:HA	3:AC:135:LYS:HG2	1.95	0.48
22:BA:1386:C:H2'	22:BA:1387:A:C8	2.49	0.48
23:BB:79:G:N7	43:BV:14:LYS:NZ	2.58	0.48
28:BG:42:GLU:HA	28:BG:55:ARG:HH21	1.78	0.48
1:AA:6:G:HO2'	1:AA:7:A:H8	1.61	0.48
22:BA:172:A:H2'	22:BA:173:A:C8	2.49	0.48
22:BA:414:C:H2'	22:BA:415:A:C8	2.48	0.48
22:BA:463:G:N2	22:BA:466:A:OP2	2.39	0.48
22:BA:687:C:H1'	50:B2:4:THR:HG22	1.96	0.48
25:BD:184:ARG:HG3	25:BD:186:LEU:HG	1.94	0.48
27:BF:103:LEU:HA	27:BF:107:ALA:HB3	1.96	0.48
34:BM:64:TRP:HB2	34:BM:104:GLU:HB2	1.95	0.48
47:BZ:4:THR:HG21	47:BZ:37:GLU:HG3	1.95	0.48
7:AG:40:GLU:HA	7:AG:43:VAL:HG12	1.96	0.47
22:BA:2233:U:H2'	22:BA:2234:G:C8	2.49	0.47
29:BH:78:VAL:HG23	29:BH:144:VAL:HG23	1.95	0.47
22:BA:2305:U:H5''	27:BF:131:GLY:HA3	1.96	0.47
29:BH:116:ARG:HD3	29:BH:133:GLN:HG2	1.97	0.47
1:AA:664:G:H22	1:AA:741:G:H1	1.61	0.47
1:AA:486:U:H2'	1:AA:487:A:C8	2.49	0.47
18:AR:41:PRO:HG2	18:AR:44:ILE:HG12	1.96	0.47
22:BA:1791:A:N6	22:BA:1828:G:O2'	2.43	0.47
22:BA:2106:U:H2'	22:BA:2107:G:C8	2.49	0.47
22:BA:2183:A:H2'	22:BA:2184:A:C8	2.49	0.47
23:BB:5:U:OP1	23:BB:61:G:O2'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1213:A:O2'	1:AA:1215:G:N7	2.39	0.47
12:AL:114:ARG:HB2	12:AL:119:VAL:HB	1.96	0.47
13:AM:71:ARG:HH12	27:BF:115:ARG:NH2	2.07	0.47
22:BA:414:C:H2'	22:BA:415:A:H8	1.79	0.47
22:BA:2291:U:H2'	22:BA:2292:U:C6	2.49	0.47
46:BY:56:LEU:HA	46:BY:59:GLU:HG2	1.95	0.47
1:AA:216:U:H2'	1:AA:217:C:C6	2.49	0.47
1:AA:1005:A:H3'	1:AA:1006:G:H8	1.79	0.47
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.49	0.47
1:AA:1493:A:H4'	56:D4:7:U:H6	1.79	0.47
1:AA:17:U:C1'	1:AA:1080:A:H1'	2.44	0.47
1:AA:79:G:H2'	1:AA:80:A:H8	1.79	0.47
1:AA:865:A:H5'	1:AA:1078:U:O4	2.14	0.47
5:AE:34:THR:HG22	5:AE:52:LYS:HG2	1.97	0.47
22:BA:1796:U:H2'	22:BA:1797:G:H8	1.79	0.47
22:BA:1864:U:OP1	22:BA:2410:G:O2'	2.28	0.47
22:BA:2547:A:H2'	22:BA:2548:U:C6	2.50	0.47
24:BC:157:SER:OG	24:BC:158:ALA:N	2.48	0.47
26:BE:16:GLU:O	26:BE:20:GLY:N	2.47	0.47
43:BV:40:ILE:HD12	43:BV:42:LEU:HD21	1.96	0.47
54:D2:15:G:N1	54:D2:48:C:N3	2.45	0.47
55:D3:8:4SU:HN3	55:D3:14:A:H62	1.62	0.47
3:AC:63:SER:OG	3:AC:64:ILE:N	2.48	0.47
9:AI:30:ILE:HG23	9:AI:65:ILE:HB	1.96	0.47
42:BU:88:GLU:HG2	42:BU:93:VAL:HG11	1.97	0.47
55:D3:16:H2U:H4'	55:D3:18:G:OP2	2.15	0.47
4:AD:95:GLU:HA	4:AD:100:ASN:ND2	2.30	0.47
22:BA:155:A:H2'	22:BA:156:A:C8	2.50	0.47
22:BA:249:C:O2	51:B3:12:LYS:NZ	2.47	0.47
22:BA:1592:C:H2'	22:BA:1593:A:C8	2.49	0.47
38:BQ:97:ASP:OD2	39:BR:13:ARG:NH2	2.40	0.47
41:BT:54:GLU:HB3	41:BT:88:LYS:HD2	1.97	0.47
49:B1:11:LEU:HB3	49:B1:49:TYR:HB3	1.96	0.47
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.50	0.47
14:AN:63:ARG:NH1	14:AN:68:GLY:O	2.47	0.47
22:BA:1667:G:O2'	22:BA:1991:U:O4	2.26	0.47
22:BA:2127:G:H2'	22:BA:2128:G:C8	2.50	0.47
42:BU:28:VAL:HG22	42:BU:34:VAL:HG12	1.97	0.47
3:AC:22:TRP:NE1	3:AC:36:ASP:OD2	2.46	0.46
8:AH:40:LEU:HD21	8:AH:129:VAL:HG21	1.97	0.46
19:AS:6:LYS:HZ2	30:BI:63:ARG:HD3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:674:G:H1'	26:BE:69:ARG:HD3	1.96	0.46
24:BC:5:LYS:HG3	24:BC:17:VAL:HG22	1.96	0.46
24:BC:133:ARG:HB3	24:BC:186:ALA:HB1	1.97	0.46
38:BQ:50:ARG:O	38:BQ:54:LYS:NZ	2.46	0.46
1:AA:382:A:H2'	1:AA:383:A:C8	2.50	0.46
1:AA:481:G:O2'	1:AA:483:C:N4	2.45	0.46
1:AA:1106:G:H2'	1:AA:1107:C:C6	2.50	0.46
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.96	0.46
22:BA:597:G:O2'	33:BL:11:GLY:O	2.26	0.46
22:BA:2246:G:H2'	22:BA:2247:A:C8	2.50	0.46
29:BH:68:ARG:HD3	29:BH:134:VAL:HG21	1.98	0.46
1:AA:1124:G:H5''	10:AJ:37:ARG:HD2	1.96	0.46
3:AC:138:VAL:HG21	3:AC:168:TYR:HD2	1.80	0.46
4:AD:8:LYS:HG2	4:AD:21:LEU:HD12	1.98	0.46
7:AG:78:ARG:NH1	7:AG:87:VAL:HG21	2.30	0.46
22:BA:545:U:O2'	22:BA:546:U:O4'	2.34	0.46
22:BA:917:A:H5''	22:BA:2268:A:H61	1.80	0.46
22:BA:1434:A:H2'	22:BA:1435:G:H8	1.80	0.46
52:B4:15:LYS:HB3	52:B4:15:LYS:HE2	1.70	0.46
1:AA:920:U:O4'	1:AA:1080:A:N1	2.49	0.46
8:AH:22:LYS:O	8:AH:65:TYR:OH	2.23	0.46
13:AM:66:GLU:O	13:AM:69:LEU:N	2.48	0.46
22:BA:589:U:H2'	22:BA:590:A:C8	2.50	0.46
22:BA:1476:U:H2'	22:BA:1477:A:H8	1.80	0.46
4:AD:167:LYS:HA	4:AD:167:LYS:HD3	1.67	0.46
22:BA:288:U:H2'	22:BA:289:G:H8	1.81	0.46
1:AA:204:G:H2'	1:AA:205:A:C4	2.51	0.46
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.48	0.46
7:AG:79:ARG:CG	7:AG:79:ARG:NH2	2.73	0.46
22:BA:2167:U:N3	22:BA:2170:A:OP2	2.43	0.46
28:BG:47:ASP:OD1	28:BG:47:ASP:N	2.49	0.46
1:AA:1078:U:C6	5:AE:90:THR:HG21	2.50	0.46
8:AH:90:ASP:OD1	8:AH:90:ASP:N	2.36	0.46
10:AJ:80:THR:O	10:AJ:83:THR:OG1	2.24	0.46
17:AQ:54:GLY:N	17:AQ:57:ASP:OD2	2.48	0.46
22:BA:1:G:H2'	22:BA:2:G:C8	2.49	0.46
22:BA:639:U:H2'	22:BA:640:C:C6	2.50	0.46
22:BA:659:G:O2'	26:BE:95:LYS:O	2.33	0.46
22:BA:1156:A:C8	38:BQ:51:ARG:HG2	2.51	0.46
27:BF:44:ILE:HG21	27:BF:79:ILE:HG22	1.98	0.46
1:AA:1098:C:P	2:AB:139:ARG:HH22	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:79:ARG:NH2	30:BI:56:ARG:HH22	2.13	0.46
22:BA:2328:A:H2'	22:BA:2329:U:C6	2.51	0.46
35:BN:79:LEU:HD23	35:BN:83:LEU:HD12	1.98	0.46
1:AA:1238:A:OP1	1:AA:1335:U:O2'	2.25	0.46
10:AJ:30:LYS:HE3	10:AJ:36:VAL:HG22	1.99	0.46
11:AK:35:THR:OG1	11:AK:36:ASP:N	2.49	0.46
22:BA:1570:A:H2'	22:BA:1571:A:C8	2.50	0.46
1:AA:521:G:OP2	12:AL:51:LYS:NZ	2.49	0.45
22:BA:1590:A:H2'	22:BA:1591:A:C8	2.51	0.45
34:BM:18:ARG:HE	34:BM:18:ARG:HB3	1.61	0.45
13:AM:44:LYS:O	13:AM:48:LEU:HD12	2.17	0.45
19:AS:11:ILE:HG13	19:AS:38:SER:HB3	1.97	0.45
22:BA:285:G:H1	22:BA:355:U:H3	1.64	0.45
58:BA:3001:ERY:O8	58:BA:3001:ERY:H293	2.16	0.45
48:B0:38:HIS:ND1	48:B0:39:LEU:O	2.50	0.45
1:AA:294:U:OP1	1:AA:610:U:O2'	2.26	0.45
1:AA:310:G:H5''	16:AP:31:ARG:HB2	1.98	0.45
1:AA:1021:A:H2'	1:AA:1022:A:C8	2.51	0.45
1:AA:1027:C:O2	1:AA:1034:G:N1	2.50	0.45
12:AL:43:LYS:HD3	12:AL:91:PRO:HG3	1.98	0.45
3:AC:164:ARG:NH1	3:AC:166:GLU:OE2	2.49	0.45
22:BA:1275:A:OP2	22:BA:1646:C:N4	2.45	0.45
13:AM:8:ASN:ND2	13:AM:23:TYR:H	2.14	0.45
15:AO:24:SER:OG	15:AO:26:GLU:OE1	2.35	0.45
22:BA:1571:A:H2'	22:BA:1572:A:C8	2.52	0.45
22:BA:2189:U:H2'	22:BA:2190:G:H8	1.81	0.45
1:AA:720:C:H5''	18:AR:41:PRO:HB3	1.99	0.45
33:BL:64:PHE:HB3	51:B3:25:LYS:HD3	1.98	0.45
1:AA:1086:U:H3	1:AA:1099:G:H1	1.65	0.45
13:AM:64:VAL:O	13:AM:69:LEU:HB2	2.17	0.45
19:AS:5:LEU:HD11	19:AS:7:LYS:HB2	1.96	0.45
22:BA:2273:A:H2'	22:BA:2274:A:C8	2.51	0.45
26:BE:83:VAL:HB	26:BE:86:ALA:HB2	1.97	0.45
30:BI:14:ALA:O	30:BI:22:MET:N	2.50	0.45
49:B1:17:THR:HG22	49:B1:19:HIS:H	1.81	0.45
1:AA:407:U:H2'	1:AA:408:A:C8	2.51	0.45
1:AA:492:C:H2'	1:AA:493:A:C8	2.52	0.45
1:AA:1175:G:H2'	1:AA:1176:A:C8	2.52	0.45
22:BA:151:C:H2'	22:BA:152:A:C8	2.52	0.45
22:BA:286:U:H2'	22:BA:287:G:H8	1.81	0.45
22:BA:721:A:H2'	22:BA:722:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1590:A:H2'	22:BA:1591:A:H8	1.81	0.45
22:BA:2619:C:H5''	25:BD:157:LYS:HG2	1.99	0.45
33:BL:20:GLY:HA2	33:BL:28:GLY:HA2	1.99	0.45
55:D3:62:C:H2'	55:D3:63:G:C8	2.48	0.45
1:AA:723:U:OP1	21:AU:55:ARG:NH1	2.34	0.45
1:AA:1040:U:H2'	1:AA:1041:G:C8	2.52	0.45
9:AI:55:VAL:HG22	9:AI:94:LEU:HD22	1.99	0.45
19:AS:30:PRO:HA	19:AS:48:THR:O	2.17	0.45
22:BA:1013:C:H2'	22:BA:1014:A:H8	1.82	0.45
9:AI:55:VAL:HG12	9:AI:57:MET:HG2	1.98	0.45
22:BA:277:G:H4'	22:BA:278:A:C5	2.52	0.45
22:BA:307:G:N1	22:BA:310:A:OP2	2.45	0.45
22:BA:2898:U:H2'	22:BA:2899:A:C8	2.53	0.45
31:BJ:8:PRO:HG3	31:BJ:48:VAL:HG13	1.98	0.45
41:BT:68:LYS:HG3	41:BT:77:ARG:HH21	1.82	0.45
54:D2:23:A:H2'	54:D2:24:G:C8	2.52	0.45
1:AA:1326:U:H2'	1:AA:1327:C:C6	2.53	0.44
10:AJ:11:LYS:HA	10:AJ:70:HIS:O	2.17	0.44
45:BX:43:GLU:OE1	45:BX:45:ARG:NH2	2.49	0.44
9:AI:34:SER:OG	9:AI:35:LEU:N	2.50	0.44
22:BA:239:C:HO2'	22:BA:622:G:HO2'	1.61	0.44
22:BA:668:A:H2'	22:BA:670:A:H62	1.82	0.44
27:BF:22:TYR:OH	27:BF:165:GLU:OE2	2.27	0.44
37:BP:87:LYS:HA	37:BP:87:LYS:HD3	1.83	0.44
7:AG:23:LEU:HD23	7:AG:23:LEU:HA	1.69	0.44
3:AC:57:ILE:H	3:AC:57:ILE:HG12	1.58	0.44
6:AF:97:THR:N	6:AF:98:GLU:OE1	2.48	0.44
9:AI:7:TYR:CE1	9:AI:18:ARG:HB2	2.44	0.44
22:BA:2579:C:O2'	25:BD:136:ASN:OD1	2.34	0.44
46:BY:9:LYS:HD3	46:BY:13:GLU:HG2	1.99	0.44
3:AC:66:VAL:HG13	3:AC:66:VAL:O	2.18	0.44
15:AO:89:ARG:HH22	22:BA:712:G:H3'	1.83	0.44
22:BA:397:U:OP2	45:BX:10:LYS:NZ	2.42	0.44
34:BM:58:LYS:O	34:BM:60:GLN:NE2	2.38	0.44
51:B3:31:HIS:O	51:B3:33:LEU:N	2.51	0.44
55:D3:60:U:H5''	55:D3:61:C:H5	1.83	0.44
1:AA:1037:C:H2'	1:AA:1038:C:C6	2.53	0.44
1:AA:1273:C:H2'	1:AA:1274:A:O4'	2.17	0.44
6:AF:10:VAL:HB	6:AF:58:HIS:HB3	2.00	0.44
10:AJ:37:ARG:HA	10:AJ:37:ARG:HD3	1.85	0.44
22:BA:581:C:H2'	22:BA:582:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:2141:G:H2'	22:BA:2142:A:C8	2.52	0.44
55:D3:16:H2U:N3	55:D3:60:U:H1'	2.33	0.44
1:AA:1098:C:OP1	2:AB:139:ARG:NH2	2.50	0.44
1:AA:1308:U:H2'	1:AA:1309:G:C8	2.52	0.44
3:AC:64:ILE:HG22	3:AC:97:VAL:HG23	1.99	0.44
3:AC:148:GLY:HA2	3:AC:171:GLY:HA3	1.99	0.44
4:AD:78:GLU:OE2	4:AD:81:ARG:NH2	2.39	0.44
8:AH:11:LEU:HD22	8:AH:75:ILE:HD11	1.99	0.44
16:AP:19:VAL:HG22	16:AP:37:GLY:C	2.39	0.44
17:AQ:57:ASP:OD1	17:AQ:82:ALA:N	2.50	0.44
22:BA:1266:G:O2'	22:BA:2012:G:O6	2.30	0.44
22:BA:1412:U:H2'	22:BA:1413:A:C8	2.53	0.44
22:BA:1802:A:H2'	22:BA:1803:A:C8	2.53	0.44
1:AA:736:C:H2'	1:AA:737:C:C6	2.53	0.44
1:AA:999:C:H2'	1:AA:1000:A:C8	2.53	0.44
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.53	0.44
23:BB:66:A:OP2	23:BB:108:A:N6	2.50	0.44
1:AA:1072:G:OP1	5:AE:62:LYS:NZ	2.51	0.43
7:AG:79:ARG:NH2	7:AG:79:ARG:HG3	2.33	0.43
9:AI:129:LYS:HE3	9:AI:129:LYS:HB2	1.78	0.43
22:BA:1386:C:H2'	22:BA:1387:A:H8	1.84	0.43
22:BA:1729:U:O2	22:BA:1731:G:N2	2.44	0.43
29:BH:14:SER:N	29:BH:17:ASP:OD2	2.44	0.43
29:BH:69:ALA:O	29:BH:73:ASN:N	2.48	0.43
54:D2:1:G:H2'	54:D2:2:G:H8	1.83	0.43
1:AA:1375:A:P	7:AG:28:ASN:HD22	2.41	0.43
12:AL:44:LYS:HD2	12:AL:44:LYS:HA	1.85	0.43
13:AM:113:ARG:H	13:AM:113:ARG:HG2	1.62	0.43
22:BA:155:A:H2'	22:BA:156:A:H8	1.83	0.43
22:BA:500:G:N1	22:BA:503:A:OP2	2.48	0.43
22:BA:1101:U:H2'	22:BA:1102:C:C6	2.53	0.43
22:BA:1278:C:H2'	22:BA:1279:G:H8	1.83	0.43
22:BA:2107:G:O6	22:BA:2182:U:O4	2.35	0.43
23:BB:49:C:H2'	23:BB:50:A:C8	2.53	0.43
51:B3:31:HIS:C	51:B3:33:LEU:H	2.22	0.43
55:D3:36:A:H2	56:D4:1:U:H5	1.61	0.43
1:AA:928:G:C2	1:AA:1390:U:O2	2.70	0.43
6:AF:18:VAL:HG21	6:AF:58:HIS:CD2	2.53	0.43
10:AJ:47:GLU:OE2	14:AN:76:LYS:NZ	2.50	0.43
14:AN:33:VAL:HG13	14:AN:41:ARG:HH12	1.83	0.43
22:BA:13:A:O2'	22:BA:15:G:N7	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:743:A:O2'	22:BA:1659:G:OP1	2.32	0.43
22:BA:1651:G:H4'	35:BN:39:PRO:HG2	2.00	0.43
1:AA:458:U:H2'	1:AA:459:A:H8	1.83	0.43
11:AK:22:HIS:HD2	11:AK:85:MET:HB2	1.84	0.43
17:AQ:59:VAL:HG21	17:AQ:75:LEU:HD11	2.00	0.43
35:BN:117:ASP:OD1	35:BN:117:ASP:N	2.46	0.43
9:AI:12:ARG:HD2	9:AI:12:ARG:HA	1.78	0.43
22:BA:848:C:H2'	22:BA:849:A:H8	1.83	0.43
55:D3:35:A:N6	56:D4:2:U:C4	2.70	0.43
1:AA:746:A:H2'	1:AA:747:A:C8	2.53	0.43
1:AA:1028:C:O2'	1:AA:1030:U:O4	2.29	0.43
3:AC:54:ARG:HB3	3:AC:69:HIS:HB2	2.01	0.43
13:AM:79:ARG:HH22	30:BI:56:ARG:HH22	1.67	0.43
22:BA:288:U:H2'	22:BA:289:G:C8	2.54	0.43
22:BA:581:C:H2'	22:BA:582:A:H8	1.83	0.43
22:BA:720:U:H2'	22:BA:721:A:C8	2.54	0.43
22:BA:1734:G:H2'	22:BA:1735:A:H8	1.83	0.43
26:BE:41:GLN:NE2	26:BE:43:THR:OG1	2.37	0.43
28:BG:158:LYS:HB2	28:BG:160:LYS:HG3	2.01	0.43
1:AA:18:C:H5'	1:AA:1079:G:H1'	1.99	0.43
1:AA:1286:U:O2'	1:AA:1287:A:H5'	2.19	0.43
1:AA:1412:C:H2'	1:AA:1413:A:C8	2.53	0.43
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.18	0.43
22:BA:172:A:H2'	22:BA:173:A:H8	1.83	0.43
22:BA:1796:U:H2'	22:BA:1797:G:C8	2.53	0.43
22:BA:2291:U:OP1	22:BA:2380:C:O2'	2.35	0.43
54:D2:1:G:H2'	54:D2:2:G:C8	2.54	0.43
54:D2:23:A:H2'	54:D2:24:G:H8	1.84	0.43
1:AA:356:A:N3	1:AA:368:U:O2'	2.39	0.43
1:AA:674:G:H2'	1:AA:675:A:C8	2.54	0.43
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.48	0.43
2:AB:94:HIS:CE1	2:AB:146:ASN:HB2	2.54	0.43
10:AJ:36:VAL:HG12	10:AJ:76:ILE:HG13	2.01	0.43
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.58	0.43
13:AM:2:ALA:HB1	13:AM:53:ILE:HG12	2.01	0.43
14:AN:20:PHE:C	14:AN:22:LYS:H	2.21	0.43
19:AS:5:LEU:CD1	19:AS:7:LYS:CB	2.93	0.43
29:BH:135:HIS:CG	29:BH:136:SER:H	2.37	0.43
2:AB:70:VAL:HB	2:AB:163:VAL:HG22	2.00	0.43
10:AJ:52:LEU:HD11	10:AJ:59:LYS:HD2	2.01	0.43
22:BA:602:A:HO2'	22:BA:604:G:HO2'	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1419:A:O2'	22:BA:1421:G:N7	2.41	0.43
22:BA:1794:A:H2'	22:BA:1795:C:C6	2.54	0.43
2:AB:159:ASP:OD1	2:AB:159:ASP:N	2.51	0.43
3:AC:66:VAL:HG13	3:AC:101:ILE:HD13	1.99	0.43
11:AK:87:LYS:HG3	11:AK:115:PRO:HD3	2.00	0.43
22:BA:538:A:H4'	31:BJ:7:LYS:HG2	2.00	0.43
3:AC:114:LYS:HA	3:AC:114:LYS:HD2	1.84	0.42
7:AG:37:SER:HA	7:AG:40:GLU:HG2	2.00	0.42
22:BA:438:G:H2'	22:BA:439:A:C8	2.55	0.42
22:BA:2515:C:H2'	22:BA:2516:A:C8	2.54	0.42
33:BL:57:LEU:HD22	51:B3:54:ASP:HB3	2.01	0.42
1:AA:1027:C:H2'	1:AA:1028:C:C6	2.54	0.42
4:AD:107:PHE:CG	4:AD:145:ILE:HD11	2.54	0.42
7:AG:15:ASP:OD1	7:AG:44:TYR:OH	2.27	0.42
24:BC:21:ASN:HB3	24:BC:24:LEU:HD13	2.01	0.42
1:AA:447:G:N1	1:AA:486:U:OP2	2.38	0.42
3:AC:132:ARG:HA	3:AC:135:LYS:HE2	2.01	0.42
5:AE:150:PRO:HB2	5:AE:164:ILE:HG23	2.01	0.42
13:AM:22:ILE:HB	13:AM:25:VAL:HG22	2.01	0.42
22:BA:598:U:H2'	22:BA:599:A:H8	1.84	0.42
22:BA:837:C:N3	22:BA:941:A:N6	2.67	0.42
22:BA:930:G:H1'	47:BZ:25:LEU:HD21	2.01	0.42
22:BA:1058:U:H2'	22:BA:1059:G:C8	2.54	0.42
22:BA:1869:G:N2	22:BA:1871:A:O2'	2.51	0.42
22:BA:2529:G:H4'	28:BG:175:LYS:HD2	2.01	0.42
29:BH:80:ILE:HB	29:BH:146:VAL:HG12	2.01	0.42
46:BY:2:LYS:HD2	46:BY:6:LEU:HD21	2.00	0.42
55:D3:35:A:N6	56:D4:2:U:H3	2.17	0.42
1:AA:458:U:H2'	1:AA:459:A:C8	2.55	0.42
1:AA:1032:G:C5	1:AA:1033:G:H1'	2.54	0.42
1:AA:1338:G:H2'	1:AA:1339:A:C4	2.55	0.42
10:AJ:66:GLU:HB3	14:AN:99:ALA:HB2	2.01	0.42
22:BA:598:U:H2'	22:BA:599:A:C8	2.54	0.42
22:BA:1672:A:C2	22:BA:2582:G:H5'	2.55	0.42
22:BA:2291:U:O2'	22:BA:2374:C:O2	2.38	0.42
26:BE:21:ARG:HD3	26:BE:106:LYS:HB3	2.02	0.42
37:BP:100:LEU:HD11	37:BP:110:ILE:HD11	2.00	0.42
39:BR:16:GLU:HG3	39:BR:101:ILE:HG12	2.01	0.42
1:AA:936:C:C2	1:AA:937:A:C8	3.07	0.42
1:AA:299:G:H2'	1:AA:300:A:C8	2.54	0.42
1:AA:921:U:H5''	1:AA:1082:A:OP1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.54	0.42
1:AA:1316:G:H22	1:AA:1319:A:H5''	1.84	0.42
2:AB:126:PHE:CZ	2:AB:137:ARG:HD2	2.54	0.42
3:AC:33:LEU:HD11	14:AN:93:ILE:HD13	2.01	0.42
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	2.02	0.42
22:BA:742:A:H2'	22:BA:743:A:C8	2.54	0.42
22:BA:1847:A:O2'	22:BA:1848:A:H8	2.02	0.42
47:BZ:23:THR:HG23	47:BZ:47:MET:HG2	2.02	0.42
1:AA:925:G:C6	1:AA:1392:G:C6	3.07	0.42
22:BA:197:A:H62	22:BA:2430:A:H2'	1.84	0.42
22:BA:911:A:N6	34:BM:11:LYS:O	2.52	0.42
58:BA:3001:ERY:H353	58:BA:3001:ERY:H10	1.76	0.42
40:BS:24:ILE:HD13	40:BS:36:LEU:HD11	2.00	0.42
1:AA:56:U:H2'	1:AA:57:G:C8	2.54	0.42
9:AI:61:LEU:HD13	9:AI:61:LEU:HA	1.87	0.42
22:BA:962:G:P	59:BA:3202:HOH:O	2.75	0.42
28:BG:85:LYS:HE2	28:BG:85:LYS:HB2	1.96	0.42
41:BT:17:SER:OG	41:BT:18:GLU:N	2.52	0.42
1:AA:1010:U:H2'	1:AA:1011:C:C6	2.55	0.42
2:AB:97:LEU:H	2:AB:100:MET:HE3	1.85	0.42
22:BA:1105:U:H2'	22:BA:1106:G:H8	1.84	0.42
22:BA:1326:U:H2'	22:BA:1327:A:H8	1.85	0.42
24:BC:133:ARG:NH2	24:BC:187:ASP:OD1	2.53	0.42
34:BM:38:ARG:HB3	34:BM:98:PRO:HD3	2.02	0.42
1:AA:88:U:H1'	1:AA:89:U:H5	1.85	0.42
1:AA:950:U:H2'	1:AA:951:G:C8	2.55	0.42
1:AA:1130:A:H2'	1:AA:1131:G:H8	1.85	0.42
6:AF:2:ARG:HD3	6:AF:91:ARG:HE	1.84	0.42
9:AI:10:GLY:HA2	9:AI:81:HIS:ND1	2.35	0.42
11:AK:87:LYS:HB2	11:AK:113:VAL:HG13	2.00	0.42
17:AQ:68:SER:HB3	17:AQ:71:LYS:HB2	2.02	0.42
22:BA:1914:C:H2'	22:BA:1915:3TD:H6	2.01	0.42
22:BA:2100:G:H4'	22:BA:2100:G:OP1	2.19	0.42
55:D3:61:C:H2'	55:D3:62:C:C6	2.55	0.42
1:AA:1287:A:H2'	1:AA:1288:A:C8	2.54	0.41
3:AC:49:LYS:HD3	3:AC:49:LYS:HA	1.91	0.41
6:AF:100:SER:O	6:AF:104:LYS:HG2	2.20	0.41
8:AH:108:LYS:HD3	8:AH:108:LYS:HA	1.86	0.41
13:AM:43:VAL:CG2	13:AM:48:LEU:CG	2.98	0.41
18:AR:37:GLY:O	18:AR:63:ARG:NH2	2.50	0.41
22:BA:646:U:O2'	22:BA:647:G:O4'	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:1429:G:H2'	22:BA:1430:G:H8	1.85	0.41
22:BA:1808:A:H3'	22:BA:1809:A:C8	2.55	0.41
22:BA:1851:U:O2'	55:D3:71:G:O2'	2.34	0.41
22:BA:2418:A:OP1	51:B3:45:ARG:NH1	2.48	0.41
35:BN:106:ASP:OD1	35:BN:106:ASP:N	2.53	0.41
3:AC:10:ILE:HD12	3:AC:10:ILE:HA	1.83	0.41
13:AM:107:ARG:NH2	13:AM:110:LYS:HE2	2.35	0.41
22:BA:494:G:H4'	40:BS:6:LYS:HB2	2.02	0.41
22:BA:1645:G:H5''	22:BA:1646:C:H5'	2.02	0.41
22:BA:2179:C:H2'	22:BA:2180:U:H6	1.84	0.41
29:BH:100:ALA:HA	29:BH:103:VAL:HG12	2.01	0.41
1:AA:79:G:H2'	1:AA:80:A:C8	2.55	0.41
1:AA:235:C:H2'	1:AA:236:A:C8	2.56	0.41
1:AA:254:G:OP1	17:AQ:68:SER:OG	2.36	0.41
1:AA:1166:G:H22	1:AA:1169:A:H5''	1.85	0.41
3:AC:19:ASN:O	3:AC:40:ARG:NH2	2.52	0.41
13:AM:79:ARG:HH12	30:BI:56:ARG:NH2	2.17	0.41
22:BA:4:U:H2'	22:BA:5:A:H8	1.85	0.41
22:BA:1316:U:H2'	22:BA:1317:G:C8	2.54	0.41
22:BA:1682:G:H2'	22:BA:1683:U:C6	2.55	0.41
22:BA:2567:G:H2'	22:BA:2568:U:C6	2.55	0.41
32:BK:17:ARG:HD3	32:BK:17:ARG:HA	1.88	0.41
32:BK:121:GLU:OE1	37:BP:65:SER:OG	2.29	0.41
1:AA:920:U:O4'	1:AA:1080:A:C2	2.74	0.41
1:AA:935:A:O2'	1:AA:1383:C:O2	2.38	0.41
13:AM:113:ARG:HH11	13:AM:113:ARG:HD3	1.75	0.41
15:AO:29:VAL:O	15:AO:33:THR:HG23	2.20	0.41
22:BA:566:U:H5''	33:BL:29:LYS:HE3	2.02	0.41
27:BF:147:ASP:N	27:BF:147:ASP:OD1	2.53	0.41
54:D2:37:T6A:N1	54:D2:37:T6A:N11	2.69	0.41
1:AA:28:A:O2'	1:AA:296:U:OP1	2.26	0.41
1:AA:253:A:O2'	17:AQ:17:MET:SD	2.77	0.41
1:AA:927:G:OP1	1:AA:1505:G:N2	2.42	0.41
2:AB:119:THR:O	2:AB:124:GLY:N	2.41	0.41
13:AM:7:ILE:CD1	27:BF:112:ARG:HB3	2.50	0.41
22:BA:26:G:H1'	22:BA:514:A:N6	2.36	0.41
22:BA:1476:U:H2'	22:BA:1477:A:C8	2.55	0.41
59:BA:3213:HOH:O	53:D1:1:FME:HE2	2.17	0.41
1:AA:588:G:P	59:AA:1711:HOH:O	2.78	0.41
1:AA:1380:U:O2'	7:AG:3:ARG:NH1	2.46	0.41
7:AG:86:GLN:NE2	7:AG:148:ASN:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:145:C:H2'	22:BA:146:A:C8	2.56	0.41
22:BA:698:C:O2'	22:BA:734:A:N6	2.54	0.41
22:BA:1992:G:N2	22:BA:1996:C:O2'	2.53	0.41
22:BA:2898:U:H2'	22:BA:2899:A:H8	1.85	0.41
4:AD:9:LEU:HD23	4:AD:22:LYS:HD2	2.03	0.41
4:AD:22:LYS:HD3	4:AD:31:LYS:HE2	2.03	0.41
10:AJ:28:THR:HA	10:AJ:31:ARG:HG2	2.03	0.41
13:AM:39:ILE:HD13	13:AM:56:LEU:HD21	2.03	0.41
22:BA:195:A:H8	59:BA:3391:HOH:O	1.99	0.41
22:BA:363:G:H2'	22:BA:364:C:C6	2.56	0.41
22:BA:1071:G:N2	22:BA:1091:G:OP2	2.54	0.41
22:BA:1300:G:H4'	22:BA:1301:A:H5''	2.02	0.41
28:BG:7:ALA:HA	28:BG:8:PRO:HD3	1.95	0.41
54:D2:50:C:H2'	54:D2:51:A:C8	2.56	0.41
1:AA:744:C:H2'	1:AA:745:G:C8	2.56	0.41
1:AA:1004:A:N6	1:AA:1025:U:OP1	2.52	0.41
1:AA:1026:G:H22	1:AA:1034:G:H1	1.69	0.41
7:AG:47:LEU:HD23	7:AG:47:LEU:HA	1.91	0.41
22:BA:1353:A:H2'	22:BA:1354:A:C8	2.56	0.41
22:BA:1548:A:H2'	22:BA:1549:A:C8	2.55	0.41
26:BE:176:ASP:OD1	26:BE:179:SER:OG	2.30	0.41
41:BT:69:ARG:NH1	41:BT:72:GLN:O	2.54	0.41
1:AA:1016:A:O2'	1:AA:1217:C:O2'	2.35	0.41
1:AA:1020:G:H8	1:AA:1020:G:OP2	2.03	0.41
1:AA:1119:C:H2'	1:AA:1120:C:H6	1.86	0.41
6:AF:38:ARG:HG2	6:AF:63:ASN:HB2	2.02	0.41
7:AG:60:GLU:OE1	7:AG:60:GLU:N	2.54	0.41
9:AI:107:ASP:OD2	9:AI:109:ARG:NH1	2.53	0.41
10:AJ:40:ILE:HG13	10:AJ:73:LEU:HB3	2.01	0.41
22:BA:1683:U:H2'	22:BA:1684:G:H8	1.85	0.41
22:BA:2243:U:H2'	22:BA:2244:U:C6	2.56	0.41
22:BA:2329:U:H2'	22:BA:2330:G:C8	2.56	0.41
22:BA:2728:U:HO2'	22:BA:2729:G:H8	1.68	0.41
27:BF:64:LYS:HA	27:BF:65:PRO:HD3	1.91	0.41
27:BF:144:ASP:N	27:BF:144:ASP:OD1	2.39	0.41
1:AA:500:G:H2'	1:AA:501:C:C6	2.56	0.41
1:AA:1011:C:H2'	1:AA:1012:A:H8	1.85	0.41
1:AA:1023:U:H2'	1:AA:1024:G:N3	2.36	0.41
1:AA:1048:G:OP1	14:AN:3:GLN:HB2	2.21	0.41
2:AB:128:LYS:HB2	2:AB:128:LYS:HE2	1.82	0.41
15:AO:32:LEU:HD23	15:AO:32:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:67:LEU:HD23	15:AO:67:LEU:HA	1.86	0.41
17:AQ:29:VAL:O	17:AQ:37:PHE:HA	2.21	0.41
22:BA:1734:G:H2'	22:BA:1735:A:C8	2.56	0.41
25:BD:109:VAL:HG22	25:BD:203:VAL:HG13	2.03	0.41
46:BY:19:LEU:HD23	46:BY:19:LEU:HA	1.94	0.41
1:AA:255:G:O3'	17:AQ:19:LYS:NZ	2.42	0.40
1:AA:384:G:H2'	1:AA:385:C:C6	2.56	0.40
1:AA:821:G:H2'	1:AA:822:U:C6	2.56	0.40
1:AA:1188:A:H2'	1:AA:1189:U:O4'	2.21	0.40
22:BA:848:C:H2'	22:BA:849:A:C8	2.56	0.40
22:BA:1174:U:H1'	22:BA:1177:G:C2	2.56	0.40
48:B0:39:LEU:HD23	48:B0:39:LEU:HA	1.90	0.40
1:AA:96:U:H2'	1:AA:97:G:C8	2.57	0.40
3:AC:87:LEU:HD23	3:AC:87:LEU:HA	1.85	0.40
4:AD:126:ASN:ND2	4:AD:142:VAL:H	2.18	0.40
19:AS:43:ASN:OD1	19:AS:43:ASN:N	2.42	0.40
22:BA:20:C:H2'	22:BA:21:A:H8	1.86	0.40
22:BA:1224:U:H2'	22:BA:1225:G:C8	2.56	0.40
22:BA:1405:U:H2'	22:BA:1406:U:C6	2.56	0.40
22:BA:2036:C:H2'	22:BA:2037:A:C8	2.56	0.40
40:BS:23:LEU:HD22	48:B0:24:ALA:HB2	2.02	0.40
1:AA:715:A:H2'	1:AA:716:A:C8	2.57	0.40
4:AD:48:LEU:HD22	4:AD:52:GLY:HA3	2.02	0.40
11:AK:47:ALA:HB1	11:AK:62:ALA:HB1	2.02	0.40
18:AR:68:LEU:HD23	18:AR:68:LEU:HA	1.84	0.40
22:BA:1636:U:H2'	22:BA:1637:A:H8	1.84	0.40
22:BA:2115:G:H2'	22:BA:2117:A:N7	2.37	0.40
22:BA:2233:U:H2'	22:BA:2234:G:H8	1.86	0.40
22:BA:2809:A:H2'	22:BA:2810:A:C8	2.56	0.40
39:BR:38:VAL:HG23	39:BR:54:VAL:HB	2.02	0.40
3:AC:79:LYS:HA	3:AC:79:LYS:HD3	1.96	0.40
4:AD:85:ASN:HB3	4:AD:88:GLU:HG2	2.04	0.40
7:AG:57:SER:HB3	7:AG:60:GLU:HB2	2.02	0.40
22:BA:2586:U:OP2	53:D1:1:FME:N	2.55	0.40
54:D2:30:C:H2'	54:D2:31:A:H8	1.87	0.40
1:AA:1254:A:H2'	1:AA:1255:G:H8	1.86	0.40
1:AA:1409:C:H2'	1:AA:1410:A:C8	2.57	0.40
4:AD:3:ARG:HH11	4:AD:3:ARG:HD3	1.75	0.40
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	2.03	0.40
10:AJ:11:LYS:HE2	10:AJ:71:LEU:HD21	2.04	0.40
10:AJ:52:LEU:HD21	10:AJ:59:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:20:C:H2'	22:BA:21:A:C8	2.57	0.40
22:BA:284:U:H3	22:BA:356:G:H1	1.69	0.40
22:BA:876:C:H2'	22:BA:877:A:O4'	2.22	0.40
22:BA:1038:G:H2'	22:BA:1039:A:C8	2.57	0.40
22:BA:1485:U:H2'	22:BA:1486:U:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
3	AC	204/233 (88%)	192 (94%)	11 (5%)	1 (0%)	29	68
4	AD	203/206 (98%)	192 (95%)	11 (5%)	0	100	100
5	AE	153/167 (92%)	143 (94%)	10 (6%)	0	100	100
6	AF	104/135 (77%)	100 (96%)	4 (4%)	0	100	100
7	AG	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
8	AH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	AI	125/130 (96%)	110 (88%)	14 (11%)	1 (1%)	19	57
10	AJ	97/103 (94%)	92 (95%)	4 (4%)	1 (1%)	15	53
11	AK	115/129 (89%)	106 (92%)	9 (8%)	0	100	100
12	AL	120/124 (97%)	111 (92%)	8 (7%)	1 (1%)	19	57
13	AM	112/118 (95%)	102 (91%)	9 (8%)	1 (1%)	17	55
14	AN	99/102 (97%)	83 (84%)	16 (16%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	AP	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
17	AQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	53/75 (71%)	50 (94%)	3 (6%)	0	100	100
19	AS	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
20	AT	84/87 (97%)	84 (100%)	0	0	100	100
21	AU	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
24	BC	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
25	BD	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	29	68
26	BE	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
27	BF	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
28	BG	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
31	BJ	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
32	BK	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	BL	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
34	BM	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
35	BN	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
36	BO	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
37	BP	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
40	BS	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
41	BT	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
42	BU	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
43	BV	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
44	BW	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
45	BX	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
46	BY	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
47	BZ	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
48	B0	54/57 (95%)	54 (100%)	0	0	100	100
49	B1	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
50	B2	44/46 (96%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	B3	62/65 (95%)	57 (92%)	3 (5%)	2 (3%)	4	22
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	D1	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	5579/5920 (94%)	5322 (95%)	249 (4%)	8 (0%)	54	85

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AL	102	LEU
25	BD	149	ASN
51	B3	32	ILE
10	AJ	57	VAL
51	B3	33	LEU
3	AC	61	ALA
9	AI	25	ASN
13	AM	66	GLU

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	
2	AB	186/199 (94%)	186 (100%)	0	100	100
3	AC	170/190 (90%)	169 (99%)	1 (1%)	86	95
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	118/126 (94%)	118 (100%)	0	100	100
6	AF	92/116 (79%)	92 (100%)	0	100	100
7	AG	124/147 (84%)	119 (96%)	5 (4%)	31	68
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	103 (98%)	2 (2%)	57	84
10	AJ	87/90 (97%)	86 (99%)	1 (1%)	73	90
11	AK	90/99 (91%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	102/103 (99%)	101 (99%)	1 (1%)	76	91
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	76/77 (99%)	76 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	73 (99%)	1 (1%)	67	88
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	71/79 (90%)	70 (99%)	1 (1%)	67	88
20	AT	65/66 (98%)	64 (98%)	1 (2%)	65	87
21	AU	48/61 (79%)	48 (100%)	0	100	100
24	BC	216/218 (99%)	215 (100%)	1 (0%)	88	96
25	BD	163/163 (100%)	162 (99%)	1 (1%)	86	95
26	BE	165/165 (100%)	164 (99%)	1 (1%)	86	95
27	BF	148/150 (99%)	148 (100%)	0	100	100
28	BG	137/138 (99%)	137 (100%)	0	100	100
29	BH	114/114 (100%)	113 (99%)	1 (1%)	78	92
30	BI	59/62 (95%)	58 (98%)	1 (2%)	60	85
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	78	92
32	BK	104/104 (100%)	104 (100%)	0	100	100
33	BL	103/103 (100%)	103 (100%)	0	100	100
34	BM	108/108 (100%)	107 (99%)	1 (1%)	78	92
35	BN	98/103 (95%)	98 (100%)	0	100	100
36	BO	87/87 (100%)	87 (100%)	0	100	100
37	BP	99/100 (99%)	99 (100%)	0	100	100
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	84 (100%)	0	100	100
40	BS	93/93 (100%)	93 (100%)	0	100	100
41	BT	80/84 (95%)	80 (100%)	0	100	100
42	BU	83/85 (98%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	78 (100%)	0	100	100
44	BW	57/63 (90%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BX	67/68 (98%)	67 (100%)	0	100	100
46	BY	54/55 (98%)	54 (100%)	0	100	100
47	BZ	48/49 (98%)	48 (100%)	0	100	100
48	B0	47/48 (98%)	46 (98%)	1 (2%)	53	82
49	B1	45/49 (92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	38 (100%)	0	100	100
51	B3	51/52 (98%)	51 (100%)	0	100	100
52	B4	34/34 (100%)	34 (100%)	0	100	100
53	D1	5/5 (100%)	5 (100%)	0	100	100
All	All	4638/4832 (96%)	4617 (100%)	21 (0%)	89	96

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AC	127	ARG
7	AG	30	LEU
7	AG	79	ARG
7	AG	148	ASN
7	AG	149	LYS
7	AG	151	PHE
9	AI	18	ARG
9	AI	106	ARG
10	AJ	69	THR
12	AL	64	THR
17	AQ	28	PHE
19	AS	69	HIS
20	AT	10	ARG
24	BC	262	ARG
25	BD	1	MET
26	BE	188	MET
29	BH	27	ARG
30	BI	16	CYS
31	BJ	92	MET
34	BM	12	MET
48	B0	40	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	177	ASN
4	AD	116	GLN
4	AD	126	ASN
4	AD	136	GLN
5	AE	89	HIS
7	AG	86	GLN
9	AI	110	GLN
12	AL	5	ASN
12	AL	73	ASN
13	AM	8	ASN
15	AO	28	GLN
20	AT	70	ASN
21	AU	56	HIS
24	BC	200	HIS
24	BC	260	ASN
27	BF	21	ASN
28	BG	22	GLN
28	BG	104	ASN
28	BG	139	GLN
32	BK	88	ASN
36	BO	100	HIS
46	BY	20	ASN
47	BZ	20	HIS
48	B0	42	HIS
49	B1	45	GLN
50	B2	26	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	267 (17%)	4 (0%)
22	BA	2891/2903 (99%)	413 (14%)	16 (0%)
23	BB	119/120 (99%)	15 (12%)	0
54	D2	73/77 (94%)	17 (23%)	3 (4%)
55	D3	74/76 (97%)	43 (58%)	3 (4%)
56	D4	8/9 (88%)	4 (50%)	0
All	All	4695/4719 (99%)	759 (16%)	26 (0%)

All (759) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U

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Mol	Chain	Res	Type
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	15	G
1	AA	22	G
1	AA	29	U
1	AA	32	A
1	AA	39	G
1	AA	44	A
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	70	U
1	AA	71	A
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	87	C
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	98	A
1	AA	116	A
1	AA	121	U
1	AA	122	G
1	AA	128	G
1	AA	130	A
1	AA	131	A
1	AA	141	G
1	AA	144	G
1	AA	159	G
1	AA	163	C
1	AA	164	G
1	AA	167	A
1	AA	181	A
1	AA	183	C
1	AA	197	A

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Mol	Chain	Res	Type
1	AA	205	A
1	AA	210	C
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	280	C
1	AA	289	G
1	AA	316	C
1	AA	321	A
1	AA	327	A
1	AA	328	C
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	384	G
1	AA	390	U
1	AA	392	C
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	428	G
1	AA	429	U
1	AA	436	C
1	AA	437	U
1	AA	439	U
1	AA	465	A
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	469	C
1	AA	478	A
1	AA	479	U
1	AA	481	G
1	AA	482	A

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Mol	Chain	Res	Type
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	496	A
1	AA	499	A
1	AA	511	C
1	AA	515	G
1	AA	517	G
1	AA	518	C
1	AA	521	G
1	AA	527	G7M
1	AA	529	G
1	AA	532	A
1	AA	533	A
1	AA	542	G
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	607	A
1	AA	631	C
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	665	A
1	AA	687	A
1	AA	688	G
1	AA	694	A
1	AA	695	A
1	AA	702	A
1	AA	703	G
1	AA	721	G
1	AA	722	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	758	C

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Mol	Chain	Res	Type
1	AA	760	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	799	G
1	AA	810	C
1	AA	815	A
1	AA	817	C
1	AA	819	A
1	AA	820	U
1	AA	821	G
1	AA	828	U
1	AA	829	G
1	AA	832	G
1	AA	840	C
1	AA	841	C
1	AA	843	U
1	AA	845	A
1	AA	846	G
1	AA	871	U
1	AA	889	A
1	AA	914	A
1	AA	929	G
1	AA	930	C
1	AA	934	C
1	AA	935	A
1	AA	942	G
1	AA	960	U
1	AA	966	2MG
1	AA	968	A
1	AA	969	A
1	AA	971	G
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	983	A
1	AA	989	U
1	AA	991	U
1	AA	992	U
1	AA	993	G
1	AA	1004	A

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Mol	Chain	Res	Type
1	AA	1008	U
1	AA	1009	U
1	AA	1018	G
1	AA	1019	A
1	AA	1020	G
1	AA	1021	A
1	AA	1022	A
1	AA	1023	U
1	AA	1024	G
1	AA	1025	U
1	AA	1026	G
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1036	A
1	AA	1043	G
1	AA	1044	A
1	AA	1045	C
1	AA	1065	U
1	AA	1070	U
1	AA	1085	U
1	AA	1089	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1127	G
1	AA	1132	C
1	AA	1133	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1143	G
1	AA	1154	G
1	AA	1158	C
1	AA	1159	U
1	AA	1168	U
1	AA	1169	A
1	AA	1171	A
1	AA	1172	C
1	AA	1173	U

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Mol	Chain	Res	Type
1	AA	1181	G
1	AA	1184	G
1	AA	1187	G
1	AA	1191	A
1	AA	1196	A
1	AA	1197	A
1	AA	1201	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1241	G
1	AA	1248	A
1	AA	1257	A
1	AA	1260	G
1	AA	1274	A
1	AA	1279	G
1	AA	1280	A
1	AA	1287	A
1	AA	1297	G
1	AA	1298	U
1	AA	1299	A
1	AA	1302	C
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
1	AA	1320	C
1	AA	1322	C
1	AA	1335	U
1	AA	1338	G
1	AA	1345	U
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1378	C
1	AA	1390	U
1	AA	1391	U
1	AA	1397	C
1	AA	1419	G

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Mol	Chain	Res	Type
1	AA	1429	A
1	AA	1432	G
1	AA	1441	A
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1497	G
1	AA	1502	A
1	AA	1505	G
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
22	BA	14	A
22	BA	15	G
22	BA	34	U
22	BA	35	G
22	BA	63	A
22	BA	71	A
22	BA	74	A
22	BA	75	G
22	BA	84	A
22	BA	91	A
22	BA	101	A
22	BA	103	A
22	BA	118	A
22	BA	119	A
22	BA	120	U
22	BA	162	U
22	BA	163	C
22	BA	165	A
22	BA	181	A
22	BA	186	G
22	BA	196	A
22	BA	197	A
22	BA	204	A
22	BA	215	G
22	BA	216	A
22	BA	221	A
22	BA	222	A
22	BA	223	A

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Mol	Chain	Res	Type
22	BA	233	A
22	BA	241	A
22	BA	248	G
22	BA	264	C
22	BA	265	A
22	BA	276	U
22	BA	278	A
22	BA	299	A
22	BA	302	C
22	BA	303	G
22	BA	311	A
22	BA	324	A
22	BA	330	A
22	BA	353	C
22	BA	361	G
22	BA	362	A
22	BA	386	G
22	BA	396	G
22	BA	406	G
22	BA	411	G
22	BA	412	A
22	BA	457	A
22	BA	467	G
22	BA	477	A
22	BA	480	A
22	BA	481	G
22	BA	491	G
22	BA	504	A
22	BA	505	A
22	BA	508	A
22	BA	509	C
22	BA	529	A
22	BA	531	C
22	BA	532	A
22	BA	533	G
22	BA	546	U
22	BA	547	A
22	BA	548	G
22	BA	549	G
22	BA	550	C
22	BA	563	A
22	BA	573	U

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Mol	Chain	Res	Type
22	BA	575	A
22	BA	577	G
22	BA	588	U
22	BA	602	A
22	BA	603	A
22	BA	613	A
22	BA	614	A
22	BA	615	U
22	BA	616	A
22	BA	634	C
22	BA	637	A
22	BA	645	C
22	BA	647	G
22	BA	653	U
22	BA	654	A
22	BA	668	A
22	BA	670	A
22	BA	685	A
22	BA	686	U
22	BA	702	U
22	BA	724	U
22	BA	730	A
22	BA	738	G
22	BA	747	5MU
22	BA	748	G
22	BA	764	A
22	BA	765	C
22	BA	775	G
22	BA	776	G
22	BA	782	A
22	BA	784	G
22	BA	785	G
22	BA	789	A
22	BA	791	C
22	BA	792	A
22	BA	793	A
22	BA	794	A
22	BA	805	G
22	BA	812	C
22	BA	827	U
22	BA	828	U
22	BA	830	G

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Mol	Chain	Res	Type
22	BA	845	A
22	BA	846	U
22	BA	859	G
22	BA	869	G
22	BA	884	U
22	BA	885	C
22	BA	895	U
22	BA	896	A
22	BA	897	C
22	BA	907	G
22	BA	910	A
22	BA	927	A
22	BA	946	C
22	BA	961	C
22	BA	974	G
22	BA	983	A
22	BA	985	C
22	BA	996	A
22	BA	999	U
22	BA	1005	C
22	BA	1009	A
22	BA	1012	U
22	BA	1013	C
22	BA	1022	G
22	BA	1026	G
22	BA	1033	U
22	BA	1046	A
22	BA	1047	G
22	BA	1054	A
22	BA	1057	A
22	BA	1061	U
22	BA	1069	A
22	BA	1070	A
22	BA	1077	A
22	BA	1087	G
22	BA	1088	A
22	BA	1089	A
22	BA	1090	A
22	BA	1094	U
22	BA	1110	G
22	BA	1112	G
22	BA	1126	A

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Mol	Chain	Res	Type
22	BA	1130	U
22	BA	1132	U
22	BA	1133	A
22	BA	1135	C
22	BA	1141	U
22	BA	1142	A
22	BA	1156	A
22	BA	1168	G
22	BA	1173	U
22	BA	1174	U
22	BA	1175	A
22	BA	1176	U
22	BA	1204	A
22	BA	1205	A
22	BA	1212	G
22	BA	1236	G
22	BA	1250	G
22	BA	1253	A
22	BA	1256	G
22	BA	1268	A
22	BA	1271	G
22	BA	1272	A
22	BA	1275	A
22	BA	1287	A
22	BA	1300	G
22	BA	1301	A
22	BA	1302	A
22	BA	1313	U
22	BA	1321	A
22	BA	1329	U
22	BA	1352	U
22	BA	1359	A
22	BA	1365	A
22	BA	1379	U
22	BA	1383	A
22	BA	1386	C
22	BA	1387	A
22	BA	1403	A
22	BA	1416	G
22	BA	1428	C
22	BA	1434	A
22	BA	1437	C

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Mol	Chain	Res	Type
22	BA	1452	G
22	BA	1453	A
22	BA	1482	G
22	BA	1493	C
22	BA	1497	U
22	BA	1508	A
22	BA	1509	A
22	BA	1515	A
22	BA	1524	G
22	BA	1535	A
22	BA	1536	C
22	BA	1544	A
22	BA	1558	C
22	BA	1559	U
22	BA	1566	A
22	BA	1569	A
22	BA	1578	U
22	BA	1583	A
22	BA	1608	A
22	BA	1610	A
22	BA	1619	G
22	BA	1626	A
22	BA	1634	A
22	BA	1647	U
22	BA	1648	U
22	BA	1649	G
22	BA	1654	A
22	BA	1664	A
22	BA	1674	G
22	BA	1677	A
22	BA	1698	A
22	BA	1699	G
22	BA	1713	A
22	BA	1729	U
22	BA	1730	C
22	BA	1732	C
22	BA	1744	A
22	BA	1757	A
22	BA	1758	U
22	BA	1764	C
22	BA	1773	A
22	BA	1781	U

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Mol	Chain	Res	Type
22	BA	1786	A
22	BA	1800	C
22	BA	1801	A
22	BA	1802	A
22	BA	1808	A
22	BA	1811	G
22	BA	1816	C
22	BA	1829	A
22	BA	1847	A
22	BA	1862	G
22	BA	1870	C
22	BA	1871	A
22	BA	1872	A
22	BA	1873	G
22	BA	1900	A
22	BA	1906	G
22	BA	1914	C
22	BA	1929	G
22	BA	1930	G
22	BA	1936	A
22	BA	1937	A
22	BA	1938	A
22	BA	1939	5MU
22	BA	1955	U
22	BA	1960	A
22	BA	1967	C
22	BA	1970	A
22	BA	1971	U
22	BA	1972	G
22	BA	1991	U
22	BA	1993	U
22	BA	1996	C
22	BA	2004	G
22	BA	2020	A
22	BA	2023	C
22	BA	2031	A
22	BA	2033	A
22	BA	2036	C
22	BA	2043	C
22	BA	2055	C
22	BA	2056	G
22	BA	2060	A

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Mol	Chain	Res	Type
22	BA	2061	G
22	BA	2062	A
22	BA	2069	G7M
22	BA	2077	A
22	BA	2080	A
22	BA	2093	G
22	BA	2099	U
22	BA	2100	G
22	BA	2101	A
22	BA	2108	A
22	BA	2110	G
22	BA	2111	U
22	BA	2113	U
22	BA	2115	G
22	BA	2116	G
22	BA	2117	A
22	BA	2118	U
22	BA	2119	A
22	BA	2121	G
22	BA	2123	G
22	BA	2124	G
22	BA	2125	G
22	BA	2126	A
22	BA	2128	G
22	BA	2131	U
22	BA	2132	U
22	BA	2133	G
22	BA	2137	U
22	BA	2146	C
22	BA	2147	A
22	BA	2158	A
22	BA	2161	C
22	BA	2162	G
22	BA	2163	A
22	BA	2164	C
22	BA	2165	C
22	BA	2167	U
22	BA	2169	A
22	BA	2171	A
22	BA	2172	U
22	BA	2173	A
22	BA	2189	U

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Mol	Chain	Res	Type
22	BA	2190	G
22	BA	2195	U
22	BA	2198	A
22	BA	2203	U
22	BA	2204	G
22	BA	2211	A
22	BA	2225	A
22	BA	2238	G
22	BA	2239	G
22	BA	2243	U
22	BA	2266	A
22	BA	2267	A
22	BA	2268	A
22	BA	2278	A
22	BA	2283	C
22	BA	2287	A
22	BA	2288	A
22	BA	2305	U
22	BA	2307	G
22	BA	2308	G
22	BA	2312	U
22	BA	2322	A
22	BA	2325	G
22	BA	2333	A
22	BA	2336	A
22	BA	2340	A
22	BA	2345	G
22	BA	2347	C
22	BA	2350	C
22	BA	2383	G
22	BA	2385	C
22	BA	2406	A
22	BA	2425	A
22	BA	2426	A
22	BA	2429	G
22	BA	2430	A
22	BA	2435	A
22	BA	2436	G
22	BA	2441	U
22	BA	2448	A
22	BA	2469	A
22	BA	2476	A

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Mol	Chain	Res	Type
22	BA	2491	U
22	BA	2498	OMC
22	BA	2502	G
22	BA	2504	PSU
22	BA	2505	G
22	BA	2518	A
22	BA	2520	C
22	BA	2529	G
22	BA	2535	G
22	BA	2547	A
22	BA	2566	A
22	BA	2567	G
22	BA	2584	U
22	BA	2585	U
22	BA	2602	A
22	BA	2603	G
22	BA	2609	U
22	BA	2613	U
22	BA	2615	U
22	BA	2623	G
22	BA	2629	U
22	BA	2630	G
22	BA	2646	C
22	BA	2660	A
22	BA	2661	G
22	BA	2663	G
22	BA	2689	U
22	BA	2690	U
22	BA	2714	G
22	BA	2726	A
22	BA	2727	A
22	BA	2732	G
22	BA	2733	A
22	BA	2744	G
22	BA	2748	A
22	BA	2765	A
22	BA	2778	A
22	BA	2800	A
22	BA	2818	U
22	BA	2820	A
22	BA	2821	A
22	BA	2835	A

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Mol	Chain	Res	Type
22	BA	2850	A
22	BA	2861	U
22	BA	2880	C
22	BA	2883	A
22	BA	2884	U
22	BA	2885	G
22	BA	2891	U
23	BB	9	G
23	BB	24	G
23	BB	35	C
23	BB	37	C
23	BB	41	G
23	BB	42	C
23	BB	45	A
23	BB	52	A
23	BB	56	G
23	BB	57	A
23	BB	67	G
23	BB	89	U
23	BB	90	C
23	BB	105	G
23	BB	109	A
54	D2	7	G
54	D2	8	4SU
54	D2	13	C
54	D2	14	A
54	D2	16	H2U
54	D2	17	H2U
54	D2	17(A)	OMG
54	D2	18	G
54	D2	19	H2U
54	D2	20	H2U
54	D2	21	A
54	D2	23	A
54	D2	37	T6A
54	D2	46	G7M
54	D2	54	5MU
54	D2	59	A
54	D2	76	A
55	D3	2	C
55	D3	6	G
55	D3	7	A

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Mol	Chain	Res	Type
55	D3	8	4SU
55	D3	9	A
55	D3	11	C
55	D3	13	C
55	D3	14	A
55	D3	15	G
55	D3	16	H2U
55	D3	17	C
55	D3	18	G
55	D3	19	G
55	D3	20	H2U
55	D3	21	A
55	D3	22	G
55	D3	23	A
55	D3	26	A
55	D3	27	G
55	D3	34	G
55	D3	35	A
55	D3	36	A
55	D3	38	A
55	D3	40	C
55	D3	44	G
55	D3	46	G
55	D3	49	C
55	D3	50	U
55	D3	53	G
55	D3	55	PSU
55	D3	56	C
55	D3	57	G
55	D3	58	A
55	D3	59	U
55	D3	62	C
55	D3	64	A
55	D3	67	C
55	D3	68	C
55	D3	70	G
55	D3	71	G
55	D3	72	C
55	D3	74	C
55	D3	76	A
56	D4	4	A
56	D4	7	U

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Mol	Chain	Res	Type
56	D4	8	A
56	D4	9	A

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	81	A
1	AA	428	G
1	AA	722	G
1	AA	1493	A
22	BA	125	A
22	BA	196	A
22	BA	221	A
22	BA	764	A
22	BA	984	A
22	BA	1046	A
22	BA	1089	A
22	BA	1142	A
22	BA	1275	A
22	BA	1634	A
22	BA	1900	A
22	BA	2116	G
22	BA	2189	U
22	BA	2468	A
22	BA	2602	A
22	BA	2873	A
54	D2	16	H2U
54	D2	17	H2U
54	D2	17(A)	OMG
55	D3	1	G
55	D3	8	4SU
55	D3	58	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
54	H2U	D2	20	54	18,21,22	3.02	5 (27%)	21,30,33	2.12	5 (23%)
22	PSU	BA	2504	22	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
1	MA6	AA	1519	1	18,26,27	1.25	1 (5%)	19,38,41	4.21	3 (15%)
1	G7M	AA	527	1	20,26,27	2.10	6 (30%)	17,39,42	1.22	1 (5%)
22	2MG	BA	2445	22	18,26,27	2.56	6 (33%)	16,38,41	1.53	4 (25%)
22	6MZ	BA	1618	22	18,25,26	2.00	3 (16%)	16,36,39	2.15	3 (18%)
55	4SU	D3	8	55	18,21,22	3.69	8 (44%)	26,30,33	2.24	5 (19%)
54	H2U	D2	19	54	18,21,22	3.27	4 (22%)	21,30,33	1.77	5 (23%)
22	PSU	BA	1911	22	18,21,22	1.02	1 (5%)	22,30,33	1.85	4 (18%)
22	OMC	BA	2498	57,22	19,22,23	2.73	7 (36%)	26,31,34	0.98	1 (3%)
22	PSU	BA	955	22	18,21,22	1.09	1 (5%)	22,30,33	1.78	4 (18%)
54	PSU	D2	39	54	18,21,22	0.93	1 (5%)	22,30,33	1.66	4 (18%)
55	H2U	D3	16	55	18,21,22	3.19	5 (27%)	21,30,33	1.65	4 (19%)
22	3TD	BA	1915	22	18,22,23	4.18	6 (33%)	22,32,35	1.69	3 (13%)
54	PSU	D2	55	54	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
1	2MG	AA	1516	1	18,26,27	2.40	6 (33%)	16,38,41	1.63	4 (25%)
22	5MU	BA	747	22	19,22,23	4.72	7 (36%)	28,32,35	3.70	9 (32%)
1	PSU	AA	516	57,1	18,21,22	1.03	3 (16%)	22,30,33	1.92	4 (18%)
54	5MU	D2	54	54	19,22,23	4.83	7 (36%)	28,32,35	3.68	9 (32%)
55	PSU	D3	55	55	18,21,22	1.15	1 (5%)	22,30,33	1.63	4 (18%)
22	6MZ	BA	2030	22	18,25,26	1.92	2 (11%)	16,36,39	2.91	3 (18%)
53	FME	D1	1	53	8,9,10	0.59	0	7,9,11	1.10	1 (14%)
34	4D4	BM	81	34	9,11,12	2.03	2 (22%)	8,13,15	1.97	3 (37%)
22	1MG	BA	745	22	18,26,27	2.54	5 (27%)	19,39,42	1.52	3 (15%)
1	2MG	AA	1207	1	18,26,27	2.45	6 (33%)	16,38,41	1.50	2 (12%)
22	PSU	BA	2580	22	18,21,22	1.10	3 (16%)	22,30,33	1.90	5 (22%)
22	PSU	BA	2604	22	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
54	OMG	D2	17(A)	54	18,26,27	2.65	8 (44%)	19,38,41	1.55	4 (21%)
54	G7M	D2	46	54	20,26,27	2.23	7 (35%)	17,39,42	1.15	1 (5%)
54	H2U	D2	17	54	18,21,22	3.06	5 (27%)	21,30,33	2.03	5 (23%)
54	4AC	D2	34	54	21,24,25	3.25	9 (42%)	29,34,37	2.03	9 (31%)
1	2MG	AA	966	1	18,26,27	2.36	5 (27%)	16,38,41	1.61	4 (25%)
12	D2T	AL	89	12	7,9,10	1.37	1 (14%)	6,11,13	1.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	5MU	BA	1939	22	19,22,23	4.66	7 (36%)	28,32,35	3.72	9 (32%)
22	OMU	BA	2552	22	19,22,23	2.99	8 (42%)	26,31,34	1.78	5 (19%)
1	5MC	AA	1407	1	18,22,23	3.18	7 (38%)	26,32,35	1.05	1 (3%)
55	H2U	D3	20	55	18,21,22	3.15	5 (27%)	21,30,33	1.90	4 (19%)
55	PSU	D3	32	55	18,21,22	1.11	1 (5%)	22,30,33	1.72	5 (22%)
1	UR3	AA	1498	1	19,22,23	2.60	6 (31%)	26,32,35	1.28	2 (7%)
22	2MG	BA	1835	22	18,26,27	2.56	6 (33%)	16,38,41	1.51	4 (25%)
1	4OC	AA	1402	1	20,23,24	2.89	8 (40%)	26,32,35	0.97	1 (3%)
22	PSU	BA	1917	22	18,21,22	1.00	1 (5%)	22,30,33	1.65	4 (18%)
54	H2U	D2	16	54	18,21,22	3.21	5 (27%)	21,30,33	1.77	5 (23%)
22	2MA	BA	2503	57,22	17,25,26	2.31	5 (29%)	17,37,40	1.40	3 (17%)
1	MA6	AA	1518	1	18,26,27	1.18	1 (5%)	19,38,41	4.21	3 (15%)
22	PSU	BA	2457	22	18,21,22	1.00	1 (5%)	22,30,33	1.91	4 (18%)
22	PSU	BA	2605	22	18,21,22	0.99	1 (5%)	22,30,33	1.77	3 (13%)
1	5MC	AA	967	1	18,22,23	3.25	7 (38%)	26,32,35	1.15	1 (3%)
25	MEQ	BD	150	25	8,9,10	0.93	0	5,10,12	0.75	0
55	PSU	D3	39	55	18,21,22	1.06	1 (5%)	22,30,33	1.74	5 (22%)
22	OMG	BA	2251	54,22	18,26,27	2.44	8 (44%)	19,38,41	1.48	4 (21%)
22	H2U	BA	2449	22	18,21,22	2.86	5 (27%)	21,30,33	2.01	5 (23%)
54	4SU	D2	8	54	18,21,22	3.61	8 (44%)	26,30,33	2.14	5 (19%)
22	5MC	BA	1962	22	18,22,23	3.31	7 (38%)	26,32,35	1.02	2 (7%)
22	G7M	BA	2069	22	20,26,27	2.16	7 (35%)	17,39,42	1.20	3 (17%)
54	T6A	D2	37	54	27,34,35	1.10	3 (11%)	29,49,52	2.17	8 (27%)
22	PSU	BA	746	57,22	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)
55	5MU	D3	54	55	19,22,23	4.88	7 (36%)	28,32,35	3.58	9 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	H2U	D2	20	54	-	3/7/38/39	0/2/2/2
22	PSU	BA	2504	22	-	2/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	2MG	BA	2445	22	-	2/5/27/28	0/3/3/3
22	6MZ	BA	1618	22	-	2/5/27/28	0/3/3/3
55	4SU	D3	8	55	-	7/7/25/26	0/2/2/2
54	H2U	D2	19	54	-	6/7/38/39	0/2/2/2
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
22	OMC	BA	2498	57,22	-	1/9/27/28	0/2/2/2
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
54	PSU	D2	39	54	-	3/7/25/26	0/2/2/2
55	H2U	D3	16	55	-	2/7/38/39	0/2/2/2
22	3TD	BA	1915	22	-	0/7/25/26	0/2/2/2
54	PSU	D2	55	54	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
22	5MU	BA	747	22	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	57,1	-	0/7/25/26	0/2/2/2
54	5MU	D2	54	54	-	2/7/25/26	0/2/2/2
55	PSU	D3	55	55	-	4/7/25/26	0/2/2/2
22	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
53	FME	D1	1	53	-	3/7/9/11	-
34	4D4	BM	81	34	-	3/11/12/14	-
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
22	PSU	BA	2580	22	-	2/7/25/26	0/2/2/2
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
54	OMG	D2	17(A)	54	-	0/5/27/28	0/3/3/3
54	G7M	D2	46	54	-	2/3/25/26	0/3/3/3
54	H2U	D2	17	54	-	1/7/38/39	0/2/2/2
54	4AC	D2	34	54	-	5/11/29/30	0/2/2/2
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
22	5MU	BA	1939	22	-	2/7/25/26	0/2/2/2
22	OMU	BA	2552	22	-	0/9/27/28	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
55	H2U	D3	20	55	-	4/7/38/39	0/2/2/2
55	PSU	D3	32	55	-	2/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	2/9/29/30	0/2/2/2
22	PSU	BA	1917	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	H2U	D2	16	54	-	5/7/38/39	0/2/2/2
22	2MA	BA	2503	57,22	-	2/3/25/26	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
25	MEQ	BD	150	25	-	3/8/9/11	-
55	PSU	D3	39	55	-	0/7/25/26	0/2/2/2
22	OMG	BA	2251	54,22	-	0/5/27/28	0/3/3/3
22	H2U	BA	2449	22	-	0/7/38/39	0/2/2/2
54	4SU	D2	8	54	-	2/7/25/26	0/2/2/2
22	5MC	BA	1962	22	-	0/7/25/26	0/2/2/2
22	G7M	BA	2069	22	-	3/3/25/26	0/3/3/3
54	T6A	D2	37	54	-	7/19/41/42	0/3/3/3
22	PSU	BA	746	57,22	-	1/7/25/26	0/2/2/2
55	5MU	D3	54	55	-	2/7/25/26	0/2/2/2

All (250) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C6-C5	12.07	1.49	1.35
54	D2	54	5MU	C2-N1	11.23	1.56	1.38
55	D3	54	5MU	C2-N1	11.22	1.56	1.38
55	D3	54	5MU	C6-N1	10.79	1.56	1.38
55	D3	16	H2U	C2-N1	10.54	1.50	1.35
54	D2	19	H2U	C2-N1	10.45	1.50	1.35
22	BA	747	5MU	C2-N1	10.40	1.55	1.38
54	D2	54	5MU	C6-N1	10.29	1.55	1.38
54	D2	16	H2U	C2-N1	10.22	1.50	1.35
22	BA	1939	5MU	C2-N1	10.19	1.54	1.38
22	BA	747	5MU	C6-N1	10.19	1.55	1.38
22	BA	1939	5MU	C6-N1	10.00	1.55	1.38
54	D2	54	5MU	C4-C5	9.90	1.61	1.44
55	D3	20	H2U	C2-N1	9.89	1.49	1.35
55	D3	54	5MU	C4-C5	9.86	1.61	1.44
22	BA	1939	5MU	C4-C5	9.55	1.60	1.44
22	BA	747	5MU	C4-C5	9.49	1.60	1.44
54	D2	17	H2U	C2-N1	9.31	1.48	1.35
54	D2	20	H2U	C2-N1	9.27	1.48	1.35
22	BA	1915	3TD	C2-N1	9.02	1.48	1.37
1	AA	967	5MC	C6-C5	8.69	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2449	H2U	C2-N1	8.50	1.47	1.35
22	BA	747	5MU	C4-N3	-8.32	1.23	1.38
22	BA	1962	5MC	C6-C5	8.29	1.48	1.34
22	BA	1939	5MU	C4-N3	-8.25	1.23	1.38
1	AA	1407	5MC	C6-C5	8.05	1.47	1.34
54	D2	54	5MU	C4-N3	-7.94	1.24	1.38
55	D3	54	5MU	C4-N3	-7.78	1.24	1.38
55	D3	8	4SU	C4-N3	7.42	1.45	1.37
22	BA	1618	6MZ	C6-N6	7.32	1.47	1.35
55	D3	8	4SU	C2-N1	7.23	1.50	1.38
54	D2	8	4SU	C4-N3	7.19	1.45	1.37
54	D2	8	4SU	C2-N1	7.16	1.49	1.38
22	BA	2552	OMU	C2-N3	7.01	1.50	1.38
22	BA	2503	2MA	C2-N3	7.00	1.46	1.31
55	D3	8	4SU	C2-N3	6.89	1.50	1.38
22	BA	2030	6MZ	C6-N6	6.89	1.46	1.35
54	D2	34	4AC	C4-N3	6.87	1.44	1.32
54	D2	8	4SU	C2-N3	6.61	1.49	1.38
54	D2	19	H2U	C2-N3	6.58	1.49	1.38
55	D3	20	H2U	C2-N3	6.56	1.49	1.38
54	D2	16	H2U	C2-N3	6.52	1.49	1.38
54	D2	17	H2U	C2-N3	6.46	1.49	1.38
1	AA	1207	2MG	C2-N2	6.37	1.47	1.33
22	BA	2552	OMU	C2-N1	6.36	1.48	1.38
54	D2	20	H2U	C2-N3	6.34	1.49	1.38
1	AA	1498	UR3	C6-C5	6.33	1.49	1.35
22	BA	1835	2MG	C2-N2	6.30	1.47	1.33
1	AA	1498	UR3	C2-N1	6.25	1.47	1.38
22	BA	1962	5MC	C4-N3	6.16	1.44	1.34
22	BA	2445	2MG	C2-N2	6.15	1.47	1.33
55	D3	16	H2U	C2-N3	6.11	1.48	1.38
22	BA	745	1MG	C2-N3	6.10	1.45	1.34
55	D3	54	5MU	C6-C5	6.07	1.44	1.34
54	D2	34	4AC	C6-C5	6.02	1.49	1.35
22	BA	2449	H2U	C2-N3	5.93	1.48	1.38
1	AA	966	2MG	C2-N2	5.92	1.46	1.33
22	BA	1962	5MC	C2-N3	5.87	1.48	1.36
54	D2	34	4AC	C2-N3	5.82	1.48	1.36
1	AA	1516	2MG	C2-N2	5.80	1.46	1.33
54	D2	54	5MU	C6-C5	5.79	1.44	1.34
22	BA	745	1MG	C2-N2	5.78	1.44	1.34
22	BA	2552	OMU	C6-C5	5.77	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	747	5MU	C6-C5	5.74	1.44	1.34
55	D3	8	4SU	C6-C5	5.69	1.48	1.35
1	AA	1407	5MC	C4-N3	5.66	1.43	1.34
22	BA	2498	OMC	C2-N3	5.63	1.47	1.36
54	D2	8	4SU	C6-C5	5.63	1.48	1.35
22	BA	2498	OMC	C6-C5	5.57	1.48	1.35
1	AA	1407	5MC	C2-N3	5.54	1.47	1.36
54	D2	17(A)	OMG	C2-N3	5.54	1.46	1.33
22	BA	1939	5MU	C6-C5	5.52	1.43	1.34
1	AA	967	5MC	C4-N3	5.46	1.43	1.34
22	BA	1915	3TD	C6-N1	5.45	1.45	1.36
1	AA	1402	4OC	C2-N3	5.43	1.47	1.36
1	AA	1402	4OC	C4-N3	5.42	1.42	1.32
1	AA	1402	4OC	C6-C5	5.35	1.47	1.35
1	AA	967	5MC	C2-N3	5.32	1.47	1.36
54	D2	17(A)	OMG	C4-N3	5.06	1.49	1.37
22	BA	1915	3TD	C2-N3	5.05	1.49	1.38
54	D2	19	H2U	C4-N3	5.00	1.46	1.37
22	BA	1835	2MG	C4-N3	4.99	1.49	1.37
54	D2	17	H2U	C4-N3	4.96	1.46	1.37
55	D3	20	H2U	C4-N3	4.93	1.46	1.37
1	AA	1402	4OC	C4-N4	4.91	1.46	1.35
54	D2	34	4AC	C7-N4	4.89	1.46	1.37
54	D2	46	G7M	C2-N2	4.87	1.45	1.34
22	BA	2445	2MG	C4-N3	4.87	1.49	1.37
54	D2	16	H2U	C4-N3	4.86	1.45	1.37
54	D2	20	H2U	C4-N3	4.86	1.45	1.37
22	BA	2251	OMG	C2-N3	4.86	1.45	1.33
22	BA	1835	2MG	C2-N1	4.84	1.44	1.36
54	D2	17(A)	OMG	C2-N2	4.83	1.45	1.34
55	D3	8	4SU	C5-C4	4.74	1.48	1.42
34	BM	81	4D4	CZ-NE	4.71	1.42	1.33
54	D2	34	4AC	C4-N4	4.67	1.46	1.39
22	BA	745	1MG	C4-N3	4.67	1.48	1.37
22	BA	2069	G7M	C2-N2	4.66	1.45	1.34
54	D2	8	4SU	C4-S4	-4.66	1.59	1.68
22	BA	2445	2MG	C2-N1	4.65	1.44	1.36
22	BA	2251	OMG	C4-N3	4.64	1.48	1.37
1	AA	527	G7M	C2-N2	4.60	1.45	1.34
1	AA	1498	UR3	C2-N3	4.59	1.47	1.39
55	D3	16	H2U	C4-N3	4.55	1.45	1.37
22	BA	2251	OMG	C2-N2	4.52	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2503	2MA	C4-N3	4.51	1.48	1.37
22	BA	2498	OMC	C4-N4	4.50	1.44	1.33
55	D3	8	4SU	C4-S4	-4.47	1.59	1.68
1	AA	1516	2MG	C4-N3	4.46	1.48	1.37
1	AA	1402	4OC	O2-C2	-4.42	1.15	1.23
1	AA	1207	2MG	C4-N3	4.38	1.48	1.37
54	D2	8	4SU	C5-C4	4.31	1.48	1.42
22	BA	2498	OMC	C4-N3	4.31	1.43	1.34
54	D2	34	4AC	C2-N1	4.30	1.49	1.40
54	D2	46	G7M	C4-N3	4.30	1.47	1.37
1	AA	1516	2MG	C2-N1	4.29	1.43	1.36
22	BA	2449	H2U	C4-N3	4.28	1.44	1.37
22	BA	2552	OMU	C4-N3	4.25	1.46	1.38
22	BA	2498	OMC	C2-N1	4.20	1.49	1.40
1	AA	966	2MG	C4-N3	4.20	1.47	1.37
22	BA	1962	5MC	C4-N4	4.16	1.44	1.34
1	AA	1207	2MG	C2-N1	4.13	1.43	1.36
54	D2	46	G7M	C2-N3	4.11	1.43	1.33
1	AA	966	2MG	C2-N1	4.11	1.43	1.36
22	BA	2069	G7M	C4-N3	4.09	1.47	1.37
22	BA	1915	3TD	O2-C2	-4.03	1.15	1.23
1	AA	967	5MC	C4-N4	3.98	1.44	1.34
22	BA	1962	5MC	C6-N1	3.96	1.44	1.38
1	AA	1407	5MC	C6-N1	3.94	1.44	1.38
54	D2	34	4AC	C5-C4	3.94	1.49	1.40
1	AA	527	G7M	C4-N3	3.88	1.46	1.37
55	D3	55	PSU	C6-C5	3.83	1.39	1.35
1	AA	1519	MA6	C5-C4	-3.82	1.30	1.40
54	D2	17(A)	OMG	C6-N1	3.82	1.43	1.37
1	AA	1407	5MC	C4-N4	3.80	1.44	1.34
1	AA	967	5MC	C6-N1	3.72	1.44	1.38
22	BA	1962	5MC	C2-N1	3.67	1.48	1.40
1	AA	527	G7M	C2-N3	3.66	1.42	1.33
55	D3	32	PSU	C6-C5	3.60	1.39	1.35
1	AA	967	5MC	O2-C2	-3.59	1.17	1.23
22	BA	2069	G7M	C2-N3	3.58	1.41	1.33
1	AA	527	G7M	O6-C6	-3.55	1.16	1.23
1	AA	1518	MA6	C5-C4	-3.55	1.31	1.40
1	AA	1402	4OC	C2-N1	3.42	1.47	1.40
1	AA	1407	5MC	C2-N1	3.42	1.47	1.40
54	D2	55	PSU	C6-C5	3.41	1.39	1.35
22	BA	2069	G7M	O6-C6	-3.39	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	D3	39	PSU	C6-C5	3.37	1.39	1.35
22	BA	2251	OMG	C6-N1	3.34	1.42	1.37
1	AA	966	2MG	C5-C4	-3.22	1.34	1.43
54	D2	17(A)	OMG	C5-C6	3.18	1.53	1.47
54	D2	46	G7M	O6-C6	-3.16	1.16	1.23
22	BA	1835	2MG	C6-N1	3.15	1.42	1.37
1	AA	1516	2MG	C5-C4	-3.14	1.35	1.43
1	AA	1407	5MC	O2-C2	-3.13	1.17	1.23
1	AA	967	5MC	C2-N1	3.13	1.46	1.40
22	BA	2445	2MG	C6-N1	3.13	1.42	1.37
1	AA	1207	2MG	C5-C4	-3.12	1.35	1.43
22	BA	955	PSU	C6-C5	3.10	1.38	1.35
1	AA	1402	4OC	C5-C4	3.10	1.47	1.40
22	BA	1911	PSU	C6-C5	3.09	1.38	1.35
1	AA	1402	4OC	CM4-N4	3.06	1.51	1.45
22	BA	745	1MG	C5-C4	-3.05	1.35	1.43
22	BA	2251	OMG	C5-C4	-3.04	1.35	1.43
54	D2	34	4AC	C6-N1	3.04	1.45	1.38
1	AA	1516	2MG	C6-N1	3.02	1.42	1.37
34	BM	81	4D4	CZ-NH2	2.98	1.44	1.32
22	BA	747	5MU	O2-C2	-2.96	1.17	1.23
22	BA	2498	OMC	O2-C2	-2.95	1.18	1.23
22	BA	746	PSU	C6-C5	2.94	1.38	1.35
22	BA	747	5MU	O4-C4	-2.94	1.18	1.23
22	BA	2445	2MG	C5-C4	-2.93	1.35	1.43
22	BA	2504	PSU	C6-C5	2.91	1.38	1.35
22	BA	1962	5MC	O2-C2	-2.91	1.18	1.23
22	BA	1939	5MU	O4-C4	-2.91	1.18	1.23
54	D2	46	G7M	C2-N1	2.90	1.44	1.37
22	BA	2445	2MG	C5-C6	2.90	1.53	1.47
55	D3	8	4SU	C6-N1	2.89	1.45	1.38
22	BA	1917	PSU	C6-C5	2.88	1.38	1.35
22	BA	1835	2MG	C5-C6	2.86	1.53	1.47
22	BA	2552	OMU	C6-N1	2.85	1.44	1.38
22	BA	2604	PSU	C6-C5	2.84	1.38	1.35
54	D2	34	4AC	O2-C2	-2.82	1.18	1.23
54	D2	17(A)	OMG	C2-N1	2.82	1.44	1.37
54	D2	46	G7M	C6-N1	2.78	1.42	1.37
54	D2	8	4SU	C6-N1	2.78	1.44	1.38
22	BA	1939	5MU	O2-C2	-2.76	1.18	1.23
54	D2	54	5MU	O4-C4	-2.75	1.18	1.23
22	BA	2449	H2U	O2-C2	-2.74	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2580	PSU	C6-C5	2.74	1.38	1.35
22	BA	2069	G7M	C2-N1	2.73	1.44	1.37
22	BA	2030	6MZ	C5-C4	-2.73	1.33	1.40
54	D2	39	PSU	C6-C5	2.73	1.38	1.35
22	BA	2552	OMU	O2-C2	-2.71	1.18	1.23
22	BA	2498	OMC	C6-N1	2.67	1.44	1.38
1	AA	1498	UR3	O4-C4	-2.63	1.17	1.23
22	BA	1835	2MG	C5-C4	-2.62	1.36	1.43
22	BA	2069	G7M	C6-N1	2.61	1.41	1.37
54	D2	8	4SU	O2-C2	-2.59	1.18	1.23
1	AA	1498	UR3	C6-N1	2.58	1.44	1.38
22	BA	2251	OMG	O6-C6	-2.58	1.18	1.23
54	D2	19	H2U	O2-C2	-2.57	1.18	1.23
54	D2	17(A)	OMG	C5-C4	-2.56	1.36	1.43
1	AA	1207	2MG	C6-N1	2.55	1.41	1.37
55	D3	54	5MU	O4-C4	-2.54	1.18	1.23
54	D2	46	G7M	C5-C6	2.54	1.52	1.45
54	D2	16	H2U	O2-C2	-2.54	1.18	1.23
22	BA	2449	H2U	O4-C4	-2.52	1.18	1.23
22	BA	2503	2MA	C5-C4	-2.51	1.36	1.43
54	D2	20	H2U	O2-C2	-2.48	1.18	1.23
1	AA	527	G7M	C2-N1	2.47	1.43	1.37
22	BA	2605	PSU	C6-C5	2.46	1.38	1.35
55	D3	54	5MU	O2-C2	-2.46	1.18	1.23
54	D2	17	H2U	O2-C2	-2.46	1.18	1.23
55	D3	16	H2U	O2-C2	-2.43	1.18	1.23
22	BA	2251	OMG	C5-C6	2.42	1.52	1.47
22	BA	2503	2MA	C2-N1	2.40	1.44	1.36
22	BA	1915	3TD	O4-C4	-2.40	1.18	1.23
1	AA	1516	2MG	C5-C6	2.38	1.52	1.47
22	BA	745	1MG	O6-C6	-2.38	1.17	1.22
22	BA	2251	OMG	C2-N1	2.38	1.43	1.37
55	D3	20	H2U	O2-C2	-2.35	1.18	1.23
55	D3	8	4SU	O2-C2	-2.35	1.18	1.23
54	D2	37	T6A	C10-N6	-2.34	1.32	1.37
22	BA	1618	6MZ	C5-C4	-2.33	1.34	1.40
22	BA	2552	OMU	C5-C4	2.31	1.48	1.43
22	BA	2580	PSU	O4'-C1'	-2.29	1.40	1.43
1	AA	527	G7M	C6-N1	2.27	1.41	1.37
1	AA	966	2MG	C6-N1	2.25	1.41	1.37
54	D2	54	5MU	O2-C2	-2.24	1.18	1.23
54	D2	17(A)	OMG	O6-C6	-2.21	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2552	OMU	O4-C4	-2.19	1.20	1.24
22	BA	2503	2MA	C6-N1	2.19	1.42	1.38
1	AA	1207	2MG	C5-C6	2.18	1.51	1.47
22	BA	2457	PSU	C6-C5	2.18	1.37	1.35
54	D2	20	H2U	O4-C4	-2.17	1.18	1.23
22	BA	1618	6MZ	C2-N3	2.17	1.35	1.32
1	AA	516	PSU	C6-C5	2.16	1.37	1.35
12	AL	89	D2T	CB1-SB	-2.14	1.75	1.79
22	BA	2069	G7M	C5-C6	2.14	1.51	1.45
54	D2	17	H2U	O4-C4	-2.14	1.18	1.23
54	D2	16	H2U	O4-C4	-2.13	1.18	1.23
55	D3	20	H2U	O4-C4	-2.12	1.19	1.23
54	D2	37	T6A	C2'-C1'	-2.12	1.50	1.53
55	D3	16	H2U	O4-C4	-2.10	1.19	1.23
1	AA	516	PSU	C4-C5	-2.08	1.38	1.44
1	AA	516	PSU	O4'-C1'	-2.06	1.41	1.43
1	AA	1498	UR3	O2-C2	-2.05	1.18	1.22
54	D2	37	T6A	C5-C4	2.05	1.46	1.40
22	BA	2580	PSU	C4-C5	-2.02	1.38	1.44

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	MA6	C1'-N9-C4	12.74	149.02	126.64
54	D2	54	5MU	C5-C4-N3	12.41	125.90	115.31
22	BA	1939	5MU	C5-C4-N3	12.30	125.81	115.31
22	BA	747	5MU	C5-C4-N3	12.19	125.72	115.31
55	D3	54	5MU	C5-C4-N3	12.13	125.66	115.31
1	AA	1519	MA6	N1-C6-N6	-12.08	104.34	117.06
1	AA	1519	MA6	C1'-N9-C4	12.01	147.75	126.64
1	AA	1518	MA6	N1-C6-N6	-11.59	104.86	117.06
22	BA	1939	5MU	C5-C6-N1	-10.47	112.57	123.34
22	BA	747	5MU	C5-C6-N1	-10.31	112.74	123.34
55	D3	54	5MU	C5-C6-N1	-9.93	113.12	123.34
54	D2	54	5MU	C5-C6-N1	-9.92	113.13	123.34
22	BA	2030	6MZ	C9-N6-C6	-8.59	115.47	122.87
55	D3	8	4SU	C4-N3-C2	-7.64	119.92	127.34
54	D2	20	H2U	C4-N3-C2	-7.43	119.62	125.79
54	D2	17	H2U	C4-N3-C2	-7.05	119.95	125.79
22	BA	2449	H2U	C4-N3-C2	-7.03	119.96	125.79
54	D2	8	4SU	C4-N3-C2	-6.94	120.60	127.34
54	D2	34	4AC	CM7-C7-N4	6.75	126.97	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D3	20	H2U	C4-N3-C2	-6.51	120.39	125.79
22	BA	2030	6MZ	N3-C2-N1	-5.92	119.42	128.68
1	AA	1519	MA6	N3-C2-N1	-5.84	119.56	128.68
54	D2	37	T6A	N6-C10-N11	5.79	121.85	113.76
54	D2	16	H2U	C4-N3-C2	-5.77	121.01	125.79
22	BA	2552	OMU	C4-N3-C2	-5.59	119.21	126.58
1	AA	1518	MA6	N3-C2-N1	-5.57	119.97	128.68
54	D2	19	H2U	C4-N3-C2	-5.49	121.23	125.79
22	BA	1915	3TD	N1-C2-N3	5.35	120.36	116.14
22	BA	1618	6MZ	C9-N6-C6	-5.31	118.30	122.87
22	BA	1618	6MZ	N3-C2-N1	-5.29	120.41	128.68
22	BA	1939	5MU	C4-N3-C2	-5.19	120.63	127.35
55	D3	54	5MU	O4-C4-C5	-5.17	118.91	124.90
22	BA	747	5MU	C4-N3-C2	-5.15	120.69	127.35
54	D2	54	5MU	O4-C4-C5	-5.12	118.97	124.90
22	BA	747	5MU	O4-C4-C5	-5.11	118.98	124.90
22	BA	1939	5MU	O4-C4-C5	-5.11	118.98	124.90
54	D2	8	4SU	C5-C4-N3	5.10	119.42	114.69
54	D2	37	T6A	C2-N1-C6	5.05	120.92	116.59
55	D3	8	4SU	C5-C4-N3	5.05	119.38	114.69
22	BA	2457	PSU	N1-C2-N3	5.04	120.84	115.13
22	BA	747	5MU	N3-C2-N1	4.96	121.47	114.89
22	BA	2580	PSU	N1-C2-N3	4.91	120.69	115.13
54	D2	54	5MU	C4-N3-C2	-4.89	121.02	127.35
22	BA	2457	PSU	C4-N3-C2	-4.88	119.31	126.34
22	BA	1911	PSU	C4-N3-C2	-4.87	119.32	126.34
22	BA	2605	PSU	C4-N3-C2	-4.87	119.33	126.34
1	AA	516	PSU	N1-C2-N3	4.85	120.63	115.13
22	BA	1911	PSU	N1-C2-N3	4.83	120.60	115.13
55	D3	54	5MU	C4-N3-C2	-4.82	121.12	127.35
1	AA	516	PSU	C4-N3-C2	-4.78	119.45	126.34
22	BA	1939	5MU	N3-C2-N1	4.72	121.16	114.89
22	BA	955	PSU	C4-N3-C2	-4.66	119.63	126.34
22	BA	746	PSU	C4-N3-C2	-4.64	119.65	126.34
55	D3	54	5MU	N3-C2-N1	4.62	121.02	114.89
22	BA	2504	PSU	N1-C2-N3	4.60	120.34	115.13
54	D2	55	PSU	C4-N3-C2	-4.55	119.78	126.34
22	BA	955	PSU	N1-C2-N3	4.55	120.28	115.13
54	D2	55	PSU	N1-C2-N3	4.52	120.25	115.13
1	AA	1498	UR3	C4-N3-C2	-4.52	120.31	124.56
54	D2	39	PSU	C4-N3-C2	-4.52	119.83	126.34
22	BA	2604	PSU	N1-C2-N3	4.50	120.23	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D3	39	PSU	C4-N3-C2	-4.49	119.87	126.34
22	BA	2605	PSU	N1-C2-N3	4.46	120.18	115.13
1	AA	967	5MC	C5-C6-N1	-4.44	118.77	123.34
55	D3	32	PSU	C4-N3-C2	-4.44	119.94	126.34
55	D3	39	PSU	N1-C2-N3	4.44	120.16	115.13
22	BA	2580	PSU	C4-N3-C2	-4.41	119.98	126.34
22	BA	2030	6MZ	C2-N1-C6	4.39	120.35	116.59
22	BA	746	PSU	N1-C2-N3	4.36	120.08	115.13
22	BA	745	1MG	C5-C6-N1	4.34	120.42	113.90
55	D3	16	H2U	C4-N3-C2	-4.33	122.20	125.79
22	BA	2604	PSU	C4-N3-C2	-4.29	120.16	126.34
54	D2	54	5MU	N3-C2-N1	4.28	120.58	114.89
55	D3	32	PSU	N1-C2-N3	4.27	119.97	115.13
22	BA	2504	PSU	C4-N3-C2	-4.26	120.19	126.34
22	BA	1917	PSU	N1-C2-N3	4.26	119.95	115.13
1	AA	1207	2MG	C5-C6-N1	4.24	121.44	113.95
54	D2	37	T6A	N6-C6-N1	4.20	124.34	118.72
54	D2	54	5MU	C5M-C5-C4	4.18	123.37	118.77
54	D2	54	5MU	C5M-C5-C6	-4.16	117.29	122.85
55	D3	55	PSU	N1-C2-N3	4.09	119.77	115.13
55	D3	8	4SU	N3-C2-N1	4.09	120.32	114.89
22	BA	2552	OMU	N3-C2-N1	4.07	120.29	114.89
22	BA	1917	PSU	C4-N3-C2	-4.05	120.50	126.34
54	D2	39	PSU	N1-C2-N3	4.05	119.72	115.13
22	BA	1915	3TD	C4-N3-C2	-4.01	120.26	124.61
55	D3	55	PSU	C4-N3-C2	-3.95	120.65	126.34
22	BA	2503	2MA	C5-C6-N1	3.85	120.67	114.02
22	BA	1939	5MU	C5M-C5-C6	-3.84	117.72	122.85
22	BA	1835	2MG	C5-C6-N1	3.78	120.63	113.95
1	AA	966	2MG	CM2-N2-C2	-3.75	115.58	123.86
22	BA	747	5MU	C5M-C5-C6	-3.71	117.90	122.85
1	AA	966	2MG	C5-C6-N1	3.68	120.46	113.95
22	BA	2445	2MG	C5-C6-N1	3.65	120.40	113.95
54	D2	8	4SU	N3-C2-N1	3.64	119.72	114.89
1	AA	1516	2MG	CM2-N2-C2	-3.57	115.97	123.86
1	AA	1516	2MG	C5-C6-N1	3.56	120.23	113.95
22	BA	1939	5MU	C5M-C5-C4	3.55	122.68	118.77
54	D2	34	4AC	O7-C7-N4	-3.45	116.22	121.82
1	AA	516	PSU	O2-C2-N1	-3.44	119.00	122.79
55	D3	8	4SU	C5-C4-S4	-3.43	120.05	124.47
22	BA	2552	OMU	C5-C4-N3	3.42	119.95	114.84
34	BM	81	4D4	NE-CZ-NH2	-3.41	114.69	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D2	17(A)	OMG	C5-C6-N1	3.41	119.97	113.95
55	D3	54	5MU	C5M-C5-C6	-3.35	118.37	122.85
22	BA	2251	OMG	C5-C6-N1	3.34	119.84	113.95
22	BA	1618	6MZ	C2-N1-C6	3.34	119.45	116.59
54	D2	8	4SU	C5-C4-S4	-3.33	120.18	124.47
54	D2	19	H2U	C5-C6-N1	3.32	122.55	111.61
22	BA	747	5MU	C5M-C5-C4	3.31	122.41	118.77
54	D2	20	H2U	N3-C2-N1	3.29	120.13	116.65
55	D3	16	H2U	C5-C6-N1	3.26	122.35	111.61
22	BA	2449	H2U	N3-C2-N1	3.23	120.06	116.65
54	D2	17	H2U	N3-C2-N1	3.22	120.06	116.65
22	BA	2580	PSU	C6-N1-C2	-3.19	119.42	122.68
55	D3	16	H2U	O2-C2-N3	-3.19	115.56	121.50
1	AA	527	G7M	C2-N1-C6	-3.15	119.30	125.10
55	D3	20	H2U	N3-C2-N1	3.07	119.90	116.65
34	BM	81	4D4	NH1-CZ-NE	3.07	126.27	119.19
55	D3	54	5MU	C5M-C5-C4	3.05	122.12	118.77
22	BA	2445	2MG	CM2-N2-C2	-3.04	117.14	123.86
54	D2	37	T6A	O10-C10-N6	-3.04	118.47	123.62
54	D2	16	H2U	C5-C6-N1	3.04	121.61	111.61
54	D2	8	4SU	C1'-N1-C2	3.01	123.03	117.57
54	D2	17(A)	OMG	C8-N7-C5	3.01	108.73	102.99
54	D2	16	H2U	N3-C2-N1	3.00	119.83	116.65
54	D2	34	4AC	C5-C4-N3	-2.99	117.77	122.59
54	D2	19	H2U	N3-C2-N1	2.99	119.81	116.65
54	D2	20	H2U	C5-C4-N3	2.98	120.00	116.65
54	D2	46	G7M	C2-N1-C6	-2.97	119.64	125.10
54	D2	34	4AC	C1'-N1-C2	2.91	124.91	118.42
22	BA	747	5MU	O2-C2-N1	-2.91	118.92	122.79
22	BA	2251	OMG	C2-N1-C6	-2.90	119.75	125.10
22	BA	2457	PSU	O2-C2-N1	-2.89	119.61	122.79
54	D2	55	PSU	O2-C2-N1	-2.84	119.66	122.79
22	BA	1962	5MC	C5-C6-N1	-2.83	120.42	123.34
54	D2	34	4AC	O7-C7-CM7	-2.83	116.81	122.06
54	D2	34	4AC	C6-C5-C4	2.82	120.41	116.96
54	D2	17	H2U	C5-C4-N3	2.82	119.81	116.65
55	D3	20	H2U	C5-C6-N1	2.81	120.89	111.61
54	D2	17(A)	OMG	C2-N1-C6	-2.81	119.93	125.10
22	BA	1939	5MU	O2-C2-N1	-2.80	119.07	122.79
22	BA	2552	OMU	O4-C4-C5	-2.79	120.25	125.16
54	D2	37	T6A	N3-C2-N1	-2.79	124.32	128.68
54	D2	34	4AC	O2-C2-N3	-2.76	117.84	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2504	PSU	O2-C2-N1	-2.75	119.77	122.79
22	BA	2504	PSU	C6-N1-C2	-2.73	119.90	122.68
22	BA	1917	PSU	C6-N1-C2	-2.72	119.90	122.68
22	BA	2580	PSU	O2-C2-N1	-2.72	119.80	122.79
1	AA	1516	2MG	O6-C6-C5	-2.71	119.07	124.37
53	D1	1	FME	O-C-CA	-2.71	117.68	124.78
22	BA	2445	2MG	C8-N7-C5	2.71	108.14	102.99
1	AA	1407	5MC	C5-C6-N1	-2.71	120.56	123.34
22	BA	2251	OMG	C8-N7-C5	2.69	108.12	102.99
22	BA	1835	2MG	CM2-N2-C2	-2.69	117.92	123.86
22	BA	2503	2MA	C8-N7-C5	2.67	108.08	102.99
22	BA	2449	H2U	C5-C4-N3	2.65	119.63	116.65
22	BA	2069	G7M	C2-N1-C6	-2.63	120.26	125.10
22	BA	745	1MG	C8-N7-C5	2.62	107.99	102.99
22	BA	1917	PSU	O2-C2-N1	-2.62	119.91	122.79
22	BA	2457	PSU	C6-N1-C2	-2.62	120.00	122.68
54	D2	17	H2U	C5-C6-N1	2.62	120.24	111.61
1	AA	1207	2MG	O6-C6-C5	-2.60	119.28	124.37
1	AA	516	PSU	C6-N1-C2	-2.60	120.02	122.68
54	D2	54	5MU	O4-C4-N3	-2.60	115.13	120.12
54	D2	37	T6A	C4-C5-N7	-2.60	106.69	109.40
22	BA	2498	OMC	O2-C2-N3	-2.59	118.12	122.33
22	BA	955	PSU	O2-C2-N1	-2.59	119.94	122.79
54	D2	17	H2U	O2-C2-N1	-2.58	119.87	123.11
54	D2	20	H2U	O2-C2-N1	-2.57	119.88	123.11
55	D3	20	H2U	C5-C4-N3	2.57	119.53	116.65
54	D2	37	T6A	C3'-C2'-C1'	2.57	104.84	100.98
22	BA	1939	5MU	O4-C4-N3	-2.56	115.20	120.12
22	BA	2449	H2U	C5-C6-N1	2.56	120.05	111.61
22	BA	1911	PSU	O2-C2-N1	-2.54	119.99	122.79
55	D3	55	PSU	C6-N1-C2	-2.54	120.09	122.68
55	D3	55	PSU	O2-C2-N1	-2.52	120.02	122.79
22	BA	747	5MU	O4-C4-N3	-2.51	115.30	120.12
22	BA	746	PSU	O2-C2-N1	-2.51	120.03	122.79
22	BA	2604	PSU	O2-C2-N1	-2.49	120.05	122.79
54	D2	19	H2U	O2-C2-N3	-2.49	116.87	121.50
22	BA	2580	PSU	O4'-C1'-C2'	2.47	108.63	105.14
54	D2	20	H2U	C5-C6-N1	2.46	119.73	111.61
22	BA	2069	G7M	N2-C2-N1	2.46	121.96	116.71
22	BA	745	1MG	O6-C6-C5	-2.46	119.83	124.19
55	D3	39	PSU	O2-C2-N1	-2.46	120.08	122.79
22	BA	2552	OMU	O2-C2-N1	-2.46	119.52	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	D3	54	5MU	O4-C4-N3	-2.45	115.42	120.12
22	BA	1835	2MG	C8-N7-C5	2.44	107.64	102.99
55	D3	16	H2U	N3-C2-N1	2.43	119.22	116.65
22	BA	1835	2MG	O6-C6-C5	-2.41	119.67	124.37
1	AA	966	2MG	O6-C6-C5	-2.39	119.70	124.37
1	AA	1402	4OC	C6-C5-C4	2.38	119.87	116.96
22	BA	2604	PSU	C6-N1-C2	-2.35	120.28	122.68
54	D2	55	PSU	C6-N1-C2	-2.34	120.29	122.68
55	D3	54	5MU	O2-C2-N1	-2.33	119.69	122.79
22	BA	955	PSU	C6-N1-C2	-2.31	120.32	122.68
1	AA	1516	2MG	C8-N7-C5	2.30	107.37	102.99
22	BA	2449	H2U	O2-C2-N1	-2.30	120.22	123.11
54	D2	34	4AC	C5-C4-N4	2.29	126.90	122.92
55	D3	32	PSU	C6-N1-C2	-2.24	120.39	122.68
22	BA	1911	PSU	C6-N1-C2	-2.23	120.40	122.68
22	BA	2445	2MG	O6-C6-C5	-2.23	120.02	124.37
55	D3	32	PSU	O2-C2-N1	-2.22	120.35	122.79
22	BA	2251	OMG	O6-C6-C5	-2.21	120.05	124.37
34	BM	81	4D4	O-C-CA	-2.20	119.02	124.78
1	AA	966	2MG	C8-N7-C5	2.19	107.16	102.99
54	D2	16	H2U	C5-C4-N3	2.18	119.10	116.65
55	D3	8	4SU	C1'-N1-C2	2.18	121.52	117.57
22	BA	746	PSU	C6-N1-C2	-2.18	120.45	122.68
54	D2	16	H2U	O2-C2-N3	-2.18	117.45	121.50
22	BA	1915	3TD	C6-C5-C4	2.17	119.72	118.22
1	AA	1498	UR3	C6-N1-C2	-2.17	119.85	121.79
54	D2	17(A)	OMG	O6-C6-C5	-2.14	120.19	124.37
54	D2	19	H2U	C5-C4-N3	2.13	119.04	116.65
55	D3	39	PSU	O4'-C1'-C2'	2.11	108.12	105.14
22	BA	1962	5MC	CM5-C5-C6	-2.11	120.03	122.85
54	D2	34	4AC	C1'-N1-C6	-2.09	116.29	120.84
55	D3	39	PSU	C6-N1-C2	-2.08	120.56	122.68
54	D2	39	PSU	O4-C4-N3	-2.07	116.16	120.12
54	D2	39	PSU	O2-C2-N1	-2.06	120.52	122.79
22	BA	2069	G7M	N1-C2-N3	-2.06	119.46	123.32
22	BA	2605	PSU	O2-C2-N1	-2.06	120.52	122.79
54	D2	54	5MU	O2-C2-N1	-2.04	120.07	122.79
55	D3	32	PSU	O4'-C1'-C2'	2.04	108.02	105.14
54	D2	37	T6A	C13-C12-N11	2.03	114.71	110.28
22	BA	2503	2MA	CM2-C2-N1	2.01	120.70	116.23

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
22	BA	1618	6MZ	O4'-C4'-C5'-O5'
22	BA	1618	6MZ	C3'-C4'-C5'-O5'
22	BA	2030	6MZ	O4'-C4'-C5'-O5'
22	BA	2030	6MZ	C3'-C4'-C5'-O5'
34	BM	81	4D4	NE-CD-CG-CB
53	D1	1	FME	O1-CN-N-CA
53	D1	1	FME	CA-CB-CG-SD
54	D2	16	H2U	O4'-C1'-N1-C2
54	D2	16	H2U	O4'-C1'-N1-C6
54	D2	34	4AC	O4'-C4'-C5'-O5'
54	D2	37	T6A	C3'-C4'-C5'-O5'
54	D2	39	PSU	C2'-C1'-C5-C4
54	D2	39	PSU	O4'-C1'-C5-C4
54	D2	39	PSU	O4'-C1'-C5-C6
54	D2	54	5MU	C3'-C4'-C5'-O5'
54	D2	54	5MU	O4'-C4'-C5'-O5'
55	D3	8	4SU	C2'-C1'-N1-C2
55	D3	8	4SU	C2'-C1'-N1-C6
55	D3	16	H2U	O4'-C1'-N1-C2
55	D3	16	H2U	O4'-C1'-N1-C6
55	D3	20	H2U	O4'-C4'-C5'-O5'
55	D3	32	PSU	C2'-C1'-C5-C4
54	D2	19	H2U	C2'-C1'-N1-C2
1	AA	966	2MG	C3'-C4'-C5'-O5'
1	AA	1402	4OC	O4'-C4'-C5'-O5'
54	D2	19	H2U	O4'-C4'-C5'-O5'
54	D2	34	4AC	C3'-C4'-C5'-O5'
55	D3	20	H2U	C3'-C4'-C5'-O5'
55	D3	54	5MU	C3'-C4'-C5'-O5'
54	D2	8	4SU	O4'-C4'-C5'-O5'
54	D2	16	H2U	O4'-C4'-C5'-O5'
54	D2	16	H2U	C3'-C4'-C5'-O5'
54	D2	19	H2U	C3'-C4'-C5'-O5'
54	D2	20	H2U	O4'-C4'-C5'-O5'
55	D3	54	5MU	O4'-C4'-C5'-O5'
54	D2	19	H2U	C2'-C1'-N1-C6
54	D2	20	H2U	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	D2	37	T6A	C14-C12-C13-ODA
1	AA	1402	4OC	C3'-C4'-C5'-O5'
22	BA	2445	2MG	C3'-C4'-C5'-O5'
54	D2	8	4SU	C3'-C4'-C5'-O5'
54	D2	37	T6A	N11-C12-C13-ODA
22	BA	2069	G7M	O4'-C4'-C5'-O5'
22	BA	2069	G7M	C3'-C4'-C5'-O5'
22	BA	2504	PSU	O4'-C4'-C5'-O5'
54	D2	37	T6A	O4'-C4'-C5'-O5'
55	D3	8	4SU	O4'-C4'-C5'-O5'
22	BA	2580	PSU	O4'-C4'-C5'-O5'
55	D3	8	4SU	O4'-C1'-N1-C6
34	BM	81	4D4	OB-CB-CG-CD
55	D3	8	4SU	O4'-C1'-N1-C2
53	D1	1	FME	CB-CG-SD-CE
54	D2	37	T6A	C14-C12-C13-ODB
25	BD	150	MEQ	OE1-CD-CG-CB
54	D2	34	4AC	O7-C7-N4-C4
54	D2	34	4AC	CM7-C7-N4-C4
25	BD	150	MEQ	NE2-CD-CG-CB
22	BA	1939	5MU	O4'-C4'-C5'-O5'
22	BA	2503	2MA	O4'-C4'-C5'-O5'
54	D2	37	T6A	N11-C12-C13-ODB
54	D2	16	H2U	C4'-C5'-O5'-P
54	D2	17	H2U	C4'-C5'-O5'-P
55	D3	8	4SU	C3'-C4'-C5'-O5'
54	D2	46	G7M	C4'-C5'-O5'-P
55	D3	8	4SU	C4'-C5'-O5'-P
55	D3	55	PSU	C4'-C5'-O5'-P
25	BD	150	MEQ	N-CA-CB-CG
55	D3	55	PSU	C3'-C4'-C5'-O5'
55	D3	55	PSU	O4'-C4'-C5'-O5'
22	BA	2069	G7M	C4'-C5'-O5'-P
54	D2	19	H2U	C4'-C5'-O5'-P
22	BA	2445	2MG	O4'-C4'-C5'-O5'
22	BA	1939	5MU	C3'-C4'-C5'-O5'
34	BM	81	4D4	CA-CB-CG-CD
54	D2	20	H2U	C2'-C1'-N1-C6
54	D2	37	T6A	N11-C12-C14-O14
22	BA	2498	OMC	O4'-C4'-C5'-O5'
22	BA	2503	2MA	C3'-C4'-C5'-O5'
22	BA	2504	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
22	BA	2580	PSU	C3'-C4'-C5'-O5'
54	D2	34	4AC	C2'-C1'-N1-C2
54	D2	46	G7M	C3'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
22	BA	746	PSU	O4'-C1'-C5-C6
55	D3	32	PSU	O4'-C1'-C5-C6
55	D3	55	PSU	O4'-C1'-C5-C6
54	D2	19	H2U	O4'-C1'-N1-C2
55	D3	20	H2U	C2'-C1'-N1-C2
55	D3	20	H2U	C4'-C5'-O5'-P

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	D3	8	4SU	1	0
55	D3	16	H2U	6	0
22	BA	1915	3TD	1	0
55	D3	55	PSU	1	0
22	BA	2030	6MZ	1	0
53	D1	1	FME	5	0
54	D2	46	G7M	1	0
55	D3	32	PSU	1	0
22	BA	2503	2MA	1	0
54	D2	37	T6A	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 173 ligands modelled in this entry, 172 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	ERY	BA	3001	-	53,53,53	0.43	0	82,82,82	0.95	5 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	ERY	BA	3001	-	-	7/72/107/107	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	BA	3001	ERY	C12-C11-C10	-4.27	111.08	116.43
58	BA	3001	ERY	O5-C16-C15	-2.64	108.73	112.96
58	BA	3001	ERY	O7-C5-C6	2.33	109.26	106.39
58	BA	3001	ERY	C16-C15-C14	-2.30	111.08	115.07
58	BA	3001	ERY	C6-C5-C4	-2.12	111.04	114.05

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	ERY	C23-C24-N1-C29
58	BA	3001	ERY	C25-C24-N1-C28
58	BA	3001	ERY	C23-C24-N1-C28
58	BA	3001	ERY	C25-C24-N1-C29
58	BA	3001	ERY	O2-C13-C36-C37
58	BA	3001	ERY	C12-C13-C36-C37
58	BA	3001	ERY	C30-C2-C3-C4

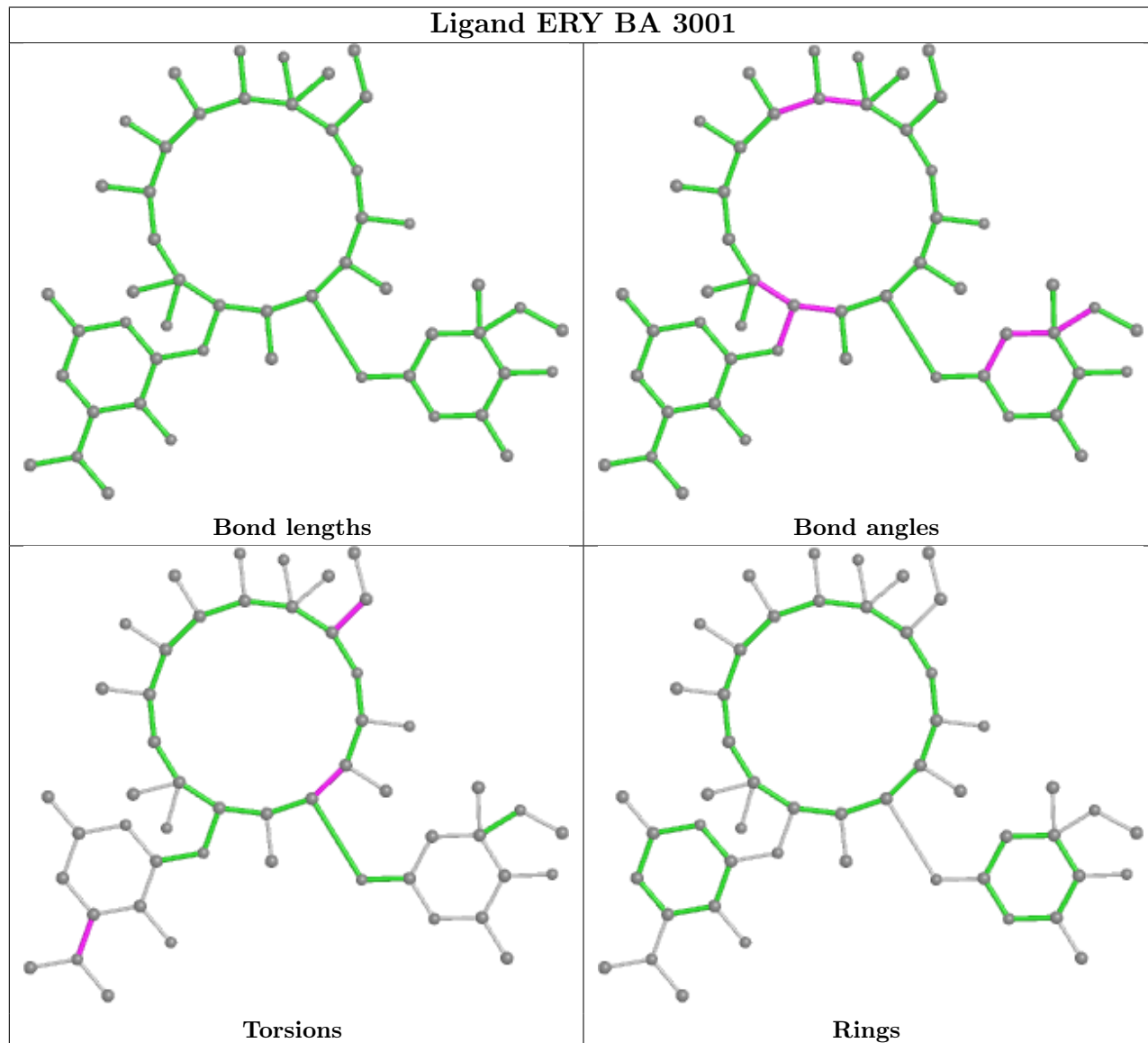
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	BA	3001	ERY	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

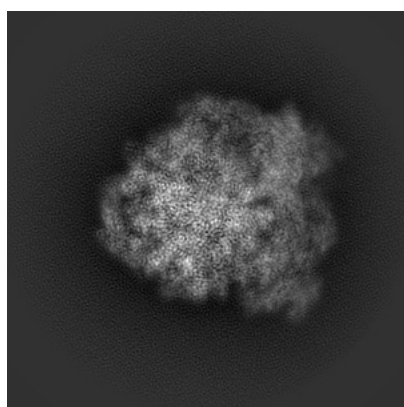
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13805. These allow visual inspection of the internal detail of the map and identification of artifacts.

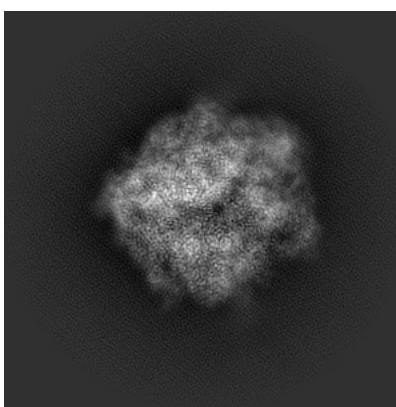
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

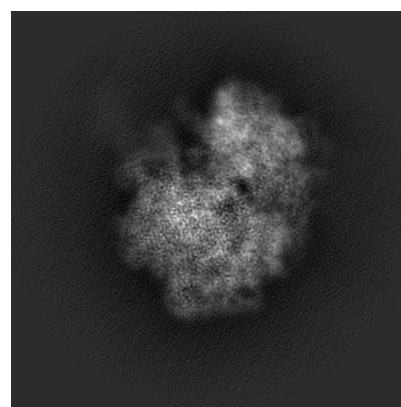
6.1.1 Primary map



X



Y

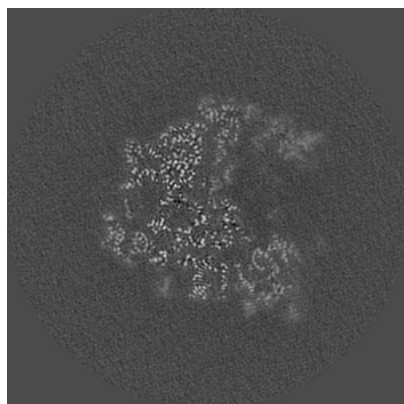


Z

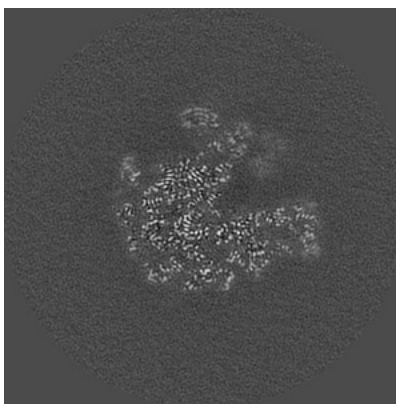
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

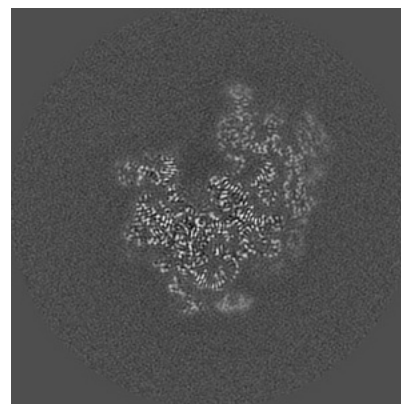
6.2.1 Primary map



X Index: 180



Y Index: 180

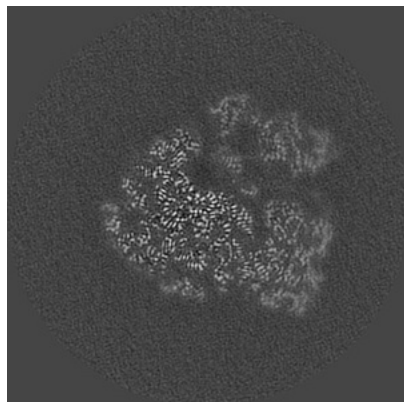


Z Index: 180

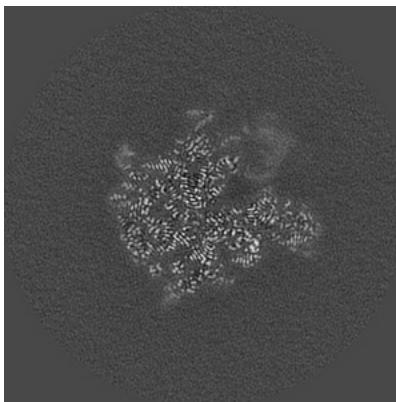
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

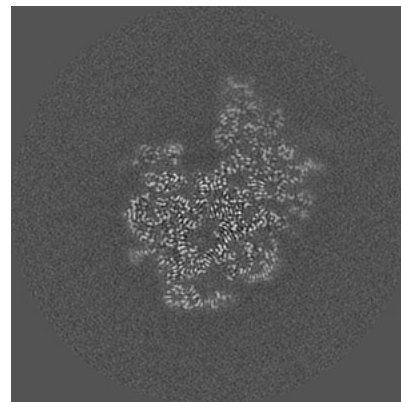
6.3.1 Primary map



X Index: 190



Y Index: 172

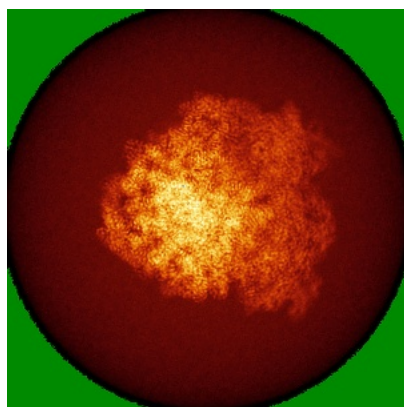


Z Index: 169

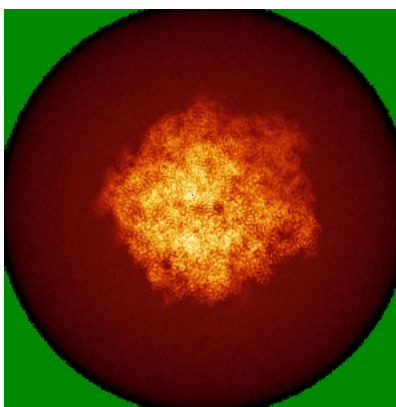
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

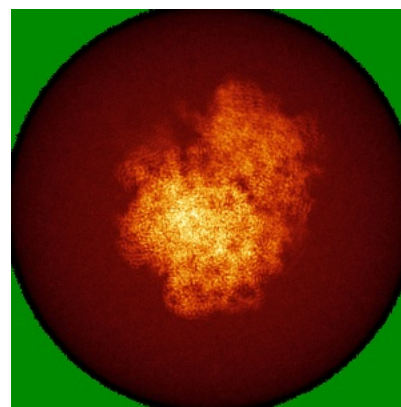
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

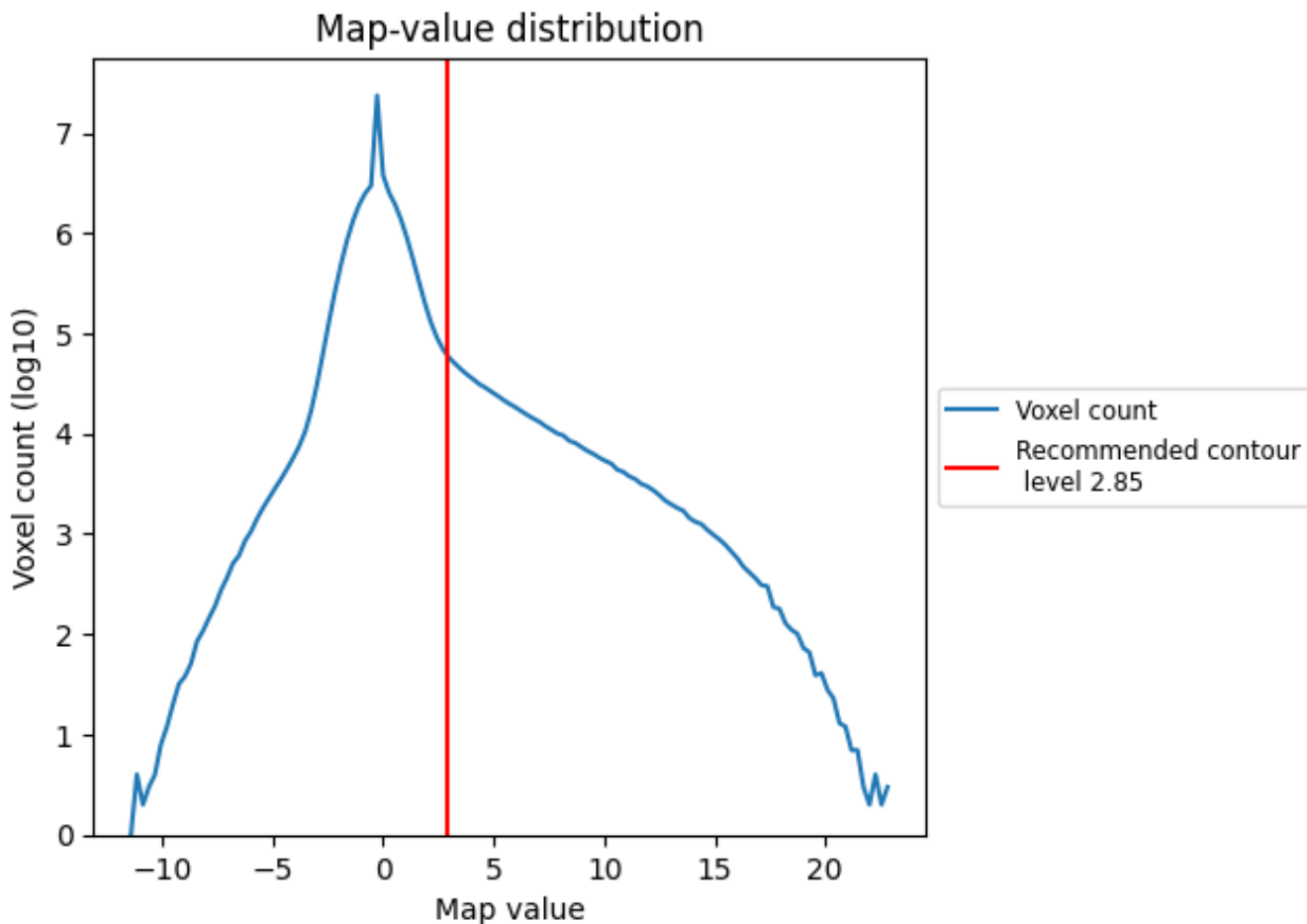
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

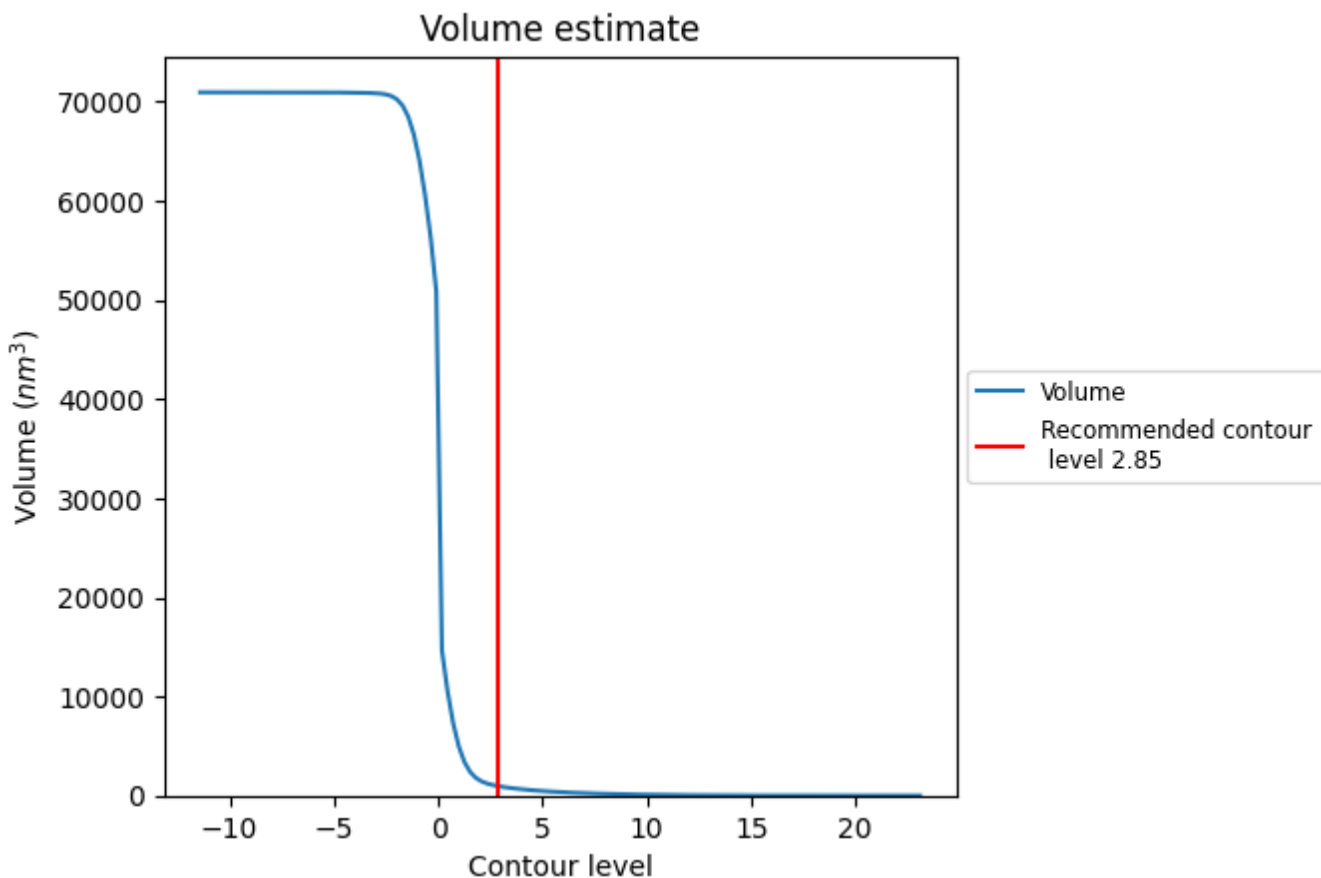
This section contains the results of statistical analysis of the map.

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.

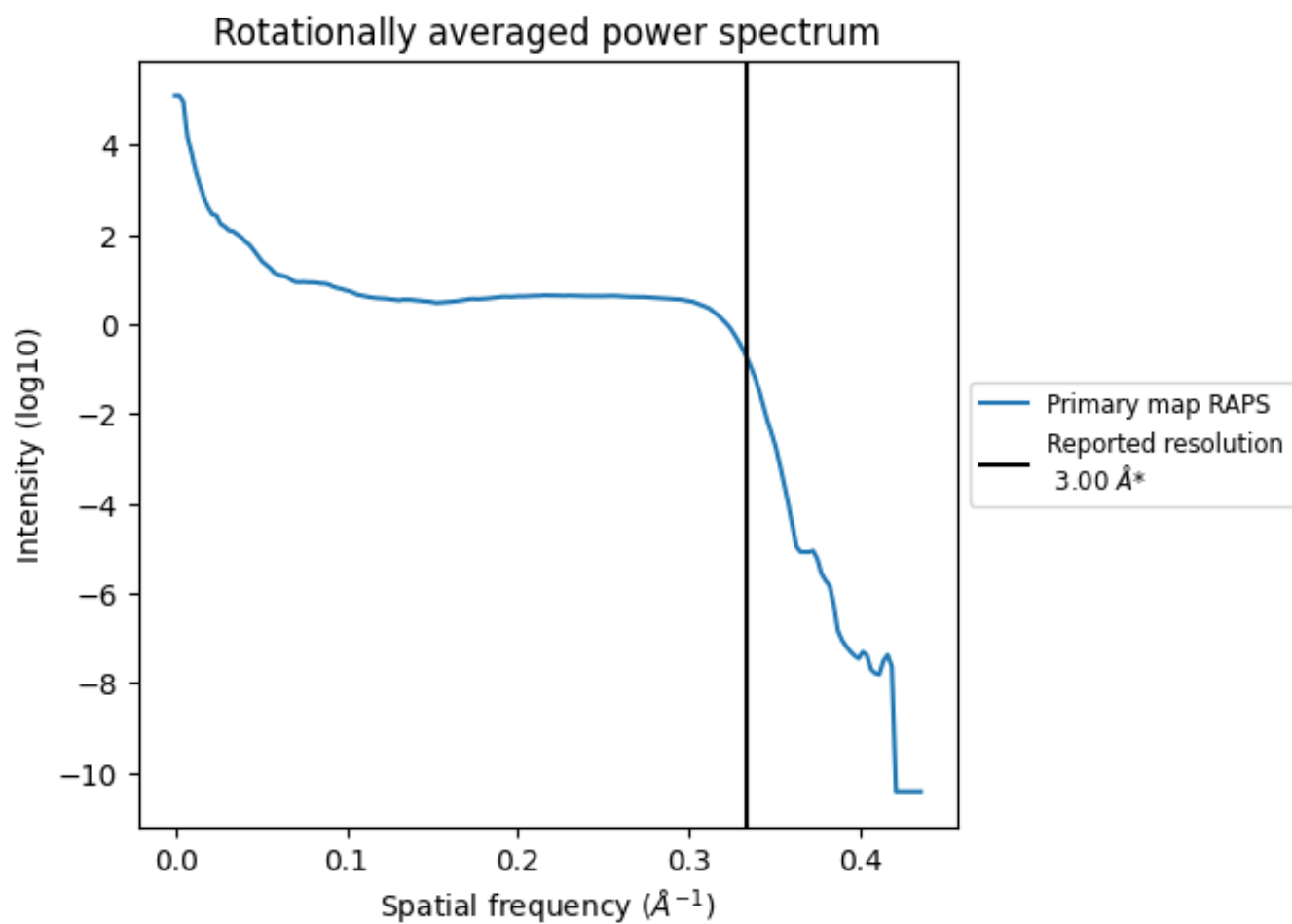
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 959 nm³; this corresponds to an approximate mass of 866 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 0.333 Å⁻¹

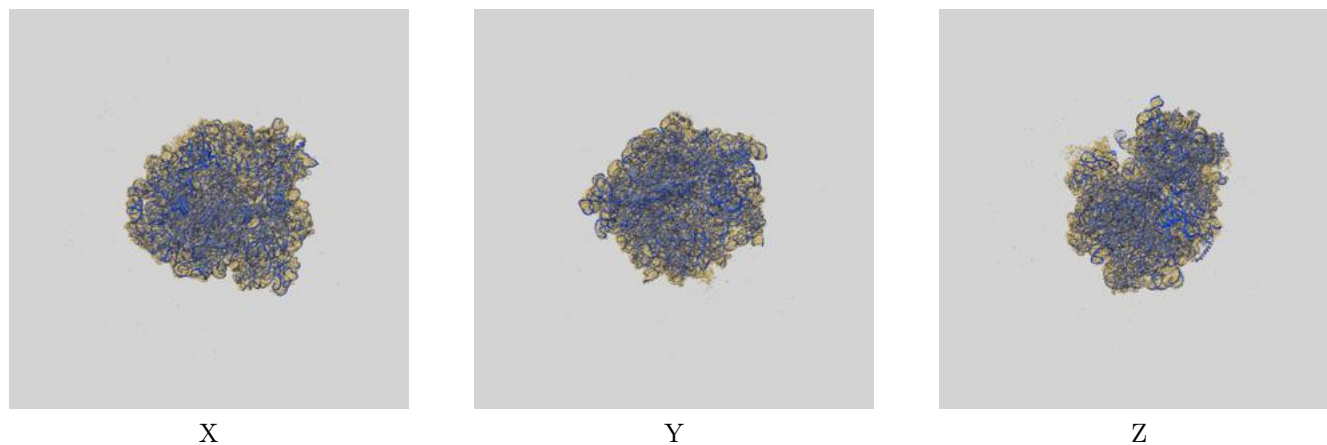
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

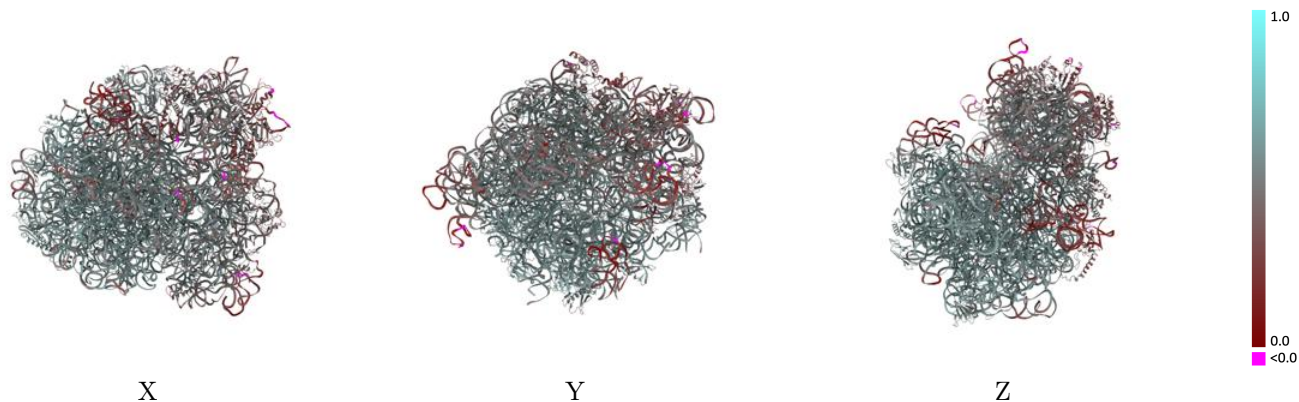
This section contains information regarding the fit between EMDB map EMD-13805 and PDB model 7Q4K. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

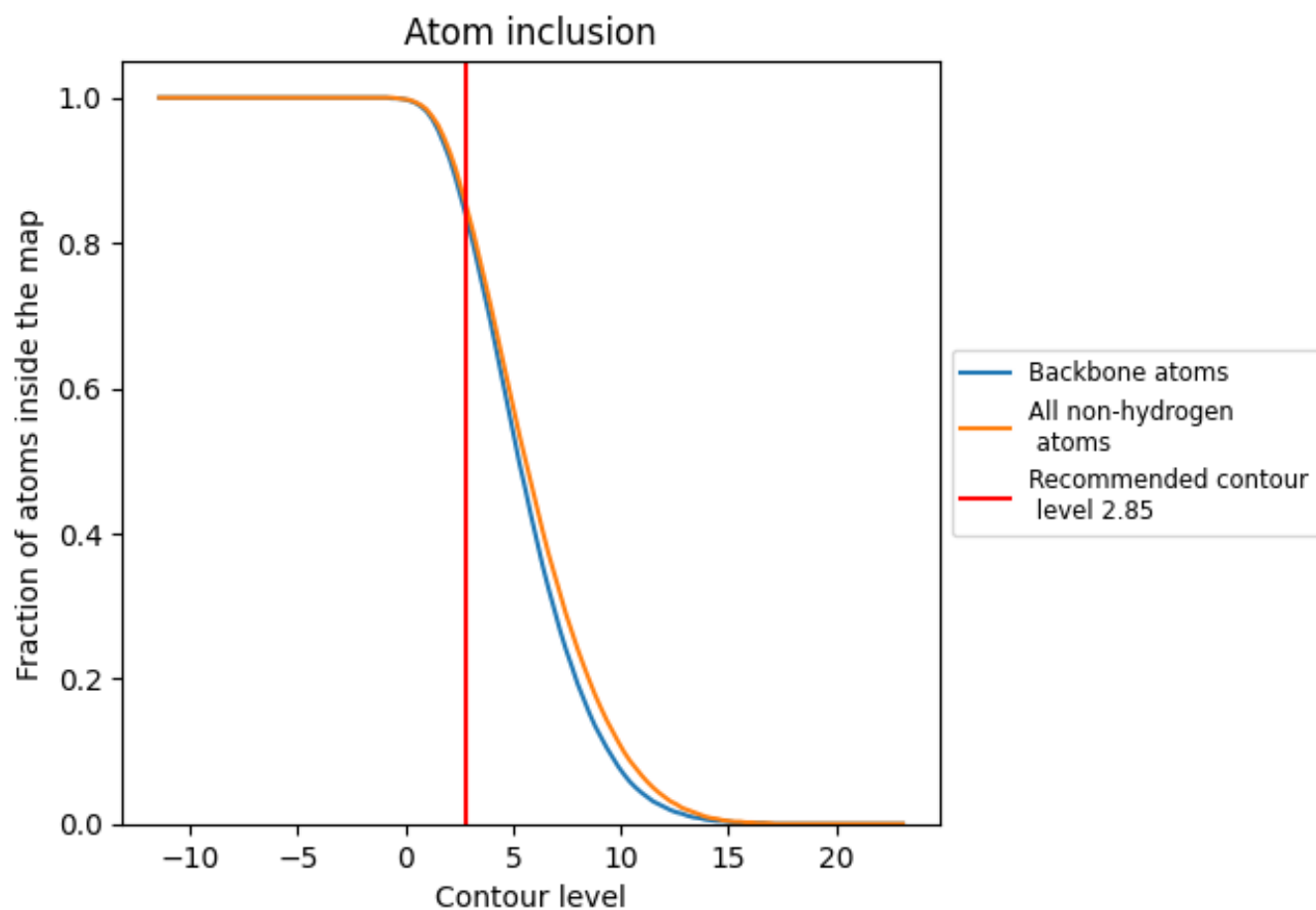


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary













































The table lists the average atom inclusion at the recommended contour level (2.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8490	 0.5140
AA	 0.8790	 0.4770
AB	 0.4950	 0.3570
AC	 0.6150	 0.4030
AD	 0.6160	 0.4130
AE	 0.7280	 0.4880
AF	 0.6710	 0.4290
AG	 0.5470	 0.3450
AH	 0.7160	 0.4960
AI	 0.6330	 0.3880
AJ	 0.5050	 0.3260
AK	 0.7350	 0.4870
AL	 0.7280	 0.5090
AM	 0.6490	 0.3910
AN	 0.6760	 0.4110
AO	 0.7590	 0.4920
AP	 0.7030	 0.4730
AQ	 0.6710	 0.4810
AR	 0.7390	 0.4760
AS	 0.6550	 0.4090
AT	 0.7360	 0.4740
AU	 0.6080	 0.4160
B0	 0.8600	 0.5770
B1	 0.8080	 0.5600
B2	 0.8840	 0.5990
B3	 0.9180	 0.5890
B4	 0.8870	 0.5830
BA	 0.9240	 0.5500
BB	 0.9420	 0.5430
BC	 0.8800	 0.5770
BD	 0.8780	 0.5810
BE	 0.8180	 0.5560
BF	 0.7400	 0.4930
BG	 0.7810	 0.5250
BH	 0.3300	 0.4060



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Chain	Atom inclusion	Q-score
BI	 0.5700	 0.3970
BJ	 0.8900	 0.5850
BK	 0.8360	 0.5700
BL	 0.8560	 0.5630
BM	 0.8630	 0.5740
BN	 0.9320	 0.5940
BO	 0.8520	 0.5480
BP	 0.8420	 0.5740
BQ	 0.9000	 0.5860
BR	 0.8630	 0.5730
BS	 0.8730	 0.5780
BT	 0.8120	 0.5570
BU	 0.8270	 0.5500
BV	 0.8360	 0.5560
BW	 0.8920	 0.5760
BX	 0.8650	 0.5680
BY	 0.8240	 0.5540
BZ	 0.8440	 0.5680
D1	 0.7680	 0.5620
D2	 0.7750	 0.4750
D3	 0.1840	 0.3060
D4	 0.7090	 0.4500