



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 02:27 pm GMT

PDB ID : 6TBV
EMDB ID : EMD-10453
Title : Cryo-EM structure of an Escherichia coli ribosome-SpeFL complex stalled in response to L-ornithine (Replicate 2)
Authors : Herrero del Valle, A.; Innis, C.A.
Deposited on : 2019-11-04
Resolution : 2.70 Å(reported)
Based on initial model : 4YBB

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

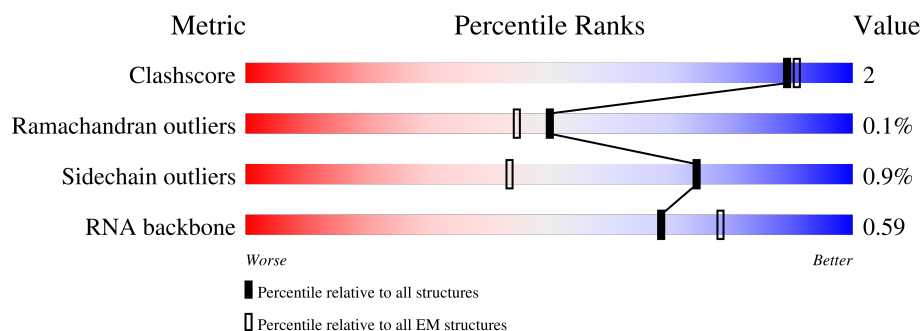
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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



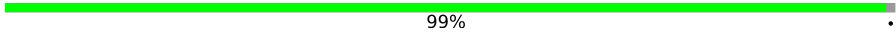
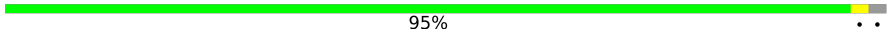
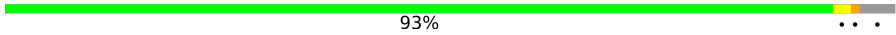

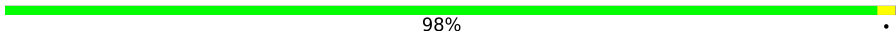
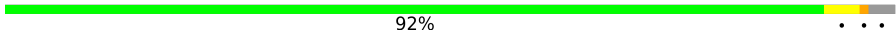
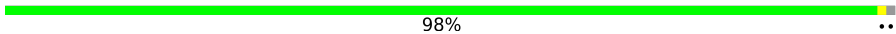
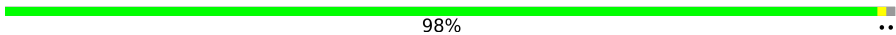
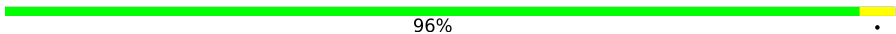
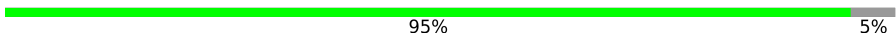


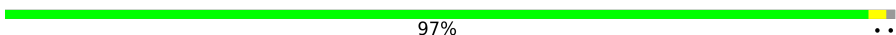



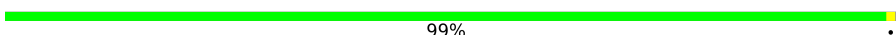
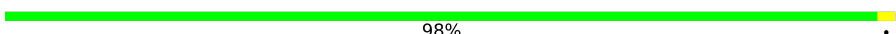
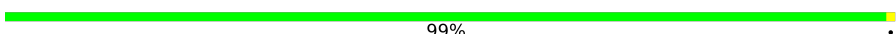
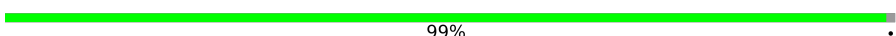
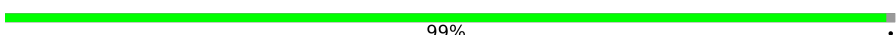
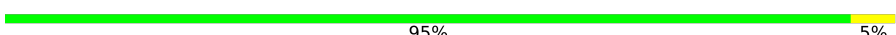

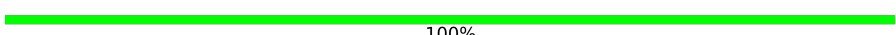
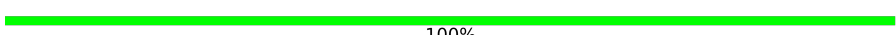
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	16S1	1534	<div> <div>65%</div> <div>30%</div> <div>5%</div> </div>
2	S021	241	<div> <div>90%</div> <div>7%</div> </div>
3	S031	233	<div> <div>88%</div> <div>12%</div> </div>
4	S041	206	<div> <div>97%</div> </div>
5	S051	167	<div> <div>92%</div> <div>7%</div> </div>
6	S061	135	<div> <div>79%</div> <div>21%</div> </div>
7	S071	179	<div> <div>82%</div> <div>16%</div> </div>

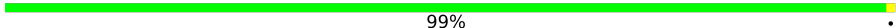
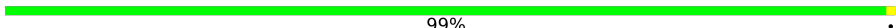

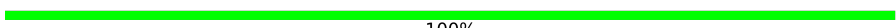
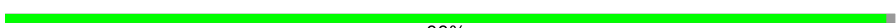








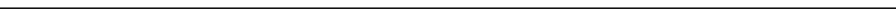

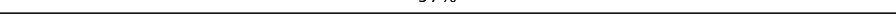
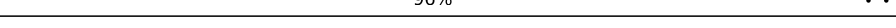

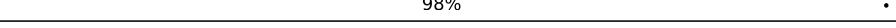
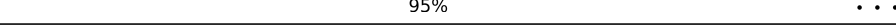
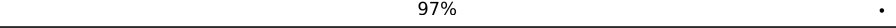


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	S081	130	
9	S091	130	
10	S101	103	
11	S111	129	
12	S121	124	
13	S131	118	
14	S141	102	
15	S151	89	
16	S161	82	
17	S171	84	
18	S181	75	
19	S191	92	
20	S201	87	
21	S211	71	
22	23S1	2897	
23	05S1	120	
24	L021	273	
25	L031	209	
26	L041	201	
27	L051	179	
28	L061	177	
29	L091	149	
30	L311	70	
31	L131	142	
32	L141	123	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	L151	144	 99% .
34	L161	136	 99% .
35	L171	127	 92% . 7%
36	L181	117	 100%
37	L191	115	 99% .
38	L201	118	 98% ..
39	L211	103	 100%
40	L221	110	 99% .
41	L231	100	 92% . 7%
42	L241	104	 97% ..
43	L251	94	 100%
44	L271	85	 89% 11%
45	L281	78	 96% ..
46	L291	63	 98% .
47	L301	59	 97% ..
48	L321	57	 96% ..
49	L331	55	 91% . 7%
50	L341	46	 98% .
51	L351	65	 95% ...
52	L361	38	 97% .
53	SPE1	34	 88% 12%
54	MRN1	7	 43% 43% 14%
55	PTR1	76	 59% 32% 9%

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 146672 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
1	16S1	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S021	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S031	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S041	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S051	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S061	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S071	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S081	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S091	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S101	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S111	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S121	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S131	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S141	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S141	35	ALA	-	insertion	UNP P0AG59

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S151	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S161	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S171	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S181	55	Total	C	N	O	0	0
			455	288	86	81		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S191	82	Total	C	N	O	S	0	0
			656	419	125	110	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S201	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	S211	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	23S1	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	05S1	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	L021	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	L031	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	L041	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L051	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L061	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L091	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L311	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L131	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L141	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L151	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L161	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L171	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L181	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L191	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	L201	117	Total	C	N	O	0	0
			947	604	192	151		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L211	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L221	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	L231	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	L241	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	L251	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	L271	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	L281	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	L291	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	L301	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L321	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L331	51	Total	C	N	O		0	0
			414	266	76	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L341	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	L351	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	L361	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called SpeFL.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SPE1	34	Total	C	N	O	S	0	0
			300	187	62	48	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SPE1	5	SER	ASN	conflict	UNP A0A4S4NWS2
SPE1	7	THR	LEU	conflict	UNP A0A4S4NWS2

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	MRN1	7	Total	C	N	O	P	0	0
			146	65	23	51	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
55	PTR1	76	Total	C	N	O	P	S	0	0
			1627	727	294	528	76	2		

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

Mol	Chain	Residues	Atoms		AltConf
56	16S1	87	Total	Mg	0
			87	87	
56	23S1	250	Total	Mg	0
			250	250	
56	L231	1	Total	Mg	0
			1	1	
56	PTR1	1	Total	Mg	0
			1	1	

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	16S1	39	Total	K	0
			39	39	
57	23S1	105	Total	K	0
			105	105	
57	05S1	1	Total	K	0
			1	1	
57	L031	1	Total	K	0
			1	1	
57	L161	1	Total	K	0
			1	1	

- Molecule 58 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
58	16S1	148	Total	X	0
			148	148	
58	S021	1	Total	X	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	S031	1	Total 1	X 1	0
58	S111	2	Total 2	X 2	0
58	S131	1	Total 1	X 1	0
58	S171	1	Total 1	X 1	0
58	23S1	919	Total 919	X 919	0
58	05S1	9	Total 9	X 9	0
58	L021	20	Total 20	X 20	0
58	L031	14	Total 14	X 14	0
58	L041	10	Total 10	X 10	0
58	L131	5	Total 5	X 5	0
58	L141	7	Total 7	X 7	0
58	L151	4	Total 4	X 4	0
58	L161	3	Total 3	X 3	0
58	L171	5	Total 5	X 5	0
58	L181	1	Total 1	X 1	0
58	L191	4	Total 4	X 4	0
58	L201	7	Total 7	X 7	0
58	L211	1	Total 1	X 1	0
58	L221	8	Total 8	X 8	0
58	L231	1	Total 1	X 1	0
58	L241	2	Total 2	X 2	0

Continued on next page...

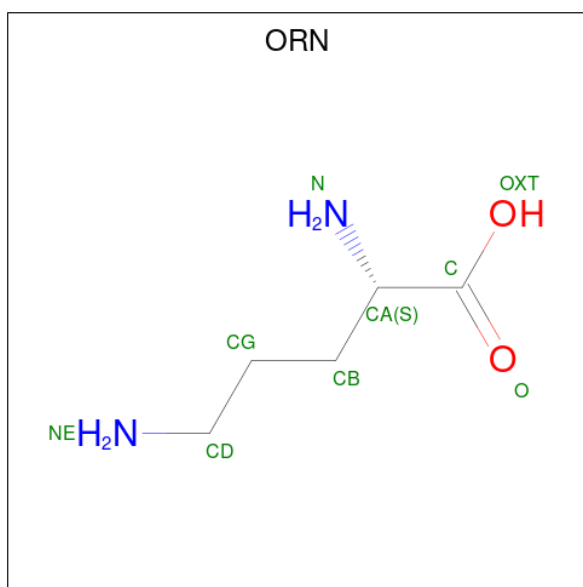
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	L251	1	Total 1	X 1	0
58	L271	1	Total 1	X 1	0
58	L281	1	Total 1	X 1	0
58	L321	2	Total 2	X 2	0
58	L331	1	Total 1	X 1	0
58	L341	7	Total 7	X 7	0
58	L351	4	Total 4	X 4	0
58	SPE1	6	Total 6	X 6	0
58	MRN1	1	Total 1	X 1	0
58	PTR1	3	Total 3	X 3	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	S021	1	Total 1	Zn 1	0
59	L311	1	Total 1	Zn 1	0
59	L361	1	Total 1	Zn 1	0

- Molecule 60 is L-ornithine (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				AltConf
60	23S1	1	Total	C	N	O	0
			9	5	2	2	

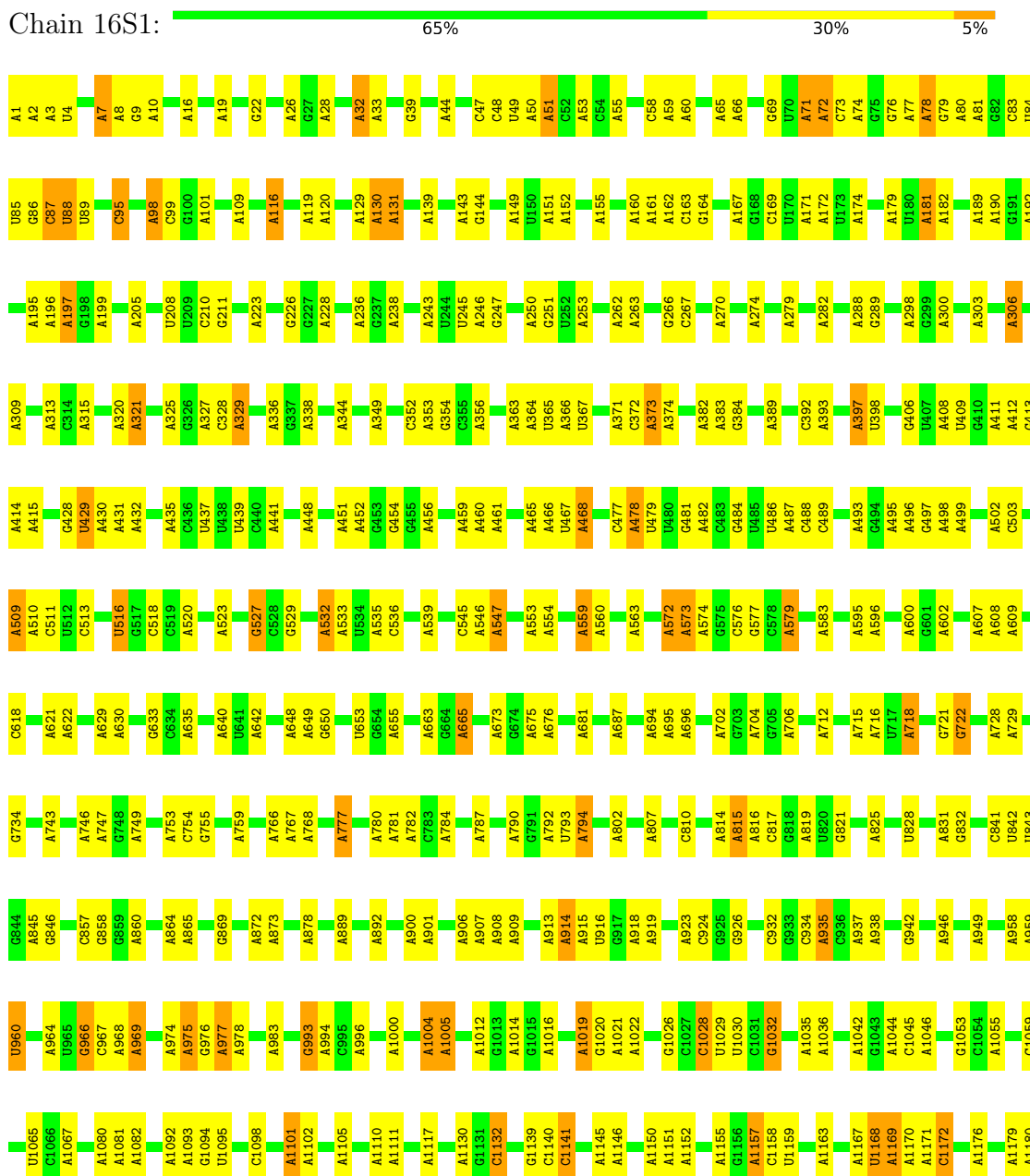
- Molecule 61 is water.

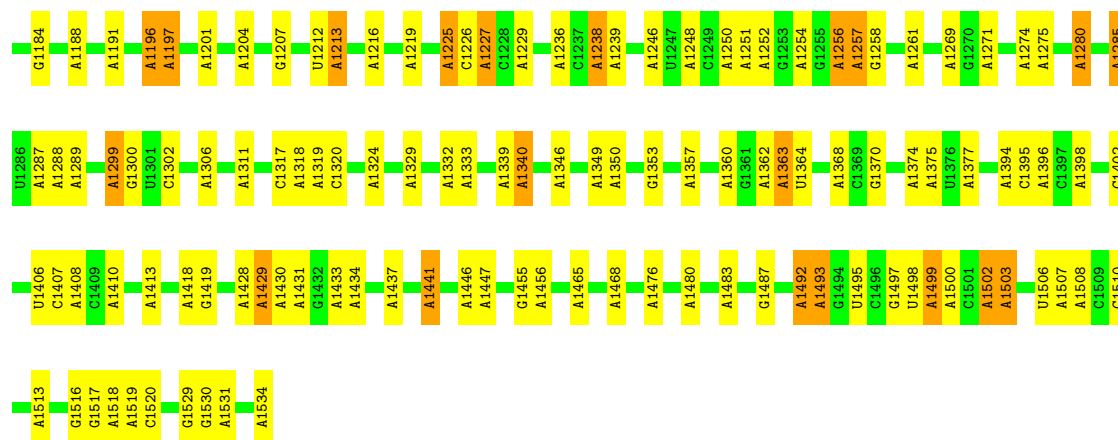
Mol	Chain	Residues	Atoms		AltConf
61	16S1	165	Total	O	0
			165	165	
61	S111	1	Total	O	0
			1	1	
61	S131	2	Total	O	0
			2	2	
61	S141	3	Total	O	0
			3	3	
61	S171	1	Total	O	0
			1	1	
61	23S1	616	Total	O	0
			616	616	
61	L021	6	Total	O	0
			6	6	
61	L031	2	Total	O	0
			2	2	
61	L151	2	Total	O	0
			2	2	
61	L171	2	Total	O	0
			2	2	

3 Residue-property plots

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

• Molecule 1: 16S rRNA

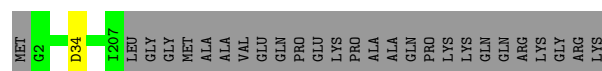




- Molecule 2: 30S ribosomal protein S2



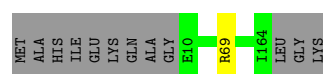
- Molecule 3: 30S ribosomal protein S3



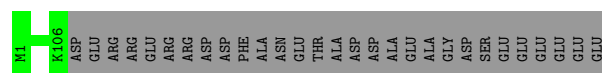
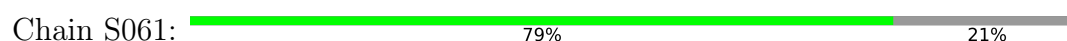
- Molecule 4: 30S ribosomal protein S4




- Molecule 5: 30S ribosomal protein S5

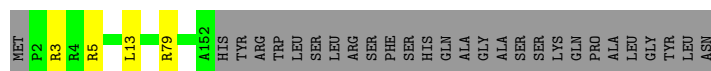


- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

Chain S071:  82% 16%



- Molecule 8: 30S ribosomal protein S8

Chain S081:  99%



- Molecule 9: 30S ribosomal protein S9

Chain S091:  95%



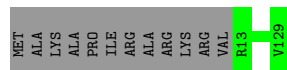
- Molecule 10: 30S ribosomal protein S10

Chain S101:  93%



- Molecule 11: 30S ribosomal protein S11

Chain S111:  91% 9%



- Molecule 12: 30S ribosomal protein S12

Chain S121:  98%



- Molecule 13: 30S ribosomal protein S13

Chain S131:  92%



- Molecule 14: 30S ribosomal protein S14

Chain S141:  98% ..



- Molecule 15: 30S ribosomal protein S15

Chain S151:  98% ..



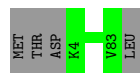
- Molecule 16: 30S ribosomal protein S16

Chain S161:  96% .




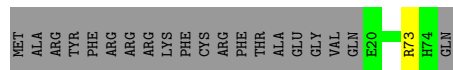
- Molecule 17: 30S ribosomal protein S17

Chain S171:  95% 5%



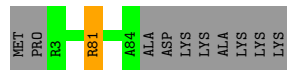
- Molecule 18: 30S ribosomal protein S18

Chain S181:  72% . 27%



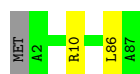
- Molecule 19: 30S ribosomal protein S19

Chain S191:  88% . 11%




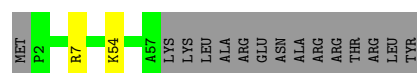
- Molecule 20: 30S ribosomal protein S20

Chain S201:  97% ..



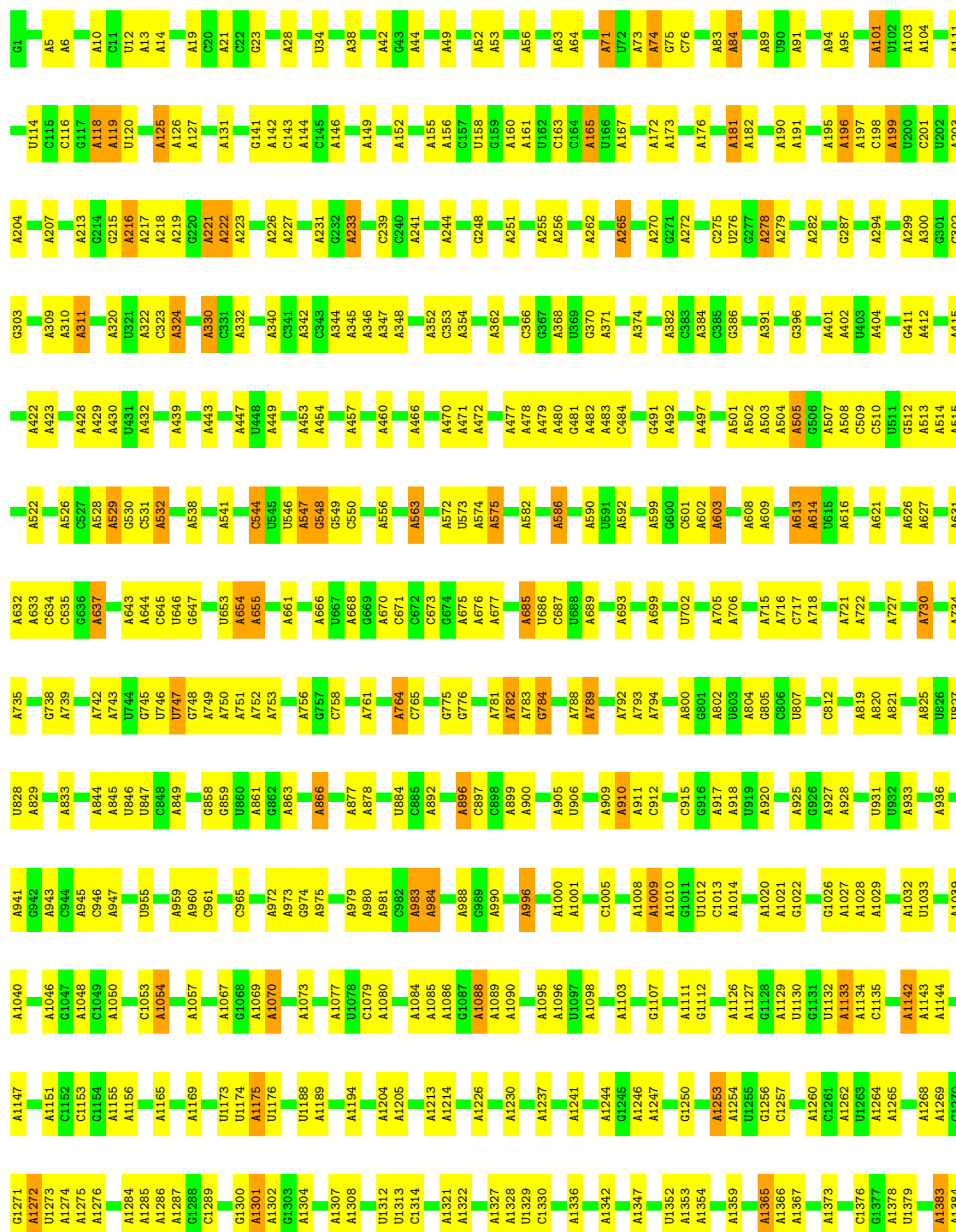
- Molecule 21: 30S ribosomal protein S21

Chain S211:  76% 21%



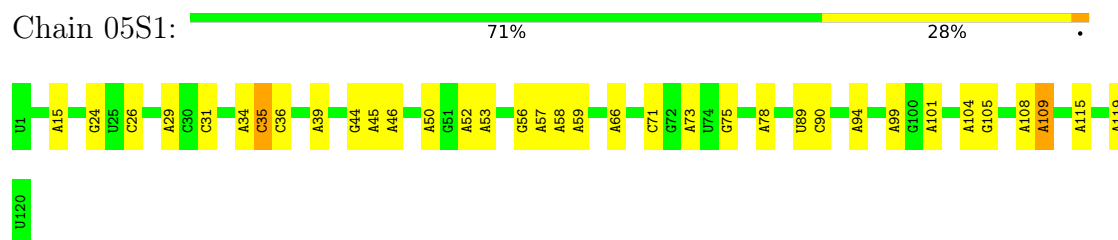
• Molecule 22: 23S rRNA

Chain 23S1:  64% 31% 5%



A2899	G2777	G2445	G2345	G2388	G2128	A2052	A1953	A1819	C1730	A1630	A1525	A1385
A2900	A2778	G2446	G2346	A2241	U2131	G2053	G1954	U1820	C1735	G1631	A1528	C1386
U2903	A2781	A2447	C2347	A2242	U2132	C2055	U1955	A1821	A1735	A1632	A1529	A1387
		A2448		U2243	G2133	G2056	A1960	A1829	G1738	A1634	A1532	A1392
		U2449	C2350	G2243	A2134	G2057	G1961	G1835	A1739	A1635	A1535	A1393
		A2450	G2351	A2247	A2135	A2058	C1962			U1636		U1394
		A2451	A2352		G2136	A2059			A1744	A1637	A1535	A1395
		C2452	G2353	G2251	U2137	A2060	A1966	A1847	A1745	A1644	A1544	
		A2453	C2354	G2252	A2142	A2062	C1967	A1848	A1746	A1641	G1546	C1398
		U2457					G1968				G1547	A1403
		G2458	A2358	A2266	C2146	G2069	A1969	A1853	A1749	C1644	A1548	
		A2459	A2366	A2267	A2147		A1970	A1854			A1549	
		U2460	G2367	A2268			U1971		A1754		G1550	
		A2461	C2368	G2269	C2150	A2071	G1972	A1858	A1755	U1647	G1546	
			A2369	A2270		A2072	A1977	A1866	A1757	U1649	A1551	
		A2468	A2376	A2273	A2154	C2073	A1978		U1758	A1650	A1552	
		A2469	A2377	A2274				A1871	A1759	G1651	A1553	
		G2470	A2378		G2157	A2077	A1981	A1872		A1652		A1420
		A2471	A2379	A2278	A2158			G1873	A1762	G1653	A1566	
		A2476	A2381	A2279		A2080	A1987		A1763	A1654	A1569	
		U2477	G2382	G2281	G2162	U2081	A1987	A1876	C1764	A1655	A1570	
		A2478	G2383	G2282	A2163	A2082	U1991	A1877		A1656	A1571	
		G2479	U2384	A2284	C2165		G1992		A1772		A1572	
		C2480	C2385	C2285		A2088	U1993	A1885	A1773	A1664		G1432
		G2481	G2386	G2286	A2169	C2089			A1774	A1665		A1433
		A2482	U2387	A2287	A2170	A2090	C1997	A1889	C1774	A1668	U1578	
			A2388	A2288	A2171		A1998	A1890	A1775	A1669	A1580	
		U2491			U2172	G2093	A2003	A1899	U1779	C1670		U1437
		A2497	A2392	A2287	A2173	A2095	G2004	A1900	A1780	U1671	A1583	U1438
		C2498	U2402	A2288		C2096	A2005	A1901	A1781	A1672	U1584	A1439
		G2502	A2406	G2306	A2176	U2098	C2006		A1782	G1673	C1585	
		A2503	A2407	G2307	U2182	G2100		G1906	A1783	A1674	A1586	G1452
		U2504	A2407	G2308	A2183	G2109	A2009	U1911	A1784	C1675	A1590	A1453
		G2505	A2407	A2309	A2184	A2101	A2013	A1912	A1785	A1676	A1591	A1469
			A2411	A2309			A2014	A1913	A1786	A1677	A1592	A1470
		A2513	A2412	G2311	U2188	G2107	A2015	3TD1915	A1787	A1678	G1593	
			A2418	A2311	G2190	U2109	A2019	U1917	C1788	A1679	A1596	
		C2517	A2418	A2314	A2191	U2111	A2020	A1918	A1789		A1597	
		A2518	A2425			G2112		A1919	G1790	A1689	A1598	A1490
			A2426	A2317	U2195	U2113	C2023	C1920	A1794	A1690		
		G2529		U2321	C2196	U2113				A1698	A1603	A1494
		A2531	G2429	A2322	U2197	A2114	G2027	A1927	C1800	G1699	A1496	
			U2431	A2322	A2198	G2115	A2030	A1928	A1801	A1700	C1606	
		A2534	A2432	G2325	A2199	G2116	A2031	G1929	A1802	A1701	G1607	A1502
			A2433	G2326		A2117	G2032	G1930	A1803	A1705	A1608	A1503
		C2540	A2434	A2327	G2204	U2118	A2033	U1931	C1804	A1705	A1609	A1504
		A2541	A2435	A2328	A2205	U2119	G2033	A1932	A1805		A1610	A1505
		A2542			A2211	G2120	A2037			A1711	A1614	
			A2439	A2333	A2212	G2121		A1936	A1808	U1712	G1615	A1508
		A2547	U2344	U2334	A2212	G2123	A2042	A1937	A1809	A1713	A1615	A1509
			U2441	A2335	A2225	G2124	C2043	A1938	A1810	A1717	C1617	
		U2552	A2336	A2336	A2226	G2125	C2044	U1939	G1811		A1613	A1515
			C2443	A2227		A2126			A1815	A1722		
		A2560	G2444	A2340	G2127		A2051	A1952	C1816		A1626	A1522

- 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

Chain L311:  89% 6% 6%



- Molecule 31: 50S ribosomal protein L13

Chain L131:  100%

There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L14

Chain L141:  100%

There are no outlier residues recorded for this chain.

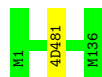
- Molecule 33: 50S ribosomal protein L15

Chain L151:  99% .



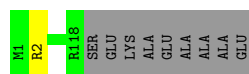
- Molecule 34: 50S ribosomal protein L16

Chain L161:  99% .



- Molecule 35: 50S ribosomal protein L17

Chain L171:  92% . 7%



- Molecule 36: 50S ribosomal protein L18

Chain L181:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: 50S ribosomal protein L19

Chain L191:  99%



- Molecule 38: 50S ribosomal protein L20

Chain L201:  98%



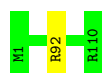
- Molecule 39: 50S ribosomal protein L21

Chain L211:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 50S ribosomal protein L22

Chain L221:  99%



- Molecule 41: 50S ribosomal protein L23

Chain L231:  92%



- Molecule 42: 50S ribosomal protein L24

Chain L241:  97%



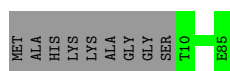
- Molecule 43: 50S ribosomal protein L25

Chain L251:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L27

Chain L271:  89%



- Molecule 45: 50S ribosomal protein L28

Chain L281: 96% ..



- Molecule 46: 50S ribosomal protein L29

Chain L291: 98% .



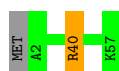
- Molecule 47: 50S ribosomal protein L30

Chain L301: 97% ..



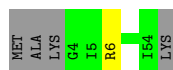
- Molecule 48: 50S ribosomal protein L32

Chain L321: 96% ..



- Molecule 49: 50S ribosomal protein L33

Chain L331: 91% . 7%



- Molecule 50: 50S ribosomal protein L34

Chain L341: 98% .



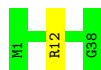
- Molecule 51: 50S ribosomal protein L35

Chain L351: 95% ...



- Molecule 52: 50S ribosomal protein L36

Chain L361: 97%



- Molecule 53: SpeFL

Chain SPE1: 88%



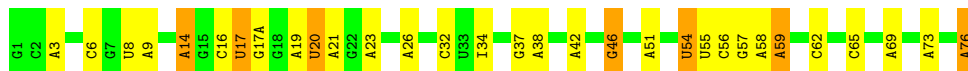
- Molecule 54: mRNA

Chain MRN1: 43%



- Molecule 55: P-site Arg-tRNA

Chain PTR1: 59%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	137494	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29.6	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	16S1	1.46	1103/36593 (3.0%)	3.48	4366/57081 (7.6%)
2	S021	0.68	0/1784	0.72	5/2403 (0.2%)
3	S031	0.78	0/1651	0.58	1/2225 (0.0%)
4	S041	0.83	0/1665	0.61	2/2227 (0.1%)
5	S051	0.72	0/1157	0.60	0/1557
6	S061	0.71	0/881	0.57	0/1189
7	S071	0.85	0/1195	0.65	1/1602 (0.1%)
8	S081	0.67	0/989	0.56	0/1326
9	S091	0.99	0/1034	0.83	0/1375
10	S101	0.88	0/805	0.70	1/1089 (0.1%)
11	S111	0.80	0/893	0.63	0/1205
12	S121	0.89	0/960	0.62	0/1286
13	S131	0.95	1/892 (0.1%)	0.78	1/1193 (0.1%)
14	S141	0.91	0/811	0.62	0/1081
15	S151	0.87	0/722	0.51	0/964
16	S161	0.87	0/659	0.68	0/884
17	S171	0.76	0/657	0.56	0/881
18	S181	0.87	0/462	0.56	0/621
19	S191	0.77	0/672	0.59	0/904
20	S201	0.72	0/676	0.53	1/895 (0.1%)
21	S211	1.01	0/472	0.53	0/627
22	23S1	1.53	2027/69120 (2.9%)	3.56	8534/107824 (7.9%)
23	05S1	1.32	71/2872 (2.5%)	3.09	276/4478 (6.2%)
24	L021	0.84	0/2121	0.60	1/2852 (0.0%)
25	L031	0.73	2/1576 (0.1%)	0.75	4/2119 (0.2%)
26	L041	0.70	0/1571	0.54	0/2113
27	L051	0.78	0/1434	0.63	0/1926
28	L061	0.65	0/1343	0.56	0/1816
29	L091	0.76	1/1121 (0.1%)	0.88	4/1515 (0.3%)
30	L311	0.77	0/531	0.87	3/709 (0.4%)
31	L131	0.72	0/1152	0.50	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	L141	0.81	0/955	0.58	0/1279
33	L151	0.81	0/1062	0.55	0/1413
34	L161	0.79	0/1081	0.54	0/1443
35	L171	0.94	0/958	0.60	0/1281
36	L181	0.83	0/910	0.52	0/1219
37	L191	0.84	0/929	0.52	0/1242
38	L201	0.90	0/960	0.50	0/1278
39	L211	0.73	0/829	0.54	0/1107
40	L221	0.78	0/864	0.54	0/1156
41	L231	0.72	0/744	0.61	0/994
42	L241	0.68	0/787	0.60	1/1051 (0.1%)
43	L251	0.66	0/766	0.53	0/1025
44	L271	0.83	0/587	0.49	0/776
45	L281	0.96	0/635	0.55	0/848
46	L291	0.77	0/502	0.48	0/667
47	L301	0.82	0/453	0.56	0/605
48	L321	0.89	0/450	0.69	1/599 (0.2%)
49	L331	0.67	0/421	0.68	1/561 (0.2%)
50	L341	1.14	0/380	0.69	1/498 (0.2%)
51	L351	0.77	0/513	0.64	1/676 (0.1%)
52	L361	0.91	0/303	0.52	0/397
53	SPE1	0.91	0/299	0.71	0/399
54	MRN1	0.61	0/161	1.28	1/248 (0.4%)
55	PTR1	1.65	56/1672 (3.3%)	3.19	173/2598 (6.7%)
All	All	1.34	3261/155692 (2.1%)	3.04	13379/232878 (5.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	S021	0	3
9	S091	0	1
10	S101	0	2
13	S131	0	3
19	S191	0	1
21	S211	0	1
29	L091	0	2
33	L151	0	1
47	L301	0	1
51	L351	0	1
All	All	0	16

All (3261) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	20	U	C5-C6	23.07	1.54	1.34
55	PTR1	17	U	C5-C6	22.09	1.54	1.34
22	23S1	2449	U	C5-C6	20.84	1.52	1.34
55	PTR1	17	U	N1-C6	10.44	1.47	1.38
55	PTR1	20	U	N1-C6	10.04	1.47	1.38
1	16S1	412	A	C8-N7	9.99	1.38	1.31
22	23S1	2451	A	C8-N7	9.69	1.38	1.31
55	PTR1	20	U	C4-C5	8.93	1.51	1.43
22	23S1	2872	A	C8-N7	8.22	1.37	1.31
25	L031	74	GLU	CD-OE2	-8.22	1.16	1.25
1	16S1	152	A	C8-N7	8.16	1.37	1.31
22	23S1	2101	A	C8-N7	8.07	1.37	1.31
55	PTR1	51	A	C8-N7	8.02	1.37	1.31
1	16S1	845	A	C8-N7	8.01	1.37	1.31
22	23S1	195	A	C8-N7	8.00	1.37	1.31
1	16S1	431	A	C8-N7	7.98	1.37	1.31
22	23S1	1434	A	C8-N7	7.96	1.37	1.31
1	16S1	1213	A	C8-N7	7.94	1.37	1.31
55	PTR1	59	A	C8-N7	7.92	1.37	1.31
22	23S1	2449	U	N1-C6	7.92	1.45	1.38
55	PTR1	17	U	C4-C5	7.90	1.50	1.43
1	16S1	74	A	C8-N7	7.88	1.37	1.31
22	23S1	1067	A	C8-N7	7.87	1.37	1.31
1	16S1	1145	A	C8-N7	7.84	1.37	1.31
22	23S1	2147	A	C8-N7	7.84	1.37	1.31
29	L091	149	GLU	CG-CD	7.83	1.63	1.51
22	23S1	2820	A	C8-N7	7.80	1.37	1.31
22	23S1	1090	A	C8-N7	7.78	1.36	1.31
1	16S1	468	A	C8-N7	7.77	1.36	1.31
55	PTR1	34	I	N3-C4	7.77	1.51	1.35
22	23S1	354	A	C8-N7	7.72	1.36	1.31
1	16S1	81	A	C8-N7	7.70	1.36	1.31
23	05S1	119	A	C8-N7	7.68	1.36	1.31
1	16S1	195	A	C8-N7	7.67	1.36	1.31
22	23S1	1096	A	C8-N7	7.66	1.36	1.31
1	16S1	1035	A	C8-N7	7.64	1.36	1.31
1	16S1	1	A	C8-N7	7.64	1.36	1.31
1	16S1	151	A	C8-N7	7.63	1.36	1.31
1	16S1	622	A	C8-N7	7.59	1.36	1.31
22	23S1	892	A	N3-C4	7.59	1.39	1.34
22	23S1	900	A	C8-N7	7.56	1.36	1.31
22	23S1	1077	A	C8-N7	7.54	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1515	A	C8-N7	7.53	1.36	1.31
22	23S1	1046	A	C8-N7	7.53	1.36	1.31
22	23S1	2163	A	C8-N7	7.52	1.36	1.31
1	16S1	1101	A	C8-N7	7.51	1.36	1.31
22	23S1	1080	A	C8-N7	7.51	1.36	1.31
22	23S1	878	A	C8-N7	7.50	1.36	1.31
1	16S1	411	A	C8-N7	7.50	1.36	1.31
1	16S1	1441	A	C8-N7	7.50	1.36	1.31
22	23S1	905	A	C8-N7	7.50	1.36	1.31
22	23S1	792	A	C5-C4	-7.49	1.33	1.38
22	23S1	2211	A	C8-N7	7.49	1.36	1.31
22	23S1	507	A	C8-N7	7.49	1.36	1.31
22	23S1	1570	A	C5-C4	-7.48	1.33	1.38
55	PTR1	17	U	C2-N3	7.47	1.43	1.37
22	23S1	2126	A	C8-N7	7.47	1.36	1.31
1	16S1	171	A	C8-N7	7.46	1.36	1.31
22	23S1	2117	A	C8-N7	7.46	1.36	1.31
55	PTR1	20	U	C2-N3	7.46	1.43	1.37
55	PTR1	26	A	C8-N7	7.43	1.36	1.31
22	23S1	2134	A	C8-N7	7.42	1.36	1.31
1	16S1	649	A	C8-N7	7.42	1.36	1.31
1	16S1	532	A	C8-N7	7.42	1.36	1.31
22	23S1	2602	A	C8-N7	7.39	1.36	1.31
22	23S1	1583	A	C8-N7	7.39	1.36	1.31
22	23S1	654	A	C8-N7	7.39	1.36	1.31
1	16S1	1012	A	C8-N7	7.38	1.36	1.31
22	23S1	1057	A	C8-N7	7.37	1.36	1.31
22	23S1	896	A	C8-N7	7.36	1.36	1.31
1	16S1	1299	A	C8-N7	7.36	1.36	1.31
22	23S1	1073	A	C8-N7	7.36	1.36	1.31
1	16S1	80	A	C8-N7	7.35	1.36	1.31
22	23S1	1028	A	C5-C4	-7.35	1.33	1.38
22	23S1	2184	A	C8-N7	7.35	1.36	1.31
1	16S1	1493	A	C8-N7	7.33	1.36	1.31
22	23S1	282	A	C8-N7	7.33	1.36	1.31
1	16S1	978	A	C8-N7	7.32	1.36	1.31
1	16S1	1534	A	C8-N7	7.32	1.36	1.31
22	23S1	1735	A	C8-N7	7.32	1.36	1.31
22	23S1	2095	A	C8-N7	7.32	1.36	1.31
22	23S1	1095	A	C8-N7	7.31	1.36	1.31
22	23S1	2154	A	C8-N7	7.31	1.36	1.31
1	16S1	1216	A	C8-N7	7.31	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1069	A	C8-N7	7.30	1.36	1.31
1	16S1	996	A	C8-N7	7.29	1.36	1.31
1	16S1	1274	A	C8-N7	7.29	1.36	1.31
22	23S1	2660	A	C8-N7	7.28	1.36	1.31
22	23S1	1419	A	C8-N7	7.28	1.36	1.31
22	23S1	165	A	C8-N7	7.27	1.36	1.31
1	16S1	465	A	C8-N7	7.26	1.36	1.31
22	23S1	2183	A	C8-N7	7.26	1.36	1.31
1	16S1	1021	A	C8-N7	7.25	1.36	1.31
22	23S1	161	A	C8-N7	7.25	1.36	1.31
22	23S1	821	A	C5-C4	-7.24	1.33	1.38
1	16S1	461	A	C8-N7	7.24	1.36	1.31
55	PTR1	23	A	C8-N7	7.24	1.36	1.31
1	16S1	80	A	N3-C4	7.23	1.39	1.34
22	23S1	2572	A	C5-C4	-7.23	1.33	1.38
1	16S1	640	A	C8-N7	7.22	1.36	1.31
1	16S1	845	A	N3-C4	7.22	1.39	1.34
1	16S1	414	A	C8-N7	7.21	1.36	1.31
1	16S1	495	A	C8-N7	7.21	1.36	1.31
1	16S1	1005	A	C8-N7	7.21	1.36	1.31
22	23S1	207	A	C5-C4	-7.21	1.33	1.38
22	23S1	1509	A	C8-N7	7.21	1.36	1.31
1	16S1	196	A	C8-N7	7.21	1.36	1.31
22	23S1	2309	A	C8-N7	7.21	1.36	1.31
22	23S1	368	A	C8-N7	7.21	1.36	1.31
22	23S1	504	A	C8-N7	7.20	1.36	1.31
22	23S1	1502	A	C8-N7	7.20	1.36	1.31
22	23S1	2014	A	C5-C4	-7.20	1.33	1.38
22	23S1	1505	A	C8-N7	7.20	1.36	1.31
23	05S1	34	A	C8-N7	7.19	1.36	1.31
1	16S1	704	A	C8-N7	7.19	1.36	1.31
22	23S1	172	A	C8-N7	7.19	1.36	1.31
1	16S1	172	A	C8-N7	7.18	1.36	1.31
22	23S1	1535	A	C8-N7	7.18	1.36	1.31
22	23S1	1853	A	C5-C4	-7.18	1.33	1.38
22	23S1	119	A	C8-N7	7.17	1.36	1.31
1	16S1	435	A	C8-N7	7.17	1.36	1.31
22	23S1	689	A	C5-C4	-7.17	1.33	1.38
22	23S1	547	A	C8-N7	7.17	1.36	1.31
22	23S1	2657	A	C8-N7	7.17	1.36	1.31
1	16S1	7	A	C8-N7	7.16	1.36	1.31
1	16S1	1044	A	C8-N7	7.16	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1155	A	C8-N7	7.16	1.36	1.31
22	23S1	2758	A	C8-N7	7.16	1.36	1.31
22	23S1	84	A	C8-N7	7.16	1.36	1.31
22	23S1	2749	A	C8-N7	7.16	1.36	1.31
1	16S1	374	A	C8-N7	7.15	1.36	1.31
22	23S1	1040	A	C8-N7	7.15	1.36	1.31
22	23S1	2311	A	C8-N7	7.14	1.36	1.31
22	23S1	1050	A	C8-N7	7.14	1.36	1.31
1	16S1	520	A	C8-N7	7.13	1.36	1.31
1	16S1	1036	A	C8-N7	7.13	1.36	1.31
22	23S1	1070	A	C8-N7	7.12	1.36	1.31
1	16S1	408	A	C8-N7	7.12	1.36	1.31
22	23S1	1175	A	C8-N7	7.12	1.36	1.31
22	23S1	1084	A	C8-N7	7.11	1.36	1.31
22	23S1	2142	A	N3-C4	7.11	1.39	1.34
22	23S1	10	A	C8-N7	7.11	1.36	1.31
22	23S1	2108	A	C8-N7	7.11	1.36	1.31
22	23S1	404	A	C8-N7	7.09	1.36	1.31
1	16S1	1410	A	C8-N7	7.09	1.36	1.31
22	23S1	278	A	C8-N7	7.09	1.36	1.31
22	23S1	2119	A	C8-N7	7.09	1.36	1.31
22	23S1	613	A	C8-N7	7.08	1.36	1.31
22	23S1	352	A	C8-N7	7.08	1.36	1.31
22	23S1	1086	A	C8-N7	7.08	1.36	1.31
22	23S1	1913	A	C8-N7	7.08	1.36	1.31
1	16S1	815	A	C5-C4	-7.08	1.33	1.38
22	23S1	1420	A	C8-N7	7.07	1.36	1.31
22	23S1	1213	A	C5-C4	-7.07	1.33	1.38
1	16S1	274	A	C8-N7	7.07	1.36	1.31
23	05S1	66	A	C8-N7	7.07	1.36	1.31
55	PTR1	9	A	C8-N7	7.06	1.36	1.31
55	PTR1	69	A	C8-N7	7.06	1.36	1.31
1	16S1	466	A	C8-N7	7.06	1.36	1.31
22	23S1	1169	A	C8-N7	7.05	1.36	1.31
1	16S1	143	A	C8-N7	7.05	1.36	1.31
22	23S1	1876	A	C8-N7	7.05	1.36	1.31
22	23S1	1413	A	C8-N7	7.05	1.36	1.31
22	23S1	655	A	C8-N7	7.05	1.36	1.31
22	23S1	2158	A	C8-N7	7.05	1.36	1.31
22	23S1	2134	A	N3-C4	7.05	1.39	1.34
22	23S1	344	A	C8-N7	7.04	1.36	1.31
22	23S1	761	A	C8-N7	7.04	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	554	A	C8-N7	7.04	1.36	1.31
55	PTR1	73	A	C8-N7	7.04	1.36	1.31
1	16S1	250	A	C8-N7	7.04	1.36	1.31
1	16S1	1257	A	C8-N7	7.04	1.36	1.31
1	16S1	1238	A	C8-N7	7.03	1.36	1.31
1	16S1	3	A	C8-N7	7.03	1.36	1.31
22	23S1	2542	A	C5-C4	-7.02	1.33	1.38
22	23S1	2516	A	C5-C4	-7.02	1.33	1.38
1	16S1	189	A	C8-N7	7.02	1.36	1.31
1	16S1	1169	A	C8-N7	7.02	1.36	1.31
22	23S1	2119	A	N3-C4	7.02	1.39	1.34
1	16S1	1329	A	C8-N7	7.01	1.36	1.31
22	23S1	345	A	C8-N7	7.01	1.36	1.31
1	16S1	1176	A	C8-N7	7.01	1.36	1.31
22	23S1	899	A	C8-N7	7.01	1.36	1.31
55	PTR1	3	A	C8-N7	7.01	1.36	1.31
22	23S1	892	A	C8-N7	7.00	1.36	1.31
22	23S1	1247	A	C5-C4	-7.00	1.33	1.38
22	23S1	2003	A	C5-C4	-7.00	1.33	1.38
1	16S1	167	A	C8-N7	7.00	1.36	1.31
1	16S1	300	A	N7-C5	-7.00	1.35	1.39
1	16S1	320	A	C8-N7	6.99	1.36	1.31
1	16S1	478	A	N3-C4	6.99	1.39	1.34
1	16S1	583	A	C8-N7	6.99	1.36	1.31
1	16S1	179	A	C8-N7	6.99	1.36	1.31
22	23S1	1504	A	C8-N7	6.99	1.36	1.31
1	16S1	1261	A	C8-N7	6.99	1.36	1.31
1	16S1	460	A	C8-N7	6.99	1.36	1.31
1	16S1	1179	A	C8-N7	6.99	1.36	1.31
22	23S1	1453	A	C8-N7	6.99	1.36	1.31
22	23S1	2721	A	C5-C4	-6.98	1.33	1.38
55	PTR1	34	I	C5-C6	6.98	1.53	1.39
22	23S1	213	A	C8-N7	6.98	1.36	1.31
22	23S1	279	A	C8-N7	6.98	1.36	1.31
22	23S1	693	A	C5-C4	-6.98	1.33	1.38
22	23S1	514	A	C5-C4	-6.98	1.33	1.38
22	23S1	1847	A	C8-N7	6.98	1.36	1.31
22	23S1	715	A	C8-N7	6.98	1.36	1.31
22	23S1	2052	A	C5-C4	-6.97	1.33	1.38
22	23S1	2101	A	N3-C4	6.97	1.39	1.34
22	23S1	1591	A	C8-N7	6.97	1.36	1.31
22	23S1	2883	A	C5-C4	-6.97	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	279	A	C8-N7	6.97	1.36	1.31
22	23S1	1749	A	C8-N7	6.97	1.36	1.31
1	16S1	1333	A	C8-N7	6.96	1.36	1.31
1	16S1	1150	A	C8-N7	6.96	1.36	1.31
22	23S1	1503	A	C8-N7	6.96	1.36	1.31
22	23S1	2170	A	C8-N7	6.96	1.36	1.31
1	16S1	1019	A	C8-N7	6.96	1.36	1.31
1	16S1	131	A	C8-N7	6.95	1.36	1.31
1	16S1	1042	A	C8-N7	6.95	1.36	1.31
22	23S1	979	A	C5-C4	-6.95	1.33	1.38
1	16S1	415	A	C8-N7	6.95	1.36	1.31
22	23S1	563	A	C5-C4	-6.95	1.33	1.38
22	23S1	676	A	C5-C4	-6.95	1.33	1.38
22	23S1	2176	A	C8-N7	6.95	1.36	1.31
22	23S1	2900	A	C8-N7	6.95	1.36	1.31
22	23S1	668	A	C5-C4	-6.95	1.33	1.38
22	23S1	1264	A	C5-C4	-6.94	1.33	1.38
22	23S1	1089	A	C8-N7	6.94	1.36	1.31
1	16S1	1022	A	C8-N7	6.93	1.36	1.31
22	23S1	1205	A	C8-N7	6.93	1.36	1.31
1	16S1	602	A	C8-N7	6.93	1.36	1.31
22	23S1	1744	A	C8-N7	6.93	1.36	1.31
1	16S1	306	A	C8-N7	6.93	1.36	1.31
22	23S1	1810	A	N7-C5	-6.93	1.35	1.39
22	23S1	1383	A	C8-N7	6.93	1.36	1.31
1	16S1	432	A	C8-N7	6.93	1.36	1.31
1	16S1	487	A	C8-N7	6.93	1.36	1.31
1	16S1	1468	A	C5-C4	-6.93	1.33	1.38
1	16S1	648	A	C8-N7	6.92	1.36	1.31
1	16S1	1000	A	C8-N7	6.92	1.36	1.31
22	23S1	181	A	C8-N7	6.92	1.36	1.31
22	23S1	2060	A	C5-C4	-6.92	1.33	1.38
22	23S1	2054	A	C5-C4	-6.92	1.33	1.38
22	23S1	1254	A	C5-C4	-6.91	1.33	1.38
1	16S1	1227	A	C8-N7	6.91	1.36	1.31
22	23S1	1039	A	C8-N7	6.91	1.36	1.31
1	16S1	78	A	C8-N7	6.91	1.36	1.31
22	23S1	1532	A	C8-N7	6.91	1.36	1.31
22	23S1	2654	A	C8-N7	6.91	1.36	1.31
1	16S1	1447	A	C8-N7	6.91	1.36	1.31
22	23S1	2740	A	C5-C4	-6.90	1.33	1.38
1	16S1	149	A	C8-N7	6.90	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	665	A	C8-N7	6.90	1.36	1.31
1	16S1	1456	A	C8-N7	6.90	1.36	1.31
22	23S1	1495	A	C8-N7	6.90	1.36	1.31
22	23S1	2469	A	C5-C4	-6.90	1.33	1.38
22	23S1	1353	A	C5-C4	-6.90	1.33	1.38
22	23S1	204	A	C5-C4	-6.89	1.33	1.38
22	23S1	1095	A	N3-C4	6.89	1.39	1.34
22	23S1	342	A	C8-N7	6.89	1.36	1.31
22	23S1	1586	A	C8-N7	6.89	1.36	1.31
1	16S1	1319	A	C8-N7	6.88	1.36	1.31
22	23S1	1877	A	C8-N7	6.88	1.36	1.31
1	16S1	1016	A	C8-N7	6.88	1.36	1.31
22	23S1	2317	A	C8-N7	6.88	1.36	1.31
22	23S1	1784	A	C5-C4	-6.87	1.33	1.38
22	23S1	1020	A	C8-N7	6.87	1.36	1.31
22	23S1	1579	A	C8-N7	6.87	1.36	1.31
22	23S1	508	A	C8-N7	6.87	1.36	1.31
1	16S1	1248	A	C8-N7	6.87	1.36	1.31
1	16S1	1332	A	C8-N7	6.86	1.36	1.31
1	16S1	182	A	C8-N7	6.86	1.36	1.31
1	16S1	456	A	C8-N7	6.86	1.36	1.31
1	16S1	1105	A	C5-C4	-6.86	1.33	1.38
1	16S1	1239	A	C8-N7	6.86	1.36	1.31
23	05S1	109	A	C8-N7	6.86	1.36	1.31
22	23S1	324	A	C5-C4	-6.86	1.33	1.38
22	23S1	575	A	C5-C4	-6.85	1.33	1.38
22	23S1	819	A	C5-C4	-6.85	1.33	1.38
22	23S1	2753	A	C8-N7	6.85	1.36	1.31
22	23S1	613	A	N3-C4	6.85	1.39	1.34
22	23S1	2173	A	N3-C4	6.85	1.39	1.34
1	16S1	1225	A	N3-C4	6.84	1.39	1.34
1	16S1	1251	A	C8-N7	6.84	1.36	1.31
22	23S1	1590	A	C8-N7	6.84	1.36	1.31
1	16S1	1151	A	C8-N7	6.84	1.36	1.31
22	23S1	2097	A	C8-N7	6.84	1.36	1.31
1	16S1	155	A	C8-N7	6.84	1.36	1.31
1	16S1	223	A	C8-N7	6.83	1.36	1.31
1	16S1	1346	A	C8-N7	6.83	1.36	1.31
22	23S1	2169	A	N3-C4	6.83	1.39	1.34
22	23S1	586	A	C5-C4	-6.83	1.33	1.38
1	16S1	1196	A	C8-N7	6.82	1.36	1.31
1	16S1	493	A	C8-N7	6.82	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1175	A	N3-C4	6.82	1.39	1.34
22	23S1	1772	A	C5-C4	-6.82	1.33	1.38
22	23S1	750	A	C5-C4	-6.82	1.33	1.38
1	16S1	547	A	C8-N7	6.81	1.36	1.31
1	16S1	1492	A	C8-N7	6.81	1.36	1.31
1	16S1	8	A	C8-N7	6.81	1.36	1.31
1	16S1	1000	A	N3-C4	6.81	1.39	1.34
1	16S1	441	A	C8-N7	6.81	1.36	1.31
22	23S1	2792	A	C8-N7	6.81	1.36	1.31
1	16S1	1105	A	C8-N7	6.81	1.36	1.31
22	23S1	1359	A	C8-N7	6.80	1.36	1.31
22	23S1	1544	A	C8-N7	6.80	1.36	1.31
22	23S1	111	A	C8-N7	6.80	1.36	1.31
23	05S1	46	A	C8-N7	6.80	1.36	1.31
22	23S1	845	A	N3-C4	6.80	1.39	1.34
1	16S1	16	A	C5-C4	-6.80	1.33	1.38
22	23S1	156	A	C8-N7	6.80	1.36	1.31
22	23S1	2281	A	C5-C4	-6.79	1.33	1.38
22	23S1	1494	A	C8-N7	6.79	1.36	1.31
23	05S1	78	A	C8-N7	6.79	1.36	1.31
1	16S1	681	A	C8-N7	6.79	1.36	1.31
22	23S1	2114	A	N3-C4	6.79	1.39	1.34
22	23S1	104	A	C8-N7	6.78	1.36	1.31
22	23S1	160	A	C8-N7	6.78	1.36	1.31
22	23S1	614	A	C8-N7	6.78	1.36	1.31
23	05S1	29	A	C8-N7	6.78	1.36	1.31
1	16S1	1360	A	C8-N7	6.78	1.36	1.31
22	23S1	144	A	C8-N7	6.78	1.36	1.31
22	23S1	155	A	C8-N7	6.78	1.36	1.31
22	23S1	1960	A	C5-C4	-6.78	1.34	1.38
22	23S1	2154	A	N3-C4	6.78	1.39	1.34
22	23S1	2183	A	N3-C4	6.78	1.39	1.34
1	16S1	60	A	C8-N7	6.77	1.36	1.31
1	16S1	915	A	C5-C4	-6.77	1.34	1.38
1	16S1	1130	A	C8-N7	6.77	1.36	1.31
22	23S1	603	A	C8-N7	6.77	1.36	1.31
1	16S1	572	A	C5-C4	-6.77	1.34	1.38
22	23S1	504	A	C5-C4	-6.77	1.34	1.38
22	23S1	2173	A	C8-N7	6.77	1.36	1.31
1	16S1	452	A	C8-N7	6.77	1.36	1.31
1	16S1	766	A	C5-C4	-6.77	1.34	1.38
22	23S1	2071	A	C5-C4	-6.77	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2247	A	C5-C4	-6.77	1.34	1.38
22	23S1	362	A	N3-C4	6.76	1.39	1.34
23	05S1	15	A	C8-N7	6.76	1.36	1.31
22	23S1	1088	A	C8-N7	6.76	1.36	1.31
1	16S1	353	A	C8-N7	6.75	1.36	1.31
22	23S1	2726	A	C8-N7	6.75	1.36	1.31
22	23S1	1953	A	C5-C4	-6.75	1.34	1.38
1	16S1	382	A	C8-N7	6.75	1.36	1.31
22	23S1	1871	A	C8-N7	6.75	1.36	1.31
22	23S1	270	A	C8-N7	6.75	1.36	1.31
22	23S1	661	A	C5-C4	-6.75	1.34	1.38
1	16S1	243	A	C8-N7	6.75	1.36	1.31
1	16S1	1246	A	C8-N7	6.75	1.36	1.31
22	23S1	272	A	C8-N7	6.75	1.36	1.31
22	23S1	2088	A	C5-C4	-6.74	1.34	1.38
22	23S1	1652	A	C5-C4	-6.74	1.34	1.38
22	23S1	2566	A	C8-N7	6.74	1.36	1.31
1	16S1	72	A	C8-N7	6.74	1.36	1.31
1	16S1	747	A	C8-N7	6.74	1.36	1.31
22	23S1	457	A	C5-C4	-6.74	1.34	1.38
23	05S1	50	A	C8-N7	6.74	1.36	1.31
22	23S1	347	A	C8-N7	6.73	1.36	1.31
22	23S1	515	A	C5-C4	-6.73	1.34	1.38
22	23S1	980	A	C5-C4	-6.73	1.34	1.38
22	23S1	2381	A	C5-C4	-6.73	1.34	1.38
22	23S1	1204	A	C8-N7	6.73	1.36	1.31
22	23S1	1354	A	C5-C4	-6.73	1.34	1.38
22	23S1	2314	A	C8-N7	6.73	1.36	1.31
22	23S1	2577	A	C5-C4	-6.73	1.34	1.38
1	16S1	309	A	C8-N7	6.73	1.36	1.31
1	16S1	1311	A	C8-N7	6.72	1.36	1.31
22	23S1	2171	A	N3-C4	6.72	1.38	1.34
1	16S1	1408	A	C8-N7	6.72	1.36	1.31
22	23S1	1569	A	C5-C4	-6.72	1.34	1.38
22	23S1	2418	A	C5-C4	-6.72	1.34	1.38
23	05S1	39	A	C8-N7	6.72	1.36	1.31
55	PTR1	42	A	C8-N7	6.72	1.36	1.31
22	23S1	348	A	C8-N7	6.72	1.36	1.31
22	23S1	1214	A	C5-C4	-6.72	1.34	1.38
22	23S1	1672	A	C5-C4	-6.72	1.34	1.38
1	16S1	129	A	C8-N7	6.71	1.36	1.31
1	16S1	767	A	C5-C4	-6.71	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1395	A	C5-C4	-6.71	1.34	1.38
22	23S1	2632	A	C8-N7	6.71	1.36	1.31
1	16S1	2	A	C8-N7	6.71	1.36	1.31
22	23S1	191	A	C5-C4	-6.71	1.34	1.38
22	23S1	734	A	C5-C4	-6.71	1.34	1.38
22	23S1	1086	A	N3-C4	6.71	1.38	1.34
22	23S1	2534	A	C8-N7	6.71	1.36	1.31
22	23S1	2809	A	C8-N7	6.71	1.36	1.31
23	05S1	58	A	C8-N7	6.71	1.36	1.31
22	23S1	599	A	C5-C4	-6.71	1.34	1.38
22	23S1	432	A	C8-N7	6.71	1.36	1.31
22	23S1	2589	A	C5-C4	-6.71	1.34	1.38
1	16S1	1019	A	N3-C4	6.71	1.38	1.34
22	23S1	896	A	N3-C4	6.71	1.38	1.34
22	23S1	1144	A	C5-C4	-6.71	1.34	1.38
1	16S1	160	A	C8-N7	6.70	1.36	1.31
22	23S1	1001	A	C5-C4	-6.70	1.34	1.38
22	23S1	1593	A	C8-N7	6.70	1.36	1.31
22	23S1	1655	A	C5-C4	-6.70	1.34	1.38
22	23S1	2082	A	C5-C4	-6.70	1.34	1.38
22	23S1	2459	A	C5-C4	-6.70	1.34	1.38
23	05S1	59	A	C8-N7	6.70	1.36	1.31
1	16S1	270	A	C8-N7	6.70	1.36	1.31
1	16S1	600	A	C8-N7	6.70	1.36	1.31
22	23S1	310	A	C5-C4	-6.70	1.34	1.38
22	23S1	63	A	C8-N7	6.70	1.36	1.31
1	16S1	1204	A	C8-N7	6.70	1.36	1.31
22	23S1	1048	A	C8-N7	6.70	1.36	1.31
22	23S1	2725	A	C5-C4	-6.70	1.34	1.38
22	23S1	1794	A	C5-C4	-6.69	1.34	1.38
1	16S1	199	A	C8-N7	6.69	1.36	1.31
1	16S1	98	A	C8-N7	6.69	1.36	1.31
1	16S1	120	A	C8-N7	6.69	1.36	1.31
22	23S1	1103	A	N3-C4	6.69	1.38	1.34
22	23S1	197	A	C5-C4	-6.69	1.34	1.38
1	16S1	749	A	C8-N7	6.68	1.36	1.31
22	23S1	1545	A	C8-N7	6.68	1.36	1.31
22	23S1	592	A	C5-C4	-6.67	1.34	1.38
22	23S1	1978	A	C5-C4	-6.67	1.34	1.38
22	23S1	5	A	C8-N7	6.67	1.36	1.31
22	23S1	2675	A	C5-C4	-6.67	1.34	1.38
1	16S1	19	A	C5-C4	-6.67	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	101	A	C8-N7	6.67	1.36	1.31
1	16S1	65	A	C8-N7	6.67	1.36	1.31
1	16S1	553	A	C5-C4	-6.67	1.34	1.38
1	16S1	1534	A	N3-C4	6.67	1.38	1.34
1	16S1	448	A	C8-N7	6.67	1.36	1.31
1	16S1	792	A	C5-C4	-6.67	1.34	1.38
22	23S1	2169	A	C8-N7	6.67	1.36	1.31
1	16S1	1035	A	N3-C4	6.66	1.38	1.34
1	16S1	906	A	C5-C4	-6.66	1.34	1.38
22	23S1	1089	A	N3-C4	6.66	1.38	1.34
22	23S1	2887	A	C5-C4	-6.66	1.34	1.38
1	16S1	596	A	C8-N7	6.66	1.36	1.31
1	16S1	784	A	C5-C4	-6.66	1.34	1.38
22	23S1	1000	A	C5-C4	-6.66	1.34	1.38
22	23S1	1054	A	C8-N7	6.66	1.36	1.31
22	23S1	2590	A	C5-C4	-6.66	1.34	1.38
1	16S1	71	A	C8-N7	6.66	1.36	1.31
22	23S1	1668	A	C5-C4	-6.66	1.34	1.38
22	23S1	2734	A	C8-N7	6.66	1.36	1.31
22	23S1	1342	A	C5-C4	-6.65	1.34	1.38
22	23S1	1809	A	C5-C4	-6.65	1.34	1.38
1	16S1	325	A	C8-N7	6.65	1.36	1.31
1	16S1	498	A	C8-N7	6.65	1.36	1.31
22	23S1	265	A	C8-N7	6.65	1.36	1.31
22	23S1	1431	A	C5-C4	-6.65	1.34	1.38
22	23S1	2142	A	C8-N7	6.65	1.36	1.31
22	23S1	722	A	C8-N7	6.65	1.36	1.31
22	23S1	2070	A	C8-N7	6.65	1.36	1.31
22	23S1	1616	A	C5-C4	-6.65	1.34	1.38
22	23S1	2761	A	C8-N7	6.65	1.36	1.31
22	23S1	1111	A	C8-N7	6.65	1.36	1.31
22	23S1	2270	A	C5-C4	-6.65	1.34	1.38
22	23S1	1134	A	C8-N7	6.64	1.36	1.31
22	23S1	1385	A	C5-C4	-6.64	1.34	1.38
22	23S1	1786	A	C5-C4	-6.64	1.34	1.38
1	16S1	918	A	C5-C4	-6.64	1.34	1.38
1	16S1	1398	A	C8-N7	6.64	1.36	1.31
1	16S1	371	A	C8-N7	6.64	1.36	1.31
22	23S1	1490	A	N3-C4	6.64	1.38	1.34
22	23S1	945	A	C8-N7	6.64	1.36	1.31
22	23S1	1746	A	C8-N7	6.64	1.36	1.31
1	16S1	1229	A	C8-N7	6.64	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2826	A	C5-C4	-6.64	1.34	1.38
1	16S1	26	A	C5-C4	-6.63	1.34	1.38
22	23S1	2013	A	C5-C4	-6.63	1.34	1.38
22	23S1	2171	A	C8-N7	6.63	1.36	1.31
1	16S1	728	A	C5-C4	-6.63	1.34	1.38
1	16S1	900	A	C5-C4	-6.63	1.34	1.38
22	23S1	1596	A	C8-N7	6.63	1.36	1.31
22	23S1	2392	A	C5-C4	-6.63	1.34	1.38
1	16S1	238	A	C8-N7	6.63	1.36	1.31
22	23S1	95	A	C8-N7	6.63	1.36	1.31
1	16S1	1280	A	C8-N7	6.63	1.36	1.31
22	23S1	626	A	C8-N7	6.63	1.36	1.31
1	16S1	958	A	C8-N7	6.63	1.36	1.31
22	23S1	1522	A	C8-N7	6.63	1.36	1.31
22	23S1	1952	A	C5-C4	-6.63	1.34	1.38
22	23S1	1966	A	C5-C4	-6.63	1.34	1.38
22	23S1	1490	A	C8-N7	6.62	1.36	1.31
22	23S1	222	A	C8-N7	6.62	1.36	1.31
22	23S1	1597	A	C8-N7	6.62	1.36	1.31
22	23S1	1819	A	C5-C4	-6.62	1.34	1.38
1	16S1	253	A	C8-N7	6.62	1.36	1.31
22	23S1	1572	A	C5-C4	-6.62	1.34	1.38
1	16S1	1146	A	C8-N7	6.62	1.36	1.31
1	16S1	1289	A	C8-N7	6.62	1.36	1.31
22	23S1	1700	A	C5-C4	-6.62	1.34	1.38
1	16S1	1256	A	C8-N7	6.62	1.36	1.31
22	23S1	2212	A	C8-N7	6.62	1.36	1.31
22	23S1	2602	A	N3-C4	6.62	1.38	1.34
1	16S1	1092	A	C8-N7	6.61	1.36	1.31
22	23S1	1268	A	C5-C4	-6.61	1.34	1.38
22	23S1	2406	A	C8-N7	6.61	1.36	1.31
22	23S1	2741	A	C5-C4	-6.61	1.34	1.38
1	16S1	205	A	C8-N7	6.61	1.36	1.31
22	23S1	637	A	C8-N7	6.61	1.36	1.31
22	23S1	1253	A	C8-N7	6.61	1.36	1.31
22	23S1	1630	A	C8-N7	6.61	1.36	1.31
22	23S1	1650	A	C5-C4	-6.61	1.34	1.38
1	16S1	935	A	C5-C4	-6.61	1.34	1.38
22	23S1	861	A	C5-C4	-6.61	1.34	1.38
22	23S1	1522	A	C5-C4	-6.61	1.34	1.38
22	23S1	1969	A	C5-C4	-6.61	1.34	1.38
1	16S1	889	A	C8-N7	6.60	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	181	A	C8-N7	6.60	1.36	1.31
1	16S1	461	A	N3-C4	6.60	1.38	1.34
1	16S1	746	A	C8-N7	6.60	1.36	1.31
23	05S1	108	A	C5-C4	-6.60	1.34	1.38
22	23S1	199	A	C5-C4	-6.60	1.34	1.38
1	16S1	1163	A	C8-N7	6.60	1.36	1.31
22	23S1	1014	A	C8-N7	6.60	1.36	1.31
22	23S1	1098	A	C8-N7	6.60	1.36	1.31
22	23S1	547	A	N3-C4	6.60	1.38	1.34
1	16S1	1250	A	C8-N7	6.59	1.36	1.31
22	23S1	947	A	C5-C4	-6.59	1.34	1.38
1	16S1	969	A	C8-N7	6.59	1.36	1.31
22	23S1	1385	A	C8-N7	6.59	1.36	1.31
22	23S1	1275	A	C5-C4	-6.59	1.34	1.38
22	23S1	322	A	C8-N7	6.59	1.36	1.31
22	23S1	632	A	C5-C4	-6.59	1.34	1.38
22	23S1	1566	A	C5-C4	-6.59	1.34	1.38
22	23S1	2378	A	C8-N7	6.59	1.36	1.31
22	23S1	1762	A	C5-C4	-6.58	1.34	1.38
22	23S1	2094	A	C8-N7	6.58	1.36	1.31
22	23S1	983	A	C5-C4	-6.58	1.34	1.38
22	23S1	761	A	C5-C4	-6.58	1.34	1.38
1	16S1	116	A	C5-C4	-6.58	1.34	1.38
22	23S1	443	A	C5-C4	-6.58	1.34	1.38
22	23S1	825	A	C5-C4	-6.58	1.34	1.38
22	23S1	909	A	C8-N7	6.58	1.36	1.31
55	PTR1	38	A	C5-C4	-6.58	1.34	1.38
1	16S1	715	A	C5-C4	-6.58	1.34	1.38
22	23S1	2205	A	C8-N7	6.58	1.36	1.31
1	16S1	44	A	C8-N7	6.58	1.36	1.31
22	23S1	677	A	C5-C4	-6.58	1.34	1.38
1	16S1	1349	A	C5-C4	-6.57	1.34	1.38
22	23S1	262	A	C8-N7	6.57	1.36	1.31
1	16S1	1044	A	N3-C4	6.57	1.38	1.34
22	23S1	439	A	C8-N7	6.57	1.36	1.31
1	16S1	1046	A	C8-N7	6.57	1.36	1.31
1	16S1	1377	A	C8-N7	6.57	1.36	1.31
22	23S1	621	A	C8-N7	6.57	1.36	1.31
22	23S1	2835	A	C8-N7	6.57	1.36	1.31
22	23S1	829	A	C5-C4	-6.57	1.34	1.38
22	23S1	1088	A	N3-C4	6.57	1.38	1.34
22	23S1	1890	A	C5-C4	-6.57	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	05S1	52	A	C8-N7	6.57	1.36	1.31
22	23S1	2682	A	C5-C4	-6.57	1.34	1.38
1	16S1	1476	A	C8-N7	6.56	1.36	1.31
22	23S1	1678	A	C5-C4	-6.56	1.34	1.38
22	23S1	2448	A	C5-C4	-6.56	1.34	1.38
1	16S1	53	A	C8-N7	6.56	1.36	1.31
22	23S1	1069	A	N3-C4	6.56	1.38	1.34
22	23S1	21	A	C5-C4	-6.56	1.34	1.38
22	23S1	582	A	C5-C4	-6.56	1.34	1.38
1	16S1	1269	A	C8-N7	6.56	1.36	1.31
22	23S1	1151	A	C5-C4	-6.56	1.34	1.38
1	16S1	303	A	C8-N7	6.56	1.36	1.31
1	16S1	1236	A	C8-N7	6.56	1.36	1.31
22	23S1	227	A	C5-C4	-6.56	1.34	1.38
1	16S1	139	A	C8-N7	6.55	1.36	1.31
22	23S1	103	A	C8-N7	6.55	1.36	1.31
22	23S1	125	A	C8-N7	6.55	1.36	1.31
22	23S1	526	A	C5-C4	-6.55	1.34	1.38
22	23S1	1916	A	C8-N7	6.55	1.36	1.31
1	16S1	282	A	C8-N7	6.55	1.36	1.31
22	23S1	28	A	C5-C4	-6.55	1.34	1.38
22	23S1	278	A	N3-C4	6.55	1.38	1.34
22	23S1	219	A	C5-C4	-6.55	1.34	1.38
22	23S1	990	A	C5-C4	-6.55	1.34	1.38
22	23S1	1477	A	C8-N7	6.55	1.36	1.31
22	23S1	2738	A	C5-C4	-6.55	1.34	1.38
22	23S1	2887	A	C8-N7	6.55	1.36	1.31
1	16S1	1167	A	C8-N7	6.55	1.36	1.31
22	23S1	91	A	C8-N7	6.55	1.36	1.31
22	23S1	428	A	C5-C4	-6.55	1.34	1.38
22	23S1	1885	A	C8-N7	6.55	1.36	1.31
22	23S1	453	A	C5-C4	-6.55	1.34	1.38
22	23S1	2090	A	C5-C4	-6.55	1.34	1.38
1	16S1	539	A	C8-N7	6.55	1.36	1.31
55	PTR1	58	A	C8-N7	6.55	1.36	1.31
1	16S1	1363	A	C8-N7	6.54	1.36	1.31
22	23S1	1046	A	N3-C4	6.54	1.38	1.34
1	16S1	130	A	C8-N7	6.54	1.36	1.31
22	23S1	1321	A	C8-N7	6.54	1.36	1.31
22	23S1	1927	A	C5-C4	-6.54	1.34	1.38
1	16S1	344	A	C8-N7	6.54	1.36	1.31
22	23S1	2736	A	C8-N7	6.54	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1285	A	C8-N7	6.54	1.36	1.31
22	23S1	422	A	C5-C4	-6.54	1.34	1.38
22	23S1	2814	A	C8-N7	6.54	1.36	1.31
1	16S1	814	A	C5-C4	-6.54	1.34	1.38
22	23S1	1098	A	N3-C4	6.54	1.38	1.34
22	23S1	1937	A	C8-N7	6.54	1.36	1.31
22	23S1	2733	A	C8-N7	6.54	1.36	1.31
22	23S1	783	A	N3-C4	6.53	1.38	1.34
22	23S1	2070	A	C5-C4	-6.53	1.34	1.38
22	23S1	616	A	C8-N7	6.53	1.36	1.31
1	16S1	228	A	C8-N7	6.53	1.36	1.31
1	16S1	411	A	C5-C4	-6.53	1.34	1.38
1	16S1	831	A	C8-N7	6.53	1.36	1.31
1	16S1	901	A	N7-C5	-6.53	1.35	1.39
1	16S1	1201	A	C8-N7	6.53	1.36	1.31
1	16S1	1271	A	C8-N7	6.53	1.36	1.31
22	23S1	2547	A	C8-N7	6.53	1.36	1.31
1	16S1	262	A	C8-N7	6.53	1.36	1.31
22	23S1	960	A	N7-C5	-6.53	1.35	1.39
22	23S1	1508	A	C8-N7	6.53	1.36	1.31
22	23S1	2077	A	C5-C4	-6.53	1.34	1.38
22	23S1	2706	A	C5-C4	-6.53	1.34	1.38
22	23S1	2800	A	C8-N7	6.53	1.36	1.31
22	23S1	1392	A	C8-N7	6.53	1.36	1.31
22	23S1	2184	A	N3-C4	6.53	1.38	1.34
1	16S1	59	A	C8-N7	6.52	1.36	1.31
22	23S1	42	A	C8-N7	6.52	1.36	1.31
22	23S1	621	A	C5-C4	-6.52	1.34	1.38
1	16S1	629	A	C8-N7	6.52	1.36	1.31
1	16S1	190	A	N3-C4	6.52	1.38	1.34
22	23S1	1189	A	C5-C4	-6.52	1.34	1.38
22	23S1	2015	A	C5-C4	-6.52	1.34	1.38
22	23S1	1307	A	C5-C4	-6.52	1.34	1.38
22	23S1	1535	A	N3-C4	6.52	1.38	1.34
22	23S1	216	A	C8-N7	6.51	1.36	1.31
22	23S1	925	A	C8-N7	6.51	1.36	1.31
22	23S1	2670	A	C5-C4	-6.51	1.34	1.38
1	16S1	109	A	C5-C4	-6.51	1.34	1.38
22	23S1	1677	A	C5-C4	-6.51	1.34	1.38
22	23S1	2469	A	C8-N7	6.51	1.36	1.31
23	05S1	115	A	C8-N7	6.51	1.36	1.31
1	16S1	1005	A	N3-C4	6.51	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1754	A	C5-C4	-6.51	1.34	1.38
22	23S1	1717	A	C8-N7	6.51	1.36	1.31
22	23S1	2033	A	C8-N7	6.51	1.36	1.31
22	23S1	1260	A	C5-C4	-6.51	1.34	1.38
22	23S1	423	A	C8-N7	6.50	1.36	1.31
22	23S1	1395	A	C8-N7	6.50	1.36	1.31
22	23S1	2541	A	C5-C4	-6.50	1.34	1.38
22	23S1	1090	A	N3-C4	6.50	1.38	1.34
22	23S1	2170	A	N3-C4	6.50	1.38	1.34
22	23S1	1287	A	C5-C4	-6.50	1.34	1.38
22	23S1	1532	A	N3-C4	6.50	1.38	1.34
22	23S1	2309	A	N3-C4	6.50	1.38	1.34
1	16S1	825	A	C5-C4	-6.50	1.34	1.38
22	23S1	1640	A	C8-N7	6.50	1.36	1.31
1	16S1	782	A	C5-C4	-6.50	1.34	1.38
22	23S1	675	A	C5-C4	-6.50	1.34	1.38
22	23S1	1419	A	C5-C4	-6.50	1.34	1.38
22	23S1	1571	A	C5-C4	-6.50	1.34	1.38
22	23S1	1928	A	C5-C4	-6.50	1.34	1.38
1	16S1	607	A	C8-N7	6.49	1.36	1.31
22	23S1	2851	A	C5-C4	-6.49	1.34	1.38
22	23S1	2882	A	C5-C4	-6.49	1.34	1.38
1	16S1	766	A	C8-N7	6.49	1.36	1.31
1	16S1	994	A	C8-N7	6.49	1.36	1.31
22	23S1	471	A	C5-C4	-6.49	1.34	1.38
22	23S1	718	A	C8-N7	6.49	1.36	1.31
22	23S1	794	A	C5-C4	-6.49	1.34	1.38
22	23S1	2042	A	C5-C4	-6.49	1.34	1.38
1	16S1	743	A	C5-C4	-6.49	1.34	1.38
22	23S1	526	A	C8-N7	6.49	1.36	1.31
22	23S1	756	A	C5-C4	-6.49	1.34	1.38
1	16S1	873	A	C5-C4	-6.49	1.34	1.38
22	23S1	1070	A	N3-C4	6.49	1.38	1.34
22	23S1	1808	A	C8-N7	6.49	1.36	1.31
1	16S1	716	A	C8-N7	6.49	1.36	1.31
22	23S1	332	A	C8-N7	6.49	1.36	1.31
22	23S1	2062	A	N3-C4	6.49	1.38	1.34
22	23S1	2388	A	C5-C4	-6.49	1.34	1.38
22	23S1	2823	A	C5-C4	-6.49	1.34	1.38
1	16S1	702	A	C8-N7	6.48	1.36	1.31
22	23S1	749	A	C5-C4	-6.48	1.34	1.38
22	23S1	1103	A	C8-N7	6.48	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1396	A	C5-C4	-6.48	1.34	1.38
22	23S1	74	A	C8-N7	6.48	1.36	1.31
22	23S1	1054	A	N3-C4	6.48	1.38	1.34
1	16S1	383	A	N7-C5	-6.48	1.35	1.39
22	23S1	739	A	C5-C4	-6.48	1.34	1.38
22	23S1	502	A	C5-C4	-6.48	1.34	1.38
22	23S1	2117	A	N3-C4	6.48	1.38	1.34
1	16S1	523	A	C8-N7	6.48	1.36	1.31
22	23S1	146	A	C8-N7	6.48	1.36	1.31
22	23S1	788	A	C5-C4	-6.48	1.34	1.38
22	23S1	2531	A	C8-N7	6.47	1.36	1.31
1	16S1	553	A	C8-N7	6.47	1.36	1.31
22	23S1	1665	A	C5-C4	-6.47	1.34	1.38
22	23S1	309	A	C5-C4	-6.47	1.34	1.38
22	23S1	1080	A	N3-C4	6.47	1.38	1.34
22	23S1	752	A	C8-N7	6.47	1.36	1.31
22	23S1	2005	A	C5-C4	-6.47	1.34	1.38
22	23S1	2748	A	C8-N7	6.47	1.36	1.31
23	05S1	59	A	C2-N3	6.47	1.39	1.33
22	23S1	1302	A	C5-C4	-6.46	1.34	1.38
22	23S1	1580	A	C8-N7	6.46	1.36	1.31
22	23S1	2435	A	C5-C4	-6.46	1.34	1.38
22	23S1	2736	A	C5-C4	-6.46	1.34	1.38
22	23S1	2564	A	C5-C4	-6.46	1.34	1.38
22	23S1	753	A	C5-C4	-6.46	1.34	1.38
22	23S1	927	A	C8-N7	6.46	1.36	1.31
22	23S1	2471	A	C8-N7	6.46	1.36	1.31
1	16S1	753	A	C8-N7	6.45	1.36	1.31
22	23S1	1165	A	C8-N7	6.45	1.36	1.31
22	23S1	1286	A	C8-N7	6.45	1.36	1.31
22	23S1	1427	A	C8-N7	6.45	1.36	1.31
22	23S1	2430	A	C8-N7	6.45	1.36	1.31
1	16S1	77	A	C8-N7	6.45	1.36	1.31
1	16S1	459	A	N3-C4	6.45	1.38	1.34
22	23S1	1308	A	C5-C4	-6.45	1.34	1.38
1	16S1	78	A	N3-C4	6.45	1.38	1.34
1	16S1	964	A	C8-N7	6.45	1.36	1.31
22	23S1	222	A	C5-C4	-6.45	1.34	1.38
22	23S1	1981	A	C5-C4	-6.45	1.34	1.38
1	16S1	1288	A	C8-N7	6.45	1.36	1.31
22	23S1	2565	A	C5-C4	-6.45	1.34	1.38
22	23S1	804	A	C5-C4	-6.44	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2566	A	C5-C4	-6.44	1.34	1.38
55	PTR1	69	A	N3-C4	6.44	1.38	1.34
22	23S1	2147	A	N3-C4	6.44	1.38	1.34
1	16S1	192	A	C8-N7	6.44	1.36	1.31
22	23S1	1889	A	C8-N7	6.44	1.36	1.31
23	05S1	104	A	C8-N7	6.44	1.36	1.31
1	16S1	1368	A	C8-N7	6.44	1.36	1.31
22	23S1	943	A	C5-C4	-6.44	1.34	1.38
22	23S1	1085	A	N3-C4	6.44	1.38	1.34
1	16S1	338	A	C8-N7	6.44	1.36	1.31
22	23S1	221	A	C5-C4	-6.44	1.34	1.38
22	23S1	2587	A	C5-C4	-6.44	1.34	1.38
22	23S1	2766	A	N3-C4	6.44	1.38	1.34
22	23S1	2679	A	C5-C4	-6.43	1.34	1.38
22	23S1	282	A	N3-C4	6.43	1.38	1.34
22	23S1	960	A	C5-C4	-6.43	1.34	1.38
22	23S1	1067	A	N3-C4	6.43	1.38	1.34
22	23S1	1194	A	C8-N7	6.43	1.36	1.31
22	23S1	2273	A	C5-C4	-6.43	1.34	1.38
1	16S1	1431	A	C5-C4	-6.43	1.34	1.38
22	23S1	1847	A	N3-C4	6.43	1.38	1.34
1	16S1	573	A	C5-C4	-6.43	1.34	1.38
22	23S1	479	A	C5-C4	-6.43	1.34	1.38
1	16S1	349	A	C5-C4	-6.43	1.34	1.38
22	23S1	415	A	C5-C4	-6.43	1.34	1.38
22	23S1	19	A	C5-C4	-6.42	1.34	1.38
22	23S1	1009	A	C5-C4	-6.42	1.34	1.38
22	23S1	1247	A	C8-N7	6.42	1.36	1.31
22	23S1	2478	A	C5-C4	-6.42	1.34	1.38
1	16S1	482	A	C8-N7	6.42	1.36	1.31
22	23S1	2450	A	C8-N7	6.42	1.36	1.31
22	23S1	2478	A	C8-N7	6.42	1.36	1.31
1	16S1	694	A	C5-C4	-6.42	1.34	1.38
1	16S1	1287	A	C8-N7	6.42	1.36	1.31
22	23S1	866	A	C8-N7	6.42	1.36	1.31
22	23S1	1050	A	N3-C4	6.42	1.38	1.34
22	23S1	1590	A	N3-C4	6.42	1.38	1.34
22	23S1	1705	A	C5-C4	-6.42	1.34	1.38
1	16S1	393	A	C8-N7	6.41	1.36	1.31
22	23S1	721	A	C8-N7	6.41	1.36	1.31
22	23S1	789	A	C5-C4	-6.41	1.34	1.38
1	16S1	315	A	C5-C4	-6.41	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	101	A	N3-C4	6.41	1.38	1.34
1	16S1	459	A	C8-N7	6.41	1.36	1.31
22	23S1	1783	A	C5-C4	-6.41	1.34	1.38
22	23S1	2850	A	C5-C4	-6.41	1.34	1.38
22	23S1	654	A	N3-C4	6.41	1.38	1.34
22	23S1	299	A	C8-N7	6.41	1.36	1.31
22	23S1	1230	A	C5-C4	-6.41	1.34	1.38
22	23S1	1366	A	C8-N7	6.41	1.36	1.31
22	23S1	2135	A	N3-C4	6.41	1.38	1.34
23	05S1	53	A	C8-N7	6.41	1.36	1.31
22	23S1	2750	A	C8-N7	6.40	1.36	1.31
1	16S1	787	A	C5-C4	-6.40	1.34	1.38
22	23S1	2080	A	C5-C4	-6.40	1.34	1.38
22	23S1	2893	A	C8-N7	6.40	1.36	1.31
1	16S1	909	A	C8-N7	6.40	1.36	1.31
22	23S1	752	A	C5-C4	-6.40	1.34	1.38
22	23S1	1413	A	N3-C4	6.40	1.38	1.34
22	23S1	299	A	C5-C4	-6.40	1.34	1.38
1	16S1	364	A	C8-N7	6.40	1.36	1.31
1	16S1	414	A	N3-C4	6.40	1.38	1.34
1	16S1	759	A	C8-N7	6.40	1.36	1.31
1	16S1	1394	A	C5-C4	-6.40	1.34	1.38
22	23S1	1253	A	C5-C4	-6.40	1.34	1.38
22	23S1	1960	A	C8-N7	6.40	1.36	1.31
1	16S1	729	A	C5-C4	-6.39	1.34	1.38
22	23S1	167	A	C8-N7	6.39	1.36	1.31
22	23S1	1900	A	C5-C4	-6.39	1.34	1.38
22	23S1	2670	A	C8-N7	6.39	1.36	1.31
1	16S1	994	A	N3-C4	6.39	1.38	1.34
22	23S1	2191	A	C8-N7	6.39	1.36	1.31
22	23S1	2461	A	C8-N7	6.39	1.36	1.31
1	16S1	197	A	C8-N7	6.39	1.36	1.31
22	23S1	877	A	C8-N7	6.39	1.36	1.31
22	23S1	1970	A	C5-C4	-6.39	1.34	1.38
1	16S1	383	A	N3-C4	6.39	1.38	1.34
1	16S1	635	A	C8-N7	6.39	1.36	1.31
22	23S1	221	A	C8-N7	6.39	1.36	1.31
1	16S1	1014	A	C8-N7	6.39	1.36	1.31
22	23S1	1155	A	C5-C4	-6.39	1.34	1.38
22	23S1	541	A	C8-N7	6.39	1.36	1.31
22	23S1	1194	A	C5-C4	-6.39	1.34	1.38
22	23S1	984	A	N3-C4	6.38	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2020	A	C5-C4	-6.38	1.34	1.38
22	23S1	590	A	C5-C4	-6.38	1.34	1.38
1	16S1	535	A	C8-N7	6.38	1.36	1.31
22	23S1	1927	A	C8-N7	6.38	1.36	1.31
23	05S1	73	A	N3-C4	6.38	1.38	1.34
1	16S1	313	A	C8-N7	6.38	1.36	1.31
22	23S1	666	A	C5-C4	-6.38	1.34	1.38
23	05S1	45	A	C8-N7	6.38	1.36	1.31
1	16S1	1201	A	C5-C4	-6.37	1.34	1.38
22	23S1	1439	A	C8-N7	6.37	1.36	1.31
22	23S1	2600	A	C5-C4	-6.37	1.34	1.38
1	16S1	1254	A	C8-N7	6.37	1.36	1.31
1	16S1	1493	A	N3-C4	6.37	1.38	1.34
22	23S1	457	A	C8-N7	6.37	1.36	1.31
22	23S1	2198	A	C5-C4	-6.37	1.34	1.38
22	23S1	2386	A	C5-C4	-6.37	1.34	1.38
22	23S1	497	A	C8-N7	6.37	1.36	1.31
22	23S1	2328	A	C5-C4	-6.37	1.34	1.38
22	23S1	2376	A	C8-N7	6.37	1.36	1.31
1	16S1	1171	A	C8-N7	6.37	1.36	1.31
1	16S1	1225	A	C8-N7	6.37	1.36	1.31
22	23S1	782	A	C5-C4	-6.37	1.34	1.38
22	23S1	1701	A	C5-C4	-6.37	1.34	1.38
1	16S1	1433	A	C8-N7	6.37	1.36	1.31
22	23S1	1272	A	C5-C4	-6.37	1.34	1.38
22	23S1	1525	A	C8-N7	6.37	1.36	1.31
22	23S1	1552	A	C5-C4	-6.37	1.34	1.38
22	23S1	2738	A	C8-N7	6.37	1.36	1.31
55	PTR1	21	A	C8-N7	6.37	1.36	1.31
22	23S1	800	A	C5-C4	-6.36	1.34	1.38
22	23S1	1918	A	C8-N7	6.36	1.36	1.31
22	23S1	2711	A	C5-C4	-6.36	1.34	1.38
1	16S1	1021	A	N3-C4	6.36	1.38	1.34
22	23S1	502	A	C8-N7	6.36	1.36	1.31
22	23S1	1237	A	C5-C4	-6.36	1.34	1.38
1	16S1	329	A	C5-C4	-6.36	1.34	1.38
22	23S1	382	A	C5-C4	-6.36	1.34	1.38
22	23S1	833	A	C5-C4	-6.36	1.34	1.38
22	23S1	844	A	C8-N7	6.36	1.36	1.31
22	23S1	1427	A	C5-C4	-6.36	1.34	1.38
1	16S1	298	A	C8-N7	6.36	1.36	1.31
22	23S1	84	A	C5-C4	-6.36	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	447	A	C5-C4	-6.36	1.34	1.38
22	23S1	743	A	C5-C4	-6.36	1.34	1.38
22	23S1	2476	A	C8-N7	6.36	1.36	1.31
1	16S1	1428	A	C8-N7	6.36	1.35	1.31
22	23S1	2225	A	C8-N7	6.36	1.35	1.31
22	23S1	13	A	C8-N7	6.35	1.35	1.31
22	23S1	2227	A	C5-C4	-6.35	1.34	1.38
1	16S1	1500	A	C8-N7	6.35	1.35	1.31
22	23S1	83	A	C8-N7	6.35	1.35	1.31
22	23S1	1551	A	C8-N7	6.35	1.35	1.31
22	23S1	2899	A	C8-N7	6.35	1.35	1.31
1	16S1	26	A	C8-N7	6.35	1.35	1.31
1	16S1	1441	A	N3-C4	6.35	1.38	1.34
22	23S1	1632	A	C8-N7	6.35	1.35	1.31
22	23S1	2198	A	C8-N7	6.35	1.35	1.31
22	23S1	2471	A	C5-C4	-6.35	1.34	1.38
22	23S1	2700	A	C5-C4	-6.35	1.34	1.38
22	23S1	928	A	C5-C4	-6.34	1.34	1.38
1	16S1	32	A	C5-C4	-6.34	1.34	1.38
22	23S1	574	A	C5-C4	-6.34	1.34	1.38
22	23S1	608	A	C5-C4	-6.34	1.34	1.38
22	23S1	705	A	C5-C4	-6.34	1.34	1.38
1	16S1	389	A	C8-N7	6.34	1.35	1.31
1	16S1	872	A	C8-N7	6.34	1.35	1.31
22	23S1	6	A	C8-N7	6.34	1.35	1.31
22	23S1	1679	A	C5-C4	-6.34	1.34	1.38
22	23S1	1073	A	N3-C4	6.34	1.38	1.34
22	23S1	1032	A	C8-N7	6.33	1.35	1.31
22	23S1	2882	A	C8-N7	6.33	1.35	1.31
1	16S1	1081	A	C5-C4	-6.33	1.34	1.38
22	23S1	1614	A	C5-C4	-6.33	1.34	1.38
22	23S1	44	A	C8-N7	6.33	1.35	1.31
22	23S1	802	A	C5-C4	-6.33	1.34	1.38
22	23S1	1304	A	C8-N7	6.33	1.35	1.31
22	23S1	2163	A	N3-C4	6.33	1.38	1.34
22	23S1	176	A	C8-N7	6.33	1.35	1.31
22	23S1	1690	A	C5-C4	-6.33	1.34	1.38
22	23S1	2336	A	C8-N7	6.33	1.35	1.31
22	23S1	1815	A	C8-N7	6.33	1.35	1.31
22	23S1	602	A	C5-C4	-6.32	1.34	1.38
22	23S1	1583	A	N3-C4	6.32	1.38	1.34
23	05S1	57	A	C8-N7	6.32	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1147	A	C8-N7	6.32	1.35	1.31
22	23S1	2135	A	C8-N7	6.32	1.35	1.31
22	23S1	706	A	C5-C4	-6.32	1.34	1.38
22	23S1	2468	A	C8-N7	6.32	1.35	1.31
1	16S1	349	A	C8-N7	6.32	1.35	1.31
1	16S1	456	A	N3-C4	6.32	1.38	1.34
1	16S1	1480	A	C5-C4	-6.32	1.34	1.38
22	23S1	118	A	C5-C4	-6.32	1.34	1.38
22	23S1	1246	A	C5-C4	-6.32	1.34	1.38
22	23S1	2114	A	C8-N7	6.32	1.35	1.31
1	16S1	1055	A	C8-N7	6.32	1.35	1.31
22	23S1	2266	A	C5-C4	-6.32	1.34	1.38
22	23S1	127	A	C5-C4	-6.31	1.34	1.38
22	23S1	190	A	C5-C4	-6.31	1.34	1.38
22	23S1	844	A	C5-C4	-6.31	1.34	1.38
22	23S1	1008	A	C5-C4	-6.31	1.34	1.38
22	23S1	1640	A	C5-C4	-6.31	1.34	1.38
22	23S1	2298	A	C8-N7	6.31	1.35	1.31
22	23S1	146	A	C5-C4	-6.31	1.34	1.38
22	23S1	1129	A	C5-C4	-6.31	1.34	1.38
1	16S1	977	A	N3-C4	6.31	1.38	1.34
22	23S1	371	A	C8-N7	6.31	1.35	1.31
22	23S1	699	A	C5-C4	-6.31	1.34	1.38
1	16S1	1275	A	C8-N7	6.30	1.35	1.31
22	23S1	64	A	C8-N7	6.30	1.35	1.31
22	23S1	1755	A	C5-C4	-6.30	1.34	1.38
22	23S1	251	A	N7-C5	-6.30	1.35	1.39
22	23S1	2450	A	C5-C4	-6.30	1.34	1.38
22	23S1	73	A	C5-C4	-6.30	1.34	1.38
22	23S1	449	A	C8-N7	6.30	1.35	1.31
22	23S1	670	A	C5-C4	-6.30	1.34	1.38
22	23S1	981	A	C5-C4	-6.30	1.34	1.38
22	23S1	1322	A	C5-C4	-6.30	1.34	1.38
22	23S1	2530	A	C8-N7	6.30	1.35	1.31
1	16S1	546	A	C8-N7	6.30	1.35	1.31
1	16S1	1500	A	C5-C4	-6.30	1.34	1.38
22	23S1	529	A	C8-N7	6.30	1.35	1.31
22	23S1	53	A	C8-N7	6.29	1.35	1.31
22	23S1	2726	A	C5-C4	-6.29	1.34	1.38
1	16S1	533	A	C8-N7	6.29	1.35	1.31
22	23S1	152	A	C8-N7	6.29	1.35	1.31
22	23S1	1365	A	C8-N7	6.29	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1759	A	C8-N7	6.29	1.35	1.31
55	PTR1	23	A	N3-C4	6.29	1.38	1.34
1	16S1	1157	A	C8-N7	6.29	1.35	1.31
22	23S1	2425	A	C5-C4	-6.29	1.34	1.38
22	23S1	1127	A	C5-C4	-6.29	1.34	1.38
1	16S1	119	A	C8-N7	6.29	1.35	1.31
1	16S1	246	A	C8-N7	6.29	1.35	1.31
1	16S1	1480	A	C8-N7	6.29	1.35	1.31
22	23S1	374	A	C5-C4	-6.29	1.34	1.38
22	23S1	928	A	C8-N7	6.29	1.35	1.31
22	23S1	1912	A	C5-C4	-6.29	1.34	1.38
1	16S1	496	A	C8-N7	6.28	1.35	1.31
1	16S1	1257	A	N3-C4	6.28	1.38	1.34
1	16S1	1287	A	C5-C4	-6.28	1.34	1.38
22	23S1	1477	A	N3-C4	6.28	1.38	1.34
1	16S1	1111	A	C8-N7	6.28	1.35	1.31
22	23S1	2225	A	C5-C4	-6.28	1.34	1.38
1	16S1	50	A	C8-N7	6.28	1.35	1.31
1	16S1	320	A	C5-C4	-6.28	1.34	1.38
1	16S1	807	A	C5-C4	-6.28	1.34	1.38
22	23S1	2799	A	N3-C4	6.28	1.38	1.34
22	23S1	1057	A	N3-C4	6.28	1.38	1.34
22	23S1	89	A	C5-C4	-6.28	1.34	1.38
22	23S1	412	A	C5-C4	-6.28	1.34	1.38
1	16S1	878	A	C5-C4	-6.28	1.34	1.38
1	16S1	1067	A	C8-N7	6.28	1.35	1.31
22	23S1	637	A	C5-C4	-6.28	1.34	1.38
22	23S1	1749	A	C5-C4	-6.28	1.34	1.38
22	23S1	2837	A	C5-C4	-6.28	1.34	1.38
22	23S1	71	A	C8-N7	6.27	1.35	1.31
22	23S1	513	A	C5-C4	-6.27	1.34	1.38
22	23S1	1676	A	C5-C4	-6.27	1.34	1.38
22	23S1	2333	A	C5-C4	-6.27	1.34	1.38
22	23S1	1871	A	N3-C4	6.27	1.38	1.34
1	16S1	655	A	C8-N7	6.27	1.35	1.31
22	23S1	2560	A	C5-C4	-6.27	1.34	1.38
1	16S1	777	A	C5-C4	-6.27	1.34	1.38
1	16S1	802	A	C5-C4	-6.27	1.34	1.38
1	16S1	937	A	C8-N7	6.27	1.35	1.31
1	16S1	1428	A	C5-C4	-6.27	1.34	1.38
22	23S1	231	A	C8-N7	6.27	1.35	1.31
22	23S1	1085	A	C8-N7	6.27	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	449	A	C5-C4	-6.27	1.34	1.38
1	16S1	313	A	C5-C4	-6.26	1.34	1.38
1	16S1	675	A	C8-N7	6.26	1.35	1.31
1	16S1	1299	A	N3-C4	6.26	1.38	1.34
22	23S1	685	A	C5-C4	-6.26	1.34	1.38
22	23S1	751	A	C5-C4	-6.26	1.34	1.38
22	23S1	2377	A	C5-C4	-6.26	1.34	1.38
22	23S1	2270	A	C8-N7	6.26	1.35	1.31
22	23S1	2829	A	C8-N7	6.26	1.35	1.31
22	23S1	1603	A	C5-C4	-6.26	1.34	1.38
22	23S1	1403	A	C5-C4	-6.26	1.34	1.38
55	PTR1	76	A	C5-C4	-6.26	1.34	1.38
1	16S1	663	A	C5-C4	-6.26	1.34	1.38
1	16S1	913	A	C8-N7	6.26	1.35	1.31
22	23S1	300	A	C8-N7	6.26	1.35	1.31
22	23S1	1853	A	C8-N7	6.26	1.35	1.31
22	23S1	2433	A	C5-C4	-6.26	1.34	1.38
1	16S1	66	A	C8-N7	6.25	1.35	1.31
1	16S1	327	A	C5-C4	-6.25	1.34	1.38
1	16S1	595	A	C8-N7	6.25	1.35	1.31
22	23S1	340	A	C8-N7	6.25	1.35	1.31
55	PTR1	59	A	N3-C4	6.25	1.38	1.34
22	23S1	1214	A	C8-N7	6.25	1.35	1.31
55	PTR1	21	A	N3-C4	6.25	1.38	1.34
1	16S1	1339	A	C5-C4	-6.25	1.34	1.38
1	16S1	509	A	C8-N7	6.25	1.35	1.31
1	16S1	935	A	C8-N7	6.25	1.35	1.31
1	16S1	1117	A	C8-N7	6.25	1.35	1.31
22	23S1	1336	A	C8-N7	6.25	1.35	1.31
22	23S1	1610	A	C5-C4	-6.25	1.34	1.38
22	23S1	2288	A	C8-N7	6.25	1.35	1.31
1	16S1	1502	A	C5-C4	-6.25	1.34	1.38
22	23S1	173	A	C8-N7	6.25	1.35	1.31
22	23S1	727	A	C5-C4	-6.25	1.34	1.38
22	23S1	1735	A	N3-C4	6.25	1.38	1.34
22	23S1	2411	A	C5-C4	-6.25	1.34	1.38
1	16S1	554	A	C5-C4	-6.25	1.34	1.38
22	23S1	1626	A	C5-C4	-6.25	1.34	1.38
1	16S1	77	A	N3-C4	6.24	1.38	1.34
1	16S1	263	A	C8-N7	6.24	1.35	1.31
1	16S1	1446	A	C8-N7	6.24	1.35	1.31
22	23S1	1347	A	C8-N7	6.24	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	182	A	C8-N7	6.24	1.35	1.31
1	16S1	174	A	C8-N7	6.24	1.35	1.31
22	23S1	925	A	C5-C4	-6.24	1.34	1.38
22	23S1	1347	A	C5-C4	-6.24	1.34	1.38
1	16S1	728	A	C8-N7	6.24	1.35	1.31
22	23S1	1000	A	C8-N7	6.24	1.35	1.31
22	23S1	1308	A	C8-N7	6.24	1.35	1.31
22	23S1	2639	A	C8-N7	6.24	1.35	1.31
1	16S1	787	A	C8-N7	6.24	1.35	1.31
1	16S1	819	A	C8-N7	6.24	1.35	1.31
22	23S1	479	A	C8-N7	6.24	1.35	1.31
1	16S1	781	A	C5-C4	-6.24	1.34	1.38
22	23S1	972	A	C5-C4	-6.24	1.34	1.38
22	23S1	1854	A	C5-C4	-6.23	1.34	1.38
22	23S1	1285	A	C5-C4	-6.23	1.34	1.38
1	16S1	10	A	C5-C4	-6.23	1.34	1.38
1	16S1	356	A	C5-C4	-6.23	1.34	1.38
1	16S1	579	A	C8-N7	6.23	1.35	1.31
1	16S1	1188	A	C5-C4	-6.23	1.34	1.38
1	16S1	1430	A	C8-N7	6.23	1.35	1.31
22	23S1	402	A	C5-C4	-6.23	1.34	1.38
22	23S1	1284	A	C8-N7	6.23	1.35	1.31
22	23S1	1711	A	C8-N7	6.23	1.35	1.31
22	23S1	1858	A	C8-N7	6.23	1.35	1.31
22	23S1	1919	A	C5-C4	-6.23	1.34	1.38
1	16S1	864	A	C5-C4	-6.23	1.34	1.38
22	23S1	53	A	C5-C4	-6.23	1.34	1.38
22	23S1	1384	A	C8-N7	6.22	1.35	1.31
22	23S1	1937	A	C5-C4	-6.22	1.34	1.38
1	16S1	768	A	C5-C4	-6.22	1.34	1.38
22	23S1	1392	A	C5-C4	-6.22	1.34	1.38
1	16S1	51	A	C5-C4	-6.22	1.34	1.38
1	16S1	460	A	N3-C4	6.22	1.38	1.34
1	16S1	983	A	C8-N7	6.22	1.35	1.31
22	23S1	909	A	N3-C4	6.22	1.38	1.34
22	23S1	2062	A	C8-N7	6.22	1.35	1.31
22	23S1	2434	A	C5-C4	-6.22	1.34	1.38
23	05S1	108	A	C8-N7	6.21	1.35	1.31
1	16S1	288	A	C8-N7	6.21	1.35	1.31
1	16S1	336	A	C8-N7	6.21	1.35	1.31
1	16S1	1188	A	C8-N7	6.21	1.35	1.31
22	23S1	1327	A	C5-C4	-6.21	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2322	A	C8-N7	6.21	1.35	1.31
22	23S1	2705	A	C5-C4	-6.21	1.34	1.38
22	23S1	532	A	C5-C4	-6.21	1.34	1.38
22	23S1	1286	A	C5-C4	-6.21	1.34	1.38
22	23S1	2278	A	C5-C4	-6.21	1.34	1.38
1	16S1	1191	A	C8-N7	6.21	1.35	1.31
22	23S1	432	A	C5-C4	-6.21	1.34	1.38
22	23S1	2340	A	C5-C4	-6.21	1.34	1.38
1	16S1	411	A	N3-C4	6.20	1.38	1.34
22	23S1	2468	A	C5-C4	-6.20	1.34	1.38
1	16S1	199	A	N3-C4	6.20	1.38	1.34
22	23S1	1032	A	C5-C4	-6.20	1.34	1.38
22	23S1	1634	A	C8-N7	6.20	1.35	1.31
22	23S1	1635	A	C5-C4	-6.20	1.34	1.38
1	16S1	533	A	N3-C4	6.20	1.38	1.34
22	23S1	764	A	C8-N7	6.20	1.35	1.31
22	23S1	1932	A	C8-N7	6.20	1.35	1.31
1	16S1	1155	A	N3-C4	6.20	1.38	1.34
1	16S1	1434	A	C5-C4	-6.20	1.34	1.38
22	23S1	910	A	C5-C4	-6.20	1.34	1.38
22	23S1	988	A	C5-C4	-6.20	1.34	1.38
22	23S1	1304	A	C5-C4	-6.20	1.34	1.38
1	16S1	353	A	C5-C4	-6.20	1.34	1.38
22	23S1	223	A	C5-C4	-6.20	1.34	1.38
22	23S1	454	A	C8-N7	6.20	1.35	1.31
22	23S1	94	A	C8-N7	6.20	1.35	1.31
22	23S1	176	A	C5-C4	-6.20	1.34	1.38
22	23S1	1328	A	C8-N7	6.20	1.35	1.31
22	23S1	2776	A	C8-N7	6.20	1.35	1.31
1	16S1	451	A	C5-C4	-6.19	1.34	1.38
1	16S1	892	A	C5-C4	-6.19	1.34	1.38
1	16S1	1163	A	N3-C4	6.19	1.38	1.34
22	23S1	1821	A	C8-N7	6.19	1.35	1.31
1	16S1	465	A	N3-C4	6.19	1.38	1.34
1	16S1	560	A	C5-C4	-6.19	1.34	1.38
1	16S1	675	A	C5-C4	-6.19	1.34	1.38
1	16S1	673	A	C5-C4	-6.19	1.34	1.38
1	16S1	694	A	C8-N7	6.19	1.35	1.31
22	23S1	204	A	C8-N7	6.19	1.35	1.31
22	23S1	1373	A	C5-C4	-6.19	1.34	1.38
22	23S1	1755	A	C8-N7	6.19	1.35	1.31
22	23S1	346	A	C8-N7	6.19	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1669	A	N3-C4	6.18	1.38	1.34
22	23S1	1759	A	C5-C4	-6.18	1.34	1.38
22	23S1	1848	A	C8-N7	6.18	1.35	1.31
22	23S1	2019	A	C5-C4	-6.18	1.34	1.38
22	23S1	2031	A	C5-C4	-6.18	1.34	1.38
22	23S1	2241	A	C5-C4	-6.18	1.34	1.38
1	16S1	1042	A	N3-C4	6.18	1.38	1.34
22	23S1	142	A	C8-N7	6.18	1.35	1.31
22	23S1	508	A	N3-C4	6.18	1.38	1.34
22	23S1	975	A	C5-C4	-6.18	1.34	1.38
22	23S1	2369	A	C5-C4	-6.18	1.34	1.38
22	23S1	2426	A	C5-C4	-6.18	1.34	1.38
22	23S1	42	A	C5-C4	-6.18	1.34	1.38
22	23S1	2740	A	C8-N7	6.18	1.35	1.31
1	16S1	1201	A	N3-C4	6.18	1.38	1.34
22	23S1	6	A	C5-C4	-6.18	1.34	1.38
22	23S1	941	A	C5-C4	-6.18	1.34	1.38
1	16S1	1082	A	C8-N7	6.18	1.35	1.31
1	16S1	373	A	N3-C4	6.18	1.38	1.34
22	23S1	466	A	C5-C4	-6.18	1.34	1.38
22	23S1	1872	A	N3-C4	6.18	1.38	1.34
23	05S1	115	A	C5-C4	-6.18	1.34	1.38
22	23S1	2813	A	C8-N7	6.17	1.35	1.31
22	23S1	2829	A	N3-C4	6.17	1.38	1.34
1	16S1	300	A	N3-C4	6.17	1.38	1.34
22	23S1	320	A	C8-N7	6.17	1.35	1.31
22	23S1	2267	A	N3-C4	6.17	1.38	1.34
22	23S1	1439	A	C5-C4	-6.17	1.34	1.38
22	23S1	2705	A	C8-N7	6.17	1.35	1.31
1	16S1	510	A	C5-C4	-6.17	1.34	1.38
1	16S1	712	A	C8-N7	6.17	1.35	1.31
23	05S1	45	A	C5-C4	-6.17	1.34	1.38
22	23S1	14	A	C5-C4	-6.17	1.34	1.38
22	23S1	920	A	C8-N7	6.17	1.35	1.31
22	23S1	1156	A	C5-C4	-6.17	1.34	1.38
22	23S1	1803	A	C5-C4	-6.17	1.34	1.38
23	05S1	59	A	N3-C4	6.17	1.38	1.34
1	16S1	1437	A	C8-N7	6.17	1.35	1.31
22	23S1	1938	A	C5-C4	-6.17	1.34	1.38
22	23S1	2381	A	C8-N7	6.17	1.35	1.31
1	16S1	532	A	N3-C4	6.16	1.38	1.34
22	23S1	2497	A	C5-C4	-6.16	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2758	A	C5-C4	-6.16	1.34	1.38
22	23S1	735	A	C5-C4	-6.16	1.34	1.38
22	23S1	2322	A	C5-C4	-6.16	1.34	1.38
22	23S1	2432	A	C8-N7	6.16	1.35	1.31
22	23S1	1508	A	N3-C4	6.16	1.38	1.34
1	16S1	298	A	C5-C4	-6.16	1.34	1.38
22	23S1	706	A	C8-N7	6.16	1.35	1.31
22	23S1	899	A	N3-C4	6.16	1.38	1.34
22	23S1	1366	A	C5-C4	-6.16	1.34	1.38
22	23S1	2340	A	C8-N7	6.16	1.35	1.31
1	16S1	1306	A	C8-N7	6.16	1.35	1.31
23	05S1	73	A	C8-N7	6.16	1.35	1.31
1	16S1	1413	A	C8-N7	6.16	1.35	1.31
22	23S1	1805	A	C5-C4	-6.16	1.34	1.38
22	23S1	1987	A	C5-C4	-6.16	1.34	1.38
22	23S1	2297	A	C8-N7	6.16	1.35	1.31
1	16S1	205	A	N3-C4	6.15	1.38	1.34
1	16S1	1324	A	C8-N7	6.15	1.35	1.31
22	23S1	602	A	C8-N7	6.15	1.35	1.31
22	23S1	2191	A	N3-C4	6.15	1.38	1.34
22	23S1	2212	A	C5-C4	-6.15	1.34	1.38
1	16S1	452	A	N3-C4	6.15	1.38	1.34
1	16S1	938	A	C8-N7	6.15	1.35	1.31
22	23S1	900	A	N3-C4	6.15	1.38	1.34
22	23S1	1096	A	N3-C4	6.15	1.38	1.34
22	23S1	1552	A	C8-N7	6.15	1.35	1.31
1	16S1	825	A	C8-N7	6.15	1.35	1.31
22	23S1	199	A	C8-N7	6.15	1.35	1.31
22	23S1	532	A	N3-C4	6.15	1.38	1.34
22	23S1	2856	A	C8-N7	6.15	1.35	1.31
23	05S1	101	A	N3-C4	6.15	1.38	1.34
22	23S1	1890	A	C8-N7	6.15	1.35	1.31
22	23S1	2560	A	C8-N7	6.15	1.35	1.31
1	16S1	665	A	C5-C4	-6.14	1.34	1.38
22	23S1	1785	A	C8-N7	6.14	1.35	1.31
22	23S1	2727	A	C5-C4	-6.14	1.34	1.38
1	16S1	1318	A	C8-N7	6.14	1.35	1.31
22	23S1	631	A	C5-C4	-6.14	1.34	1.38
1	16S1	430	A	C8-N7	6.14	1.35	1.31
22	23S1	362	A	C5-C4	-6.14	1.34	1.38
22	23S1	1664	A	C5-C4	-6.14	1.34	1.38
22	23S1	1977	A	C5-C4	-6.14	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2764	A	C8-N7	6.14	1.35	1.31
1	16S1	780	A	C5-C4	-6.13	1.34	1.38
22	23S1	1147	A	C5-C4	-6.13	1.34	1.38
22	23S1	1384	A	C5-C4	-6.13	1.34	1.38
1	16S1	983	A	N3-C4	6.13	1.38	1.34
55	PTR1	58	A	N3-C4	6.13	1.38	1.34
1	16S1	315	A	C8-N7	6.13	1.35	1.31
1	16S1	498	A	N3-C4	6.13	1.38	1.34
22	23S1	119	A	C5-C4	-6.13	1.34	1.38
22	23S1	262	A	C5-C4	-6.13	1.34	1.38
22	23S1	1378	A	C8-N7	6.13	1.35	1.31
22	23S1	2352	A	C5-C4	-6.13	1.34	1.38
1	16S1	718	A	C8-N7	6.13	1.35	1.31
1	16S1	1429	A	C5-C4	-6.13	1.34	1.38
22	23S1	1754	A	C8-N7	6.13	1.35	1.31
1	16S1	621	A	C8-N7	6.13	1.35	1.31
1	16S1	1167	A	N3-C4	6.13	1.38	1.34
22	23S1	2284	A	C8-N7	6.13	1.35	1.31
22	23S1	2800	A	C5-C4	-6.13	1.34	1.38
22	23S1	71	A	C5-C4	-6.12	1.34	1.38
22	23S1	428	A	C8-N7	6.12	1.35	1.31
22	23S1	866	A	C5-C4	-6.12	1.34	1.38
1	16S1	630	A	C8-N7	6.12	1.35	1.31
1	16S1	908	A	C5-C4	-6.12	1.34	1.38
1	16S1	1431	A	C8-N7	6.12	1.35	1.31
22	23S1	1987	A	C8-N7	6.12	1.35	1.31
22	23S1	2333	A	C8-N7	6.12	1.35	1.31
1	16S1	1465	A	C8-N7	6.12	1.35	1.31
22	23S1	256	A	C8-N7	6.12	1.35	1.31
22	23S1	332	A	C5-C4	-6.12	1.34	1.38
22	23S1	1913	A	N3-C4	6.12	1.38	1.34
1	16S1	560	A	C8-N7	6.12	1.35	1.31
1	16S1	1092	A	C5-C4	-6.12	1.34	1.38
22	23S1	2274	A	C5-C4	-6.12	1.34	1.38
55	PTR1	76	A	C8-N7	6.12	1.35	1.31
1	16S1	161	A	C8-N7	6.11	1.35	1.31
1	16S1	373	A	C8-N7	6.11	1.35	1.31
1	16S1	499	A	N3-C4	6.11	1.38	1.34
23	05S1	94	A	C5-C4	-6.11	1.34	1.38
1	16S1	579	A	C5-C4	-6.11	1.34	1.38
1	16S1	608	A	C8-N7	6.11	1.35	1.31
1	16S1	1434	A	C8-N7	6.11	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1773	A	C5-C4	-6.11	1.34	1.38
22	23S1	2241	A	C8-N7	6.11	1.35	1.31
22	23S1	2513	A	C8-N7	6.11	1.35	1.31
22	23S1	1801	A	C8-N7	6.11	1.35	1.31
22	23S1	2809	A	C5-C4	-6.11	1.34	1.38
1	16S1	408	A	N3-C4	6.10	1.38	1.34
22	23S1	2837	A	C8-N7	6.10	1.35	1.31
22	23S1	118	A	C8-N7	6.10	1.35	1.31
22	23S1	310	A	C8-N7	6.10	1.35	1.31
22	23S1	2778	A	C5-C4	-6.10	1.34	1.38
22	23S1	501	A	C8-N7	6.10	1.35	1.31
22	23S1	730	A	C5-C4	-6.10	1.34	1.38
22	23S1	1165	A	C5-C4	-6.10	1.34	1.38
22	23S1	644	A	C5-C4	-6.10	1.34	1.38
22	23S1	2781	A	C5-C4	-6.10	1.34	1.38
23	05S1	78	A	C5-C4	-6.10	1.34	1.38
1	16S1	1256	A	N3-C4	6.10	1.38	1.34
22	23S1	231	A	C5-C4	-6.10	1.34	1.38
22	23S1	482	A	C5-C4	-6.10	1.34	1.38
22	23S1	863	A	C5-C4	-6.10	1.34	1.38
22	23S1	1789	A	C5-C4	-6.10	1.34	1.38
22	23S1	2453	A	C5-C4	-6.10	1.34	1.38
1	16S1	1340	A	C8-N7	6.10	1.35	1.31
22	23S1	167	A	C5-C4	-6.10	1.34	1.38
1	16S1	1362	A	C5-C4	-6.09	1.34	1.38
22	23S1	218	A	C8-N7	6.09	1.35	1.31
22	23S1	2448	A	C8-N7	6.09	1.35	1.31
1	16S1	448	A	N3-C4	6.09	1.38	1.34
22	23S1	2439	A	C5-C4	-6.09	1.34	1.38
1	16S1	908	A	C8-N7	6.09	1.35	1.31
22	23S1	227	A	C8-N7	6.09	1.35	1.31
22	23S1	1204	A	N3-C4	6.09	1.38	1.34
22	23S1	1237	A	C8-N7	6.09	1.35	1.31
22	23S1	2377	A	C8-N7	6.09	1.35	1.31
22	23S1	56	A	C5-C4	-6.09	1.34	1.38
22	23S1	505	A	C5-C4	-6.09	1.34	1.38
22	23S1	936	A	C8-N7	6.09	1.35	1.31
22	23S1	2158	A	N3-C4	6.09	1.38	1.34
22	23S1	1230	A	C8-N7	6.08	1.35	1.31
1	16S1	496	A	N3-C4	6.08	1.38	1.34
1	16S1	794	A	C5-C4	-6.08	1.34	1.38
1	16S1	1197	A	C8-N7	6.08	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1319	A	N3-C4	6.08	1.38	1.34
22	23S1	627	A	C8-N7	6.08	1.35	1.31
22	23S1	1142	A	C5-C4	-6.08	1.34	1.38
22	23S1	1698	A	C5-C4	-6.08	1.34	1.38
22	23S1	2268	A	C5-C4	-6.08	1.34	1.38
1	16S1	1483	A	C5-C4	-6.08	1.34	1.38
22	23S1	920	A	C5-C4	-6.08	1.34	1.38
22	23S1	2564	A	C8-N7	6.08	1.35	1.31
23	05S1	39	A	N3-C4	6.08	1.38	1.34
23	05S1	101	A	C2-N3	6.08	1.39	1.33
22	23S1	2856	A	C5-C4	-6.08	1.34	1.38
1	16S1	1408	A	C5-C4	-6.08	1.34	1.38
22	23S1	73	A	C8-N7	6.08	1.35	1.31
22	23S1	89	A	C8-N7	6.08	1.35	1.31
22	23S1	241	A	C8-N7	6.08	1.35	1.31
22	23S1	1608	A	C5-C4	-6.08	1.34	1.38
1	16S1	642	A	C8-N7	6.08	1.35	1.31
22	23S1	2037	A	C5-C4	-6.08	1.34	1.38
1	16S1	1012	A	N3-C4	6.08	1.38	1.34
22	23S1	219	A	C8-N7	6.08	1.35	1.31
22	23S1	265	A	C5-C4	-6.08	1.34	1.38
22	23S1	627	A	C5-C4	-6.08	1.34	1.38
22	23S1	1274	A	C8-N7	6.08	1.35	1.31
22	23S1	1634	A	C5-C4	-6.08	1.34	1.38
22	23S1	2734	A	C5-C4	-6.08	1.34	1.38
1	16S1	1275	A	C5-C4	-6.07	1.34	1.38
22	23S1	131	A	N3-C4	6.07	1.38	1.34
22	23S1	1889	A	C5-C4	-6.07	1.34	1.38
1	16S1	19	A	C8-N7	6.07	1.35	1.31
22	23S1	2434	A	C8-N7	6.07	1.35	1.31
22	23S1	2635	A	C5-C4	-6.07	1.34	1.38
22	23S1	793	A	C8-N7	6.07	1.35	1.31
22	23S1	1302	A	C8-N7	6.07	1.35	1.31
1	16S1	1146	A	N3-C4	6.07	1.38	1.34
22	23S1	2298	A	C5-C4	-6.07	1.34	1.38
22	23S1	149	A	C8-N7	6.07	1.35	1.31
22	23S1	244	A	C5-C4	-6.07	1.34	1.38
22	23S1	311	A	C5-C4	-6.07	1.34	1.38
22	23S1	2860	A	C5-C4	-6.06	1.34	1.38
1	16S1	468	A	N3-C4	6.06	1.38	1.34
22	23S1	933	A	C8-N7	6.06	1.35	1.31
22	23S1	1133	A	C8-N7	6.06	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2009	A	C5-C4	-6.06	1.34	1.38
22	23S1	2733	A	N3-C4	6.06	1.38	1.34
23	05S1	119	A	N3-C4	6.06	1.38	1.34
1	16S1	574	A	C5-C4	-6.06	1.34	1.38
1	16S1	919	A	C5-C4	-6.06	1.34	1.38
22	23S1	933	A	N3-C4	6.06	1.38	1.34
22	23S1	2267	A	C5-C4	-6.06	1.34	1.38
22	23S1	2634	A	C5-C4	-6.06	1.34	1.38
1	16S1	274	A	C5-C4	-6.06	1.34	1.38
1	16S1	309	A	C5-C4	-6.06	1.34	1.38
22	23S1	10	A	C5-C4	-6.06	1.34	1.38
22	23S1	1593	A	N3-C4	6.06	1.38	1.34
22	23S1	1858	A	C5-C4	-6.06	1.34	1.38
22	23S1	2033	A	C5-C4	-6.06	1.34	1.38
1	16S1	1507	A	C8-N7	6.06	1.35	1.31
22	23S1	2386	A	C8-N7	6.06	1.35	1.31
22	23S1	144	A	C5-C4	-6.05	1.34	1.38
22	23S1	878	A	N3-C4	6.05	1.38	1.34
22	23S1	1246	A	C8-N7	6.05	1.35	1.31
22	23S1	1336	A	C5-C4	-6.05	1.34	1.38
22	23S1	2336	A	C5-C4	-6.05	1.34	1.38
1	16S1	371	A	C5-C4	-6.05	1.34	1.38
1	16S1	889	A	C5-C4	-6.05	1.34	1.38
22	23S1	233	A	C5-C4	-6.05	1.34	1.38
22	23S1	988	A	C8-N7	6.05	1.35	1.31
22	23S1	1133	A	C5-C4	-6.05	1.34	1.38
22	23S1	1367	A	C5-C4	-6.05	1.34	1.38
22	23S1	1496	A	C8-N7	6.05	1.35	1.31
1	16S1	499	A	C8-N7	6.05	1.35	1.31
1	16S1	1311	A	N3-C4	6.05	1.38	1.34
22	23S1	1566	A	C8-N7	6.05	1.35	1.31
55	PTR1	42	A	N3-C4	6.05	1.38	1.34
1	16S1	81	A	N3-C4	6.05	1.38	1.34
22	23S1	460	A	C5-C4	-6.05	1.34	1.38
1	16S1	356	A	C8-N7	6.04	1.35	1.31
22	23S1	609	A	C5-C4	-6.04	1.34	1.38
22	23S1	1654	A	C5-C4	-6.04	1.34	1.38
1	16S1	969	A	C5-C4	-6.04	1.34	1.38
22	23S1	111	A	C5-C4	-6.04	1.34	1.38
22	23S1	541	A	C5-C4	-6.04	1.34	1.38
22	23S1	1285	A	C8-N7	6.04	1.35	1.31
22	23S1	1698	A	C8-N7	6.04	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2635	A	C8-N7	6.04	1.35	1.31
1	16S1	498	A	C5-C4	-6.04	1.34	1.38
1	16S1	1236	A	C5-C4	-6.04	1.34	1.38
1	16S1	1377	A	C5-C4	-6.04	1.34	1.38
22	23S1	1276	A	C5-C4	-6.04	1.34	1.38
1	16S1	236	A	C8-N7	6.04	1.35	1.31
22	23S1	294	A	C8-N7	6.04	1.35	1.31
22	23S1	1548	A	C8-N7	6.04	1.35	1.31
22	23S1	1757	A	C8-N7	6.04	1.35	1.31
22	23S1	2572	A	C8-N7	6.04	1.35	1.31
1	16S1	502	A	C8-N7	6.04	1.35	1.31
1	16S1	1093	A	C5-C4	-6.04	1.34	1.38
1	16S1	53	A	N3-C4	6.04	1.38	1.34
1	16S1	181	A	N3-C4	6.04	1.38	1.34
1	16S1	715	A	C8-N7	6.04	1.35	1.31
22	23S1	454	A	C5-C4	-6.04	1.34	1.38
22	23S1	2298	A	N3-C4	6.04	1.38	1.34
1	16S1	451	A	C8-N7	6.03	1.35	1.31
22	23S1	49	A	N3-C4	6.03	1.38	1.34
22	23S1	255	A	C5-C4	-6.03	1.34	1.38
22	23S1	391	A	C5-C4	-6.03	1.34	1.38
22	23S1	845	A	C8-N7	6.03	1.35	1.31
22	23S1	959	A	C5-C4	-6.03	1.34	1.38
22	23S1	1433	A	C8-N7	6.03	1.35	1.31
22	23S1	1641	A	C8-N7	6.03	1.35	1.31
1	16S1	430	A	N3-C4	6.03	1.38	1.34
22	23S1	2820	A	N3-C4	6.03	1.38	1.34
1	16S1	120	A	C5-C4	-6.03	1.34	1.38
1	16S1	303	A	C5-C4	-6.03	1.34	1.38
1	16S1	974	A	C8-N7	6.03	1.35	1.31
22	23S1	1021	A	C5-C4	-6.03	1.34	1.38
22	23S1	1274	A	C5-C4	-6.03	1.34	1.38
1	16S1	28	A	C8-N7	6.02	1.35	1.31
1	16S1	596	A	C5-C4	-6.02	1.34	1.38
22	23S1	1630	A	C5-C4	-6.02	1.34	1.38
1	16S1	329	A	C8-N7	6.02	1.35	1.31
1	16S1	1437	A	C5-C4	-6.02	1.34	1.38
22	23S1	503	A	C5-C4	-6.02	1.34	1.38
22	23S1	1469	A	C5-C4	-6.02	1.34	1.38
22	23S1	2810	A	C8-N7	6.02	1.35	1.31
1	16S1	729	A	C8-N7	6.02	1.35	1.31
22	23S1	1525	A	C5-C4	-6.02	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1744	A	N3-C4	6.02	1.38	1.34
1	16S1	746	A	N3-C4	6.01	1.38	1.34
22	23S1	522	A	C5-C4	-6.01	1.34	1.38
22	23S1	1713	A	C5-C4	-6.01	1.34	1.38
22	23S1	2590	A	C8-N7	6.01	1.35	1.31
22	23S1	2757	A	N3-C4	6.01	1.38	1.34
1	16S1	975	A	C5-C4	-6.01	1.34	1.38
22	23S1	2518	A	C5-C4	-6.01	1.34	1.38
1	16S1	1239	A	C5-C4	-6.01	1.34	1.38
22	23S1	203	A	C5-C4	-6.01	1.34	1.38
22	23S1	430	A	C8-N7	6.01	1.35	1.31
22	23S1	1509	A	N3-C4	6.01	1.38	1.34
1	16S1	498	A	C2-N3	6.01	1.39	1.33
1	16S1	968	A	C8-N7	6.01	1.35	1.31
1	16S1	600	A	C5-C4	-6.01	1.34	1.38
1	16S1	635	A	C5-C4	-6.01	1.34	1.38
1	16S1	1080	A	C5-C4	-6.01	1.34	1.38
1	16S1	1513	A	C8-N7	6.01	1.35	1.31
22	23S1	742	A	C5-C4	-6.01	1.34	1.38
22	23S1	2829	A	C5-C4	-6.01	1.34	1.38
22	23S1	2482	A	C8-N7	6.00	1.35	1.31
22	23S1	1378	A	C5-C4	-6.00	1.34	1.38
22	23S1	1787	A	C5-C4	-6.00	1.34	1.38
22	23S1	2407	A	C8-N7	6.00	1.35	1.31
1	16S1	161	A	N3-C4	6.00	1.38	1.34
1	16S1	321	A	C8-N7	6.00	1.35	1.31
1	16S1	949	A	C5-C4	-6.00	1.34	1.38
22	23S1	279	A	N3-C4	6.00	1.38	1.34
22	23S1	2327	A	C5-C4	-6.00	1.34	1.38
22	23S1	1504	A	N3-C4	6.00	1.38	1.34
1	16S1	975	A	C8-N7	6.00	1.35	1.31
22	23S1	1711	A	C5-C4	-6.00	1.34	1.38
22	23S1	2108	A	N3-C4	6.00	1.38	1.34
1	16S1	28	A	C5-C4	-6.00	1.34	1.38
1	16S1	949	A	C8-N7	6.00	1.35	1.31
1	16S1	1363	A	N3-C4	6.00	1.38	1.34
22	23S1	371	A	C5-C4	-6.00	1.34	1.38
22	23S1	2766	A	C5-C4	-6.00	1.34	1.38
22	23S1	64	A	C5-C4	-6.00	1.34	1.38
22	23S1	616	A	C5-C4	-6.00	1.34	1.38
1	16S1	282	A	C5-C4	-5.99	1.34	1.38
22	23S1	300	A	C5-C4	-5.99	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2682	A	C8-N7	5.99	1.35	1.31
1	16S1	1117	A	N3-C4	5.99	1.38	1.34
1	16S1	892	A	C8-N7	5.99	1.35	1.31
1	16S1	1340	A	N3-C4	5.99	1.38	1.34
22	23S1	1027	A	C5-C4	-5.99	1.34	1.38
1	16S1	197	A	N3-C4	5.99	1.38	1.34
22	23S1	126	A	C5-C4	-5.99	1.34	1.38
22	23S1	165	A	N3-C4	5.99	1.38	1.34
22	23S1	2432	A	C5-C4	-5.99	1.34	1.38
1	16S1	901	A	C5-C4	-5.99	1.34	1.38
22	23S1	152	A	N3-C4	5.99	1.38	1.34
22	23S1	1010	A	C5-C4	-5.99	1.34	1.38
1	16S1	1250	A	C5-C4	-5.99	1.34	1.38
22	23S1	270	A	N3-C4	5.99	1.38	1.34
22	23S1	945	A	C5-C4	-5.99	1.34	1.38
22	23S1	1048	A	N3-C4	5.99	1.38	1.34
1	16S1	262	A	C5-C4	-5.98	1.34	1.38
22	23S1	294	A	C5-C4	-5.98	1.34	1.38
22	23S1	1591	A	C5-C4	-5.98	1.34	1.38
23	05S1	29	A	N3-C4	5.98	1.38	1.34
1	16S1	816	A	C5-C4	-5.98	1.34	1.38
13	S131	65	VAL	CB-CG2	-5.98	1.40	1.52
22	23S1	311	A	C8-N7	5.98	1.35	1.31
22	23S1	2598	A	C5-C4	-5.98	1.34	1.38
1	16S1	250	A	N3-C4	5.98	1.38	1.34
22	23S1	1336	A	N3-C4	5.98	1.38	1.34
22	23S1	1393	A	C5-C4	-5.98	1.34	1.38
22	23S1	1469	A	C8-N7	5.98	1.35	1.31
23	05S1	104	A	C5-C4	-5.98	1.34	1.38
1	16S1	1346	A	N3-C4	5.98	1.38	1.34
22	23S1	104	A	N3-C4	5.98	1.38	1.34
22	23S1	226	A	C8-N7	5.98	1.35	1.31
1	16S1	743	A	C8-N7	5.98	1.35	1.31
22	23S1	423	A	C5-C4	-5.98	1.34	1.38
22	23S1	1549	A	C8-N7	5.98	1.35	1.31
22	23S1	2886	A	C5-C4	-5.98	1.34	1.38
22	23S1	38	A	C8-N7	5.98	1.35	1.31
22	23S1	2750	A	C5-C4	-5.98	1.34	1.38
22	23S1	716	A	C8-N7	5.97	1.35	1.31
22	23S1	849	A	C8-N7	5.97	1.35	1.31
22	23S1	1155	A	C8-N7	5.97	1.35	1.31
1	16S1	435	A	N3-C4	5.97	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1507	A	C5-C4	-5.97	1.34	1.38
22	23S1	529	A	C5-C4	-5.97	1.34	1.38
1	16S1	109	A	C8-N7	5.97	1.35	1.31
22	23S1	1745	A	C8-N7	5.97	1.35	1.31
1	16S1	629	A	N3-C4	5.97	1.38	1.34
1	16S1	790	A	C5-C4	-5.97	1.34	1.38
1	16S1	1022	A	N3-C4	5.97	1.38	1.34
22	23S1	342	A	C5-C4	-5.97	1.34	1.38
22	23S1	781	A	C5-C4	-5.97	1.34	1.38
22	23S1	1630	A	N3-C4	5.97	1.38	1.34
1	16S1	397	A	N3-C4	5.97	1.38	1.34
22	23S1	2314	A	N3-C4	5.97	1.38	1.34
22	23S1	2531	A	N3-C4	5.97	1.38	1.34
1	16S1	602	A	C5-C4	-5.97	1.34	1.38
1	16S1	663	A	C8-N7	5.97	1.35	1.31
1	16S1	1465	A	C5-C4	-5.97	1.34	1.38
22	23S1	217	A	C8-N7	5.97	1.35	1.31
22	23S1	478	A	C5-C4	-5.97	1.34	1.38
22	23S1	941	A	C8-N7	5.97	1.35	1.31
1	16S1	831	A	C5-C4	-5.96	1.34	1.38
1	16S1	1157	A	N3-C4	5.96	1.38	1.34
55	PTR1	73	A	N3-C4	5.96	1.38	1.34
1	16S1	288	A	C5-C4	-5.96	1.34	1.38
1	16S1	1531	A	C8-N7	5.96	1.35	1.31
22	23S1	1244	A	C5-C4	-5.96	1.34	1.38
22	23S1	1359	A	C5-C4	-5.96	1.34	1.38
1	16S1	807	A	C8-N7	5.96	1.35	1.31
1	16S1	946	A	C8-N7	5.96	1.35	1.31
22	23S1	401	A	C8-N7	5.96	1.35	1.31
22	23S1	505	A	C8-N7	5.96	1.35	1.31
22	23S1	1722	A	N3-C4	5.96	1.38	1.34
22	23S1	1916	A	N3-C4	5.96	1.38	1.34
22	23S1	2534	A	C5-C4	-5.96	1.34	1.38
22	23S1	2835	A	C5-C4	-5.96	1.34	1.38
1	16S1	192	A	N3-C4	5.96	1.38	1.34
1	16S1	306	A	N3-C4	5.96	1.38	1.34
1	16S1	1252	A	C5-C4	-5.96	1.34	1.38
22	23S1	1241	A	C5-C4	-5.96	1.34	1.38
1	16S1	907	A	C5-C4	-5.96	1.34	1.38
22	23S1	1027	A	C8-N7	5.96	1.35	1.31
22	23S1	1548	A	N3-C4	5.96	1.38	1.34
22	23S1	1609	A	C8-N7	5.96	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2094	A	C5-C4	-5.96	1.34	1.38
1	16S1	1180	A	C5-C4	-5.96	1.34	1.38
22	23S1	1899	A	C5-C4	-5.96	1.34	1.38
1	16S1	974	A	N3-C4	5.95	1.38	1.34
22	23S1	1301	A	C5-C4	-5.95	1.34	1.38
22	23S1	1780	A	C8-N7	5.95	1.35	1.31
1	16S1	1093	A	N3-C4	5.95	1.38	1.34
22	23S1	492	A	N3-C4	5.95	1.38	1.34
1	16S1	865	A	C5-C4	-5.95	1.34	1.38
1	16S1	1499	A	C8-N7	5.95	1.35	1.31
22	23S1	1433	A	C5-C4	-5.95	1.34	1.38
22	23S1	1544	A	C5-C4	-5.95	1.34	1.38
22	23S1	1548	A	C5-C4	-5.95	1.34	1.38
1	16S1	130	A	C5-C4	-5.95	1.34	1.38
1	16S1	412	A	N3-C4	5.95	1.38	1.34
22	23S1	217	A	C5-C4	-5.95	1.34	1.38
22	23S1	1204	A	C5-C4	-5.95	1.34	1.38
22	23S1	1284	A	C5-C4	-5.95	1.34	1.38
1	16S1	1274	A	N3-C4	5.95	1.38	1.34
22	23S1	877	A	N3-C4	5.95	1.38	1.34
1	16S1	792	A	N3-C4	5.95	1.38	1.34
1	16S1	1350	A	C8-N7	5.95	1.35	1.31
22	23S1	156	A	C5-C4	-5.95	1.34	1.38
22	23S1	1632	A	C5-C4	-5.95	1.34	1.38
22	23S1	1932	A	C5-C4	-5.95	1.34	1.38
1	16S1	321	A	C5-C4	-5.94	1.34	1.38
22	23S1	1805	A	C8-N7	5.94	1.35	1.31
22	23S1	2346	A	C8-N7	5.94	1.35	1.31
22	23S1	2412	A	C5-C4	-5.94	1.34	1.38
1	16S1	1151	A	N3-C4	5.94	1.38	1.34
22	23S1	382	A	N3-C4	5.94	1.38	1.34
22	23S1	2335	A	C8-N7	5.94	1.35	1.31
1	16S1	246	A	C5-C4	-5.94	1.34	1.38
22	23S1	14	A	C8-N7	5.94	1.35	1.31
22	23S1	340	A	C5-C4	-5.94	1.34	1.38
1	16S1	72	A	N3-C4	5.94	1.38	1.34
22	23S1	513	A	N7-C5	-5.94	1.35	1.39
1	16S1	66	A	N3-C4	5.94	1.38	1.34
22	23S1	429	A	C8-N7	5.94	1.35	1.31
22	23S1	936	A	C5-C4	-5.94	1.34	1.38
22	23S1	2095	A	C5-C4	-5.93	1.34	1.38
22	23S1	2376	A	C5-C4	-5.93	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	630	A	N3-C4	5.93	1.38	1.34
22	23S1	2126	A	N3-C4	5.93	1.38	1.34
22	23S1	1143	A	C5-C4	-5.93	1.34	1.38
22	23S1	52	A	C5-C4	-5.93	1.34	1.38
1	16S1	695	A	C5-C4	-5.93	1.34	1.38
1	16S1	1499	A	C5-C4	-5.93	1.34	1.38
22	23S1	1938	A	C8-N7	5.93	1.35	1.31
1	16S1	914	A	C8-N7	5.93	1.35	1.31
1	16S1	1171	A	N3-C4	5.93	1.38	1.34
1	16S1	1360	A	C5-C4	-5.93	1.34	1.38
22	23S1	1713	A	C8-N7	5.93	1.35	1.31
22	23S1	1998	A	C8-N7	5.93	1.35	1.31
22	23S1	2314	A	C5-C4	-5.93	1.34	1.38
22	23S1	2814	A	C5-C4	-5.93	1.34	1.38
1	16S1	53	A	C5-C4	-5.92	1.34	1.38
1	16S1	366	A	C8-N7	5.92	1.35	1.31
1	16S1	441	A	N3-C4	5.92	1.38	1.34
1	16S1	1433	A	C5-C4	-5.92	1.34	1.38
22	23S1	131	A	C8-N7	5.92	1.35	1.31
22	23S1	1265	A	C5-C4	-5.92	1.34	1.38
22	23S1	2059	A	C8-N7	5.92	1.35	1.31
1	16S1	366	A	C5-C4	-5.92	1.34	1.38
22	23S1	984	A	C5-C4	-5.92	1.34	1.38
22	23S1	1918	A	C5-C4	-5.92	1.34	1.38
1	16S1	309	A	N3-C4	5.92	1.38	1.34
1	16S1	749	A	N3-C4	5.92	1.38	1.34
22	23S1	213	A	C5-C4	-5.92	1.34	1.38
22	23S1	1353	A	C8-N7	5.92	1.35	1.31
22	23S1	2407	A	C5-C4	-5.92	1.34	1.38
22	23S1	2639	A	C5-C4	-5.92	1.34	1.38
22	23S1	2886	A	C8-N7	5.92	1.35	1.31
22	23S1	256	A	C5-C4	-5.92	1.34	1.38
1	16S1	640	A	N3-C4	5.92	1.38	1.34
1	16S1	1110	A	C5-C4	-5.92	1.34	1.38
1	16S1	1329	A	C5-C4	-5.92	1.34	1.38
1	16S1	1374	A	C5-C4	-5.92	1.34	1.38
1	16S1	1513	A	C5-C4	-5.92	1.34	1.38
22	23S1	1495	A	C5-C4	-5.92	1.34	1.38
1	16S1	389	A	N3-C4	5.92	1.38	1.34
1	16S1	583	A	C5-C4	-5.92	1.34	1.38
1	16S1	706	A	C5-C4	-5.92	1.34	1.38
1	16S1	959	A	C8-N7	5.92	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	213	A	N3-C4	5.92	1.38	1.34
22	23S1	216	A	C5-C4	-5.92	1.34	1.38
22	23S1	538	A	C8-N7	5.92	1.35	1.31
22	23S1	749	A	C8-N7	5.92	1.35	1.31
22	23S1	979	A	C8-N7	5.92	1.35	1.31
1	16S1	189	A	N3-C4	5.92	1.38	1.34
1	16S1	1306	A	C5-C4	-5.92	1.34	1.38
22	23S1	1151	A	C8-N7	5.92	1.35	1.31
1	16S1	397	A	C5-C4	-5.91	1.34	1.38
1	16S1	1081	A	C8-N7	5.91	1.35	1.31
22	23S1	503	A	C8-N7	5.91	1.35	1.31
22	23S1	670	A	C8-N7	5.91	1.35	1.31
22	23S1	909	A	C5-C4	-5.91	1.34	1.38
1	16S1	1219	A	N3-C4	5.91	1.38	1.34
22	23S1	753	A	C8-N7	5.91	1.35	1.31
22	23S1	2665	A	C8-N7	5.91	1.35	1.31
1	16S1	1219	A	C5-C4	-5.91	1.34	1.38
1	16S1	1349	A	C8-N7	5.91	1.35	1.31
22	23S1	2700	A	C8-N7	5.91	1.35	1.31
1	16S1	243	A	C5-C4	-5.91	1.34	1.38
22	23S1	28	A	C8-N7	5.91	1.35	1.31
22	23S1	556	A	C5-C4	-5.91	1.34	1.38
22	23S1	2748	A	C5-C4	-5.91	1.34	1.38
22	23S1	820	A	C5-C4	-5.91	1.34	1.38
1	16S1	50	A	N3-C4	5.91	1.38	1.34
1	16S1	563	A	C5-C4	-5.91	1.34	1.38
1	16S1	782	A	C8-N7	5.90	1.35	1.31
22	23S1	10	A	N3-C4	5.90	1.38	1.34
22	23S1	38	A	C5-C4	-5.90	1.34	1.38
22	23S1	804	A	C8-N7	5.90	1.35	1.31
1	16S1	155	A	N3-C4	5.90	1.38	1.34
1	16S1	236	A	N3-C4	5.90	1.38	1.34
1	16S1	621	A	C5-C4	-5.90	1.34	1.38
22	23S1	556	A	C8-N7	5.90	1.35	1.31
22	23S1	643	A	C8-N7	5.90	1.35	1.31
22	23S1	1272	A	C8-N7	5.90	1.35	1.31
22	23S1	2821	A	C5-C4	-5.90	1.34	1.38
23	05S1	94	A	N3-C4	5.90	1.38	1.34
1	16S1	946	A	C5-C4	-5.90	1.34	1.38
1	16S1	1346	A	C5-C4	-5.90	1.34	1.38
1	16S1	1368	A	C5-C4	-5.90	1.34	1.38
1	16S1	382	A	N3-C4	5.90	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1020	A	C5-C4	-5.90	1.34	1.38
22	23S1	2358	A	C5-C4	-5.90	1.34	1.38
1	16S1	958	A	C5-C4	-5.90	1.34	1.38
22	23S1	1545	A	C5-C4	-5.90	1.34	1.38
22	23S1	2614	A	C8-N7	5.90	1.35	1.31
22	23S1	1591	A	N3-C4	5.89	1.38	1.34
22	23S1	2776	A	C5-C4	-5.89	1.34	1.38
22	23S1	471	A	N3-C4	5.89	1.38	1.34
22	23S1	866	A	N3-C4	5.89	1.38	1.34
22	23S1	1127	A	C8-N7	5.89	1.35	1.31
1	16S1	432	A	N3-C4	5.89	1.38	1.34
22	23S1	233	A	C8-N7	5.89	1.35	1.31
22	23S1	1701	A	C8-N7	5.89	1.35	1.31
22	23S1	2366	A	C8-N7	5.89	1.35	1.31
1	16S1	1508	A	C5-C4	-5.89	1.34	1.38
22	23S1	309	A	C8-N7	5.89	1.35	1.31
22	23S1	793	A	C5-C4	-5.89	1.34	1.38
22	23S1	1126	A	C5-C4	-5.89	1.34	1.38
22	23S1	1596	A	C5-C4	-5.89	1.34	1.38
22	23S1	1690	A	C8-N7	5.89	1.35	1.31
22	23S1	2288	A	C5-C4	-5.89	1.34	1.38
1	16S1	336	A	C5-C4	-5.89	1.34	1.38
22	23S1	470	A	C5-C4	-5.89	1.34	1.38
1	16S1	263	A	N3-C4	5.88	1.38	1.34
1	16S1	371	A	N3-C4	5.88	1.38	1.34
1	16S1	676	A	C8-N7	5.88	1.35	1.31
22	23S1	483	A	C8-N7	5.88	1.35	1.31
22	23S1	1866	A	N3-C4	5.88	1.38	1.34
1	16S1	223	A	N3-C4	5.88	1.38	1.34
22	23S1	2097	A	N3-C4	5.88	1.38	1.34
1	16S1	573	A	C8-N7	5.88	1.35	1.31
1	16S1	1429	A	C8-N7	5.88	1.35	1.31
1	16S1	1430	A	C5-C4	-5.88	1.34	1.38
22	23S1	1040	A	C5-C4	-5.88	1.34	1.38
22	23S1	1134	A	C5-C4	-5.88	1.34	1.38
22	23S1	1276	A	C8-N7	5.88	1.35	1.31
22	23S1	2679	A	C8-N7	5.88	1.35	1.31
22	23S1	2411	A	C8-N7	5.88	1.35	1.31
1	16S1	1219	A	C8-N7	5.88	1.35	1.31
22	23S1	152	A	C5-C4	-5.88	1.34	1.38
22	23S1	368	A	C5-C4	-5.88	1.34	1.38
22	23S1	528	A	C5-C4	-5.88	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1328	A	C5-C4	-5.88	1.34	1.38
1	16S1	687	A	C8-N7	5.88	1.35	1.31
1	16S1	1196	A	C5-C4	-5.88	1.34	1.38
1	16S1	964	A	C5-C4	-5.87	1.34	1.38
1	16S1	1396	A	C8-N7	5.87	1.35	1.31
22	23S1	590	A	C8-N7	5.87	1.35	1.31
22	23S1	603	A	C5-C4	-5.87	1.34	1.38
22	23S1	1641	A	C5-C4	-5.87	1.34	1.38
22	23S1	2764	A	C5-C4	-5.87	1.34	1.38
1	16S1	509	A	C5-C4	-5.87	1.34	1.38
1	16S1	1004	A	C5-C4	-5.87	1.34	1.38
22	23S1	362	A	C8-N7	5.87	1.35	1.31
22	23S1	1269	A	C5-C4	-5.87	1.34	1.38
22	23S1	270	A	C5-C4	-5.87	1.34	1.38
1	16S1	274	A	N3-C4	5.87	1.38	1.34
1	16S1	535	A	C5-C4	-5.87	1.34	1.38
1	16S1	792	A	C8-N7	5.87	1.35	1.31
1	16S1	1067	A	N3-C4	5.87	1.38	1.34
1	16S1	1280	A	C5-C4	-5.87	1.34	1.38
1	16S1	1413	A	C5-C4	-5.87	1.34	1.38
1	16S1	59	A	N3-C4	5.87	1.38	1.34
1	16S1	718	A	N3-C4	5.87	1.38	1.34
1	16S1	1508	A	N3-C4	5.87	1.38	1.34
22	23S1	294	A	N3-C4	5.87	1.38	1.34
22	23S1	382	A	C8-N7	5.87	1.35	1.31
22	23S1	1496	A	C5-C4	-5.87	1.34	1.38
22	23S1	2227	A	C8-N7	5.87	1.35	1.31
22	23S1	2665	A	N3-C4	5.87	1.38	1.34
1	16S1	197	A	C5-C4	-5.86	1.34	1.38
1	16S1	923	A	C5-C4	-5.86	1.34	1.38
1	16S1	1271	A	C5-C4	-5.86	1.34	1.38
22	23S1	927	A	C5-C4	-5.86	1.34	1.38
22	23S1	996	A	C8-N7	5.86	1.35	1.31
1	16S1	435	A	C5-C4	-5.86	1.34	1.38
22	23S1	173	A	C5-C4	-5.86	1.34	1.38
1	16S1	609	A	C8-N7	5.86	1.35	1.31
1	16S1	1110	A	C8-N7	5.86	1.35	1.31
22	23S1	5	A	N3-C4	5.86	1.38	1.34
22	23S1	2439	A	C8-N7	5.86	1.35	1.31
1	16S1	1	A	N3-C4	5.86	1.38	1.34
1	16S1	1362	A	C8-N7	5.86	1.35	1.31
22	23S1	1327	A	C8-N7	5.86	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1689	A	C5-C4	-5.86	1.34	1.38
1	16S1	356	A	N3-C4	5.86	1.38	1.34
1	16S1	1082	A	C5-C4	-5.86	1.34	1.38
22	23S1	1321	A	C5-C4	-5.86	1.34	1.38
1	16S1	171	A	C5-C4	-5.86	1.34	1.38
1	16S1	860	A	C8-N7	5.86	1.35	1.31
22	23S1	439	A	C5-C4	-5.86	1.34	1.38
22	23S1	538	A	N3-C4	5.86	1.38	1.34
22	23S1	917	A	C5-C4	-5.86	1.34	1.38
22	23S1	2634	A	C8-N7	5.86	1.35	1.31
1	16S1	539	A	N3-C4	5.85	1.38	1.34
1	16S1	155	A	C5-C4	-5.85	1.34	1.38
22	23S1	443	A	C8-N7	5.85	1.35	1.31
22	23S1	718	A	N3-C4	5.85	1.38	1.34
22	23S1	2281	A	C8-N7	5.85	1.35	1.31
22	23S1	2366	A	C5-C4	-5.85	1.34	1.38
1	16S1	8	A	C5-C4	-5.85	1.34	1.38
1	16S1	174	A	N3-C4	5.85	1.38	1.34
1	16S1	784	A	C8-N7	5.85	1.35	1.31
22	23S1	2005	A	C8-N7	5.85	1.35	1.31
1	16S1	777	A	C8-N7	5.85	1.35	1.31
1	16S1	1271	A	N3-C4	5.85	1.38	1.34
1	16S1	1275	A	N3-C4	5.85	1.38	1.34
22	23S1	241	A	C5-C4	-5.85	1.34	1.38
23	05S1	34	A	C5-C4	-5.85	1.34	1.38
22	23S1	1244	A	C8-N7	5.84	1.35	1.31
23	05S1	94	A	C8-N7	5.84	1.35	1.31
55	PTR1	26	A	N3-C4	5.84	1.38	1.34
22	23S1	633	A	N3-C4	5.84	1.38	1.34
22	23S1	1021	A	N3-C4	5.84	1.38	1.34
22	23S1	1722	A	C8-N7	5.84	1.35	1.31
1	16S1	246	A	N3-C4	5.84	1.38	1.34
1	16S1	648	A	C5-C4	-5.84	1.34	1.38
22	23S1	94	A	N3-C4	5.84	1.38	1.34
22	23S1	2051	A	C5-C4	-5.84	1.34	1.38
22	23S1	2346	A	C5-C4	-5.84	1.34	1.38
22	23S1	2657	A	C5-C4	-5.84	1.34	1.38
1	16S1	996	A	N3-C4	5.84	1.38	1.34
22	23S1	330	A	C8-N7	5.84	1.35	1.31
22	23S1	633	A	C5-C4	-5.84	1.34	1.38
22	23S1	1039	A	C5-C4	-5.84	1.34	1.38
22	23S1	1111	A	N3-C4	5.84	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1226	A	C5-C4	-5.84	1.34	1.38
22	23S1	2059	A	N3-C4	5.84	1.38	1.34
22	23S1	504	A	N9-C4	-5.84	1.34	1.37
1	16S1	236	A	C5-C4	-5.84	1.34	1.38
1	16S1	759	A	C5-C4	-5.84	1.34	1.38
22	23S1	497	A	C5-C4	-5.84	1.34	1.38
22	23S1	1515	A	C5-C4	-5.83	1.34	1.38
23	05S1	99	A	C5-C4	-5.83	1.34	1.38
22	23S1	764	A	C5-C4	-5.83	1.34	1.38
22	23S1	2042	A	C8-N7	5.83	1.35	1.31
1	16S1	759	A	N3-C4	5.83	1.38	1.34
22	23S1	346	A	C5-C4	-5.83	1.34	1.38
22	23S1	472	A	C8-N7	5.83	1.35	1.31
22	23S1	917	A	C8-N7	5.83	1.35	1.31
1	16S1	937	A	C5-C4	-5.83	1.34	1.38
1	16S1	1117	A	C5-C4	-5.83	1.34	1.38
1	16S1	478	A	C8-N7	5.83	1.35	1.31
1	16S1	1288	A	N3-C4	5.83	1.38	1.34
22	23S1	1143	A	N3-C4	5.83	1.38	1.34
22	23S1	1144	A	C8-N7	5.83	1.35	1.31
22	23S1	1551	A	N3-C4	5.83	1.38	1.34
22	23S1	1635	A	C8-N7	5.83	1.35	1.31
22	23S1	1762	A	C8-N7	5.83	1.35	1.31
22	23S1	2792	A	C5-C4	-5.83	1.34	1.38
22	23S1	430	A	C5-C4	-5.83	1.34	1.38
22	23S1	1717	A	C5-C4	-5.83	1.34	1.38
1	16S1	149	A	N3-C4	5.83	1.38	1.34
1	16S1	968	A	N3-C4	5.83	1.38	1.34
22	23S1	330	A	C5-C4	-5.83	1.34	1.38
22	23S1	721	A	C5-C4	-5.83	1.34	1.38
22	23S1	918	A	C8-N7	5.83	1.35	1.31
22	23S1	2287	A	C5-C4	-5.83	1.34	1.38
1	16S1	1252	A	C8-N7	5.82	1.35	1.31
22	23S1	346	A	N3-C4	5.82	1.38	1.34
22	23S1	1616	A	C8-N7	5.82	1.35	1.31
1	16S1	238	A	C5-C4	-5.82	1.34	1.38
1	16S1	1394	A	C8-N7	5.82	1.35	1.31
22	23S1	44	A	C5-C4	-5.82	1.34	1.38
22	23S1	56	A	C8-N7	5.82	1.35	1.31
22	23S1	2542	A	C8-N7	5.82	1.35	1.31
1	16S1	1410	A	C5-C4	-5.82	1.34	1.38
22	23S1	2199	A	C5-C4	-5.82	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2726	A	N3-C4	5.82	1.38	1.34
22	23S1	1241	A	N3-C4	5.82	1.38	1.34
22	23S1	1387	A	C5-C4	-5.82	1.34	1.38
22	23S1	1598	A	C8-N7	5.82	1.35	1.31
22	23S1	384	A	C5-C4	-5.81	1.34	1.38
1	16S1	162	A	N7-C5	-5.81	1.35	1.39
1	16S1	819	A	C5-C4	-5.81	1.34	1.38
22	23S1	637	A	N3-C4	5.81	1.38	1.34
22	23S1	2412	A	C8-N7	5.81	1.35	1.31
1	16S1	1152	A	C8-N7	5.81	1.35	1.31
22	23S1	981	A	C8-N7	5.81	1.35	1.31
22	23S1	1365	A	C5-C4	-5.81	1.34	1.38
22	23S1	1609	A	C5-C4	-5.81	1.34	1.38
22	23S1	1829	A	C8-N7	5.81	1.35	1.31
1	16S1	749	A	C5-C4	-5.81	1.34	1.38
1	16S1	872	A	N3-C4	5.81	1.38	1.34
1	16S1	1288	A	C5-C4	-5.81	1.34	1.38
22	23S1	156	A	N3-C4	5.81	1.38	1.34
22	23S1	1901	A	C5-C4	-5.81	1.34	1.38
22	23S1	2058	A	C5-C4	-5.81	1.34	1.38
1	16S1	253	A	N3-C4	5.81	1.38	1.34
1	16S1	1180	A	C8-N7	5.81	1.35	1.31
1	16S1	753	A	C5-C4	-5.80	1.34	1.38
22	23S1	2821	A	C8-N7	5.80	1.35	1.31
1	16S1	119	A	C5-C4	-5.80	1.34	1.38
22	23S1	402	A	C8-N7	5.80	1.35	1.31
1	16S1	167	A	C5-C4	-5.80	1.34	1.38
1	16S1	913	A	C5-C4	-5.80	1.34	1.38
1	16S1	1130	A	N3-C4	5.80	1.38	1.34
1	16S1	315	A	N3-C4	5.80	1.38	1.34
1	16S1	415	A	N3-C4	5.80	1.38	1.34
1	16S1	938	A	C5-C4	-5.80	1.34	1.38
1	16S1	1374	A	N3-C4	5.80	1.38	1.34
1	16S1	1499	A	N3-C4	5.80	1.38	1.34
22	23S1	89	A	N3-C4	5.80	1.38	1.34
1	16S1	635	A	N3-C4	5.80	1.38	1.34
1	16S1	1150	A	N3-C4	5.80	1.38	1.34
22	23S1	572	A	C5-C4	-5.80	1.34	1.38
1	16S1	363	A	C8-N7	5.80	1.35	1.31
1	16S1	767	A	C8-N7	5.80	1.35	1.31
1	16S1	914	A	C5-C4	-5.79	1.34	1.38
1	16S1	1170	A	C5-C4	-5.79	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	492	A	C5-C4	-5.79	1.34	1.38
22	23S1	1711	A	N3-C4	5.79	1.38	1.34
1	16S1	172	A	N3-C4	5.79	1.38	1.34
1	16S1	572	A	C8-N7	5.79	1.35	1.31
1	16S1	1191	A	C5-C4	-5.79	1.34	1.38
1	16S1	1238	A	C5-C4	-5.79	1.34	1.38
1	16S1	1246	A	N3-C4	5.79	1.38	1.34
22	23S1	101	A	C8-N7	5.79	1.35	1.31
22	23S1	1821	A	C5-C4	-5.79	1.34	1.38
22	23S1	2632	A	C5-C4	-5.79	1.34	1.38
22	23S1	1029	A	C5-C4	-5.79	1.34	1.38
22	23S1	2060	A	C8-N7	5.79	1.35	1.31
22	23S1	2449	U	C4-C5	5.79	1.48	1.43
22	23S1	2899	A	N3-C4	5.79	1.38	1.34
1	16S1	622	A	C5-C4	-5.79	1.34	1.38
22	23S1	63	A	N3-C4	5.79	1.38	1.34
22	23S1	1301	A	C8-N7	5.79	1.35	1.31
1	16S1	918	A	C8-N7	5.79	1.35	1.31
1	16S1	1101	A	C5-C4	-5.79	1.34	1.38
22	23S1	1142	A	N3-C4	5.79	1.38	1.34
1	16S1	3	A	N3-C4	5.79	1.38	1.34
1	16S1	182	A	N3-C4	5.79	1.38	1.34
22	23S1	800	A	C8-N7	5.79	1.35	1.31
22	23S1	1528	A	N3-C4	5.79	1.38	1.34
1	16S1	790	A	C8-N7	5.78	1.35	1.31
22	23S1	1801	A	C5-C4	-5.78	1.34	1.38
1	16S1	559	A	C5-C4	-5.78	1.34	1.38
1	16S1	1046	A	N3-C4	5.78	1.38	1.34
1	16S1	1252	A	N3-C4	5.78	1.38	1.34
22	23S1	1802	A	C5-C4	-5.78	1.34	1.38
22	23S1	2340	A	N3-C4	5.78	1.38	1.34
22	23S1	2471	A	N3-C4	5.78	1.38	1.34
1	16S1	1004	A	C8-N7	5.78	1.35	1.31
22	23S1	1383	A	C5-C4	-5.78	1.34	1.38
23	05S1	45	A	N3-C4	5.78	1.38	1.34
22	23S1	2287	A	N3-C4	5.78	1.38	1.34
22	23S1	2761	A	C5-C4	-5.78	1.34	1.38
22	23S1	911	A	C5-C4	-5.77	1.34	1.38
22	23S1	2378	A	C5-C4	-5.77	1.34	1.38
22	23S1	2530	A	C5-C4	-5.77	1.34	1.38
22	23S1	172	A	N3-C4	5.77	1.38	1.34
22	23S1	1757	A	C5-C4	-5.77	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2297	A	C5-C4	-5.77	1.34	1.38
1	16S1	695	A	C8-N7	5.77	1.35	1.31
1	16S1	1093	A	C8-N7	5.77	1.35	1.31
22	23S1	195	A	C5-C4	-5.77	1.34	1.38
22	23S1	1453	A	C5-C4	-5.77	1.34	1.38
22	23S1	2632	A	N3-C4	5.77	1.38	1.34
1	16S1	33	A	C5-C4	-5.77	1.34	1.38
1	16S1	630	A	C5-C4	-5.77	1.34	1.38
1	16S1	1254	A	C5-C4	-5.77	1.34	1.38
22	23S1	13	A	C5-C4	-5.77	1.34	1.38
22	23S1	483	A	C5-C4	-5.77	1.34	1.38
22	23S1	1322	A	C8-N7	5.77	1.35	1.31
1	16S1	270	A	N3-C4	5.77	1.38	1.34
22	23S1	501	A	C5-C4	-5.77	1.34	1.38
22	23S1	1885	A	C5-C4	-5.77	1.34	1.38
22	23S1	2893	A	C5-C4	-5.77	1.34	1.38
22	23S1	2899	A	C5-C4	-5.77	1.34	1.38
55	PTR1	9	A	C5-C4	-5.77	1.34	1.38
1	16S1	10	A	C8-N7	5.76	1.35	1.31
1	16S1	790	A	N3-C4	5.76	1.38	1.34
1	16S1	909	A	C5-C4	-5.76	1.34	1.38
22	23S1	1593	A	C5-C4	-5.76	1.34	1.38
22	23S1	1998	A	C5-C4	-5.76	1.34	1.38
22	23S1	734	A	C8-N7	5.76	1.35	1.31
22	23S1	272	A	C5-C4	-5.76	1.34	1.38
22	23S1	330	A	N3-C4	5.76	1.38	1.34
22	23S1	973	A	C8-N7	5.76	1.35	1.31
22	23S1	2534	A	N3-C4	5.76	1.38	1.34
22	23S1	1791	A	C5-C4	-5.76	1.34	1.38
22	23S1	2665	A	C5-C4	-5.76	1.34	1.38
1	16S1	768	A	C8-N7	5.76	1.35	1.31
1	16S1	1418	A	N3-C4	5.76	1.38	1.34
22	23S1	149	A	C5-C4	-5.76	1.34	1.38
22	23S1	391	A	C8-N7	5.76	1.35	1.31
22	23S1	2883	A	C8-N7	5.76	1.35	1.31
1	16S1	1246	A	C5-C4	-5.76	1.34	1.38
22	23S1	5	A	C5-C4	-5.76	1.34	1.38
1	16S1	33	A	C8-N7	5.75	1.35	1.31
1	16S1	1502	A	C8-N7	5.75	1.35	1.31
22	23S1	415	A	C8-N7	5.75	1.35	1.31
22	23S1	1739	A	C8-N7	5.75	1.35	1.31
23	05S1	39	A	C5-C4	-5.75	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	65	A	N3-C4	5.75	1.38	1.34
1	16S1	190	A	C2-N3	5.75	1.38	1.33
22	23S1	643	A	C5-C4	-5.75	1.34	1.38
22	23S1	716	A	C5-C4	-5.75	1.34	1.38
22	23S1	1387	A	C8-N7	5.75	1.35	1.31
22	23S1	1420	A	N3-C4	5.75	1.38	1.34
22	23S1	2430	A	N7-C5	-5.75	1.35	1.39
23	05S1	46	A	C5-C4	-5.75	1.34	1.38
1	16S1	139	A	N3-C4	5.75	1.38	1.34
1	16S1	681	A	N3-C4	5.75	1.38	1.34
1	16S1	1155	A	C5-C4	-5.75	1.34	1.38
1	16S1	1507	A	N3-C4	5.75	1.38	1.34
22	23S1	661	A	C8-N7	5.75	1.35	1.31
22	23S1	1262	A	C8-N7	5.75	1.35	1.31
22	23S1	1810	A	C5-C4	-5.75	1.34	1.38
23	05S1	115	A	N3-C4	5.75	1.38	1.34
1	16S1	1216	A	C5-C4	-5.75	1.34	1.38
22	23S1	1084	A	N3-C4	5.75	1.38	1.34
1	16S1	559	A	C8-N7	5.74	1.35	1.31
1	16S1	600	A	N3-C4	5.74	1.38	1.34
1	16S1	915	A	C8-N7	5.74	1.35	1.31
22	23S1	244	A	C8-N7	5.74	1.35	1.31
22	23S1	626	A	C5-C4	-5.74	1.34	1.38
22	23S1	1014	A	C5-C4	-5.74	1.34	1.38
1	16S1	1285	A	C5-C4	-5.74	1.34	1.38
22	23S1	1470	A	C5-C4	-5.74	1.34	1.38
22	23S1	1919	A	N3-C4	5.74	1.38	1.34
1	16S1	101	A	C5-C4	-5.74	1.34	1.38
1	16S1	563	A	C8-N7	5.74	1.35	1.31
1	16S1	1398	A	C5-C4	-5.74	1.34	1.38
1	16S1	1447	A	C5-C4	-5.74	1.34	1.38
22	23S1	49	A	C8-N7	5.74	1.35	1.31
22	23S1	71	A	N3-C4	5.74	1.38	1.34
1	16S1	1046	A	C5-C4	-5.74	1.34	1.38
1	16S1	1179	A	N3-C4	5.74	1.38	1.34
22	23S1	614	A	N3-C4	5.74	1.38	1.34
22	23S1	1553	A	C8-N7	5.74	1.35	1.31
22	23S1	1977	A	C8-N7	5.74	1.35	1.31
22	23S1	1757	A	N3-C4	5.74	1.38	1.34
1	16S1	101	A	N3-C4	5.74	1.38	1.34
1	16S1	1357	A	C8-N7	5.74	1.35	1.31
1	16S1	1456	A	N3-C4	5.74	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	196	A	N3-C4	5.73	1.38	1.34
22	23S1	2761	A	N3-C4	5.73	1.38	1.34
1	16S1	747	A	C5-C4	-5.73	1.34	1.38
1	16S1	1374	A	C8-N7	5.73	1.35	1.31
22	23S1	1307	A	C8-N7	5.73	1.35	1.31
22	23S1	226	A	C5-C4	-5.73	1.34	1.38
1	16S1	502	A	N3-C4	5.73	1.38	1.34
1	16S1	968	A	C5-C4	-5.73	1.34	1.38
22	23S1	126	A	C8-N7	5.73	1.35	1.31
22	23S1	182	A	N3-C4	5.73	1.38	1.34
22	23S1	861	A	C8-N7	5.73	1.35	1.31
22	23S1	1569	A	C8-N7	5.73	1.35	1.31
22	23S1	2639	A	N3-C4	5.73	1.38	1.34
22	23S1	2358	A	C8-N7	5.73	1.35	1.31
1	16S1	1340	A	C5-C4	-5.72	1.34	1.38
22	23S1	207	A	C8-N7	5.72	1.35	1.31
22	23S1	472	A	C5-C4	-5.72	1.34	1.38
22	23S1	2741	A	C8-N7	5.72	1.35	1.31
1	16S1	523	A	C5-C4	-5.72	1.34	1.38
1	16S1	1055	A	C5-C4	-5.72	1.34	1.38
1	16S1	1067	A	C5-C4	-5.72	1.34	1.38
1	16S1	1261	A	N3-C4	5.72	1.38	1.34
22	23S1	479	A	N3-C4	5.72	1.38	1.34
22	23S1	1419	A	N3-C4	5.72	1.38	1.34
22	23S1	2090	A	C8-N7	5.72	1.35	1.31
22	23S1	2518	A	C8-N7	5.72	1.35	1.31
1	16S1	1418	A	C5-C4	-5.72	1.34	1.38
22	23S1	789	A	N3-C4	5.72	1.38	1.34
22	23S1	1987	A	N3-C4	5.72	1.38	1.34
22	23S1	2031	A	C8-N7	5.72	1.35	1.31
22	23S1	2799	A	C8-N7	5.72	1.35	1.31
22	23S1	2868	A	N3-C4	5.72	1.38	1.34
1	16S1	167	A	N3-C4	5.72	1.38	1.34
22	23S1	347	A	C5-C4	-5.72	1.34	1.38
22	23S1	592	A	C8-N7	5.72	1.35	1.31
22	23S1	1901	A	N3-C4	5.72	1.38	1.34
22	23S1	2009	A	C8-N7	5.72	1.35	1.31
1	16S1	151	A	C5-C4	-5.72	1.34	1.38
1	16S1	595	A	C5-C4	-5.72	1.34	1.38
22	23S1	599	A	C8-N7	5.72	1.35	1.31
22	23S1	1705	A	C8-N7	5.72	1.35	1.31
22	23S1	2461	A	C5-C4	-5.72	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	55	A	N3-C4	5.71	1.38	1.34
1	16S1	1036	A	N3-C4	5.71	1.38	1.34
1	16S1	1229	A	N3-C4	5.71	1.38	1.34
22	23S1	155	A	C5-C4	-5.71	1.34	1.38
22	23S1	643	A	N3-C4	5.71	1.38	1.34
22	23S1	996	A	C5-C4	-5.71	1.34	1.38
22	23S1	1608	A	C8-N7	5.71	1.35	1.31
22	23S1	1637	A	C8-N7	5.71	1.35	1.31
22	23S1	1689	A	C8-N7	5.71	1.35	1.31
22	23S1	1794	A	C8-N7	5.71	1.35	1.31
22	23S1	1901	A	C8-N7	5.71	1.35	1.31
1	16S1	608	A	C5-C4	-5.71	1.34	1.38
1	16S1	1503	A	C5-C4	-5.71	1.34	1.38
22	23S1	125	A	N3-C4	5.71	1.38	1.34
1	16S1	1201	A	C2-N3	5.71	1.38	1.33
1	16S1	1375	A	C5-C4	-5.71	1.34	1.38
22	23S1	1829	A	C5-C4	-5.71	1.34	1.38
22	23S1	515	A	C8-N7	5.71	1.35	1.31
22	23S1	1626	A	C8-N7	5.71	1.35	1.31
1	16S1	282	A	N3-C4	5.71	1.38	1.34
1	16S1	383	A	C2-N3	5.71	1.38	1.33
1	16S1	1375	A	C8-N7	5.71	1.35	1.31
22	23S1	21	A	C8-N7	5.71	1.35	1.31
22	23S1	574	A	C8-N7	5.71	1.35	1.31
22	23S1	1142	A	C8-N7	5.71	1.35	1.31
1	16S1	182	A	C5-C4	-5.70	1.34	1.38
1	16S1	782	A	N3-C4	5.70	1.38	1.34
22	23S1	344	A	N3-C4	5.70	1.38	1.34
22	23S1	528	A	N3-C4	5.70	1.38	1.34
1	16S1	162	A	N3-C4	5.70	1.38	1.34
1	16S1	171	A	N3-C4	5.70	1.38	1.34
1	16S1	1324	A	N3-C4	5.70	1.38	1.34
23	05S1	52	A	C5-C4	-5.70	1.34	1.38
1	16S1	32	A	C8-N7	5.70	1.35	1.31
1	16S1	878	A	C8-N7	5.70	1.35	1.31
1	16S1	676	A	C5-C4	-5.70	1.34	1.38
1	16S1	1152	A	N3-C4	5.70	1.38	1.34
22	23S1	103	A	C5-C4	-5.70	1.34	1.38
22	23S1	1268	A	C8-N7	5.70	1.35	1.31
22	23S1	1876	A	N3-C4	5.70	1.38	1.34
22	23S1	91	A	C5-C4	-5.69	1.34	1.38
22	23S1	477	A	C8-N7	5.69	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	139	A	C5-C4	-5.69	1.34	1.38
1	16S1	712	A	C5-C4	-5.69	1.34	1.38
22	23S1	918	A	C5-C4	-5.69	1.34	1.38
22	23S1	2317	A	C5-C4	-5.69	1.34	1.38
22	23S1	2432	A	N3-C4	5.69	1.38	1.34
1	16S1	129	A	N3-C4	5.69	1.38	1.34
22	23S1	556	A	N3-C4	5.69	1.38	1.34
22	23S1	1129	A	C8-N7	5.69	1.35	1.31
22	23S1	1668	A	C8-N7	5.69	1.35	1.31
1	16S1	655	A	C5-C4	-5.69	1.34	1.38
23	05S1	58	A	N3-C4	5.69	1.38	1.34
22	23S1	83	A	N3-C4	5.69	1.38	1.34
22	23S1	821	A	C8-N7	5.69	1.35	1.31
22	23S1	1009	A	C8-N7	5.69	1.35	1.31
22	23S1	1610	A	C8-N7	5.69	1.35	1.31
22	23S1	1815	A	C5-C4	-5.69	1.34	1.38
22	23S1	2080	A	C8-N7	5.69	1.35	1.31
55	PTR1	3	A	N3-C4	5.69	1.38	1.34
1	16S1	482	A	N3-C4	5.68	1.38	1.34
22	23S1	789	A	C8-N7	5.68	1.35	1.31
22	23S1	1262	A	C5-C4	-5.68	1.34	1.38
22	23S1	2826	A	N3-C4	5.68	1.38	1.34
1	16S1	802	A	C8-N7	5.68	1.35	1.31
22	23S1	223	A	C8-N7	5.68	1.35	1.31
22	23S1	538	A	C5-C4	-5.68	1.34	1.38
22	23S1	2810	A	C5-C4	-5.68	1.34	1.38
22	23S1	320	A	N7-C5	-5.68	1.35	1.39
22	23S1	1496	A	N3-C4	5.68	1.38	1.34
1	16S1	878	A	N3-C4	5.68	1.38	1.34
1	16S1	1196	A	N3-C4	5.68	1.38	1.34
22	23S1	217	A	N3-C4	5.68	1.38	1.34
22	23S1	631	A	C8-N7	5.68	1.35	1.31
22	23S1	1504	A	C5-C4	-5.68	1.34	1.38
22	23S1	2776	A	N3-C4	5.68	1.38	1.34
22	23S1	1342	A	C8-N7	5.68	1.35	1.31
1	16S1	996	A	C5-C4	-5.68	1.34	1.38
22	23S1	2476	A	C5-C4	-5.68	1.34	1.38
1	16S1	366	A	N3-C4	5.67	1.38	1.34
22	23S1	1246	A	N3-C4	5.67	1.38	1.34
22	23S1	1678	A	C8-N7	5.67	1.35	1.31
22	23S1	2868	A	C5-C4	-5.67	1.34	1.38
1	16S1	1171	A	C5-C4	-5.67	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	55	A	C8-N7	5.67	1.35	1.31
1	16S1	152	A	N3-C4	5.67	1.38	1.34
1	16S1	1357	A	C5-C4	-5.67	1.34	1.38
22	23S1	2757	A	C8-N7	5.67	1.35	1.31
22	23S1	324	A	C8-N7	5.67	1.35	1.31
22	23S1	1654	A	C8-N7	5.67	1.35	1.31
22	23S1	1912	A	C8-N7	5.67	1.35	1.31
22	23S1	2541	A	C8-N7	5.67	1.35	1.31
1	16S1	495	A	N3-C4	5.67	1.38	1.34
22	23S1	125	A	C5-C4	-5.67	1.34	1.38
22	23S1	2513	A	N3-C4	5.67	1.38	1.34
1	16S1	704	A	N3-C4	5.67	1.38	1.34
22	23S1	819	A	N3-C4	5.67	1.38	1.34
22	23S1	1866	A	C8-N7	5.67	1.35	1.31
1	16S1	71	A	C5-C4	-5.66	1.34	1.38
1	16S1	1014	A	N3-C4	5.66	1.38	1.34
22	23S1	272	A	N3-C4	5.66	1.38	1.34
22	23S1	528	A	C8-N7	5.66	1.35	1.31
22	23S1	655	A	C5-C4	-5.66	1.34	1.38
22	23S1	2725	A	C8-N7	5.66	1.35	1.31
22	23S1	131	A	C5-C4	-5.66	1.34	1.38
22	23S1	322	A	C5-C4	-5.66	1.34	1.38
22	23S1	1156	A	C8-N7	5.66	1.35	1.31
22	23S1	1936	A	C5-C4	-5.66	1.34	1.38
22	23S1	155	A	N3-C4	5.66	1.38	1.34
22	23S1	460	A	C8-N7	5.66	1.35	1.31
22	23S1	1580	A	C5-C4	-5.66	1.34	1.38
22	23S1	1746	A	N3-C4	5.66	1.38	1.34
22	23S1	1759	A	N3-C4	5.66	1.38	1.34
22	23S1	1981	A	C8-N7	5.66	1.35	1.31
1	16S1	288	A	N3-C4	5.66	1.38	1.34
1	16S1	609	A	C5-C4	-5.66	1.34	1.38
22	23S1	730	A	C8-N7	5.66	1.35	1.31
22	23S1	1913	A	C5-C4	-5.66	1.34	1.38
23	05S1	109	A	N3-C4	5.66	1.38	1.34
55	PTR1	9	A	N3-C4	5.66	1.38	1.34
1	16S1	327	A	C8-N7	5.66	1.35	1.31
1	16S1	673	A	N3-C4	5.66	1.38	1.34
22	23S1	666	A	C8-N7	5.66	1.35	1.31
22	23S1	1503	A	N3-C4	5.66	1.38	1.34
1	16S1	1197	A	C5-C4	-5.65	1.34	1.38
1	16S1	1357	A	N3-C4	5.65	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	768	A	N3-C4	5.65	1.38	1.34
22	23S1	655	A	N3-C4	5.65	1.38	1.34
1	16S1	563	A	N3-C4	5.65	1.38	1.34
1	16S1	1102	A	C8-N7	5.65	1.35	1.31
1	16S1	1311	A	C5-C4	-5.65	1.34	1.38
22	23S1	182	A	C5-C4	-5.65	1.34	1.38
22	23S1	1477	A	C5-C4	-5.65	1.34	1.38
1	16S1	325	A	C5-C4	-5.65	1.34	1.38
22	23S1	2211	A	N3-C4	5.65	1.38	1.34
22	23S1	2813	A	C5-C4	-5.65	1.34	1.38
23	05S1	50	A	C5-C4	-5.65	1.34	1.38
1	16S1	412	A	C5-C4	-5.65	1.34	1.38
22	23S1	49	A	C5-C4	-5.65	1.34	1.38
22	23S1	1637	A	C5-C4	-5.65	1.34	1.38
23	05S1	50	A	N3-C4	5.65	1.38	1.34
1	16S1	1503	A	C8-N7	5.65	1.35	1.31
22	23S1	181	A	N3-C4	5.65	1.38	1.34
22	23S1	478	A	C8-N7	5.65	1.35	1.31
22	23S1	2765	A	N3-C4	5.65	1.38	1.34
1	16S1	338	A	C5-C4	-5.64	1.34	1.38
22	23S1	345	A	C5-C4	-5.64	1.34	1.38
1	16S1	16	A	C8-N7	5.64	1.35	1.31
1	16S1	1251	A	C5-C4	-5.64	1.34	1.38
22	23S1	716	A	N3-C4	5.64	1.38	1.34
22	23S1	1021	A	N7-C5	-5.64	1.35	1.39
22	23S1	2311	A	C5-C4	-5.64	1.34	1.38
22	23S1	160	A	C5-C4	-5.64	1.34	1.38
1	16S1	364	A	N3-C4	5.64	1.38	1.34
1	16S1	642	A	C5-C4	-5.64	1.34	1.38
22	23S1	1652	A	C8-N7	5.64	1.35	1.31
22	23S1	1866	A	C5-C4	-5.64	1.34	1.38
1	16S1	975	A	N3-C4	5.64	1.38	1.34
1	16S1	1102	A	C5-C4	-5.64	1.34	1.38
22	23S1	63	A	C5-C4	-5.64	1.34	1.38
22	23S1	172	A	C5-C4	-5.64	1.34	1.38
22	23S1	905	A	N3-C4	5.64	1.38	1.34
22	23S1	1597	A	C5-C4	-5.64	1.34	1.38
22	23S1	2778	A	N3-C4	5.64	1.38	1.34
1	16S1	363	A	C5-C4	-5.64	1.34	1.38
22	23S1	863	A	C8-N7	5.64	1.35	1.31
22	23S1	2778	A	C8-N7	5.64	1.35	1.31
1	16S1	374	A	C5-C4	-5.63	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	441	A	C5-C4	-5.63	1.34	1.38
1	16S1	1333	A	C5-C4	-5.63	1.34	1.38
22	23S1	2205	A	C5-C4	-5.63	1.34	1.38
22	23S1	482	A	N3-C4	5.63	1.38	1.34
1	16S1	502	A	C5-C4	-5.63	1.34	1.38
22	23S1	632	A	C8-N7	5.63	1.35	1.31
1	16S1	547	A	C5-C4	-5.63	1.34	1.38
22	23S1	522	A	C8-N7	5.63	1.35	1.31
22	23S1	927	A	N3-C4	5.63	1.38	1.34
22	23S1	1700	A	N3-C4	5.63	1.38	1.34
55	PTR1	14	A	N3-C4	5.63	1.38	1.34
1	16S1	2	A	N3-C4	5.63	1.38	1.34
22	23S1	83	A	C5-C4	-5.63	1.34	1.38
22	23S1	480	A	N3-C4	5.63	1.38	1.34
22	23S1	990	A	C8-N7	5.63	1.35	1.31
1	16S1	1375	A	N3-C4	5.62	1.38	1.34
23	05S1	57	A	C5-C4	-5.62	1.34	1.38
1	16S1	228	A	N3-C4	5.62	1.38	1.34
22	23S1	973	A	C5-C4	-5.62	1.34	1.38
22	23S1	1403	A	C8-N7	5.62	1.35	1.31
22	23S1	1885	A	N3-C4	5.62	1.38	1.34
55	PTR1	14	A	C8-N7	5.62	1.35	1.31
22	23S1	1040	A	N3-C4	5.62	1.38	1.34
22	23S1	1549	A	N3-C4	5.62	1.38	1.34
22	23S1	1553	A	C5-C4	-5.62	1.34	1.38
22	23S1	19	A	C8-N7	5.62	1.35	1.31
22	23S1	342	A	N3-C4	5.62	1.38	1.34
22	23S1	668	A	C8-N7	5.62	1.35	1.31
22	23S1	1470	A	N3-C4	5.62	1.38	1.34
1	16S1	32	A	N3-C4	5.62	1.38	1.34
1	16S1	1476	A	C5-C4	-5.62	1.34	1.38
22	23S1	1570	A	C8-N7	5.62	1.35	1.31
1	16S1	913	A	N3-C4	5.62	1.38	1.34
1	16S1	179	A	N3-C4	5.62	1.38	1.34
1	16S1	1261	A	C5-C4	-5.62	1.34	1.38
1	16S1	1150	A	C5-C4	-5.61	1.34	1.38
1	16S1	1251	A	N3-C4	5.61	1.38	1.34
1	16S1	1289	A	C5-C4	-5.61	1.34	1.38
22	23S1	142	A	C5-C4	-5.61	1.34	1.38
22	23S1	1275	A	C8-N7	5.61	1.35	1.31
22	23S1	2266	A	C8-N7	5.61	1.35	1.31
22	23S1	2267	A	C8-N7	5.61	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	673	A	C8-N7	5.61	1.35	1.31
22	23S1	127	A	C8-N7	5.61	1.35	1.31
1	16S1	1170	A	N3-C4	5.61	1.38	1.34
1	16S1	1456	A	C5-C4	-5.61	1.34	1.38
22	23S1	1655	A	N3-C4	5.61	1.38	1.34
22	23S1	1679	A	C8-N7	5.61	1.35	1.31
22	23S1	2425	A	C8-N7	5.61	1.35	1.31
22	23S1	2058	A	N3-C4	5.61	1.38	1.34
22	23S1	2873	A	C8-N7	5.61	1.35	1.31
1	16S1	44	A	C5-C4	-5.61	1.34	1.38
1	16S1	1350	A	C5-C4	-5.61	1.34	1.38
22	23S1	905	A	C5-C4	-5.61	1.34	1.38
22	23S1	1265	A	C8-N7	5.61	1.35	1.31
22	23S1	2317	A	N3-C4	5.61	1.38	1.34
22	23S1	2476	A	N3-C4	5.61	1.38	1.34
1	16S1	344	A	N3-C4	5.60	1.38	1.34
1	16S1	629	A	C5-C4	-5.60	1.34	1.38
1	16S1	1204	A	C5-C4	-5.60	1.34	1.38
1	16S1	195	A	N3-C4	5.60	1.38	1.34
1	16S1	696	A	C5-C4	-5.60	1.34	1.38
22	23S1	2530	A	N3-C4	5.60	1.38	1.34
22	23S1	2868	A	C8-N7	5.60	1.35	1.31
1	16S1	459	A	C5-C4	-5.60	1.34	1.38
22	23S1	1515	A	N3-C4	5.60	1.38	1.34
22	23S1	2352	A	N3-C4	5.60	1.38	1.34
1	16S1	129	A	C5-C4	-5.60	1.34	1.38
22	23S1	849	A	C5-C4	-5.60	1.34	1.38
22	23S1	2873	A	C5-C4	-5.60	1.34	1.38
55	PTR1	42	A	C5-C4	-5.60	1.34	1.38
1	16S1	7	A	C5-C4	-5.59	1.34	1.38
1	16S1	10	A	N3-C4	5.59	1.38	1.34
22	23S1	104	A	C5-C4	-5.59	1.34	1.38
22	23S1	626	A	N3-C4	5.59	1.38	1.34
22	23S1	1876	A	C5-C4	-5.59	1.34	1.38
1	16S1	55	A	C5-C4	-5.59	1.34	1.38
1	16S1	174	A	C5-C4	-5.59	1.34	1.38
1	16S1	819	A	N3-C4	5.59	1.38	1.34
22	23S1	721	A	N3-C4	5.59	1.38	1.34
22	23S1	1553	A	N3-C4	5.59	1.38	1.34
22	23S1	348	A	N3-C4	5.59	1.38	1.34
22	23S1	603	A	N3-C4	5.59	1.38	1.34
22	23S1	1672	A	N3-C4	5.59	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2287	A	C8-N7	5.59	1.35	1.31
1	16S1	1239	A	N3-C4	5.59	1.38	1.34
22	23S1	21	A	N3-C4	5.59	1.38	1.34
22	23S1	173	A	N3-C4	5.59	1.38	1.34
22	23S1	2418	A	C8-N7	5.59	1.35	1.31
22	23S1	2851	A	C8-N7	5.59	1.35	1.31
1	16S1	306	A	C5-C4	-5.59	1.34	1.38
23	05S1	99	A	C8-N7	5.59	1.35	1.31
22	23S1	677	A	C8-N7	5.59	1.35	1.31
22	23S1	1147	A	N3-C4	5.59	1.38	1.34
22	23S1	1354	A	N7-C5	-5.59	1.35	1.39
1	16S1	510	A	C8-N7	5.58	1.35	1.31
1	16S1	906	A	C8-N7	5.58	1.35	1.31
1	16S1	949	A	N3-C4	5.58	1.38	1.34
1	16S1	1468	A	N3-C4	5.58	1.38	1.34
22	23S1	324	A	N3-C4	5.58	1.38	1.34
22	23S1	1494	A	C5-C4	-5.58	1.34	1.38
22	23S1	1502	A	N3-C4	5.58	1.38	1.34
22	23S1	2749	A	C5-C4	-5.58	1.34	1.38
1	16S1	160	A	N3-C4	5.58	1.38	1.34
1	16S1	681	A	C5-C4	-5.58	1.34	1.38
1	16S1	946	A	N3-C4	5.58	1.38	1.34
22	23S1	910	A	C8-N7	5.58	1.35	1.31
22	23S1	401	A	C5-C4	-5.58	1.34	1.38
22	23S1	1551	A	C5-C4	-5.58	1.34	1.38
22	23S1	2426	A	C8-N7	5.58	1.35	1.31
1	16S1	523	A	N3-C4	5.58	1.38	1.34
1	16S1	579	A	N3-C4	5.58	1.38	1.34
22	23S1	722	A	N3-C4	5.58	1.38	1.34
22	23S1	1028	A	C8-N7	5.58	1.35	1.31
22	23S1	2516	A	C8-N7	5.58	1.35	1.31
22	23S1	2711	A	C8-N7	5.58	1.35	1.31
1	16S1	495	A	C5-C4	-5.58	1.34	1.38
1	16S1	1248	A	N3-C4	5.58	1.38	1.34
1	16S1	1492	A	N3-C4	5.58	1.38	1.34
22	23S1	412	A	C8-N7	5.58	1.35	1.31
22	23S1	1676	A	N3-C4	5.58	1.38	1.34
22	23S1	1705	A	N3-C4	5.58	1.38	1.34
22	23S1	1367	A	C8-N7	5.57	1.35	1.31
22	23S1	1700	A	C8-N7	5.57	1.35	1.31
22	23S1	1918	A	N3-C4	5.57	1.38	1.34
1	16S1	900	A	C8-N7	5.57	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1176	A	N3-C4	5.57	1.38	1.34
1	16S1	1368	A	N3-C4	5.57	1.38	1.34
22	23S1	1169	A	C5-C4	-5.57	1.34	1.38
22	23S1	1739	A	N3-C4	5.57	1.38	1.34
1	16S1	496	A	C5-C4	-5.57	1.34	1.38
1	16S1	609	A	N3-C4	5.57	1.38	1.34
22	23S1	251	A	C5-C4	-5.57	1.34	1.38
22	23S1	374	A	C8-N7	5.57	1.35	1.31
22	23S1	1872	A	C2-N3	5.57	1.38	1.33
22	23S1	844	A	N3-C4	5.57	1.38	1.34
22	23S1	975	A	N3-C4	5.57	1.38	1.34
22	23S1	2879	A	C5-C4	-5.57	1.34	1.38
22	23S1	2725	A	N3-C4	5.56	1.38	1.34
22	23S1	1780	A	N3-C4	5.56	1.38	1.34
22	23S1	2377	A	N3-C4	5.56	1.38	1.34
1	16S1	648	A	N3-C4	5.56	1.38	1.34
22	23S1	146	A	N3-C4	5.56	1.38	1.34
22	23S1	1307	A	N3-C4	5.56	1.38	1.34
1	16S1	1430	A	N3-C4	5.56	1.38	1.34
22	23S1	1597	A	N3-C4	5.56	1.38	1.34
22	23S1	1603	A	N3-C4	5.56	1.38	1.34
22	23S1	1641	A	N3-C4	5.56	1.38	1.34
1	16S1	959	A	N3-C4	5.56	1.38	1.34
22	23S1	2614	A	C5-C4	-5.56	1.34	1.38
1	16S1	794	A	N3-C4	5.56	1.38	1.34
1	16S1	44	A	N3-C4	5.55	1.38	1.34
22	23S1	1029	A	N3-C4	5.55	1.38	1.34
22	23S1	2142	A	C2-N3	5.55	1.38	1.33
22	23S1	936	A	N3-C4	5.55	1.38	1.34
1	16S1	130	A	N3-C4	5.55	1.38	1.34
1	16S1	344	A	C5-C4	-5.55	1.34	1.38
22	23S1	2820	A	C5-C4	-5.55	1.34	1.38
1	16S1	364	A	C5-C4	-5.55	1.34	1.38
22	23S1	1808	A	N3-C4	5.55	1.38	1.34
22	23S1	2406	A	C5-C4	-5.55	1.34	1.38
1	16S1	907	A	C8-N7	5.54	1.35	1.31
1	16S1	190	A	N7-C5	-5.54	1.35	1.39
1	16S1	499	A	C5-C4	-5.54	1.34	1.38
1	16S1	655	A	N3-C4	5.54	1.38	1.34
1	16S1	977	A	C8-N7	5.54	1.35	1.31
22	23S1	917	A	N3-C4	5.54	1.38	1.34
22	23S1	2821	A	N3-C4	5.54	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	716	A	C5-C4	-5.54	1.34	1.38
1	16S1	915	A	N3-C4	5.54	1.38	1.34
1	16S1	1289	A	N3-C4	5.54	1.38	1.34
1	16S1	389	A	C5-C4	-5.54	1.34	1.38
22	23S1	1780	A	C5-C4	-5.54	1.34	1.38
22	23S1	2388	A	N3-C4	5.54	1.38	1.34
1	16S1	238	A	N3-C4	5.54	1.38	1.34
1	16S1	909	A	N3-C4	5.54	1.38	1.34
1	16S1	373	A	C5-C4	-5.54	1.34	1.38
22	23S1	1077	A	N3-C4	5.54	1.38	1.34
22	23S1	1439	A	N3-C4	5.54	1.38	1.34
22	23S1	1528	A	C8-N7	5.54	1.35	1.31
22	23S1	1635	A	N3-C4	5.54	1.38	1.34
55	PTR1	38	A	N3-C4	5.54	1.38	1.34
22	23S1	144	A	N3-C4	5.53	1.38	1.34
25	L031	33	ARG	CZ-NH2	5.53	1.40	1.33
1	16S1	451	A	N3-C4	5.53	1.38	1.34
22	23S1	2518	A	N3-C4	5.53	1.38	1.34
22	23S1	2733	A	C5-C4	-5.53	1.34	1.38
22	23S1	2900	A	N3-C4	5.53	1.38	1.34
22	23S1	95	A	C5-C4	-5.53	1.34	1.38
22	23S1	447	A	C8-N7	5.53	1.35	1.31
22	23S1	1126	A	C8-N7	5.53	1.35	1.31
22	23S1	1321	A	N3-C4	5.53	1.38	1.34
1	16S1	583	A	N3-C4	5.53	1.38	1.34
1	16S1	687	A	N3-C4	5.53	1.38	1.34
1	16S1	1465	A	N3-C4	5.53	1.38	1.34
23	05S1	78	A	N3-C4	5.53	1.38	1.34
1	16S1	181	A	C5-C4	-5.52	1.34	1.38
1	16S1	1145	A	N3-C4	5.52	1.38	1.34
22	23S1	602	A	N3-C4	5.52	1.38	1.34
22	23S1	1169	A	N3-C4	5.52	1.38	1.34
22	23S1	1952	A	C8-N7	5.52	1.35	1.31
22	23S1	1966	A	C8-N7	5.52	1.35	1.31
22	23S1	412	A	N3-C4	5.52	1.38	1.34
22	23S1	2823	A	C8-N7	5.52	1.35	1.31
1	16S1	676	A	N3-C4	5.52	1.38	1.34
1	16S1	1362	A	N3-C4	5.52	1.38	1.34
22	23S1	1785	A	N3-C4	5.52	1.38	1.34
55	PTR1	34	I	C2-N3	5.52	1.47	1.35
1	16S1	547	A	N3-C4	5.52	1.38	1.34
1	16S1	974	A	C5-C4	-5.52	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	753	A	N3-C4	5.52	1.38	1.34
22	23S1	1453	A	N3-C4	5.52	1.38	1.34
22	23S1	514	A	C8-N7	5.51	1.35	1.31
22	23S1	960	A	N3-C4	5.51	1.38	1.34
22	23S1	2327	A	C8-N7	5.51	1.35	1.31
22	23S1	2700	A	N3-C4	5.51	1.38	1.34
22	23S1	2799	A	C5-C4	-5.51	1.34	1.38
22	23S1	2826	A	C8-N7	5.51	1.35	1.31
1	16S1	493	A	C5-C4	-5.51	1.34	1.38
1	16S1	923	A	N3-C4	5.51	1.38	1.34
22	23S1	928	A	N3-C4	5.51	1.38	1.34
22	23S1	1373	A	C8-N7	5.51	1.35	1.31
22	23S1	1787	A	N3-C4	5.51	1.38	1.34
22	23S1	2411	A	N3-C4	5.51	1.38	1.34
22	23S1	1111	A	C5-C4	-5.51	1.34	1.38
22	23S1	1789	A	N3-C4	5.51	1.38	1.34
22	23S1	2058	A	C8-N7	5.51	1.35	1.31
22	23S1	2281	A	N3-C4	5.51	1.38	1.34
22	23S1	2482	A	C5-C4	-5.51	1.34	1.38
22	23S1	2757	A	C5-C4	-5.51	1.34	1.38
1	16S1	487	A	N3-C4	5.51	1.38	1.34
1	16S1	1197	A	N3-C4	5.51	1.38	1.34
22	23S1	368	A	N3-C4	5.51	1.38	1.34
22	23S1	699	A	C8-N7	5.51	1.35	1.31
22	23S1	781	A	C8-N7	5.51	1.35	1.31
1	16S1	977	A	C5-C4	-5.50	1.34	1.38
1	16S1	393	A	C5-C4	-5.50	1.34	1.38
22	23S1	44	A	N3-C4	5.50	1.38	1.34
22	23S1	975	A	C8-N7	5.50	1.35	1.31
22	23S1	1819	A	C8-N7	5.50	1.35	1.31
22	23S1	2758	A	N3-C4	5.50	1.38	1.34
22	23S1	311	A	N3-C4	5.50	1.38	1.34
22	23S1	1579	A	N3-C4	5.50	1.38	1.34
22	23S1	2378	A	N3-C4	5.50	1.38	1.34
55	PTR1	38	A	C8-N7	5.50	1.35	1.31
1	16S1	1483	A	N3-C4	5.50	1.38	1.34
22	23S1	1848	A	C5-C4	-5.50	1.34	1.38
1	16S1	179	A	C5-C4	-5.50	1.34	1.38
22	23S1	1586	A	N3-C4	5.50	1.38	1.34
22	23S1	2205	A	N3-C4	5.50	1.38	1.34
23	05S1	59	A	N1-C2	5.50	1.39	1.34
1	16S1	1111	A	C5-C4	-5.50	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	348	A	C5-C4	-5.50	1.34	1.38
22	23S1	1244	A	N3-C4	5.50	1.38	1.34
22	23S1	1701	A	N3-C4	5.50	1.38	1.34
22	23S1	2077	A	N3-C4	5.50	1.38	1.34
22	23S1	2675	A	C8-N7	5.50	1.35	1.31
23	05S1	57	A	N3-C4	5.50	1.38	1.34
22	23S1	384	A	C8-N7	5.50	1.35	1.31
22	23S1	2547	A	C5-C4	-5.50	1.34	1.38
1	16S1	1151	A	C5-C4	-5.49	1.34	1.38
1	16S1	1236	A	N3-C4	5.49	1.38	1.34
1	16S1	1254	A	N3-C4	5.49	1.38	1.34
22	23S1	195	A	N3-C4	5.49	1.38	1.34
22	23S1	42	A	N3-C4	5.49	1.38	1.34
22	23S1	2851	A	N3-C4	5.49	1.38	1.34
1	16S1	539	A	C5-C4	-5.49	1.34	1.38
1	16S1	1111	A	N3-C4	5.49	1.38	1.34
22	23S1	1603	A	C8-N7	5.49	1.35	1.31
22	23S1	1579	A	C5-C4	-5.49	1.34	1.38
1	16S1	1434	A	N3-C4	5.49	1.38	1.34
22	23S1	345	A	N3-C4	5.49	1.38	1.34
22	23S1	1027	A	N3-C4	5.49	1.38	1.34
1	16S1	535	A	N3-C4	5.48	1.38	1.34
1	16S1	696	A	N3-C4	5.48	1.38	1.34
22	23S1	1287	A	C8-N7	5.48	1.35	1.31
22	23S1	2059	A	C5-C4	-5.48	1.34	1.38
1	16S1	60	A	C5-C4	-5.48	1.34	1.38
1	16S1	1531	A	N3-C4	5.48	1.38	1.34
23	05S1	73	A	C5-C4	-5.48	1.34	1.38
55	PTR1	69	A	C5-C4	-5.48	1.34	1.38
22	23S1	819	A	N7-C5	-5.48	1.35	1.39
22	23S1	1254	A	C8-N7	5.48	1.35	1.31
22	23S1	1301	A	N3-C4	5.48	1.38	1.34
22	23S1	1434	A	C5-C4	-5.48	1.34	1.38
22	23S1	2886	A	N3-C4	5.48	1.38	1.34
22	23S1	608	A	C8-N7	5.48	1.35	1.31
22	23S1	1745	A	C5-C4	-5.48	1.34	1.38
22	23S1	2278	A	N3-C4	5.48	1.38	1.34
1	16S1	109	A	N3-C4	5.47	1.38	1.34
1	16S1	456	A	C5-C4	-5.47	1.34	1.38
1	16S1	7	A	N3-C4	5.47	1.38	1.34
22	23S1	354	A	N3-C4	5.47	1.38	1.34
22	23S1	2433	A	C8-N7	5.47	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1269	A	C5-C4	-5.47	1.34	1.38
22	23S1	2451	A	C5-C4	-5.47	1.34	1.38
1	16S1	270	A	C5-C4	-5.47	1.34	1.38
1	16S1	607	A	C5-C4	-5.47	1.34	1.38
22	23S1	111	A	N3-C4	5.47	1.38	1.34
22	23S1	574	A	N3-C4	5.47	1.38	1.34
22	23S1	2860	A	N3-C4	5.47	1.38	1.34
23	05S1	101	A	C8-N7	5.47	1.35	1.31
1	16S1	642	A	N3-C4	5.47	1.38	1.34
1	16S1	706	A	C8-N7	5.47	1.35	1.31
1	16S1	1250	A	N3-C4	5.46	1.38	1.34
22	23S1	118	A	N3-C4	5.46	1.38	1.34
22	23S1	507	A	N3-C4	5.46	1.38	1.34
1	16S1	546	A	N3-C4	5.46	1.38	1.34
22	23S1	218	A	N3-C4	5.46	1.38	1.34
22	23S1	735	A	N3-C4	5.46	1.38	1.34
1	16S1	65	A	C5-C4	-5.46	1.34	1.38
1	16S1	59	A	C5-C4	-5.46	1.34	1.38
1	16S1	712	A	N3-C4	5.46	1.38	1.34
22	23S1	825	A	C8-N7	5.46	1.35	1.31
1	16S1	695	A	N3-C4	5.46	1.38	1.34
1	16S1	1179	A	C5-C4	-5.46	1.34	1.38
22	23S1	64	A	N3-C4	5.46	1.38	1.34
1	16S1	1169	A	C5-C4	-5.46	1.34	1.38
22	23S1	167	A	N3-C4	5.46	1.38	1.34
22	23S1	1664	A	N3-C4	5.46	1.38	1.34
22	23S1	1854	A	N3-C4	5.46	1.38	1.34
22	23S1	1998	A	N3-C4	5.46	1.38	1.34
1	16S1	595	A	N3-C4	5.45	1.38	1.34
1	16S1	663	A	N3-C4	5.45	1.38	1.34
22	23S1	1260	A	C8-N7	5.45	1.35	1.31
22	23S1	722	A	C5-C4	-5.45	1.34	1.38
1	16S1	1169	A	N3-C4	5.45	1.38	1.34
1	16S1	1324	A	C5-C4	-5.45	1.34	1.38
22	23S1	165	A	C5-C4	-5.45	1.34	1.38
1	16S1	51	A	C8-N7	5.45	1.35	1.31
22	23S1	756	A	C8-N7	5.45	1.35	1.31
23	05S1	58	A	C5-C4	-5.45	1.34	1.38
1	16S1	205	A	C5-C4	-5.45	1.34	1.38
22	23S1	241	A	N3-C4	5.45	1.38	1.34
1	16S1	815	A	C8-N7	5.44	1.35	1.31
22	23S1	1598	A	C5-C4	-5.44	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2094	A	N3-C4	5.44	1.38	1.34
1	16S1	223	A	C5-C4	-5.44	1.34	1.38
22	23S1	470	A	N3-C4	5.44	1.38	1.34
22	23S1	750	A	C8-N7	5.44	1.35	1.31
22	23S1	2335	A	N3-C4	5.44	1.38	1.34
1	16S1	3	A	C5-C4	-5.44	1.34	1.38
1	16S1	320	A	N3-C4	5.44	1.38	1.34
1	16S1	1146	A	C5-C4	-5.44	1.34	1.38
22	23S1	190	A	C8-N7	5.44	1.35	1.31
23	05S1	99	A	N3-C4	5.44	1.38	1.34
22	23S1	1535	A	C2-N3	5.44	1.38	1.33
1	16S1	919	A	C8-N7	5.44	1.35	1.31
1	16S1	1318	A	N3-C4	5.44	1.38	1.34
22	23S1	2662	A	N3-C4	5.44	1.38	1.34
22	23S1	74	A	C5-C4	-5.44	1.34	1.38
22	23S1	1403	A	N3-C4	5.44	1.38	1.34
22	23S1	1598	A	N3-C4	5.44	1.38	1.34
22	23S1	2513	A	C5-C4	-5.44	1.34	1.38
1	16S1	1080	A	C8-N7	5.43	1.35	1.31
1	16S1	1350	A	N3-C4	5.43	1.38	1.34
22	23S1	706	A	N3-C4	5.43	1.38	1.34
22	23S1	1205	A	C5-C4	-5.43	1.34	1.38
22	23S1	2765	A	C5-C4	-5.43	1.34	1.38
1	16S1	131	A	C5-C4	-5.43	1.34	1.38
1	16S1	864	A	C8-N7	5.43	1.35	1.31
1	16S1	1204	A	N3-C4	5.43	1.38	1.34
22	23S1	1230	A	N3-C4	5.43	1.38	1.34
22	23S1	1393	A	C8-N7	5.43	1.35	1.31
22	23S1	1808	A	C5-C4	-5.43	1.34	1.38
22	23S1	2088	A	C8-N7	5.43	1.35	1.31
22	23S1	2478	A	N3-C4	5.43	1.38	1.34
23	05S1	15	A	N3-C4	5.43	1.38	1.34
22	23S1	2459	A	C8-N7	5.43	1.35	1.31
22	23S1	845	A	C5-C4	-5.43	1.34	1.38
1	16S1	860	A	C5-C4	-5.42	1.34	1.38
22	23S1	2860	A	C8-N7	5.42	1.35	1.31
23	05S1	53	A	C5-C4	-5.42	1.34	1.38
22	23S1	1689	A	N3-C4	5.42	1.38	1.34
22	23S1	2176	A	N3-C4	5.42	1.38	1.34
22	23S1	2381	A	N3-C4	5.42	1.38	1.34
22	23S1	52	A	C8-N7	5.42	1.35	1.31
22	23S1	503	A	N3-C4	5.42	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1713	A	N3-C4	5.42	1.38	1.34
1	16S1	71	A	N3-C4	5.42	1.38	1.34
1	16S1	1318	A	C5-C4	-5.42	1.34	1.38
22	23S1	103	A	N3-C4	5.42	1.38	1.34
22	23S1	529	A	N3-C4	5.42	1.38	1.34
22	23S1	1583	A	C5-C4	-5.42	1.34	1.38
22	23S1	2199	A	N3-C4	5.42	1.38	1.34
1	16S1	1349	A	N3-C4	5.42	1.38	1.34
22	23S1	161	A	N3-C4	5.42	1.38	1.34
22	23S1	344	A	C5-C4	-5.42	1.34	1.38
22	23S1	439	A	N3-C4	5.42	1.38	1.34
1	16S1	2	A	C5-C4	-5.42	1.34	1.38
1	16S1	338	A	N3-C4	5.42	1.38	1.34
1	16S1	718	A	C5-C4	-5.42	1.34	1.38
1	16S1	825	A	N3-C4	5.42	1.38	1.34
1	16S1	1339	A	C8-N7	5.42	1.35	1.31
22	23S1	477	A	C5-C4	-5.41	1.34	1.38
23	05S1	101	A	N1-C2	5.41	1.39	1.34
55	PTR1	23	A	C5-C4	-5.41	1.34	1.38
22	23S1	251	A	N3-C4	5.41	1.38	1.34
55	PTR1	59	A	C5-C4	-5.41	1.34	1.38
1	16S1	8	A	N3-C4	5.41	1.38	1.34
1	16S1	729	A	N3-C4	5.41	1.38	1.34
22	23S1	2654	A	N3-C4	5.41	1.38	1.34
23	05S1	109	A	C5-C4	-5.41	1.34	1.38
22	23S1	1596	A	N3-C4	5.41	1.38	1.34
1	16S1	192	A	C5-C4	-5.41	1.34	1.38
22	23S1	218	A	C5-C4	-5.41	1.34	1.38
1	16S1	160	A	C5-C4	-5.40	1.34	1.38
1	16S1	706	A	N3-C4	5.40	1.38	1.34
22	23S1	227	A	N3-C4	5.40	1.38	1.34
22	23S1	718	A	C5-C4	-5.40	1.34	1.38
22	23S1	2657	A	N3-C4	5.40	1.38	1.34
1	16S1	596	A	N3-C4	5.40	1.38	1.34
1	16S1	1055	A	N3-C4	5.40	1.38	1.34
22	23S1	676	A	C8-N7	5.40	1.35	1.31
22	23S1	918	A	N3-C4	5.40	1.38	1.34
1	16S1	196	A	C5-C4	-5.40	1.34	1.38
1	16S1	374	A	N3-C4	5.40	1.38	1.34
22	23S1	447	A	N3-C4	5.40	1.38	1.34
1	16S1	702	A	C5-C4	-5.40	1.34	1.38
22	23S1	480	A	C8-N7	5.40	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2037	A	C8-N7	5.40	1.35	1.31
22	23S1	2386	A	N3-C4	5.40	1.38	1.34
23	05S1	15	A	C5-C4	-5.40	1.34	1.38
22	23S1	513	A	N3-C4	5.40	1.38	1.34
22	23S1	609	A	C8-N7	5.40	1.35	1.31
22	23S1	2336	A	N3-C4	5.40	1.38	1.34
1	16S1	1248	A	C5-C4	-5.39	1.34	1.38
1	16S1	1413	A	N3-C4	5.39	1.38	1.34
23	05S1	104	A	N3-C4	5.39	1.38	1.34
1	16S1	746	A	C2-N3	5.39	1.38	1.33
22	23S1	1953	A	N7-C5	-5.39	1.36	1.39
22	23S1	2273	A	N3-C4	5.39	1.38	1.34
23	05S1	101	A	C5-C4	-5.39	1.34	1.38
1	16S1	172	A	C5-C4	-5.39	1.34	1.38
22	23S1	2322	A	N3-C4	5.39	1.38	1.34
1	16S1	1167	A	C5-C4	-5.39	1.34	1.38
22	23S1	689	A	N3-C4	5.39	1.38	1.34
22	23S1	2095	A	N3-C4	5.39	1.38	1.34
22	23S1	2856	A	N3-C4	5.39	1.38	1.34
1	16S1	1019	A	C5-C4	-5.39	1.34	1.38
1	16S1	1157	A	C5-C4	-5.39	1.34	1.38
1	16S1	1306	A	N3-C4	5.39	1.38	1.34
1	16S1	1468	A	C8-N7	5.38	1.35	1.31
22	23S1	1241	A	C8-N7	5.38	1.35	1.31
22	23S1	2749	A	N3-C4	5.38	1.38	1.34
1	16S1	60	A	N3-C4	5.38	1.38	1.34
22	23S1	223	A	N3-C4	5.38	1.38	1.34
22	23S1	1571	A	N7-C5	-5.38	1.36	1.39
1	16S1	1503	A	N3-C4	5.38	1.38	1.34
22	23S1	391	A	N3-C4	5.38	1.38	1.34
22	23S1	2850	A	C8-N7	5.38	1.35	1.31
1	16S1	781	A	C8-N7	5.38	1.35	1.31
1	16S1	906	A	N3-C4	5.38	1.38	1.34
1	16S1	1285	A	N3-C4	5.38	1.38	1.34
22	23S1	911	A	N3-C4	5.38	1.38	1.34
22	23S1	1977	A	N3-C4	5.38	1.38	1.34
22	23S1	2062	A	C5-C4	-5.38	1.34	1.38
22	23S1	2211	A	C5-C4	-5.38	1.34	1.38
22	23S1	2837	A	N3-C4	5.38	1.38	1.34
1	16S1	559	A	N3-C4	5.38	1.38	1.34
22	23S1	1978	A	C8-N7	5.38	1.35	1.31
1	16S1	560	A	N3-C4	5.37	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	687	A	C5-C4	-5.37	1.34	1.38
22	23S1	608	A	N3-C4	5.37	1.38	1.34
1	16S1	414	A	C5-C4	-5.37	1.34	1.38
22	23S1	1387	A	N3-C4	5.37	1.38	1.34
55	PTR1	73	A	C5-C4	-5.37	1.34	1.38
1	16S1	908	A	N3-C4	5.37	1.38	1.34
22	23S1	947	A	N3-C4	5.37	1.38	1.34
22	23S1	1528	A	C5-C4	-5.37	1.34	1.38
22	23S1	1858	A	N3-C4	5.37	1.38	1.34
22	23S1	2792	A	N3-C4	5.37	1.38	1.34
22	23S1	422	A	N3-C4	5.37	1.38	1.34
1	16S1	1229	A	C5-C4	-5.37	1.34	1.38
1	16S1	1256	A	C5-C4	-5.37	1.34	1.38
22	23S1	374	A	N3-C4	5.37	1.38	1.34
1	16S1	195	A	C5-C4	-5.36	1.34	1.38
1	16S1	781	A	N3-C4	5.36	1.38	1.34
22	23S1	2335	A	C5-C4	-5.36	1.34	1.38
22	23S1	2531	A	C5-C4	-5.36	1.34	1.38
1	16S1	746	A	C5-C4	-5.36	1.34	1.38
22	23S1	675	A	C8-N7	5.36	1.35	1.31
1	16S1	1176	A	C5-C4	-5.36	1.34	1.38
22	23S1	310	A	N3-C4	5.36	1.38	1.34
22	23S1	401	A	N3-C4	5.36	1.38	1.34
22	23S1	959	A	C8-N7	5.36	1.35	1.31
22	23S1	1050	A	C5-C4	-5.36	1.34	1.38
22	23S1	1572	A	N3-C4	5.36	1.38	1.34
22	23S1	1810	A	N3-C4	5.36	1.38	1.34
22	23S1	2052	A	C8-N7	5.36	1.35	1.31
22	23S1	2266	A	N3-C4	5.36	1.38	1.34
22	23S1	2169	A	C2-N3	5.36	1.38	1.33
1	16S1	74	A	C5-C4	-5.36	1.34	1.38
22	23S1	756	A	N3-C4	5.36	1.38	1.34
22	23S1	2426	A	N3-C4	5.36	1.38	1.34
23	05S1	29	A	C5-C4	-5.36	1.35	1.38
22	23S1	256	A	N3-C4	5.36	1.38	1.34
22	23S1	1802	A	N3-C4	5.36	1.38	1.34
22	23S1	1189	A	N3-C4	5.35	1.38	1.34
22	23S1	1354	A	N3-C4	5.35	1.38	1.34
22	23S1	1665	A	C8-N7	5.35	1.35	1.31
22	23S1	2198	A	N3-C4	5.35	1.38	1.34
1	16S1	1014	A	C5-C4	-5.35	1.35	1.38
22	23S1	1213	A	N7-C5	-5.35	1.36	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	685	A	C8-N7	5.35	1.35	1.31
22	23S1	1373	A	N3-C4	5.35	1.38	1.34
22	23S1	2199	A	C8-N7	5.35	1.35	1.31
1	16S1	482	A	C5-C4	-5.35	1.35	1.38
1	16S1	889	A	N3-C4	5.35	1.38	1.34
22	23S1	161	A	C5-C4	-5.35	1.35	1.38
22	23S1	443	A	N3-C4	5.35	1.38	1.34
22	23S1	1791	A	N3-C4	5.35	1.38	1.34
22	23S1	2879	A	N3-C4	5.35	1.38	1.34
1	16S1	872	A	C5-C4	-5.35	1.35	1.38
22	23S1	477	A	N3-C4	5.35	1.38	1.34
22	23S1	2037	A	N3-C4	5.35	1.38	1.34
22	23S1	2247	A	C8-N7	5.35	1.35	1.31
1	16S1	228	A	C5-C4	-5.34	1.35	1.38
22	23S1	699	A	N3-C4	5.34	1.38	1.34
22	23S1	1505	A	N3-C4	5.34	1.38	1.34
22	23S1	2753	A	C5-C4	-5.34	1.35	1.38
22	23S1	715	A	C5-C4	-5.34	1.35	1.38
22	23S1	743	A	C8-N7	5.34	1.35	1.31
1	16S1	602	A	N3-C4	5.34	1.38	1.34
1	16S1	958	A	N3-C4	5.34	1.38	1.34
22	23S1	95	A	N3-C4	5.34	1.38	1.34
22	23S1	255	A	N3-C4	5.34	1.38	1.34
22	23S1	480	A	C5-C4	-5.34	1.35	1.38
22	23S1	2003	A	N3-C4	5.34	1.38	1.34
1	16S1	363	A	N3-C4	5.34	1.38	1.34
1	16S1	533	A	C5-C4	-5.34	1.35	1.38
22	23S1	833	A	C8-N7	5.34	1.35	1.31
55	PTR1	58	A	C5-C4	-5.34	1.35	1.38
1	16S1	329	A	N3-C4	5.34	1.38	1.34
22	23S1	2654	A	C5-C4	-5.34	1.35	1.38
22	23S1	2893	A	N3-C4	5.34	1.38	1.34
22	23S1	983	A	C8-N7	5.34	1.35	1.31
22	23S1	1900	A	C8-N7	5.34	1.35	1.31
22	23S1	2435	A	C8-N7	5.34	1.35	1.31
1	16S1	1180	A	N3-C4	5.33	1.38	1.34
22	23S1	1522	A	N3-C4	5.33	1.38	1.34
22	23S1	1871	A	C2-N3	5.33	1.38	1.33
22	23S1	2453	A	C8-N7	5.33	1.35	1.31
1	16S1	553	A	N3-C4	5.33	1.38	1.34
22	23S1	1746	A	C5-C4	-5.33	1.35	1.38
22	23S1	1785	A	C5-C4	-5.33	1.35	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	994	A	C5-C4	-5.33	1.35	1.38
1	16S1	1377	A	N3-C4	5.33	1.38	1.34
22	23S1	91	A	N3-C4	5.33	1.38	1.34
22	23S1	244	A	N3-C4	5.33	1.38	1.34
22	23S1	429	A	C5-C4	-5.33	1.35	1.38
22	23S1	2736	A	N3-C4	5.33	1.38	1.34
23	05S1	53	A	N3-C4	5.33	1.38	1.34
55	PTR1	21	A	C5-C4	-5.33	1.35	1.38
1	16S1	199	A	C5-C4	-5.33	1.35	1.38
1	16S1	938	A	N3-C4	5.33	1.38	1.34
22	23S1	362	A	C2-N3	5.33	1.38	1.33
1	16S1	1012	A	C5-C4	-5.33	1.35	1.38
55	PTR1	23	A	C2-N3	5.33	1.38	1.33
22	23S1	1571	A	N3-C4	5.33	1.38	1.34
1	16S1	1394	A	N3-C4	5.32	1.38	1.34
22	23S1	1783	A	C8-N7	5.32	1.35	1.31
22	23S1	1919	A	C8-N7	5.32	1.35	1.31
22	23S1	2077	A	N7-C5	-5.32	1.36	1.39
22	23S1	483	A	N3-C4	5.32	1.38	1.34
22	23S1	2406	A	N3-C4	5.32	1.38	1.34
1	16S1	1513	A	N3-C4	5.32	1.38	1.34
22	23S1	352	A	C5-C4	-5.32	1.35	1.38
22	23S1	572	A	C8-N7	5.32	1.35	1.31
22	23S1	742	A	N3-C4	5.32	1.38	1.34
22	23S1	1010	A	N7-C5	-5.32	1.36	1.39
22	23S1	1342	A	N3-C4	5.32	1.38	1.34
22	23S1	1772	A	N3-C4	5.32	1.38	1.34
22	23S1	2171	A	C2-N3	5.32	1.38	1.33
22	23S1	2660	A	N3-C4	5.32	1.38	1.34
22	23S1	322	A	N3-C4	5.32	1.38	1.34
22	23S1	616	A	N3-C4	5.32	1.38	1.34
22	23S1	742	A	C8-N7	5.32	1.35	1.31
22	23S1	1029	A	N7-C5	-5.32	1.36	1.39
22	23S1	2284	A	N3-C4	5.32	1.38	1.34
22	23S1	792	A	C8-N7	5.32	1.35	1.31
1	16S1	80	A	C2-N3	5.31	1.38	1.33
1	16S1	466	A	N3-C4	5.31	1.38	1.34
1	16S1	914	A	N3-C4	5.31	1.38	1.34
22	23S1	627	A	N3-C4	5.31	1.38	1.34
22	23S1	753	A	N3-C4	5.31	1.38	1.34
22	23S1	1090	A	C2-N3	5.31	1.38	1.33
1	16S1	1000	A	C2-N3	5.31	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1446	A	C5-C4	-5.31	1.35	1.38
1	16S1	161	A	C5-C4	-5.31	1.35	1.38
1	16S1	393	A	N3-C4	5.31	1.38	1.34
1	16S1	1429	A	N3-C4	5.31	1.38	1.34
22	23S1	739	A	C8-N7	5.31	1.35	1.31
22	23S1	1057	A	C5-C4	-5.31	1.35	1.38
22	23S1	2288	A	N3-C4	5.31	1.38	1.34
22	23S1	2670	A	N3-C4	5.31	1.38	1.34
22	23S1	2900	A	C5-C4	-5.31	1.35	1.38
1	16S1	460	A	C2-N3	5.31	1.38	1.33
1	16S1	814	A	C8-N7	5.31	1.35	1.31
1	16S1	831	A	N3-C4	5.31	1.38	1.34
1	16S1	1191	A	N3-C4	5.31	1.38	1.34
22	23S1	829	A	C8-N7	5.31	1.35	1.31
22	23S1	1433	A	N3-C4	5.31	1.38	1.34
1	16S1	1437	A	N3-C4	5.30	1.38	1.34
22	23S1	1237	A	N3-C4	5.30	1.38	1.34
22	23S1	2765	A	N7-C5	-5.30	1.36	1.39
1	16S1	143	A	N3-C4	5.30	1.38	1.34
22	23S1	2097	A	C5-C4	-5.30	1.35	1.38
22	23S1	233	A	N3-C4	5.30	1.38	1.34
22	23S1	1509	A	C5-C4	-5.30	1.35	1.38
22	23S1	1650	A	C8-N7	5.30	1.35	1.31
22	23S1	1722	A	C5-C4	-5.30	1.35	1.38
22	23S1	1739	A	C5-C4	-5.30	1.35	1.38
22	23S1	1848	A	N3-C4	5.30	1.38	1.34
22	23S1	2346	A	N3-C4	5.30	1.38	1.34
22	23S1	2660	A	C5-C4	-5.30	1.35	1.38
55	PTR1	14	A	C2-N3	5.30	1.38	1.33
22	23S1	216	A	N3-C4	5.30	1.38	1.34
22	23S1	1098	A	C2-N3	5.30	1.38	1.33
22	23S1	735	A	C8-N7	5.29	1.35	1.31
1	16S1	199	A	C2-N3	5.29	1.38	1.33
22	23S1	633	A	C8-N7	5.29	1.35	1.31
22	23S1	2015	A	N3-C4	5.29	1.38	1.34
22	23S1	2547	A	N3-C4	5.29	1.38	1.34
1	16S1	253	A	C5-C4	-5.29	1.35	1.38
22	23S1	541	A	N3-C4	5.29	1.38	1.34
22	23S1	996	A	N3-C4	5.29	1.38	1.34
22	23S1	1431	A	C8-N7	5.29	1.35	1.31
22	23S1	2013	A	C8-N7	5.29	1.35	1.31
1	16S1	50	A	C5-C4	-5.29	1.35	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1854	A	N7-C5	-5.29	1.36	1.39
1	16S1	196	A	N3-C4	5.29	1.38	1.34
1	16S1	694	A	N7-C5	-5.29	1.36	1.39
22	23S1	1505	A	C5-C4	-5.29	1.35	1.38
22	23S1	1877	A	C5-C4	-5.29	1.35	1.38
22	23S1	1877	A	N3-C4	5.29	1.38	1.34
22	23S1	2734	A	N3-C4	5.29	1.38	1.34
22	23S1	2835	A	N3-C4	5.28	1.38	1.34
1	16S1	325	A	N3-C4	5.28	1.38	1.34
1	16S1	814	A	N3-C4	5.28	1.38	1.34
1	16S1	1339	A	N3-C4	5.28	1.38	1.34
22	23S1	863	A	N3-C4	5.28	1.38	1.34
22	23S1	933	A	C5-C4	-5.28	1.35	1.38
22	23S1	1572	A	C8-N7	5.28	1.35	1.31
22	23S1	1772	A	C8-N7	5.28	1.35	1.31
55	PTR1	51	A	C5-C4	-5.28	1.35	1.38
1	16S1	243	A	N3-C4	5.28	1.38	1.34
22	23S1	197	A	C8-N7	5.28	1.35	1.31
22	23S1	526	A	N3-C4	5.28	1.38	1.34
22	23S1	1669	A	C5-C4	-5.28	1.35	1.38
22	23S1	1745	A	N3-C4	5.28	1.38	1.34
22	23S1	2497	A	C8-N7	5.28	1.35	1.31
1	16S1	649	A	C5-C4	-5.28	1.35	1.38
22	23S1	1614	A	C8-N7	5.28	1.35	1.31
1	16S1	1280	A	N3-C4	5.28	1.38	1.34
22	23S1	1143	A	C8-N7	5.28	1.35	1.31
22	23S1	1717	A	N3-C4	5.28	1.38	1.34
22	23S1	196	A	C5-C4	-5.27	1.35	1.38
22	23S1	1872	A	C8-N7	5.27	1.35	1.31
1	16S1	1396	A	N3-C4	5.27	1.38	1.34
22	23S1	453	A	C8-N7	5.27	1.35	1.31
22	23S1	1655	A	C8-N7	5.27	1.35	1.31
22	23S1	2706	A	C8-N7	5.27	1.35	1.31
22	23S1	1226	A	N3-C4	5.27	1.38	1.34
22	23S1	1269	A	C8-N7	5.27	1.35	1.31
22	23S1	84	A	N3-C4	5.27	1.38	1.34
1	16S1	461	A	C5-C4	-5.26	1.35	1.38
22	23S1	347	A	N3-C4	5.26	1.38	1.34
22	23S1	1226	A	C8-N7	5.26	1.35	1.31
22	23S1	1265	A	N3-C4	5.26	1.38	1.34
22	23S1	2741	A	N3-C4	5.26	1.38	1.34
22	23S1	984	A	N7-C5	-5.26	1.36	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1284	A	N3-C4	5.26	1.38	1.34
1	16S1	816	A	C8-N7	5.26	1.35	1.31
22	23S1	705	A	N3-C4	5.26	1.38	1.34
22	23S1	727	A	N3-C4	5.26	1.38	1.34
22	23S1	1469	A	N3-C4	5.26	1.38	1.34
1	16S1	116	A	C8-N7	5.26	1.35	1.31
1	16S1	382	A	C5-C4	-5.26	1.35	1.38
1	16S1	907	A	N3-C4	5.26	1.38	1.34
1	16S1	1163	A	C5-C4	-5.26	1.35	1.38
1	16S1	1360	A	N3-C4	5.26	1.38	1.34
22	23S1	181	A	C5-C4	-5.26	1.35	1.38
22	23S1	563	A	C8-N7	5.26	1.35	1.31
22	23S1	1014	A	N3-C4	5.26	1.38	1.34
22	23S1	2268	A	C8-N7	5.26	1.35	1.31
1	16S1	452	A	C5-C4	-5.25	1.35	1.38
1	16S1	608	A	N3-C4	5.25	1.38	1.34
22	23S1	471	A	C8-N7	5.25	1.35	1.31
22	23S1	783	A	C8-N7	5.25	1.35	1.31
22	23S1	1073	A	C2-N3	5.25	1.38	1.33
22	23S1	2392	A	N3-C4	5.25	1.38	1.34
22	23S1	2469	A	N3-C4	5.25	1.38	1.34
1	16S1	327	A	N3-C4	5.25	1.38	1.34
22	23S1	925	A	N3-C4	5.25	1.38	1.34
22	23S1	2020	A	C8-N7	5.25	1.35	1.31
1	16S1	143	A	C5-C4	-5.25	1.35	1.38
1	16S1	860	A	N3-C4	5.25	1.38	1.34
1	16S1	1446	A	N3-C4	5.25	1.38	1.34
22	23S1	1089	A	C2-N3	5.25	1.38	1.33
1	16S1	383	A	N1-C2	5.25	1.39	1.34
22	23S1	2366	A	N3-C4	5.25	1.38	1.34
1	16S1	493	A	N3-C4	5.24	1.38	1.34
1	16S1	937	A	N3-C4	5.24	1.38	1.34
22	23S1	1502	A	C5-C4	-5.24	1.35	1.38
1	16S1	1016	A	C5-C4	-5.24	1.35	1.38
22	23S1	644	A	C8-N7	5.24	1.35	1.31
22	23S1	1590	A	C5-C4	-5.24	1.35	1.38
1	16S1	675	A	N3-C4	5.24	1.38	1.34
22	23S1	56	A	N3-C4	5.24	1.38	1.34
22	23S1	947	A	C8-N7	5.24	1.35	1.31
22	23S1	1665	A	N3-C4	5.24	1.38	1.34
22	23S1	2060	A	N3-C4	5.24	1.38	1.34
22	23S1	2799	A	C2-N3	5.24	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	116	A	N3-C4	5.24	1.38	1.34
22	23S1	644	A	N3-C4	5.24	1.38	1.34
1	16S1	349	A	N3-C4	5.23	1.38	1.34
1	16S1	901	A	N3-C4	5.23	1.38	1.34
22	23S1	196	A	C8-N7	5.23	1.35	1.31
1	16S1	607	A	N3-C4	5.23	1.38	1.34
22	23S1	384	A	N3-C4	5.23	1.38	1.34
22	23S1	1698	A	N3-C4	5.23	1.38	1.34
1	16S1	155	A	C2-N3	5.23	1.38	1.33
22	23S1	877	A	C5-C4	-5.23	1.35	1.38
22	23S1	1359	A	N3-C4	5.23	1.38	1.34
22	23S1	1803	A	N3-C4	5.23	1.38	1.34
22	23S1	2033	A	N3-C4	5.23	1.38	1.34
22	23S1	1420	A	C5-C4	-5.23	1.35	1.38
1	16S1	353	A	N3-C4	5.23	1.38	1.34
1	16S1	461	A	C2-N3	5.23	1.38	1.33
1	16S1	1042	A	C5-C4	-5.23	1.35	1.38
22	23S1	825	A	N3-C4	5.23	1.38	1.34
22	23S1	2015	A	C8-N7	5.23	1.35	1.31
22	23S1	2388	A	C8-N7	5.23	1.35	1.31
22	23S1	2439	A	N3-C4	5.23	1.38	1.34
55	PTR1	14	A	C5-C4	-5.23	1.35	1.38
1	16S1	1213	A	N3-C4	5.23	1.38	1.34
22	23S1	1254	A	N3-C4	5.23	1.38	1.34
1	16S1	1170	A	N7-C5	-5.22	1.36	1.39
22	23S1	715	A	N3-C4	5.22	1.38	1.34
22	23S1	2809	A	N3-C4	5.22	1.38	1.34
1	16S1	66	A	C5-C4	-5.22	1.35	1.38
1	16S1	1102	A	N3-C4	5.22	1.38	1.34
22	23S1	404	A	C5-C4	-5.22	1.35	1.38
22	23S1	1308	A	N3-C4	5.22	1.38	1.34
1	16S1	546	A	C5-C4	-5.22	1.35	1.38
1	16S1	1044	A	C5-C4	-5.22	1.35	1.38
22	23S1	74	A	N3-C4	5.22	1.38	1.34
22	23S1	1151	A	N3-C4	5.22	1.38	1.34
22	23S1	1669	A	C8-N7	5.22	1.35	1.31
22	23S1	2014	A	N3-C4	5.22	1.38	1.34
1	16S1	1333	A	N3-C4	5.22	1.38	1.34
22	23S1	2082	A	C8-N7	5.22	1.35	1.31
22	23S1	582	A	N3-C4	5.22	1.38	1.34
1	16S1	120	A	N3-C4	5.21	1.38	1.34
1	16S1	649	A	N3-C4	5.21	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	497	A	N3-C4	5.21	1.38	1.34
22	23S1	2135	A	C2-N3	5.21	1.38	1.33
22	23S1	2572	A	N3-C4	5.21	1.38	1.34
1	16S1	747	A	N3-C4	5.21	1.38	1.34
22	23S1	2879	A	C8-N7	5.21	1.35	1.31
23	05S1	66	A	C5-C4	-5.21	1.35	1.38
22	23S1	2158	A	C2-N3	5.21	1.38	1.33
22	23S1	2598	A	N3-C4	5.21	1.38	1.34
23	05S1	52	A	N3-C4	5.21	1.38	1.34
1	16S1	263	A	C5-C4	-5.21	1.35	1.38
22	23S1	1580	A	N3-C4	5.21	1.38	1.34
22	23S1	2748	A	N3-C4	5.21	1.38	1.34
1	16S1	1130	A	C5-C4	-5.21	1.35	1.38
22	23S1	504	A	N3-C4	5.21	1.38	1.34
22	23S1	1008	A	N3-C4	5.21	1.38	1.34
1	16S1	716	A	N3-C4	5.21	1.38	1.34
1	16S1	892	A	N3-C4	5.21	1.38	1.34
22	23S1	764	A	N3-C4	5.21	1.38	1.34
22	23S1	1264	A	C8-N7	5.21	1.35	1.31
22	23S1	1470	A	C8-N7	5.21	1.35	1.31
22	23S1	1640	A	N3-C4	5.21	1.38	1.34
1	16S1	397	A	C8-N7	5.20	1.35	1.31
22	23S1	1327	A	N3-C4	5.20	1.38	1.34
22	23S1	1637	A	N3-C4	5.20	1.38	1.34
22	23S1	1786	A	C8-N7	5.20	1.35	1.31
22	23S1	2278	A	C8-N7	5.20	1.35	1.31
1	16S1	640	A	C5-C4	-5.20	1.35	1.38
22	23S1	1735	A	C5-C4	-5.20	1.35	1.38
1	16S1	743	A	N3-C4	5.20	1.38	1.34
1	16S1	1269	A	N3-C4	5.20	1.38	1.34
22	23S1	282	A	C5-C4	-5.20	1.35	1.38
22	23S1	429	A	N3-C4	5.20	1.38	1.34
22	23S1	482	A	N7-C5	-5.20	1.36	1.39
22	23S1	920	A	N3-C4	5.20	1.38	1.34
22	23S1	2822	G	C8-N7	-5.20	1.27	1.30
1	16S1	574	A	C8-N7	5.20	1.35	1.31
1	16S1	784	A	N3-C4	5.20	1.38	1.34
22	23S1	1276	A	N3-C4	5.20	1.38	1.34
1	16S1	704	A	C5-C4	-5.20	1.35	1.38
22	23S1	1503	A	C5-C4	-5.20	1.35	1.38
22	23S1	127	A	N3-C4	5.19	1.38	1.34
22	23S1	1528	A	N7-C5	-5.19	1.36	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	222	A	N3-C4	5.19	1.38	1.34
22	23S1	614	A	C5-C4	-5.19	1.35	1.38
22	23S1	661	A	N3-C4	5.19	1.38	1.34
22	23S1	1392	A	N3-C4	5.19	1.38	1.34
1	16S1	78	A	C5-C4	-5.19	1.35	1.38
22	23S1	262	A	N3-C4	5.19	1.38	1.34
1	16S1	298	A	N3-C4	5.19	1.38	1.34
1	16S1	533	A	C2-N3	5.19	1.38	1.33
22	23S1	941	A	N3-C4	5.19	1.38	1.34
22	23S1	1773	A	C8-N7	5.19	1.35	1.31
1	16S1	865	A	C8-N7	5.18	1.35	1.31
22	23S1	2170	A	C5-C4	-5.18	1.35	1.38
22	23S1	532	A	C8-N7	5.18	1.35	1.31
22	23S1	2247	A	N3-C4	5.18	1.38	1.34
1	16S1	959	A	C5-C4	-5.18	1.35	1.38
22	23S1	6	A	N3-C4	5.18	1.38	1.34
22	23S1	1634	A	N3-C4	5.18	1.38	1.34
1	16S1	621	A	N3-C4	5.18	1.38	1.34
1	16S1	1004	A	N3-C4	5.17	1.38	1.34
22	23S1	2800	A	N3-C4	5.17	1.38	1.34
1	16S1	807	A	N3-C4	5.17	1.38	1.34
1	16S1	1257	A	C5-C4	-5.17	1.35	1.38
22	23S1	191	A	N7-C5	-5.17	1.36	1.39
22	23S1	820	A	N3-C4	5.17	1.38	1.34
22	23S1	2587	A	N3-C4	5.17	1.38	1.34
22	23S1	2682	A	N3-C4	5.17	1.38	1.34
1	16S1	1105	A	N3-C4	5.17	1.38	1.34
22	23S1	190	A	N7-C5	-5.17	1.36	1.39
22	23S1	693	A	C8-N7	5.17	1.35	1.31
22	23S1	572	A	N3-C4	5.17	1.38	1.34
22	23S1	2635	A	N3-C4	5.17	1.38	1.34
22	23S1	207	A	N3-C4	5.17	1.38	1.34
22	23S1	693	A	N3-C4	5.17	1.38	1.34
1	16S1	978	A	N3-C4	5.17	1.38	1.34
1	16S1	1500	A	N3-C4	5.17	1.38	1.34
22	23S1	788	A	N3-C4	5.17	1.38	1.34
22	23S1	1155	A	N3-C4	5.17	1.38	1.34
1	16S1	430	A	C5-C4	-5.16	1.35	1.38
22	23S1	430	A	N3-C4	5.16	1.38	1.34
22	23S1	734	A	N3-C4	5.16	1.38	1.34
22	23S1	1608	A	N3-C4	5.16	1.38	1.34
22	23S1	460	A	N3-C4	5.16	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	77	A	C2-N3	5.16	1.38	1.33
1	16S1	1046	A	C2-N3	5.16	1.38	1.33
22	23S1	1008	A	C8-N7	5.16	1.35	1.31
22	23S1	1347	A	N3-C4	5.16	1.38	1.34
22	23S1	1784	A	C8-N7	5.16	1.35	1.31
22	23S1	1784	A	N3-C4	5.16	1.38	1.34
22	23S1	2003	A	C8-N7	5.16	1.35	1.31
22	23S1	2241	A	N3-C4	5.16	1.38	1.34
1	16S1	1287	A	N3-C4	5.16	1.38	1.34
55	PTR1	26	A	C5-C4	-5.16	1.35	1.38
22	23S1	1532	A	C2-N3	5.16	1.38	1.33
1	16S1	162	A	C5-C4	-5.15	1.35	1.38
22	23S1	730	A	N3-C4	5.15	1.38	1.34
22	23S1	2600	A	C8-N7	5.15	1.35	1.31
22	23S1	621	A	N3-C4	5.15	1.38	1.34
22	23S1	2119	A	C2-N3	5.15	1.38	1.33
22	23S1	2706	A	N3-C4	5.15	1.38	1.34
1	16S1	262	A	N3-C4	5.15	1.38	1.34
22	23S1	1626	A	N3-C4	5.15	1.38	1.34
1	16S1	459	A	C2-N3	5.14	1.38	1.33
1	16S1	1035	A	C2-N3	5.14	1.38	1.33
22	23S1	101	A	C5-C4	-5.14	1.35	1.38
1	16S1	1329	A	N3-C4	5.14	1.38	1.34
22	23S1	1672	A	C8-N7	5.14	1.35	1.31
22	23S1	1912	A	N3-C4	5.14	1.38	1.34
23	05S1	59	A	C5-C4	-5.14	1.35	1.38
22	23S1	804	A	N3-C4	5.14	1.38	1.34
22	23S1	1001	A	C8-N7	5.14	1.35	1.31
22	23S1	2005	A	N3-C4	5.14	1.38	1.34
1	16S1	300	A	C5-C4	-5.14	1.35	1.38
1	16S1	1080	A	N3-C4	5.14	1.38	1.34
22	23S1	727	A	C8-N7	5.14	1.35	1.31
22	23S1	1791	A	N7-C5	-5.14	1.36	1.39
1	16S1	1000	A	C5-C4	-5.14	1.35	1.38
22	23S1	231	A	N3-C4	5.14	1.38	1.34
22	23S1	1899	A	N7-C5	-5.14	1.36	1.39
1	16S1	964	A	N3-C4	5.13	1.38	1.34
1	16S1	1476	A	N3-C4	5.13	1.38	1.34
22	23S1	94	A	C5-C4	-5.13	1.35	1.38
22	23S1	1969	A	N3-C4	5.13	1.38	1.34
22	23S1	2009	A	N3-C4	5.13	1.38	1.34
1	16S1	74	A	N3-C4	5.13	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	522	A	N3-C4	5.13	1.38	1.34
22	23S1	352	A	N3-C4	5.13	1.38	1.34
22	23S1	899	A	C5-C4	-5.13	1.35	1.38
22	23S1	2051	A	N7-C5	-5.13	1.36	1.39
22	23S1	2101	A	C2-N3	5.13	1.38	1.33
23	05S1	119	A	C2-N3	5.13	1.38	1.33
55	PTR1	3	A	C5-C4	-5.13	1.35	1.38
22	23S1	203	A	N7-C5	-5.13	1.36	1.39
1	16S1	1363	A	C5-C4	-5.12	1.35	1.38
22	23S1	1046	A	C2-N3	5.12	1.38	1.33
22	23S1	1794	A	N3-C4	5.12	1.38	1.34
22	23S1	2154	A	C2-N3	5.12	1.38	1.33
22	23S1	2587	A	C8-N7	5.12	1.35	1.31
1	16S1	149	A	C5-C4	-5.12	1.35	1.38
1	16S1	460	A	C5-C4	-5.12	1.35	1.38
1	16S1	694	A	N3-C4	5.12	1.38	1.34
22	23S1	599	A	N3-C4	5.12	1.38	1.34
22	23S1	802	A	C8-N7	5.12	1.35	1.31
55	PTR1	3	A	C2-N3	5.12	1.38	1.33
22	23S1	802	A	N3-C4	5.12	1.38	1.34
22	23S1	1247	A	N3-C4	5.12	1.38	1.34
22	23S1	1367	A	N3-C4	5.12	1.38	1.34
22	23S1	1552	A	N3-C4	5.12	1.38	1.34
22	23S1	2225	A	N3-C4	5.12	1.38	1.34
55	PTR1	76	A	N3-C4	5.12	1.38	1.34
22	23S1	1080	A	C2-N3	5.12	1.38	1.33
22	23S1	2589	A	N3-C4	5.12	1.38	1.34
22	23S1	2602	A	C5-C4	-5.12	1.35	1.38
1	16S1	510	A	N3-C4	5.12	1.38	1.34
1	16S1	1163	A	C2-N3	5.12	1.38	1.33
1	16S1	1480	A	N3-C4	5.12	1.38	1.34
22	23S1	878	A	C5-C4	-5.12	1.35	1.38
23	05S1	34	A	N3-C4	5.12	1.38	1.34
1	16S1	487	A	C5-C4	-5.11	1.35	1.38
1	16S1	983	A	C5-C4	-5.11	1.35	1.38
1	16S1	1016	A	N3-C4	5.11	1.38	1.34
1	16S1	1502	A	N3-C4	5.11	1.38	1.34
22	23S1	149	A	N3-C4	5.11	1.38	1.34
1	16S1	665	A	N3-C4	5.11	1.38	1.34
22	23S1	265	A	N3-C4	5.11	1.38	1.34
22	23S1	1722	A	C2-N3	5.11	1.38	1.33
22	23S1	2019	A	C8-N7	5.11	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2142	A	C5-C4	-5.11	1.35	1.38
22	23S1	1133	A	N3-C4	5.11	1.38	1.34
22	23S1	1960	A	N3-C4	5.11	1.38	1.34
22	23S1	2461	A	N3-C4	5.11	1.38	1.34
1	16S1	131	A	N3-C4	5.11	1.38	1.34
22	23S1	472	A	N3-C4	5.11	1.38	1.34
1	16S1	1145	A	C5-C4	-5.11	1.35	1.38
22	23S1	1928	A	C8-N7	5.11	1.35	1.31
1	16S1	1110	A	N3-C4	5.10	1.38	1.34
22	23S1	2142	A	N1-C2	5.10	1.39	1.34
22	23S1	2577	A	C8-N7	5.10	1.35	1.31
1	16S1	448	A	C5-C4	-5.10	1.35	1.38
22	23S1	1054	A	C2-N3	5.10	1.38	1.33
1	16S1	72	A	C5-C4	-5.10	1.35	1.38
22	23S1	1801	A	N3-C4	5.10	1.38	1.34
1	16S1	1493	A	C2-N3	5.10	1.38	1.33
22	23S1	676	A	N3-C4	5.10	1.38	1.34
22	23S1	279	A	C5-C4	-5.10	1.35	1.38
22	23S1	515	A	N3-C4	5.10	1.38	1.34
22	23S1	1744	A	C5-C4	-5.10	1.35	1.38
22	23S1	2369	A	N3-C4	5.10	1.38	1.34
22	23S1	2516	A	N3-C4	5.10	1.38	1.34
22	23S1	1021	A	C8-N7	5.10	1.35	1.31
22	23S1	2134	A	C2-N3	5.09	1.38	1.33
22	23S1	2781	A	C8-N7	5.09	1.35	1.31
22	23S1	2813	A	N3-C4	5.09	1.38	1.34
1	16S1	1410	A	N3-C4	5.09	1.38	1.34
22	23S1	142	A	N3-C4	5.09	1.38	1.34
22	23S1	1590	A	C2-N3	5.09	1.38	1.33
22	23S1	1969	A	N7-C5	-5.09	1.36	1.39
22	23S1	492	A	N7-C5	-5.09	1.36	1.39
22	23S1	1354	A	C8-N7	5.09	1.35	1.31
1	16S1	696	A	C8-N7	5.09	1.35	1.31
22	23S1	453	A	N3-C4	5.09	1.38	1.34
22	23S1	983	A	N3-C4	5.08	1.38	1.34
1	16S1	336	A	N3-C4	5.08	1.37	1.34
22	23S1	1916	A	C5-C4	-5.08	1.35	1.38
1	16S1	777	A	N3-C4	5.08	1.37	1.34
22	23S1	1274	A	N3-C4	5.08	1.37	1.34
23	05S1	108	A	N3-C4	5.08	1.37	1.34
22	23S1	470	A	C8-N7	5.08	1.35	1.31
22	23S1	782	A	C8-N7	5.08	1.35	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	69	A	C2-N3	5.08	1.38	1.33
22	23S1	354	A	C5-C4	-5.08	1.35	1.38
22	23S1	829	A	N3-C4	5.08	1.37	1.34
22	23S1	466	A	N7-C5	-5.07	1.36	1.39
22	23S1	1020	A	N3-C4	5.07	1.37	1.34
22	23S1	2727	A	N3-C4	5.07	1.37	1.34
1	16S1	1216	A	N3-C4	5.07	1.37	1.34
22	23S1	300	A	N3-C4	5.07	1.37	1.34
22	23S1	705	A	N7-C5	-5.07	1.36	1.39
22	23S1	861	A	N3-C4	5.07	1.37	1.34
22	23S1	1165	A	N3-C4	5.07	1.37	1.34
22	23S1	1427	A	N3-C4	5.07	1.37	1.34
22	23S1	2602	A	C2-N3	5.07	1.38	1.33
1	16S1	1433	A	N3-C4	5.07	1.37	1.34
22	23S1	2882	A	N3-C4	5.07	1.37	1.34
1	16S1	1225	A	C5-C4	-5.06	1.35	1.38
22	23S1	1569	A	N3-C4	5.06	1.37	1.34
22	23S1	2872	A	C5-C4	-5.06	1.35	1.38
1	16S1	640	A	C2-N3	5.06	1.38	1.33
1	16S1	816	A	N3-C4	5.06	1.37	1.34
1	16S1	715	A	N3-C4	5.06	1.37	1.34
22	23S1	1809	A	C8-N7	5.06	1.35	1.31
1	16S1	16	A	N3-C4	5.06	1.37	1.34
22	23S1	547	A	C5-C4	-5.06	1.35	1.38
22	23S1	631	A	N3-C4	5.06	1.37	1.34
22	23S1	1264	A	N3-C4	5.06	1.37	1.34
22	23S1	2679	A	N3-C4	5.06	1.37	1.34
22	23S1	119	A	N3-C4	5.05	1.37	1.34
22	23S1	1532	A	C5-C4	-5.05	1.35	1.38
1	16S1	465	A	C5-C4	-5.05	1.35	1.38
22	23S1	782	A	N3-C4	5.05	1.37	1.34
22	23S1	340	A	N3-C4	5.05	1.37	1.34
22	23S1	911	A	C8-N7	5.05	1.35	1.31
22	23S1	1936	A	C8-N7	5.05	1.35	1.31
1	16S1	1081	A	N3-C4	5.05	1.37	1.34
22	23S1	309	A	N3-C4	5.05	1.37	1.34
22	23S1	2352	A	C8-N7	5.05	1.35	1.31
22	23S1	783	A	C5-C4	-5.05	1.35	1.38
22	23S1	1609	A	N3-C4	5.05	1.37	1.34
1	16S1	190	A	N1-C2	5.04	1.38	1.34
22	23S1	900	A	C5-C4	-5.04	1.35	1.38
22	23S1	1048	A	C5-C4	-5.04	1.35	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16S1	1238	A	N3-C4	5.04	1.37	1.34
1	16S1	1408	A	N3-C4	5.04	1.37	1.34
22	23S1	52	A	N3-C4	5.04	1.37	1.34
22	23S1	1304	A	N3-C4	5.04	1.37	1.34
22	23S1	2268	A	N3-C4	5.04	1.37	1.34
22	23S1	2662	A	C2-N3	5.04	1.38	1.33
22	23S1	53	A	N3-C4	5.04	1.37	1.34
22	23S1	1009	A	N3-C4	5.04	1.37	1.34
22	23S1	1803	A	N7-C5	-5.04	1.36	1.39
22	23S1	1847	A	C2-N3	5.04	1.38	1.33
22	23S1	2435	A	N3-C4	5.04	1.37	1.34
22	23S1	2565	A	N7-C5	-5.04	1.36	1.39
22	23S1	2738	A	N3-C4	5.04	1.37	1.34
1	16S1	1012	A	C2-N3	5.04	1.38	1.33
1	16S1	1019	A	C2-N3	5.04	1.38	1.33
22	23S1	2425	A	N3-C4	5.04	1.37	1.34
22	23S1	750	A	N3-C4	5.03	1.37	1.34
22	23S1	1664	A	C8-N7	5.03	1.35	1.31
22	23S1	2158	A	C5-C4	-5.03	1.35	1.38
22	23S1	2792	A	C2-N3	5.03	1.38	1.33
22	23S1	2184	A	C2-N3	5.03	1.38	1.33
22	23S1	478	A	N3-C4	5.03	1.37	1.34
22	23S1	1088	A	C2-N3	5.03	1.38	1.33
1	16S1	78	A	C2-N3	5.03	1.38	1.33
22	23S1	751	A	C8-N7	5.03	1.35	1.31
22	23S1	1525	A	N3-C4	5.02	1.37	1.34
1	16S1	969	A	N3-C4	5.02	1.37	1.34
1	16S1	1319	A	C5-C4	-5.02	1.35	1.38
22	23S1	219	A	N3-C4	5.02	1.37	1.34
22	23S1	910	A	N3-C4	5.02	1.37	1.34
22	23S1	981	A	N3-C4	5.02	1.37	1.34
22	23S1	1899	A	N3-C4	5.02	1.37	1.34
22	23S1	2297	A	N3-C4	5.02	1.37	1.34
1	16S1	923	A	N7-C5	-5.02	1.36	1.39
22	23S1	371	A	N3-C4	5.02	1.37	1.34
22	23S1	1650	A	N3-C4	5.02	1.37	1.34
22	23S1	2147	A	C2-N3	5.02	1.38	1.33
22	23S1	2274	A	C8-N7	5.02	1.35	1.31
1	16S1	1508	A	C8-N7	5.02	1.35	1.31
22	23S1	1549	A	C5-C4	-5.02	1.35	1.38
22	23S1	788	A	C8-N7	5.02	1.35	1.31
22	23S1	197	A	N7-C5	-5.01	1.36	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	972	A	C8-N7	5.01	1.35	1.31
22	23S1	1938	A	N3-C4	5.01	1.37	1.34
22	23S1	2711	A	N3-C4	5.01	1.37	1.34
1	16S1	300	A	N1-C2	5.01	1.38	1.34
1	16S1	466	A	C5-C4	-5.01	1.35	1.38
22	23S1	2369	A	C8-N7	5.01	1.35	1.31
1	16S1	1428	A	N3-C4	5.01	1.37	1.34
22	23S1	176	A	N3-C4	5.01	1.37	1.34
22	23S1	689	A	C8-N7	5.01	1.35	1.31
22	23S1	979	A	N3-C4	5.01	1.37	1.34
22	23S1	1508	A	C5-C4	-5.01	1.35	1.38
1	16S1	1492	A	C2-N3	5.01	1.38	1.33
22	23S1	1586	A	C5-C4	-5.01	1.35	1.38
22	23S1	2071	A	C8-N7	5.01	1.35	1.31
1	16S1	1431	A	N3-C4	5.00	1.37	1.34
22	23S1	943	A	N3-C4	5.00	1.37	1.34
22	23S1	2451	A	N3-C4	5.00	1.37	1.34
1	16S1	1	A	C2-N3	5.00	1.38	1.33
22	23S1	492	A	C8-N7	5.00	1.35	1.31
22	23S1	959	A	N3-C4	5.00	1.37	1.34
22	23S1	1032	A	N3-C4	5.00	1.37	1.34
22	23S1	2082	A	N3-C4	5.00	1.37	1.34
22	23S1	2662	A	C8-N7	5.00	1.35	1.31
22	23S1	2662	A	N7-C5	-5.00	1.36	1.39
1	16S1	162	A	C2-N3	5.00	1.38	1.33
1	16S1	794	A	C8-N7	5.00	1.35	1.31
22	23S1	1773	A	N7-C5	-5.00	1.36	1.39

All (13379) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2189	U	O5'-P-OP1	-28.80	76.14	110.70
22	23S1	2872	A	N1-C6-N6	-26.88	102.47	118.60
22	23S1	2887	A	C2-N3-C4	26.20	123.70	110.60
22	23S1	504	A	N1-C2-N3	-25.31	116.65	129.30
22	23S1	1434	A	N1-C6-N6	-24.56	103.86	118.60
22	23S1	1937	A	N1-C6-N6	-23.59	104.45	118.60
22	23S1	783	A	C2-N3-C4	23.50	122.35	110.60
22	23S1	2887	A	N1-C2-N3	-23.35	117.63	129.30
1	16S1	151	A	N1-C6-N6	-23.05	104.77	118.60
1	16S1	1225	A	C2-N3-C4	22.90	122.05	110.60
22	23S1	1515	A	N1-C6-N6	-22.84	104.90	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2173	A	C2-N3-C4	22.82	122.01	110.60
1	16S1	151	A	C2-N3-C4	22.72	121.96	110.60
1	16S1	431	A	N1-C6-N6	-22.69	104.99	118.60
22	23S1	1000	A	C2-N3-C4	22.50	121.85	110.60
1	16S1	498	A	N1-C6-N6	-22.42	105.15	118.60
22	23S1	845	A	C2-N3-C4	22.42	121.81	110.60
1	16S1	389	A	C2-N3-C4	22.41	121.81	110.60
22	23S1	84	A	N1-C2-N3	-22.39	118.11	129.30
1	16S1	1004	A	C2-N3-C4	22.36	121.78	110.60
22	23S1	783	A	N1-C6-N6	-22.22	105.27	118.60
22	23S1	2740	A	C2-N3-C4	22.21	121.70	110.60
22	23S1	2451	A	N1-C6-N6	-22.14	105.31	118.60
22	23S1	1028	A	C2-N3-C4	22.06	121.63	110.60
1	16S1	412	A	N1-C6-N6	-21.98	105.41	118.60
22	23S1	1544	A	C2-N3-C4	21.97	121.58	110.60
22	23S1	299	A	C2-N3-C4	21.96	121.58	110.60
22	23S1	983	A	N1-C2-N3	-21.91	118.35	129.30
22	23S1	1021	A	C2-N3-C4	21.87	121.54	110.60
1	16S1	716	A	N1-C6-N6	-21.87	105.48	118.60
22	23S1	160	A	C2-N3-C4	21.84	121.52	110.60
22	23S1	2060	A	N1-C2-N3	-21.82	118.39	129.30
22	23S1	1755	A	N1-C6-N6	-21.76	105.55	118.60
1	16S1	1213	A	N1-C6-N6	-21.73	105.56	118.60
22	23S1	10	A	N1-C6-N6	-21.71	105.57	118.60
1	16S1	554	A	N1-C6-N6	-21.71	105.57	118.60
1	16S1	704	A	N1-C6-N6	-21.71	105.58	118.60
22	23S1	2887	A	N1-C6-N6	-21.70	105.58	118.60
22	23S1	613	A	C2-N3-C4	21.69	121.44	110.60
1	16S1	520	A	N1-C6-N6	-21.65	105.61	118.60
1	16S1	977	A	C2-N3-C4	21.59	121.40	110.60
23	05S1	59	A	C2-N3-C4	21.57	121.39	110.60
22	23S1	1809	A	C2-N3-C4	21.56	121.38	110.60
22	23S1	1669	A	C2-N3-C4	21.50	121.35	110.60
1	16S1	498	A	C2-N3-C4	21.49	121.35	110.60
22	23S1	1919	A	N1-C2-N3	-21.47	118.56	129.30
22	23S1	119	A	N1-C6-N6	-21.47	105.72	118.60
1	16S1	397	A	C2-N3-C4	21.44	121.32	110.60
1	16S1	496	A	N1-C2-N3	-21.44	118.58	129.30
22	23S1	2765	A	C2-N3-C4	21.43	121.31	110.60
22	23S1	1392	A	C2-N3-C4	21.42	121.31	110.60
1	16S1	2	A	C2-N3-C4	21.39	121.29	110.60
1	16S1	716	A	C2-N3-C4	21.38	121.29	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	465	A	C2-N3-C4	21.37	121.29	110.60
22	23S1	1020	A	N1-C2-N3	-21.37	118.61	129.30
22	23S1	1028	A	N1-C2-N3	-21.37	118.61	129.30
22	23S1	1086	A	C2-N3-C4	21.37	121.29	110.60
22	23S1	563	A	C2-N3-C4	21.37	121.28	110.60
22	23S1	2267	A	C2-N3-C4	21.37	121.28	110.60
22	23S1	984	A	C2-N3-C4	21.36	121.28	110.60
22	23S1	643	A	N1-C2-N3	-21.35	118.62	129.30
22	23S1	221	A	N1-C2-N3	-21.35	118.63	129.30
22	23S1	1353	A	C2-N3-C4	21.34	121.27	110.60
22	23S1	514	A	C2-N3-C4	21.33	121.27	110.60
22	23S1	1490	A	C2-N3-C4	21.29	121.25	110.60
22	23S1	1328	A	N1-C6-N6	-21.27	105.84	118.60
22	23S1	320	A	N1-C2-N3	-21.27	118.67	129.30
22	23S1	2566	A	N1-C2-N3	-21.25	118.68	129.30
22	23S1	2758	A	N1-C6-N6	-21.25	105.85	118.60
1	16S1	1500	A	N1-C2-N3	-21.20	118.70	129.30
22	23S1	1927	A	C2-N3-C4	21.19	121.20	110.60
22	23S1	2657	A	N1-C2-N3	-21.19	118.71	129.30
22	23S1	2273	A	C2-N3-C4	21.17	121.19	110.60
22	23S1	196	A	C2-N3-C4	21.16	121.18	110.60
1	16S1	1333	A	C2-N3-C4	21.14	121.17	110.60
22	23S1	2823	A	N1-C2-N3	-21.12	118.74	129.30
22	23S1	981	A	N1-C2-N3	-21.11	118.75	129.30
1	16S1	431	A	N1-C2-N3	-21.11	118.75	129.30
22	23S1	514	A	N1-C2-N3	-21.10	118.75	129.30
22	23S1	892	A	C2-N3-C4	21.10	121.15	110.60
22	23S1	821	A	N1-C6-N6	-21.09	105.95	118.60
22	23S1	196	A	N1-C6-N6	-21.08	105.95	118.60
22	23S1	2740	A	N1-C2-N3	-21.08	118.76	129.30
22	23S1	1214	A	N1-C2-N3	-21.08	118.76	129.30
1	16S1	563	A	C2-N3-C4	21.07	121.14	110.60
1	16S1	1101	A	N1-C6-N6	-21.07	105.96	118.60
22	23S1	2033	A	N1-C6-N6	-21.07	105.96	118.60
22	23S1	1353	A	N1-C6-N6	-21.07	105.96	118.60
22	23S1	1088	A	C2-N3-C4	21.06	121.13	110.60
1	16S1	914	A	N1-C2-N3	-21.06	118.77	129.30
1	16S1	704	A	N1-C2-N3	-21.04	118.78	129.30
22	23S1	675	A	C2-N3-C4	21.04	121.12	110.60
1	16S1	621	A	C2-N3-C4	21.03	121.12	110.60
22	23S1	1214	A	C2-N3-C4	21.03	121.12	110.60
22	23S1	118	A	N1-C2-N3	-21.01	118.79	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	412	A	N1-C2-N3	-21.00	118.80	129.30
1	16S1	16	A	N1-C2-N3	-20.98	118.81	129.30
22	23S1	529	A	N1-C6-N6	-20.97	106.02	118.60
22	23S1	2542	A	N1-C6-N6	-20.94	106.04	118.60
22	23S1	532	A	C2-N3-C4	20.93	121.07	110.60
22	23S1	2564	A	N1-C6-N6	-20.93	106.04	118.60
22	23S1	526	A	N1-C6-N6	-20.92	106.05	118.60
1	16S1	389	A	N1-C6-N6	-20.90	106.06	118.60
22	23S1	1214	A	N1-C6-N6	-20.89	106.07	118.60
22	23S1	2518	A	C2-N3-C4	20.88	121.04	110.60
1	16S1	1004	A	N1-C6-N6	-20.88	106.07	118.60
22	23S1	207	A	N1-C2-N3	-20.87	118.87	129.30
22	23S1	1308	A	N1-C6-N6	-20.85	106.09	118.60
22	23S1	1630	A	N1-C6-N6	-20.85	106.09	118.60
22	23S1	299	A	N1-C2-N3	-20.84	118.88	129.30
22	23S1	1262	A	N1-C6-N6	-20.84	106.10	118.60
22	23S1	1754	A	N1-C2-N3	-20.83	118.89	129.30
1	16S1	1225	A	N1-C6-N6	-20.82	106.11	118.60
1	16S1	622	A	N1-C6-N6	-20.82	106.11	118.60
22	23S1	2311	A	N1-C6-N6	-20.80	106.12	118.60
22	23S1	1952	A	C2-N3-C4	20.80	121.00	110.60
22	23S1	2564	A	C2-N3-C4	20.80	121.00	110.60
22	23S1	1000	A	N1-C2-N3	-20.79	118.90	129.30
22	23S1	1784	A	N1-C2-N3	-20.79	118.91	129.30
22	23S1	2738	A	N1-C2-N3	-20.76	118.92	129.30
1	16S1	356	A	C2-N3-C4	20.76	120.98	110.60
1	16S1	1145	A	N1-C6-N6	-20.76	106.14	118.60
22	23S1	2062	A	C2-N3-C4	20.75	120.98	110.60
1	16S1	728	A	C2-N3-C4	20.74	120.97	110.60
22	23S1	1175	A	C2-N3-C4	20.73	120.97	110.60
22	23S1	1544	A	N1-C6-N6	-20.73	106.16	118.60
22	23S1	800	A	N1-C6-N6	-20.72	106.17	118.60
22	23S1	195	A	N1-C2-N3	-20.71	118.94	129.30
22	23S1	449	A	C2-N3-C4	20.71	120.96	110.60
22	23S1	764	A	N1-C2-N3	-20.71	118.95	129.30
22	23S1	1395	A	N1-C6-N6	-20.70	106.18	118.60
22	23S1	2451	A	C2-N3-C4	20.70	120.95	110.60
22	23S1	73	A	N1-C2-N3	-20.70	118.95	129.30
22	23S1	1668	A	N1-C6-N6	-20.69	106.19	118.60
22	23S1	432	A	C2-N3-C4	20.68	120.94	110.60
22	23S1	973	A	N1-C6-N6	-20.68	106.19	118.60
1	16S1	1363	A	C2-N3-C4	20.67	120.93	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	983	A	C2-N3-C4	20.66	120.93	110.60
22	23S1	1419	A	N1-C2-N3	-20.65	118.97	129.30
22	23S1	1359	A	N1-C6-N6	-20.65	106.21	118.60
22	23S1	1253	A	N1-C6-N6	-20.64	106.22	118.60
1	16S1	1333	A	N1-C6-N6	-20.64	106.22	118.60
22	23S1	1787	A	C2-N3-C4	20.63	120.92	110.60
1	16S1	81	A	N1-C6-N6	-20.62	106.23	118.60
22	23S1	1427	A	N1-C6-N6	-20.62	106.23	118.60
22	23S1	502	A	N1-C6-N6	-20.60	106.24	118.60
22	23S1	2101	A	N1-C6-N6	-20.59	106.25	118.60
1	16S1	1067	A	N1-C2-N3	-20.57	119.01	129.30
1	16S1	978	A	N1-C6-N6	-20.56	106.26	118.60
22	23S1	2288	A	N1-C2-N3	-20.56	119.02	129.30
1	16S1	815	A	N1-C2-N3	-20.56	119.02	129.30
22	23S1	2740	A	N1-C6-N6	-20.56	106.26	118.60
22	23S1	675	A	N1-C2-N3	-20.56	119.02	129.30
22	23S1	1155	A	N1-C6-N6	-20.56	106.27	118.60
22	23S1	216	A	N1-C6-N6	-20.55	106.27	118.60
22	23S1	1285	A	N1-C6-N6	-20.55	106.27	118.60
22	23S1	654	A	C2-N3-C4	20.54	120.87	110.60
1	16S1	509	A	C2-N3-C4	20.54	120.87	110.60
22	23S1	2809	A	C2-N3-C4	20.53	120.87	110.60
22	23S1	1815	A	N1-C6-N6	-20.53	106.28	118.60
1	16S1	179	A	N1-C6-N6	-20.52	106.29	118.60
22	23S1	910	A	C2-N3-C4	20.52	120.86	110.60
22	23S1	959	A	C2-N3-C4	20.52	120.86	110.60
22	23S1	432	A	N1-C2-N3	-20.51	119.05	129.30
22	23S1	909	A	C2-N3-C4	20.51	120.86	110.60
22	23S1	802	A	N1-C2-N3	-20.51	119.05	129.30
1	16S1	282	A	N1-C6-N6	-20.50	106.30	118.60
1	16S1	1446	A	C2-N3-C4	20.50	120.85	110.60
22	23S1	1805	A	C2-N3-C4	20.50	120.85	110.60
1	16S1	573	A	C2-N3-C4	20.50	120.85	110.60
22	23S1	933	A	C2-N3-C4	20.50	120.85	110.60
1	16S1	371	A	C2-N3-C4	20.49	120.84	110.60
1	16S1	151	A	N1-C2-N3	-20.48	119.06	129.30
1	16S1	1346	A	N1-C6-N6	-20.48	106.31	118.60
22	23S1	2766	A	C2-N3-C4	20.48	120.84	110.60
22	23S1	1927	A	N1-C6-N6	-20.47	106.32	118.60
22	23S1	1632	A	C2-N3-C4	20.46	120.83	110.60
22	23S1	739	A	C2-N3-C4	20.46	120.83	110.60
23	05S1	101	A	C2-N3-C4	20.45	120.83	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	814	A	C2-N3-C4	20.45	120.83	110.60
22	23S1	2450	A	N1-C2-N3	-20.45	119.08	129.30
22	23S1	1086	A	N1-C2-N3	-20.44	119.08	129.30
22	23S1	2212	A	C2-N3-C4	20.44	120.82	110.60
22	23S1	127	A	N1-C2-N3	-20.43	119.08	129.30
22	23S1	1652	A	N1-C6-N6	-20.43	106.34	118.60
22	23S1	207	A	C2-N3-C4	20.43	120.82	110.60
22	23S1	749	A	N1-C6-N6	-20.43	106.34	118.60
22	23S1	675	A	N1-C6-N6	-20.42	106.35	118.60
22	23S1	1009	A	C2-N3-C4	20.42	120.81	110.60
22	23S1	1998	A	C2-N3-C4	20.41	120.81	110.60
55	PTR1	76	A	N1-C2-N3	-20.41	119.09	129.30
22	23S1	1392	A	N1-C6-N6	-20.41	106.36	118.60
22	23S1	1515	A	N1-C2-N3	-20.41	119.10	129.30
1	16S1	607	A	N1-C2-N3	-20.40	119.10	129.30
22	23S1	2566	A	N1-C6-N6	-20.40	106.36	118.60
1	16S1	579	A	C2-N3-C4	20.40	120.80	110.60
22	23S1	1655	A	C2-N3-C4	20.40	120.80	110.60
1	16S1	889	A	N1-C6-N6	-20.39	106.37	118.60
22	23S1	1655	A	N1-C2-N3	-20.38	119.11	129.30
22	23S1	2823	A	C2-N3-C4	20.38	120.79	110.60
22	23S1	1853	A	C2-N3-C4	20.37	120.78	110.60
22	23S1	2311	A	C2-N3-C4	20.37	120.78	110.60
22	23S1	219	A	C2-N3-C4	20.36	120.78	110.60
22	23S1	1347	A	N1-C6-N6	-20.36	106.38	118.60
22	23S1	621	A	N1-C6-N6	-20.36	106.38	118.60
22	23S1	1853	A	N1-C6-N6	-20.36	106.39	118.60
22	23S1	71	A	C2-N3-C4	20.36	120.78	110.60
22	23S1	1419	A	N1-C6-N6	-20.35	106.39	118.60
1	16S1	572	A	N1-C6-N6	-20.35	106.39	118.60
22	23S1	1287	A	N1-C2-N3	-20.35	119.13	129.30
22	23S1	2119	A	N1-C6-N6	-20.34	106.39	118.60
22	23S1	1129	A	N1-C2-N3	-20.34	119.13	129.30
22	23S1	1204	A	N1-C6-N6	-20.34	106.39	118.60
1	16S1	448	A	C2-N3-C4	20.34	120.77	110.60
22	23S1	84	A	N1-C6-N6	-20.34	106.40	118.60
22	23S1	204	A	N1-C6-N6	-20.34	106.39	118.60
22	23S1	668	A	N1-C2-N3	-20.34	119.13	129.30
1	16S1	465	A	N1-C6-N6	-20.34	106.40	118.60
22	23S1	2823	A	N1-C6-N6	-20.33	106.40	118.60
22	23S1	1254	A	N1-C2-N3	-20.33	119.14	129.30
1	16S1	687	A	N1-C2-N3	-20.32	119.14	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1759	A	C2-N3-C4	20.32	120.76	110.60
22	23S1	160	A	N1-C6-N6	-20.32	106.41	118.60
1	16S1	766	A	N1-C6-N6	-20.31	106.41	118.60
22	23S1	689	A	C2-N3-C4	20.31	120.76	110.60
22	23S1	1919	A	N1-C6-N6	-20.31	106.41	118.60
22	23S1	1668	A	N1-C2-N3	-20.30	119.15	129.30
1	16S1	171	A	N1-C6-N6	-20.30	106.42	118.60
22	23S1	2031	A	C2-N3-C4	20.30	120.75	110.60
1	16S1	845	A	C2-N3-C4	20.29	120.75	110.60
22	23S1	195	A	N1-C6-N6	-20.29	106.43	118.60
22	23S1	1275	A	N1-C2-N3	-20.29	119.16	129.30
1	16S1	815	A	C2-N3-C4	20.29	120.75	110.60
1	16S1	913	A	N1-C2-N3	-20.29	119.16	129.30
22	23S1	1253	A	N1-C2-N3	-20.29	119.16	129.30
22	23S1	2241	A	C2-N3-C4	20.29	120.75	110.60
23	05S1	73	A	C2-N3-C4	20.28	120.74	110.60
22	23S1	454	A	N1-C6-N6	-20.28	106.43	118.60
22	23S1	753	A	C2-N3-C4	20.28	120.74	110.60
1	16S1	975	A	N1-C2-N3	-20.27	119.17	129.30
22	23S1	2781	A	N1-C2-N3	-20.27	119.17	129.30
1	16S1	3	A	N1-C2-N3	-20.26	119.17	129.30
1	16S1	78	A	N1-C6-N6	-20.26	106.44	118.60
1	16S1	1428	A	N1-C6-N6	-20.26	106.44	118.60
1	16S1	872	A	C2-N3-C4	20.26	120.73	110.60
1	16S1	1499	A	C2-N3-C4	20.26	120.73	110.60
22	23S1	278	A	C2-N3-C4	20.26	120.73	110.60
22	23S1	973	A	N1-C2-N3	-20.26	119.17	129.30
22	23S1	2173	A	N1-C2-N3	-20.26	119.17	129.30
1	16S1	313	A	C2-N3-C4	20.25	120.73	110.60
1	16S1	1299	A	C2-N3-C4	20.25	120.72	110.60
22	23S1	825	A	C2-N3-C4	20.25	120.72	110.60
1	16S1	452	A	C2-N3-C4	20.22	120.71	110.60
22	23S1	2883	A	N1-C2-N3	-20.22	119.19	129.30
1	16S1	19	A	C2-N3-C4	20.21	120.71	110.60
22	23S1	457	A	N1-C2-N3	-20.21	119.19	129.30
22	23S1	761	A	N1-C6-N6	-20.21	106.47	118.60
22	23S1	1789	A	N1-C6-N6	-20.21	106.47	118.60
22	23S1	104	A	N1-C6-N6	-20.21	106.48	118.60
22	23S1	1302	A	N1-C2-N3	-20.20	119.20	129.30
22	23S1	2173	A	N1-C6-N6	-20.20	106.48	118.60
1	16S1	994	A	C2-N3-C4	20.20	120.70	110.60
22	23S1	2614	A	C2-N3-C4	20.20	120.70	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1333	A	N1-C2-N3	-20.19	119.21	129.30
22	23S1	802	A	C2-N3-C4	20.19	120.69	110.60
1	16S1	130	A	N1-C2-N3	-20.19	119.21	129.30
22	23S1	899	A	C2-N3-C4	20.18	120.69	110.60
22	23S1	794	A	C2-N3-C4	20.18	120.69	110.60
22	23S1	792	A	N1-C2-N3	-20.18	119.21	129.30
22	23S1	1937	A	C2-N3-C4	20.18	120.69	110.60
1	16S1	1360	A	N1-C6-N6	-20.17	106.50	118.60
1	16S1	1046	A	C2-N3-C4	20.17	120.69	110.60
23	05S1	99	A	N1-C6-N6	-20.17	106.50	118.60
1	16S1	728	A	N1-C6-N6	-20.17	106.50	118.60
1	16S1	938	A	C2-N3-C4	20.17	120.68	110.60
22	23S1	1156	A	N1-C2-N3	-20.17	119.22	129.30
22	23S1	2872	A	N1-C2-N3	-20.17	119.22	129.30
22	23S1	2013	A	C2-N3-C4	20.16	120.68	110.60
1	16S1	468	A	N1-C6-N6	-20.16	106.50	118.60
1	16S1	1360	A	C2-N3-C4	20.16	120.68	110.60
1	16S1	602	A	C2-N3-C4	20.15	120.68	110.60
22	23S1	1927	A	N1-C2-N3	-20.15	119.22	129.30
22	23S1	74	A	C2-N3-C4	20.15	120.68	110.60
22	23S1	2453	A	C2-N3-C4	20.15	120.67	110.60
1	16S1	649	A	N1-C6-N6	-20.14	106.51	118.60
22	23S1	161	A	N1-C6-N6	-20.14	106.52	118.60
22	23S1	2114	A	C2-N3-C4	20.14	120.67	110.60
22	23S1	1597	A	N1-C6-N6	-20.13	106.52	118.60
1	16S1	665	A	N1-C6-N6	-20.13	106.52	118.60
1	16S1	414	A	C2-N3-C4	20.12	120.66	110.60
22	23S1	2753	A	N1-C6-N6	-20.12	106.53	118.60
1	16S1	313	A	N1-C6-N6	-20.11	106.53	118.60
1	16S1	1219	A	C2-N3-C4	20.11	120.66	110.60
22	23S1	165	A	N1-C6-N6	-20.11	106.53	118.60
22	23S1	1749	A	N1-C6-N6	-20.11	106.53	118.60
22	23S1	528	A	C2-N3-C4	20.11	120.65	110.60
22	23S1	2005	A	N1-C6-N6	-20.11	106.53	118.60
1	16S1	1179	A	N1-C2-N3	-20.11	119.25	129.30
22	23S1	2757	A	N1-C2-N3	-20.11	119.25	129.30
1	16S1	496	A	C2-N3-C4	20.11	120.65	110.60
22	23S1	241	A	N1-C6-N6	-20.10	106.54	118.60
22	23S1	1938	A	N1-C2-N3	-20.10	119.25	129.30
22	23S1	621	A	N1-C2-N3	-20.10	119.25	129.30
22	23S1	515	A	N1-C6-N6	-20.10	106.54	118.60
22	23S1	2358	A	N1-C6-N6	-20.10	106.54	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1238	A	C2-N3-C4	20.09	120.64	110.60
22	23S1	1392	A	N1-C2-N3	-20.09	119.26	129.30
1	16S1	149	A	N1-C6-N6	-20.08	106.55	118.60
22	23S1	1213	A	C2-N3-C4	20.08	120.64	110.60
22	23S1	1794	A	C2-N3-C4	20.08	120.64	110.60
22	23S1	2117	A	N1-C2-N3	-20.08	119.26	129.30
22	23S1	1000	A	N1-C6-N6	-20.08	106.55	118.60
1	16S1	243	A	N1-C6-N6	-20.08	106.55	118.60
22	23S1	878	A	N1-C6-N6	-20.08	106.55	118.60
22	23S1	1700	A	C2-N3-C4	20.08	120.64	110.60
22	23S1	526	A	N1-C2-N3	-20.08	119.26	129.30
22	23S1	2434	A	N1-C6-N6	-20.08	106.55	118.60
1	16S1	1499	A	N1-C6-N6	-20.07	106.56	118.60
22	23S1	1786	A	C2-N3-C4	20.07	120.64	110.60
23	05S1	99	A	C2-N3-C4	20.07	120.64	110.60
22	23S1	13	A	N1-C6-N6	-20.07	106.56	118.60
22	23S1	749	A	N1-C2-N3	-20.07	119.27	129.30
22	23S1	1165	A	N1-C2-N3	-20.07	119.27	129.30
22	23S1	38	A	N1-C6-N6	-20.07	106.56	118.60
22	23S1	2198	A	N1-C2-N3	-20.06	119.27	129.30
22	23S1	973	A	C2-N3-C4	20.06	120.63	110.60
22	23S1	2407	A	C2-N3-C4	20.06	120.63	110.60
1	16S1	1201	A	C2-N3-C4	20.05	120.62	110.60
1	16S1	1431	A	C2-N3-C4	20.05	120.62	110.60
22	23S1	1755	A	C2-N3-C4	20.05	120.63	110.60
22	23S1	294	A	N1-C2-N3	-20.05	119.28	129.30
22	23S1	980	A	C2-N3-C4	20.05	120.62	110.60
22	23S1	265	A	N1-C2-N3	-20.05	119.28	129.30
1	16S1	152	A	N1-C6-N6	-20.04	106.57	118.60
1	16S1	766	A	N1-C2-N3	-20.04	119.28	129.30
22	23S1	1630	A	C2-N3-C4	20.04	120.62	110.60
22	23S1	14	A	N1-C6-N6	-20.04	106.58	118.60
22	23S1	613	A	N1-C6-N6	-20.04	106.58	118.60
1	16S1	478	A	C2-N3-C4	20.04	120.62	110.60
22	23S1	503	A	C2-N3-C4	20.03	120.62	110.60
22	23S1	1522	A	N1-C6-N6	-20.03	106.58	118.60
22	23S1	507	A	N1-C6-N6	-20.03	106.58	118.60
22	23S1	1502	A	N1-C6-N6	-20.03	106.58	118.60
22	23S1	2070	A	N1-C6-N6	-20.03	106.58	118.60
22	23S1	2679	A	C2-N3-C4	20.03	120.61	110.60
22	23S1	190	A	C2-N3-C4	20.02	120.61	110.60
1	16S1	665	A	N1-C2-N3	-20.02	119.29	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	44	A	N1-C6-N6	-20.01	106.59	118.60
1	16S1	583	A	N1-C6-N6	-20.01	106.59	118.60
22	23S1	631	A	C2-N3-C4	20.01	120.61	110.60
1	16S1	533	A	C2-N3-C4	20.01	120.60	110.60
1	16S1	768	A	N1-C2-N3	-20.01	119.30	129.30
22	23S1	676	A	N1-C2-N3	-20.01	119.30	129.30
1	16S1	172	A	N1-C6-N6	-20.01	106.60	118.60
22	23S1	637	A	N1-C2-N3	-20.01	119.30	129.30
55	PTR1	51	A	N1-C6-N6	-20.00	106.60	118.60
22	23S1	670	A	C2-N3-C4	20.00	120.60	110.60
22	23S1	1754	A	N1-C6-N6	-20.00	106.60	118.60
22	23S1	1744	A	C2-N3-C4	20.00	120.60	110.60
22	23S1	2761	A	C2-N3-C4	19.99	120.60	110.60
22	23S1	2461	A	C2-N3-C4	19.99	120.59	110.60
22	23S1	346	A	C2-N3-C4	19.99	120.59	110.60
1	16S1	282	A	C2-N3-C4	19.98	120.59	110.60
22	23S1	1286	A	N1-C6-N6	-19.98	106.61	118.60
22	23S1	74	A	N1-C6-N6	-19.98	106.61	118.60
22	23S1	227	A	N1-C2-N3	-19.98	119.31	129.30
22	23S1	1698	A	N1-C6-N6	-19.98	106.61	118.60
22	23S1	2267	A	N1-C2-N3	-19.98	119.31	129.30
22	23S1	502	A	N1-C2-N3	-19.97	119.32	129.30
22	23S1	2589	A	N1-C2-N3	-19.97	119.32	129.30
23	05S1	34	A	N1-C6-N6	-19.97	106.62	118.60
22	23S1	1809	A	N1-C2-N3	-19.97	119.32	129.30
1	16S1	1428	A	C2-N3-C4	19.96	120.58	110.60
1	16S1	1101	A	N1-C2-N3	-19.96	119.32	129.30
22	23S1	983	A	C2-N3-C4	19.96	120.58	110.60
22	23S1	602	A	C2-N3-C4	19.96	120.58	110.60
22	23S1	1525	A	N1-C6-N6	-19.96	106.62	118.60
22	23S1	345	A	N1-C6-N6	-19.95	106.63	118.60
22	23S1	1365	A	C2-N3-C4	19.95	120.57	110.60
22	23S1	2327	A	C2-N3-C4	19.95	120.58	110.60
55	PTR1	21	A	N1-C2-N3	-19.95	119.33	129.30
22	23S1	1805	A	N1-C6-N6	-19.94	106.64	118.60
22	23S1	1919	A	C2-N3-C4	19.94	120.57	110.60
22	23S1	2336	A	N1-C2-N3	-19.94	119.33	129.30
1	16S1	1346	A	N1-C2-N3	-19.94	119.33	129.30
22	23S1	1021	A	N1-C6-N6	-19.94	106.64	118.60
1	16S1	1285	A	N1-C2-N3	-19.94	119.33	129.30
22	23S1	10	A	N1-C2-N3	-19.94	119.33	129.30
22	23S1	804	A	N1-C2-N3	-19.93	119.33	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2101	A	C2-N3-C4	19.93	120.57	110.60
22	23S1	14	A	N1-C2-N3	-19.93	119.33	129.30
22	23S1	756	A	C2-N3-C4	19.93	120.56	110.60
1	16S1	382	A	C2-N3-C4	19.93	120.56	110.60
1	16S1	802	A	N1-C2-N3	-19.93	119.33	129.30
22	23S1	750	A	C2-N3-C4	19.93	120.56	110.60
22	23S1	1668	A	C2-N3-C4	19.93	120.56	110.60
22	23S1	2287	A	C2-N3-C4	19.93	120.56	110.60
22	23S1	2758	A	C2-N3-C4	19.93	120.56	110.60
22	23S1	739	A	N1-C2-N3	-19.93	119.34	129.30
1	16S1	814	A	N1-C2-N3	-19.92	119.34	129.30
22	23S1	1522	A	N1-C2-N3	-19.92	119.34	129.30
23	05S1	29	A	N1-C6-N6	-19.92	106.65	118.60
1	16S1	583	A	N1-C2-N3	-19.91	119.34	129.30
22	23S1	603	A	N1-C2-N3	-19.91	119.34	129.30
22	23S1	507	A	N1-C2-N3	-19.91	119.34	129.30
1	16S1	59	A	C2-N3-C4	19.91	120.56	110.60
22	23S1	751	A	N1-C2-N3	-19.91	119.34	129.30
22	23S1	984	A	N1-C6-N6	-19.91	106.66	118.60
22	23S1	1284	A	C2-N3-C4	19.91	120.55	110.60
22	23S1	1359	A	N1-C2-N3	-19.91	119.35	129.30
22	23S1	892	A	N1-C6-N6	-19.90	106.66	118.60
1	16S1	1250	A	C2-N3-C4	19.90	120.55	110.60
22	23S1	563	A	N1-C6-N6	-19.89	106.67	118.60
22	23S1	2497	A	C2-N3-C4	19.89	120.54	110.60
1	16S1	1238	A	N1-C6-N6	-19.89	106.67	118.60
1	16S1	414	A	N1-C6-N6	-19.88	106.67	118.60
22	23S1	2572	A	N1-C2-N3	-19.88	119.36	129.30
1	16S1	781	A	N1-C6-N6	-19.88	106.67	118.60
1	16S1	909	A	N1-C6-N6	-19.88	106.67	118.60
22	23S1	789	A	N1-C2-N3	-19.88	119.36	129.30
22	23S1	1353	A	N1-C2-N3	-19.88	119.36	129.30
1	16S1	640	A	N1-C6-N6	-19.88	106.67	118.60
22	23S1	216	A	C2-N3-C4	19.88	120.54	110.60
22	23S1	943	A	C2-N3-C4	19.88	120.54	110.60
22	23S1	1321	A	C2-N3-C4	19.88	120.54	110.60
22	23S1	1544	A	N1-C2-N3	-19.88	119.36	129.30
1	16S1	1216	A	N1-C6-N6	-19.87	106.68	118.60
55	PTR1	59	A	N1-C6-N6	-19.87	106.68	118.60
1	16S1	262	A	C2-N3-C4	19.87	120.53	110.60
1	16S1	914	A	N1-C6-N6	-19.87	106.68	118.60
22	23S1	975	A	N1-C2-N3	-19.87	119.37	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1998	A	N1-C6-N6	-19.87	106.68	118.60
22	23S1	2388	A	N1-C2-N3	-19.87	119.37	129.30
22	23S1	119	A	N1-C2-N3	-19.87	119.37	129.30
22	23S1	905	A	N1-C6-N6	-19.86	106.68	118.60
1	16S1	781	A	N1-C2-N3	-19.86	119.37	129.30
22	23S1	160	A	N1-C2-N3	-19.86	119.37	129.30
22	23S1	2114	A	N1-C6-N6	-19.86	106.69	118.60
1	16S1	78	A	C2-N3-C4	19.86	120.53	110.60
22	23S1	345	A	C2-N3-C4	19.86	120.53	110.60
22	23S1	346	A	N1-C6-N6	-19.86	106.69	118.60
22	23S1	863	A	C2-N3-C4	19.86	120.53	110.60
1	16S1	195	A	N1-C6-N6	-19.85	106.69	118.60
1	16S1	718	A	C2-N3-C4	19.85	120.53	110.60
22	23S1	752	A	N1-C6-N6	-19.85	106.69	118.60
22	23S1	2054	A	C2-N3-C4	19.85	120.53	110.60
22	23S1	2281	A	C2-N3-C4	19.85	120.53	110.60
22	23S1	1246	A	C2-N3-C4	19.85	120.52	110.60
22	23S1	2590	A	N1-C2-N3	-19.85	119.38	129.30
22	23S1	299	A	N1-C6-N6	-19.84	106.69	118.60
22	23S1	354	A	N1-C6-N6	-19.84	106.69	118.60
1	16S1	648	A	C2-N3-C4	19.84	120.52	110.60
22	23S1	1142	A	C2-N3-C4	19.84	120.52	110.60
1	16S1	171	A	C2-N3-C4	19.84	120.52	110.60
22	23S1	677	A	C2-N3-C4	19.84	120.52	110.60
22	23S1	2764	A	N1-C6-N6	-19.84	106.70	118.60
22	23S1	637	A	C2-N3-C4	19.83	120.52	110.60
22	23S1	2450	A	N1-C6-N6	-19.83	106.70	118.60
55	PTR1	59	A	C2-N3-C4	19.83	120.51	110.60
1	16S1	315	A	N1-C2-N3	-19.83	119.39	129.30
22	23S1	219	A	N1-C2-N3	-19.83	119.39	129.30
22	23S1	330	A	C2-N3-C4	19.83	120.51	110.60
22	23S1	1786	A	N1-C2-N3	-19.83	119.39	129.30
22	23S1	1354	A	C2-N3-C4	19.83	120.51	110.60
22	23S1	2274	A	N1-C2-N3	-19.83	119.39	129.30
1	16S1	729	A	N1-C2-N3	-19.82	119.39	129.30
22	23S1	2037	A	C2-N3-C4	19.82	120.51	110.60
22	23S1	2726	A	N1-C6-N6	-19.82	106.71	118.60
1	16S1	1500	A	C2-N3-C4	19.81	120.51	110.60
1	16S1	80	A	C2-N3-C4	19.81	120.51	110.60
22	23S1	443	A	N1-C6-N6	-19.81	106.71	118.60
22	23S1	1354	A	N1-C2-N3	-19.81	119.39	129.30
22	23S1	1477	A	N1-C2-N3	-19.81	119.40	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	05S1	29	A	C2-N3-C4	19.80	120.50	110.60
1	16S1	909	A	C2-N3-C4	19.80	120.50	110.60
22	23S1	28	A	N1-C2-N3	-19.80	119.40	129.30
1	16S1	509	A	N1-C6-N6	-19.80	106.72	118.60
1	16S1	900	A	N1-C6-N6	-19.80	106.72	118.60
22	23S1	972	A	C2-N3-C4	19.80	120.50	110.60
22	23S1	1569	A	N1-C6-N6	-19.80	106.72	118.60
22	23S1	1127	A	N1-C2-N3	-19.80	119.40	129.30
22	23S1	582	A	C2-N3-C4	19.80	120.50	110.60
22	23S1	1395	A	N1-C2-N3	-19.80	119.40	129.30
22	23S1	2513	A	C2-N3-C4	19.80	120.50	110.60
22	23S1	1637	A	C2-N3-C4	19.80	120.50	110.60
22	23S1	1928	A	N1-C6-N6	-19.80	106.72	118.60
1	16S1	1225	A	N1-C2-N3	-19.79	119.40	129.30
22	23S1	1570	A	N1-C2-N3	-19.79	119.40	129.30
1	16S1	787	A	N1-C2-N3	-19.79	119.40	129.30
1	16S1	1500	A	N1-C6-N6	-19.79	106.72	118.60
22	23S1	1570	A	N1-C6-N6	-19.79	106.72	118.60
22	23S1	1853	A	N1-C2-N3	-19.79	119.40	129.30
22	23S1	429	A	C2-N3-C4	19.79	120.50	110.60
1	16S1	60	A	N1-C6-N6	-19.79	106.73	118.60
1	16S1	918	A	C2-N3-C4	19.79	120.50	110.60
1	16S1	1004	A	N1-C2-N3	-19.79	119.41	129.30
22	23S1	1889	A	N1-C2-N3	-19.79	119.41	129.30
22	23S1	2062	A	N1-C2-N3	-19.79	119.41	129.30
22	23S1	2741	A	N1-C2-N3	-19.78	119.41	129.30
22	23S1	783	A	N1-C2-N3	-19.78	119.41	129.30
1	16S1	1145	A	N1-C2-N3	-19.78	119.41	129.30
22	23S1	1981	A	N1-C6-N6	-19.78	106.73	118.60
1	16S1	448	A	N1-C2-N3	-19.78	119.41	129.30
1	16S1	915	A	N1-C6-N6	-19.78	106.73	118.60
22	23S1	1378	A	N1-C6-N6	-19.78	106.73	118.60
1	16S1	130	A	C2-N3-C4	19.78	120.49	110.60
22	23S1	804	A	N1-C6-N6	-19.78	106.73	118.60
22	23S1	111	A	N1-C6-N6	-19.77	106.74	118.60
22	23S1	2005	A	N1-C2-N3	-19.77	119.41	129.30
22	23S1	352	A	N1-C6-N6	-19.77	106.74	118.60
22	23S1	941	A	C2-N3-C4	19.77	120.48	110.60
22	23S1	631	A	N1-C2-N3	-19.77	119.42	129.30
22	23S1	204	A	N1-C2-N3	-19.77	119.42	129.30
22	23S1	449	A	N1-C6-N6	-19.76	106.74	118.60
22	23S1	1165	A	C2-N3-C4	19.76	120.48	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	602	A	N1-C2-N3	-19.76	119.42	129.30
22	23S1	402	A	N1-C2-N3	-19.76	119.42	129.30
22	23S1	983	A	N1-C6-N6	-19.76	106.75	118.60
22	23S1	927	A	N1-C6-N6	-19.76	106.75	118.60
1	16S1	53	A	C2-N3-C4	19.75	120.48	110.60
22	23S1	1640	A	N1-C6-N6	-19.75	106.75	118.60
1	16S1	715	A	N1-C2-N3	-19.75	119.42	129.30
22	23S1	1749	A	C2-N3-C4	19.75	120.47	110.60
22	23S1	1889	A	C2-N3-C4	19.75	120.47	110.60
22	23S1	2095	A	N1-C6-N6	-19.75	106.75	118.60
1	16S1	59	A	N1-C6-N6	-19.75	106.75	118.60
1	16S1	621	A	N1-C2-N3	-19.75	119.43	129.30
22	23S1	515	A	N1-C2-N3	-19.75	119.43	129.30
22	23S1	2013	A	N1-C6-N6	-19.75	106.75	118.60
22	23S1	2031	A	N1-C6-N6	-19.74	106.75	118.60
22	23S1	103	A	N1-C6-N6	-19.74	106.75	118.60
22	23S1	655	A	N1-C2-N3	-19.74	119.43	129.30
22	23S1	1090	A	N1-C2-N3	-19.74	119.43	129.30
22	23S1	2726	A	N1-C2-N3	-19.74	119.43	129.30
1	16S1	195	A	N1-C2-N3	-19.74	119.43	129.30
22	23S1	2080	A	C2-N3-C4	19.74	120.47	110.60
22	23S1	2426	A	N1-C2-N3	-19.74	119.43	129.30
22	23S1	1901	A	C2-N3-C4	19.74	120.47	110.60
1	16S1	1191	A	C2-N3-C4	19.73	120.47	110.60
22	23S1	945	A	N1-C6-N6	-19.73	106.76	118.60
22	23S1	980	A	N1-C2-N3	-19.73	119.43	129.30
22	23S1	1515	A	C2-N3-C4	19.73	120.47	110.60
22	23S1	1932	A	N1-C6-N6	-19.73	106.76	118.60
22	23S1	2757	A	C2-N3-C4	19.73	120.47	110.60
22	23S1	430	A	C2-N3-C4	19.73	120.46	110.60
22	23S1	1677	A	N1-C2-N3	-19.73	119.44	129.30
22	23S1	101	A	C2-N3-C4	19.72	120.46	110.60
22	23S1	800	A	N1-C2-N3	-19.72	119.44	129.30
22	23S1	223	A	N1-C2-N3	-19.72	119.44	129.30
22	23S1	1952	A	N1-C2-N3	-19.72	119.44	129.30
22	23S1	2860	A	N1-C2-N3	-19.72	119.44	129.30
22	23S1	1040	A	C2-N3-C4	19.72	120.46	110.60
1	16S1	408	A	C2-N3-C4	19.72	120.46	110.60
1	16S1	964	A	N1-C2-N3	-19.72	119.44	129.30
1	16S1	1251	A	C2-N3-C4	19.71	120.46	110.60
22	23S1	910	A	N1-C6-N6	-19.71	106.77	118.60
22	23S1	1545	A	N1-C6-N6	-19.71	106.77	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	964	A	C2-N3-C4	19.71	120.45	110.60
22	23S1	2333	A	N1-C2-N3	-19.71	119.44	129.30
1	16S1	306	A	C2-N3-C4	19.71	120.45	110.60
1	16S1	777	A	C2-N3-C4	19.71	120.45	110.60
1	16S1	1251	A	N1-C6-N6	-19.71	106.77	118.60
22	23S1	131	A	C2-N3-C4	19.71	120.45	110.60
22	23S1	918	A	N1-C2-N3	-19.71	119.45	129.30
22	23S1	761	A	N1-C2-N3	-19.70	119.45	129.30
22	23S1	990	A	C2-N3-C4	19.70	120.45	110.60
22	23S1	1385	A	N1-C6-N6	-19.70	106.78	118.60
22	23S1	497	A	N1-C6-N6	-19.70	106.78	118.60
1	16S1	1410	A	C2-N3-C4	19.70	120.45	110.60
22	23S1	1700	A	N1-C2-N3	-19.70	119.45	129.30
22	23S1	529	A	C2-N3-C4	19.70	120.45	110.60
22	23S1	1785	A	N1-C2-N3	-19.70	119.45	129.30
1	16S1	1019	A	C2-N3-C4	19.70	120.45	110.60
1	16S1	1329	A	N1-C6-N6	-19.70	106.78	118.60
1	16S1	1410	A	N1-C6-N6	-19.70	106.78	118.60
22	23S1	191	A	C2-N3-C4	19.70	120.45	110.60
22	23S1	1237	A	N1-C2-N3	-19.69	119.45	129.30
1	16S1	460	A	C2-N3-C4	19.69	120.45	110.60
1	16S1	845	A	N1-C6-N6	-19.69	106.78	118.60
22	23S1	892	A	N1-C2-N3	-19.69	119.45	129.30
22	23S1	1307	A	N1-C2-N3	-19.69	119.45	129.30
22	23S1	1632	A	N1-C6-N6	-19.69	106.79	118.60
22	23S1	1635	A	N1-C2-N3	-19.69	119.46	129.30
1	16S1	681	A	C2-N3-C4	19.68	120.44	110.60
22	23S1	1189	A	C2-N3-C4	19.68	120.44	110.60
22	23S1	2015	A	N1-C2-N3	-19.68	119.46	129.30
1	16S1	949	A	C2-N3-C4	19.68	120.44	110.60
22	23S1	2564	A	N1-C2-N3	-19.68	119.46	129.30
22	23S1	2572	A	N1-C6-N6	-19.68	106.79	118.60
55	PTR1	59	A	N1-C2-N3	-19.68	119.46	129.30
1	16S1	459	A	C2-N3-C4	19.68	120.44	110.60
1	16S1	958	A	N1-C6-N6	-19.68	106.79	118.60
22	23S1	532	A	N1-C6-N6	-19.68	106.79	118.60
22	23S1	2211	A	N1-C2-N3	-19.68	119.46	129.30
22	23S1	2882	A	N1-C6-N6	-19.68	106.79	118.60
1	16S1	648	A	N1-C2-N3	-19.67	119.46	129.30
1	16S1	860	A	N1-C6-N6	-19.67	106.80	118.60
22	23S1	789	A	C2-N3-C4	19.67	120.44	110.60
22	23S1	988	A	N1-C6-N6	-19.67	106.80	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1251	A	N1-C2-N3	-19.67	119.47	129.30
22	23S1	1676	A	N1-C2-N3	-19.67	119.47	129.30
22	23S1	1890	A	N1-C6-N6	-19.67	106.80	118.60
22	23S1	788	A	N1-C2-N3	-19.66	119.47	129.30
22	23S1	1522	A	C2-N3-C4	19.66	120.43	110.60
1	16S1	539	A	C2-N3-C4	19.66	120.43	110.60
22	23S1	1608	A	C2-N3-C4	19.66	120.43	110.60
22	23S1	1794	A	N1-C2-N3	-19.66	119.47	129.30
22	23S1	2212	A	N1-C6-N6	-19.66	106.81	118.60
22	23S1	990	A	N1-C6-N6	-19.66	106.81	118.60
1	16S1	246	A	N1-C2-N3	-19.66	119.47	129.30
22	23S1	501	A	N1-C6-N6	-19.65	106.81	118.60
22	23S1	502	A	C2-N3-C4	19.65	120.42	110.60
22	23S1	793	A	N1-C6-N6	-19.65	106.81	118.60
1	16S1	1280	A	N1-C2-N3	-19.65	119.48	129.30
22	23S1	222	A	C2-N3-C4	19.65	120.42	110.60
1	16S1	320	A	C2-N3-C4	19.64	120.42	110.60
1	16S1	101	A	C2-N3-C4	19.64	120.42	110.60
22	23S1	1786	A	N1-C6-N6	-19.64	106.81	118.60
1	16S1	777	A	N1-C2-N3	-19.64	119.48	129.30
1	16S1	1044	A	C2-N3-C4	19.64	120.42	110.60
22	23S1	706	A	N1-C2-N3	-19.64	119.48	129.30
22	23S1	878	A	C2-N3-C4	19.64	120.42	110.60
1	16S1	560	A	C2-N3-C4	19.64	120.42	110.60
1	16S1	716	A	N1-C2-N3	-19.64	119.48	129.30
1	16S1	781	A	C2-N3-C4	19.64	120.42	110.60
22	23S1	1593	A	N1-C2-N3	-19.64	119.48	129.30
22	23S1	1593	A	C2-N3-C4	19.63	120.42	110.60
1	16S1	1176	A	C2-N3-C4	19.63	120.42	110.60
22	23S1	2189	U	O5'-P-OP2	-19.63	87.14	110.70
1	16S1	918	A	N1-C6-N6	-19.63	106.82	118.60
22	23S1	309	A	C2-N3-C4	19.63	120.42	110.60
22	23S1	676	A	N1-C6-N6	-19.63	106.82	118.60
22	23S1	792	A	C2-N3-C4	19.63	120.42	110.60
22	23S1	2376	A	N1-C2-N3	-19.63	119.48	129.30
22	23S1	2826	A	N1-C2-N3	-19.63	119.48	129.30
1	16S1	1012	A	C2-N3-C4	19.63	120.41	110.60
1	16S1	622	A	N1-C2-N3	-19.62	119.49	129.30
22	23S1	1262	A	C2-N3-C4	19.62	120.41	110.60
22	23S1	1490	A	N1-C2-N3	-19.62	119.49	129.30
22	23S1	1496	A	C2-N3-C4	19.62	120.41	110.60
22	23S1	2052	A	C2-N3-C4	19.62	120.41	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	111	A	C2-N3-C4	19.62	120.41	110.60
22	23S1	1427	A	N1-C2-N3	-19.62	119.49	129.30
1	16S1	282	A	N1-C2-N3	-19.62	119.49	129.30
22	23S1	1393	A	N1-C2-N3	-19.61	119.49	129.30
22	23S1	1785	A	N1-C6-N6	-19.61	106.83	118.60
1	16S1	55	A	C2-N3-C4	19.61	120.41	110.60
22	23S1	1772	A	N1-C2-N3	-19.61	119.50	129.30
22	23S1	1155	A	N1-C2-N3	-19.61	119.50	129.30
22	23S1	199	A	N1-C6-N6	-19.60	106.84	118.60
22	23S1	1365	A	N1-C6-N6	-19.60	106.84	118.60
1	16S1	640	A	C2-N3-C4	19.60	120.40	110.60
22	23S1	2632	A	N1-C6-N6	-19.60	106.84	118.60
1	16S1	288	A	C2-N3-C4	19.60	120.40	110.60
1	16S1	313	A	N1-C2-N3	-19.59	119.50	129.30
22	23S1	1057	A	N1-C2-N3	-19.59	119.50	129.30
22	23S1	1226	A	N1-C2-N3	-19.59	119.50	129.30
23	05S1	119	A	C2-N3-C4	19.59	120.39	110.60
22	23S1	1434	A	N1-C2-N3	-19.59	119.51	129.30
22	23S1	1032	A	N1-C6-N6	-19.59	106.85	118.60
1	16S1	768	A	C2-N3-C4	19.59	120.39	110.60
22	23S1	1156	A	C2-N3-C4	19.59	120.39	110.60
22	23S1	216	A	N1-C2-N3	-19.58	119.51	129.30
23	05S1	108	A	N1-C2-N3	-19.58	119.51	129.30
1	16S1	199	A	C2-N3-C4	19.58	120.39	110.60
22	23S1	2247	A	C2-N3-C4	19.58	120.39	110.60
1	16S1	909	A	N1-C2-N3	-19.58	119.51	129.30
22	23S1	2270	A	N1-C6-N6	-19.58	106.85	118.60
1	16S1	131	A	N1-C6-N6	-19.58	106.85	118.60
1	16S1	958	A	C2-N3-C4	19.57	120.39	110.60
22	23S1	241	A	N1-C2-N3	-19.57	119.51	129.30
22	23S1	632	A	C2-N3-C4	19.57	120.39	110.60
1	16S1	412	A	C2-N3-C4	19.57	120.39	110.60
22	23S1	563	A	N1-C2-N3	-19.57	119.51	129.30
22	23S1	2682	A	N1-C2-N3	-19.57	119.51	129.30
22	23S1	155	A	C2-N3-C4	19.57	120.38	110.60
22	23S1	529	A	N1-C2-N3	-19.57	119.52	129.30
22	23S1	1610	A	N1-C2-N3	-19.57	119.52	129.30
22	23S1	1978	A	N1-C2-N3	-19.57	119.52	129.30
22	23S1	2381	A	N1-C2-N3	-19.57	119.52	129.30
22	23S1	1787	A	N1-C2-N3	-19.57	119.52	129.30
1	16S1	502	A	C2-N3-C4	19.57	120.38	110.60
22	23S1	2547	A	N1-C6-N6	-19.57	106.86	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1632	A	N1-C2-N3	-19.56	119.52	129.30
22	23S1	2247	A	N1-C2-N3	-19.56	119.52	129.30
1	16S1	1413	A	N1-C2-N3	-19.56	119.52	129.30
22	23S1	590	A	C2-N3-C4	19.56	120.38	110.60
22	23S1	1010	A	N1-C2-N3	-19.56	119.52	129.30
22	23S1	2829	A	C2-N3-C4	19.56	120.38	110.60
1	16S1	807	A	N1-C6-N6	-19.56	106.86	118.60
22	23S1	1247	A	N1-C6-N6	-19.56	106.87	118.60
22	23S1	1495	A	N1-C2-N3	-19.56	119.52	129.30
22	23S1	278	A	N1-C6-N6	-19.55	106.87	118.60
22	23S1	1327	A	N1-C2-N3	-19.55	119.52	129.30
1	16S1	109	A	N1-C2-N3	-19.55	119.52	129.30
1	16S1	802	A	C2-N3-C4	19.55	120.38	110.60
22	23S1	423	A	N1-C2-N3	-19.55	119.52	129.30
1	16S1	1394	A	N1-C2-N3	-19.55	119.52	129.30
22	23S1	900	A	N1-C6-N6	-19.55	106.87	118.60
1	16S1	1179	A	C2-N3-C4	19.55	120.37	110.60
22	23S1	1655	A	N1-C6-N6	-19.55	106.87	118.60
22	23S1	1304	A	N1-C6-N6	-19.54	106.88	118.60
22	23S1	1829	A	C2-N3-C4	19.54	120.37	110.60
22	23S1	2727	A	C2-N3-C4	19.54	120.37	110.60
1	16S1	1502	A	N1-C2-N3	-19.54	119.53	129.30
22	23S1	1819	A	N1-C6-N6	-19.54	106.88	118.60
1	16S1	262	A	N1-C2-N3	-19.54	119.53	129.30
1	16S1	288	A	N1-C2-N3	-19.54	119.53	129.30
22	23S1	1603	A	C2-N3-C4	19.54	120.37	110.60
22	23S1	1789	A	N1-C2-N3	-19.54	119.53	129.30
22	23S1	2478	A	N1-C2-N3	-19.54	119.53	129.30
1	16S1	435	A	C2-N3-C4	19.54	120.37	110.60
1	16S1	72	A	C2-N3-C4	19.53	120.37	110.60
22	23S1	1759	A	N1-C2-N3	-19.53	119.53	129.30
22	23S1	1301	A	C2-N3-C4	19.53	120.37	110.60
1	16S1	629	A	C2-N3-C4	19.53	120.36	110.60
22	23S1	572	A	C2-N3-C4	19.53	120.36	110.60
1	16S1	728	A	N1-C2-N3	-19.52	119.54	129.30
22	23S1	197	A	N1-C6-N6	-19.52	106.89	118.60
22	23S1	1001	A	N1-C2-N3	-19.52	119.54	129.30
22	23S1	10	A	C2-N3-C4	19.52	120.36	110.60
22	23S1	514	A	N1-C6-N6	-19.52	106.89	118.60
22	23S1	936	A	C2-N3-C4	19.52	120.36	110.60
1	16S1	172	A	N1-C2-N3	-19.52	119.54	129.30
1	16S1	802	A	N1-C6-N6	-19.52	106.89	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	346	A	N1-C2-N3	-19.52	119.54	129.30
1	16S1	1248	A	N1-C6-N6	-19.52	106.89	118.60
1	16S1	1311	A	C2-N3-C4	19.52	120.36	110.60
22	23S1	44	A	C2-N3-C4	19.52	120.36	110.60
22	23S1	1789	A	C2-N3-C4	19.52	120.36	110.60
22	23S1	2014	A	C2-N3-C4	19.52	120.36	110.60
22	23S1	804	A	C2-N3-C4	19.52	120.36	110.60
22	23S1	900	A	C2-N3-C4	19.52	120.36	110.60
22	23S1	244	A	C2-N3-C4	19.51	120.36	110.60
22	23S1	2298	A	N1-C2-N3	-19.51	119.54	129.30
22	23S1	2826	A	C2-N3-C4	19.51	120.36	110.60
1	16S1	303	A	N1-C6-N6	-19.51	106.89	118.60
22	23S1	1630	A	N1-C2-N3	-19.51	119.55	129.30
22	23S1	2314	A	C2-N3-C4	19.51	120.35	110.60
1	16S1	1204	A	N1-C6-N6	-19.51	106.90	118.60
1	16S1	1250	A	N1-C6-N6	-19.51	106.89	118.60
22	23S1	1551	A	C2-N3-C4	19.50	120.35	110.60
22	23S1	1803	A	N1-C2-N3	-19.50	119.55	129.30
22	23S1	627	A	N1-C2-N3	-19.50	119.55	129.30
22	23S1	1253	A	C2-N3-C4	19.50	120.35	110.60
23	05S1	104	A	C2-N3-C4	19.50	120.35	110.60
1	16S1	197	A	N1-C2-N3	-19.50	119.55	129.30
22	23S1	2005	A	C2-N3-C4	19.50	120.35	110.60
1	16S1	1191	A	N1-C2-N3	-19.50	119.55	129.30
22	23S1	2451	A	N1-C2-N3	-19.50	119.55	129.30
55	PTR1	69	A	C2-N3-C4	19.50	120.35	110.60
1	16S1	320	A	N1-C6-N6	-19.50	106.90	118.60
1	16S1	7	A	N1-C6-N6	-19.50	106.90	118.60
1	16S1	816	A	C2-N3-C4	19.50	120.35	110.60
22	23S1	734	A	N1-C2-N3	-19.50	119.55	129.30
22	23S1	833	A	C2-N3-C4	19.50	120.35	110.60
1	16S1	149	A	N1-C2-N3	-19.49	119.55	129.30
1	16S1	1163	A	C2-N3-C4	19.49	120.35	110.60
1	16S1	673	A	C2-N3-C4	19.49	120.35	110.60
1	16S1	1408	A	N1-C6-N6	-19.49	106.90	118.60
22	23S1	1858	A	N1-C6-N6	-19.49	106.91	118.60
1	16S1	819	A	C2-N3-C4	19.49	120.34	110.60
22	23S1	71	A	N1-C6-N6	-19.49	106.91	118.60
1	16S1	743	A	C2-N3-C4	19.49	120.34	110.60
22	23S1	1496	A	N1-C2-N3	-19.49	119.56	129.30
1	16S1	572	A	N1-C2-N3	-19.49	119.56	129.30
22	23S1	910	A	N1-C2-N3	-19.49	119.56	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	825	A	N1-C6-N6	-19.48	106.91	118.60
22	23S1	899	A	N1-C2-N3	-19.48	119.56	129.30
1	16S1	574	A	N1-C2-N3	-19.48	119.56	129.30
1	16S1	1396	A	C2-N3-C4	19.48	120.34	110.60
22	23S1	693	A	C2-N3-C4	19.48	120.34	110.60
22	23S1	1260	A	C2-N3-C4	19.48	120.34	110.60
22	23S1	2587	A	N1-C2-N3	-19.48	119.56	129.30
1	16S1	629	A	N1-C2-N3	-19.48	119.56	129.30
22	23S1	199	A	C2-N3-C4	19.47	120.34	110.60
22	23S1	1265	A	C2-N3-C4	19.47	120.34	110.60
22	23S1	1155	A	C2-N3-C4	19.47	120.34	110.60
1	16S1	1288	A	C2-N3-C4	19.47	120.33	110.60
22	23S1	127	A	N1-C6-N6	-19.47	106.92	118.60
22	23S1	1899	A	N1-C6-N6	-19.47	106.92	118.60
22	23S1	972	A	N1-C2-N3	-19.47	119.56	129.30
22	23S1	1378	A	N1-C2-N3	-19.47	119.57	129.30
22	23S1	1936	A	C2-N3-C4	19.47	120.33	110.60
22	23S1	2031	A	N1-C2-N3	-19.47	119.57	129.30
22	23S1	2560	A	C2-N3-C4	19.47	120.33	110.60
1	16S1	2	A	N1-C6-N6	-19.47	106.92	118.60
22	23S1	443	A	N1-C2-N3	-19.47	119.57	129.30
22	23S1	632	A	N1-C2-N3	-19.47	119.57	129.30
22	23S1	1048	A	N1-C2-N3	-19.47	119.57	129.30
22	23S1	1383	A	N1-C6-N6	-19.47	106.92	118.60
22	23S1	1780	A	N1-C2-N3	-19.47	119.57	129.30
22	23S1	2886	A	C2-N3-C4	19.47	120.33	110.60
22	23S1	332	A	N1-C6-N6	-19.46	106.92	118.60
22	23S1	1900	A	N1-C2-N3	-19.46	119.57	129.30
1	16S1	766	A	C2-N3-C4	19.46	120.33	110.60
1	16S1	468	A	C2-N3-C4	19.46	120.33	110.60
22	23S1	866	A	N1-C2-N3	-19.46	119.57	129.30
1	16S1	59	A	N1-C2-N3	-19.46	119.57	129.30
1	16S1	1067	A	N1-C6-N6	-19.46	106.93	118.60
22	23S1	621	A	C2-N3-C4	19.46	120.33	110.60
22	23S1	1286	A	N1-C2-N3	-19.46	119.57	129.30
1	16S1	1204	A	N1-C2-N3	-19.45	119.57	129.30
22	23S1	825	A	N1-C6-N6	-19.45	106.93	118.60
22	23S1	947	A	N1-C2-N3	-19.45	119.57	129.30
22	23S1	2366	A	N1-C2-N3	-19.45	119.57	129.30
1	16S1	389	A	N1-C2-N3	-19.45	119.57	129.30
1	16S1	510	A	N1-C2-N3	-19.45	119.57	129.30
1	16S1	1155	A	C2-N3-C4	19.45	120.33	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2273	A	N1-C2-N3	-19.45	119.58	129.30
23	05S1	115	A	N1-C2-N3	-19.45	119.57	129.30
1	16S1	26	A	N1-C2-N3	-19.45	119.58	129.30
1	16S1	1374	A	C2-N3-C4	19.45	120.33	110.60
1	16S1	1534	A	N1-C2-N3	-19.45	119.58	129.30
22	23S1	1713	A	N1-C2-N3	-19.45	119.58	129.30
22	23S1	928	A	N1-C2-N3	-19.45	119.58	129.30
22	23S1	2042	A	N1-C2-N3	-19.45	119.58	129.30
22	23S1	1503	A	N1-C6-N6	-19.45	106.93	118.60
1	16S1	495	A	N1-C2-N3	-19.44	119.58	129.30
22	23S1	1551	A	N1-C6-N6	-19.44	106.94	118.60
22	23S1	457	A	N1-C6-N6	-19.44	106.94	118.60
22	23S1	1342	A	N1-C2-N3	-19.44	119.58	129.30
22	23S1	1918	A	N1-C6-N6	-19.44	106.94	118.60
22	23S1	371	A	N1-C6-N6	-19.44	106.94	118.60
22	23S1	1077	A	N1-C6-N6	-19.44	106.94	118.60
22	23S1	1635	A	C2-N3-C4	19.44	120.32	110.60
22	23S1	2736	A	C2-N3-C4	19.44	120.32	110.60
55	PTR1	23	A	C2-N3-C4	19.44	120.32	110.60
1	16S1	182	A	N1-C2-N3	-19.44	119.58	129.30
1	16S1	792	A	N1-C2-N3	-19.44	119.58	129.30
1	16S1	315	A	C2-N3-C4	19.43	120.32	110.60
1	16S1	1446	A	N1-C2-N3	-19.43	119.58	129.30
22	23S1	975	A	C2-N3-C4	19.43	120.32	110.60
1	16S1	171	A	N1-C2-N3	-19.43	119.58	129.30
1	16S1	560	A	N1-C6-N6	-19.43	106.94	118.60
1	16S1	1261	A	N1-C2-N3	-19.43	119.58	129.30
22	23S1	213	A	N1-C6-N6	-19.43	106.94	118.60
22	23S1	764	A	C2-N3-C4	19.43	120.31	110.60
22	23S1	1342	A	N1-C6-N6	-19.43	106.94	118.60
22	23S1	391	A	C2-N3-C4	19.43	120.31	110.60
22	23S1	782	A	C2-N3-C4	19.43	120.31	110.60
22	23S1	222	A	N1-C2-N3	-19.43	119.59	129.30
22	23S1	735	A	N1-C2-N3	-19.43	119.59	129.30
22	23S1	2837	A	C2-N3-C4	19.43	120.31	110.60
22	23S1	644	A	C2-N3-C4	19.42	120.31	110.60
22	23S1	727	A	N1-C2-N3	-19.42	119.59	129.30
22	23S1	735	A	C2-N3-C4	19.42	120.31	110.60
22	23S1	447	A	N1-C2-N3	-19.42	119.59	129.30
1	16S1	1398	A	N1-C6-N6	-19.42	106.95	118.60
22	23S1	53	A	N1-C2-N3	-19.42	119.59	129.30
22	23S1	1090	A	C2-N3-C4	19.42	120.31	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2212	A	N1-C2-N3	-19.42	119.59	129.30
22	23S1	918	A	C2-N3-C4	19.42	120.31	110.60
22	23S1	2882	A	C2-N3-C4	19.42	120.31	110.60
22	23S1	2513	A	N1-C6-N6	-19.42	106.95	118.60
22	23S1	2700	A	C2-N3-C4	19.42	120.31	110.60
1	16S1	553	A	C2-N3-C4	19.41	120.31	110.60
22	23S1	2071	A	C2-N3-C4	19.41	120.31	110.60
22	23S1	2142	A	C2-N3-C4	19.41	120.31	110.60
22	23S1	2577	A	N1-C2-N3	-19.41	119.59	129.30
22	23S1	2882	A	N1-C2-N3	-19.41	119.59	129.30
22	23S1	146	A	C2-N3-C4	19.41	120.31	110.60
22	23S1	792	A	N1-C6-N6	-19.41	106.95	118.60
22	23S1	311	A	N1-C6-N6	-19.41	106.95	118.60
22	23S1	821	A	N1-C2-N3	-19.41	119.59	129.30
22	23S1	845	A	N1-C2-N3	-19.41	119.59	129.30
1	16S1	74	A	N1-C6-N6	-19.41	106.95	118.60
1	16S1	573	A	N1-C2-N3	-19.41	119.59	129.30
1	16S1	889	A	C2-N3-C4	19.41	120.31	110.60
1	16S1	782	A	N1-C6-N6	-19.41	106.95	118.60
22	23S1	2476	A	C2-N3-C4	19.41	120.31	110.60
1	16S1	223	A	C2-N3-C4	19.41	120.30	110.60
22	23S1	743	A	C2-N3-C4	19.41	120.30	110.60
22	23S1	984	A	N1-C2-N3	-19.41	119.60	129.30
22	23S1	2471	A	C2-N3-C4	19.41	120.30	110.60
22	23S1	2657	A	N1-C6-N6	-19.41	106.96	118.60
1	16S1	787	A	C2-N3-C4	19.40	120.30	110.60
1	16S1	845	A	N1-C2-N3	-19.40	119.60	129.30
22	23S1	2835	A	N1-C6-N6	-19.40	106.96	118.60
22	23S1	981	A	N1-C6-N6	-19.40	106.96	118.60
1	16S1	1408	A	N1-C2-N3	-19.40	119.60	129.30
1	16S1	935	A	C2-N3-C4	19.40	120.30	110.60
22	23S1	1204	A	N1-C2-N3	-19.40	119.60	129.30
22	23S1	1431	A	C2-N3-C4	19.40	120.30	110.60
22	23S1	2541	A	N1-C6-N6	-19.40	106.96	118.60
22	23S1	374	A	N1-C2-N3	-19.40	119.60	129.30
22	23S1	861	A	C2-N3-C4	19.40	120.30	110.60
22	23S1	1821	A	N1-C6-N6	-19.40	106.96	118.60
1	16S1	1431	A	N1-C6-N6	-19.39	106.96	118.60
22	23S1	1403	A	C2-N3-C4	19.39	120.30	110.60
22	23S1	1690	A	N1-C6-N6	-19.39	106.96	118.60
1	16S1	98	A	C2-N3-C4	19.39	120.30	110.60
22	23S1	590	A	N1-C2-N3	-19.39	119.60	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	782	A	C2-N3-C4	19.39	120.30	110.60
22	23S1	1890	A	N1-C2-N3	-19.39	119.61	129.30
1	16S1	608	A	C2-N3-C4	19.39	120.29	110.60
22	23S1	909	A	N1-C2-N3	-19.39	119.61	129.30
22	23S1	2376	A	C2-N3-C4	19.39	120.29	110.60
1	16S1	696	A	N1-C2-N3	-19.39	119.61	129.30
22	23S1	526	A	C2-N3-C4	19.39	120.29	110.60
22	23S1	1001	A	N1-C6-N6	-19.39	106.97	118.60
1	16S1	807	A	C2-N3-C4	19.38	120.29	110.60
22	23S1	2835	A	N1-C2-N3	-19.38	119.61	129.30
1	16S1	873	A	N1-C2-N3	-19.38	119.61	129.30
22	23S1	528	A	N1-C2-N3	-19.38	119.61	129.30
22	23S1	2418	A	C2-N3-C4	19.38	120.29	110.60
22	23S1	761	A	C2-N3-C4	19.38	120.29	110.60
22	23S1	1477	A	C2-N3-C4	19.38	120.29	110.60
22	23S1	1634	A	N1-C6-N6	-19.38	106.97	118.60
22	23S1	2433	A	C2-N3-C4	19.38	120.29	110.60
1	16S1	80	A	N1-C6-N6	-19.38	106.97	118.60
22	23S1	918	A	N1-C6-N6	-19.38	106.97	118.60
22	23S1	2060	A	N1-C6-N6	-19.38	106.97	118.60
22	23S1	2088	A	C2-N3-C4	19.38	120.29	110.60
22	23S1	2590	A	N1-C6-N6	-19.38	106.97	118.60
22	23S1	699	A	N1-C2-N3	-19.38	119.61	129.30
1	16S1	2	A	N1-C2-N3	-19.37	119.61	129.30
22	23S1	332	A	N1-C2-N3	-19.37	119.61	129.30
22	23S1	1048	A	N1-C6-N6	-19.37	106.98	118.60
23	05S1	78	A	C2-N3-C4	19.37	120.29	110.60
22	23S1	1572	A	N1-C2-N3	-19.37	119.61	129.30
22	23S1	2033	A	C2-N3-C4	19.37	120.28	110.60
22	23S1	706	A	C2-N3-C4	19.37	120.28	110.60
22	23S1	990	A	N1-C2-N3	-19.37	119.62	129.30
22	23S1	2019	A	C2-N3-C4	19.37	120.28	110.60
1	16S1	1196	A	N1-C2-N3	-19.36	119.62	129.30
1	16S1	1238	A	N1-C2-N3	-19.36	119.62	129.30
22	23S1	670	A	N1-C2-N3	-19.36	119.62	129.30
22	23S1	1347	A	C2-N3-C4	19.36	120.28	110.60
22	23S1	2435	A	N1-C6-N6	-19.36	106.98	118.60
22	23S1	2706	A	C2-N3-C4	19.36	120.28	110.60
1	16S1	149	A	C2-N3-C4	19.36	120.28	110.60
1	16S1	694	A	N1-C2-N3	-19.36	119.62	129.30
22	23S1	21	A	C2-N3-C4	19.36	120.28	110.60
22	23S1	735	A	N1-C6-N6	-19.36	106.98	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1616	A	N1-C2-N3	-19.36	119.62	129.30
22	23S1	2328	A	C2-N3-C4	19.36	120.28	110.60
23	05S1	99	A	N1-C2-N3	-19.36	119.62	129.30
22	23S1	941	A	N1-C2-N3	-19.36	119.62	129.30
22	23S1	2734	A	N1-C2-N3	-19.36	119.62	129.30
1	16S1	746	A	C2-N3-C4	19.36	120.28	110.60
22	23S1	793	A	C2-N3-C4	19.36	120.28	110.60
22	23S1	1503	A	C2-N3-C4	19.36	120.28	110.60
22	23S1	1570	A	C2-N3-C4	19.36	120.28	110.60
22	23S1	2154	A	C2-N3-C4	19.36	120.28	110.60
22	23S1	2317	A	C2-N3-C4	19.36	120.28	110.60
22	23S1	861	A	N1-C2-N3	-19.36	119.62	129.30
22	23S1	917	A	C2-N3-C4	19.36	120.28	110.60
22	23S1	866	A	C2-N3-C4	19.35	120.28	110.60
22	23S1	1365	A	N1-C2-N3	-19.35	119.62	129.30
22	23S1	1960	A	C2-N3-C4	19.35	120.28	110.60
1	16S1	768	A	N1-C6-N6	-19.35	106.99	118.60
1	16S1	1150	A	N1-C6-N6	-19.35	106.99	118.60
22	23S1	1268	A	C2-N3-C4	19.35	120.28	110.60
22	23S1	1552	A	N1-C2-N3	-19.35	119.62	129.30
22	23S1	2381	A	C2-N3-C4	19.35	120.28	110.60
22	23S1	2868	A	C2-N3-C4	19.35	120.28	110.60
1	16S1	753	A	N1-C2-N3	-19.35	119.63	129.30
22	23S1	1773	A	C2-N3-C4	19.35	120.27	110.60
22	23S1	613	A	N1-C2-N3	-19.35	119.63	129.30
22	23S1	1014	A	C2-N3-C4	19.35	120.27	110.60
22	23S1	1165	A	N1-C6-N6	-19.35	106.99	118.60
23	05S1	73	A	N1-C2-N3	-19.35	119.63	129.30
22	23S1	2013	A	N1-C2-N3	-19.35	119.63	129.30
1	16S1	152	A	N1-C2-N3	-19.34	119.63	129.30
22	23S1	1569	A	N1-C2-N3	-19.34	119.63	129.30
22	23S1	1918	A	C2-N3-C4	19.34	120.27	110.60
23	05S1	108	A	C2-N3-C4	19.34	120.27	110.60
1	16S1	468	A	N1-C2-N3	-19.34	119.63	129.30
22	23S1	309	A	N1-C2-N3	-19.34	119.63	129.30
22	23S1	1308	A	C2-N3-C4	19.34	120.27	110.60
22	23S1	1641	A	C2-N3-C4	19.34	120.27	110.60
1	16S1	298	A	N1-C2-N3	-19.34	119.63	129.30
22	23S1	322	A	N1-C6-N6	-19.34	107.00	118.60
22	23S1	479	A	N1-C2-N3	-19.34	119.63	129.30
22	23S1	1665	A	C2-N3-C4	19.34	120.27	110.60
1	16S1	753	A	C2-N3-C4	19.34	120.27	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	374	A	C2-N3-C4	19.34	120.27	110.60
22	23S1	2758	A	N1-C2-N3	-19.34	119.63	129.30
1	16S1	461	A	C2-N3-C4	19.34	120.27	110.60
22	23S1	2660	A	N1-C6-N6	-19.34	107.00	118.60
1	16S1	371	A	N1-C2-N3	-19.34	119.63	129.30
22	23S1	727	A	C2-N3-C4	19.34	120.27	110.60
22	23S1	2311	A	N1-C2-N3	-19.34	119.63	129.30
22	23S1	226	A	N1-C2-N3	-19.33	119.63	129.30
22	23S1	63	A	N1-C2-N3	-19.33	119.63	129.30
22	23S1	182	A	C2-N3-C4	19.33	120.27	110.60
22	23S1	1815	A	N1-C2-N3	-19.33	119.63	129.30
1	16S1	1480	A	N1-C6-N6	-19.33	107.00	118.60
22	23S1	2227	A	N1-C2-N3	-19.33	119.64	129.30
1	16S1	706	A	C2-N3-C4	19.33	120.27	110.60
22	23S1	819	A	C2-N3-C4	19.33	120.27	110.60
22	23S1	2003	A	C2-N3-C4	19.33	120.26	110.60
22	23S1	2051	A	N1-C6-N6	-19.33	107.00	118.60
22	23S1	2829	A	N1-C2-N3	-19.33	119.64	129.30
23	05S1	78	A	N1-C6-N6	-19.33	107.00	118.60
1	16S1	327	A	N1-C2-N3	-19.33	119.64	129.30
22	23S1	582	A	N1-C2-N3	-19.33	119.64	129.30
23	05S1	45	A	N1-C2-N3	-19.33	119.64	129.30
1	16S1	174	A	C2-N3-C4	19.32	120.26	110.60
22	23S1	947	A	C2-N3-C4	19.32	120.26	110.60
22	23S1	1552	A	C2-N3-C4	19.32	120.26	110.60
1	16S1	411	A	N1-C2-N3	-19.32	119.64	129.30
22	23S1	49	A	C2-N3-C4	19.32	120.26	110.60
22	23S1	203	A	C2-N3-C4	19.32	120.26	110.60
22	23S1	2766	A	N1-C2-N3	-19.32	119.64	129.30
1	16S1	1252	A	C2-N3-C4	19.32	120.26	110.60
1	16S1	1429	A	C2-N3-C4	19.32	120.26	110.60
22	23S1	666	A	N1-C2-N3	-19.32	119.64	129.30
1	16S1	663	A	C2-N3-C4	19.32	120.26	110.60
22	23S1	190	A	N1-C2-N3	-19.32	119.64	129.30
22	23S1	972	A	N1-C6-N6	-19.32	107.01	118.60
22	23S1	1268	A	N1-C6-N6	-19.32	107.01	118.60
22	23S1	2090	A	C2-N3-C4	19.31	120.26	110.60
22	23S1	412	A	N1-C2-N3	-19.31	119.64	129.30
22	23S1	1284	A	N1-C2-N3	-19.31	119.64	129.30
22	23S1	2284	A	C2-N3-C4	19.31	120.25	110.60
1	16S1	1274	A	N1-C6-N6	-19.31	107.01	118.60
1	16S1	1433	A	C2-N3-C4	19.31	120.25	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1805	A	N1-C2-N3	-19.31	119.64	129.30
1	16S1	1329	A	C2-N3-C4	19.31	120.25	110.60
22	23S1	231	A	N1-C6-N6	-19.31	107.02	118.60
1	16S1	393	A	C2-N3-C4	19.31	120.25	110.60
22	23S1	471	A	N1-C2-N3	-19.31	119.65	129.30
22	23S1	2270	A	N1-C2-N3	-19.31	119.65	129.30
22	23S1	2675	A	C2-N3-C4	19.30	120.25	110.60
1	16S1	1155	A	N1-C2-N3	-19.30	119.65	129.30
22	23S1	1067	A	C2-N3-C4	19.30	120.25	110.60
22	23S1	1264	A	C2-N3-C4	19.30	120.25	110.60
22	23S1	1701	A	N1-C2-N3	-19.30	119.65	129.30
1	16S1	1229	A	C2-N3-C4	19.30	120.25	110.60
22	23S1	300	A	N1-C2-N3	-19.30	119.65	129.30
1	16S1	532	A	C2-N3-C4	19.30	120.25	110.60
22	23S1	2516	A	N1-C2-N3	-19.30	119.65	129.30
22	23S1	42	A	C2-N3-C4	19.30	120.25	110.60
22	23S1	1566	A	C2-N3-C4	19.30	120.25	110.60
22	23S1	125	A	N1-C2-N3	-19.30	119.65	129.30
22	23S1	1384	A	N1-C2-N3	-19.30	119.65	129.30
22	23S1	1711	A	C2-N3-C4	19.30	120.25	110.60
1	16S1	1499	A	N1-C2-N3	-19.29	119.65	129.30
22	23S1	979	A	N1-C6-N6	-19.29	107.02	118.60
22	23S1	2266	A	N1-C6-N6	-19.29	107.02	118.60
22	23S1	1268	A	N1-C2-N3	-19.29	119.65	129.30
22	23S1	1469	A	C2-N3-C4	19.29	120.25	110.60
22	23S1	1254	A	C2-N3-C4	19.29	120.25	110.60
22	23S1	2211	A	N1-C6-N6	-19.29	107.03	118.60
22	23S1	1439	A	C2-N3-C4	19.29	120.24	110.60
22	23S1	1690	A	C2-N3-C4	19.29	120.24	110.60
1	16S1	1236	A	C2-N3-C4	19.29	120.24	110.60
22	23S1	1264	A	N1-C2-N3	-19.29	119.66	129.30
1	16S1	129	A	N1-C2-N3	-19.28	119.66	129.30
1	16S1	456	A	C2-N3-C4	19.28	120.24	110.60
22	23S1	199	A	N1-C2-N3	-19.28	119.66	129.30
22	23S1	599	A	N1-C2-N3	-19.28	119.66	129.30
22	23S1	1757	A	N1-C2-N3	-19.28	119.66	129.30
22	23S1	2639	A	N1-C2-N3	-19.28	119.66	129.30
1	16S1	461	A	N1-C2-N3	-19.28	119.66	129.30
1	16S1	1465	A	C2-N3-C4	19.28	120.24	110.60
22	23S1	943	A	N1-C2-N3	-19.28	119.66	129.30
22	23S1	1230	A	C2-N3-C4	19.28	120.24	110.60
1	16S1	19	A	N1-C6-N6	-19.28	107.03	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1084	A	C2-N3-C4	19.28	120.24	110.60
22	23S1	1127	A	N1-C6-N6	-19.27	107.03	118.60
22	23S1	1654	A	C2-N3-C4	19.27	120.24	110.60
22	23S1	2266	A	N1-C2-N3	-19.27	119.66	129.30
22	23S1	1276	A	C2-N3-C4	19.27	120.23	110.60
1	16S1	1	A	N1-C6-N6	-19.27	107.04	118.60
22	23S1	14	A	C2-N3-C4	19.27	120.23	110.60
22	23S1	330	A	N1-C2-N3	-19.27	119.67	129.30
22	23S1	2776	A	N1-C2-N3	-19.27	119.67	129.30
1	16S1	1246	A	C2-N3-C4	19.27	120.23	110.60
22	23S1	176	A	C2-N3-C4	19.27	120.23	110.60
22	23S1	833	A	N1-C2-N3	-19.27	119.67	129.30
22	23S1	1260	A	N1-C2-N3	-19.27	119.67	129.30
55	PTR1	42	A	C2-N3-C4	19.27	120.23	110.60
22	23S1	402	A	N1-C6-N6	-19.26	107.04	118.60
22	23S1	1966	A	N1-C2-N3	-19.26	119.67	129.30
22	23S1	2589	A	C2-N3-C4	19.26	120.23	110.60
22	23S1	715	A	C2-N3-C4	19.26	120.23	110.60
22	23S1	497	A	N1-C2-N3	-19.26	119.67	129.30
22	23S1	592	A	C2-N3-C4	19.26	120.23	110.60
22	23S1	2602	A	N1-C2-N3	-19.26	119.67	129.30
22	23S1	1525	A	C2-N3-C4	19.26	120.23	110.60
1	16S1	1456	A	N1-C2-N3	-19.26	119.67	129.30
22	23S1	1274	A	C2-N3-C4	19.26	120.23	110.60
22	23S1	1439	A	N1-C2-N3	-19.26	119.67	129.30
22	23S1	1932	A	C2-N3-C4	19.25	120.23	110.60
22	23S1	2675	A	N1-C2-N3	-19.25	119.67	129.30
22	23S1	2851	A	N1-C2-N3	-19.25	119.67	129.30
1	16S1	1275	A	N1-C2-N3	-19.25	119.67	129.30
22	23S1	1579	A	N1-C6-N6	-19.25	107.05	118.60
22	23S1	1583	A	N1-C2-N3	-19.25	119.67	129.30
22	23S1	1847	A	C2-N3-C4	19.25	120.23	110.60
22	23S1	1916	A	C2-N3-C4	19.25	120.23	110.60
22	23S1	2241	A	N1-C6-N6	-19.25	107.05	118.60
22	23S1	2469	A	N1-C2-N3	-19.25	119.67	129.30
22	23S1	322	A	N1-C2-N3	-19.25	119.68	129.30
22	23S1	920	A	C2-N3-C4	19.25	120.22	110.60
22	23S1	2270	A	C2-N3-C4	19.25	120.22	110.60
22	23S1	2298	A	C2-N3-C4	19.25	120.22	110.60
22	23S1	71	A	N1-C2-N3	-19.25	119.68	129.30
22	23S1	2097	A	C2-N3-C4	19.25	120.22	110.60
1	16S1	1476	A	C2-N3-C4	19.25	120.22	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1678	A	N1-C2-N3	-19.25	119.68	129.30
22	23S1	1434	A	C2-N3-C4	19.24	120.22	110.60
22	23S1	1504	A	C2-N3-C4	19.24	120.22	110.60
1	16S1	1150	A	C2-N3-C4	19.24	120.22	110.60
22	23S1	478	A	C2-N3-C4	19.24	120.22	110.60
1	16S1	238	A	C2-N3-C4	19.24	120.22	110.60
1	16S1	1513	A	C2-N3-C4	19.24	120.22	110.60
22	23S1	300	A	C2-N3-C4	19.24	120.22	110.60
22	23S1	547	A	N1-C2-N3	-19.24	119.68	129.30
22	23S1	1095	A	C2-N3-C4	19.24	120.22	110.60
22	23S1	1762	A	C2-N3-C4	19.24	120.22	110.60
1	16S1	923	A	C2-N3-C4	19.24	120.22	110.60
1	16S1	1480	A	C2-N3-C4	19.24	120.22	110.60
22	23S1	196	A	N1-C2-N3	-19.24	119.68	129.30
22	23S1	1284	A	N1-C6-N6	-19.24	107.06	118.60
22	23S1	1287	A	C2-N3-C4	19.24	120.22	110.60
22	23S1	959	A	N1-C2-N3	-19.23	119.68	129.30
22	23S1	1809	A	N1-C6-N6	-19.23	107.06	118.60
22	23S1	227	A	C2-N3-C4	19.23	120.22	110.60
1	16S1	977	A	N1-C2-N3	-19.23	119.68	129.30
1	16S1	864	A	N1-C6-N6	-19.23	107.06	118.60
1	16S1	1441	A	N1-C2-N3	-19.23	119.69	129.30
22	23S1	2665	A	C2-N3-C4	19.23	120.22	110.60
22	23S1	1591	A	N1-C2-N3	-19.23	119.69	129.30
22	23S1	1175	A	N1-C2-N3	-19.23	119.69	129.30
22	23S1	1977	A	N1-C2-N3	-19.23	119.69	129.30
1	16S1	1150	A	N1-C2-N3	-19.22	119.69	129.30
22	23S1	1088	A	N1-C2-N3	-19.22	119.69	129.30
22	23S1	1144	A	C2-N3-C4	19.22	120.21	110.60
22	23S1	1535	A	N1-C6-N6	-19.22	107.07	118.60
22	23S1	2657	A	C2-N3-C4	19.22	120.21	110.60
1	16S1	1433	A	N1-C6-N6	-19.22	107.07	118.60
22	23S1	89	A	C2-N3-C4	19.22	120.21	110.60
22	23S1	1858	A	C2-N3-C4	19.22	120.21	110.60
22	23S1	2336	A	N1-C6-N6	-19.22	107.07	118.60
1	16S1	1349	A	N1-C2-N3	-19.22	119.69	129.30
1	16S1	1434	A	N1-C2-N3	-19.22	119.69	129.30
22	23S1	146	A	N1-C2-N3	-19.22	119.69	129.30
22	23S1	1009	A	N1-C2-N3	-19.22	119.69	129.30
22	23S1	1603	A	N1-C2-N3	-19.22	119.69	129.30
22	23S1	2199	A	N1-C2-N3	-19.22	119.69	129.30
55	PTR1	26	A	N1-C2-N3	-19.22	119.69	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1180	A	C2-N3-C4	19.22	120.21	110.60
22	23S1	126	A	N1-C6-N6	-19.22	107.07	118.60
1	16S1	1196	A	C2-N3-C4	19.22	120.21	110.60
22	23S1	742	A	C2-N3-C4	19.22	120.21	110.60
22	23S1	1347	A	N1-C2-N3	-19.22	119.69	129.30
22	23S1	2450	A	C2-N3-C4	19.22	120.21	110.60
1	16S1	1349	A	N1-C6-N6	-19.21	107.07	118.60
1	16S1	583	A	C2-N3-C4	19.21	120.21	110.60
22	23S1	2094	A	C2-N3-C4	19.21	120.21	110.60
22	23S1	2725	A	C2-N3-C4	19.21	120.21	110.60
1	16S1	969	A	N1-C2-N3	-19.21	119.69	129.30
1	16S1	958	A	N1-C2-N3	-19.21	119.69	129.30
1	16S1	1368	A	C2-N3-C4	19.21	120.20	110.60
22	23S1	13	A	C2-N3-C4	19.21	120.21	110.60
22	23S1	1829	A	N1-C6-N6	-19.21	107.07	118.60
1	16S1	3	A	N1-C6-N6	-19.21	107.08	118.60
1	16S1	167	A	N1-C2-N3	-19.21	119.70	129.30
22	23S1	1598	A	C2-N3-C4	19.21	120.20	110.60
22	23S1	2225	A	C2-N3-C4	19.21	120.20	110.60
22	23S1	1247	A	C2-N3-C4	19.21	120.20	110.60
22	23S1	1265	A	N1-C6-N6	-19.21	107.08	118.60
22	23S1	2134	A	C2-N3-C4	19.21	120.20	110.60
1	16S1	32	A	C2-N3-C4	19.20	120.20	110.60
1	16S1	892	A	C2-N3-C4	19.20	120.20	110.60
22	23S1	231	A	C2-N3-C4	19.20	120.20	110.60
22	23S1	2721	A	N1-C2-N3	-19.20	119.70	129.30
22	23S1	1069	A	N1-C2-N3	-19.20	119.70	129.30
22	23S1	2227	A	N1-C6-N6	-19.20	107.08	118.60
22	23S1	2600	A	N1-C6-N6	-19.20	107.08	118.60
22	23S1	1342	A	C2-N3-C4	19.20	120.20	110.60
22	23S1	1439	A	N1-C6-N6	-19.20	107.08	118.60
22	23S1	2227	A	C2-N3-C4	19.20	120.20	110.60
22	23S1	91	A	N1-C2-N3	-19.20	119.70	129.30
22	23S1	255	A	C2-N3-C4	19.20	120.20	110.60
22	23S1	83	A	N1-C2-N3	-19.20	119.70	129.30
1	16S1	309	A	C2-N3-C4	19.20	120.20	110.60
22	23S1	429	A	N1-C2-N3	-19.20	119.70	129.30
22	23S1	439	A	C2-N3-C4	19.20	120.20	110.60
22	23S1	2835	A	C2-N3-C4	19.20	120.20	110.60
22	23S1	631	A	N1-C6-N6	-19.20	107.08	118.60
22	23S1	1969	A	N1-C2-N3	-19.19	119.70	129.30
22	23S1	2577	A	C2-N3-C4	19.19	120.20	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2765	A	N1-C6-N6	-19.19	107.08	118.60
22	23S1	2899	A	C2-N3-C4	19.19	120.20	110.60
1	16S1	196	A	N1-C2-N3	-19.19	119.70	129.30
1	16S1	983	A	N1-C6-N6	-19.19	107.08	118.60
1	16S1	1431	A	N1-C2-N3	-19.19	119.70	129.30
22	23S1	608	A	C2-N3-C4	19.19	120.20	110.60
22	23S1	666	A	C2-N3-C4	19.19	120.19	110.60
22	23S1	1591	A	C2-N3-C4	19.19	120.19	110.60
22	23S1	1701	A	C2-N3-C4	19.19	120.19	110.60
22	23S1	2682	A	C2-N3-C4	19.19	120.19	110.60
22	23S1	2297	A	N1-C6-N6	-19.19	107.09	118.60
22	23S1	2340	A	N1-C2-N3	-19.19	119.70	129.30
1	16S1	306	A	N1-C2-N3	-19.19	119.71	129.30
1	16S1	1000	A	C2-N3-C4	19.19	120.19	110.60
22	23S1	38	A	C2-N3-C4	19.19	120.19	110.60
22	23S1	347	A	N1-C6-N6	-19.19	107.09	118.60
22	23S1	2060	A	C2-N3-C4	19.19	120.19	110.60
1	16S1	1019	A	N1-C2-N3	-19.18	119.71	129.30
22	23S1	83	A	N1-C6-N6	-19.18	107.09	118.60
22	23S1	270	A	C2-N3-C4	19.18	120.19	110.60
1	16S1	155	A	C2-N3-C4	19.18	120.19	110.60
22	23S1	1548	A	C2-N3-C4	19.18	120.19	110.60
1	16S1	784	A	C2-N3-C4	19.18	120.19	110.60
1	16S1	865	A	N1-C6-N6	-19.18	107.09	118.60
1	16S1	1082	A	C2-N3-C4	19.18	120.19	110.60
22	23S1	928	A	C2-N3-C4	19.18	120.19	110.60
1	16S1	195	A	C2-N3-C4	19.18	120.19	110.60
22	23S1	2033	A	N1-C2-N3	-19.18	119.71	129.30
1	16S1	1476	A	N1-C6-N6	-19.18	107.09	118.60
22	23S1	222	A	N1-C6-N6	-19.18	107.09	118.60
22	23S1	716	A	N1-C2-N3	-19.18	119.71	129.30
22	23S1	1664	A	C2-N3-C4	19.18	120.19	110.60
22	23S1	1876	A	N1-C2-N3	-19.18	119.71	129.30
22	23S1	1901	A	N1-C2-N3	-19.18	119.71	129.30
22	23S1	1928	A	N1-C2-N3	-19.18	119.71	129.30
1	16S1	1280	A	N1-C6-N6	-19.18	107.09	118.60
22	23S1	1987	A	N1-C2-N3	-19.18	119.71	129.30
1	16S1	547	A	N1-C2-N3	-19.18	119.71	129.30
1	16S1	630	A	N1-C2-N3	-19.18	119.71	129.30
22	23S1	19	A	N1-C6-N6	-19.18	107.09	118.60
22	23S1	104	A	N1-C2-N3	-19.18	119.71	129.30
22	23S1	340	A	C2-N3-C4	19.18	120.19	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1640	A	C2-N3-C4	19.18	120.19	110.60
22	23S1	149	A	C2-N3-C4	19.17	120.19	110.60
22	23S1	1387	A	C2-N3-C4	19.17	120.19	110.60
22	23S1	2376	A	N1-C6-N6	-19.17	107.09	118.60
22	23S1	878	A	N1-C2-N3	-19.17	119.71	129.30
22	23S1	1525	A	N1-C2-N3	-19.17	119.71	129.30
22	23S1	2014	A	N1-C2-N3	-19.17	119.71	129.30
22	23S1	2654	A	N1-C6-N6	-19.17	107.10	118.60
22	23S1	2749	A	N1-C6-N6	-19.17	107.10	118.60
1	16S1	937	A	C2-N3-C4	19.17	120.19	110.60
22	23S1	896	A	N1-C6-N6	-19.17	107.10	118.60
22	23S1	1490	A	N1-C6-N6	-19.17	107.10	118.60
22	23S1	522	A	C2-N3-C4	19.17	120.19	110.60
1	16S1	28	A	C2-N3-C4	19.17	120.18	110.60
1	16S1	270	A	C2-N3-C4	19.17	120.18	110.60
22	23S1	371	A	C2-N3-C4	19.17	120.18	110.60
22	23S1	670	A	N1-C6-N6	-19.17	107.10	118.60
22	23S1	575	A	N1-C2-N3	-19.17	119.72	129.30
22	23S1	1566	A	N1-C2-N3	-19.17	119.72	129.30
22	23S1	2199	A	C2-N3-C4	19.17	120.18	110.60
22	23S1	2682	A	N1-C6-N6	-19.17	107.10	118.60
1	16S1	695	A	C2-N3-C4	19.16	120.18	110.60
1	16S1	906	A	C2-N3-C4	19.16	120.18	110.60
1	16S1	1157	A	C2-N3-C4	19.16	120.18	110.60
1	16S1	1246	A	N1-C2-N3	-19.16	119.72	129.30
22	23S1	213	A	N1-C2-N3	-19.16	119.72	129.30
22	23S1	219	A	N1-C6-N6	-19.16	107.10	118.60
22	23S1	979	A	C2-N3-C4	19.16	120.18	110.60
22	23S1	1937	A	N1-C2-N3	-19.16	119.72	129.30
22	23S1	2287	A	N1-C2-N3	-19.16	119.72	129.30
22	23S1	1504	A	N1-C2-N3	-19.16	119.72	129.30
1	16S1	325	A	N1-C2-N3	-19.16	119.72	129.30
22	23S1	1978	A	C2-N3-C4	19.16	120.18	110.60
22	23S1	94	A	C2-N3-C4	19.16	120.18	110.60
1	16S1	831	A	N1-C6-N6	-19.16	107.11	118.60
22	23S1	2476	A	N1-C2-N3	-19.16	119.72	129.30
1	16S1	1197	A	C2-N3-C4	19.16	120.18	110.60
22	23S1	368	A	N1-C2-N3	-19.16	119.72	129.30
1	16S1	630	A	C2-N3-C4	19.16	120.18	110.60
1	16S1	1016	A	C2-N3-C4	19.16	120.18	110.60
22	23S1	1327	A	C2-N3-C4	19.16	120.18	110.60
22	23S1	2266	A	C2-N3-C4	19.16	120.18	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	712	A	C2-N3-C4	19.15	120.18	110.60
22	23S1	655	A	N1-C6-N6	-19.15	107.11	118.60
1	16S1	205	A	C2-N3-C4	19.15	120.18	110.60
1	16S1	747	A	N1-C6-N6	-19.15	107.11	118.60
22	23S1	1654	A	N1-C2-N3	-19.15	119.72	129.30
1	16S1	487	A	C2-N3-C4	19.15	120.17	110.60
1	16S1	1167	A	N1-C2-N3	-19.15	119.72	129.30
22	23S1	2082	A	C2-N3-C4	19.15	120.17	110.60
1	16S1	167	A	C2-N3-C4	19.15	120.17	110.60
1	16S1	160	A	N1-C2-N3	-19.15	119.73	129.30
1	16S1	1306	A	C2-N3-C4	19.15	120.17	110.60
22	23S1	213	A	C2-N3-C4	19.15	120.17	110.60
22	23S1	1635	A	N1-C6-N6	-19.15	107.11	118.60
22	23S1	979	A	N1-C2-N3	-19.14	119.73	129.30
22	23S1	6	A	C2-N3-C4	19.14	120.17	110.60
22	23S1	270	A	N1-C2-N3	-19.14	119.73	129.30
22	23S1	282	A	N1-C2-N3	-19.14	119.73	129.30
22	23S1	2478	A	N1-C6-N6	-19.14	107.11	118.60
23	05S1	104	A	N1-C2-N3	-19.14	119.73	129.30
1	16S1	996	A	C2-N3-C4	19.14	120.17	110.60
1	16S1	1271	A	C2-N3-C4	19.14	120.17	110.60
22	23S1	73	A	N1-C6-N6	-19.14	107.12	118.60
22	23S1	348	A	C2-N3-C4	19.14	120.17	110.60
1	16S1	946	A	C2-N3-C4	19.14	120.17	110.60
22	23S1	2516	A	C2-N3-C4	19.14	120.17	110.60
22	23S1	2749	A	N1-C2-N3	-19.14	119.73	129.30
55	PTR1	69	A	N1-C2-N3	-19.14	119.73	129.30
1	16S1	8	A	N1-C2-N3	-19.14	119.73	129.30
1	16S1	1288	A	N1-C2-N3	-19.14	119.73	129.30
22	23S1	165	A	N1-C2-N3	-19.14	119.73	129.30
22	23S1	515	A	C2-N3-C4	19.14	120.17	110.60
22	23S1	750	A	N1-C2-N3	-19.14	119.73	129.30
22	23S1	1579	A	N1-C2-N3	-19.14	119.73	129.30
1	16S1	364	A	C2-N3-C4	19.13	120.17	110.60
22	23S1	104	A	C2-N3-C4	19.13	120.17	110.60
22	23S1	310	A	N1-C2-N3	-19.13	119.73	129.30
22	23S1	513	A	C2-N3-C4	19.13	120.17	110.60
22	23S1	1147	A	C2-N3-C4	19.13	120.17	110.60
22	23S1	1307	A	C2-N3-C4	19.13	120.17	110.60
22	23S1	2809	A	N1-C2-N3	-19.13	119.73	129.30
22	23S1	1032	A	N1-C2-N3	-19.13	119.73	129.30
1	16S1	1151	A	C2-N3-C4	19.13	120.17	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	432	A	N1-C6-N6	-19.13	107.12	118.60
22	23S1	1204	A	C2-N3-C4	19.13	120.16	110.60
1	16S1	327	A	C2-N3-C4	19.13	120.16	110.60
1	16S1	1256	A	N1-C2-N3	-19.13	119.74	129.30
22	23S1	155	A	N1-C6-N6	-19.13	107.12	118.60
22	23S1	1048	A	C2-N3-C4	19.13	120.16	110.60
1	16S1	1180	A	N1-C2-N3	-19.12	119.74	129.30
22	23S1	217	A	N1-C6-N6	-19.12	107.13	118.60
22	23S1	917	A	N1-C6-N6	-19.12	107.12	118.60
1	16S1	356	A	N1-C2-N3	-19.12	119.74	129.30
1	16S1	539	A	N1-C2-N3	-19.12	119.74	129.30
22	23S1	2660	A	N1-C2-N3	-19.12	119.74	129.30
22	23S1	262	A	C2-N3-C4	19.12	120.16	110.60
22	23S1	802	A	N1-C6-N6	-19.12	107.13	118.60
1	16S1	704	A	C2-N3-C4	19.12	120.16	110.60
22	23S1	749	A	C2-N3-C4	19.12	120.16	110.60
22	23S1	2052	A	N1-C6-N6	-19.12	107.13	118.60
22	23S1	2809	A	N1-C6-N6	-19.12	107.13	118.60
22	23S1	118	A	C2-N3-C4	19.11	120.16	110.60
22	23S1	1126	A	C2-N3-C4	19.11	120.16	110.60
22	23S1	1494	A	N1-C6-N6	-19.11	107.13	118.60
22	23S1	2518	A	N1-C6-N6	-19.11	107.13	118.60
22	23S1	2679	A	N1-C2-N3	-19.11	119.74	129.30
1	16S1	119	A	N1-C2-N3	-19.11	119.74	129.30
1	16S1	274	A	C2-N3-C4	19.11	120.16	110.60
22	23S1	119	A	C2-N3-C4	19.11	120.16	110.60
1	16S1	456	A	N1-C2-N3	-19.11	119.75	129.30
1	16S1	787	A	N1-C6-N6	-19.11	107.13	118.60
22	23S1	2352	A	C2-N3-C4	19.11	120.16	110.60
55	PTR1	9	A	N1-C2-N3	-19.11	119.75	129.30
1	16S1	892	A	N1-C2-N3	-19.11	119.75	129.30
1	16S1	1329	A	N1-C2-N3	-19.11	119.75	129.30
22	23S1	167	A	N1-C2-N3	-19.11	119.75	129.30
22	23S1	1960	A	N1-C2-N3	-19.11	119.75	129.30
22	23S1	1384	A	C2-N3-C4	19.11	120.15	110.60
1	16S1	338	A	N1-C2-N3	-19.11	119.75	129.30
22	23S1	1932	A	N1-C2-N3	-19.11	119.75	129.30
22	23S1	1336	A	C2-N3-C4	19.10	120.15	110.60
22	23S1	2071	A	N1-C6-N6	-19.10	107.14	118.60
22	23S1	2335	A	C2-N3-C4	19.10	120.15	110.60
1	16S1	435	A	N1-C2-N3	-19.10	119.75	129.30
1	16S1	1250	A	N1-C2-N3	-19.10	119.75	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2366	A	C2-N3-C4	19.10	120.15	110.60
1	16S1	782	A	N1-C2-N3	-19.10	119.75	129.30
1	16S1	1111	A	N1-C2-N3	-19.10	119.75	129.30
22	23S1	1650	A	C2-N3-C4	19.10	120.15	110.60
23	05S1	94	A	C2-N3-C4	19.10	120.15	110.60
1	16S1	553	A	N1-C6-N6	-19.10	107.14	118.60
1	16S1	825	A	N1-C2-N3	-19.10	119.75	129.30
22	23S1	371	A	N1-C2-N3	-19.10	119.75	129.30
1	16S1	665	A	C2-N3-C4	19.10	120.15	110.60
1	16S1	1179	A	N1-C6-N6	-19.10	107.14	118.60
22	23S1	309	A	N1-C6-N6	-19.10	107.14	118.60
22	23S1	362	A	C2-N3-C4	19.10	120.15	110.60
22	23S1	1637	A	N1-C2-N3	-19.10	119.75	129.30
22	23S1	1866	A	C2-N3-C4	19.10	120.15	110.60
22	23S1	2468	A	C2-N3-C4	19.10	120.15	110.60
1	16S1	1	A	C2-N3-C4	19.10	120.15	110.60
1	16S1	1261	A	C2-N3-C4	19.09	120.15	110.60
22	23S1	466	A	N1-C2-N3	-19.09	119.75	129.30
22	23S1	829	A	N1-C2-N3	-19.09	119.75	129.30
22	23S1	1952	A	N1-C6-N6	-19.09	107.14	118.60
1	16S1	600	A	C2-N3-C4	19.09	120.15	110.60
1	16S1	1377	A	N1-C2-N3	-19.09	119.75	129.30
22	23S1	626	A	N1-C2-N3	-19.09	119.75	129.30
22	23S1	1054	A	C2-N3-C4	19.09	120.15	110.60
22	23S1	1129	A	N1-C6-N6	-19.09	107.15	118.60
23	05S1	50	A	C2-N3-C4	19.09	120.15	110.60
22	23S1	513	A	N1-C2-N3	-19.09	119.75	129.30
22	23S1	941	A	N1-C6-N6	-19.09	107.15	118.60
22	23S1	2820	A	N1-C6-N6	-19.09	107.15	118.60
1	16S1	1016	A	N1-C2-N3	-19.09	119.76	129.30
1	16S1	1111	A	C2-N3-C4	19.09	120.14	110.60
1	16S1	1275	A	C2-N3-C4	19.09	120.14	110.60
1	16S1	1287	A	N1-C6-N6	-19.09	107.15	118.60
23	05S1	101	A	N1-C6-N6	-19.09	107.15	118.60
22	23S1	144	A	C2-N3-C4	19.09	120.14	110.60
22	23S1	2386	A	C2-N3-C4	19.09	120.14	110.60
1	16S1	373	A	C2-N3-C4	19.09	120.14	110.60
1	16S1	1081	A	C2-N3-C4	19.09	120.14	110.60
22	23S1	752	A	C2-N3-C4	19.09	120.14	110.60
22	23S1	1701	A	N1-C6-N6	-19.09	107.15	118.60
22	23S1	603	A	N1-C6-N6	-19.08	107.15	118.60
22	23S1	1634	A	N1-C2-N3	-19.08	119.76	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1755	A	N1-C2-N3	-19.08	119.76	129.30
1	16S1	116	A	N1-C2-N3	-19.08	119.76	129.30
22	23S1	126	A	C2-N3-C4	19.08	120.14	110.60
22	23S1	1413	A	N1-C2-N3	-19.08	119.76	129.30
22	23S1	1690	A	N1-C2-N3	-19.08	119.76	129.30
23	05S1	78	A	N1-C2-N3	-19.08	119.76	129.30
22	23S1	706	A	N1-C6-N6	-19.08	107.15	118.60
22	23S1	1328	A	C2-N3-C4	19.08	120.14	110.60
1	16S1	729	A	C2-N3-C4	19.08	120.14	110.60
1	16S1	1256	A	C2-N3-C4	19.08	120.14	110.60
22	23S1	825	A	N1-C2-N3	-19.08	119.76	129.30
22	23S1	1189	A	N1-C2-N3	-19.08	119.76	129.30
1	16S1	414	A	N1-C2-N3	-19.08	119.76	129.30
1	16S1	906	A	N1-C2-N3	-19.08	119.76	129.30
1	16S1	1213	A	N1-C2-N3	-19.08	119.76	129.30
22	23S1	1095	A	N1-C2-N3	-19.08	119.76	129.30
22	23S1	2183	A	N1-C2-N3	-19.08	119.76	129.30
22	23S1	2872	A	C2-N3-C4	19.08	120.14	110.60
1	16S1	547	A	N1-C6-N6	-19.08	107.15	118.60
1	16S1	907	A	C2-N3-C4	19.08	120.14	110.60
22	23S1	1744	A	N1-C6-N6	-19.08	107.16	118.60
1	16S1	1480	A	N1-C2-N3	-19.07	119.76	129.30
22	23S1	49	A	N1-C2-N3	-19.07	119.76	129.30
22	23S1	633	A	N1-C2-N3	-19.07	119.76	129.30
22	23S1	1067	A	N1-C2-N3	-19.07	119.76	129.30
22	23S1	1070	A	N1-C2-N3	-19.07	119.76	129.30
23	05S1	34	A	C2-N3-C4	19.07	120.14	110.60
1	16S1	1332	A	N1-C6-N6	-19.07	107.16	118.60
22	23S1	1819	A	C2-N3-C4	19.07	120.14	110.60
22	23S1	1495	A	C2-N3-C4	19.07	120.14	110.60
22	23S1	28	A	C2-N3-C4	19.07	120.14	110.60
22	23S1	508	A	N1-C2-N3	-19.07	119.77	129.30
1	16S1	694	A	C2-N3-C4	19.07	120.13	110.60
1	16S1	889	A	N1-C2-N3	-19.07	119.77	129.30
22	23S1	347	A	C2-N3-C4	19.07	120.13	110.60
22	23S1	1757	A	N1-C6-N6	-19.07	107.16	118.60
1	16S1	1117	A	N1-C2-N3	-19.07	119.77	129.30
22	23S1	1096	A	N1-C2-N3	-19.07	119.77	129.30
22	23S1	1672	A	N1-C2-N3	-19.07	119.77	129.30
22	23S1	2009	A	N1-C2-N3	-19.07	119.77	129.30
22	23S1	2635	A	C2-N3-C4	19.07	120.13	110.60
22	23S1	2872	A	C5-C6-N6	19.07	138.95	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	499	A	N1-C2-N3	-19.06	119.77	129.30
1	16S1	1080	A	N1-C2-N3	-19.06	119.77	129.30
1	16S1	1239	A	N1-C2-N3	-19.06	119.77	129.30
22	23S1	1039	A	N1-C6-N6	-19.06	107.16	118.60
1	16S1	533	A	N1-C6-N6	-19.06	107.16	118.60
22	23S1	1194	A	N1-C6-N6	-19.06	107.16	118.60
22	23S1	2377	A	N1-C2-N3	-19.06	119.77	129.30
22	23S1	586	A	N1-C2-N3	-19.06	119.77	129.30
22	23S1	753	A	N1-C2-N3	-19.06	119.77	129.30
22	23S1	1420	A	C2-N3-C4	19.06	120.13	110.60
22	23S1	1772	A	C2-N3-C4	19.06	120.13	110.60
22	23S1	2635	A	N1-C6-N6	-19.06	107.16	118.60
23	05S1	45	A	C2-N3-C4	19.06	120.13	110.60
22	23S1	699	A	C2-N3-C4	19.06	120.13	110.60
1	16S1	466	A	C2-N3-C4	19.06	120.13	110.60
1	16S1	767	A	C2-N3-C4	19.06	120.13	110.60
1	16S1	915	A	N1-C2-N3	-19.06	119.77	129.30
1	16S1	996	A	N1-C6-N6	-19.06	107.17	118.60
22	23S1	905	A	N1-C2-N3	-19.06	119.77	129.30
22	23S1	1151	A	C2-N3-C4	19.06	120.13	110.60
22	23S1	1321	A	N1-C2-N3	-19.06	119.77	129.30
22	23S1	1413	A	C2-N3-C4	19.06	120.13	110.60
22	23S1	1640	A	N1-C2-N3	-19.06	119.77	129.30
22	23S1	2333	A	C2-N3-C4	19.06	120.13	110.60
22	23S1	2425	A	C2-N3-C4	19.06	120.13	110.60
1	16S1	1105	A	C2-N3-C4	19.05	120.13	110.60
22	23S1	2317	A	N1-C6-N6	-19.05	107.17	118.60
22	23S1	715	A	N1-C6-N6	-19.05	107.17	118.60
22	23S1	1194	A	N1-C2-N3	-19.05	119.77	129.30
22	23S1	2711	A	N1-C6-N6	-19.05	107.17	118.60
22	23S1	203	A	N1-C2-N3	-19.05	119.77	129.30
22	23S1	2070	A	C2-N3-C4	19.05	120.13	110.60
1	16S1	465	A	N1-C2-N3	-19.05	119.78	129.30
1	16S1	1016	A	N1-C6-N6	-19.05	107.17	118.60
22	23S1	218	A	C2-N3-C4	19.05	120.13	110.60
1	16S1	309	A	N1-C6-N6	-19.05	107.17	118.60
22	23S1	42	A	N1-C2-N3	-19.05	119.78	129.30
22	23S1	945	A	C2-N3-C4	19.05	120.12	110.60
22	23S1	1032	A	C2-N3-C4	19.05	120.12	110.60
22	23S1	2358	A	N1-C2-N3	-19.05	119.78	129.30
22	23S1	614	A	N1-C2-N3	-19.05	119.78	129.30
22	23S1	1244	A	C2-N3-C4	19.05	120.12	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2278	A	C2-N3-C4	19.05	120.12	110.60
22	23S1	2327	A	N1-C6-N6	-19.05	107.17	118.60
22	23S1	1067	A	N1-C6-N6	-19.04	107.17	118.60
22	23S1	1373	A	C2-N3-C4	19.04	120.12	110.60
22	23S1	2461	A	N1-C6-N6	-19.04	107.17	118.60
1	16S1	1311	A	N1-C2-N3	-19.04	119.78	129.30
22	23S1	454	A	N1-C2-N3	-19.04	119.78	129.30
22	23S1	996	A	C2-N3-C4	19.04	120.12	110.60
22	23S1	1566	A	N1-C6-N6	-19.04	107.18	118.60
1	16S1	1055	A	C2-N3-C4	19.04	120.12	110.60
1	16S1	10	A	C2-N3-C4	19.04	120.12	110.60
22	23S1	226	A	N1-C6-N6	-19.04	107.18	118.60
22	23S1	2886	A	N1-C2-N3	-19.04	119.78	129.30
1	16S1	1236	A	N1-C2-N3	-19.03	119.78	129.30
22	23S1	5	A	C2-N3-C4	19.03	120.12	110.60
22	23S1	752	A	N1-C2-N3	-19.03	119.78	129.30
22	23S1	1783	A	N1-C2-N3	-19.03	119.78	129.30
22	23S1	2052	A	N1-C2-N3	-19.03	119.78	129.30
1	16S1	1082	A	N1-C6-N6	-19.03	107.18	118.60
1	16S1	790	A	C2-N3-C4	19.03	120.11	110.60
1	16S1	1248	A	N1-C2-N3	-19.03	119.78	129.30
1	16S1	1287	A	N1-C2-N3	-19.03	119.78	129.30
22	23S1	197	A	C2-N3-C4	19.03	120.12	110.60
22	23S1	233	A	N1-C2-N3	-19.03	119.78	129.30
22	23S1	608	A	N1-C2-N3	-19.03	119.78	129.30
22	23S1	2095	A	N1-C2-N3	-19.03	119.78	129.30
1	16S1	946	A	N1-C2-N3	-19.03	119.79	129.30
1	16S1	563	A	N1-C2-N3	-19.03	119.79	129.30
22	23S1	155	A	N1-C2-N3	-19.03	119.79	129.30
22	23S1	156	A	C2-N3-C4	19.03	120.11	110.60
22	23S1	1762	A	N1-C2-N3	-19.03	119.79	129.30
1	16S1	792	A	N1-C6-N6	-19.03	107.19	118.60
22	23S1	821	A	C2-N3-C4	19.02	120.11	110.60
22	23S1	1213	A	N1-C2-N3	-19.02	119.79	129.30
22	23S1	1579	A	C2-N3-C4	19.02	120.11	110.60
22	23S1	2119	A	N1-C2-N3	-19.02	119.79	129.30
22	23S1	2560	A	N1-C6-N6	-19.02	107.19	118.60
1	16S1	532	A	N1-C2-N3	-19.02	119.79	129.30
22	23S1	1111	A	N1-C2-N3	-19.02	119.79	129.30
22	23S1	1274	A	N1-C2-N3	-19.02	119.79	129.30
22	23S1	1641	A	N1-C2-N3	-19.02	119.79	129.30
22	23S1	2541	A	C2-N3-C4	19.02	120.11	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	120	A	N1-C6-N6	-19.02	107.19	118.60
1	16S1	994	A	N1-C2-N3	-19.02	119.79	129.30
22	23S1	300	A	N1-C6-N6	-19.02	107.19	118.60
22	23S1	661	A	C2-N3-C4	19.02	120.11	110.60
22	23S1	83	A	C2-N3-C4	19.02	120.11	110.60
22	23S1	1453	A	C2-N3-C4	19.02	120.11	110.60
22	23S1	1453	A	N1-C2-N3	-19.02	119.79	129.30
1	16S1	1408	A	C2-N3-C4	19.02	120.11	110.60
22	23S1	1689	A	C2-N3-C4	19.02	120.11	110.60
1	16S1	1169	A	N1-C2-N3	-19.01	119.79	129.30
22	23S1	412	A	C2-N3-C4	19.01	120.11	110.60
22	23S1	730	A	C2-N3-C4	19.01	120.11	110.60
22	23S1	1700	A	N1-C6-N6	-19.01	107.19	118.60
22	23S1	2518	A	N1-C2-N3	-19.01	119.79	129.30
22	23S1	217	A	C2-N3-C4	19.01	120.11	110.60
22	23S1	2837	A	N1-C2-N3	-19.01	119.79	129.30
22	23S1	311	A	C2-N3-C4	19.01	120.11	110.60
22	23S1	479	A	C2-N3-C4	19.01	120.11	110.60
22	23S1	1669	A	N1-C6-N6	-19.01	107.19	118.60
22	23S1	152	A	C2-N3-C4	19.01	120.10	110.60
22	23S1	2378	A	N1-C2-N3	-19.01	119.80	129.30
22	23S1	2513	A	N1-C2-N3	-19.01	119.80	129.30
1	16S1	26	A	C2-N3-C4	19.00	120.10	110.60
1	16S1	181	A	C2-N3-C4	19.00	120.10	110.60
1	16S1	459	A	N1-C2-N3	-19.00	119.80	129.30
1	16S1	864	A	C2-N3-C4	19.00	120.10	110.60
22	23S1	905	A	C2-N3-C4	19.00	120.10	110.60
22	23S1	1597	A	C2-N3-C4	19.00	120.10	110.60
1	16S1	129	A	C2-N3-C4	19.00	120.10	110.60
1	16S1	1346	A	C2-N3-C4	19.00	120.10	110.60
22	23S1	945	A	N1-C2-N3	-19.00	119.80	129.30
22	23S1	1427	A	C2-N3-C4	19.00	120.10	110.60
1	16S1	1111	A	N1-C6-N6	-19.00	107.20	118.60
22	23S1	311	A	N1-C2-N3	-19.00	119.80	129.30
22	23S1	616	A	N1-C6-N6	-19.00	107.20	118.60
22	23S1	1050	A	N1-C2-N3	-19.00	119.80	129.30
22	23S1	2042	A	C2-N3-C4	19.00	120.10	110.60
1	16S1	535	A	N1-C2-N3	-19.00	119.80	129.30
22	23S1	2711	A	C2-N3-C4	19.00	120.10	110.60
1	16S1	482	A	N1-C2-N3	-19.00	119.80	129.30
22	23S1	781	A	N1-C6-N6	-19.00	107.20	118.60
1	16S1	1014	A	N1-C2-N3	-19.00	119.80	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2062	A	N1-C6-N6	-19.00	107.20	118.60
22	23S1	2879	A	C2-N3-C4	19.00	120.10	110.60
1	16S1	1035	A	C2-N3-C4	19.00	120.10	110.60
22	23S1	429	A	N1-C6-N6	-19.00	107.20	118.60
22	23S1	734	A	C2-N3-C4	19.00	120.10	110.60
22	23S1	2101	A	N1-C2-N3	-19.00	119.80	129.30
22	23S1	2369	A	C2-N3-C4	19.00	120.10	110.60
1	16S1	554	A	C2-N3-C4	18.99	120.10	110.60
1	16S1	759	A	N1-C6-N6	-18.99	107.20	118.60
22	23S1	2134	A	N1-C2-N3	-18.99	119.80	129.30
1	16S1	559	A	N1-C2-N3	-18.99	119.80	129.30
22	23S1	279	A	N1-C2-N3	-18.99	119.80	129.30
22	23S1	423	A	C2-N3-C4	18.99	120.10	110.60
22	23S1	685	A	C2-N3-C4	18.99	120.10	110.60
55	PTR1	73	A	N1-C2-N3	-18.99	119.80	129.30
1	16S1	865	A	C2-N3-C4	18.99	120.10	110.60
22	23S1	2547	A	C2-N3-C4	18.99	120.10	110.60
22	23S1	56	A	C2-N3-C4	18.99	120.09	110.60
22	23S1	111	A	N1-C2-N3	-18.99	119.81	129.30
22	23S1	2634	A	C2-N3-C4	18.99	120.09	110.60
22	23S1	2814	A	N1-C2-N3	-18.99	119.81	129.30
1	16S1	243	A	N1-C2-N3	-18.99	119.81	129.30
1	16S1	382	A	N1-C2-N3	-18.99	119.81	129.30
1	16S1	1285	A	N1-C6-N6	-18.99	107.21	118.60
22	23S1	415	A	C2-N3-C4	18.99	120.09	110.60
22	23S1	1205	A	N1-C6-N6	-18.98	107.21	118.60
22	23S1	782	A	N1-C6-N6	-18.98	107.21	118.60
55	PTR1	26	A	C2-N3-C4	18.98	120.09	110.60
1	16S1	1433	A	N1-C2-N3	-18.98	119.81	129.30
22	23S1	1156	A	N1-C6-N6	-18.98	107.21	118.60
1	16S1	364	A	N1-C6-N6	-18.98	107.21	118.60
1	16S1	825	A	C2-N3-C4	18.98	120.09	110.60
22	23S1	89	A	N1-C2-N3	-18.98	119.81	129.30
22	23S1	382	A	C2-N3-C4	18.98	120.09	110.60
22	23S1	1269	A	C2-N3-C4	18.98	120.09	110.60
22	23S1	1419	A	C2-N3-C4	18.98	120.09	110.60
22	23S1	191	A	N1-C2-N3	-18.98	119.81	129.30
22	23S1	342	A	C2-N3-C4	18.97	120.09	110.60
22	23S1	2183	A	C2-N3-C4	18.97	120.09	110.60
1	16S1	44	A	C2-N3-C4	18.97	120.09	110.60
1	16S1	872	A	N1-C6-N6	-18.97	107.22	118.60
1	16S1	969	A	C2-N3-C4	18.97	120.09	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1014	A	C2-N3-C4	18.97	120.09	110.60
1	16S1	1430	A	N1-C2-N3	-18.97	119.81	129.30
55	PTR1	38	A	N1-C2-N3	-18.97	119.81	129.30
55	PTR1	42	A	N1-C2-N3	-18.97	119.81	129.30
1	16S1	553	A	N1-C2-N3	-18.97	119.81	129.30
1	16S1	949	A	N1-C6-N6	-18.97	107.22	118.60
1	16S1	1289	A	N1-C6-N6	-18.97	107.22	118.60
22	23S1	2184	A	N1-C6-N6	-18.97	107.22	118.60
1	16S1	749	A	C2-N3-C4	18.97	120.08	110.60
22	23S1	592	A	N1-C6-N6	-18.97	107.22	118.60
22	23S1	685	A	N1-C2-N3	-18.97	119.81	129.30
22	23S1	1084	A	N1-C6-N6	-18.97	107.22	118.60
22	23S1	1096	A	N1-C6-N6	-18.97	107.22	118.60
22	23S1	1142	A	N1-C6-N6	-18.97	107.22	118.60
22	23S1	1246	A	N1-C6-N6	-18.97	107.22	118.60
22	23S1	614	A	C2-N3-C4	18.97	120.08	110.60
22	23S1	1395	A	C2-N3-C4	18.97	120.08	110.60
1	16S1	65	A	N1-C2-N3	-18.97	119.82	129.30
22	23S1	575	A	C2-N3-C4	18.97	120.08	110.60
22	23S1	2119	A	C2-N3-C4	18.97	120.08	110.60
22	23S1	2377	A	C2-N3-C4	18.97	120.08	110.60
22	23S1	538	A	N1-C2-N3	-18.96	119.82	129.30
22	23S1	2577	A	N1-C6-N6	-18.96	107.22	118.60
22	23S1	322	A	C2-N3-C4	18.96	120.08	110.60
22	23S1	340	A	N1-C2-N3	-18.96	119.82	129.30
1	16S1	344	A	N1-C2-N3	-18.96	119.82	129.30
1	16S1	374	A	N1-C6-N6	-18.96	107.22	118.60
1	16S1	1362	A	N1-C2-N3	-18.96	119.82	129.30
22	23S1	324	A	N1-C2-N3	-18.96	119.82	129.30
22	23S1	384	A	N1-C6-N6	-18.96	107.22	118.60
1	16S1	1306	A	N1-C2-N3	-18.96	119.82	129.30
22	23S1	63	A	C2-N3-C4	18.96	120.08	110.60
22	23S1	181	A	N1-C2-N3	-18.96	119.82	129.30
22	23S1	1889	A	N1-C6-N6	-18.96	107.22	118.60
22	23S1	2097	A	N1-C6-N6	-18.96	107.22	118.60
1	16S1	298	A	C2-N3-C4	18.96	120.08	110.60
1	16S1	415	A	N1-C6-N6	-18.96	107.23	118.60
1	16S1	1021	A	C2-N3-C4	18.96	120.08	110.60
22	23S1	2868	A	N1-C2-N3	-18.96	119.82	129.30
1	16S1	1396	A	N1-C2-N3	-18.96	119.82	129.30
22	23S1	340	A	N1-C6-N6	-18.96	107.23	118.60
22	23S1	637	A	N1-C6-N6	-18.96	107.23	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	126	A	N1-C2-N3	-18.95	119.82	129.30
22	23S1	454	A	C2-N3-C4	18.95	120.08	110.60
22	23S1	2077	A	C2-N3-C4	18.95	120.08	110.60
1	16S1	1	A	N1-C2-N3	-18.95	119.82	129.30
1	16S1	1204	A	C2-N3-C4	18.95	120.08	110.60
22	23S1	654	A	N1-C6-N6	-18.95	107.23	118.60
22	23S1	959	A	N1-C6-N6	-18.95	107.23	118.60
22	23S1	1433	A	C2-N3-C4	18.95	120.08	110.60
22	23S1	2126	A	N1-C6-N6	-18.95	107.23	118.60
22	23S1	2837	A	N1-C6-N6	-18.95	107.23	118.60
22	23S1	2734	A	C2-N3-C4	18.95	120.08	110.60
22	23S1	2792	A	C2-N3-C4	18.95	120.08	110.60
1	16S1	559	A	C2-N3-C4	18.95	120.07	110.60
1	16S1	579	A	N1-C2-N3	-18.95	119.83	129.30
1	16S1	1456	A	C2-N3-C4	18.95	120.07	110.60
22	23S1	233	A	C2-N3-C4	18.95	120.07	110.60
22	23S1	1301	A	N1-C2-N3	-18.95	119.83	129.30
1	16S1	288	A	N1-C6-N6	-18.95	107.23	118.60
1	16S1	1534	A	C2-N3-C4	18.95	120.07	110.60
22	23S1	2850	A	C2-N3-C4	18.95	120.07	110.60
23	05S1	115	A	C2-N3-C4	18.95	120.07	110.60
1	16S1	655	A	C2-N3-C4	18.94	120.07	110.60
22	23S1	172	A	C2-N3-C4	18.94	120.07	110.60
22	23S1	1308	A	N1-C2-N3	-18.94	119.83	129.30
22	23S1	1596	A	C2-N3-C4	18.94	120.07	110.60
1	16S1	523	A	C2-N3-C4	18.94	120.07	110.60
22	23S1	262	A	N1-C6-N6	-18.94	107.23	118.60
22	23S1	541	A	C2-N3-C4	18.94	120.07	110.60
22	23S1	590	A	N1-C6-N6	-18.94	107.24	118.60
22	23S1	1453	A	N1-C6-N6	-18.94	107.24	118.60
22	23S1	1802	A	C2-N3-C4	18.94	120.07	110.60
22	23S1	2418	A	N1-C2-N3	-18.94	119.83	129.30
22	23S1	1705	A	C2-N3-C4	18.94	120.07	110.60
22	23S1	1872	A	C2-N3-C4	18.94	120.07	110.60
22	23S1	2169	A	C2-N3-C4	18.94	120.07	110.60
22	23S1	310	A	N1-C6-N6	-18.93	107.24	118.60
22	23S1	1532	A	C2-N3-C4	18.93	120.07	110.60
1	16S1	816	A	N1-C2-N3	-18.93	119.83	129.30
1	16S1	1036	A	C2-N3-C4	18.93	120.06	110.60
22	23S1	28	A	N1-C6-N6	-18.93	107.24	118.60
22	23S1	661	A	N1-C2-N3	-18.93	119.83	129.30
22	23S1	1147	A	N1-C2-N3	-18.93	119.83	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1265	A	N1-C2-N3	-18.93	119.83	129.30
22	23S1	1735	A	C2-N3-C4	18.93	120.07	110.60
1	16S1	373	A	N1-C2-N3	-18.93	119.84	129.30
1	16S1	807	A	N1-C2-N3	-18.93	119.84	129.30
1	16S1	814	A	N1-C6-N6	-18.93	107.24	118.60
1	16S1	1035	A	N1-C6-N6	-18.93	107.24	118.60
1	16S1	1377	A	C2-N3-C4	18.93	120.06	110.60
22	23S1	2340	A	C2-N3-C4	18.93	120.06	110.60
1	16S1	411	A	C2-N3-C4	18.93	120.06	110.60
1	16S1	974	A	C2-N3-C4	18.93	120.06	110.60
1	16S1	1269	A	N1-C2-N3	-18.93	119.84	129.30
22	23S1	1070	A	C2-N3-C4	18.93	120.06	110.60
22	23S1	1046	A	N1-C2-N3	-18.93	119.84	129.30
22	23S1	1494	A	N1-C2-N3	-18.93	119.84	129.30
22	23S1	2158	A	N1-C2-N3	-18.93	119.84	129.30
22	23S1	602	A	N1-C6-N6	-18.92	107.25	118.60
22	23S1	1151	A	N1-C2-N3	-18.92	119.84	129.30
1	16S1	493	A	N1-C2-N3	-18.92	119.84	129.30
22	23S1	1912	A	C2-N3-C4	18.92	120.06	110.60
22	23S1	2821	A	N1-C2-N3	-18.92	119.84	129.30
1	16S1	363	A	C2-N3-C4	18.92	120.06	110.60
1	16S1	408	A	N1-C6-N6	-18.92	107.25	118.60
1	16S1	1042	A	N1-C2-N3	-18.92	119.84	129.30
22	23S1	925	A	C2-N3-C4	18.92	120.06	110.60
22	23S1	1272	A	N1-C2-N3	-18.92	119.84	129.30
22	23S1	2572	A	C2-N3-C4	18.92	120.06	110.60
22	23S1	217	A	N1-C2-N3	-18.92	119.84	129.30
22	23S1	218	A	N1-C6-N6	-18.92	107.25	118.60
22	23S1	1854	A	N1-C2-N3	-18.92	119.84	129.30
22	23S1	2497	A	N1-C6-N6	-18.92	107.25	118.60
22	23S1	508	A	C2-N3-C4	18.92	120.06	110.60
22	23S1	2225	A	N1-C6-N6	-18.92	107.25	118.60
1	16S1	696	A	C2-N3-C4	18.91	120.06	110.60
1	16S1	702	A	N1-C6-N6	-18.91	107.25	118.60
22	23S1	478	A	N1-C2-N3	-18.91	119.84	129.30
22	23S1	532	A	N1-C2-N3	-18.91	119.84	129.30
22	23S1	1808	A	N1-C2-N3	-18.91	119.84	129.30
1	16S1	1229	A	N1-C6-N6	-18.91	107.25	118.60
22	23S1	1366	A	N1-C6-N6	-18.91	107.25	118.60
22	23S1	2459	A	C2-N3-C4	18.91	120.06	110.60
23	05S1	59	A	N1-C6-N6	-18.91	107.25	118.60
1	16S1	325	A	C2-N3-C4	18.91	120.06	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2471	A	N1-C2-N3	-18.91	119.84	129.30
1	16S1	10	A	N1-C6-N6	-18.91	107.25	118.60
1	16S1	642	A	C2-N3-C4	18.91	120.05	110.60
22	23S1	1773	A	N1-C2-N3	-18.91	119.85	129.30
22	23S1	2003	A	N1-C6-N6	-18.91	107.26	118.60
1	16S1	969	A	N1-C6-N6	-18.91	107.26	118.60
22	23S1	764	A	N1-C6-N6	-18.91	107.26	118.60
22	23S1	789	A	N1-C6-N6	-18.91	107.26	118.60
22	23S1	793	A	N1-C2-N3	-18.91	119.85	129.30
22	23S1	819	A	N1-C2-N3	-18.91	119.85	129.30
22	23S1	1262	A	N1-C2-N3	-18.91	119.85	129.30
22	23S1	705	A	C2-N3-C4	18.90	120.05	110.60
1	16S1	238	A	N1-C6-N6	-18.90	107.26	118.60
22	23S1	344	A	N1-C2-N3	-18.90	119.85	129.30
22	23S1	1652	A	N1-C2-N3	-18.90	119.85	129.30
22	23S1	2426	A	C2-N3-C4	18.90	120.05	110.60
1	16S1	831	A	N1-C2-N3	-18.90	119.85	129.30
22	23S1	1384	A	N1-C6-N6	-18.90	107.26	118.60
1	16S1	353	A	N1-C2-N3	-18.90	119.85	129.30
1	16S1	535	A	C2-N3-C4	18.90	120.05	110.60
1	16S1	139	A	N1-C2-N3	-18.90	119.85	129.30
1	16S1	448	A	N1-C6-N6	-18.90	107.26	118.60
22	23S1	1780	A	C2-N3-C4	18.90	120.05	110.60
1	16S1	152	A	C2-N3-C4	18.89	120.05	110.60
1	16S1	753	A	N1-C6-N6	-18.89	107.26	118.60
1	16S1	1318	A	C2-N3-C4	18.89	120.05	110.60
1	16S1	72	A	N1-C2-N3	-18.89	119.85	129.30
22	23S1	716	A	C2-N3-C4	18.89	120.05	110.60
1	16S1	1492	A	C2-N3-C4	18.89	120.05	110.60
22	23S1	1050	A	N1-C6-N6	-18.89	107.27	118.60
22	23S1	44	A	N1-C6-N6	-18.89	107.27	118.60
22	23S1	64	A	C2-N3-C4	18.89	120.05	110.60
22	23S1	342	A	N1-C2-N3	-18.89	119.85	129.30
22	23S1	556	A	N1-C2-N3	-18.89	119.86	129.30
22	23S1	1027	A	N1-C2-N3	-18.89	119.85	129.30
22	23S1	1269	A	N1-C6-N6	-18.89	107.27	118.60
1	16S1	1447	A	N1-C2-N3	-18.89	119.86	129.30
1	16S1	1447	A	N1-C6-N6	-18.89	107.27	118.60
22	23S1	1783	A	N1-C6-N6	-18.89	107.27	118.60
1	16S1	495	A	N1-C6-N6	-18.89	107.27	118.60
1	16S1	1093	A	N1-C2-N3	-18.89	119.86	129.30
22	23S1	794	A	N1-C6-N6	-18.89	107.27	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	616	A	C2-N3-C4	18.89	120.04	110.60
22	23S1	1103	A	N1-C2-N3	-18.89	119.86	129.30
22	23S1	2169	A	N1-C6-N6	-18.89	107.27	118.60
22	23S1	1509	A	N1-C2-N3	-18.88	119.86	129.30
22	23S1	2820	A	N1-C2-N3	-18.88	119.86	129.30
22	23S1	320	A	C2-N3-C4	18.88	120.04	110.60
22	23S1	430	A	N1-C2-N3	-18.88	119.86	129.30
22	23S1	477	A	C2-N3-C4	18.88	120.04	110.60
22	23S1	911	A	N1-C2-N3	-18.88	119.86	129.30
22	23S1	2639	A	N1-C6-N6	-18.88	107.27	118.60
23	05S1	39	A	N1-C2-N3	-18.88	119.86	129.30
1	16S1	1377	A	N1-C6-N6	-18.88	107.27	118.60
22	23S1	2478	A	C2-N3-C4	18.88	120.04	110.60
22	23S1	2726	A	C2-N3-C4	18.88	120.04	110.60
1	16S1	635	A	C2-N3-C4	18.88	120.04	110.60
1	16S1	767	A	N1-C2-N3	-18.88	119.86	129.30
1	16S1	364	A	N1-C2-N3	-18.88	119.86	129.30
1	16S1	792	A	C2-N3-C4	18.88	120.04	110.60
22	23S1	1433	A	N1-C2-N3	-18.88	119.86	129.30
1	16S1	600	A	N1-C2-N3	-18.87	119.86	129.30
1	16S1	996	A	N1-C2-N3	-18.87	119.86	129.30
22	23S1	1505	A	C2-N3-C4	18.87	120.04	110.60
1	16S1	432	A	C2-N3-C4	18.87	120.03	110.60
22	23S1	574	A	C2-N3-C4	18.87	120.03	110.60
22	23S1	1596	A	N1-C6-N6	-18.87	107.28	118.60
22	23S1	1877	A	N1-C6-N6	-18.87	107.28	118.60
22	23S1	2135	A	C2-N3-C4	18.87	120.04	110.60
22	23S1	2899	A	N1-C2-N3	-18.87	119.86	129.30
1	16S1	749	A	N1-C2-N3	-18.87	119.86	129.30
22	23S1	404	A	N1-C2-N3	-18.87	119.87	129.30
23	05S1	46	A	N1-C6-N6	-18.87	107.28	118.60
1	16S1	120	A	N1-C2-N3	-18.87	119.87	129.30
1	16S1	572	A	C2-N3-C4	18.87	120.03	110.60
1	16S1	1110	A	N1-C2-N3	-18.87	119.87	129.30
22	23S1	820	A	C2-N3-C4	18.87	120.03	110.60
22	23S1	1966	A	C2-N3-C4	18.87	120.03	110.60
1	16S1	560	A	N1-C2-N3	-18.87	119.87	129.30
22	23S1	244	A	N1-C2-N3	-18.87	119.87	129.30
22	23S1	1637	A	N1-C6-N6	-18.87	107.28	118.60
22	23S1	165	A	C2-N3-C4	18.86	120.03	110.60
22	23S1	1134	A	N1-C6-N6	-18.86	107.28	118.60
1	16S1	1428	A	N1-C2-N3	-18.86	119.87	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1468	A	C2-N3-C4	18.86	120.03	110.60
22	23S1	1127	A	C2-N3-C4	18.86	120.03	110.60
22	23S1	1698	A	C2-N3-C4	18.86	120.03	110.60
22	23S1	1746	A	C2-N3-C4	18.86	120.03	110.60
22	23S1	2530	A	C2-N3-C4	18.86	120.03	110.60
22	23S1	2184	A	C2-N3-C4	18.86	120.03	110.60
22	23S1	2358	A	C2-N3-C4	18.86	120.03	110.60
22	23S1	2453	A	N1-C6-N6	-18.86	107.29	118.60
1	16S1	878	A	C2-N3-C4	18.86	120.03	110.60
1	16S1	1171	A	C2-N3-C4	18.86	120.03	110.60
22	23S1	896	A	C2-N3-C4	18.86	120.03	110.60
1	16S1	509	A	N1-C2-N3	-18.85	119.87	129.30
1	16S1	695	A	N1-C2-N3	-18.85	119.87	129.30
22	23S1	53	A	N1-C6-N6	-18.85	107.29	118.60
22	23S1	125	A	C2-N3-C4	18.85	120.03	110.60
22	23S1	1470	A	N1-C2-N3	-18.85	119.87	129.30
1	16S1	1146	A	C2-N3-C4	18.85	120.03	110.60
22	23S1	909	A	N1-C6-N6	-18.85	107.29	118.60
1	16S1	1363	A	N1-C6-N6	-18.85	107.29	118.60
22	23S1	1385	A	N1-C2-N3	-18.85	119.88	129.30
1	16S1	983	A	N1-C2-N3	-18.85	119.88	129.30
22	23S1	1050	A	C2-N3-C4	18.85	120.02	110.60
22	23S1	1264	A	N1-C6-N6	-18.85	107.29	118.60
22	23S1	2764	A	N1-C2-N3	-18.85	119.88	129.30
22	23S1	592	A	N1-C2-N3	-18.84	119.88	129.30
22	23S1	715	A	N1-C2-N3	-18.84	119.88	129.30
22	23S1	430	A	N1-C6-N6	-18.84	107.30	118.60
22	23S1	1885	A	C2-N3-C4	18.84	120.02	110.60
1	16S1	119	A	N1-C6-N6	-18.84	107.30	118.60
22	23S1	1626	A	N1-C2-N3	-18.84	119.88	129.30
22	23S1	2327	A	N1-C2-N3	-18.84	119.88	129.30
55	PTR1	3	A	N1-C2-N3	-18.84	119.88	129.30
1	16S1	718	A	N1-C2-N3	-18.84	119.88	129.30
22	23S1	1008	A	N1-C2-N3	-18.84	119.88	129.30
1	16S1	1042	A	C2-N3-C4	18.84	120.02	110.60
22	23S1	734	A	N1-C6-N6	-18.84	107.30	118.60
22	23S1	1367	A	N1-C6-N6	-18.84	107.30	118.60
22	23S1	2322	A	C2-N3-C4	18.84	120.02	110.60
1	16S1	1035	A	N1-C2-N3	-18.83	119.88	129.30
1	16S1	1362	A	C2-N3-C4	18.83	120.02	110.60
22	23S1	391	A	N1-C2-N3	-18.83	119.88	129.30
22	23S1	1142	A	N1-C2-N3	-18.83	119.88	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1366	A	N1-C2-N3	-18.83	119.88	129.30
22	23S1	2670	A	C2-N3-C4	18.83	120.02	110.60
22	23S1	654	A	N1-C2-N3	-18.83	119.89	129.30
22	23S1	693	A	N1-C2-N3	-18.83	119.89	129.30
22	23S1	2448	A	N1-C6-N6	-18.83	107.30	118.60
1	16S1	729	A	N1-C6-N6	-18.83	107.30	118.60
22	23S1	685	A	N1-C6-N6	-18.83	107.30	118.60
22	23S1	1008	A	C2-N3-C4	18.83	120.01	110.60
22	23S1	1689	A	N1-C2-N3	-18.83	119.89	129.30
22	23S1	2654	A	N1-C2-N3	-18.83	119.89	129.30
22	23S1	149	A	N1-C6-N6	-18.83	107.31	118.60
22	23S1	204	A	C2-N3-C4	18.83	120.01	110.60
1	16S1	532	A	N1-C6-N6	-18.82	107.31	118.60
1	16S1	546	A	C2-N3-C4	18.82	120.01	110.60
1	16S1	759	A	N1-C2-N3	-18.82	119.89	129.30
1	16S1	1105	A	N1-C2-N3	-18.82	119.89	129.30
22	23S1	470	A	C2-N3-C4	18.82	120.01	110.60
22	23S1	1938	A	C2-N3-C4	18.82	120.01	110.60
22	23S1	1286	A	C2-N3-C4	18.82	120.01	110.60
22	23S1	2241	A	N1-C2-N3	-18.82	119.89	129.30
1	16S1	78	A	N1-C2-N3	-18.82	119.89	129.30
1	16S1	1374	A	N1-C6-N6	-18.82	107.31	118.60
22	23S1	1378	A	C2-N3-C4	18.82	120.01	110.60
22	23S1	1785	A	C2-N3-C4	18.82	120.01	110.60
22	23S1	1885	A	N1-C6-N6	-18.82	107.31	118.60
1	16S1	274	A	N1-C2-N3	-18.82	119.89	129.30
1	16S1	1188	A	N1-C2-N3	-18.82	119.89	129.30
22	23S1	1096	A	C2-N3-C4	18.82	120.01	110.60
22	23S1	1126	A	N1-C6-N6	-18.82	107.31	118.60
22	23S1	1244	A	N1-C2-N3	-18.82	119.89	129.30
22	23S1	1553	A	C2-N3-C4	18.82	120.01	110.60
22	23S1	1085	A	N1-C2-N3	-18.82	119.89	129.30
22	23S1	1626	A	C2-N3-C4	18.82	120.01	110.60
22	23S1	2566	A	C2-N3-C4	18.82	120.01	110.60
1	16S1	19	A	N1-C2-N3	-18.82	119.89	129.30
1	16S1	101	A	N1-C2-N3	-18.82	119.89	129.30
22	23S1	556	A	C2-N3-C4	18.81	120.01	110.60
1	16S1	451	A	N1-C2-N3	-18.81	119.89	129.30
1	16S1	1340	A	C2-N3-C4	18.81	120.01	110.60
22	23S1	74	A	N1-C2-N3	-18.81	119.89	129.30
22	23S1	348	A	N1-C6-N6	-18.81	107.31	118.60
22	23S1	457	A	C2-N3-C4	18.81	120.01	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	750	A	N1-C6-N6	-18.81	107.31	118.60
1	16S1	1188	A	N1-C6-N6	-18.81	107.31	118.60
1	16S1	441	A	C2-N3-C4	18.81	120.00	110.60
1	16S1	595	A	N1-C2-N3	-18.81	119.89	129.30
1	16S1	831	A	C2-N3-C4	18.81	120.00	110.60
22	23S1	2037	A	N1-C2-N3	-18.81	119.90	129.30
22	23S1	2309	A	N1-C2-N3	-18.81	119.89	129.30
22	23S1	899	A	N1-C6-N6	-18.81	107.31	118.60
22	23S1	1652	A	C2-N3-C4	18.81	120.00	110.60
22	23S1	2284	A	N1-C6-N6	-18.81	107.31	118.60
1	16S1	71	A	N1-C2-N3	-18.81	119.90	129.30
1	16S1	167	A	N1-C6-N6	-18.81	107.32	118.60
1	16S1	1021	A	N1-C2-N3	-18.81	119.90	129.30
1	16S1	1252	A	N1-C2-N3	-18.81	119.90	129.30
22	23S1	19	A	C2-N3-C4	18.81	120.00	110.60
22	23S1	265	A	N1-C6-N6	-18.81	107.32	118.60
22	23S1	1571	A	N1-C2-N3	-18.81	119.90	129.30
22	23S1	1757	A	C2-N3-C4	18.81	120.00	110.60
22	23S1	2660	A	C2-N3-C4	18.81	120.00	110.60
22	23S1	2761	A	N1-C6-N6	-18.81	107.32	118.60
1	16S1	938	A	N1-C6-N6	-18.80	107.32	118.60
23	05S1	109	A	C2-N3-C4	18.80	120.00	110.60
1	16S1	72	A	N1-C6-N6	-18.80	107.32	118.60
1	16S1	1274	A	C2-N3-C4	18.80	120.00	110.60
1	16S1	1368	A	N1-C2-N3	-18.80	119.90	129.30
22	23S1	541	A	N1-C6-N6	-18.80	107.32	118.60
22	23S1	1009	A	N1-C6-N6	-18.80	107.32	118.60
22	23S1	1912	A	N1-C6-N6	-18.80	107.32	118.60
1	16S1	321	A	N1-C6-N6	-18.80	107.32	118.60
1	16S1	937	A	N1-C2-N3	-18.80	119.90	129.30
22	23S1	1678	A	C2-N3-C4	18.80	120.00	110.60
22	23S1	676	A	C2-N3-C4	18.80	120.00	110.60
22	23S1	2600	A	C2-N3-C4	18.80	120.00	110.60
22	23S1	2705	A	C2-N3-C4	18.80	120.00	110.60
22	23S1	2736	A	N1-C2-N3	-18.80	119.90	129.30
22	23S1	2497	A	N1-C2-N3	-18.80	119.90	129.30
1	16S1	263	A	C2-N3-C4	18.80	120.00	110.60
22	23S1	324	A	C2-N3-C4	18.80	120.00	110.60
22	23S1	896	A	N1-C2-N3	-18.80	119.90	129.30
22	23S1	2542	A	N1-C2-N3	-18.80	119.90	129.30
22	23S1	1241	A	C2-N3-C4	18.80	120.00	110.60
22	23S1	1590	A	C2-N3-C4	18.80	120.00	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2776	A	N1-C6-N6	-18.80	107.32	118.60
1	16S1	1429	A	N1-C2-N3	-18.79	119.90	129.30
1	16S1	238	A	N1-C2-N3	-18.79	119.90	129.30
1	16S1	432	A	N1-C6-N6	-18.79	107.33	118.60
22	23S1	2432	A	N1-C2-N3	-18.79	119.90	129.30
1	16S1	452	A	N1-C2-N3	-18.79	119.91	129.30
22	23S1	2314	A	N1-C2-N3	-18.79	119.90	129.30
1	16S1	1289	A	C2-N3-C4	18.79	119.99	110.60
1	16S1	900	A	N1-C2-N3	-18.79	119.91	129.30
1	16S1	1093	A	C2-N3-C4	18.79	119.99	110.60
22	23S1	443	A	C2-N3-C4	18.79	119.99	110.60
22	23S1	1144	A	N1-C2-N3	-18.79	119.91	129.30
23	05S1	29	A	N1-C2-N3	-18.79	119.91	129.30
1	16S1	1357	A	C2-N3-C4	18.79	119.99	110.60
22	23S1	2211	A	C2-N3-C4	18.78	119.99	110.60
1	16S1	523	A	N1-C2-N3	-18.78	119.91	129.30
22	23S1	1772	A	N1-C6-N6	-18.78	107.33	118.60
22	23S1	1791	A	N1-C2-N3	-18.78	119.91	129.30
23	05S1	39	A	C2-N3-C4	18.78	119.99	110.60
1	16S1	181	A	N1-C2-N3	-18.78	119.91	129.30
1	16S1	228	A	C2-N3-C4	18.78	119.99	110.60
22	23S1	1169	A	C2-N3-C4	18.78	119.99	110.60
22	23S1	1783	A	C2-N3-C4	18.78	119.99	110.60
22	23S1	453	A	C2-N3-C4	18.78	119.99	110.60
22	23S1	988	A	N1-C2-N3	-18.78	119.91	129.30
1	16S1	579	A	N1-C6-N6	-18.78	107.33	118.60
1	16S1	978	A	N1-C2-N3	-18.78	119.91	129.30
22	23S1	1420	A	N1-C2-N3	-18.78	119.91	129.30
1	16S1	160	A	N1-C6-N6	-18.77	107.34	118.60
1	16S1	1502	A	C2-N3-C4	18.77	119.99	110.60
22	23S1	1586	A	C2-N3-C4	18.77	119.99	110.60
22	23S1	1194	A	C2-N3-C4	18.77	119.99	110.60
22	23S1	1876	A	C2-N3-C4	18.77	119.99	110.60
22	23S1	149	A	N1-C2-N3	-18.77	119.91	129.30
22	23S1	1572	A	C2-N3-C4	18.77	119.99	110.60
22	23S1	1598	A	N1-C6-N6	-18.77	107.34	118.60
22	23S1	2019	A	N1-C2-N3	-18.77	119.92	129.30
22	23S1	2388	A	N1-C6-N6	-18.77	107.34	118.60
1	16S1	918	A	N1-C2-N3	-18.77	119.92	129.30
22	23S1	330	A	N1-C6-N6	-18.77	107.34	118.60
22	23S1	345	A	N1-C2-N3	-18.77	119.92	129.30
22	23S1	1848	A	C2-N3-C4	18.77	119.98	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	600	A	N1-C6-N6	-18.77	107.34	118.60
1	16S1	681	A	N1-C6-N6	-18.77	107.34	118.60
1	16S1	1374	A	N1-C2-N3	-18.77	119.92	129.30
22	23S1	422	A	N1-C2-N3	-18.77	119.92	129.30
22	23S1	1040	A	N1-C2-N3	-18.77	119.92	129.30
55	PTR1	14	A	C2-N3-C4	18.77	119.98	110.60
1	16S1	784	A	N1-C6-N6	-18.76	107.34	118.60
22	23S1	574	A	N1-C2-N3	-18.76	119.92	129.30
22	23S1	877	A	N1-C2-N3	-18.76	119.92	129.30
22	23S1	988	A	C2-N3-C4	18.76	119.98	110.60
22	23S1	1073	A	C2-N3-C4	18.76	119.98	110.60
22	23S1	1654	A	N1-C6-N6	-18.76	107.34	118.60
1	16S1	382	A	N1-C6-N6	-18.76	107.34	118.60
22	23S1	1502	A	C2-N3-C4	18.76	119.98	110.60
22	23S1	2733	A	C2-N3-C4	18.76	119.98	110.60
1	16S1	908	A	C2-N3-C4	18.76	119.98	110.60
1	16S1	1349	A	C2-N3-C4	18.76	119.98	110.60
22	23S1	2015	A	C2-N3-C4	18.76	119.98	110.60
22	23S1	2080	A	N1-C6-N6	-18.76	107.34	118.60
22	23S1	2171	A	N1-C2-N3	-18.76	119.92	129.30
22	23S1	2158	A	C2-N3-C4	18.75	119.98	110.60
22	23S1	2741	A	C2-N3-C4	18.75	119.98	110.60
23	05S1	46	A	N1-C2-N3	-18.75	119.92	129.30
1	16S1	196	A	N1-C6-N6	-18.75	107.35	118.60
1	16S1	1188	A	C2-N3-C4	18.75	119.98	110.60
22	23S1	2765	A	N1-C2-N3	-18.75	119.92	129.30
22	23S1	2799	A	C2-N3-C4	18.75	119.98	110.60
22	23S1	460	A	C2-N3-C4	18.75	119.97	110.60
1	16S1	1280	A	C2-N3-C4	18.75	119.97	110.60
22	23S1	460	A	N1-C2-N3	-18.75	119.93	129.30
22	23S1	1383	A	C2-N3-C4	18.75	119.97	110.60
22	23S1	2670	A	N1-C2-N3	-18.75	119.93	129.30
1	16S1	179	A	C2-N3-C4	18.75	119.97	110.60
22	23S1	6	A	N1-C6-N6	-18.75	107.35	118.60
22	23S1	2753	A	C2-N3-C4	18.75	119.97	110.60
1	16S1	143	A	N1-C6-N6	-18.74	107.35	118.60
22	23S1	2813	A	N1-C2-N3	-18.74	119.93	129.30
1	16S1	139	A	C2-N3-C4	18.74	119.97	110.60
22	23S1	173	A	N1-C2-N3	-18.74	119.93	129.30
55	PTR1	58	A	C2-N3-C4	18.74	119.97	110.60
1	16S1	196	A	C2-N3-C4	18.74	119.97	110.60
22	23S1	471	A	C2-N3-C4	18.74	119.97	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	927	A	C2-N3-C4	18.74	119.97	110.60
22	23S1	2147	A	C2-N3-C4	18.74	119.97	110.60
22	23S1	279	A	N1-C6-N6	-18.74	107.36	118.60
1	16S1	325	A	N1-C6-N6	-18.74	107.36	118.60
22	23S1	415	A	N1-C2-N3	-18.73	119.93	129.30
22	23S1	1713	A	C2-N3-C4	18.73	119.97	110.60
22	23S1	1505	A	N1-C6-N6	-18.73	107.36	118.60
1	16S1	8	A	C2-N3-C4	18.73	119.97	110.60
1	16S1	236	A	N1-C2-N3	-18.73	119.93	129.30
1	16S1	596	A	N1-C2-N3	-18.73	119.94	129.30
22	23S1	2003	A	N1-C2-N3	-18.73	119.93	129.30
22	23S1	2147	A	N1-C6-N6	-18.73	107.36	118.60
22	23S1	2748	A	N1-C2-N3	-18.73	119.93	129.30
55	PTR1	21	A	C2-N3-C4	18.73	119.97	110.60
22	23S1	226	A	C2-N3-C4	18.73	119.97	110.60
1	16S1	819	A	N1-C2-N3	-18.73	119.94	129.30
22	23S1	1759	A	N1-C6-N6	-18.73	107.36	118.60
55	PTR1	3	A	C2-N3-C4	18.73	119.96	110.60
1	16S1	1513	A	N1-C2-N3	-18.73	119.94	129.30
22	23S1	279	A	C2-N3-C4	18.73	119.96	110.60
22	23S1	501	A	C2-N3-C4	18.73	119.96	110.60
22	23S1	699	A	N1-C6-N6	-18.73	107.36	118.60
22	23S1	721	A	N1-C2-N3	-18.73	119.94	129.30
22	23S1	1359	A	C2-N3-C4	18.73	119.96	110.60
1	16S1	573	A	N1-C6-N6	-18.72	107.37	118.60
22	23S1	1254	A	N1-C6-N6	-18.72	107.37	118.60
22	23S1	1960	A	N1-C6-N6	-18.72	107.36	118.60
1	16S1	747	A	C2-N3-C4	18.72	119.96	110.60
22	23S1	2225	A	N1-C2-N3	-18.72	119.94	129.30
22	23S1	2469	A	C2-N3-C4	18.72	119.96	110.60
22	23S1	2639	A	C2-N3-C4	18.72	119.96	110.60
22	23S1	1077	A	C2-N3-C4	18.72	119.96	110.60
22	23S1	2051	A	C2-N3-C4	18.72	119.96	110.60
1	16S1	482	A	C2-N3-C4	18.72	119.96	110.60
1	16S1	974	A	N1-C2-N3	-18.72	119.94	129.30
1	16S1	1257	A	N1-C2-N3	-18.72	119.94	129.30
22	23S1	294	A	C2-N3-C4	18.72	119.96	110.60
1	16S1	189	A	C2-N3-C4	18.72	119.96	110.60
1	16S1	777	A	N1-C6-N6	-18.72	107.37	118.60
1	16S1	1213	A	C2-N3-C4	18.72	119.96	110.60
1	16S1	1437	A	N1-C2-N3	-18.72	119.94	129.30
22	23S1	127	A	C2-N3-C4	18.72	119.96	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	668	A	C2-N3-C4	18.72	119.96	110.60
22	23S1	53	A	C2-N3-C4	18.71	119.96	110.60
22	23S1	1977	A	C2-N3-C4	18.71	119.96	110.60
22	23S1	2883	A	N1-C6-N6	-18.71	107.37	118.60
22	23S1	1134	A	N1-C2-N3	-18.71	119.94	129.30
22	23S1	2080	A	N1-C2-N3	-18.71	119.94	129.30
22	23S1	2154	A	N1-C2-N3	-18.71	119.94	129.30
22	23S1	181	A	C2-N3-C4	18.71	119.96	110.60
1	16S1	1285	A	C2-N3-C4	18.71	119.95	110.60
22	23S1	1890	A	C2-N3-C4	18.71	119.95	110.60
22	23S1	2665	A	N1-C2-N3	-18.71	119.94	129.30
22	23S1	2733	A	N1-C6-N6	-18.71	107.37	118.60
22	23S1	453	A	N1-C2-N3	-18.71	119.94	129.30
22	23S1	756	A	N1-C2-N3	-18.71	119.95	129.30
22	23S1	1672	A	C2-N3-C4	18.71	119.95	110.60
22	23S1	2435	A	C2-N3-C4	18.71	119.95	110.60
22	23S1	2705	A	N1-C2-N3	-18.71	119.95	129.30
1	16S1	143	A	C2-N3-C4	18.70	119.95	110.60
22	23S1	1598	A	N1-C2-N3	-18.70	119.95	129.30
1	16S1	306	A	N1-C6-N6	-18.70	107.38	118.60
22	23S1	1098	A	C2-N3-C4	18.70	119.95	110.60
22	23S1	1287	A	N1-C6-N6	-18.70	107.38	118.60
1	16S1	236	A	C2-N3-C4	18.70	119.95	110.60
22	23S1	310	A	C2-N3-C4	18.70	119.95	110.60
22	23S1	2411	A	N1-C2-N3	-18.70	119.95	129.30
22	23S1	1634	A	C2-N3-C4	18.70	119.95	110.60
22	23S1	1913	A	C2-N3-C4	18.70	119.95	110.60
1	16S1	33	A	N1-C2-N3	-18.70	119.95	129.30
22	23S1	144	A	N1-C2-N3	-18.70	119.95	129.30
22	23S1	483	A	N1-C6-N6	-18.70	107.38	118.60
22	23S1	1230	A	N1-C2-N3	-18.70	119.95	129.30
1	16S1	253	A	C2-N3-C4	18.69	119.95	110.60
1	16S1	415	A	C2-N3-C4	18.69	119.95	110.60
1	16S1	495	A	C2-N3-C4	18.69	119.95	110.60
1	16S1	1046	A	N1-C6-N6	-18.69	107.38	118.60
1	16S1	1493	A	N1-C6-N6	-18.69	107.38	118.60
22	23S1	449	A	N1-C2-N3	-18.69	119.95	129.30
22	23S1	572	A	N1-C6-N6	-18.69	107.38	118.60
22	23S1	722	A	C2-N3-C4	18.69	119.95	110.60
22	23S1	2191	A	N1-C6-N6	-18.69	107.38	118.60
22	23S1	2602	A	C2-N3-C4	18.69	119.95	110.60
1	16S1	487	A	N1-C6-N6	-18.69	107.39	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	401	A	N1-C6-N6	-18.69	107.39	118.60
22	23S1	1509	A	N1-C6-N6	-18.69	107.39	118.60
22	23S1	103	A	N1-C2-N3	-18.69	119.96	129.30
22	23S1	173	A	C2-N3-C4	18.69	119.94	110.60
22	23S1	716	A	N1-C6-N6	-18.69	107.39	118.60
1	16S1	1022	A	N1-C6-N6	-18.69	107.39	118.60
22	23S1	95	A	C2-N3-C4	18.69	119.94	110.60
1	16S1	1271	A	N1-C2-N3	-18.68	119.96	129.30
22	23S1	1431	A	N1-C2-N3	-18.68	119.96	129.30
22	23S1	2721	A	C2-N3-C4	18.68	119.94	110.60
22	23S1	2856	A	C2-N3-C4	18.68	119.94	110.60
22	23S1	1246	A	N1-C2-N3	-18.68	119.96	129.30
23	05S1	15	A	N1-C2-N3	-18.68	119.96	129.30
1	16S1	329	A	N1-C2-N3	-18.68	119.96	129.30
22	23S1	1085	A	C2-N3-C4	18.68	119.94	110.60
22	23S1	2813	A	C2-N3-C4	18.68	119.94	110.60
22	23S1	1847	A	N1-C2-N3	-18.68	119.96	129.30
22	23S1	616	A	N1-C2-N3	-18.68	119.96	129.30
22	23S1	1247	A	N1-C2-N3	-18.68	119.96	129.30
22	23S1	753	A	N1-C6-N6	-18.68	107.39	118.60
1	16S1	1005	A	C2-N3-C4	18.68	119.94	110.60
1	16S1	1289	A	N1-C2-N3	-18.68	119.96	129.30
22	23S1	1614	A	N1-C2-N3	-18.68	119.96	129.30
22	23S1	332	A	C2-N3-C4	18.67	119.94	110.60
22	23S1	1735	A	N1-C2-N3	-18.67	119.97	129.30
22	23S1	2750	A	N1-C6-N6	-18.67	107.40	118.60
1	16S1	1151	A	N1-C6-N6	-18.67	107.40	118.60
1	16S1	596	A	C2-N3-C4	18.67	119.93	110.60
1	16S1	794	A	N1-C6-N6	-18.67	107.40	118.60
22	23S1	21	A	N1-C2-N3	-18.67	119.97	129.30
22	23S1	1470	A	C2-N3-C4	18.67	119.93	110.60
1	16S1	228	A	N1-C6-N6	-18.67	107.40	118.60
1	16S1	33	A	C2-N3-C4	18.66	119.93	110.60
1	16S1	309	A	N1-C2-N3	-18.66	119.97	129.30
1	16S1	320	A	N1-C2-N3	-18.66	119.97	129.30
22	23S1	195	A	C2-N3-C4	18.66	119.93	110.60
22	23S1	643	A	C2-N3-C4	18.66	119.93	110.60
22	23S1	1678	A	N1-C6-N6	-18.66	107.40	118.60
22	23S1	2019	A	N1-C6-N6	-18.66	107.40	118.60
1	16S1	676	A	C2-N3-C4	18.66	119.93	110.60
22	23S1	2147	A	N1-C2-N3	-18.66	119.97	129.30
23	05S1	57	A	C2-N3-C4	18.66	119.93	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	648	A	N1-C6-N6	-18.66	107.40	118.60
22	23S1	721	A	C2-N3-C4	18.66	119.93	110.60
22	23S1	2534	A	N1-C2-N3	-18.66	119.97	129.30
1	16S1	1176	A	N1-C2-N3	-18.66	119.97	129.30
22	23S1	118	A	N1-C6-N6	-18.66	107.41	118.60
22	23S1	255	A	N1-C2-N3	-18.66	119.97	129.30
22	23S1	2126	A	C2-N3-C4	18.66	119.93	110.60
1	16S1	65	A	C2-N3-C4	18.66	119.93	110.60
22	23S1	788	A	N1-C6-N6	-18.65	107.41	118.60
22	23S1	1717	A	N1-C2-N3	-18.65	119.97	129.30
22	23S1	256	A	C2-N3-C4	18.65	119.93	110.60
22	23S1	38	A	N1-C2-N3	-18.65	119.97	129.30
22	23S1	2725	A	N1-C2-N3	-18.65	119.97	129.30
22	23S1	920	A	N1-C2-N3	-18.65	119.97	129.30
22	23S1	2468	A	N1-C2-N3	-18.65	119.97	129.30
22	23S1	2799	A	N1-C2-N3	-18.65	119.97	129.30
22	23S1	2829	A	N1-C6-N6	-18.65	107.41	118.60
23	05S1	94	A	N1-C2-N3	-18.65	119.98	129.30
1	16S1	1350	A	C2-N3-C4	18.65	119.92	110.60
22	23S1	1916	A	N1-C2-N3	-18.65	119.98	129.30
22	23S1	2750	A	N1-C2-N3	-18.65	119.98	129.30
22	23S1	925	A	N1-C2-N3	-18.64	119.98	129.30
1	16S1	279	A	N1-C2-N3	-18.64	119.98	129.30
1	16S1	1022	A	C2-N3-C4	18.64	119.92	110.60
1	16S1	1248	A	C2-N3-C4	18.64	119.92	110.60
22	23S1	1274	A	N1-C6-N6	-18.64	107.41	118.60
22	23S1	1871	A	C2-N3-C4	18.64	119.92	110.60
22	23S1	2534	A	C2-N3-C4	18.64	119.92	110.60
22	23S1	2800	A	N1-C2-N3	-18.64	119.98	129.30
1	16S1	1287	A	C2-N3-C4	18.64	119.92	110.60
1	16S1	349	A	C2-N3-C4	18.64	119.92	110.60
1	16S1	1257	A	C2-N3-C4	18.64	119.92	110.60
22	23S1	172	A	N1-C2-N3	-18.64	119.98	129.30
22	23S1	344	A	C2-N3-C4	18.64	119.92	110.60
22	23S1	1090	A	N1-C6-N6	-18.64	107.42	118.60
22	23S1	1175	A	N1-C6-N6	-18.64	107.42	118.60
22	23S1	1717	A	C2-N3-C4	18.64	119.92	110.60
22	23S1	2108	A	C2-N3-C4	18.64	119.92	110.60
1	16S1	935	A	N1-C2-N3	-18.64	119.98	129.30
1	16S1	1410	A	N1-C2-N3	-18.64	119.98	129.30
22	23S1	262	A	N1-C2-N3	-18.64	119.98	129.30
22	23S1	599	A	C2-N3-C4	18.64	119.92	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	917	A	N1-C2-N3	-18.64	119.98	129.30
22	23S1	2163	A	C2-N3-C4	18.64	119.92	110.60
22	23S1	1077	A	N1-C2-N3	-18.63	119.98	129.30
22	23S1	2632	A	C2-N3-C4	18.63	119.92	110.60
1	16S1	16	A	C2-N3-C4	18.63	119.92	110.60
1	16S1	1005	A	N1-C2-N3	-18.63	119.98	129.30
1	16S1	1398	A	N1-C2-N3	-18.63	119.98	129.30
22	23S1	2170	A	C2-N3-C4	18.63	119.92	110.60
1	16S1	160	A	C2-N3-C4	18.63	119.92	110.60
1	16S1	1465	A	N1-C2-N3	-18.63	119.98	129.30
1	16S1	161	A	N1-C6-N6	-18.63	107.42	118.60
1	16S1	816	A	N1-C6-N6	-18.63	107.42	118.60
22	23S1	541	A	N1-C2-N3	-18.63	119.99	129.30
22	23S1	609	A	C2-N3-C4	18.63	119.92	110.60
22	23S1	705	A	N1-C2-N3	-18.63	119.99	129.30
22	23S1	1801	A	N1-C2-N3	-18.63	119.99	129.30
22	23S1	2778	A	N1-C2-N3	-18.63	119.99	129.30
1	16S1	1513	A	N1-C6-N6	-18.63	107.42	118.60
22	23S1	1095	A	N1-C6-N6	-18.63	107.42	118.60
22	23S1	2530	A	N1-C2-N3	-18.63	119.99	129.30
22	23S1	2778	A	C2-N3-C4	18.63	119.91	110.60
23	05S1	57	A	N1-C2-N3	-18.63	119.99	129.30
1	16S1	784	A	N1-C2-N3	-18.62	119.99	129.30
1	16S1	1092	A	N1-C6-N6	-18.62	107.42	118.60
1	16S1	1146	A	N1-C6-N6	-18.62	107.42	118.60
22	23S1	1508	A	N1-C2-N3	-18.62	119.99	129.30
22	23S1	1794	A	N1-C6-N6	-18.62	107.42	118.60
1	16S1	702	A	N1-C2-N3	-18.62	119.99	129.30
1	16S1	938	A	N1-C2-N3	-18.62	119.99	129.30
1	16S1	1110	A	C2-N3-C4	18.62	119.91	110.60
22	23S1	1373	A	N1-C2-N3	-18.62	119.99	129.30
1	16S1	1176	A	N1-C6-N6	-18.62	107.43	118.60
1	16S1	1434	A	C2-N3-C4	18.62	119.91	110.60
22	23S1	1677	A	C2-N3-C4	18.62	119.91	110.60
22	23S1	2058	A	C2-N3-C4	18.62	119.91	110.60
22	23S1	2418	A	N1-C6-N6	-18.62	107.43	118.60
23	05S1	34	A	N1-C2-N3	-18.62	119.99	129.30
22	23S1	256	A	N1-C2-N3	-18.62	119.99	129.30
1	16S1	8	A	N1-C6-N6	-18.62	107.43	118.60
1	16S1	780	A	C2-N3-C4	18.62	119.91	110.60
22	23S1	142	A	N1-C2-N3	-18.62	119.99	129.30
22	23S1	2322	A	N1-C6-N6	-18.62	107.43	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1913	A	N1-C2-N3	-18.61	119.99	129.30
22	23S1	2388	A	C2-N3-C4	18.61	119.91	110.60
1	16S1	1117	A	C2-N3-C4	18.61	119.91	110.60
22	23S1	900	A	N1-C2-N3	-18.61	119.99	129.30
22	23S1	2297	A	C2-N3-C4	18.61	119.91	110.60
22	23S1	2820	A	C2-N3-C4	18.61	119.91	110.60
1	16S1	338	A	C2-N3-C4	18.61	119.91	110.60
1	16S1	907	A	N1-C2-N3	-18.61	120.00	129.30
1	16S1	937	A	N1-C6-N6	-18.61	107.43	118.60
22	23S1	1385	A	C2-N3-C4	18.61	119.91	110.60
22	23S1	2598	A	N1-C2-N3	-18.61	119.99	129.30
22	23S1	64	A	N1-C2-N3	-18.61	120.00	129.30
22	23S1	2734	A	N1-C6-N6	-18.61	107.44	118.60
1	16S1	649	A	C2-N3-C4	18.61	119.90	110.60
1	16S1	1434	A	N1-C6-N6	-18.61	107.44	118.60
1	16S1	179	A	N1-C2-N3	-18.61	120.00	129.30
1	16S1	205	A	N1-C2-N3	-18.61	120.00	129.30
1	16S1	959	A	C2-N3-C4	18.61	119.90	110.60
1	16S1	1101	A	C2-N3-C4	18.61	119.90	110.60
22	23S1	788	A	C2-N3-C4	18.61	119.90	110.60
22	23S1	1535	A	C2-N3-C4	18.61	119.90	110.60
22	23S1	2753	A	N1-C2-N3	-18.61	120.00	129.30
23	05S1	15	A	N1-C6-N6	-18.61	107.44	118.60
22	23S1	849	A	C2-N3-C4	18.61	119.90	110.60
22	23S1	1413	A	N1-C6-N6	-18.61	107.44	118.60
22	23S1	2700	A	N1-C2-N3	-18.60	120.00	129.30
22	23S1	2430	A	N1-C6-N6	-18.60	107.44	118.60
22	23S1	2736	A	N1-C6-N6	-18.60	107.44	118.60
22	23S1	1039	A	N1-C2-N3	-18.60	120.00	129.30
22	23S1	1111	A	C2-N3-C4	18.60	119.90	110.60
22	23S1	1133	A	N1-C2-N3	-18.60	120.00	129.30
22	23S1	1528	A	C2-N3-C4	18.60	119.90	110.60
22	23S1	1705	A	N1-C2-N3	-18.60	120.00	129.30
22	23S1	2095	A	C2-N3-C4	18.60	119.90	110.60
22	23S1	609	A	N1-C6-N6	-18.60	107.44	118.60
22	23S1	2278	A	N1-C2-N3	-18.60	120.00	129.30
1	16S1	1299	A	N1-C6-N6	-18.60	107.44	118.60
22	23S1	2850	A	N1-C2-N3	-18.60	120.00	129.30
1	16S1	1146	A	N1-C2-N3	-18.59	120.00	129.30
1	16S1	1152	A	C2-N3-C4	18.59	119.90	110.60
1	16S1	1493	A	N1-C2-N3	-18.59	120.00	129.30
22	23S1	368	A	N1-C6-N6	-18.59	107.44	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1987	A	C2-N3-C4	18.59	119.90	110.60
1	16S1	298	A	N1-C6-N6	-18.59	107.45	118.60
22	23S1	928	A	N1-C6-N6	-18.59	107.44	118.60
1	16S1	393	A	N1-C6-N6	-18.59	107.45	118.60
1	16S1	607	A	N1-C6-N6	-18.59	107.45	118.60
1	16S1	635	A	N1-C2-N3	-18.59	120.00	129.30
22	23S1	5	A	N1-C6-N6	-18.59	107.45	118.60
1	16S1	197	A	N1-C6-N6	-18.59	107.45	118.60
22	23S1	1129	A	C2-N3-C4	18.59	119.89	110.60
22	23S1	501	A	N1-C2-N3	-18.59	120.01	129.30
1	16S1	1446	A	N1-C6-N6	-18.59	107.45	118.60
22	23S1	73	A	C2-N3-C4	18.59	119.89	110.60
22	23S1	2587	A	C2-N3-C4	18.59	119.89	110.60
1	16S1	120	A	C2-N3-C4	18.58	119.89	110.60
22	23S1	181	A	N1-C6-N6	-18.58	107.45	118.60
22	23S1	423	A	N1-C6-N6	-18.58	107.45	118.60
22	23S1	1069	A	C2-N3-C4	18.58	119.89	110.60
22	23S1	2893	A	C2-N3-C4	18.58	119.89	110.60
22	23S1	1586	A	N1-C6-N6	-18.58	107.45	118.60
1	16S1	1493	A	C2-N3-C4	18.58	119.89	110.60
1	16S1	1507	A	C2-N3-C4	18.58	119.89	110.60
22	23S1	1549	A	C2-N3-C4	18.58	119.89	110.60
22	23S1	1616	A	N1-C6-N6	-18.58	107.45	118.60
22	23S1	2893	A	N1-C2-N3	-18.58	120.01	129.30
1	16S1	1239	A	N1-C6-N6	-18.58	107.45	118.60
22	23S1	1143	A	N1-C2-N3	-18.58	120.01	129.30
22	23S1	1571	A	C2-N3-C4	18.58	119.89	110.60
22	23S1	2406	A	C2-N3-C4	18.58	119.89	110.60
1	16S1	50	A	N1-C2-N3	-18.57	120.01	129.30
1	16S1	780	A	N1-C2-N3	-18.57	120.01	129.30
22	23S1	176	A	N1-C6-N6	-18.57	107.45	118.60
1	16S1	759	A	C2-N3-C4	18.57	119.89	110.60
22	23S1	2534	A	N1-C6-N6	-18.57	107.46	118.60
23	05S1	15	A	C2-N3-C4	18.57	119.89	110.60
22	23S1	2058	A	N1-C6-N6	-18.57	107.46	118.60
1	16S1	892	A	N1-C6-N6	-18.57	107.46	118.60
22	23S1	384	A	N1-C2-N3	-18.57	120.02	129.30
22	23S1	603	A	C2-N3-C4	18.57	119.88	110.60
22	23S1	1953	A	N1-C2-N3	-18.57	120.02	129.30
22	23S1	2090	A	N1-C6-N6	-18.57	107.46	118.60
22	23S1	2614	A	N1-C6-N6	-18.57	107.46	118.60
22	23S1	2851	A	C2-N3-C4	18.57	119.88	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	161	A	N1-C2-N3	-18.57	120.02	129.30
1	16S1	250	A	C2-N3-C4	18.57	119.88	110.60
22	23S1	1089	A	N1-C2-N3	-18.57	120.02	129.30
22	23S1	1304	A	C2-N3-C4	18.57	119.88	110.60
22	23S1	2750	A	C2-N3-C4	18.57	119.88	110.60
1	16S1	1145	A	C2-N3-C4	18.56	119.88	110.60
1	16S1	336	A	C2-N3-C4	18.56	119.88	110.60
22	23S1	478	A	N1-C6-N6	-18.56	107.46	118.60
22	23S1	2058	A	N1-C2-N3	-18.56	120.02	129.30
22	23S1	2748	A	C2-N3-C4	18.56	119.88	110.60
1	16S1	16	A	N1-C6-N6	-18.56	107.46	118.60
1	16S1	1044	A	N1-C2-N3	-18.56	120.02	129.30
1	16S1	1171	A	N1-C2-N3	-18.56	120.02	129.30
22	23S1	428	A	C2-N3-C4	18.56	119.88	110.60
55	PTR1	73	A	N1-C6-N6	-18.56	107.47	118.60
1	16S1	860	A	C2-N3-C4	18.56	119.88	110.60
22	23S1	2009	A	C2-N3-C4	18.56	119.88	110.60
1	16S1	44	A	N1-C2-N3	-18.56	120.02	129.30
22	23S1	44	A	N1-C2-N3	-18.56	120.02	129.30
22	23S1	1169	A	N1-C2-N3	-18.56	120.02	129.30
22	23S1	2059	A	C2-N3-C4	18.55	119.88	110.60
22	23S1	1545	A	N1-C2-N3	-18.55	120.02	129.30
22	23S1	1133	A	N1-C6-N6	-18.55	107.47	118.60
1	16S1	1441	A	C2-N3-C4	18.55	119.87	110.60
22	23S1	42	A	N1-C6-N6	-18.55	107.47	118.60
22	23S1	472	A	C2-N3-C4	18.55	119.87	110.60
22	23S1	1057	A	C2-N3-C4	18.55	119.87	110.60
22	23S1	1749	A	N1-C2-N3	-18.55	120.03	129.30
22	23S1	2425	A	N1-C2-N3	-18.54	120.03	129.30
1	16S1	609	A	C2-N3-C4	18.54	119.87	110.60
1	16S1	977	A	N1-C6-N6	-18.54	107.47	118.60
22	23S1	2530	A	N1-C6-N6	-18.54	107.47	118.60
1	16S1	1456	A	N1-C6-N6	-18.54	107.47	118.60
22	23S1	142	A	C2-N3-C4	18.54	119.87	110.60
22	23S1	1039	A	C2-N3-C4	18.54	119.87	110.60
1	16S1	7	A	N1-C2-N3	-18.54	120.03	129.30
1	16S1	430	A	C2-N3-C4	18.54	119.87	110.60
22	23S1	1590	A	N1-C2-N3	-18.54	120.03	129.30
22	23S1	1815	A	C2-N3-C4	18.54	119.87	110.60
1	16S1	53	A	N1-C2-N3	-18.54	120.03	129.30
1	16S1	559	A	N1-C6-N6	-18.54	107.48	118.60
22	23S1	1383	A	N1-C2-N3	-18.54	120.03	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1858	A	N1-C2-N3	-18.54	120.03	129.30
22	23S1	2482	A	C2-N3-C4	18.54	119.87	110.60
1	16S1	676	A	N1-C2-N3	-18.54	120.03	129.30
22	23S1	2054	A	N1-C2-N3	-18.54	120.03	129.30
1	16S1	535	A	N1-C6-N6	-18.53	107.48	118.60
22	23S1	718	A	N1-C6-N6	-18.53	107.48	118.60
22	23S1	2542	A	C2-N3-C4	18.53	119.87	110.60
22	23S1	718	A	C2-N3-C4	18.53	119.86	110.60
22	23S1	1877	A	N1-C2-N3	-18.53	120.03	129.30
22	23S1	472	A	N1-C2-N3	-18.53	120.04	129.30
22	23S1	1086	A	N1-C6-N6	-18.53	107.48	118.60
1	16S1	143	A	N1-C2-N3	-18.53	120.04	129.30
22	23S1	401	A	C2-N3-C4	18.53	119.86	110.60
1	16S1	681	A	N1-C2-N3	-18.52	120.04	129.30
1	16S1	908	A	N1-C2-N3	-18.52	120.04	129.30
22	23S1	1367	A	C2-N3-C4	18.52	119.86	110.60
1	16S1	349	A	N1-C2-N3	-18.52	120.04	129.30
1	16S1	336	A	N1-C2-N3	-18.52	120.04	129.30
1	16S1	1081	A	N1-C2-N3	-18.52	120.04	129.30
22	23S1	756	A	N1-C6-N6	-18.52	107.49	118.60
22	23S1	866	A	N1-C6-N6	-18.52	107.49	118.60
22	23S1	936	A	N1-C2-N3	-18.52	120.04	129.30
22	23S1	2267	A	N1-C6-N6	-18.52	107.49	118.60
22	23S1	1583	A	N1-C6-N6	-18.52	107.49	118.60
22	23S1	1900	A	C2-N3-C4	18.52	119.86	110.60
22	23S1	2090	A	N1-C2-N3	-18.52	120.04	129.30
22	23S1	152	A	N1-C2-N3	-18.52	120.04	129.30
22	23S1	1322	A	N1-C6-N6	-18.52	107.49	118.60
22	23S1	1551	A	N1-C2-N3	-18.52	120.04	129.30
1	16S1	81	A	C2-N3-C4	18.51	119.86	110.60
1	16S1	374	A	N1-C2-N3	-18.51	120.04	129.30
1	16S1	1254	A	N1-C2-N3	-18.51	120.04	129.30
22	23S1	626	A	C2-N3-C4	18.51	119.86	110.60
22	23S1	1322	A	N1-C2-N3	-18.51	120.04	129.30
22	23S1	1784	A	C2-N3-C4	18.51	119.86	110.60
22	23S1	2814	A	N1-C6-N6	-18.51	107.49	118.60
22	23S1	1508	A	C2-N3-C4	18.51	119.86	110.60
22	23S1	1366	A	C2-N3-C4	18.51	119.86	110.60
22	23S1	2097	A	N1-C2-N3	-18.51	120.05	129.30
22	23S1	2711	A	N1-C2-N3	-18.51	120.04	129.30
22	23S1	751	A	C2-N3-C4	18.51	119.85	110.60
1	16S1	968	A	N1-C2-N3	-18.51	120.05	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	422	A	C2-N3-C4	18.50	119.85	110.60
22	23S1	632	A	N1-C6-N6	-18.50	107.50	118.60
22	23S1	1080	A	N1-C2-N3	-18.50	120.05	129.30
22	23S1	1609	A	C2-N3-C4	18.50	119.85	110.60
1	16S1	554	A	N1-C2-N3	-18.50	120.05	129.30
1	16S1	1340	A	N1-C2-N3	-18.50	120.05	129.30
1	16S1	675	A	N1-C2-N3	-18.50	120.05	129.30
1	16S1	1531	A	N1-C2-N3	-18.50	120.05	129.30
22	23S1	1275	A	N1-C6-N6	-18.50	107.50	118.60
22	23S1	2749	A	C2-N3-C4	18.50	119.85	110.60
22	23S1	1495	A	N1-C6-N6	-18.50	107.50	118.60
22	23S1	1912	A	N1-C2-N3	-18.50	120.05	129.30
22	23S1	2281	A	N1-C2-N3	-18.50	120.05	129.30
1	16S1	1219	A	N1-C2-N3	-18.50	120.05	129.30
1	16S1	1274	A	N1-C2-N3	-18.50	120.05	129.30
1	16S1	1492	A	N1-C6-N6	-18.50	107.50	118.60
22	23S1	272	A	N1-C2-N3	-18.50	120.05	129.30
22	23S1	1669	A	N1-C2-N3	-18.50	120.05	129.30
1	16S1	747	A	N1-C2-N3	-18.49	120.05	129.30
22	23S1	1021	A	N1-C2-N3	-18.49	120.05	129.30
22	23S1	2268	A	C2-N3-C4	18.49	119.85	110.60
22	23S1	2565	A	N1-C2-N3	-18.49	120.05	129.30
1	16S1	676	A	N1-C6-N6	-18.49	107.51	118.60
1	16S1	1340	A	N1-C6-N6	-18.49	107.50	118.60
22	23S1	347	A	N1-C2-N3	-18.49	120.06	129.30
1	16S1	116	A	C2-N3-C4	18.49	119.84	110.60
1	16S1	374	A	C2-N3-C4	18.49	119.84	110.60
22	23S1	103	A	C2-N3-C4	18.49	119.84	110.60
22	23S1	362	A	N1-C2-N3	-18.49	120.06	129.30
22	23S1	1970	A	N1-C2-N3	-18.49	120.06	129.30
22	23S1	1046	A	C2-N3-C4	18.48	119.84	110.60
1	16S1	321	A	C2-N3-C4	18.48	119.84	110.60
22	23S1	197	A	N1-C2-N3	-18.48	120.06	129.30
22	23S1	439	A	N1-C6-N6	-18.48	107.51	118.60
22	23S1	1304	A	N1-C2-N3	-18.48	120.06	129.30
22	23S1	1583	A	C2-N3-C4	18.48	119.84	110.60
23	05S1	52	A	C2-N3-C4	18.48	119.84	110.60
22	23S1	2322	A	N1-C2-N3	-18.48	120.06	129.30
1	16S1	77	A	C2-N3-C4	18.48	119.84	110.60
1	16S1	695	A	N1-C6-N6	-18.48	107.51	118.60
22	23S1	482	A	C2-N3-C4	18.48	119.84	110.60
22	23S1	1089	A	C2-N3-C4	18.48	119.84	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1711	A	N1-C2-N3	-18.48	120.06	129.30
22	23S1	2020	A	C2-N3-C4	18.48	119.84	110.60
22	23S1	1819	A	N1-C2-N3	-18.48	120.06	129.30
22	23S1	2009	A	N1-C6-N6	-18.48	107.51	118.60
22	23S1	2406	A	N1-C6-N6	-18.48	107.51	118.60
1	16S1	223	A	N1-C6-N6	-18.48	107.51	118.60
22	23S1	497	A	C2-N3-C4	18.48	119.84	110.60
22	23S1	1998	A	N1-C2-N3	-18.48	120.06	129.30
22	23S1	2335	A	N1-C2-N3	-18.48	120.06	129.30
23	05S1	53	A	N1-C2-N3	-18.47	120.06	129.30
22	23S1	401	A	N1-C2-N3	-18.47	120.06	129.30
22	23S1	2560	A	N1-C2-N3	-18.47	120.06	129.30
22	23S1	1027	A	C2-N3-C4	18.47	119.83	110.60
22	23S1	1854	A	C2-N3-C4	18.47	119.83	110.60
23	05S1	52	A	N1-C2-N3	-18.47	120.06	129.30
22	23S1	125	A	N1-C6-N6	-18.47	107.52	118.60
22	23S1	609	A	N1-C2-N3	-18.47	120.07	129.30
22	23S1	2297	A	N1-C2-N3	-18.47	120.07	129.30
1	16S1	3	A	C2-N3-C4	18.46	119.83	110.60
22	23S1	368	A	C2-N3-C4	18.46	119.83	110.60
22	23S1	439	A	N1-C2-N3	-18.46	120.07	129.30
22	23S1	1336	A	N1-C2-N3	-18.46	120.07	129.30
22	23S1	2873	A	N1-C2-N3	-18.46	120.07	129.30
23	05S1	50	A	N1-C2-N3	-18.46	120.07	129.30
22	23S1	182	A	N1-C6-N6	-18.46	107.52	118.60
22	23S1	627	A	C2-N3-C4	18.46	119.83	110.60
22	23S1	693	A	N1-C6-N6	-18.46	107.52	118.60
1	16S1	353	A	N1-C6-N6	-18.46	107.52	118.60
22	23S1	480	A	C2-N3-C4	18.46	119.83	110.60
22	23S1	505	A	C2-N3-C4	18.46	119.83	110.60
23	05S1	108	A	N1-C6-N6	-18.46	107.52	118.60
22	23S1	1676	A	C2-N3-C4	18.46	119.83	110.60
22	23S1	1801	A	C2-N3-C4	18.46	119.83	110.60
1	16S1	1180	A	N1-C6-N6	-18.46	107.53	118.60
22	23S1	1080	A	C2-N3-C4	18.46	119.83	110.60
1	16S1	435	A	N1-C6-N6	-18.46	107.53	118.60
22	23S1	172	A	N1-C6-N6	-18.46	107.53	118.60
22	23S1	218	A	N1-C2-N3	-18.46	120.07	129.30
22	23S1	1285	A	C2-N3-C4	18.46	119.83	110.60
22	23S1	344	A	N1-C6-N6	-18.46	107.53	118.60
22	23S1	483	A	C2-N3-C4	18.46	119.83	110.60
1	16S1	621	A	N1-C6-N6	-18.45	107.53	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	968	A	C2-N3-C4	18.45	119.83	110.60
1	16S1	1196	A	N1-C6-N6	-18.45	107.53	118.60
1	16S1	1269	A	C2-N3-C4	18.45	119.83	110.60
22	23S1	167	A	C2-N3-C4	18.45	119.83	110.60
22	23S1	241	A	C2-N3-C4	18.45	119.83	110.60
22	23S1	1302	A	C2-N3-C4	18.45	119.83	110.60
22	23S1	2392	A	N1-C2-N3	-18.45	120.07	129.30
1	16S1	1216	A	N1-C2-N3	-18.45	120.07	129.30
22	23S1	384	A	C2-N3-C4	18.45	119.83	110.60
1	16S1	65	A	N1-C6-N6	-18.45	107.53	118.60
1	16S1	1503	A	N1-C2-N3	-18.45	120.08	129.30
22	23S1	2094	A	N1-C2-N3	-18.45	120.08	129.30
1	16S1	1324	A	C2-N3-C4	18.45	119.82	110.60
22	23S1	95	A	N1-C6-N6	-18.45	107.53	118.60
22	23S1	1496	A	N1-C6-N6	-18.45	107.53	118.60
1	16S1	366	A	N1-C2-N3	-18.45	120.08	129.30
1	16S1	596	A	N1-C6-N6	-18.45	107.53	118.60
1	16S1	1169	A	C2-N3-C4	18.45	119.82	110.60
1	16S1	1430	A	N1-C6-N6	-18.45	107.53	118.60
22	23S1	689	A	N1-C2-N3	-18.45	120.08	129.30
23	05S1	39	A	N1-C6-N6	-18.45	107.53	118.60
22	23S1	845	A	N1-C6-N6	-18.45	107.53	118.60
1	16S1	1254	A	C2-N3-C4	18.44	119.82	110.60
1	16S1	1261	A	N1-C6-N6	-18.44	107.53	118.60
22	23S1	2392	A	C2-N3-C4	18.44	119.82	110.60
22	23S1	1762	A	N1-C6-N6	-18.44	107.53	118.60
22	23S1	2386	A	N1-C2-N3	-18.44	120.08	129.30
1	16S1	815	A	N1-C6-N6	-18.44	107.54	118.60
1	16S1	1332	A	C2-N3-C4	18.44	119.82	110.60
22	23S1	391	A	N1-C6-N6	-18.44	107.53	118.60
1	16S1	397	A	N1-C2-N3	-18.44	120.08	129.30
1	16S1	547	A	C2-N3-C4	18.44	119.82	110.60
23	05S1	119	A	N1-C6-N6	-18.44	107.54	118.60
1	16S1	60	A	N1-C2-N3	-18.44	120.08	129.30
1	16S1	250	A	N1-C2-N3	-18.44	120.08	129.30
1	16S1	1044	A	N1-C6-N6	-18.44	107.54	118.60
22	23S1	739	A	N1-C6-N6	-18.44	107.54	118.60
22	23S1	1616	A	C2-N3-C4	18.44	119.82	110.60
22	23S1	1698	A	N1-C2-N3	-18.44	120.08	129.30
1	16S1	642	A	N1-C6-N6	-18.43	107.54	118.60
22	23S1	1046	A	N1-C6-N6	-18.43	107.54	118.60
22	23S1	2336	A	C2-N3-C4	18.43	119.82	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	05S1	52	A	N1-C6-N6	-18.43	107.54	118.60
1	16S1	393	A	N1-C2-N3	-18.43	120.08	129.30
22	23S1	927	A	N1-C2-N3	-18.43	120.08	129.30
22	23S1	1885	A	N1-C2-N3	-18.43	120.08	129.30
22	23S1	2411	A	C2-N3-C4	18.43	119.82	110.60
23	05S1	53	A	C2-N3-C4	18.43	119.81	110.60
1	16S1	50	A	N1-C6-N6	-18.43	107.54	118.60
22	23S1	1596	A	N1-C2-N3	-18.43	120.08	129.30
1	16S1	1082	A	N1-C2-N3	-18.43	120.09	129.30
22	23S1	2268	A	N1-C2-N3	-18.43	120.09	129.30
22	23S1	2407	A	N1-C2-N3	-18.43	120.09	129.30
22	23S1	2776	A	C2-N3-C4	18.43	119.81	110.60
22	23S1	1580	A	C2-N3-C4	18.43	119.81	110.60
22	23S1	844	A	N1-C2-N3	-18.43	120.09	129.30
1	16S1	546	A	N1-C2-N3	-18.42	120.09	129.30
22	23S1	1548	A	N1-C2-N3	-18.42	120.09	129.30
1	16S1	408	A	N1-C2-N3	-18.42	120.09	129.30
1	16S1	1155	A	N1-C6-N6	-18.42	107.55	118.60
22	23S1	1918	A	N1-C2-N3	-18.42	120.09	129.30
22	23S1	2281	A	N1-C6-N6	-18.42	107.55	118.60
1	16S1	1318	A	N1-C2-N3	-18.42	120.09	129.30
22	23S1	1073	A	N1-C2-N3	-18.42	120.09	129.30
22	23S1	1791	A	C2-N3-C4	18.42	119.81	110.60
1	16S1	460	A	N1-C2-N3	-18.42	120.09	129.30
1	16S1	878	A	N1-C6-N6	-18.42	107.55	118.60
22	23S1	2733	A	N1-C2-N3	-18.42	120.09	129.30
1	16S1	767	A	N1-C6-N6	-18.42	107.55	118.60
1	16S1	182	A	N1-C6-N6	-18.41	107.55	118.60
22	23S1	56	A	N1-C6-N6	-18.41	107.55	118.60
22	23S1	2826	A	N1-C6-N6	-18.41	107.55	118.60
1	16S1	274	A	N1-C6-N6	-18.41	107.55	118.60
1	16S1	1430	A	C2-N3-C4	18.41	119.81	110.60
22	23S1	643	A	N1-C6-N6	-18.41	107.55	118.60
22	23S1	1665	A	N1-C2-N3	-18.41	120.09	129.30
22	23S1	2381	A	N1-C6-N6	-18.41	107.55	118.60
22	23S1	1260	A	N1-C6-N6	-18.41	107.55	118.60
22	23S1	1876	A	N1-C6-N6	-18.41	107.55	118.60
22	23S1	2333	A	N1-C6-N6	-18.41	107.55	118.60
1	16S1	1130	A	C2-N3-C4	18.41	119.81	110.60
22	23S1	528	A	N1-C6-N6	-18.41	107.56	118.60
22	23S1	1744	A	N1-C2-N3	-18.41	120.10	129.30
22	23S1	2654	A	C2-N3-C4	18.41	119.80	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1000	A	N1-C2-N3	-18.41	120.10	129.30
1	16S1	1534	A	N1-C6-N6	-18.41	107.56	118.60
22	23S1	13	A	N1-C2-N3	-18.41	120.10	129.30
1	16S1	1167	A	C2-N3-C4	18.40	119.80	110.60
22	23S1	2199	A	N1-C6-N6	-18.40	107.56	118.60
22	23S1	342	A	N1-C6-N6	-18.40	107.56	118.60
22	23S1	428	A	N1-C2-N3	-18.40	120.10	129.30
22	23S1	1073	A	N1-C6-N6	-18.40	107.56	118.60
22	23S1	1679	A	C2-N3-C4	18.40	119.80	110.60
22	23S1	2411	A	N1-C6-N6	-18.40	107.56	118.60
22	23S1	5	A	N1-C2-N3	-18.40	120.10	129.30
22	23S1	2662	A	C2-N3-C4	18.40	119.80	110.60
22	23S1	2433	A	N1-C2-N3	-18.40	120.10	129.30
1	16S1	602	A	N1-C2-N3	-18.39	120.10	129.30
22	23S1	627	A	N1-C6-N6	-18.39	107.56	118.60
22	23S1	960	A	C2-N3-C4	18.39	119.80	110.60
22	23S1	2632	A	N1-C2-N3	-18.39	120.10	129.30
22	23S1	2879	A	N1-C2-N3	-18.39	120.10	129.30
55	PTR1	38	A	C2-N3-C4	18.39	119.80	110.60
1	16S1	949	A	N1-C2-N3	-18.39	120.10	129.30
1	16S1	1447	A	C2-N3-C4	18.39	119.80	110.60
22	23S1	911	A	C2-N3-C4	18.39	119.80	110.60
22	23S1	1276	A	N1-C2-N3	-18.39	120.11	129.30
22	23S1	2317	A	N1-C2-N3	-18.39	120.11	129.30
22	23S1	2432	A	N1-C6-N6	-18.39	107.57	118.60
1	16S1	119	A	C2-N3-C4	18.39	119.79	110.60
1	16S1	794	A	C2-N3-C4	18.39	119.79	110.60
1	16S1	1269	A	N1-C6-N6	-18.39	107.57	118.60
22	23S1	2471	A	N1-C6-N6	-18.38	107.57	118.60
1	16S1	174	A	N1-C6-N6	-18.38	107.57	118.60
22	23S1	996	A	N1-C2-N3	-18.38	120.11	129.30
22	23S1	1134	A	C2-N3-C4	18.38	119.79	110.60
22	23S1	2082	A	N1-C2-N3	-18.38	120.11	129.30
22	23S1	2191	A	C2-N3-C4	18.38	119.79	110.60
22	23S1	2738	A	C2-N3-C4	18.38	119.79	110.60
22	23S1	1877	A	C2-N3-C4	18.38	119.79	110.60
22	23S1	933	A	N1-C2-N3	-18.38	120.11	129.30
55	PTR1	26	A	N1-C6-N6	-18.38	107.58	118.60
1	16S1	109	A	C2-N3-C4	18.37	119.79	110.60
22	23S1	2406	A	N1-C2-N3	-18.37	120.11	129.30
22	23S1	2468	A	N1-C6-N6	-18.37	107.58	118.60
22	23S1	2810	A	N1-C6-N6	-18.37	107.58	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	52	A	N1-C2-N3	-18.37	120.11	129.30
22	23S1	2705	A	N1-C6-N6	-18.37	107.58	118.60
1	16S1	1418	A	N1-C2-N3	-18.37	120.12	129.30
22	23S1	2764	A	C2-N3-C4	18.37	119.78	110.60
22	23S1	1469	A	N1-C2-N3	-18.37	120.12	129.30
1	16S1	7	A	C2-N3-C4	18.36	119.78	110.60
1	16S1	1507	A	N1-C2-N3	-18.36	120.12	129.30
22	23S1	1301	A	N1-C6-N6	-18.36	107.58	118.60
22	23S1	2727	A	N1-C6-N6	-18.36	107.58	118.60
1	16S1	451	A	C2-N3-C4	18.36	119.78	110.60
1	16S1	1021	A	N1-C6-N6	-18.36	107.58	118.60
22	23S1	1650	A	N1-C2-N3	-18.36	120.12	129.30
22	23S1	2738	A	N1-C6-N6	-18.36	107.58	118.60
1	16S1	1360	A	N1-C2-N3	-18.36	120.12	129.30
22	23S1	320	A	N1-C6-N6	-18.36	107.58	118.60
22	23S1	644	A	N1-C6-N6	-18.36	107.58	118.60
22	23S1	1801	A	N1-C6-N6	-18.36	107.58	118.60
22	23S1	1367	A	N1-C2-N3	-18.36	120.12	129.30
1	16S1	161	A	C2-N3-C4	18.35	119.78	110.60
1	16S1	431	A	C2-N3-C4	18.35	119.78	110.60
1	16S1	1319	A	N1-C6-N6	-18.35	107.59	118.60
22	23S1	781	A	C2-N3-C4	18.35	119.78	110.60
22	23S1	2531	A	C2-N3-C4	18.35	119.78	110.60
1	16S1	523	A	N1-C6-N6	-18.35	107.59	118.60
22	23S1	1745	A	C2-N3-C4	18.35	119.78	110.60
1	16S1	520	A	C2-N3-C4	18.35	119.78	110.60
22	23S1	1569	A	C2-N3-C4	18.35	119.78	110.60
55	PTR1	9	A	C2-N3-C4	18.35	119.78	110.60
22	23S1	244	A	N1-C6-N6	-18.35	107.59	118.60
1	16S1	321	A	N1-C2-N3	-18.34	120.13	129.30
22	23S1	689	A	N1-C6-N6	-18.34	107.59	118.60
22	23S1	1532	A	N1-C2-N3	-18.34	120.13	129.30
22	23S1	2309	A	N1-C6-N6	-18.34	107.59	118.60
22	23S1	2434	A	C2-N3-C4	18.34	119.77	110.60
22	23S1	2432	A	C2-N3-C4	18.34	119.77	110.60
1	16S1	1055	A	N1-C2-N3	-18.34	120.13	129.30
22	23S1	844	A	C2-N3-C4	18.34	119.77	110.60
22	23S1	2205	A	N1-C6-N6	-18.34	107.60	118.60
22	23S1	1773	A	N1-C6-N6	-18.34	107.60	118.60
1	16S1	174	A	N1-C2-N3	-18.34	120.13	129.30
1	16S1	794	A	N1-C2-N3	-18.34	120.13	129.30
22	23S1	1754	A	C2-N3-C4	18.34	119.77	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2205	A	C2-N3-C4	18.34	119.77	110.60
22	23S1	6	A	N1-C2-N3	-18.33	120.13	129.30
22	23S1	1608	A	N1-C6-N6	-18.33	107.60	118.60
1	16S1	655	A	N1-C6-N6	-18.33	107.60	118.60
1	16S1	1357	A	N1-C2-N3	-18.33	120.13	129.30
1	16S1	1012	A	N1-C2-N3	-18.33	120.13	129.30
1	16S1	1362	A	N1-C6-N6	-18.33	107.60	118.60
1	16S1	649	A	N1-C2-N3	-18.33	120.14	129.30
1	16S1	192	A	C2-N3-C4	18.33	119.76	110.60
1	16S1	371	A	N1-C6-N6	-18.33	107.60	118.60
22	23S1	655	A	C2-N3-C4	18.33	119.76	110.60
1	16S1	1216	A	C2-N3-C4	18.32	119.76	110.60
22	23S1	782	A	N1-C2-N3	-18.32	120.14	129.30
22	23S1	1028	A	N1-C6-N6	-18.32	107.61	118.60
1	16S1	28	A	N1-C6-N6	-18.32	107.61	118.60
1	16S1	246	A	C2-N3-C4	18.32	119.76	110.60
22	23S1	1866	A	N1-C2-N3	-18.32	120.14	129.30
22	23S1	2727	A	N1-C2-N3	-18.32	120.14	129.30
22	23S1	503	A	N1-C6-N6	-18.32	107.61	118.60
22	23S1	1014	A	N1-C6-N6	-18.32	107.61	118.60
1	16S1	432	A	N1-C2-N3	-18.32	120.14	129.30
22	23S1	231	A	N1-C2-N3	-18.32	120.14	129.30
22	23S1	507	A	C2-N3-C4	18.32	119.76	110.60
22	23S1	2346	A	N1-C6-N6	-18.32	107.61	118.60
1	16S1	574	A	C2-N3-C4	18.31	119.76	110.60
22	23S1	1847	A	N1-C6-N6	-18.31	107.61	118.60
23	05S1	58	A	N1-C2-N3	-18.31	120.14	129.30
22	23S1	547	A	N1-C6-N6	-18.31	107.61	118.60
1	16S1	900	A	C2-N3-C4	18.31	119.76	110.60
1	16S1	1092	A	N1-C2-N3	-18.31	120.14	129.30
22	23S1	2163	A	N1-C6-N6	-18.31	107.61	118.60
1	16S1	338	A	N1-C6-N6	-18.31	107.61	118.60
1	16S1	915	A	C2-N3-C4	18.31	119.75	110.60
22	23S1	2184	A	N1-C2-N3	-18.31	120.15	129.30
1	16S1	1229	A	N1-C2-N3	-18.31	120.15	129.30
22	23S1	2198	A	N1-C6-N6	-18.31	107.62	118.60
22	23S1	2298	A	N1-C6-N6	-18.31	107.62	118.60
1	16S1	263	A	N1-C2-N3	-18.30	120.15	129.30
22	23S1	1010	A	N1-C6-N6	-18.30	107.62	118.60
22	23S1	1848	A	N1-C2-N3	-18.30	120.15	129.30
22	23S1	877	A	C2-N3-C4	18.30	119.75	110.60
22	23S1	556	A	N1-C6-N6	-18.30	107.62	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2883	A	C2-N3-C4	18.30	119.75	110.60
22	23S1	742	A	N1-C6-N6	-18.30	107.62	118.60
22	23S1	1147	A	N1-C6-N6	-18.29	107.62	118.60
1	16S1	363	A	N1-C6-N6	-18.29	107.62	118.60
1	16S1	608	A	N1-C2-N3	-18.29	120.15	129.30
1	16S1	60	A	C2-N3-C4	18.29	119.75	110.60
1	16S1	205	A	N1-C6-N6	-18.29	107.62	118.60
1	16S1	466	A	N1-C2-N3	-18.29	120.16	129.30
22	23S1	1739	A	C2-N3-C4	18.29	119.74	110.60
22	23S1	2071	A	N1-C2-N3	-18.29	120.16	129.30
1	16S1	366	A	C2-N3-C4	18.29	119.74	110.60
1	16S1	1246	A	N1-C6-N6	-18.29	107.63	118.60
22	23S1	2433	A	N1-C6-N6	-18.29	107.63	118.60
1	16S1	28	A	N1-C2-N3	-18.29	120.16	129.30
1	16S1	1080	A	C2-N3-C4	18.29	119.74	110.60
22	23S1	447	A	C2-N3-C4	18.29	119.74	110.60
1	16S1	161	A	N1-C2-N3	-18.29	120.16	129.30
1	16S1	1531	A	C2-N3-C4	18.29	119.74	110.60
22	23S1	829	A	N1-C6-N6	-18.28	107.63	118.60
22	23S1	1040	A	N1-C6-N6	-18.28	107.63	118.60
22	23S1	1953	A	N1-C6-N6	-18.28	107.63	118.60
22	23S1	2439	A	C2-N3-C4	18.28	119.74	110.60
22	23S1	2378	A	C2-N3-C4	18.28	119.74	110.60
22	23S1	492	A	N1-C2-N3	-18.28	120.16	129.30
1	16S1	608	A	N1-C6-N6	-18.28	107.63	118.60
22	23S1	1008	A	N1-C6-N6	-18.28	107.63	118.60
22	23S1	2059	A	N1-C2-N3	-18.28	120.16	129.30
22	23S1	2781	A	C2-N3-C4	18.28	119.74	110.60
1	16S1	1508	A	C2-N3-C4	18.28	119.74	110.60
22	23S1	2020	A	N1-C2-N3	-18.28	120.16	129.30
22	23S1	294	A	N1-C6-N6	-18.27	107.64	118.60
22	23S1	2448	A	N1-C2-N3	-18.27	120.16	129.30
1	16S1	878	A	N1-C2-N3	-18.27	120.16	129.30
22	23S1	272	A	C2-N3-C4	18.27	119.73	110.60
1	16S1	1102	A	C2-N3-C4	18.27	119.73	110.60
22	23S1	1650	A	N1-C6-N6	-18.27	107.64	118.60
1	16S1	243	A	C2-N3-C4	18.27	119.73	110.60
22	23S1	348	A	N1-C2-N3	-18.27	120.17	129.30
23	05S1	109	A	N1-C2-N3	-18.27	120.17	129.30
22	23S1	282	A	C2-N3-C4	18.26	119.73	110.60
22	23S1	1084	A	N1-C2-N3	-18.26	120.17	129.30
22	23S1	1901	A	N1-C6-N6	-18.26	107.64	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1319	A	N1-C2-N3	-18.26	120.17	129.30
22	23S1	402	A	C2-N3-C4	18.26	119.73	110.60
22	23S1	2781	A	N1-C6-N6	-18.26	107.64	118.60
1	16S1	1468	A	N1-C2-N3	-18.26	120.17	129.30
22	23S1	1665	A	N1-C6-N6	-18.26	107.65	118.60
1	16S1	363	A	N1-C2-N3	-18.25	120.17	129.30
1	16S1	872	A	N1-C2-N3	-18.25	120.17	129.30
22	23S1	182	A	N1-C2-N3	-18.25	120.17	129.30
22	23S1	1829	A	N1-C2-N3	-18.25	120.17	129.30
22	23S1	2135	A	N1-C2-N3	-18.25	120.17	129.30
22	23S1	2183	A	N1-C6-N6	-18.25	107.65	118.60
22	23S1	2665	A	N1-C6-N6	-18.25	107.65	118.60
1	16S1	336	A	N1-C6-N6	-18.25	107.65	118.60
22	23S1	1307	A	N1-C6-N6	-18.25	107.65	118.60
22	23S1	2054	A	N1-C6-N6	-18.25	107.65	118.60
22	23S1	1597	A	N1-C2-N3	-18.25	120.18	129.30
1	16S1	994	A	N1-C6-N6	-18.24	107.65	118.60
1	16S1	478	A	N1-C2-N3	-18.24	120.18	129.30
22	23S1	1553	A	N1-C2-N3	-18.24	120.18	129.30
22	23S1	2814	A	C2-N3-C4	18.24	119.72	110.60
22	23S1	1981	A	N1-C2-N3	-18.24	120.18	129.30
1	16S1	10	A	N1-C2-N3	-18.24	120.18	129.30
22	23S1	156	A	N1-C2-N3	-18.24	120.18	129.30
55	PTR1	73	A	C2-N3-C4	18.24	119.72	110.60
1	16S1	1170	A	C2-N3-C4	18.24	119.72	110.60
22	23S1	586	A	N1-C6-N6	-18.24	107.66	118.60
22	23S1	94	A	N1-C6-N6	-18.23	107.66	118.60
1	16S1	1254	A	N1-C6-N6	-18.23	107.66	118.60
22	23S1	2810	A	N1-C2-N3	-18.23	120.19	129.30
22	23S1	2309	A	C2-N3-C4	18.23	119.71	110.60
22	23S1	2900	A	C2-N3-C4	18.23	119.71	110.60
1	16S1	452	A	N1-C6-N6	-18.23	107.67	118.60
1	16S1	1483	A	C2-N3-C4	18.23	119.71	110.60
22	23S1	190	A	N1-C6-N6	-18.23	107.66	118.60
22	23S1	270	A	N1-C6-N6	-18.23	107.66	118.60
1	16S1	1503	A	C2-N3-C4	18.22	119.71	110.60
22	23S1	101	A	N1-C2-N3	-18.22	120.19	129.30
22	23S1	1420	A	N1-C6-N6	-18.22	107.67	118.60
1	16S1	502	A	N1-C2-N3	-18.22	120.19	129.30
22	23S1	2407	A	N1-C6-N6	-18.22	107.67	118.60
22	23S1	1069	A	N1-C6-N6	-18.22	107.67	118.60
22	23S1	538	A	C2-N3-C4	18.22	119.71	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	715	A	C2-N3-C4	18.22	119.71	110.60
22	23S1	1354	A	N1-C6-N6	-18.22	107.67	118.60
22	23S1	1746	A	N1-C6-N6	-18.22	107.67	118.60
22	23S1	980	A	N1-C6-N6	-18.21	107.67	118.60
22	23S1	1014	A	N1-C2-N3	-18.21	120.19	129.30
23	05S1	104	A	N1-C6-N6	-18.21	107.67	118.60
1	16S1	131	A	C2-N3-C4	18.21	119.71	110.60
22	23S1	1010	A	C2-N3-C4	18.21	119.70	110.60
22	23S1	1722	A	C2-N3-C4	18.21	119.71	110.60
22	23S1	2134	A	N1-C6-N6	-18.21	107.67	118.60
22	23S1	2600	A	N1-C2-N3	-18.21	120.19	129.30
1	16S1	162	A	C2-N3-C4	18.21	119.70	110.60
1	16S1	1339	A	C2-N3-C4	18.21	119.70	110.60
1	16S1	609	A	N1-C2-N3	-18.21	120.20	129.30
22	23S1	1241	A	N1-C2-N3	-18.21	120.20	129.30
22	23S1	1580	A	N1-C2-N3	-18.21	120.20	129.30
22	23S1	2273	A	N1-C6-N6	-18.21	107.67	118.60
22	23S1	453	A	N1-C6-N6	-18.21	107.68	118.60
55	PTR1	58	A	N1-C2-N3	-18.21	120.20	129.30
1	16S1	228	A	N1-C2-N3	-18.20	120.20	129.30
1	16S1	819	A	N1-C6-N6	-18.20	107.68	118.60
22	23S1	743	A	N1-C2-N3	-18.20	120.20	129.30
1	16S1	1418	A	C2-N3-C4	18.20	119.70	110.60
22	23S1	251	A	N1-C2-N3	-18.20	120.20	129.30
22	23S1	2335	A	N1-C6-N6	-18.20	107.68	118.60
1	16S1	344	A	C2-N3-C4	18.20	119.70	110.60
1	16S1	478	A	N1-C6-N6	-18.20	107.68	118.60
1	16S1	1363	A	N1-C2-N3	-18.20	120.20	129.30
1	16S1	466	A	N1-C6-N6	-18.20	107.68	118.60
22	23S1	265	A	C2-N3-C4	18.20	119.70	110.60
22	23S1	404	A	N1-C6-N6	-18.20	107.68	118.60
22	23S1	1899	A	C2-N3-C4	18.20	119.70	110.60
22	23S1	479	A	N1-C6-N6	-18.20	107.68	118.60
1	16S1	270	A	N1-C2-N3	-18.20	120.20	129.30
1	16S1	353	A	C2-N3-C4	18.20	119.70	110.60
22	23S1	2386	A	N1-C6-N6	-18.20	107.68	118.60
1	16S1	1019	A	N1-C6-N6	-18.19	107.68	118.60
1	16S1	1465	A	N1-C6-N6	-18.19	107.68	118.60
22	23S1	2346	A	C2-N3-C4	18.19	119.70	110.60
1	16S1	262	A	N1-C6-N6	-18.19	107.69	118.60
22	23S1	1393	A	N1-C6-N6	-18.19	107.69	118.60
22	23S1	2314	A	N1-C6-N6	-18.19	107.69	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2378	A	N1-C6-N6	-18.19	107.69	118.60
22	23S1	2589	A	N1-C6-N6	-18.19	107.69	118.60
22	23S1	146	A	N1-C6-N6	-18.19	107.69	118.60
22	23S1	483	A	N1-C2-N3	-18.19	120.21	129.30
22	23S1	1509	A	C2-N3-C4	18.19	119.69	110.60
23	05S1	109	A	N1-C6-N6	-18.19	107.69	118.60
1	16S1	192	A	N1-C2-N3	-18.19	120.21	129.30
1	16S1	964	A	N1-C6-N6	-18.19	107.69	118.60
22	23S1	2077	A	N1-C2-N3	-18.19	120.21	129.30
22	23S1	2856	A	N1-C2-N3	-18.19	120.21	129.30
22	23S1	223	A	C2-N3-C4	18.18	119.69	110.60
1	16S1	131	A	N1-C2-N3	-18.18	120.21	129.30
1	16S1	182	A	C2-N3-C4	18.18	119.69	110.60
1	16S1	1318	A	N1-C6-N6	-18.18	107.69	118.60
22	23S1	1505	A	N1-C2-N3	-18.18	120.21	129.30
22	23S1	2369	A	N1-C2-N3	-18.18	120.21	129.30
22	23S1	2547	A	N1-C2-N3	-18.18	120.21	129.30
22	23S1	1001	A	C2-N3-C4	18.18	119.69	110.60
1	16S1	1157	A	N1-C6-N6	-18.18	107.69	118.60
22	23S1	1803	A	C2-N3-C4	18.18	119.69	110.60
1	16S1	595	A	C2-N3-C4	18.18	119.69	110.60
1	16S1	1191	A	N1-C6-N6	-18.18	107.69	118.60
22	23S1	1552	A	N1-C6-N6	-18.18	107.69	118.60
22	23S1	1969	A	C2-N3-C4	18.18	119.69	110.60
1	16S1	790	A	N1-C2-N3	-18.17	120.21	129.30
22	23S1	2274	A	N1-C6-N6	-18.17	107.70	118.60
1	16S1	172	A	C2-N3-C4	18.17	119.69	110.60
1	16S1	1375	A	C2-N3-C4	18.17	119.69	110.60
22	23S1	89	A	N1-C6-N6	-18.17	107.70	118.60
22	23S1	2059	A	N1-C6-N6	-18.17	107.70	118.60
22	23S1	751	A	N1-C6-N6	-18.17	107.70	118.60
1	16S1	253	A	N1-C2-N3	-18.17	120.22	129.30
22	23S1	575	A	N1-C6-N6	-18.17	107.70	118.60
22	23S1	1745	A	N1-C2-N3	-18.17	120.22	129.30
1	16S1	26	A	N1-C6-N6	-18.16	107.70	118.60
1	16S1	1350	A	N1-C2-N3	-18.16	120.22	129.30
22	23S1	1739	A	N1-C2-N3	-18.16	120.22	129.30
22	23S1	2117	A	C2-N3-C4	18.16	119.68	110.60
22	23S1	1504	A	N1-C6-N6	-18.16	107.70	118.60
22	23S1	2757	A	N1-C6-N6	-18.16	107.70	118.60
22	23S1	2761	A	N1-C2-N3	-18.16	120.22	129.30
1	16S1	873	A	C2-N3-C4	18.16	119.68	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1350	A	N1-C6-N6	-18.16	107.70	118.60
22	23S1	2598	A	N1-C6-N6	-18.16	107.70	118.60
1	16S1	913	A	N1-C6-N6	-18.16	107.71	118.60
1	16S1	687	A	C2-N3-C4	18.15	119.67	110.60
22	23S1	477	A	N1-C2-N3	-18.15	120.22	129.30
22	23S1	1802	A	N1-C2-N3	-18.15	120.22	129.30
22	23S1	492	A	C2-N3-C4	18.15	119.67	110.60
22	23S1	2169	A	N1-C2-N3	-18.15	120.23	129.30
22	23S1	2565	A	N1-C6-N6	-18.15	107.71	118.60
1	16S1	864	A	N1-C2-N3	-18.14	120.23	129.30
1	16S1	1437	A	C2-N3-C4	18.14	119.67	110.60
1	16S1	718	A	N1-C6-N6	-18.14	107.71	118.60
22	23S1	2015	A	N1-C6-N6	-18.14	107.71	118.60
22	23S1	1237	A	C2-N3-C4	18.14	119.67	110.60
22	23S1	2352	A	N1-C2-N3	-18.14	120.23	129.30
1	16S1	510	A	C2-N3-C4	18.14	119.67	110.60
1	16S1	978	A	C2-N3-C4	18.14	119.67	110.60
22	23S1	354	A	N1-C2-N3	-18.14	120.23	129.30
22	23S1	2482	A	N1-C6-N6	-18.14	107.72	118.60
22	23S1	1679	A	N1-C2-N3	-18.14	120.23	129.30
22	23S1	2171	A	C2-N3-C4	18.14	119.67	110.60
22	23S1	2328	A	N1-C6-N6	-18.14	107.72	118.60
1	16S1	546	A	N1-C6-N6	-18.14	107.72	118.60
1	16S1	959	A	N1-C6-N6	-18.14	107.72	118.60
1	16S1	1288	A	N1-C6-N6	-18.14	107.72	118.60
22	23S1	1746	A	N1-C2-N3	-18.14	120.23	129.30
1	16S1	197	A	C2-N3-C4	18.13	119.67	110.60
22	23S1	742	A	N1-C2-N3	-18.13	120.23	129.30
1	16S1	1036	A	N1-C6-N6	-18.13	107.72	118.60
22	23S1	2531	A	N1-C2-N3	-18.13	120.23	129.30
22	23S1	2541	A	N1-C2-N3	-18.13	120.23	129.30
22	23S1	2602	A	N1-C6-N6	-18.13	107.72	118.60
22	23S1	2748	A	N1-C6-N6	-18.13	107.72	118.60
1	16S1	574	A	N1-C6-N6	-18.13	107.72	118.60
22	23S1	2679	A	N1-C6-N6	-18.13	107.72	118.60
22	23S1	2346	A	N1-C2-N3	-18.13	120.24	129.30
1	16S1	66	A	C2-N3-C4	18.13	119.66	110.60
1	16S1	1256	A	N1-C6-N6	-18.13	107.72	118.60
22	23S1	1614	A	C2-N3-C4	18.13	119.66	110.60
22	23S1	1545	A	C2-N3-C4	18.12	119.66	110.60
1	16S1	441	A	N1-C2-N3	-18.12	120.24	129.30
1	16S1	1169	A	N1-C6-N6	-18.12	107.73	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	522	A	N1-C2-N3	-18.12	120.24	129.30
22	23S1	1677	A	N1-C6-N6	-18.12	107.73	118.60
1	16S1	303	A	C2-N3-C4	18.12	119.66	110.60
22	23S1	2634	A	N1-C2-N3	-18.12	120.24	129.30
22	23S1	2810	A	C2-N3-C4	18.12	119.66	110.60
1	16S1	74	A	C2-N3-C4	18.11	119.66	110.60
22	23S1	2850	A	N1-C6-N6	-18.11	107.73	118.60
22	23S1	470	A	N1-C2-N3	-18.11	120.24	129.30
1	16S1	66	A	N1-C2-N3	-18.11	120.24	129.30
1	16S1	315	A	N1-C6-N6	-18.11	107.73	118.60
22	23S1	538	A	N1-C6-N6	-18.11	107.73	118.60
22	23S1	1608	A	N1-C2-N3	-18.11	120.25	129.30
22	23S1	2435	A	N1-C2-N3	-18.11	120.25	129.30
1	16S1	595	A	N1-C6-N6	-18.11	107.74	118.60
1	16S1	155	A	N1-C2-N3	-18.10	120.25	129.30
22	23S1	1936	A	N1-C2-N3	-18.10	120.25	129.30
1	16S1	461	A	N1-C6-N6	-18.10	107.74	118.60
22	23S1	52	A	C2-N3-C4	18.10	119.65	110.60
22	23S1	91	A	C2-N3-C4	18.10	119.65	110.60
22	23S1	1321	A	N1-C6-N6	-18.10	107.74	118.60
1	16S1	487	A	N1-C2-N3	-18.10	120.25	129.30
1	16S1	1257	A	N1-C6-N6	-18.09	107.74	118.60
22	23S1	2170	A	N1-C2-N3	-18.09	120.25	129.30
1	16S1	914	A	C2-N3-C4	18.09	119.65	110.60
22	23S1	1787	A	N1-C6-N6	-18.09	107.75	118.60
22	23S1	1494	A	C2-N3-C4	18.09	119.64	110.60
1	16S1	1503	A	N1-C6-N6	-18.09	107.75	118.60
22	23S1	354	A	C2-N3-C4	18.09	119.64	110.60
22	23S1	718	A	N1-C2-N3	-18.09	120.26	129.30
1	16S1	906	A	N1-C6-N6	-18.09	107.75	118.60
1	16S1	303	A	N1-C2-N3	-18.09	120.26	129.30
22	23S1	2706	A	N1-C2-N3	-18.09	120.26	129.30
1	16S1	1368	A	N1-C6-N6	-18.08	107.75	118.60
22	23S1	661	A	N1-C6-N6	-18.08	107.75	118.60
22	23S1	412	A	N1-C6-N6	-18.08	107.75	118.60
1	16S1	139	A	N1-C6-N6	-18.07	107.75	118.60
1	16S1	1197	A	N1-C6-N6	-18.07	107.75	118.60
22	23S1	131	A	N1-C2-N3	-18.07	120.26	129.30
22	23S1	176	A	N1-C2-N3	-18.07	120.26	129.30
1	16S1	329	A	C2-N3-C4	18.07	119.64	110.60
22	23S1	2288	A	C2-N3-C4	18.07	119.64	110.60
1	16S1	1441	A	N1-C6-N6	-18.07	107.76	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	505	A	N1-C6-N6	-18.07	107.76	118.60
22	23S1	633	A	C2-N3-C4	18.07	119.64	110.60
22	23S1	94	A	N1-C2-N3	-18.07	120.27	129.30
22	23S1	2873	A	C2-N3-C4	18.07	119.63	110.60
22	23S1	1054	A	N1-C2-N3	-18.07	120.27	129.30
22	23S1	1610	A	C2-N3-C4	18.07	119.63	110.60
1	16S1	1299	A	N1-C2-N3	-18.06	120.27	129.30
22	23S1	1029	A	C2-N3-C4	18.06	119.63	110.60
22	23S1	2459	A	N1-C2-N3	-18.06	120.27	129.30
1	16S1	456	A	N1-C6-N6	-18.06	107.76	118.60
23	05S1	119	A	N1-C2-N3	-18.06	120.27	129.30
1	16S1	263	A	N1-C6-N6	-18.06	107.76	118.60
22	23S1	1970	A	C2-N3-C4	18.06	119.63	110.60
1	16S1	663	A	N1-C2-N3	-18.06	120.27	129.30
22	23S1	1285	A	N1-C2-N3	-18.06	120.27	129.30
22	23S1	1871	A	N1-C2-N3	-18.06	120.27	129.30
22	23S1	1609	A	N1-C2-N3	-18.05	120.27	129.30
23	05S1	73	A	N1-C6-N6	-18.05	107.77	118.60
55	PTR1	42	A	N1-C6-N6	-18.05	107.77	118.60
1	16S1	974	A	N1-C6-N6	-18.05	107.77	118.60
22	23S1	2590	A	C2-N3-C4	18.05	119.63	110.60
23	05S1	58	A	N1-C6-N6	-18.05	107.77	118.60
1	16S1	1311	A	N1-C6-N6	-18.05	107.77	118.60
22	23S1	2205	A	N1-C2-N3	-18.05	120.28	129.30
1	16S1	607	A	C2-N3-C4	18.05	119.62	110.60
22	23S1	2094	A	N1-C6-N6	-18.05	107.77	118.60
1	16S1	1152	A	N1-C2-N3	-18.05	120.28	129.30
22	23S1	1641	A	N1-C6-N6	-18.04	107.77	118.60
1	16S1	50	A	C2-N3-C4	18.04	119.62	110.60
1	16S1	1429	A	N1-C6-N6	-18.04	107.78	118.60
22	23S1	2453	A	N1-C2-N3	-18.04	120.28	129.30
1	16S1	622	A	C2-N3-C4	18.04	119.62	110.60
1	16S1	192	A	N1-C6-N6	-18.03	107.78	118.60
22	23S1	2531	A	N1-C6-N6	-18.03	107.78	118.60
23	05S1	58	A	C2-N3-C4	18.03	119.62	110.60
55	PTR1	23	A	N1-C2-N3	-18.03	120.28	129.30
1	16S1	1275	A	N1-C6-N6	-18.03	107.78	118.60
1	16S1	53	A	N1-C6-N6	-18.03	107.78	118.60
1	16S1	74	A	N1-C2-N3	-18.03	120.29	129.30
22	23S1	1664	A	N1-C6-N6	-18.03	107.78	118.60
22	23S1	2020	A	N1-C6-N6	-18.03	107.78	118.60
1	16S1	190	A	C2-N3-C4	18.02	119.61	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	996	A	N1-C6-N6	-18.02	107.79	118.60
1	16S1	694	A	N1-C6-N6	-18.02	107.79	118.60
1	16S1	430	A	N1-C2-N3	-18.02	120.29	129.30
22	23S1	1966	A	N1-C6-N6	-18.02	107.79	118.60
1	16S1	975	A	N1-C6-N6	-18.02	107.79	118.60
22	23S1	547	A	C2-N3-C4	18.02	119.61	110.60
1	16S1	1476	A	N1-C2-N3	-18.01	120.29	129.30
22	23S1	1672	A	N1-C6-N6	-18.01	107.79	118.60
22	23S1	2482	A	N1-C2-N3	-18.01	120.30	129.30
1	16S1	635	A	N1-C6-N6	-18.01	107.80	118.60
22	23S1	936	A	N1-C6-N6	-18.01	107.80	118.60
22	23S1	2070	A	N1-C2-N3	-18.01	120.30	129.30
22	23S1	668	A	N1-C6-N6	-18.00	107.80	118.60
55	PTR1	14	A	N1-C6-N6	-18.00	107.80	118.60
22	23S1	1705	A	N1-C6-N6	-18.00	107.80	118.60
22	23S1	849	A	N1-C6-N6	-18.00	107.80	118.60
22	23S1	1735	A	N1-C6-N6	-18.00	107.80	118.60
55	PTR1	58	A	N1-C6-N6	-18.00	107.80	118.60
22	23S1	1780	A	N1-C6-N6	-18.00	107.80	118.60
22	23S1	1230	A	N1-C6-N6	-18.00	107.80	118.60
1	16S1	687	A	N1-C6-N6	-18.00	107.80	118.60
22	23S1	863	A	N1-C2-N3	-18.00	120.30	129.30
22	23S1	1126	A	N1-C2-N3	-18.00	120.30	129.30
1	16S1	1197	A	N1-C2-N3	-17.99	120.30	129.30
22	23S1	572	A	N1-C2-N3	-17.99	120.30	129.30
1	16S1	780	A	N1-C6-N6	-17.99	107.81	118.60
1	16S1	1151	A	N1-C2-N3	-17.99	120.31	129.30
22	23S1	131	A	N1-C6-N6	-17.99	107.81	118.60
22	23S1	207	A	N1-C6-N6	-17.99	107.81	118.60
22	23S1	1591	A	N1-C6-N6	-17.99	107.81	118.60
22	23S1	508	A	N1-C6-N6	-17.98	107.81	118.60
22	23S1	2425	A	N1-C6-N6	-17.98	107.81	118.60
22	23S1	2439	A	N1-C2-N3	-17.98	120.31	129.30
1	16S1	1413	A	C2-N3-C4	17.98	119.59	110.60
1	16S1	1413	A	N1-C6-N6	-17.98	107.81	118.60
22	23S1	1143	A	C2-N3-C4	17.98	119.59	110.60
22	23S1	800	A	C2-N3-C4	17.98	119.59	110.60
22	23S1	1503	A	N1-C2-N3	-17.97	120.31	129.30
1	16S1	1508	A	N1-C2-N3	-17.97	120.31	129.30
22	23S1	1977	A	N1-C6-N6	-17.97	107.82	118.60
1	16S1	451	A	N1-C6-N6	-17.97	107.82	118.60
1	16S1	642	A	N1-C2-N3	-17.97	120.32	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	913	A	C2-N3-C4	17.97	119.58	110.60
22	23S1	1226	A	C2-N3-C4	17.97	119.58	110.60
22	23S1	2886	A	N1-C6-N6	-17.97	107.82	118.60
1	16S1	189	A	N1-C2-N3	-17.96	120.32	129.30
1	16S1	923	A	N1-C2-N3	-17.96	120.32	129.30
22	23S1	981	A	C2-N3-C4	17.96	119.58	110.60
22	23S1	2434	A	N1-C2-N3	-17.96	120.32	129.30
22	23S1	91	A	N1-C6-N6	-17.96	107.82	118.60
22	23S1	1088	A	N1-C6-N6	-17.96	107.82	118.60
22	23S1	382	A	N1-C6-N6	-17.96	107.83	118.60
22	23S1	722	A	N1-C2-N3	-17.96	120.32	129.30
22	23S1	960	A	N1-C2-N3	-17.96	120.32	129.30
1	16S1	415	A	N1-C2-N3	-17.95	120.32	129.30
1	16S1	749	A	N1-C6-N6	-17.95	107.83	118.60
1	16S1	1130	A	N1-C2-N3	-17.95	120.32	129.30
22	23S1	829	A	C2-N3-C4	17.95	119.58	110.60
1	16S1	32	A	N1-C2-N3	-17.95	120.33	129.30
22	23S1	191	A	N1-C6-N6	-17.95	107.83	118.60
22	23S1	833	A	N1-C6-N6	-17.95	107.83	118.60
22	23S1	2191	A	N1-C2-N3	-17.95	120.33	129.30
23	05S1	50	A	N1-C6-N6	-17.95	107.83	118.60
22	23S1	2412	A	C2-N3-C4	17.95	119.57	110.60
1	16S1	1394	A	C2-N3-C4	17.94	119.57	110.60
22	23S1	1586	A	N1-C2-N3	-17.94	120.33	129.30
22	23S1	2800	A	C2-N3-C4	17.94	119.57	110.60
22	23S1	2287	A	N1-C6-N6	-17.94	107.83	118.60
1	16S1	482	A	N1-C6-N6	-17.94	107.84	118.60
22	23S1	1549	A	N1-C6-N6	-17.94	107.83	118.60
22	23S1	2108	A	N1-C6-N6	-17.94	107.83	118.60
22	23S1	861	A	N1-C6-N6	-17.94	107.84	118.60
1	16S1	1042	A	N1-C6-N6	-17.94	107.84	118.60
22	23S1	730	A	N1-C2-N3	-17.94	120.33	129.30
22	23S1	1848	A	N1-C6-N6	-17.93	107.84	118.60
22	23S1	1916	A	N1-C6-N6	-17.93	107.84	118.60
1	16S1	80	A	N1-C2-N3	-17.93	120.33	129.30
1	16S1	129	A	N1-C6-N6	-17.93	107.84	118.60
1	16S1	499	A	C2-N3-C4	17.93	119.56	110.60
23	05S1	53	A	N1-C6-N6	-17.92	107.85	118.60
1	16S1	1502	A	N1-C6-N6	-17.92	107.85	118.60
1	16S1	706	A	N1-C2-N3	-17.92	120.34	129.30
22	23S1	1938	A	N1-C6-N6	-17.92	107.85	118.60
22	23S1	2778	A	N1-C6-N6	-17.92	107.85	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2851	A	N1-C6-N6	-17.92	107.85	118.60
22	23S1	849	A	N1-C2-N3	-17.91	120.35	129.30
22	23S1	1103	A	C2-N3-C4	17.91	119.55	110.60
22	23S1	1237	A	N1-C6-N6	-17.91	107.86	118.60
1	16S1	673	A	N1-C2-N3	-17.90	120.35	129.30
22	23S1	503	A	N1-C2-N3	-17.90	120.35	129.30
1	16S1	51	A	N1-C2-N3	-17.90	120.35	129.30
22	23S1	2247	A	N1-C6-N6	-17.90	107.86	118.60
22	23S1	2635	A	N1-C2-N3	-17.90	120.35	129.30
22	23S1	19	A	N1-C2-N3	-17.90	120.35	129.30
22	23S1	505	A	N1-C2-N3	-17.90	120.35	129.30
1	16S1	975	A	C2-N3-C4	17.89	119.54	110.60
22	23S1	2328	A	N1-C2-N3	-17.89	120.36	129.30
22	23S1	947	A	N1-C6-N6	-17.88	107.87	118.60
22	23S1	1784	A	N1-C6-N6	-17.88	107.87	118.60
55	PTR1	21	A	N1-C6-N6	-17.88	107.87	118.60
22	23S1	352	A	N1-C2-N3	-17.88	120.36	129.30
22	23S1	1626	A	N1-C6-N6	-17.88	107.87	118.60
22	23S1	84	A	C2-N3-C4	17.88	119.54	110.60
22	23S1	1433	A	N1-C6-N6	-17.88	107.88	118.60
22	23S1	1276	A	N1-C6-N6	-17.87	107.88	118.60
1	16S1	712	A	N1-C6-N6	-17.87	107.88	118.60
22	23S1	1322	A	C2-N3-C4	17.87	119.53	110.60
1	16S1	279	A	C2-N3-C4	17.87	119.53	110.60
22	23S1	2198	A	C2-N3-C4	17.87	119.53	110.60
22	23S1	666	A	N1-C6-N6	-17.86	107.88	118.60
22	23S1	2158	A	N1-C6-N6	-17.86	107.88	118.60
22	23S1	2377	A	N1-C6-N6	-17.86	107.88	118.60
1	16S1	1492	A	N1-C2-N3	-17.86	120.37	129.30
1	16S1	1319	A	C2-N3-C4	17.85	119.53	110.60
1	16S1	602	A	N1-C6-N6	-17.84	107.90	118.60
22	23S1	251	A	C2-N3-C4	17.84	119.52	110.60
1	16S1	1130	A	N1-C6-N6	-17.84	107.90	118.60
22	23S1	227	A	N1-C6-N6	-17.83	107.90	118.60
22	23S1	1431	A	N1-C6-N6	-17.83	107.90	118.60
22	23S1	2088	A	N1-C2-N3	-17.83	120.38	129.30
1	16S1	1105	A	N1-C6-N6	-17.83	107.90	118.60
22	23S1	608	A	N1-C6-N6	-17.83	107.90	118.60
22	23S1	1502	A	N1-C2-N3	-17.82	120.39	129.30
22	23S1	1029	A	N1-C2-N3	-17.82	120.39	129.30
1	16S1	223	A	N1-C2-N3	-17.82	120.39	129.30
22	23S1	1913	A	N1-C6-N6	-17.82	107.91	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	98	A	N1-C6-N6	-17.81	107.91	118.60
1	16S1	1012	A	N1-C6-N6	-17.81	107.91	118.60
1	16S1	1271	A	N1-C6-N6	-17.81	107.91	118.60
55	PTR1	23	A	N1-C6-N6	-17.81	107.91	118.60
1	16S1	630	A	N1-C6-N6	-17.81	107.91	118.60
22	23S1	614	A	N1-C6-N6	-17.81	107.92	118.60
22	23S1	2176	A	N1-C6-N6	-17.81	107.92	118.60
23	05S1	115	A	N1-C6-N6	-17.81	107.92	118.60
1	16S1	609	A	N1-C6-N6	-17.80	107.92	118.60
22	23S1	95	A	N1-C2-N3	-17.80	120.40	129.30
22	23S1	1679	A	N1-C6-N6	-17.80	107.92	118.60
1	16S1	959	A	N1-C2-N3	-17.79	120.40	129.30
1	16S1	1332	A	N1-C2-N3	-17.79	120.41	129.30
22	23S1	203	A	N1-C6-N6	-17.79	107.93	118.60
22	23S1	374	A	N1-C6-N6	-17.79	107.93	118.60
22	23S1	2163	A	N1-C2-N3	-17.79	120.41	129.30
22	23S1	447	A	N1-C6-N6	-17.78	107.93	118.60
22	23S1	920	A	N1-C6-N6	-17.78	107.93	118.60
22	23S1	2412	A	N1-C6-N6	-17.78	107.93	118.60
1	16S1	919	A	N1-C6-N6	-17.77	107.94	118.60
22	23S1	2792	A	N1-C2-N3	-17.77	120.41	129.30
22	23S1	2893	A	N1-C6-N6	-17.77	107.94	118.60
1	16S1	539	A	N1-C6-N6	-17.77	107.94	118.60
1	16S1	1005	A	N1-C6-N6	-17.77	107.94	118.60
1	16S1	1093	A	N1-C6-N6	-17.77	107.94	118.60
22	23S1	1689	A	N1-C6-N6	-17.77	107.94	118.60
1	16S1	130	A	N1-C6-N6	-17.77	107.94	118.60
22	23S1	460	A	N1-C6-N6	-17.76	107.94	118.60
22	23S1	820	A	N1-C2-N3	-17.76	120.42	129.30
22	23S1	1328	A	N1-C2-N3	-17.76	120.42	129.30
22	23S1	743	A	N1-C6-N6	-17.76	107.94	118.60
22	23S1	2516	A	N1-C6-N6	-17.76	107.94	118.60
22	23S1	2051	A	N1-C2-N3	-17.75	120.42	129.30
1	16S1	655	A	N1-C2-N3	-17.75	120.42	129.30
1	16S1	712	A	N1-C2-N3	-17.75	120.43	129.30
22	23S1	722	A	N1-C6-N6	-17.75	107.95	118.60
1	16S1	1227	A	N1-C2-N3	-17.75	120.43	129.30
22	23S1	1133	A	C2-N3-C4	17.75	119.47	110.60
22	23S1	1393	A	C2-N3-C4	17.74	119.47	110.60
22	23S1	1387	A	N1-C6-N6	-17.74	107.95	118.60
1	16S1	279	A	N1-C6-N6	-17.74	107.96	118.60
1	16S1	459	A	N1-C6-N6	-17.74	107.95	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1593	A	N1-C6-N6	-17.74	107.95	118.60
1	16S1	1483	A	N1-C2-N3	-17.74	120.43	129.30
22	23S1	64	A	N1-C6-N6	-17.74	107.96	118.60
22	23S1	382	A	N1-C2-N3	-17.74	120.43	129.30
22	23S1	471	A	N1-C6-N6	-17.73	107.96	118.60
22	23S1	727	A	N1-C6-N6	-17.73	107.96	118.60
1	16S1	1110	A	N1-C6-N6	-17.73	107.96	118.60
22	23S1	1614	A	N1-C6-N6	-17.73	107.96	118.60
22	23S1	2821	A	C2-N3-C4	17.73	119.47	110.60
1	16S1	1163	A	N1-C2-N3	-17.73	120.43	129.30
22	23S1	1664	A	N1-C2-N3	-17.73	120.43	129.30
1	16S1	493	A	C2-N3-C4	17.73	119.47	110.60
22	23S1	428	A	N1-C6-N6	-17.73	107.96	118.60
1	16S1	199	A	N1-C6-N6	-17.73	107.97	118.60
1	16S1	1080	A	N1-C6-N6	-17.73	107.97	118.60
22	23S1	794	A	N1-C2-N3	-17.73	120.44	129.30
1	16S1	901	A	C2-N3-C4	17.72	119.46	110.60
22	23S1	56	A	N1-C2-N3	-17.72	120.44	129.30
22	23S1	1713	A	N1-C6-N6	-17.72	107.97	118.60
1	16S1	366	A	N1-C6-N6	-17.72	107.97	118.60
1	16S1	629	A	N1-C6-N6	-17.72	107.97	118.60
1	16S1	675	A	C2-N3-C4	17.72	119.46	110.60
22	23S1	2042	A	N1-C6-N6	-17.72	107.97	118.60
22	23S1	2860	A	C2-N3-C4	17.72	119.46	110.60
1	16S1	1014	A	N1-C6-N6	-17.72	107.97	118.60
1	16S1	1022	A	N1-C2-N3	-17.71	120.44	129.30
1	16S1	1236	A	N1-C6-N6	-17.71	107.97	118.60
1	16S1	349	A	N1-C6-N6	-17.71	107.97	118.60
22	23S1	1610	A	N1-C6-N6	-17.71	107.97	118.60
22	23S1	933	A	N1-C6-N6	-17.71	107.97	118.60
22	23S1	1535	A	N1-C2-N3	-17.71	120.44	129.30
22	23S1	2741	A	N1-C6-N6	-17.71	107.97	118.60
1	16S1	55	A	N1-C6-N6	-17.71	107.97	118.60
1	16S1	702	A	C2-N3-C4	17.70	119.45	110.60
22	23S1	1580	A	N1-C6-N6	-17.70	107.98	118.60
22	23S1	255	A	N1-C6-N6	-17.70	107.98	118.60
22	23S1	2176	A	C2-N3-C4	17.70	119.45	110.60
22	23S1	282	A	N1-C6-N6	-17.69	107.98	118.60
22	23S1	677	A	N1-C2-N3	-17.69	120.45	129.30
1	16S1	1067	A	C2-N3-C4	17.69	119.44	110.60
1	16S1	1157	A	N1-C2-N3	-17.69	120.45	129.30
22	23S1	278	A	N1-C2-N3	-17.69	120.46	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1981	A	C2-N3-C4	17.69	119.44	110.60
22	23S1	223	A	N1-C6-N6	-17.68	107.99	118.60
22	23S1	1403	A	N1-C2-N3	-17.68	120.46	129.30
22	23S1	1821	A	C2-N3-C4	17.68	119.44	110.60
22	23S1	1144	A	N1-C6-N6	-17.68	107.99	118.60
1	16S1	189	A	N1-C6-N6	-17.68	107.99	118.60
22	23S1	1169	A	N1-C6-N6	-17.68	107.99	118.60
1	16S1	968	A	N1-C6-N6	-17.68	108.00	118.60
22	23S1	470	A	N1-C6-N6	-17.66	108.00	118.60
22	23S1	49	A	N1-C6-N6	-17.66	108.00	118.60
22	23S1	156	A	N1-C6-N6	-17.66	108.00	118.60
22	23S1	1722	A	N1-C2-N3	-17.66	120.47	129.30
1	16S1	1102	A	N1-C6-N6	-17.66	108.00	118.60
22	23S1	1953	A	C2-N3-C4	17.66	119.43	110.60
22	23S1	2873	A	N1-C6-N6	-17.66	108.00	118.60
22	23S1	2126	A	N1-C2-N3	-17.65	120.48	129.30
22	23S1	2170	A	N1-C6-N6	-17.65	108.01	118.60
22	23S1	63	A	N1-C6-N6	-17.64	108.01	118.60
22	23S1	522	A	N1-C6-N6	-17.64	108.01	118.60
22	23S1	1871	A	N1-C6-N6	-17.64	108.01	118.60
1	16S1	383	A	C2-N3-C4	17.64	119.42	110.60
1	16S1	860	A	N1-C2-N3	-17.64	120.48	129.30
22	23S1	21	A	N1-C6-N6	-17.64	108.02	118.60
22	23S1	1070	A	N1-C6-N6	-17.64	108.02	118.60
1	16S1	1375	A	N1-C2-N3	-17.63	120.48	129.30
22	23S1	2634	A	N1-C6-N6	-17.63	108.02	118.60
1	16S1	520	A	N1-C2-N3	-17.62	120.49	129.30
22	23S1	480	A	N1-C6-N6	-17.62	108.03	118.60
22	23S1	2448	A	C2-N3-C4	17.62	119.41	110.60
22	23S1	2117	A	N1-C6-N6	-17.62	108.03	118.60
55	PTR1	3	A	N1-C6-N6	-17.62	108.03	118.60
22	23S1	1808	A	N1-C6-N6	-17.62	108.03	118.60
22	23S1	1226	A	N1-C6-N6	-17.61	108.03	118.60
22	23S1	2860	A	N1-C6-N6	-17.61	108.03	118.60
22	23S1	626	A	N1-C6-N6	-17.61	108.03	118.60
22	23S1	1327	A	N1-C6-N6	-17.61	108.03	118.60
1	16S1	706	A	N1-C6-N6	-17.61	108.03	118.60
1	16S1	77	A	N1-C2-N3	-17.61	120.50	129.30
1	16S1	1324	A	N1-C2-N3	-17.60	120.50	129.30
22	23S1	1098	A	N1-C2-N3	-17.60	120.50	129.30
1	16S1	640	A	N1-C2-N3	-17.60	120.50	129.30
1	16S1	1239	A	C2-N3-C4	17.60	119.40	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	480	A	N1-C2-N3	-17.59	120.50	129.30
22	23S1	2476	A	N1-C6-N6	-17.59	108.04	118.60
22	23S1	2412	A	N1-C2-N3	-17.59	120.50	129.30
55	PTR1	69	A	N1-C6-N6	-17.59	108.05	118.60
1	16S1	71	A	N1-C6-N6	-17.59	108.05	118.60
1	16S1	743	A	N1-C2-N3	-17.58	120.51	129.30
22	23S1	2856	A	N1-C6-N6	-17.57	108.06	118.60
1	16S1	1531	A	N1-C6-N6	-17.57	108.06	118.60
22	23S1	2587	A	N1-C6-N6	-17.57	108.06	118.60
22	23S1	975	A	N1-C6-N6	-17.57	108.06	118.60
22	23S1	1791	A	N1-C6-N6	-17.56	108.06	118.60
22	23S1	2565	A	C2-N3-C4	17.56	119.38	110.60
1	16S1	71	A	C2-N3-C4	17.56	119.38	110.60
22	23S1	1528	A	N1-C2-N3	-17.56	120.52	129.30
22	23S1	472	A	N1-C6-N6	-17.56	108.06	118.60
22	23S1	582	A	N1-C6-N6	-17.56	108.06	118.60
22	23S1	256	A	N1-C6-N6	-17.56	108.07	118.60
23	05S1	57	A	N1-C6-N6	-17.55	108.07	118.60
1	16S1	493	A	N1-C6-N6	-17.55	108.07	118.60
22	23S1	1336	A	N1-C6-N6	-17.55	108.07	118.60
55	PTR1	76	A	N1-C6-N6	-17.53	108.08	118.60
1	16S1	66	A	N1-C6-N6	-17.53	108.08	118.60
22	23S1	877	A	N1-C6-N6	-17.53	108.08	118.60
1	16S1	743	A	N1-C6-N6	-17.52	108.09	118.60
22	23S1	482	A	N1-C2-N3	-17.52	120.54	129.30
22	23S1	2675	A	N1-C6-N6	-17.51	108.09	118.60
22	23S1	2278	A	N1-C6-N6	-17.51	108.09	118.60
22	23S1	925	A	N1-C6-N6	-17.51	108.09	118.60
22	23S1	1020	A	C2-N3-C4	17.51	119.35	110.60
22	23S1	152	A	N1-C6-N6	-17.50	108.10	118.60
1	16S1	510	A	N1-C6-N6	-17.50	108.10	118.60
1	16S1	460	A	N1-C6-N6	-17.50	108.10	118.60
1	16S1	790	A	N1-C6-N6	-17.50	108.10	118.60
22	23S1	1272	A	N1-C6-N6	-17.50	108.10	118.60
22	23S1	2899	A	N1-C6-N6	-17.50	108.10	118.60
1	16S1	675	A	N1-C6-N6	-17.50	108.10	118.60
55	PTR1	76	A	C2-N3-C4	17.50	119.35	110.60
22	23S1	2879	A	N1-C6-N6	-17.49	108.10	118.60
1	16S1	344	A	N1-C6-N6	-17.49	108.11	118.60
1	16S1	1357	A	N1-C6-N6	-17.49	108.11	118.60
22	23S1	1151	A	N1-C6-N6	-17.49	108.11	118.60
22	23S1	1808	A	C2-N3-C4	17.49	119.34	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2274	A	C2-N3-C4	17.49	119.34	110.60
1	16S1	1102	A	N1-C2-N3	-17.48	120.56	129.30
23	05S1	94	A	N1-C6-N6	-17.48	108.11	118.60
22	23S1	2268	A	N1-C6-N6	-17.48	108.11	118.60
1	16S1	1167	A	N1-C6-N6	-17.47	108.12	118.60
22	23S1	2439	A	N1-C6-N6	-17.47	108.12	118.60
22	23S1	1549	A	N1-C2-N3	-17.47	120.57	129.30
22	23S1	1717	A	N1-C6-N6	-17.47	108.12	118.60
22	23S1	404	A	C2-N3-C4	17.46	119.33	110.60
22	23S1	2037	A	N1-C6-N6	-17.45	108.13	118.60
1	16S1	502	A	N1-C6-N6	-17.45	108.13	118.60
22	23S1	1987	A	N1-C6-N6	-17.45	108.13	118.60
22	23S1	1810	A	C2-N3-C4	17.45	119.32	110.60
22	23S1	730	A	N1-C6-N6	-17.45	108.13	118.60
22	23S1	1900	A	N1-C6-N6	-17.44	108.14	118.60
22	23S1	2142	A	N1-C2-N3	-17.44	120.58	129.30
22	23S1	1373	A	N1-C6-N6	-17.44	108.14	118.60
22	23S1	2900	A	N1-C2-N3	-17.44	120.58	129.30
22	23S1	1508	A	N1-C6-N6	-17.43	108.14	118.60
1	16S1	901	A	N1-C2-N3	-17.43	120.58	129.30
22	23S1	1269	A	N1-C2-N3	-17.43	120.58	129.30
22	23S1	1711	A	N1-C6-N6	-17.42	108.15	118.60
22	23S1	1978	A	N1-C6-N6	-17.42	108.15	118.60
22	23S1	466	A	C2-N3-C4	17.41	119.30	110.60
22	23S1	1803	A	N1-C6-N6	-17.41	108.16	118.60
22	23S1	2813	A	N1-C6-N6	-17.40	108.16	118.60
1	16S1	101	A	N1-C6-N6	-17.40	108.16	118.60
22	23S1	781	A	N1-C2-N3	-17.40	120.60	129.30
22	23S1	1403	A	N1-C6-N6	-17.40	108.16	118.60
22	23S1	943	A	N1-C6-N6	-17.39	108.17	118.60
22	23S1	1387	A	N1-C2-N3	-17.39	120.61	129.30
23	05S1	66	A	N1-C6-N6	-17.39	108.17	118.60
1	16S1	1306	A	N1-C6-N6	-17.36	108.18	118.60
22	23S1	844	A	N1-C6-N6	-17.36	108.18	118.60
1	16S1	441	A	N1-C6-N6	-17.36	108.19	118.60
1	16S1	1375	A	N1-C6-N6	-17.36	108.18	118.60
22	23S1	2340	A	N1-C6-N6	-17.36	108.18	118.60
1	16S1	253	A	N1-C6-N6	-17.36	108.19	118.60
22	23S1	2459	A	N1-C6-N6	-17.36	108.19	118.60
22	23S1	2706	A	N1-C6-N6	-17.35	108.19	118.60
1	16S1	327	A	N1-C6-N6	-17.35	108.19	118.60
1	16S1	300	A	C2-N3-C4	17.34	119.27	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1477	A	N1-C6-N6	-17.34	108.19	118.60
1	16S1	1000	A	N1-C6-N6	-17.32	108.21	118.60
22	23S1	2284	A	N1-C2-N3	-17.31	120.64	129.30
22	23S1	2176	A	N1-C2-N3	-17.31	120.65	129.30
1	16S1	270	A	N1-C6-N6	-17.30	108.22	118.60
1	16S1	1252	A	N1-C6-N6	-17.30	108.22	118.60
22	23S1	1469	A	N1-C6-N6	-17.30	108.22	118.60
22	23S1	2461	A	N1-C2-N3	-17.30	120.65	129.30
1	16S1	1055	A	N1-C6-N6	-17.30	108.22	118.60
1	16S1	1398	A	C2-N3-C4	17.30	119.25	110.60
55	PTR1	14	A	N1-C2-N3	-17.29	120.65	129.30
1	16S1	1394	A	N1-C6-N6	-17.29	108.23	118.60
1	16S1	1170	A	N1-C2-N3	-17.28	120.66	129.30
22	23S1	2366	A	N1-C6-N6	-17.27	108.24	118.60
1	16S1	1163	A	N1-C6-N6	-17.27	108.24	118.60
22	23S1	1085	A	N1-C6-N6	-17.26	108.24	118.60
1	16S1	55	A	N1-C2-N3	-17.25	120.67	129.30
22	23S1	2088	A	N1-C6-N6	-17.25	108.25	118.60
22	23S1	2700	A	N1-C6-N6	-17.25	108.25	118.60
22	23S1	1872	A	N1-C2-N3	-17.25	120.68	129.30
1	16S1	715	A	N1-C6-N6	-17.24	108.25	118.60
22	23S1	161	A	C2-N3-C4	17.24	119.22	110.60
22	23S1	1080	A	N1-C6-N6	-17.24	108.25	118.60
22	23S1	1089	A	N1-C6-N6	-17.24	108.25	118.60
22	23S1	1027	A	N1-C6-N6	-17.24	108.26	118.60
22	23S1	1572	A	N1-C6-N6	-17.24	108.26	118.60
22	23S1	1548	A	N1-C6-N6	-17.23	108.26	118.60
1	16S1	356	A	N1-C6-N6	-17.23	108.26	118.60
1	16S1	1081	A	N1-C6-N6	-17.23	108.26	118.60
1	16S1	1437	A	N1-C6-N6	-17.23	108.26	118.60
22	23S1	167	A	N1-C6-N6	-17.23	108.26	118.60
22	23S1	2469	A	N1-C6-N6	-17.22	108.27	118.60
1	16S1	563	A	N1-C6-N6	-17.22	108.27	118.60
22	23S1	2598	A	C2-N3-C4	17.22	119.21	110.60
1	16S1	1339	A	N1-C2-N3	-17.21	120.69	129.30
22	23S1	1275	A	C2-N3-C4	17.21	119.21	110.60
22	23S1	2014	A	N1-C6-N6	-17.20	108.28	118.60
1	16S1	250	A	N1-C6-N6	-17.19	108.28	118.60
1	16S1	919	A	N1-C2-N3	-17.19	120.70	129.30
22	23S1	1057	A	N1-C6-N6	-17.19	108.29	118.60
1	16S1	373	A	N1-C6-N6	-17.18	108.29	118.60
1	16S1	1507	A	N1-C6-N6	-17.16	108.30	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1821	A	N1-C2-N3	-17.16	120.72	129.30
1	16S1	236	A	N1-C6-N6	-17.15	108.31	118.60
22	23S1	1098	A	N1-C6-N6	-17.15	108.31	118.60
22	23S1	1272	A	C2-N3-C4	17.15	119.18	110.60
22	23S1	352	A	C2-N3-C4	17.15	119.17	110.60
22	23S1	2721	A	N1-C6-N6	-17.15	108.31	118.60
22	23S1	1553	A	N1-C6-N6	-17.14	108.31	118.60
1	16S1	1483	A	N1-C6-N6	-17.14	108.32	118.60
1	16S1	51	A	C2-N3-C4	17.13	119.17	110.60
22	23S1	142	A	N1-C6-N6	-17.13	108.32	118.60
1	16S1	673	A	N1-C6-N6	-17.13	108.32	118.60
22	23S1	1590	A	N1-C6-N6	-17.12	108.33	118.60
1	16S1	33	A	N1-C6-N6	-17.11	108.33	118.60
1	16S1	935	A	N1-C6-N6	-17.10	108.34	118.60
22	23S1	2108	A	N1-C2-N3	-17.10	120.75	129.30
1	16S1	246	A	N1-C6-N6	-17.10	108.34	118.60
22	23S1	221	A	C2-N3-C4	17.10	119.15	110.60
22	23S1	1470	A	N1-C6-N6	-17.10	108.34	118.60
1	16S1	946	A	N1-C6-N6	-17.10	108.34	118.60
22	23S1	1020	A	N1-C6-N6	-17.09	108.34	118.60
1	16S1	155	A	N1-C6-N6	-17.09	108.34	118.60
1	16S1	1036	A	N1-C2-N3	-17.09	120.75	129.30
1	16S1	496	A	N1-C6-N6	-17.09	108.35	118.60
22	23S1	1603	A	N1-C6-N6	-17.09	108.35	118.60
1	16S1	98	A	N1-C2-N3	-17.08	120.76	129.30
1	16S1	908	A	N1-C6-N6	-17.08	108.35	118.60
22	23S1	2288	A	N1-C6-N6	-17.08	108.35	118.60
1	16S1	300	A	N1-C2-N3	-17.07	120.77	129.30
22	23S1	599	A	N1-C6-N6	-17.06	108.36	118.60
22	23S1	466	A	N1-C6-N6	-17.05	108.37	118.60
1	16S1	109	A	N1-C6-N6	-17.04	108.38	118.60
1	16S1	1219	A	N1-C6-N6	-17.04	108.37	118.60
22	23S1	1928	A	C2-N3-C4	17.04	119.12	110.60
1	16S1	907	A	N1-C6-N6	-17.03	108.38	118.60
23	05S1	46	A	C2-N3-C4	17.03	119.11	110.60
1	16S1	865	A	N1-C2-N3	-17.02	120.79	129.30
22	23S1	2426	A	N1-C6-N6	-17.02	108.39	118.60
1	16S1	746	A	N1-C6-N6	-17.01	108.39	118.60
23	05S1	66	A	N1-C2-N3	-17.01	120.79	129.30
1	16S1	51	A	N1-C6-N6	-17.01	108.39	118.60
22	23S1	1866	A	N1-C6-N6	-17.01	108.39	118.60
22	23S1	2868	A	N1-C6-N6	-17.00	108.40	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1324	A	N1-C6-N6	-17.00	108.40	118.60
22	23S1	1244	A	N1-C6-N6	-16.98	108.41	118.60
22	23S1	2154	A	N1-C6-N6	-16.98	108.41	118.60
1	16S1	329	A	N1-C6-N6	-16.98	108.41	118.60
22	23S1	173	A	N1-C6-N6	-16.97	108.42	118.60
22	23S1	1054	A	N1-C6-N6	-16.97	108.42	118.60
1	16S1	162	A	N1-C2-N3	-16.96	120.82	129.30
22	23S1	721	A	N1-C6-N6	-16.95	108.43	118.60
22	23S1	1609	A	N1-C6-N6	-16.95	108.43	118.60
1	16S1	1117	A	N1-C6-N6	-16.94	108.44	118.60
1	16S1	411	A	N1-C6-N6	-16.94	108.44	118.60
22	23S1	2662	A	N1-C2-N3	-16.93	120.83	129.30
55	PTR1	9	A	N1-C6-N6	-16.93	108.44	118.60
22	23S1	415	A	N1-C6-N6	-16.93	108.44	118.60
22	23S1	2114	A	N1-C2-N3	-16.92	120.84	129.30
22	23S1	1532	A	N1-C6-N6	-16.91	108.45	118.60
22	23S1	574	A	N1-C6-N6	-16.91	108.45	118.60
22	23S1	2800	A	N1-C6-N6	-16.91	108.46	118.60
1	16S1	1339	A	N1-C6-N6	-16.88	108.47	118.60
22	23S1	911	A	N1-C6-N6	-16.88	108.47	118.60
1	16S1	1092	A	C2-N3-C4	16.87	119.03	110.60
1	16S1	1227	A	C2-N3-C4	16.87	119.03	110.60
22	23S1	586	A	C2-N3-C4	16.86	119.03	110.60
22	23S1	1302	A	N1-C6-N6	-16.86	108.48	118.60
22	23S1	1189	A	N1-C6-N6	-16.86	108.48	118.60
1	16S1	199	A	N1-C2-N3	-16.86	120.87	129.30
1	16S1	431	A	C5-C6-N6	16.84	137.17	123.70
1	16S1	746	A	N1-C2-N3	-16.83	120.89	129.30
1	16S1	1201	A	N1-C6-N6	-16.82	108.51	118.60
22	23S1	477	A	N1-C6-N6	-16.81	108.51	118.60
22	23S1	1103	A	N1-C6-N6	-16.81	108.51	118.60
55	PTR1	51	A	C2-N3-C4	16.81	119.01	110.60
23	05S1	66	A	C2-N3-C4	16.81	119.00	110.60
22	23S1	1745	A	N1-C6-N6	-16.80	108.52	118.60
22	23S1	2900	A	N1-C6-N6	-16.80	108.52	118.60
22	23S1	2792	A	N1-C6-N6	-16.79	108.52	118.60
22	23S1	1899	A	N1-C2-N3	-16.79	120.90	129.30
1	16S1	663	A	N1-C6-N6	-16.79	108.53	118.60
1	16S1	1046	A	N1-C2-N3	-16.78	120.91	129.30
22	23S1	272	A	N1-C6-N6	-16.77	108.54	118.60
55	PTR1	51	A	N1-C2-N3	-16.77	120.92	129.30
1	16S1	1396	A	N1-C6-N6	-16.77	108.54	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	863	A	N1-C6-N6	-16.76	108.55	118.60
1	16S1	430	A	N1-C6-N6	-16.75	108.55	118.60
22	23S1	2082	A	N1-C6-N6	-16.75	108.55	118.60
22	23S1	1810	A	N1-C2-N3	-16.74	120.93	129.30
22	23S1	633	A	N1-C6-N6	-16.74	108.55	118.60
1	16S1	1171	A	N1-C6-N6	-16.74	108.56	118.60
22	23S1	677	A	N1-C6-N6	-16.71	108.57	118.60
22	23S1	1739	A	N1-C6-N6	-16.70	108.58	118.60
1	16S1	919	A	C2-N3-C4	16.70	118.95	110.60
22	23S1	221	A	N1-C6-N6	-16.70	108.58	118.60
22	23S1	2670	A	N1-C6-N6	-16.69	108.59	118.60
22	23S1	1676	A	N1-C6-N6	-16.67	108.60	118.60
22	23S1	1205	A	N1-C2-N3	-16.65	120.97	129.30
1	16S1	116	A	N1-C6-N6	-16.63	108.62	118.60
22	23S1	101	A	N1-C6-N6	-16.61	108.64	118.60
1	16S1	923	A	N1-C6-N6	-16.59	108.64	118.60
22	23S1	492	A	N1-C6-N6	-16.58	108.65	118.60
23	05S1	45	A	N1-C6-N6	-16.58	108.65	118.60
22	23S1	144	A	N1-C6-N6	-16.57	108.66	118.60
22	23S1	1802	A	N1-C6-N6	-16.57	108.66	118.60
22	23S1	2392	A	N1-C6-N6	-16.55	108.67	118.60
22	23S1	233	A	N1-C6-N6	-16.52	108.69	118.60
1	16S1	32	A	N1-C6-N6	-16.51	108.69	118.60
22	23S1	504	A	C2-N3-C4	16.51	118.86	110.60
1	16S1	190	A	N1-C2-N3	-16.48	121.06	129.30
22	23S1	2135	A	N1-C6-N6	-16.48	108.71	118.60
22	23S1	1936	A	N1-C6-N6	-16.47	108.72	118.60
1	16S1	77	A	N1-C6-N6	-16.46	108.72	118.60
22	23S1	644	A	N1-C2-N3	-16.45	121.08	129.30
22	23S1	1205	A	C2-N3-C4	16.43	118.82	110.60
22	23S1	422	A	N1-C6-N6	-16.41	108.75	118.60
1	16S1	181	A	N1-C6-N6	-16.39	108.76	118.60
22	23S1	52	A	N1-C6-N6	-16.38	108.77	118.60
22	23S1	2821	A	N1-C6-N6	-16.37	108.78	118.60
1	16S1	81	A	N1-C2-N3	-16.36	121.12	129.30
22	23S1	2352	A	N1-C6-N6	-16.30	108.82	118.60
1	16S1	383	A	N1-C2-N3	-16.29	121.16	129.30
1	16S1	1152	A	N1-C6-N6	-16.29	108.83	118.60
22	23S1	1213	A	N1-C6-N6	-16.28	108.83	118.60
22	23S1	1029	A	N1-C6-N6	-16.27	108.84	118.60
55	PTR1	38	A	N1-C6-N6	-16.26	108.84	118.60
1	16S1	873	A	N1-C6-N6	-16.22	108.87	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2725	A	N1-C6-N6	-16.22	108.87	118.60
1	16S1	533	A	N1-C2-N3	-16.19	121.21	129.30
22	23S1	1969	A	N1-C6-N6	-16.18	108.89	118.60
22	23S1	1434	A	C5-C6-N6	16.13	136.60	123.70
22	23S1	820	A	N1-C6-N6	-16.12	108.93	118.60
22	23S1	2369	A	N1-C6-N6	-16.05	108.97	118.60
22	23S1	1143	A	N1-C6-N6	-16.05	108.97	118.60
1	16S1	1508	A	N1-C6-N6	-16.04	108.98	118.60
22	23S1	705	A	N1-C6-N6	-15.96	109.02	118.60
22	23S1	819	A	N1-C6-N6	-15.95	109.03	118.60
22	23S1	2077	A	N1-C6-N6	-15.94	109.03	118.60
1	16S1	397	A	N1-C6-N6	-15.94	109.03	118.60
1	16S1	1201	A	N1-C2-N3	-15.80	121.40	129.30
22	23S1	1241	A	N1-C6-N6	-15.70	109.18	118.60
22	23S1	320	A	C5-C6-N6	15.67	136.24	123.70
25	L031	33	ARG	NE-CZ-NH1	-15.67	112.46	120.30
1	16S1	1418	A	N1-C6-N6	-15.64	109.22	118.60
22	23S1	2614	A	N1-C2-N3	-15.64	121.48	129.30
22	23S1	1111	A	N1-C6-N6	-15.62	109.23	118.60
22	23S1	2766	A	N1-C6-N6	-15.56	109.26	118.60
22	23S1	324	A	N1-C6-N6	-15.55	109.27	118.60
22	23S1	1970	A	N1-C6-N6	-15.49	109.31	118.60
22	23S1	2188	U	OP1-P-O3'	-15.34	71.45	105.20
22	23S1	504	A	N1-C6-N6	-15.30	109.42	118.60
1	16S1	1227	A	N1-C6-N6	-15.28	109.43	118.60
22	23S1	1872	A	N1-C6-N6	-15.20	109.48	118.60
1	16S1	696	A	N1-C6-N6	-15.06	109.56	118.60
1	16S1	1468	A	N1-C6-N6	-15.04	109.58	118.60
22	23S1	1937	A	C5-C6-N6	15.01	135.71	123.70
22	23S1	2171	A	N1-C6-N6	-14.83	109.70	118.60
1	16S1	499	A	N1-C6-N6	-14.82	109.71	118.60
22	23S1	1722	A	N1-C6-N6	-14.72	109.77	118.60
22	23S1	1854	A	N1-C6-N6	-14.71	109.77	118.60
23	05S1	59	A	N3-C4-C5	-14.62	116.56	126.80
22	23S1	504	A	N7-C8-N9	-14.61	106.50	113.80
1	16S1	520	A	C5-C6-N6	14.56	135.35	123.70
22	23S1	2799	A	N1-C6-N6	-14.55	109.87	118.60
22	23S1	2142	A	N1-C6-N6	-14.45	109.93	118.60
1	16S1	498	A	N1-C2-N3	-14.44	122.08	129.30
22	23S1	1571	A	N1-C6-N6	-14.43	109.94	118.60
23	05S1	101	A	N3-C4-C5	-14.26	116.82	126.80
22	23S1	2662	A	N1-C6-N6	-14.18	110.09	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1213	A	C5-C6-N6	14.15	135.02	123.70
22	23S1	513	A	N1-C6-N6	-14.10	110.14	118.60
1	16S1	1004	A	N7-C8-N9	-14.00	106.80	113.80
25	L031	33	ARG	NE-CZ-NH2	13.88	127.24	120.30
1	16S1	411	A	N7-C8-N9	-13.77	106.92	113.80
22	23S1	783	A	N3-C4-C5	-13.75	117.17	126.80
1	16S1	498	A	N3-C4-C5	-13.73	117.19	126.80
1	16S1	704	A	C5-C6-N6	13.62	134.60	123.70
22	23S1	800	A	C5-C6-N6	13.60	134.58	123.70
22	23S1	2572	A	N7-C8-N9	-13.54	107.03	113.80
23	05S1	59	A	N1-C2-N3	-13.50	122.55	129.30
22	23S1	1528	A	N1-C6-N6	-13.46	110.53	118.60
1	16S1	1170	A	N1-C6-N6	-13.40	110.56	118.60
22	23S1	2119	A	N7-C8-N9	-13.38	107.11	113.80
23	05S1	101	A	N1-C2-N3	-13.28	122.66	129.30
22	23S1	783	A	C5-C6-N6	13.27	134.32	123.70
22	23S1	1912	A	N7-C8-N9	-13.25	107.18	113.80
1	16S1	860	A	C5-C6-N6	13.20	134.26	123.70
1	16S1	1239	A	N7-C8-N9	-13.19	107.20	113.80
22	23S1	1515	A	C5-C6-N6	13.19	134.25	123.70
1	16S1	554	A	C5-C6-N6	13.17	134.23	123.70
1	16S1	978	A	C5-C6-N6	13.17	134.23	123.70
1	16S1	51	A	N7-C8-N9	-13.13	107.23	113.80
22	23S1	84	A	C5-C6-N6	13.13	134.21	123.70
22	23S1	196	A	C5-C6-N6	13.10	134.18	123.70
22	23S1	1928	A	C5-C6-N6	13.07	134.16	123.70
22	23S1	1021	A	N3-C4-C5	-13.06	117.65	126.80
22	23S1	792	A	N7-C8-N9	-13.06	107.27	113.80
1	16S1	383	A	C4-C5-C6	13.03	123.52	117.00
1	16S1	274	A	N7-C8-N9	-13.03	107.28	113.80
1	16S1	151	A	C5-C6-N6	13.02	134.12	123.70
1	16S1	792	A	N7-C8-N9	-13.01	107.29	113.80
1	16S1	397	A	N3-C4-C5	-13.00	117.70	126.80
22	23S1	2542	A	C5-C6-N6	12.98	134.09	123.70
1	16S1	1101	A	C5-C6-N6	12.98	134.08	123.70
22	23S1	1755	A	C5-C6-N6	12.97	134.07	123.70
22	23S1	845	A	N3-C4-C5	-12.94	117.74	126.80
22	23S1	454	A	C5-C6-N6	12.93	134.05	123.70
22	23S1	2883	A	N7-C8-N9	-12.90	107.35	113.80
22	23S1	547	A	N7-C8-N9	-12.88	107.36	113.80
22	23S1	251	A	N1-C6-N6	-12.86	110.89	118.60
22	23S1	1754	A	C5-C6-N6	12.84	133.97	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	8	A	N7-C8-N9	-12.82	107.39	113.80
22	23S1	2170	A	N7-C8-N9	-12.80	107.40	113.80
22	23S1	2887	A	N3-C4-C5	-12.79	117.85	126.80
1	16S1	914	A	C5-C6-N6	12.79	133.93	123.70
22	23S1	1669	A	N3-C4-C5	-12.78	117.86	126.80
1	16S1	179	A	C5-C6-N6	12.75	133.90	123.70
22	23S1	204	A	N7-C8-N9	-12.74	107.43	113.80
1	16S1	716	A	C5-C6-N6	12.74	133.89	123.70
1	16S1	1225	A	N3-C4-C5	-12.70	117.91	126.80
22	23S1	1272	A	N7-C8-N9	-12.69	107.45	113.80
1	16S1	81	A	C5-C6-N6	12.69	133.85	123.70
22	23S1	749	A	C5-C6-N6	12.68	133.84	123.70
22	23S1	981	A	C5-C6-N6	12.67	133.84	123.70
1	16S1	1275	A	N7-C8-N9	-12.65	107.47	113.80
1	16S1	451	A	N7-C8-N9	-12.65	107.47	113.80
22	23S1	960	A	N1-C6-N6	-12.65	111.01	118.60
1	16S1	55	A	N7-C8-N9	-12.64	107.48	113.80
22	23S1	2033	A	C5-C6-N6	12.64	133.81	123.70
22	23S1	362	A	N1-C6-N6	-12.62	111.03	118.60
1	16S1	782	A	N7-C8-N9	-12.61	107.50	113.80
22	23S1	1328	A	C5-C6-N6	12.60	133.78	123.70
55	PTR1	51	A	C5-C6-N6	12.60	133.78	123.70
22	23S1	821	A	C5-C6-N6	12.58	133.77	123.70
1	16S1	498	A	C5-C6-N1	12.56	123.98	117.70
1	16S1	383	A	N3-C4-C5	-12.56	118.01	126.80
22	23S1	2189	U	OP1-P-OP2	12.56	138.44	119.60
22	23S1	278	A	N3-C4-C5	-12.55	118.02	126.80
1	16S1	74	A	N7-C8-N9	-12.54	107.53	113.80
22	23S1	1919	A	C5-C6-N6	12.53	133.73	123.70
1	16S1	901	A	N1-C6-N6	-12.53	111.08	118.60
22	23S1	161	A	C5-C6-N6	12.51	133.71	123.70
22	23S1	1285	A	C5-C6-N6	12.50	133.70	123.70
1	16S1	1145	A	C5-C6-N6	12.50	133.70	123.70
1	16S1	815	A	N7-C8-N9	-12.50	107.55	113.80
22	23S1	352	A	C5-C6-N6	12.49	133.69	123.70
55	PTR1	76	A	N7-C8-N9	-12.49	107.56	113.80
1	16S1	1004	A	C5-N7-C8	12.48	110.14	103.90
22	23S1	644	A	N7-C8-N9	-12.48	107.56	113.80
22	23S1	2753	A	C5-C6-N6	12.48	133.69	123.70
1	16S1	572	A	N7-C8-N9	-12.48	107.56	113.80
1	16S1	1067	A	C5-C6-N6	12.47	133.68	123.70
22	23S1	2358	A	C5-C6-N6	12.47	133.67	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1308	A	N7-C8-N9	-12.46	107.57	113.80
1	16S1	1398	A	C5-C6-N6	12.46	133.67	123.70
22	23S1	1700	A	N7-C8-N9	-12.46	107.57	113.80
22	23S1	2765	A	N3-C4-C5	-12.46	118.08	126.80
1	16S1	197	A	N7-C8-N9	-12.45	107.58	113.80
22	23S1	1262	A	C5-C6-N6	12.45	133.66	123.70
22	23S1	2117	A	N7-C8-N9	-12.45	107.58	113.80
1	16S1	694	A	N7-C8-N9	-12.44	107.58	113.80
22	23S1	2114	A	N3-C4-C5	-12.44	118.09	126.80
22	23S1	2388	A	N7-C8-N9	-12.44	107.58	113.80
22	23S1	752	A	N7-C8-N9	-12.43	107.58	113.80
22	23S1	526	A	C5-C6-N6	12.43	133.65	123.70
22	23S1	983	A	C5-C6-N6	12.43	133.64	123.70
22	23S1	1247	A	N7-C8-N9	-12.43	107.59	113.80
22	23S1	1308	A	C5-C6-N6	12.43	133.64	123.70
1	16S1	149	A	C5-C6-N6	12.42	133.64	123.70
22	23S1	2101	A	C5-C6-N6	12.41	133.63	123.70
22	23S1	84	A	N7-C8-N9	-12.40	107.60	113.80
22	23S1	1385	A	N7-C8-N9	-12.39	107.60	113.80
1	16S1	977	A	N3-C4-C5	-12.39	118.13	126.80
1	16S1	622	A	C5-C6-N6	12.39	133.61	123.70
22	23S1	2602	A	N7-C8-N9	-12.38	107.61	113.80
1	16S1	309	A	N7-C8-N9	-12.38	107.61	113.80
22	23S1	443	A	N7-C8-N9	-12.38	107.61	113.80
1	16S1	243	A	C5-C6-N6	12.37	133.60	123.70
1	16S1	533	A	N3-C4-C5	-12.37	118.14	126.80
22	23S1	457	A	N7-C8-N9	-12.37	107.62	113.80
22	23S1	1069	A	N7-C8-N9	-12.37	107.62	113.80
1	16S1	1004	A	C5-C6-N6	12.36	133.59	123.70
22	23S1	1096	A	N7-C8-N9	-12.36	107.62	113.80
55	PTR1	14	A	N7-C8-N9	-12.36	107.62	113.80
22	23S1	119	A	C5-C6-N6	12.36	133.59	123.70
22	23S1	2823	A	C5-C6-N6	12.36	133.58	123.70
22	23S1	905	A	N7-C8-N9	-12.35	107.63	113.80
22	23S1	2887	A	C5-C6-N6	12.34	133.57	123.70
1	16S1	499	A	N7-C8-N9	-12.34	107.63	113.80
22	23S1	616	A	N7-C8-N9	-12.34	107.63	113.80
55	PTR1	9	A	N7-C8-N9	-12.32	107.64	113.80
22	23S1	1789	A	C5-C6-N6	12.32	133.56	123.70
1	16S1	1216	A	N7-C8-N9	-12.32	107.64	113.80
22	23S1	1583	A	N7-C8-N9	-12.31	107.64	113.80
55	PTR1	58	A	N7-C8-N9	-12.30	107.65	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	PTR1	51	A	N7-C8-N9	-12.30	107.65	113.80
22	23S1	2060	A	C5-C6-N6	12.30	133.54	123.70
22	23S1	2450	A	C5-C6-N6	12.30	133.54	123.70
22	23S1	2449	U	C5-C6-N1	-12.29	116.55	122.70
1	16S1	1503	A	N7-C8-N9	-12.27	107.66	113.80
22	23S1	973	A	C5-C6-N6	12.27	133.52	123.70
22	23S1	668	A	N7-C8-N9	-12.27	107.67	113.80
22	23S1	2173	A	N3-C4-C5	-12.27	118.21	126.80
22	23S1	127	A	C5-C6-N6	12.26	133.51	123.70
22	23S1	1046	A	N7-C8-N9	-12.26	107.67	113.80
22	23S1	2297	A	N7-C8-N9	-12.26	107.67	113.80
22	23S1	2270	A	N7-C8-N9	-12.25	107.67	113.80
1	16S1	389	A	N3-C4-C5	-12.25	118.23	126.80
23	05S1	46	A	C5-C6-N6	12.24	133.49	123.70
22	23S1	586	A	C5-C6-N6	12.24	133.49	123.70
22	23S1	750	A	N7-C8-N9	-12.24	107.68	113.80
1	16S1	1105	A	N7-C8-N9	-12.24	107.68	113.80
1	16S1	572	A	C5-C6-N6	12.23	133.49	123.70
22	23S1	2566	A	C5-C6-N6	12.23	133.48	123.70
22	23S1	1821	A	C5-C6-N6	12.23	133.48	123.70
1	16S1	1101	A	N7-C8-N9	-12.22	107.69	113.80
22	23S1	497	A	C5-C6-N6	12.22	133.48	123.70
22	23S1	800	A	N7-C8-N9	-12.22	107.69	113.80
1	16S1	162	A	N1-C6-N6	-12.21	111.27	118.60
22	23S1	2298	A	N7-C8-N9	-12.21	107.69	113.80
22	23S1	984	A	N3-C4-C5	-12.21	118.25	126.80
1	16S1	120	A	N7-C8-N9	-12.21	107.70	113.80
1	16S1	1067	A	N7-C8-N9	-12.21	107.70	113.80
22	23S1	693	A	N7-C8-N9	-12.20	107.70	113.80
22	23S1	1048	A	C5-C6-N6	12.20	133.46	123.70
22	23S1	2060	A	N7-C8-N9	-12.20	107.70	113.80
1	16S1	190	A	N3-C4-C5	-12.20	118.26	126.80
22	23S1	529	A	C5-C6-N6	12.20	133.46	123.70
1	16S1	996	A	N7-C8-N9	-12.19	107.70	113.80
22	23S1	1566	A	N7-C8-N9	-12.18	107.71	113.80
22	23S1	1913	A	N7-C8-N9	-12.18	107.71	113.80
55	PTR1	59	A	N7-C8-N9	-12.18	107.71	113.80
22	23S1	1580	A	N7-C8-N9	-12.18	107.71	113.80
1	16S1	349	A	N7-C8-N9	-12.17	107.71	113.80
22	23S1	241	A	C5-C6-N6	12.17	133.44	123.70
22	23S1	73	A	C5-C6-N6	12.17	133.44	123.70
22	23S1	1981	A	C5-C6-N6	12.16	133.43	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	165	A	C5-C6-N6	12.16	133.43	123.70
22	23S1	2632	A	N7-C8-N9	-12.16	107.72	113.80
1	16S1	16	A	N7-C8-N9	-12.16	107.72	113.80
1	16S1	353	A	N7-C8-N9	-12.16	107.72	113.80
22	23S1	502	A	C5-C6-N6	12.16	133.43	123.70
1	16S1	784	A	N7-C8-N9	-12.15	107.72	113.80
22	23S1	222	A	N7-C8-N9	-12.15	107.72	113.80
22	23S1	1353	A	C5-C6-N6	12.15	133.42	123.70
22	23S1	310	A	N7-C8-N9	-12.15	107.72	113.80
22	23S1	167	A	N7-C8-N9	-12.15	107.73	113.80
22	23S1	1815	A	C5-C6-N6	12.15	133.42	123.70
22	23S1	866	A	N7-C8-N9	-12.14	107.73	113.80
22	23S1	1050	A	N7-C8-N9	-12.14	107.73	113.80
22	23S1	2758	A	C5-C6-N6	12.14	133.41	123.70
1	16S1	1201	A	N7-C8-N9	-12.14	107.73	113.80
1	16S1	1500	A	C5-C6-N6	12.13	133.41	123.70
22	23S1	1668	A	C5-C6-N6	12.13	133.41	123.70
22	23S1	1419	A	N7-C8-N9	-12.13	107.73	113.80
22	23S1	204	A	C5-C6-N6	12.13	133.40	123.70
22	23S1	1032	A	N7-C8-N9	-12.12	107.74	113.80
22	23S1	1155	A	C5-C6-N6	12.12	133.40	123.70
22	23S1	2439	A	N7-C8-N9	-12.12	107.74	113.80
55	PTR1	73	A	N7-C8-N9	-12.11	107.74	113.80
1	16S1	60	A	C5-C6-N6	12.11	133.39	123.70
1	16S1	1004	A	N3-C4-C5	-12.11	118.32	126.80
22	23S1	945	A	C5-C6-N6	12.11	133.38	123.70
22	23S1	2297	A	C5-C6-N6	12.10	133.38	123.70
22	23S1	655	A	N7-C8-N9	-12.10	107.75	113.80
22	23S1	2590	A	N7-C8-N9	-12.09	107.75	113.80
22	23S1	479	A	N7-C8-N9	-12.09	107.75	113.80
22	23S1	1509	A	N7-C8-N9	-12.08	107.76	113.80
22	23S1	10	A	C5-C6-N6	12.08	133.36	123.70
22	23S1	2198	A	N7-C8-N9	-12.08	107.76	113.80
1	16S1	794	A	N7-C8-N9	-12.08	107.76	113.80
1	16S1	167	A	N7-C8-N9	-12.08	107.76	113.80
22	23S1	2119	A	C5-C6-N6	12.08	133.36	123.70
22	23S1	2657	A	C5-C6-N6	12.08	133.36	123.70
1	16S1	1092	A	N7-C8-N9	-12.07	107.76	113.80
22	23S1	1395	A	C5-C6-N6	12.07	133.36	123.70
1	16S1	373	A	N7-C8-N9	-12.07	107.77	113.80
1	16S1	468	A	N7-C8-N9	-12.07	107.77	113.80
1	16S1	1346	A	C5-C6-N6	12.06	133.35	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1057	A	N7-C8-N9	-12.06	107.77	113.80
1	16S1	1447	A	N7-C8-N9	-12.06	107.77	113.80
22	23S1	2736	A	N7-C8-N9	-12.05	107.77	113.80
1	16S1	1333	A	C5-C6-N6	12.05	133.34	123.70
22	23S1	262	A	N7-C8-N9	-12.05	107.78	113.80
22	23S1	1001	A	C5-C6-N6	12.05	133.34	123.70
22	23S1	1652	A	C5-C6-N6	12.05	133.34	123.70
22	23S1	1927	A	C5-C6-N6	12.05	133.34	123.70
22	23S1	2764	A	C5-C6-N6	12.05	133.34	123.70
22	23S1	1420	A	N7-C8-N9	-12.05	107.78	113.80
22	23S1	1630	A	C5-C6-N6	12.05	133.34	123.70
22	23S1	216	A	C5-C6-N6	12.04	133.34	123.70
22	23S1	538	A	N7-C8-N9	-12.04	107.78	113.80
22	23S1	1871	A	N7-C8-N9	-12.04	107.78	113.80
1	16S1	1216	A	C5-C6-N6	12.04	133.33	123.70
22	23S1	1287	A	N7-C8-N9	-12.04	107.78	113.80
22	23S1	412	A	N7-C8-N9	-12.04	107.78	113.80
1	16S1	648	A	N7-C8-N9	-12.04	107.78	113.80
22	23S1	2590	A	C5-C6-N6	12.04	133.33	123.70
22	23S1	2776	A	N7-C8-N9	-12.03	107.78	113.80
1	16S1	71	A	N7-C8-N9	-12.03	107.78	113.80
22	23S1	1088	A	N3-C4-C5	-12.03	118.38	126.80
22	23S1	1275	A	N7-C8-N9	-12.03	107.78	113.80
22	23S1	2042	A	N7-C8-N9	-12.03	107.78	113.80
22	23S1	2070	A	N7-C8-N9	-12.03	107.79	113.80
1	16S1	649	A	C5-C6-N6	12.02	133.32	123.70
22	23S1	2564	A	C5-C6-N6	12.02	133.32	123.70
22	23S1	675	A	C5-C6-N6	12.02	133.31	123.70
1	16S1	1271	A	N7-C8-N9	-12.02	107.79	113.80
22	23S1	599	A	N7-C8-N9	-12.02	107.79	113.80
22	23S1	829	A	N7-C8-N9	-12.01	107.79	113.80
22	23S1	1395	A	N7-C8-N9	-12.01	107.79	113.80
22	23S1	2311	A	C5-C6-N6	12.01	133.31	123.70
22	23S1	2614	A	N3-C4-C5	-12.01	118.39	126.80
1	16S1	554	A	N7-C8-N9	-12.01	107.80	113.80
22	23S1	2003	A	N7-C8-N9	-12.01	107.80	113.80
1	16S1	172	A	C5-C6-N6	12.01	133.31	123.70
22	23S1	38	A	C5-C6-N6	12.01	133.31	123.70
1	16S1	3	A	C5-C6-N6	12.00	133.30	123.70
1	16S1	1201	A	N3-C4-C5	-12.00	118.40	126.80
22	23S1	354	A	C5-C6-N6	12.00	133.30	123.70
22	23S1	627	A	N7-C8-N9	-12.00	107.80	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2542	A	N7-C8-N9	-12.00	107.80	113.80
1	16S1	1329	A	N7-C8-N9	-12.00	107.80	113.80
22	23S1	2095	A	N7-C8-N9	-11.99	107.80	113.80
1	16S1	412	A	C5-C6-N6	11.99	133.29	123.70
22	23S1	621	A	C5-C6-N6	11.99	133.29	123.70
1	16S1	935	A	N7-C8-N9	-11.99	107.81	113.80
22	23S1	278	A	C5-C6-N6	11.99	133.29	123.70
1	16S1	495	A	N7-C8-N9	-11.98	107.81	113.80
22	23S1	1427	A	C5-C6-N6	11.98	133.28	123.70
1	16S1	635	A	N7-C8-N9	-11.98	107.81	113.80
23	05S1	34	A	N7-C8-N9	-11.98	107.81	113.80
22	23S1	2094	A	N7-C8-N9	-11.97	107.81	113.80
23	05S1	115	A	N7-C8-N9	-11.97	107.81	113.80
22	23S1	734	A	N7-C8-N9	-11.97	107.81	113.80
22	23S1	1111	A	N7-C8-N9	-11.97	107.81	113.80
22	23S1	1127	A	C5-C6-N6	11.97	133.28	123.70
22	23S1	1872	A	N3-C4-C5	-11.97	118.42	126.80
22	23S1	2430	A	C5-C6-N6	11.97	133.28	123.70
22	23S1	2158	A	N7-C8-N9	-11.97	107.81	113.80
22	23S1	2682	A	N7-C8-N9	-11.97	107.82	113.80
1	16S1	162	A	N3-C4-C5	-11.96	118.43	126.80
22	23S1	2662	A	N3-C4-C5	-11.96	118.42	126.80
22	23S1	196	A	N3-C4-C5	-11.96	118.43	126.80
22	23S1	1020	A	N7-C8-N9	-11.96	107.82	113.80
22	23S1	2726	A	N7-C8-N9	-11.96	107.82	113.80
1	16S1	1441	A	N7-C8-N9	-11.96	107.82	113.80
22	23S1	13	A	C5-C6-N6	11.96	133.27	123.70
22	23S1	1285	A	N7-C8-N9	-11.96	107.82	113.80
22	23S1	1359	A	C5-C6-N6	11.95	133.26	123.70
1	16S1	459	A	N7-C8-N9	-11.95	107.82	113.80
22	23S1	354	A	N7-C8-N9	-11.95	107.82	113.80
22	23S1	2205	A	N7-C8-N9	-11.95	107.83	113.80
1	16S1	1145	A	N7-C8-N9	-11.94	107.83	113.80
22	23S1	2670	A	N7-C8-N9	-11.94	107.83	113.80
22	23S1	532	A	N3-C4-C5	-11.94	118.44	126.80
22	23S1	2766	A	N3-C4-C5	-11.94	118.44	126.80
22	23S1	1494	A	C5-C6-N6	11.93	133.25	123.70
22	23S1	905	A	C5-C6-N6	11.93	133.25	123.70
22	23S1	161	A	N7-C8-N9	-11.93	107.84	113.80
22	23S1	1347	A	C5-C6-N6	11.92	133.24	123.70
22	23S1	2750	A	N7-C8-N9	-11.92	107.84	113.80
22	23S1	2882	A	N7-C8-N9	-11.92	107.84	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2031	A	N7-C8-N9	-11.91	107.84	113.80
22	23S1	2013	A	N7-C8-N9	-11.91	107.84	113.80
1	16S1	313	A	C5-C6-N6	11.91	133.23	123.70
22	23S1	195	A	C5-C6-N6	11.91	133.22	123.70
1	16S1	607	A	C5-C6-N6	11.90	133.22	123.70
22	23S1	165	A	N7-C8-N9	-11.90	107.85	113.80
1	16S1	1349	A	N7-C8-N9	-11.90	107.85	113.80
22	23S1	1439	A	N7-C8-N9	-11.90	107.85	113.80
1	16S1	298	A	N7-C8-N9	-11.90	107.85	113.80
22	23S1	716	A	N7-C8-N9	-11.90	107.85	113.80
1	16S1	563	A	N3-C4-C5	-11.89	118.47	126.80
22	23S1	1275	A	C5-C6-N6	11.89	133.21	123.70
1	16S1	1005	A	N7-C8-N9	-11.89	107.86	113.80
22	23S1	718	A	N7-C8-N9	-11.89	107.86	113.80
1	16S1	1196	A	N7-C8-N9	-11.89	107.86	113.80
22	23S1	2336	A	C5-C6-N6	11.88	133.21	123.70
1	16S1	16	A	C5-C6-N6	11.88	133.21	123.70
1	16S1	44	A	C5-C6-N6	11.88	133.21	123.70
22	23S1	1890	A	C5-C6-N6	11.88	133.21	123.70
22	23S1	2274	A	C5-C6-N6	11.88	133.20	123.70
22	23S1	2572	A	C5-C6-N6	11.88	133.20	123.70
22	23S1	1591	A	N7-C8-N9	-11.87	107.86	113.80
22	23S1	1570	A	C5-C6-N6	11.87	133.20	123.70
22	23S1	2469	A	N7-C8-N9	-11.87	107.86	113.80
22	23S1	1525	A	C5-C6-N6	11.87	133.19	123.70
22	23S1	2820	A	N7-C8-N9	-11.86	107.87	113.80
1	16S1	282	A	C5-C6-N6	11.86	133.19	123.70
22	23S1	104	A	C5-C6-N6	11.86	133.19	123.70
22	23S1	2800	A	N7-C8-N9	-11.86	107.87	113.80
1	16S1	949	A	N7-C8-N9	-11.86	107.87	113.80
22	23S1	482	A	N1-C6-N6	-11.86	111.49	118.60
22	23S1	1960	A	N7-C8-N9	-11.86	107.87	113.80
22	23S1	1987	A	N7-C8-N9	-11.86	107.87	113.80
22	23S1	213	A	N7-C8-N9	-11.85	107.87	113.80
22	23S1	103	A	N7-C8-N9	-11.85	107.88	113.80
22	23S1	613	A	N3-C4-C5	-11.85	118.51	126.80
1	16S1	19	A	N7-C8-N9	-11.85	107.88	113.80
22	23S1	507	A	C5-C6-N6	11.85	133.18	123.70
22	23S1	1253	A	C5-C6-N6	11.85	133.18	123.70
1	16S1	441	A	N7-C8-N9	-11.84	107.88	113.80
22	23S1	402	A	C5-C6-N6	11.84	133.17	123.70
22	23S1	1900	A	N7-C8-N9	-11.84	107.88	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	644	A	N3-C4-C5	-11.83	118.52	126.80
22	23S1	2014	A	N7-C8-N9	-11.83	107.88	113.80
22	23S1	752	A	C5-C6-N6	11.83	133.16	123.70
22	23S1	1597	A	C5-C6-N6	11.83	133.17	123.70
22	23S1	933	A	N3-C4-C5	-11.83	118.52	126.80
22	23S1	2738	A	N7-C8-N9	-11.83	107.89	113.80
1	16S1	1257	A	N7-C8-N9	-11.83	107.89	113.80
1	16S1	1377	A	N7-C8-N9	-11.83	107.89	113.80
22	23S1	443	A	C5-C6-N6	11.82	133.16	123.70
1	16S1	1408	A	N7-C8-N9	-11.82	107.89	113.80
22	23S1	181	A	N7-C8-N9	-11.82	107.89	113.80
22	23S1	878	A	N7-C8-N9	-11.81	107.89	113.80
22	23S1	1876	A	N7-C8-N9	-11.81	107.89	113.80
22	23S1	2434	A	C5-C6-N6	11.81	133.15	123.70
1	16S1	155	A	N7-C8-N9	-11.81	107.89	113.80
22	23S1	2095	A	C5-C6-N6	11.81	133.15	123.70
55	PTR1	20	U	C5-C6-N1	-11.81	116.79	122.70
1	16S1	781	A	C5-C6-N6	11.81	133.15	123.70
1	16S1	1299	A	N3-C4-C5	-11.80	118.54	126.80
22	23S1	2758	A	N7-C8-N9	-11.80	107.90	113.80
22	23S1	1378	A	C5-C6-N6	11.80	133.14	123.70
1	16S1	1456	A	N7-C8-N9	-11.80	107.90	113.80
1	16S1	374	A	N7-C8-N9	-11.79	107.91	113.80
1	16S1	171	A	N7-C8-N9	-11.79	107.91	113.80
1	16S1	1225	A	C5-C6-N6	11.79	133.13	123.70
22	23S1	655	A	C5-C6-N6	11.79	133.13	123.70
22	23S1	352	A	N7-C8-N9	-11.78	107.91	113.80
22	23S1	1969	A	N7-C8-N9	-11.78	107.91	113.80
22	23S1	2657	A	N7-C8-N9	-11.78	107.91	113.80
22	23S1	1819	A	N7-C8-N9	-11.78	107.91	113.80
22	23S1	676	A	N7-C8-N9	-11.77	107.91	113.80
22	23S1	1385	A	C5-C6-N6	11.77	133.12	123.70
22	23S1	1504	A	N7-C8-N9	-11.77	107.91	113.80
22	23S1	1545	A	C5-C6-N6	11.77	133.12	123.70
22	23S1	1652	A	N7-C8-N9	-11.77	107.91	113.80
1	16S1	675	A	N7-C8-N9	-11.77	107.92	113.80
1	16S1	1248	A	C5-C6-N6	11.77	133.11	123.70
22	23S1	322	A	N7-C8-N9	-11.77	107.92	113.80
1	16S1	246	A	N7-C8-N9	-11.76	107.92	113.80
1	16S1	946	A	N7-C8-N9	-11.76	107.92	113.80
22	23S1	749	A	N7-C8-N9	-11.76	107.92	113.80
22	23S1	804	A	C5-C6-N6	11.76	133.11	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1366	A	N7-C8-N9	-11.76	107.92	113.80
22	23S1	2711	A	N7-C8-N9	-11.76	107.92	113.80
1	16S1	74	A	C5-C6-N6	11.76	133.11	123.70
22	23S1	101	A	N3-C4-C5	-11.76	118.57	126.80
22	23S1	1010	A	C5-C6-N6	11.76	133.10	123.70
23	05S1	108	A	N7-C8-N9	-11.76	107.92	113.80
1	16S1	831	A	N7-C8-N9	-11.75	107.92	113.80
1	16S1	468	A	C5-C6-N6	11.75	133.10	123.70
1	16S1	983	A	N3-C4-C5	-11.75	118.57	126.80
22	23S1	1853	A	N7-C8-N9	-11.75	107.92	113.80
22	23S1	2426	A	N7-C8-N9	-11.75	107.93	113.80
1	16S1	223	A	N7-C8-N9	-11.75	107.93	113.80
22	23S1	2826	A	N7-C8-N9	-11.75	107.93	113.80
22	23S1	226	A	C5-C6-N6	11.75	133.10	123.70
1	16S1	1329	A	C5-C6-N6	11.74	133.10	123.70
22	23S1	103	A	C5-C6-N6	11.74	133.10	123.70
22	23S1	2378	A	N7-C8-N9	-11.74	107.93	113.80
22	23S1	320	A	C4-C5-C6	11.74	122.87	117.00
22	23S1	2850	A	N7-C8-N9	-11.74	107.93	113.80
22	23S1	89	A	N7-C8-N9	-11.74	107.93	113.80
1	16S1	825	A	N7-C8-N9	-11.73	107.93	113.80
22	23S1	172	A	N7-C8-N9	-11.73	107.93	113.80
22	23S1	637	A	N7-C8-N9	-11.73	107.93	113.80
22	23S1	1640	A	N7-C8-N9	-11.73	107.93	113.80
22	23S1	42	A	N7-C8-N9	-11.73	107.94	113.80
1	16S1	1311	A	N7-C8-N9	-11.73	107.94	113.80
22	23S1	19	A	N7-C8-N9	-11.72	107.94	113.80
22	23S1	1392	A	C5-C6-N6	11.72	133.08	123.70
22	23S1	1634	A	N7-C8-N9	-11.72	107.94	113.80
23	05S1	29	A	C5-C6-N6	11.72	133.08	123.70
22	23S1	1237	A	N7-C8-N9	-11.72	107.94	113.80
23	05S1	34	A	C5-C6-N6	11.72	133.07	123.70
22	23S1	384	A	C5-C6-N6	11.72	133.07	123.70
22	23S1	14	A	C5-C6-N6	11.72	133.07	123.70
22	23S1	2837	A	N7-C8-N9	-11.72	107.94	113.80
22	23S1	1286	A	C5-C6-N6	11.71	133.07	123.70
22	23S1	2317	A	N7-C8-N9	-11.71	107.94	113.80
1	16S1	1285	A	N7-C8-N9	-11.71	107.94	113.80
22	23S1	2211	A	N7-C8-N9	-11.71	107.94	113.80
23	05S1	99	A	C5-C6-N6	11.71	133.07	123.70
1	16S1	547	A	N7-C8-N9	-11.71	107.95	113.80
1	16S1	1155	A	N7-C8-N9	-11.71	107.95	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2726	A	C5-C6-N6	11.71	133.07	123.70
1	16S1	728	A	C5-C6-N6	11.71	133.06	123.70
1	16S1	1046	A	N3-C4-C5	-11.70	118.61	126.80
22	23S1	1213	A	N7-C8-N9	-11.70	107.95	113.80
1	16S1	1151	A	N7-C8-N9	-11.69	107.95	113.80
1	16S1	1499	A	C5-C6-N6	11.70	133.06	123.70
22	23S1	1434	A	N7-C8-N9	-11.69	107.95	113.80
22	23S1	2381	A	N7-C8-N9	-11.70	107.95	113.80
22	23S1	2781	A	C5-C6-N6	11.70	133.06	123.70
1	16S1	802	A	C5-C6-N6	11.69	133.06	123.70
22	23S1	1129	A	C5-C6-N6	11.69	133.05	123.70
22	23S1	2005	A	C5-C6-N6	11.69	133.05	123.70
22	23S1	265	A	N7-C8-N9	-11.69	107.96	113.80
22	23S1	900	A	N7-C8-N9	-11.69	107.96	113.80
22	23S1	2322	A	N7-C8-N9	-11.69	107.96	113.80
1	16S1	465	A	N3-C4-C5	-11.69	118.62	126.80
22	23S1	1095	A	N7-C8-N9	-11.69	107.96	113.80
22	23S1	1749	A	N7-C8-N9	-11.69	107.96	113.80
22	23S1	1785	A	C5-C6-N6	11.68	133.05	123.70
22	23S1	1755	A	N7-C8-N9	-11.68	107.96	113.80
22	23S1	1938	A	N7-C8-N9	-11.68	107.96	113.80
1	16S1	1287	A	N7-C8-N9	-11.68	107.96	113.80
22	23S1	2288	A	N7-C8-N9	-11.68	107.96	113.80
22	23S1	2660	A	C5-C6-N6	11.68	133.04	123.70
22	23S1	299	A	C5-C6-N6	11.68	133.04	123.70
22	23S1	979	A	N7-C8-N9	-11.68	107.96	113.80
22	23S1	1205	A	C5-C6-N6	11.68	133.04	123.70
1	16S1	366	A	N7-C8-N9	-11.68	107.96	113.80
1	16S1	1204	A	C5-C6-N6	11.68	133.04	123.70
22	23S1	1040	A	N7-C8-N9	-11.67	107.96	113.80
22	23S1	2468	A	N7-C8-N9	-11.67	107.96	113.80
22	23S1	2577	A	N7-C8-N9	-11.67	107.96	113.80
1	16S1	1363	A	N3-C4-C5	-11.67	118.63	126.80
22	23S1	104	A	N7-C8-N9	-11.67	107.97	113.80
1	16S1	759	A	N7-C8-N9	-11.67	107.97	113.80
1	16S1	1480	A	N7-C8-N9	-11.67	107.97	113.80
1	16S1	1261	A	N7-C8-N9	-11.66	107.97	113.80
22	23S1	1039	A	N7-C8-N9	-11.66	107.97	113.80
22	23S1	1469	A	N7-C8-N9	-11.66	107.97	113.80
1	16S1	766	A	C5-C6-N6	11.66	133.03	123.70
1	16S1	1346	A	N7-C8-N9	-11.66	107.97	113.80
1	16S1	3	A	N7-C8-N9	-11.66	107.97	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	139	A	N7-C8-N9	-11.66	107.97	113.80
1	16S1	547	A	C5-C6-N6	11.66	133.03	123.70
1	16S1	600	A	N7-C8-N9	-11.66	107.97	113.80
1	16S1	889	A	C5-C6-N6	11.66	133.03	123.70
1	16S1	1246	A	N7-C8-N9	-11.66	107.97	113.80
22	23S1	1342	A	N7-C8-N9	-11.65	107.97	113.80
22	23S1	2734	A	N7-C8-N9	-11.65	107.97	113.80
23	05S1	104	A	N7-C8-N9	-11.65	107.97	113.80
1	16S1	1428	A	C5-C6-N6	11.65	133.02	123.70
22	23S1	1453	A	N7-C8-N9	-11.65	107.97	113.80
22	23S1	2632	A	C5-C6-N6	11.65	133.02	123.70
22	23S1	270	A	N7-C8-N9	-11.65	107.98	113.80
22	23S1	661	A	N7-C8-N9	-11.65	107.98	113.80
22	23S1	1616	A	N7-C8-N9	-11.65	107.98	113.80
22	23S1	2565	A	C5-C6-N6	11.65	133.02	123.70
1	16S1	320	A	N7-C8-N9	-11.64	107.98	113.80
1	16S1	478	A	N3-C4-C5	-11.64	118.65	126.80
1	16S1	729	A	N7-C8-N9	-11.64	107.98	113.80
22	23S1	371	A	C5-C6-N6	11.64	133.01	123.70
22	23S1	457	A	C5-C6-N6	11.64	133.01	123.70
22	23S1	793	A	C5-C6-N6	11.64	133.01	123.70
22	23S1	574	A	N7-C8-N9	-11.64	107.98	113.80
1	16S1	1251	A	C5-C6-N6	11.64	133.01	123.70
1	16S1	1332	A	C5-C6-N6	11.64	133.01	123.70
1	16S1	131	A	N7-C8-N9	-11.63	107.98	113.80
22	23S1	2518	A	N3-C4-C5	-11.64	118.66	126.80
22	23S1	2872	A	N7-C8-N9	-11.64	107.98	113.80
23	05S1	46	A	N7-C8-N9	-11.63	107.98	113.80
22	23S1	146	A	N7-C8-N9	-11.63	107.98	113.80
22	23S1	265	A	C5-C6-N6	11.63	133.00	123.70
22	23S1	1194	A	N7-C8-N9	-11.63	107.99	113.80
22	23S1	471	A	N7-C8-N9	-11.62	107.99	113.80
22	23S1	1698	A	C5-C6-N6	11.63	133.00	123.70
22	23S1	1937	A	N7-C8-N9	-11.62	107.99	113.80
1	16S1	915	A	N7-C8-N9	-11.62	107.99	113.80
1	16S1	1368	A	N7-C8-N9	-11.62	107.99	113.80
22	23S1	2388	A	C5-C6-N6	11.62	133.00	123.70
22	23S1	1889	A	N7-C8-N9	-11.62	107.99	113.80
22	23S1	447	A	N7-C8-N9	-11.62	107.99	113.80
1	16S1	1236	A	N7-C8-N9	-11.61	107.99	113.80
22	23S1	861	A	N7-C8-N9	-11.62	107.99	113.80
22	23S1	1810	A	N3-C4-C5	-11.61	118.67	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2471	A	N7-C8-N9	-11.61	107.99	113.80
22	23S1	1735	A	N7-C8-N9	-11.61	108.00	113.80
22	23S1	1569	A	N7-C8-N9	-11.61	108.00	113.80
1	16S1	1340	A	N7-C8-N9	-11.61	108.00	113.80
22	23S1	2513	A	C5-C6-N6	11.61	132.99	123.70
1	16S1	179	A	N7-C8-N9	-11.60	108.00	113.80
22	23S1	279	A	N7-C8-N9	-11.60	108.00	113.80
22	23S1	483	A	N7-C8-N9	-11.60	108.00	113.80
1	16S1	487	A	N7-C8-N9	-11.60	108.00	113.80
1	16S1	702	A	C5-C6-N6	11.60	132.98	123.70
22	23S1	1490	A	N3-C4-C5	-11.59	118.69	126.80
22	23S1	1077	A	C5-C6-N6	11.59	132.97	123.70
1	16S1	131	A	C5-C6-N6	11.59	132.97	123.70
55	PTR1	59	A	C5-C6-N6	11.59	132.97	123.70
1	16S1	915	A	C5-C6-N6	11.59	132.97	123.70
22	23S1	1133	A	N7-C8-N9	-11.59	108.01	113.80
1	16S1	303	A	C5-C6-N6	11.58	132.97	123.70
22	23S1	282	A	N7-C8-N9	-11.58	108.01	113.80
1	16S1	1256	A	N7-C8-N9	-11.58	108.01	113.80
22	23S1	1067	A	N7-C8-N9	-11.58	108.01	113.80
22	23S1	1302	A	N7-C8-N9	-11.58	108.01	113.80
22	23S1	1544	A	C5-C6-N6	11.58	132.97	123.70
22	23S1	1129	A	N7-C8-N9	-11.58	108.01	113.80
22	23S1	2675	A	N7-C8-N9	-11.58	108.01	113.80
22	23S1	2872	A	N9-C4-C5	11.58	110.43	105.80
1	16S1	461	A	N7-C8-N9	-11.57	108.01	113.80
22	23S1	322	A	C5-C6-N6	11.57	132.96	123.70
22	23S1	1630	A	N7-C8-N9	-11.57	108.01	113.80
55	PTR1	26	A	N7-C8-N9	-11.57	108.01	113.80
22	23S1	1214	A	C5-C6-N6	11.57	132.96	123.70
1	16S1	315	A	N7-C8-N9	-11.57	108.02	113.80
22	23S1	2134	A	N7-C8-N9	-11.57	108.02	113.80
22	23S1	2212	A	C5-C6-N6	11.57	132.96	123.70
22	23S1	2547	A	C5-C6-N6	11.57	132.96	123.70
23	05S1	39	A	N7-C8-N9	-11.57	108.02	113.80
1	16S1	900	A	C5-C6-N6	11.57	132.96	123.70
1	16S1	913	A	N7-C8-N9	-11.57	108.02	113.80
22	23S1	160	A	C5-C6-N6	11.57	132.95	123.70
22	23S1	382	A	N7-C8-N9	-11.57	108.02	113.80
22	23S1	794	A	N3-C4-C5	-11.57	118.70	126.80
22	23S1	1383	A	C5-C6-N6	11.57	132.95	123.70
22	23S1	1858	A	N7-C8-N9	-11.57	108.02	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2227	A	C5-C6-N6	11.57	132.95	123.70
22	23S1	125	A	N7-C8-N9	-11.56	108.02	113.80
22	23S1	1205	A	N7-C8-N9	-11.56	108.02	113.80
22	23S1	1668	A	N7-C8-N9	-11.56	108.02	113.80
22	23S1	2566	A	N7-C8-N9	-11.56	108.02	113.80
22	23S1	821	A	N7-C8-N9	-11.56	108.02	113.80
22	23S1	825	A	N7-C8-N9	-11.56	108.02	113.80
23	05S1	78	A	N7-C8-N9	-11.55	108.02	113.80
1	16S1	1394	A	N7-C8-N9	-11.55	108.02	113.80
1	16S1	182	A	N7-C8-N9	-11.55	108.03	113.80
22	23S1	1365	A	C5-C6-N6	11.55	132.94	123.70
22	23S1	1393	A	C5-C6-N6	11.55	132.94	123.70
22	23S1	2273	A	N3-C4-C5	-11.55	118.72	126.80
1	16S1	7	A	C5-C6-N6	11.54	132.94	123.70
22	23S1	391	A	N7-C8-N9	-11.54	108.03	113.80
22	23S1	878	A	C5-C6-N6	11.54	132.94	123.70
22	23S1	988	A	C5-C6-N6	11.54	132.94	123.70
22	23S1	1899	A	C5-C6-N6	11.54	132.93	123.70
22	23S1	2406	A	N7-C8-N9	-11.54	108.03	113.80
1	16S1	687	A	C5-C6-N6	11.54	132.93	123.70
1	16S1	2	A	N3-C4-C5	-11.54	118.72	126.80
1	16S1	65	A	N7-C8-N9	-11.54	108.03	113.80
22	23S1	1009	A	N7-C8-N9	-11.54	108.03	113.80
22	23S1	1378	A	N7-C8-N9	-11.54	108.03	113.80
22	23S1	501	A	C5-C6-N6	11.54	132.93	123.70
22	23S1	2070	A	C5-C6-N6	11.54	132.93	123.70
22	23S1	2270	A	C5-C6-N6	11.54	132.93	123.70
22	23S1	10	A	N7-C8-N9	-11.54	108.03	113.80
22	23S1	1494	A	N7-C8-N9	-11.53	108.03	113.80
1	16S1	80	A	N3-C4-C5	-11.53	118.73	126.80
22	23S1	689	A	N7-C8-N9	-11.53	108.03	113.80
22	23S1	2478	A	N7-C8-N9	-11.53	108.03	113.80
22	23S1	2883	A	C5-C6-N6	11.53	132.93	123.70
22	23S1	432	A	C5-C6-N6	11.53	132.92	123.70
22	23S1	927	A	C5-C6-N6	11.53	132.92	123.70
22	23S1	1545	A	N7-C8-N9	-11.53	108.04	113.80
22	23S1	1786	A	C5-C6-N6	11.53	132.92	123.70
22	23S1	1853	A	C5-C6-N6	11.53	132.92	123.70
22	23S1	2761	A	N7-C8-N9	-11.53	108.04	113.80
22	23S1	761	A	C5-C6-N6	11.53	132.92	123.70
22	23S1	1772	A	N7-C8-N9	-11.53	108.04	113.80
22	23S1	2740	A	C5-C6-N6	11.53	132.92	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2851	A	N7-C8-N9	-11.53	108.04	113.80
22	23S1	563	A	C5-C6-N6	11.52	132.92	123.70
22	23S1	990	A	C5-C6-N6	11.52	132.92	123.70
1	16S1	1250	A	C5-C6-N6	11.52	132.92	123.70
22	23S1	1885	A	N7-C8-N9	-11.52	108.04	113.80
22	23S1	2534	A	N7-C8-N9	-11.52	108.04	113.80
1	16S1	1499	A	N7-C8-N9	-11.52	108.04	113.80
22	23S1	1287	A	C5-C6-N6	11.51	132.91	123.70
1	16S1	665	A	C5-C6-N6	11.51	132.91	123.70
22	23S1	2281	A	N7-C8-N9	-11.51	108.05	113.80
22	23S1	1144	A	N7-C8-N9	-11.51	108.05	113.80
22	23S1	2333	A	N7-C8-N9	-11.51	108.05	113.80
1	16S1	300	A	N3-C4-C5	-11.50	118.75	126.80
1	16S1	746	A	N3-C4-C5	-11.50	118.75	126.80
22	23S1	764	A	C5-C6-N6	11.50	132.90	123.70
22	23S1	2764	A	N7-C8-N9	-11.50	108.05	113.80
22	23S1	344	A	N7-C8-N9	-11.50	108.05	113.80
22	23S1	2225	A	N7-C8-N9	-11.50	108.05	113.80
1	16S1	1042	A	N7-C8-N9	-11.50	108.05	113.80
22	23S1	2314	A	N7-C8-N9	-11.50	108.05	113.80
22	23S1	1596	A	N7-C8-N9	-11.50	108.05	113.80
1	16S1	109	A	N7-C8-N9	-11.49	108.05	113.80
1	16S1	435	A	N7-C8-N9	-11.49	108.05	113.80
1	16S1	909	A	C5-C6-N6	11.49	132.90	123.70
1	16S1	1254	A	N7-C8-N9	-11.49	108.05	113.80
22	23S1	1502	A	C5-C6-N6	11.49	132.90	123.70
22	23S1	2412	A	N7-C8-N9	-11.49	108.05	113.80
22	23S1	2792	A	N7-C8-N9	-11.49	108.05	113.80
22	23S1	788	A	N7-C8-N9	-11.49	108.05	113.80
22	23S1	64	A	N7-C8-N9	-11.49	108.06	113.80
22	23S1	1322	A	N7-C8-N9	-11.49	108.06	113.80
22	23S1	1783	A	N7-C8-N9	-11.49	108.06	113.80
22	23S1	497	A	N7-C8-N9	-11.49	108.06	113.80
22	23S1	802	A	C5-C6-N6	11.49	132.89	123.70
22	23S1	2311	A	N7-C8-N9	-11.49	108.06	113.80
1	16S1	152	A	C5-C6-N6	11.48	132.89	123.70
1	16S1	768	A	C5-C6-N6	11.48	132.89	123.70
22	23S1	345	A	C5-C6-N6	11.48	132.89	123.70
1	16S1	509	A	N7-C8-N9	-11.48	108.06	113.80
22	23S1	896	A	C5-C6-N6	11.48	132.88	123.70
22	23S1	2005	A	N7-C8-N9	-11.48	108.06	113.80
22	23S1	2191	A	C5-C6-N6	11.48	132.88	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	603	A	C5-C6-N6	11.48	132.88	123.70
22	23S1	1635	A	C5-C6-N6	11.48	132.88	123.70
1	16S1	171	A	C5-C6-N6	11.47	132.88	123.70
1	16S1	243	A	N7-C8-N9	-11.47	108.06	113.80
1	16S1	1188	A	N7-C8-N9	-11.47	108.06	113.80
22	23S1	1147	A	N7-C8-N9	-11.47	108.06	113.80
22	23S1	1156	A	C5-C6-N6	11.47	132.88	123.70
22	23S1	1632	A	C5-C6-N6	11.47	132.88	123.70
1	16S1	873	A	N7-C8-N9	-11.47	108.06	113.80
1	16S1	1170	A	N3-C4-C5	-11.47	118.77	126.80
22	23S1	1204	A	C5-C6-N6	11.47	132.87	123.70
22	23S1	1268	A	C5-C6-N6	11.47	132.88	123.70
22	23S1	111	A	C5-C6-N6	11.46	132.87	123.70
22	23S1	613	A	C5-C6-N6	11.46	132.87	123.70
22	23S1	1502	A	N7-C8-N9	-11.46	108.07	113.80
22	23S1	2054	A	N7-C8-N9	-11.46	108.07	113.80
22	23S1	735	A	N7-C8-N9	-11.46	108.07	113.80
1	16S1	60	A	N7-C8-N9	-11.46	108.07	113.80
1	16S1	238	A	N7-C8-N9	-11.46	108.07	113.80
22	23S1	676	A	C5-C6-N6	11.46	132.87	123.70
22	23S1	804	A	N7-C8-N9	-11.46	108.07	113.80
1	16S1	681	A	N7-C8-N9	-11.46	108.07	113.80
22	23S1	1634	A	C5-C6-N6	11.46	132.87	123.70
22	23S1	1928	A	N7-C8-N9	-11.46	108.07	113.80
22	23S1	2227	A	N7-C8-N9	-11.46	108.07	113.80
22	23S1	368	A	N7-C8-N9	-11.45	108.07	113.80
1	16S1	371	A	N7-C8-N9	-11.45	108.08	113.80
22	23S1	515	A	C5-C6-N6	11.45	132.86	123.70
1	16S1	553	A	N7-C8-N9	-11.45	108.08	113.80
22	23S1	1096	A	C5-C6-N6	11.45	132.86	123.70
1	16S1	1434	A	N7-C8-N9	-11.45	108.08	113.80
22	23S1	789	A	N7-C8-N9	-11.45	108.08	113.80
22	23S1	1020	A	C5-C6-N6	11.45	132.86	123.70
22	23S1	2418	A	N7-C8-N9	-11.45	108.08	113.80
1	16S1	781	A	N7-C8-N9	-11.44	108.08	113.80
22	23S1	1522	A	N7-C8-N9	-11.44	108.08	113.80
1	16S1	1012	A	N7-C8-N9	-11.44	108.08	113.80
1	16S1	1360	A	N7-C8-N9	-11.44	108.08	113.80
22	23S1	111	A	N7-C8-N9	-11.44	108.08	113.80
22	23S1	984	A	C5-C6-N6	11.44	132.85	123.70
1	16S1	716	A	N3-C4-C5	-11.44	118.80	126.80
1	16S1	495	A	C5-C6-N6	11.43	132.85	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1046	A	N7-C8-N9	-11.43	108.08	113.80
22	23S1	454	A	N7-C8-N9	-11.43	108.08	113.80
1	16S1	300	A	C4-C5-C6	11.43	122.72	117.00
1	16S1	356	A	N3-C4-C5	-11.43	118.80	126.80
22	23S1	1039	A	C5-C6-N6	11.43	132.84	123.70
1	16S1	1413	A	N7-C8-N9	-11.43	108.09	113.80
1	16S1	958	A	N7-C8-N9	-11.43	108.09	113.80
22	23S1	227	A	N7-C8-N9	-11.43	108.09	113.80
22	23S1	2340	A	N7-C8-N9	-11.43	108.09	113.80
22	23S1	53	A	N7-C8-N9	-11.43	108.09	113.80
22	23S1	371	A	N7-C8-N9	-11.43	108.09	113.80
22	23S1	1230	A	N7-C8-N9	-11.43	108.09	113.80
1	16S1	1396	A	N7-C8-N9	-11.42	108.09	113.80
22	23S1	74	A	C5-C6-N6	11.42	132.84	123.70
22	23S1	332	A	N7-C8-N9	-11.42	108.09	113.80
1	16S1	1493	A	N7-C8-N9	-11.42	108.09	113.80
1	16S1	743	A	N7-C8-N9	-11.42	108.09	113.80
22	23S1	621	A	N7-C8-N9	-11.42	108.09	113.80
22	23S1	332	A	C5-C6-N6	11.42	132.83	123.70
22	23S1	2809	A	N7-C8-N9	-11.42	108.09	113.80
22	23S1	1579	A	C5-C6-N6	11.41	132.83	123.70
22	23S1	2577	A	C5-C6-N6	11.41	132.83	123.70
22	23S1	1090	A	N7-C8-N9	-11.41	108.09	113.80
22	23S1	1165	A	C5-C6-N6	11.41	132.83	123.70
22	23S1	2101	A	N7-C8-N9	-11.41	108.09	113.80
55	PTR1	14	A	N3-C4-C5	-11.41	118.81	126.80
1	16S1	1219	A	N3-C4-C5	-11.41	118.81	126.80
22	23S1	1089	A	N7-C8-N9	-11.41	108.10	113.80
22	23S1	1307	A	N7-C8-N9	-11.41	108.10	113.80
22	23S1	272	A	N7-C8-N9	-11.41	108.10	113.80
22	23S1	2082	A	N7-C8-N9	-11.40	108.10	113.80
22	23S1	2435	A	C5-C6-N6	11.40	132.82	123.70
22	23S1	2814	A	N7-C8-N9	-11.40	108.10	113.80
1	16S1	120	A	C5-C6-N6	11.40	132.82	123.70
22	23S1	374	A	N7-C8-N9	-11.40	108.10	113.80
22	23S1	1304	A	N7-C8-N9	-11.40	108.10	113.80
22	23S1	1805	A	C5-C6-N6	11.40	132.82	123.70
22	23S1	2598	A	C5-C6-N6	11.40	132.82	123.70
1	16S1	10	A	N7-C8-N9	-11.40	108.10	113.80
1	16S1	1197	A	N7-C8-N9	-11.40	108.10	113.80
1	16S1	1513	A	N7-C8-N9	-11.40	108.10	113.80
22	23S1	983	A	N7-C8-N9	-11.40	108.10	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1347	A	N7-C8-N9	-11.40	108.10	113.80
22	23S1	1819	A	C5-C6-N6	11.40	132.82	123.70
22	23S1	1672	A	N7-C8-N9	-11.40	108.10	113.80
22	23S1	2013	A	C5-C6-N6	11.40	132.82	123.70
1	16S1	44	A	N7-C8-N9	-11.39	108.10	113.80
1	16S1	374	A	C5-C6-N6	11.39	132.81	123.70
1	16S1	1360	A	C5-C6-N6	11.39	132.82	123.70
22	23S1	1912	A	C5-C6-N6	11.39	132.81	123.70
22	23S1	1932	A	C5-C6-N6	11.39	132.81	123.70
1	16S1	195	A	C5-C6-N6	11.39	132.81	123.70
1	16S1	160	A	N7-C8-N9	-11.39	108.11	113.80
1	16S1	1428	A	N7-C8-N9	-11.39	108.11	113.80
22	23S1	1265	A	C5-C6-N6	11.39	132.81	123.70
1	16S1	59	A	C5-C6-N6	11.39	132.81	123.70
22	23S1	324	A	N7-C8-N9	-11.39	108.11	113.80
22	23S1	2654	A	C5-C6-N6	11.39	132.81	123.70
1	16S1	749	A	N7-C8-N9	-11.38	108.11	113.80
22	23S1	1690	A	C5-C6-N6	11.39	132.81	123.70
1	16S1	807	A	C5-C6-N6	11.38	132.81	123.70
22	23S1	1528	A	N3-C4-C5	-11.38	118.83	126.80
1	16S1	80	A	C5-C6-N6	11.38	132.81	123.70
22	23S1	1084	A	N7-C8-N9	-11.38	108.11	113.80
22	23S1	1783	A	C5-C6-N6	11.38	132.81	123.70
1	16S1	715	A	N7-C8-N9	-11.38	108.11	113.80
1	16S1	1035	A	N7-C8-N9	-11.38	108.11	113.80
1	16S1	190	A	C4-C5-C6	11.38	122.69	117.00
22	23S1	1978	A	N7-C8-N9	-11.38	108.11	113.80
22	23S1	342	A	N7-C8-N9	-11.38	108.11	113.80
22	23S1	910	A	C5-C6-N6	11.38	132.80	123.70
1	16S1	1250	A	N7-C8-N9	-11.37	108.11	113.80
1	16S1	767	A	N7-C8-N9	-11.37	108.11	113.80
1	16S1	1022	A	C5-C6-N6	11.37	132.80	123.70
1	16S1	1179	A	C5-C6-N6	11.37	132.80	123.70
22	23S1	643	A	C5-C6-N6	11.37	132.80	123.70
22	23S1	1569	A	C5-C6-N6	11.37	132.80	123.70
1	16S1	1248	A	N7-C8-N9	-11.37	108.11	113.80
22	23S1	900	A	C5-C6-N6	11.37	132.80	123.70
22	23S1	632	A	N7-C8-N9	-11.37	108.12	113.80
22	23S1	735	A	C5-C6-N6	11.37	132.79	123.70
22	23S1	2740	A	N7-C8-N9	-11.37	108.12	113.80
22	23S1	2821	A	N7-C8-N9	-11.37	108.12	113.80
22	23S1	1304	A	C5-C6-N6	11.37	132.79	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1532	A	N7-C8-N9	-11.37	108.12	113.80
22	23S1	925	A	N7-C8-N9	-11.36	108.12	113.80
22	23S1	1535	A	C5-C6-N6	11.36	132.79	123.70
22	23S1	1759	A	N7-C8-N9	-11.36	108.12	113.80
22	23S1	2088	A	N7-C8-N9	-11.36	108.12	113.80
22	23S1	294	A	N7-C8-N9	-11.36	108.12	113.80
22	23S1	1705	A	N7-C8-N9	-11.36	108.12	113.80
1	16S1	583	A	C5-C6-N6	11.36	132.78	123.70
22	23S1	654	A	N3-C4-C5	-11.36	118.85	126.80
22	23S1	892	A	C5-C6-N6	11.36	132.78	123.70
22	23S1	2516	A	N7-C8-N9	-11.36	108.12	113.80
22	23S1	753	A	N7-C8-N9	-11.35	108.12	113.80
22	23S1	1640	A	C5-C6-N6	11.35	132.78	123.70
22	23S1	2700	A	N7-C8-N9	-11.35	108.12	113.80
23	05S1	58	A	N7-C8-N9	-11.35	108.12	113.80
55	PTR1	3	A	N7-C8-N9	-11.35	108.12	113.80
1	16S1	1280	A	C5-C6-N6	11.35	132.78	123.70
22	23S1	221	A	N7-C8-N9	-11.35	108.12	113.80
55	PTR1	69	A	N7-C8-N9	-11.35	108.12	113.80
22	23S1	1134	A	N7-C8-N9	-11.35	108.13	113.80
22	23S1	1890	A	N7-C8-N9	-11.35	108.13	113.80
1	16S1	55	A	N3-C4-C5	-11.35	118.86	126.80
22	23S1	972	A	C5-C6-N6	11.35	132.78	123.70
1	16S1	509	A	C5-C6-N6	11.34	132.78	123.70
22	23S1	156	A	N7-C8-N9	-11.34	108.13	113.80
1	16S1	913	A	C5-C6-N6	11.34	132.77	123.70
22	23S1	402	A	N7-C8-N9	-11.34	108.13	113.80
22	23S1	1032	A	C5-C6-N6	11.34	132.77	123.70
1	16S1	872	A	N3-C4-C5	-11.34	118.86	126.80
22	23S1	482	A	N3-C4-C5	-11.34	118.86	126.80
22	23S1	2459	A	N7-C8-N9	-11.34	108.13	113.80
22	23S1	131	A	N3-C4-C5	-11.33	118.87	126.80
22	23S1	2169	A	C5-C6-N6	11.33	132.77	123.70
22	23S1	2893	A	N7-C8-N9	-11.33	108.13	113.80
1	16S1	1480	A	C5-C6-N6	11.33	132.76	123.70
22	23S1	715	A	N7-C8-N9	-11.33	108.13	113.80
22	23S1	1156	A	N7-C8-N9	-11.33	108.14	113.80
22	23S1	1981	A	N7-C8-N9	-11.33	108.14	113.80
1	16S1	1150	A	N7-C8-N9	-11.32	108.14	113.80
22	23S1	2835	A	N7-C8-N9	-11.32	108.14	113.80
1	16S1	969	A	C5-C6-N6	11.32	132.76	123.70
22	23S1	126	A	C5-C6-N6	11.32	132.76	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	311	A	C5-C6-N6	11.32	132.76	123.70
22	23S1	643	A	N7-C8-N9	-11.32	108.14	113.80
22	23S1	556	A	N7-C8-N9	-11.32	108.14	113.80
22	23S1	1276	A	N7-C8-N9	-11.32	108.14	113.80
22	23S1	2051	A	C5-C6-N6	11.32	132.75	123.70
1	16S1	860	A	N7-C8-N9	-11.32	108.14	113.80
1	16S1	596	A	N7-C8-N9	-11.32	108.14	113.80
22	23S1	2309	A	N7-C8-N9	-11.32	108.14	113.80
22	23S1	563	A	N7-C8-N9	-11.31	108.14	113.80
22	23S1	1593	A	N7-C8-N9	-11.31	108.14	113.80
22	23S1	2031	A	C5-C6-N6	11.31	132.75	123.70
1	16S1	845	A	N7-C8-N9	-11.31	108.14	113.80
22	23S1	792	A	C5-C6-N6	11.31	132.75	123.70
22	23S1	1655	A	N7-C8-N9	-11.31	108.14	113.80
1	16S1	969	A	N7-C8-N9	-11.31	108.15	113.80
22	23S1	144	A	N7-C8-N9	-11.31	108.15	113.80
22	23S1	1431	A	N7-C8-N9	-11.31	108.15	113.80
22	23S1	1503	A	N7-C8-N9	-11.31	108.15	113.80
22	23S1	2117	A	C5-C6-N6	11.31	132.74	123.70
1	16S1	906	A	N7-C8-N9	-11.30	108.15	113.80
22	23S1	947	A	N7-C8-N9	-11.30	108.15	113.80
22	23S1	1353	A	N7-C8-N9	-11.30	108.15	113.80
22	23S1	2835	A	C5-C6-N6	11.30	132.74	123.70
1	16S1	1495	U	N1-C2-O2	11.30	130.71	122.80
22	23S1	541	A	N7-C8-N9	-11.30	108.15	113.80
22	23S1	918	A	C5-C6-N6	11.30	132.74	123.70
23	05S1	119	A	N7-C8-N9	-11.30	108.15	113.80
55	PTR1	42	A	N7-C8-N9	-11.30	108.15	113.80
22	23S1	347	A	N7-C8-N9	-11.30	108.15	113.80
1	16S1	1092	A	C5-C6-N6	11.29	132.74	123.70
1	16S1	1408	A	C5-C6-N6	11.29	132.74	123.70
22	23S1	1254	A	N7-C8-N9	-11.29	108.15	113.80
1	16S1	151	A	N3-C4-C5	-11.29	118.90	126.80
22	23S1	1342	A	C5-C6-N6	11.29	132.73	123.70
22	23S1	1439	A	C5-C6-N6	11.29	132.73	123.70
22	23S1	2453	A	N3-C4-C5	-11.29	118.90	126.80
1	16S1	1	A	C5-C6-N6	11.29	132.73	123.70
1	16S1	777	A	C5-C6-N6	11.29	132.73	123.70
22	23S1	52	A	N7-C8-N9	-11.29	108.16	113.80
22	23S1	233	A	N7-C8-N9	-11.29	108.16	113.80
22	23S1	432	A	N7-C8-N9	-11.29	108.16	113.80
22	23S1	706	A	N7-C8-N9	-11.29	108.16	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	994	A	N3-C4-C5	-11.29	118.90	126.80
1	16S1	1410	A	N7-C8-N9	-11.29	108.16	113.80
22	23S1	960	A	N3-C4-C5	-11.29	118.90	126.80
22	23S1	1829	A	N7-C8-N9	-11.29	108.16	113.80
22	23S1	2733	A	N7-C8-N9	-11.29	108.16	113.80
1	16S1	344	A	N7-C8-N9	-11.29	108.16	113.80
1	16S1	432	A	N7-C8-N9	-11.28	108.16	113.80
22	23S1	602	A	N7-C8-N9	-11.28	108.16	113.80
1	16S1	321	A	C5-C6-N6	11.28	132.72	123.70
22	23S1	670	A	N7-C8-N9	-11.28	108.16	113.80
22	23S1	1000	A	N3-C4-C5	-11.28	118.90	126.80
22	23S1	1169	A	N7-C8-N9	-11.28	108.16	113.80
22	23S1	2882	A	C5-C6-N6	11.28	132.73	123.70
1	16S1	1093	A	N7-C8-N9	-11.28	108.16	113.80
22	23S1	603	A	N7-C8-N9	-11.28	108.16	113.80
22	23S1	1204	A	N7-C8-N9	-11.28	108.16	113.80
22	23S1	2448	A	C5-C6-N6	11.28	132.72	123.70
1	16S1	119	A	N7-C8-N9	-11.27	108.16	113.80
1	16S1	1319	A	C5-C6-N6	11.27	132.72	123.70
22	23S1	449	A	N3-C4-C5	-11.27	118.91	126.80
1	16S1	199	A	N3-C4-C5	-11.27	118.91	126.80
1	16S1	1274	A	C5-C6-N6	11.27	132.72	123.70
22	23S1	1808	A	N7-C8-N9	-11.27	108.16	113.80
22	23S1	118	A	N7-C8-N9	-11.27	108.17	113.80
22	23S1	404	A	N7-C8-N9	-11.27	108.17	113.80
22	23S1	2211	A	C5-C6-N6	11.27	132.72	123.70
22	23S1	2461	A	N3-C4-C5	-11.27	118.91	126.80
22	23S1	2738	A	C5-C6-N6	11.27	132.71	123.70
1	16S1	901	A	N3-C4-C5	-11.27	118.91	126.80
1	16S1	1000	A	N7-C8-N9	-11.27	108.17	113.80
1	16S1	1238	A	C5-C6-N6	11.26	132.71	123.70
22	23S1	231	A	N7-C8-N9	-11.26	108.17	113.80
22	23S1	21	A	N7-C8-N9	-11.26	108.17	113.80
22	23S1	677	A	N3-C4-C5	-11.26	118.92	126.80
22	23S1	917	A	C5-C6-N6	11.26	132.71	123.70
1	16S1	465	A	C5-C6-N6	11.26	132.71	123.70
1	16S1	753	A	N7-C8-N9	-11.26	108.17	113.80
22	23S1	1713	A	N7-C8-N9	-11.26	108.17	113.80
1	16S1	192	A	N7-C8-N9	-11.26	108.17	113.80
1	16S1	975	A	C5-C6-N6	11.26	132.70	123.70
22	23S1	2600	A	C5-C6-N6	11.26	132.70	123.70
22	23S1	1953	A	C5-C6-N6	11.25	132.70	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2425	A	N7-C8-N9	-11.25	108.17	113.80
1	16S1	288	A	C5-C6-N6	11.25	132.70	123.70
1	16S1	1081	A	N7-C8-N9	-11.25	108.17	113.80
1	16S1	1287	A	C5-C6-N6	11.25	132.70	123.70
22	23S1	207	A	N7-C8-N9	-11.25	108.17	113.80
22	23S1	936	A	N7-C8-N9	-11.25	108.17	113.80
22	23S1	2126	A	C5-C6-N6	11.25	132.70	123.70
22	23S1	2267	A	N3-C4-C5	-11.25	118.93	126.80
1	16S1	787	A	N7-C8-N9	-11.25	108.18	113.80
22	23S1	6	A	N7-C8-N9	-11.25	108.18	113.80
22	23S1	1086	A	N3-C4-C5	-11.25	118.93	126.80
22	23S1	2328	A	N3-C4-C5	-11.25	118.93	126.80
1	16S1	415	A	C5-C6-N6	11.24	132.70	123.70
22	23S1	152	A	N7-C8-N9	-11.24	108.18	113.80
22	23S1	347	A	C5-C6-N6	11.24	132.70	123.70
1	16S1	53	A	N7-C8-N9	-11.24	108.18	113.80
1	16S1	1111	A	C5-C6-N6	11.24	132.69	123.70
1	16S1	1213	A	N7-C8-N9	-11.24	108.18	113.80
22	23S1	1194	A	C5-C6-N6	11.24	132.69	123.70
22	23S1	1359	A	N7-C8-N9	-11.24	108.18	113.80
22	23S1	1525	A	N7-C8-N9	-11.24	108.18	113.80
22	23S1	2682	A	C5-C6-N6	11.24	132.69	123.70
22	23S1	505	A	N7-C8-N9	-11.24	108.18	113.80
1	16S1	560	A	C5-C6-N6	11.24	132.69	123.70
22	23S1	1690	A	N7-C8-N9	-11.24	108.18	113.80
23	05S1	50	A	N7-C8-N9	-11.24	108.18	113.80
1	16S1	1239	A	C5-C6-N6	11.23	132.69	123.70
22	23S1	217	A	C5-C6-N6	11.23	132.69	123.70
22	23S1	825	A	C5-C6-N6	11.23	132.69	123.70
22	23S1	428	A	N7-C8-N9	-11.23	108.18	113.80
22	23S1	1067	A	C5-C6-N6	11.23	132.69	123.70
22	23S1	1073	A	N7-C8-N9	-11.23	108.18	113.80
22	23S1	504	A	C8-N9-C4	11.23	110.29	105.80
22	23S1	863	A	N3-C4-C5	-11.23	118.94	126.80
22	23S1	1749	A	C5-C6-N6	11.23	132.69	123.70
22	23S1	1936	A	N3-C4-C5	-11.23	118.94	126.80
1	16S1	303	A	N7-C8-N9	-11.23	108.19	113.80
22	23S1	340	A	N7-C8-N9	-11.23	108.19	113.80
1	16S1	908	A	N7-C8-N9	-11.23	108.19	113.80
22	23S1	1080	A	N7-C8-N9	-11.23	108.19	113.80
22	23S1	1579	A	N7-C8-N9	-11.23	108.19	113.80
1	16S1	865	A	N3-C4-C5	-11.23	118.94	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1000	A	C5-C6-N6	11.23	132.68	123.70
22	23S1	1048	A	N7-C8-N9	-11.23	108.19	113.80
22	23S1	1495	A	C5-C6-N6	11.23	132.68	123.70
1	16S1	181	A	N7-C8-N9	-11.22	108.19	113.80
22	23S1	429	A	C5-C6-N6	11.22	132.68	123.70
22	23S1	1572	A	N7-C8-N9	-11.22	108.19	113.80
22	23S1	2433	A	N7-C8-N9	-11.22	108.19	113.80
22	23S1	1522	A	C5-C6-N6	11.22	132.68	123.70
1	16S1	865	A	C5-C6-N6	11.22	132.68	123.70
22	23S1	526	A	N7-C8-N9	-11.22	108.19	113.80
22	23S1	592	A	N7-C8-N9	-11.22	108.19	113.80
22	23S1	1829	A	C5-C6-N6	11.22	132.68	123.70
22	23S1	71	A	N7-C8-N9	-11.22	108.19	113.80
22	23S1	670	A	C5-C6-N6	11.22	132.67	123.70
22	23S1	1495	A	N7-C8-N9	-11.22	108.19	113.80
1	16S1	782	A	C5-C6-N6	11.21	132.67	123.70
22	23S1	590	A	N7-C8-N9	-11.21	108.19	113.80
22	23S1	1214	A	N7-C8-N9	-11.21	108.19	113.80
22	23S1	1503	A	C5-C6-N6	11.22	132.67	123.70
22	23S1	2376	A	C5-C6-N6	11.21	132.67	123.70
1	16S1	26	A	N7-C8-N9	-11.21	108.19	113.80
1	16S1	325	A	C5-C6-N6	11.21	132.67	123.70
1	16S1	389	A	C5-C6-N6	11.21	132.67	123.70
1	16S1	1375	A	N7-C8-N9	-11.21	108.19	113.80
22	23S1	155	A	N7-C8-N9	-11.21	108.19	113.80
22	23S1	2451	A	C5-C6-N6	11.21	132.67	123.70
1	16S1	321	A	N7-C8-N9	-11.21	108.20	113.80
1	16S1	1285	A	C5-C6-N6	11.21	132.67	123.70
22	23S1	346	A	C5-C6-N6	11.21	132.67	123.70
1	16S1	197	A	C5-C6-N6	11.21	132.66	123.70
1	16S1	968	A	N7-C8-N9	-11.21	108.20	113.80
22	23S1	279	A	C5-C6-N6	11.21	132.66	123.70
22	23S1	627	A	C5-C6-N6	11.21	132.66	123.70
22	23S1	1711	A	N7-C8-N9	-11.21	108.20	113.80
22	23S1	1744	A	N3-C4-C5	-11.20	118.96	126.80
22	23S1	508	A	N7-C8-N9	-11.20	108.20	113.80
22	23S1	515	A	N7-C8-N9	-11.20	108.20	113.80
22	23S1	917	A	N7-C8-N9	-11.20	108.20	113.80
22	23S1	1336	A	N7-C8-N9	-11.20	108.20	113.80
22	23S1	1419	A	C5-C6-N6	11.20	132.66	123.70
23	05S1	29	A	N7-C8-N9	-11.20	108.20	113.80
1	16S1	533	A	N7-C8-N9	-11.20	108.20	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	958	A	C5-C6-N6	11.20	132.66	123.70
1	16S1	1016	A	C5-C6-N6	11.20	132.66	123.70
23	05S1	109	A	N7-C8-N9	-11.20	108.20	113.80
1	16S1	535	A	N7-C8-N9	-11.19	108.20	113.80
1	16S1	1158	C	N1-C2-O2	11.19	125.62	118.90
22	23S1	1509	A	C5-C6-N6	11.19	132.66	123.70
22	23S1	2749	A	C5-C6-N6	11.19	132.66	123.70
1	16S1	1534	A	C5-C6-N6	11.19	132.65	123.70
22	23S1	666	A	N7-C8-N9	-11.19	108.20	113.80
22	23S1	892	A	N3-C4-C5	-11.19	118.97	126.80
22	23S1	503	A	N3-C4-C5	-11.19	118.97	126.80
22	23S1	1213	A	N3-C4-C5	-11.19	118.97	126.80
22	23S1	453	A	N7-C8-N9	-11.19	108.21	113.80
22	23S1	91	A	N7-C8-N9	-11.19	108.21	113.80
22	23S1	1598	A	C5-C6-N6	11.19	132.65	123.70
22	23S1	1665	A	N7-C8-N9	-11.19	108.21	113.80
1	16S1	673	A	N3-C4-C5	-11.18	118.97	126.80
22	23S1	197	A	C5-C6-N6	11.18	132.65	123.70
22	23S1	1899	A	N3-C4-C5	-11.18	118.97	126.80
22	23S1	2009	A	N7-C8-N9	-11.18	108.21	113.80
22	23S1	2327	A	C5-C6-N6	11.18	132.65	123.70
22	23S1	2776	A	C5-C6-N6	11.18	132.65	123.70
1	16S1	151	A	N7-C8-N9	-11.18	108.21	113.80
1	16S1	1146	A	N7-C8-N9	-11.18	108.21	113.80
22	23S1	532	A	N7-C8-N9	-11.18	108.21	113.80
22	23S1	1505	A	N7-C8-N9	-11.18	108.21	113.80
22	23S1	572	A	N3-C4-C5	-11.18	118.98	126.80
22	23S1	1678	A	N7-C8-N9	-11.18	108.21	113.80
22	23S1	423	A	N7-C8-N9	-11.18	108.21	113.80
22	23S1	2560	A	N7-C8-N9	-11.18	108.21	113.80
22	23S1	160	A	N3-C4-C5	-11.17	118.98	126.80
22	23S1	2376	A	N7-C8-N9	-11.17	108.21	113.80
22	23S1	1998	A	N3-C4-C5	-11.17	118.98	126.80
1	16S1	1251	A	N7-C8-N9	-11.17	108.21	113.80
1	16S1	1447	A	C5-C6-N6	11.17	132.64	123.70
22	23S1	2461	A	N7-C8-N9	-11.17	108.22	113.80
1	16S1	560	A	N7-C8-N9	-11.17	108.22	113.80
1	16S1	1117	A	N7-C8-N9	-11.17	108.22	113.80
1	16S1	1150	A	C5-C6-N6	11.17	132.63	123.70
1	16S1	1170	A	N7-C8-N9	-11.17	108.22	113.80
1	16S1	160	A	C5-C6-N6	11.16	132.63	123.70
22	23S1	1626	A	N7-C8-N9	-11.16	108.22	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2142	A	N7-C8-N9	-11.16	108.22	113.80
23	05S1	78	A	C5-C6-N6	11.16	132.63	123.70
1	16S1	787	A	C5-C6-N6	11.16	132.63	123.70
1	16S1	1021	A	N7-C8-N9	-11.16	108.22	113.80
1	16S1	1167	A	N7-C8-N9	-11.16	108.22	113.80
22	23S1	844	A	N7-C8-N9	-11.16	108.22	113.80
22	23S1	2062	A	N3-C4-C5	-11.16	118.99	126.80
1	16S1	143	A	N7-C8-N9	-11.16	108.22	113.80
22	23S1	38	A	N7-C8-N9	-11.16	108.22	113.80
22	23S1	191	A	N7-C8-N9	-11.16	108.22	113.80
22	23S1	256	A	N7-C8-N9	-11.16	108.22	113.80
22	23S1	979	A	C5-C6-N6	11.16	132.63	123.70
22	23S1	1794	A	N7-C8-N9	-11.16	108.22	113.80
22	23S1	460	A	N7-C8-N9	-11.16	108.22	113.80
22	23S1	1998	A	C5-C6-N6	11.16	132.63	123.70
22	23S1	1570	A	N7-C8-N9	-11.16	108.22	113.80
22	23S1	340	A	C5-C6-N6	11.16	132.62	123.70
22	23S1	2090	A	N7-C8-N9	-11.16	108.22	113.80
1	16S1	149	A	N7-C8-N9	-11.15	108.22	113.80
1	16S1	1465	A	N7-C8-N9	-11.15	108.22	113.80
22	23S1	781	A	N7-C8-N9	-11.15	108.22	113.80
22	23S1	1244	A	N7-C8-N9	-11.15	108.22	113.80
22	23S1	83	A	C5-C6-N6	11.15	132.62	123.70
22	23S1	1321	A	N7-C8-N9	-11.15	108.22	113.80
23	05S1	45	A	N7-C8-N9	-11.15	108.22	113.80
22	23S1	1366	A	C5-C6-N6	11.15	132.62	123.70
1	16S1	1	A	N7-C8-N9	-11.15	108.22	113.80
22	23S1	401	A	C5-C6-N6	11.15	132.62	123.70
22	23S1	718	A	C5-C6-N6	11.15	132.62	123.70
22	23S1	28	A	N7-C8-N9	-11.15	108.23	113.80
1	16S1	448	A	C5-C6-N6	11.14	132.62	123.70
22	23S1	5	A	N7-C8-N9	-11.14	108.23	113.80
22	23S1	1970	A	N7-C8-N9	-11.14	108.23	113.80
1	16S1	143	A	C5-C6-N6	11.14	132.61	123.70
1	16S1	364	A	N7-C8-N9	-11.14	108.23	113.80
22	23S1	502	A	N7-C8-N9	-11.14	108.23	113.80
1	16S1	119	A	C5-C6-N6	11.14	132.61	123.70
22	23S1	346	A	N7-C8-N9	-11.14	108.23	113.80
22	23S1	348	A	N7-C8-N9	-11.14	108.23	113.80
22	23S1	715	A	C5-C6-N6	11.14	132.61	123.70
1	16S1	579	A	N3-C4-C5	-11.13	119.01	126.80
22	23S1	1274	A	C5-C6-N6	11.13	132.61	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	794	A	C5-C6-N6	11.13	132.60	123.70
1	16S1	1179	A	N7-C8-N9	-11.13	108.23	113.80
22	23S1	2142	A	N3-C4-C5	-11.13	119.01	126.80
1	16S1	802	A	N7-C8-N9	-11.13	108.24	113.80
22	23S1	1367	A	C5-C6-N6	11.12	132.60	123.70
22	23S1	1754	A	N7-C8-N9	-11.12	108.24	113.80
1	16S1	78	A	C5-C6-N6	11.12	132.60	123.70
22	23S1	1810	A	C4-C5-C6	11.12	122.56	117.00
22	23S1	1427	A	N7-C8-N9	-11.12	108.24	113.80
22	23S1	1669	A	C5-C6-N6	11.12	132.60	123.70
1	16S1	329	A	N7-C8-N9	-11.12	108.24	113.80
1	16S1	640	A	N7-C8-N9	-11.12	108.24	113.80
1	16S1	728	A	N7-C8-N9	-11.12	108.24	113.80
1	16S1	918	A	C5-C6-N6	11.12	132.59	123.70
22	23S1	404	A	C5-C6-N6	11.12	132.59	123.70
22	23S1	1134	A	C5-C6-N6	11.12	132.59	123.70
22	23S1	2778	A	N7-C8-N9	-11.12	108.24	113.80
23	05S1	15	A	N7-C8-N9	-11.12	108.24	113.80
1	16S1	864	A	C5-C6-N6	11.12	132.59	123.70
1	16S1	1289	A	C5-C6-N6	11.12	132.59	123.70
22	23S1	199	A	C5-C6-N6	11.12	132.59	123.70
22	23S1	2639	A	C5-C6-N6	11.11	132.59	123.70
22	23S1	63	A	N7-C8-N9	-11.11	108.24	113.80
22	23S1	330	A	C5-C6-N6	11.11	132.59	123.70
22	23S1	756	A	N7-C8-N9	-11.11	108.24	113.80
22	23S1	1133	A	C5-C6-N6	11.11	132.59	123.70
22	23S1	1453	A	C5-C6-N6	11.11	132.59	123.70
22	23S1	1717	A	N7-C8-N9	-11.11	108.24	113.80
23	05S1	52	A	N7-C8-N9	-11.11	108.24	113.80
1	16S1	1468	A	N7-C8-N9	-11.11	108.25	113.80
22	23S1	2020	A	N7-C8-N9	-11.11	108.25	113.80
1	16S1	432	A	C5-C6-N6	11.11	132.59	123.70
22	23S1	716	A	C5-C6-N6	11.11	132.58	123.70
22	23S1	1801	A	N7-C8-N9	-11.11	108.25	113.80
22	23S1	2810	A	C5-C6-N6	11.11	132.58	123.70
22	23S1	1070	A	N7-C8-N9	-11.10	108.25	113.80
1	16S1	532	A	N7-C8-N9	-11.10	108.25	113.80
1	16S1	1431	A	N7-C8-N9	-11.10	108.25	113.80
22	23S1	781	A	C5-C6-N6	11.10	132.58	123.70
1	16S1	182	A	C5-C6-N6	11.10	132.58	123.70
1	16S1	914	A	N7-C8-N9	-11.10	108.25	113.80
1	16S1	1306	A	N7-C8-N9	-11.10	108.25	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1433	A	C5-C6-N6	11.10	132.58	123.70
22	23S1	71	A	C5-C6-N6	11.10	132.58	123.70
22	23S1	119	A	N7-C8-N9	-11.10	108.25	113.80
22	23S1	449	A	C5-C6-N6	11.10	132.58	123.70
22	23S1	2287	A	N3-C4-C5	-11.10	119.03	126.80
1	16S1	161	A	C5-C6-N6	11.10	132.58	123.70
1	16S1	574	A	C5-C6-N6	11.10	132.58	123.70
1	16S1	825	A	C5-C6-N6	11.10	132.58	123.70
1	16S1	1171	A	N7-C8-N9	-11.10	108.25	113.80
1	16S1	759	A	C5-C6-N6	11.10	132.58	123.70
1	16S1	1180	A	N7-C8-N9	-11.10	108.25	113.80
22	23S1	981	A	N7-C8-N9	-11.10	108.25	113.80
22	23S1	2541	A	C5-C6-N6	11.10	132.58	123.70
1	16S1	98	A	N3-C4-C5	-11.09	119.03	126.80
1	16S1	892	A	N7-C8-N9	-11.09	108.25	113.80
22	23S1	320	A	N3-C4-C5	-11.09	119.03	126.80
22	23S1	608	A	N7-C8-N9	-11.09	108.25	113.80
22	23S1	782	A	C5-C6-N6	11.09	132.57	123.70
1	16S1	815	A	C5-C6-N6	11.09	132.57	123.70
22	23S1	1700	A	C5-C6-N6	11.09	132.57	123.70
1	16S1	546	A	N7-C8-N9	-11.09	108.25	113.80
1	16S1	1055	A	N7-C8-N9	-11.09	108.25	113.80
22	23S1	788	A	C5-C6-N6	11.09	132.57	123.70
22	23S1	616	A	C5-C6-N6	11.09	132.57	123.70
22	23S1	1551	A	N7-C8-N9	-11.09	108.26	113.80
1	16S1	718	A	N3-C4-C5	-11.09	119.04	126.80
1	16S1	889	A	N7-C8-N9	-11.09	108.26	113.80
22	23S1	532	A	C5-C6-N6	11.09	132.57	123.70
22	23S1	1551	A	C5-C6-N6	11.09	132.57	123.70
22	23S1	2565	A	N7-C8-N9	-11.09	108.26	113.80
22	23S1	1877	A	C5-C6-N6	11.09	132.57	123.70
22	23S1	504	A	C5-C6-N6	11.08	132.57	123.70
1	16S1	196	A	C5-C6-N6	11.08	132.56	123.70
22	23S1	2377	A	N7-C8-N9	-11.08	108.26	113.80
22	23S1	2589	A	N7-C8-N9	-11.08	108.26	113.80
1	16S1	364	A	C5-C6-N6	11.08	132.56	123.70
22	23S1	251	A	N3-C4-C5	-11.08	119.04	126.80
1	16S1	414	A	N7-C8-N9	-11.08	108.26	113.80
22	23S1	2169	A	N7-C8-N9	-11.08	108.26	113.80
22	23S1	2564	A	N7-C8-N9	-11.08	108.26	113.80
1	16S1	130	A	N7-C8-N9	-11.07	108.26	113.80
1	16S1	199	A	N7-C8-N9	-11.07	108.26	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	320	A	N7-C8-N9	-11.07	108.26	113.80
22	23S1	1284	A	C5-C6-N6	11.07	132.56	123.70
1	16S1	814	A	N7-C8-N9	-11.07	108.26	113.80
22	23S1	1544	A	N3-C4-C5	-11.07	119.05	126.80
22	23S1	1966	A	N7-C8-N9	-11.07	108.26	113.80
22	23S1	2665	A	N7-C8-N9	-11.07	108.26	113.80
22	23S1	2860	A	C5-C6-N6	11.07	132.56	123.70
1	16S1	325	A	N7-C8-N9	-11.07	108.27	113.80
1	16S1	393	A	N7-C8-N9	-11.07	108.27	113.80
1	16S1	845	A	C5-C6-N6	11.07	132.55	123.70
22	23S1	311	A	N7-C8-N9	-11.07	108.27	113.80
22	23S1	1477	A	N7-C8-N9	-11.07	108.27	113.80
1	16S1	452	A	N3-C4-C5	-11.06	119.05	126.80
22	23S1	213	A	C5-C6-N6	11.06	132.55	123.70
23	05S1	73	A	N3-C4-C5	-11.06	119.05	126.80
22	23S1	2059	A	N7-C8-N9	-11.06	108.27	113.80
22	23S1	2899	A	N7-C8-N9	-11.06	108.27	113.80
1	16S1	768	A	N7-C8-N9	-11.06	108.27	113.80
1	16S1	1280	A	N7-C8-N9	-11.06	108.27	113.80
22	23S1	1773	A	C5-C6-N6	11.06	132.55	123.70
22	23S1	2856	A	N7-C8-N9	-11.06	108.27	113.80
23	05S1	15	A	C5-C6-N6	11.06	132.55	123.70
1	16S1	7	A	N7-C8-N9	-11.06	108.27	113.80
22	23S1	563	A	N3-C4-C5	-11.06	119.06	126.80
22	23S1	609	A	C5-C6-N6	11.06	132.55	123.70
22	23S1	1050	A	C5-C6-N6	11.06	132.55	123.70
22	23S1	1090	A	C5-C6-N6	11.06	132.55	123.70
22	23S1	2154	A	N7-C8-N9	-11.06	108.27	113.80
1	16S1	408	A	C5-C6-N6	11.06	132.54	123.70
22	23S1	218	A	C5-C6-N6	11.06	132.54	123.70
22	23S1	2757	A	C5-C6-N6	11.06	132.54	123.70
22	23S1	1189	A	N7-C8-N9	-11.05	108.27	113.80
1	16S1	205	A	N7-C8-N9	-11.05	108.27	113.80
1	16S1	487	A	C5-C6-N6	11.05	132.54	123.70
22	23S1	959	A	C5-C6-N6	11.05	132.54	123.70
22	23S1	2411	A	N7-C8-N9	-11.05	108.27	113.80
1	16S1	559	A	C5-C6-N6	11.05	132.54	123.70
22	23S1	1918	A	C5-C6-N6	11.05	132.54	123.70
22	23S1	2015	A	C5-C6-N6	11.05	132.54	123.70
1	16S1	1176	A	N7-C8-N9	-11.05	108.28	113.80
22	23S1	1809	A	N3-C4-C5	-11.05	119.07	126.80
1	16S1	356	A	N7-C8-N9	-11.05	108.28	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1016	A	N7-C8-N9	-11.04	108.28	113.80
22	23S1	118	A	C5-C6-N6	11.04	132.54	123.70
22	23S1	1269	A	C5-C6-N6	11.05	132.54	123.70
22	23S1	631	A	C5-C6-N6	11.04	132.53	123.70
22	23S1	941	A	C5-C6-N6	11.04	132.53	123.70
1	16S1	595	A	N7-C8-N9	-11.04	108.28	113.80
22	23S1	1722	A	N7-C8-N9	-11.04	108.28	113.80
22	23S1	2679	A	N7-C8-N9	-11.04	108.28	113.80
22	23S1	1548	A	N7-C8-N9	-11.04	108.28	113.80
22	23S1	2654	A	N7-C8-N9	-11.04	108.28	113.80
22	23S1	2247	A	N7-C8-N9	-11.04	108.28	113.80
22	23S1	2600	A	N7-C8-N9	-11.04	108.28	113.80
22	23S1	2660	A	N7-C8-N9	-11.04	108.28	113.80
1	16S1	1410	A	C5-C6-N6	11.04	132.53	123.70
22	23S1	1889	A	C5-C6-N6	11.04	132.53	123.70
22	23S1	1757	A	C5-C6-N6	11.03	132.53	123.70
1	16S1	1500	A	N7-C8-N9	-11.03	108.28	113.80
22	23S1	1084	A	C5-C6-N6	11.03	132.53	123.70
22	23S1	1142	A	N7-C8-N9	-11.03	108.28	113.80
22	23S1	1786	A	N7-C8-N9	-11.03	108.28	113.80
22	23S1	2278	A	N7-C8-N9	-11.03	108.28	113.80
1	16S1	676	A	N7-C8-N9	-11.03	108.29	113.80
22	23S1	1918	A	N7-C8-N9	-11.03	108.28	113.80
22	23S1	959	A	N3-C4-C5	-11.03	119.08	126.80
22	23S1	2266	A	C5-C6-N6	11.03	132.52	123.70
1	16S1	262	A	N7-C8-N9	-11.02	108.29	113.80
1	16S1	694	A	C5-C6-N6	11.02	132.52	123.70
1	16S1	974	A	N7-C8-N9	-11.02	108.29	113.80
1	16S1	1019	A	N7-C8-N9	-11.02	108.29	113.80
1	16S1	1157	A	N7-C8-N9	-11.02	108.29	113.80
1	16S1	1204	A	N7-C8-N9	-11.02	108.29	113.80
1	16S1	753	A	C5-C6-N6	11.02	132.51	123.70
22	23S1	513	A	N3-C4-C5	-11.02	119.09	126.80
22	23S1	1175	A	N3-C4-C5	-11.02	119.09	126.80
22	23S1	1367	A	N7-C8-N9	-11.02	108.29	113.80
22	23S1	1098	A	N3-C4-C5	-11.02	119.09	126.80
22	23S1	1322	A	C5-C6-N6	11.02	132.51	123.70
22	23S1	2241	A	N3-C4-C5	-11.02	119.09	126.80
22	23S1	2829	A	N7-C8-N9	-11.02	108.29	113.80
22	23S1	2225	A	C5-C6-N6	11.01	132.51	123.70
22	23S1	2448	A	N7-C8-N9	-11.01	108.29	113.80
22	23S1	2765	A	C5-C6-N6	11.01	132.51	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	729	A	C5-C6-N6	11.01	132.51	123.70
1	16S1	1430	A	N7-C8-N9	-11.01	108.30	113.80
22	23S1	1609	A	N7-C8-N9	-11.01	108.30	113.80
22	23S1	1858	A	C5-C6-N6	11.01	132.51	123.70
22	23S1	2711	A	C5-C6-N6	11.01	132.51	123.70
1	16S1	414	A	C5-C6-N6	11.00	132.50	123.70
22	23S1	310	A	C5-C6-N6	11.00	132.50	123.70
22	23S1	1226	A	C5-C6-N6	11.00	132.50	123.70
22	23S1	1654	A	C5-C6-N6	11.00	132.50	123.70
1	16S1	502	A	N3-C4-C5	-11.00	119.10	126.80
1	16S1	1503	A	C5-C6-N6	11.00	132.50	123.70
22	23S1	1614	A	N7-C8-N9	-11.00	108.30	113.80
22	23S1	1821	A	N7-C8-N9	-11.00	108.30	113.80
22	23S1	2335	A	C5-C6-N6	11.00	132.50	123.70
1	16S1	1377	A	C5-C6-N6	11.00	132.50	123.70
22	23S1	721	A	N7-C8-N9	-11.00	108.30	113.80
22	23S1	1635	A	N7-C8-N9	-11.00	108.30	113.80
1	16S1	649	A	N7-C8-N9	-11.00	108.30	113.80
1	16S1	983	A	C5-C6-N6	11.00	132.50	123.70
22	23S1	28	A	C5-C6-N6	11.00	132.50	123.70
22	23S1	920	A	N7-C8-N9	-11.00	108.30	113.80
22	23S1	1286	A	N7-C8-N9	-11.00	108.30	113.80
1	16S1	640	A	C5-C6-N6	10.99	132.50	123.70
1	16S1	747	A	N7-C8-N9	-10.99	108.30	113.80
1	16S1	1188	A	C5-C6-N6	10.99	132.50	123.70
22	23S1	1616	A	C5-C6-N6	10.99	132.50	123.70
1	16S1	747	A	C5-C6-N6	10.99	132.49	123.70
22	23S1	1014	A	N7-C8-N9	-10.99	108.30	113.80
22	23S1	1784	A	N7-C8-N9	-10.99	108.31	113.80
1	16S1	320	A	C5-C6-N6	10.99	132.49	123.70
1	16S1	602	A	N7-C8-N9	-10.99	108.31	113.80
1	16S1	923	A	N3-C4-C5	-10.99	119.11	126.80
22	23S1	1247	A	C5-C6-N6	10.99	132.49	123.70
22	23S1	1384	A	C5-C6-N6	10.99	132.49	123.70
1	16S1	695	A	C5-C6-N6	10.98	132.49	123.70
22	23S1	83	A	N7-C8-N9	-10.98	108.31	113.80
22	23S1	528	A	N7-C8-N9	-10.98	108.31	113.80
22	23S1	1086	A	N7-C8-N9	-10.98	108.31	113.80
22	23S1	2740	A	N3-C4-C5	-10.98	119.11	126.80
22	23S1	988	A	N7-C8-N9	-10.98	108.31	113.80
22	23S1	996	A	N7-C8-N9	-10.98	108.31	113.80
1	16S1	431	A	N7-C8-N9	-10.98	108.31	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	532	A	C5-C6-N6	10.98	132.48	123.70
22	23S1	1655	A	C5-C6-N6	10.98	132.48	123.70
22	23S1	2352	A	N3-C4-C5	-10.98	119.11	126.80
22	23S1	1103	A	N7-C8-N9	-10.98	108.31	113.80
1	16S1	408	A	N7-C8-N9	-10.97	108.31	113.80
1	16S1	792	A	C5-C6-N6	10.97	132.48	123.70
22	23S1	300	A	C5-C6-N6	10.97	132.48	123.70
22	23S1	2435	A	N7-C8-N9	-10.97	108.31	113.80
1	16S1	909	A	N7-C8-N9	-10.97	108.31	113.80
1	16S1	1413	A	C5-C6-N6	10.97	132.48	123.70
22	23S1	368	A	C5-C6-N6	10.97	132.48	123.70
22	23S1	2241	A	C5-C6-N6	10.97	132.48	123.70
22	23S1	439	A	N7-C8-N9	-10.97	108.31	113.80
22	23S1	1165	A	N7-C8-N9	-10.97	108.31	113.80
22	23S1	2198	A	C5-C6-N6	10.97	132.48	123.70
1	16S1	59	A	N7-C8-N9	-10.97	108.32	113.80
1	16S1	1082	A	C5-C6-N6	10.97	132.47	123.70
22	23S1	2761	A	N3-C4-C5	-10.97	119.12	126.80
1	16S1	949	A	C5-C6-N6	10.96	132.47	123.70
22	23S1	2453	A	C5-C6-N6	10.97	132.47	123.70
22	23S1	2634	A	N7-C8-N9	-10.97	108.32	113.80
1	16S1	978	A	N7-C8-N9	-10.96	108.32	113.80
22	23S1	699	A	C5-C6-N6	10.96	132.47	123.70
22	23S1	1490	A	C5-C6-N6	10.96	132.47	123.70
22	23S1	1597	A	N7-C8-N9	-10.96	108.32	113.80
22	23S1	1780	A	C5-C6-N6	10.96	132.47	123.70
1	16S1	937	A	N7-C8-N9	-10.96	108.32	113.80
1	16S1	1021	A	C5-C6-N6	10.96	132.47	123.70
22	23S1	309	A	C5-C6-N6	10.96	132.47	123.70
22	23S1	751	A	C5-C6-N6	10.96	132.47	123.70
22	23S1	2433	A	C5-C6-N6	10.96	132.47	123.70
1	16S1	596	A	C5-C6-N6	10.96	132.47	123.70
1	16S1	509	A	N3-C4-C5	-10.95	119.13	126.80
22	23S1	1413	A	C5-C6-N6	10.96	132.46	123.70
22	23S1	2284	A	N3-C4-C5	-10.96	119.13	126.80
1	16S1	327	A	N7-C8-N9	-10.95	108.32	113.80
22	23S1	1637	A	C5-C6-N6	10.95	132.46	123.70
22	23S1	1246	A	N7-C8-N9	-10.95	108.33	113.80
22	23S1	522	A	N7-C8-N9	-10.95	108.33	113.80
22	23S1	1268	A	N7-C8-N9	-10.95	108.33	113.80
22	23S1	1566	A	C5-C6-N6	10.95	132.46	123.70
1	16S1	288	A	N7-C8-N9	-10.95	108.33	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1269	A	C5-C6-N6	10.95	132.46	123.70
22	23S1	73	A	N7-C8-N9	-10.95	108.33	113.80
1	16S1	919	A	C5-C6-N6	10.94	132.46	123.70
1	16S1	1437	A	N7-C8-N9	-10.95	108.33	113.80
22	23S1	423	A	C5-C6-N6	10.95	132.46	123.70
22	23S1	2386	A	N7-C8-N9	-10.95	108.33	113.80
1	16S1	50	A	C5-C6-N6	10.94	132.45	123.70
1	16S1	621	A	N3-C4-C5	-10.94	119.14	126.80
1	16S1	1169	A	C5-C6-N6	10.94	132.45	123.70
22	23S1	685	A	N7-C8-N9	-10.94	108.33	113.80
1	16S1	1493	A	C5-C6-N6	10.94	132.45	123.70
22	23S1	575	A	N7-C8-N9	-10.94	108.33	113.80
22	23S1	734	A	C5-C6-N6	10.94	132.45	123.70
22	23S1	2587	A	C5-C6-N6	10.94	132.45	123.70
22	23S1	2432	A	C5-C6-N6	10.94	132.45	123.70
1	16S1	1035	A	C5-C6-N6	10.94	132.45	123.70
1	16S1	101	A	N7-C8-N9	-10.93	108.33	113.80
1	16S1	1398	A	N7-C8-N9	-10.93	108.33	113.80
22	23S1	1387	A	N3-C4-C5	-10.93	119.15	126.80
1	16S1	831	A	C5-C6-N6	10.93	132.44	123.70
22	23S1	2147	A	C5-C6-N6	10.93	132.44	123.70
55	PTR1	14	A	C5-C6-N6	10.93	132.44	123.70
1	16S1	1289	A	N7-C8-N9	-10.93	108.34	113.80
22	23S1	2336	A	N7-C8-N9	-10.93	108.34	113.80
1	16S1	892	A	C5-C6-N6	10.93	132.44	123.70
22	23S1	127	A	N7-C8-N9	-10.93	108.34	113.80
22	23S1	1802	A	N3-C4-C5	-10.93	119.15	126.80
1	16S1	1163	A	N3-C4-C5	-10.92	119.16	126.80
22	23S1	223	A	N7-C8-N9	-10.92	108.34	113.80
22	23S1	819	A	N3-C4-C5	-10.92	119.15	126.80
1	16S1	228	A	C5-C6-N6	10.92	132.44	123.70
1	16S1	250	A	N7-C8-N9	-10.92	108.34	113.80
1	16S1	408	A	N3-C4-C5	-10.92	119.16	126.80
1	16S1	1238	A	N7-C8-N9	-10.92	108.34	113.80
22	23S1	1515	A	N7-C8-N9	-10.92	108.34	113.80
1	16S1	807	A	N7-C8-N9	-10.92	108.34	113.80
22	23S1	190	A	C5-C6-N6	10.92	132.44	123.70
22	23S1	2309	A	C5-C6-N6	10.92	132.44	123.70
22	23S1	2541	A	N7-C8-N9	-10.92	108.34	113.80
1	16S1	456	A	N7-C8-N9	-10.92	108.34	113.80
23	05S1	53	A	N7-C8-N9	-10.92	108.34	113.80
22	23S1	176	A	N7-C8-N9	-10.91	108.34	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1678	A	C5-C6-N6	10.91	132.43	123.70
22	23S1	2184	A	C5-C6-N6	10.91	132.43	123.70
22	23S1	2212	A	N7-C8-N9	-10.91	108.34	113.80
22	23S1	2288	A	C5-C6-N6	10.91	132.43	123.70
1	16S1	816	A	C5-C6-N6	10.91	132.43	123.70
22	23S1	928	A	N7-C8-N9	-10.91	108.34	113.80
22	23S1	2019	A	C5-C6-N6	10.91	132.43	123.70
1	16S1	313	A	N7-C8-N9	-10.91	108.35	113.80
22	23S1	2108	A	C5-C6-N6	10.91	132.43	123.70
1	16S1	253	A	N7-C8-N9	-10.90	108.35	113.80
22	23S1	430	A	C5-C6-N6	10.90	132.42	123.70
22	23S1	483	A	C5-C6-N6	10.90	132.42	123.70
22	23S1	941	A	N7-C8-N9	-10.90	108.35	113.80
22	23S1	2052	A	N7-C8-N9	-10.90	108.35	113.80
22	23S1	2432	A	N7-C8-N9	-10.90	108.35	113.80
55	PTR1	21	A	C5-C6-N6	10.90	132.42	123.70
1	16S1	466	A	C5-C6-N6	10.90	132.42	123.70
22	23S1	654	A	C5-C6-N6	10.90	132.42	123.70
22	23S1	1008	A	N7-C8-N9	-10.90	108.35	113.80
22	23S1	1677	A	C5-C6-N6	10.90	132.42	123.70
22	23S1	1553	A	N7-C8-N9	-10.90	108.35	113.80
1	16S1	8	A	C5-C6-N6	10.90	132.42	123.70
1	16S1	51	A	C5-C6-N6	10.90	132.42	123.70
1	16S1	676	A	C5-C6-N6	10.90	132.42	123.70
22	23S1	547	A	C5-C6-N6	10.90	132.42	123.70
22	23S1	2241	A	N7-C8-N9	-10.90	108.35	113.80
22	23S1	2814	A	C5-C6-N6	10.90	132.42	123.70
22	23S1	592	A	C5-C6-N6	10.89	132.42	123.70
22	23S1	1088	A	N7-C8-N9	-10.89	108.35	113.80
55	PTR1	73	A	C5-C6-N6	10.89	132.42	123.70
1	16S1	949	A	N3-C4-C5	-10.89	119.18	126.80
22	23S1	1952	A	C5-C6-N6	10.89	132.41	123.70
22	23S1	2497	A	C5-C6-N6	10.89	132.41	123.70
1	16S1	907	A	N7-C8-N9	-10.89	108.36	113.80
22	23S1	219	A	N7-C8-N9	-10.89	108.36	113.80
22	23S1	1701	A	N7-C8-N9	-10.89	108.36	113.80
22	23S1	1787	A	N3-C4-C5	-10.89	119.18	126.80
1	16S1	743	A	N3-C4-C5	-10.88	119.18	126.80
22	23S1	2199	A	C5-C6-N6	10.88	132.41	123.70
22	23S1	2900	A	N7-C8-N9	-10.89	108.36	113.80
1	16S1	393	A	C5-C6-N6	10.88	132.40	123.70
22	23S1	222	A	C5-C6-N6	10.88	132.41	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	689	A	N3-C4-C5	-10.88	119.18	126.80
22	23S1	1073	A	C5-C6-N6	10.88	132.41	123.70
22	23S1	819	A	N7-C8-N9	-10.88	108.36	113.80
22	23S1	927	A	N7-C8-N9	-10.88	108.36	113.80
22	23S1	1095	A	C5-C6-N6	10.88	132.40	123.70
22	23S1	1805	A	N7-C8-N9	-10.88	108.36	113.80
1	16S1	1180	A	C5-C6-N6	10.88	132.40	123.70
22	23S1	2176	A	C5-C6-N6	10.88	132.40	123.70
1	16S1	1476	A	C5-C6-N6	10.87	132.40	123.70
22	23S1	217	A	N7-C8-N9	-10.87	108.36	113.80
1	16S1	238	A	C5-C6-N6	10.87	132.40	123.70
1	16S1	298	A	C5-C6-N6	10.87	132.40	123.70
1	16S1	918	A	N7-C8-N9	-10.87	108.36	113.80
22	23S1	362	A	N3-C4-C5	-10.87	119.19	126.80
22	23S1	1241	A	N3-C4-C5	-10.87	119.19	126.80
22	23S1	2478	A	C5-C6-N6	10.87	132.40	123.70
22	23S1	12	U	N3-C2-O2	-10.87	114.59	122.20
22	23S1	793	A	N7-C8-N9	-10.87	108.37	113.80
22	23S1	1241	A	N7-C8-N9	-10.87	108.37	113.80
22	23S1	1772	A	C5-C6-N6	10.87	132.40	123.70
22	23S1	1392	A	N3-C4-C5	-10.87	119.19	126.80
22	23S1	1505	A	C5-C6-N6	10.87	132.40	123.70
22	23S1	2407	A	N3-C4-C5	-10.87	119.19	126.80
1	16S1	1431	A	C5-C6-N6	10.87	132.39	123.70
22	23S1	91	A	C5-C6-N6	10.87	132.39	123.70
1	16S1	32	A	N3-C4-C5	-10.86	119.20	126.80
1	16S1	50	A	N7-C8-N9	-10.86	108.37	113.80
1	16S1	878	A	N7-C8-N9	-10.86	108.37	113.80
22	23S1	2062	A	C5-C6-N6	10.86	132.39	123.70
1	16S1	1429	A	N7-C8-N9	-10.86	108.37	113.80
1	16S1	1146	A	C5-C6-N6	10.86	132.39	123.70
22	23S1	2430	A	C2-N3-C4	10.86	116.03	110.60
1	16S1	520	A	N7-C8-N9	-10.86	108.37	113.80
22	23S1	1246	A	N3-C4-C5	-10.86	119.20	126.80
1	16S1	448	A	N7-C8-N9	-10.85	108.37	113.80
1	16S1	1036	A	N3-C4-C5	-10.85	119.20	126.80
22	23S1	181	A	C5-C6-N6	10.85	132.38	123.70
22	23S1	1801	A	C5-C6-N6	10.85	132.38	123.70
1	16S1	478	A	C5-C6-N6	10.85	132.38	123.70
22	23S1	572	A	C5-C6-N6	10.85	132.38	123.70
22	23S1	2080	A	N7-C8-N9	-10.85	108.38	113.80
1	16S1	573	A	N3-C4-C5	-10.85	119.21	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	19	A	C5-C6-N6	10.85	132.38	123.70
22	23S1	44	A	C5-C6-N6	10.85	132.38	123.70
1	16S1	602	A	N3-C4-C5	-10.85	119.21	126.80
22	23S1	2033	A	N7-C8-N9	-10.85	108.38	113.80
22	23S1	2721	A	N7-C8-N9	-10.85	108.38	113.80
22	23S1	2114	A	C5-C6-N6	10.84	132.38	123.70
1	16S1	306	A	N7-C8-N9	-10.84	108.38	113.80
1	16S1	1456	A	C5-C6-N6	10.84	132.37	123.70
1	16S1	353	A	C5-C6-N6	10.84	132.37	123.70
22	23S1	508	A	C5-C6-N6	10.84	132.37	123.70
22	23S1	1143	A	N7-C8-N9	-10.84	108.38	113.80
1	16S1	1492	A	C5-C6-N6	10.83	132.37	123.70
22	23S1	2820	A	C5-C6-N6	10.83	132.37	123.70
22	23S1	899	A	C5-C6-N6	10.83	132.37	123.70
1	16S1	1360	A	N3-C4-C5	-10.83	119.22	126.80
22	23S1	190	A	N3-C4-C5	-10.83	119.22	126.80
22	23S1	1383	A	N7-C8-N9	-10.83	108.39	113.80
22	23S1	1977	A	N7-C8-N9	-10.83	108.39	113.80
22	23S1	2327	A	N3-C4-C5	-10.83	119.22	126.80
22	23S1	2433	A	N3-C4-C5	-10.83	119.22	126.80
1	16S1	539	A	N7-C8-N9	-10.83	108.39	113.80
1	16S1	579	A	N7-C8-N9	-10.83	108.39	113.80
1	16S1	415	A	N7-C8-N9	-10.82	108.39	113.80
22	23S1	149	A	C5-C6-N6	10.82	132.36	123.70
22	23S1	538	A	C5-C6-N6	10.82	132.36	123.70
22	23S1	2163	A	C5-C6-N6	10.82	132.36	123.70
22	23S1	2333	A	C5-C6-N6	10.82	132.36	123.70
1	16S1	1157	A	N3-C4-C5	-10.82	119.23	126.80
22	23S1	1001	A	N7-C8-N9	-10.82	108.39	113.80
22	23S1	1586	A	C5-C6-N6	10.82	132.35	123.70
1	16S1	1229	A	N7-C8-N9	-10.81	108.39	113.80
22	23S1	2809	A	N3-C4-C5	-10.81	119.23	126.80
1	16S1	1446	A	N3-C4-C5	-10.81	119.23	126.80
22	23S1	706	A	C5-C6-N6	10.81	132.35	123.70
22	23S1	2378	A	C5-C6-N6	10.81	132.35	123.70
22	23S1	216	A	N7-C8-N9	-10.81	108.39	113.80
1	16S1	309	A	C5-C6-N6	10.81	132.35	123.70
1	16S1	1507	A	N7-C8-N9	-10.81	108.40	113.80
22	23S1	2071	A	C5-C6-N6	10.80	132.34	123.70
1	16S1	162	A	C4-C5-C6	10.80	122.40	117.00
22	23S1	637	A	C5-C6-N6	10.80	132.34	123.70
22	23S1	1046	A	C5-C6-N6	10.80	132.34	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	53	A	N3-C4-C5	-10.80	119.24	126.80
22	23S1	829	A	C5-C6-N6	10.80	132.34	123.70
22	23S1	1403	A	N3-C4-C5	-10.80	119.24	126.80
22	23S1	2705	A	C5-C6-N6	10.80	132.34	123.70
1	16S1	1082	A	N7-C8-N9	-10.79	108.40	113.80
22	23S1	362	A	N7-C8-N9	-10.79	108.40	113.80
22	23S1	802	A	N7-C8-N9	-10.79	108.40	113.80
22	23S1	1403	A	N7-C8-N9	-10.79	108.40	113.80
22	23S1	1664	A	N3-C4-C5	-10.79	119.24	126.80
22	23S1	528	A	C5-C6-N6	10.79	132.33	123.70
1	16S1	996	A	C5-C6-N6	10.79	132.33	123.70
22	23S1	1552	A	N7-C8-N9	-10.79	108.41	113.80
1	16S1	129	A	N7-C8-N9	-10.79	108.41	113.80
1	16S1	607	A	N7-C8-N9	-10.79	108.41	113.80
1	16S1	728	A	N3-C4-C5	-10.79	119.25	126.80
1	16S1	814	A	C5-C6-N6	10.79	132.33	123.70
1	16S1	938	A	N7-C8-N9	-10.79	108.41	113.80
22	23S1	753	A	N3-C4-C5	-10.79	119.25	126.80
22	23S1	1885	A	C5-C6-N6	10.79	132.33	123.70
22	23S1	330	A	N7-C8-N9	-10.79	108.41	113.80
22	23S1	2530	A	N7-C8-N9	-10.79	108.41	113.80
55	PTR1	26	A	C5-C6-N6	10.79	132.33	123.70
22	23S1	197	A	N7-C8-N9	-10.78	108.41	113.80
22	23S1	614	A	N7-C8-N9	-10.78	108.41	113.80
1	16S1	306	A	C5-C6-N6	10.78	132.33	123.70
22	23S1	415	A	N7-C8-N9	-10.78	108.41	113.80
22	23S1	1353	A	N3-C4-C5	-10.78	119.25	126.80
22	23S1	2476	A	N7-C8-N9	-10.78	108.41	113.80
22	23S1	2497	A	N3-C4-C5	-10.78	119.25	126.80
22	23S1	2531	A	N7-C8-N9	-10.78	108.41	113.80
55	PTR1	76	A	C5-C6-N6	10.78	132.32	123.70
1	16S1	1340	A	C5-C6-N6	10.78	132.32	123.70
22	23S1	125	A	C5-C6-N6	10.78	132.32	123.70
1	16S1	1433	A	N7-C8-N9	-10.78	108.41	113.80
22	23S1	299	A	N3-C4-C5	-10.78	119.25	126.80
22	23S1	2082	A	N3-C4-C5	-10.78	119.25	126.80
22	23S1	2750	A	C5-C6-N6	10.78	132.32	123.70
1	16S1	1169	A	N7-C8-N9	-10.78	108.41	113.80
1	16S1	1468	A	N3-C4-C5	-10.78	119.26	126.80
22	23S1	294	A	C5-C6-N6	10.78	132.32	123.70
22	23S1	685	A	C5-C6-N6	10.78	132.32	123.70
22	23S1	1759	A	N3-C4-C5	-10.78	119.26	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1876	A	C5-C6-N6	10.78	132.32	123.70
23	05S1	94	A	N7-C8-N9	-10.78	108.41	113.80
1	16S1	81	A	N3-C4-C5	-10.77	119.26	126.80
1	16S1	573	A	N7-C8-N9	-10.77	108.41	113.80
1	16S1	1333	A	N7-C8-N9	-10.77	108.41	113.80
22	23S1	910	A	N7-C8-N9	-10.77	108.42	113.80
22	23S1	2015	A	N7-C8-N9	-10.77	108.42	113.80
1	16S1	642	A	C5-C6-N6	10.77	132.31	123.70
1	16S1	994	A	N7-C8-N9	-10.77	108.42	113.80
1	16S1	65	A	C5-C6-N6	10.77	132.31	123.70
1	16S1	1349	A	C5-C6-N6	10.77	132.31	123.70
22	23S1	71	A	N3-C4-C5	-10.77	119.26	126.80
22	23S1	1610	A	C5-C6-N6	10.77	132.31	123.70
1	16S1	640	A	N3-C4-C5	-10.77	119.27	126.80
22	23S1	44	A	N7-C8-N9	-10.77	108.42	113.80
22	23S1	820	A	N3-C4-C5	-10.77	119.27	126.80
1	16S1	642	A	N7-C8-N9	-10.76	108.42	113.80
22	23S1	722	A	N7-C8-N9	-10.76	108.42	113.80
22	23S1	470	A	N3-C4-C5	-10.76	119.27	126.80
22	23S1	1373	A	N7-C8-N9	-10.76	108.42	113.80
22	23S1	2741	A	N7-C8-N9	-10.76	108.42	113.80
1	16S1	279	A	C5-C6-N6	10.76	132.31	123.70
22	23S1	345	A	N7-C8-N9	-10.76	108.42	113.80
22	23S1	2051	A	N3-C4-C5	-10.76	119.27	126.80
22	23S1	244	A	N7-C8-N9	-10.75	108.42	113.80
22	23S1	2589	A	C5-C6-N6	10.75	132.30	123.70
1	16S1	270	A	N3-C4-C5	-10.75	119.27	126.80
1	16S1	535	A	C5-C6-N6	10.75	132.30	123.70
22	23S1	644	A	C5-N7-C8	10.75	109.28	103.90
1	16S1	1374	A	N7-C8-N9	-10.75	108.43	113.80
22	23S1	1269	A	N3-C4-C5	-10.75	119.28	126.80
22	23S1	2725	A	N7-C8-N9	-10.75	108.43	113.80
22	23S1	528	A	N3-C4-C5	-10.74	119.28	126.80
22	23S1	1433	A	N7-C8-N9	-10.74	108.43	113.80
22	23S1	2635	A	C5-C6-N6	10.74	132.30	123.70
1	16S1	1513	A	C5-C6-N6	10.74	132.29	123.70
1	16S1	493	A	C5-C6-N6	10.74	132.29	123.70
1	16S1	746	A	N7-C8-N9	-10.74	108.43	113.80
22	23S1	2411	A	C5-C6-N6	10.74	132.29	123.70
22	23S1	2635	A	N7-C8-N9	-10.74	108.43	113.80
22	23S1	2088	A	N3-C4-C5	-10.74	119.28	126.80
22	23S1	2587	A	N7-C8-N9	-10.74	108.43	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	665	A	N7-C8-N9	-10.74	108.43	113.80
22	23S1	1254	A	C5-C6-N6	10.74	132.29	123.70
22	23S1	2058	A	C5-C6-N6	10.74	132.29	123.70
1	16S1	223	A	N3-C4-C5	-10.73	119.29	126.80
22	23S1	1264	A	C5-C6-N6	10.73	132.29	123.70
22	23S1	2298	A	C5-C6-N6	10.73	132.29	123.70
22	23S1	2412	A	C5-C6-N6	10.73	132.29	123.70
23	05S1	39	A	C5-C6-N6	10.73	132.29	123.70
1	16S1	382	A	C5-C6-N6	10.73	132.28	123.70
22	23S1	182	A	N7-C8-N9	-10.73	108.43	113.80
1	16S1	2	A	C5-C6-N6	10.73	132.28	123.70
22	23S1	1126	A	C5-C6-N6	10.73	132.28	123.70
1	16S1	174	A	N7-C8-N9	-10.73	108.44	113.80
22	23S1	221	A	C5-C6-N6	10.73	132.28	123.70
22	23S1	756	A	N3-C4-C5	-10.73	119.29	126.80
22	23S1	1608	A	N3-C4-C5	-10.73	119.29	126.80
22	23S1	1866	A	N3-C4-C5	-10.73	119.29	126.80
22	23S1	2727	A	N7-C8-N9	-10.73	108.44	113.80
22	23S1	2009	A	C5-C6-N6	10.72	132.28	123.70
22	23S1	2534	A	C5-C6-N6	10.72	132.28	123.70
22	23S1	1596	A	C5-C6-N6	10.72	132.28	123.70
22	23S1	1780	A	N7-C8-N9	-10.72	108.44	113.80
1	16S1	482	A	C5-C6-N6	10.72	132.28	123.70
1	16S1	510	A	C5-C6-N6	10.72	132.28	123.70
22	23S1	74	A	N3-C4-C5	-10.72	119.30	126.80
22	23S1	1142	A	N3-C4-C5	-10.72	119.30	126.80
22	23S1	1809	A	C5-C6-N6	10.72	132.28	123.70
22	23S1	1952	A	N3-C4-C5	-10.72	119.30	126.80
22	23S1	2126	A	N7-C8-N9	-10.72	108.44	113.80
1	16S1	695	A	N7-C8-N9	-10.72	108.44	113.80
1	16S1	1499	A	N3-C4-C5	-10.72	119.30	126.80
22	23S1	94	A	N3-C4-C5	-10.72	119.30	126.80
22	23S1	1272	A	C5-C6-N6	10.72	132.28	123.70
22	23S1	1321	A	N3-C4-C5	-10.72	119.30	126.80
22	23S1	1810	A	N1-C6-N6	-10.72	112.17	118.60
1	16S1	608	A	N7-C8-N9	-10.71	108.44	113.80
22	23S1	1722	A	N3-C4-C5	-10.72	119.30	126.80
22	23S1	2749	A	N7-C8-N9	-10.72	108.44	113.80
22	23S1	101	A	N7-C8-N9	-10.71	108.44	113.80
1	16S1	959	A	C5-C6-N6	10.71	132.27	123.70
1	16S1	1111	A	N7-C8-N9	-10.71	108.44	113.80
1	16S1	1446	A	C5-C6-N6	10.71	132.27	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	382	A	N3-C4-C5	-10.71	119.30	126.80
22	23S1	632	A	C5-C6-N6	10.71	132.27	123.70
22	23S1	1590	A	N7-C8-N9	-10.71	108.44	113.80
1	16S1	19	A	C5-C6-N6	10.71	132.27	123.70
22	23S1	2317	A	C5-C6-N6	10.71	132.27	123.70
22	23S1	1583	A	C5-C6-N6	10.71	132.26	123.70
22	23S1	1641	A	C5-C6-N6	10.71	132.27	123.70
22	23S1	1762	A	N7-C8-N9	-10.71	108.45	113.80
22	23S1	1603	A	N7-C8-N9	-10.71	108.45	113.80
22	23S1	1791	A	C5-C6-N6	10.71	132.26	123.70
1	16S1	573	A	C5-C6-N6	10.70	132.26	123.70
1	16S1	78	A	N3-C4-C5	-10.70	119.31	126.80
22	23S1	401	A	N7-C8-N9	-10.70	108.45	113.80
22	23S1	782	A	N7-C8-N9	-10.70	108.45	113.80
1	16S1	430	A	N7-C8-N9	-10.70	108.45	113.80
1	16S1	1531	A	C5-C6-N6	10.70	132.26	123.70
1	16S1	1534	A	N7-C8-N9	-10.70	108.45	113.80
22	23S1	56	A	N7-C8-N9	-10.70	108.45	113.80
22	23S1	1021	A	C5-C6-N6	10.70	132.26	123.70
22	23S1	2346	A	N7-C8-N9	-10.70	108.45	113.80
1	16S1	523	A	N7-C8-N9	-10.70	108.45	113.80
22	23S1	2369	A	N3-C4-C5	-10.70	119.31	126.80
22	23S1	219	A	C5-C6-N6	10.70	132.26	123.70
22	23S1	575	A	C5-C6-N6	10.69	132.25	123.70
22	23S1	2530	A	C5-C6-N6	10.70	132.26	123.70
22	23S1	2560	A	C5-C6-N6	10.69	132.25	123.70
23	05S1	66	A	N7-C8-N9	-10.70	108.45	113.80
1	16S1	767	A	C5-C6-N6	10.69	132.25	123.70
1	16S1	790	A	N7-C8-N9	-10.69	108.45	113.80
22	23S1	1701	A	C5-C6-N6	10.69	132.25	123.70
1	16S1	228	A	N7-C8-N9	-10.69	108.45	113.80
1	16S1	1374	A	C5-C6-N6	10.69	132.25	123.70
22	23S1	173	A	N7-C8-N9	-10.69	108.45	113.80
22	23S1	53	A	C5-C6-N6	10.69	132.25	123.70
22	23S1	478	A	C5-C6-N6	10.69	132.25	123.70
22	23S1	514	A	C5-C6-N6	10.69	132.25	123.70
1	16S1	766	A	N7-C8-N9	-10.69	108.46	113.80
1	16S1	964	A	C5-C6-N6	10.69	132.25	123.70
22	23S1	2169	A	N3-C4-C5	-10.69	119.32	126.80
22	23S1	2281	A	N3-C4-C5	-10.69	119.32	126.80
1	16S1	1362	A	N7-C8-N9	-10.68	108.46	113.80
22	23S1	330	A	N3-C4-C5	-10.68	119.32	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	556	A	C5-C6-N6	10.68	132.25	123.70
22	23S1	1927	A	N7-C8-N9	-10.68	108.46	113.80
22	23S1	1028	A	N7-C8-N9	-10.68	108.46	113.80
1	16S1	706	A	N3-C4-C5	-10.68	119.32	126.80
22	23S1	223	A	C5-C6-N6	10.68	132.25	123.70
22	23S1	449	A	N7-C8-N9	-10.68	108.46	113.80
22	23S1	541	A	C5-C6-N6	10.68	132.25	123.70
22	23S1	789	A	C5-C6-N6	10.68	132.25	123.70
1	16S1	382	A	N3-C4-C5	-10.68	119.33	126.80
1	16S1	1476	A	N7-C8-N9	-10.68	108.46	113.80
22	23S1	631	A	N7-C8-N9	-10.68	108.46	113.80
22	23S1	2406	A	C5-C6-N6	10.68	132.24	123.70
22	23S1	1744	A	C5-C6-N6	10.68	132.24	123.70
1	16S1	498	A	N7-C8-N9	-10.68	108.46	113.80
22	23S1	2266	A	N7-C8-N9	-10.68	108.46	113.80
1	16S1	655	A	N7-C8-N9	-10.68	108.46	113.80
1	16S1	1434	A	C5-C6-N6	10.68	132.24	123.70
22	23S1	1637	A	N7-C8-N9	-10.68	108.46	113.80
22	23S1	1469	A	N3-C4-C5	-10.67	119.33	126.80
22	23S1	1794	A	C5-C6-N6	10.67	132.24	123.70
1	16S1	583	A	N7-C8-N9	-10.67	108.47	113.80
22	23S1	1877	A	N7-C8-N9	-10.67	108.46	113.80
22	23S1	126	A	N7-C8-N9	-10.67	108.47	113.80
22	23S1	899	A	N3-C4-C5	-10.67	119.33	126.80
22	23S1	2860	A	N7-C8-N9	-10.67	108.47	113.80
22	23S1	1610	A	N7-C8-N9	-10.67	108.47	113.80
22	23S1	2191	A	N3-C4-C5	-10.66	119.33	126.80
22	23S1	2837	A	C5-C6-N6	10.66	132.23	123.70
22	23S1	244	A	C5-C6-N6	10.66	132.23	123.70
22	23S1	825	A	N3-C4-C5	-10.66	119.34	126.80
22	23S1	262	A	C5-C6-N6	10.66	132.23	123.70
22	23S1	2736	A	C5-C6-N6	10.66	132.23	123.70
22	23S1	344	A	C5-C6-N6	10.66	132.23	123.70
1	16S1	460	A	N3-C4-C5	-10.66	119.34	126.80
22	23S1	730	A	N3-C4-C5	-10.65	119.34	126.80
22	23S1	2287	A	C5-C6-N6	10.65	132.22	123.70
22	23S1	590	A	C5-C6-N6	10.65	132.22	123.70
22	23S1	1387	A	N7-C8-N9	-10.65	108.47	113.80
22	23S1	1571	A	N3-C4-C5	-10.65	119.34	126.80
22	23S1	1077	A	N7-C8-N9	-10.65	108.47	113.80
23	05S1	52	A	C5-C6-N6	10.65	132.22	123.70
22	23S1	1689	A	C5-C6-N6	10.65	132.22	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	PTR1	23	A	N3-C4-C5	-10.65	119.35	126.80
22	23S1	2170	A	C5-C6-N6	10.65	132.22	123.70
22	23S1	231	A	C5-C6-N6	10.64	132.22	123.70
22	23S1	1009	A	N3-C4-C5	-10.64	119.35	126.80
22	23S1	2513	A	N3-C4-C5	-10.64	119.35	126.80
22	23S1	1155	A	N7-C8-N9	-10.64	108.48	113.80
1	16S1	190	A	N1-C6-N6	-10.64	112.22	118.60
22	23S1	2058	A	N7-C8-N9	-10.64	108.48	113.80
22	23S1	2753	A	N7-C8-N9	-10.64	108.48	113.80
22	23S1	2173	A	C5-C6-N6	10.64	132.21	123.70
1	16S1	1196	A	C5-C6-N6	10.64	132.21	123.70
22	23S1	1086	A	C5-C6-N6	10.64	132.21	123.70
22	23S1	2706	A	N3-C4-C5	-10.64	119.35	126.80
22	23S1	2733	A	C5-C6-N6	10.64	132.21	123.70
1	16S1	236	A	N7-C8-N9	-10.63	108.48	113.80
1	16S1	860	A	N3-C4-C5	-10.63	119.36	126.80
1	16S1	1036	A	C5-C6-N6	10.63	132.21	123.70
22	23S1	1977	A	C5-C6-N6	10.63	132.21	123.70
1	16S1	510	A	N7-C8-N9	-10.63	108.48	113.80
22	23S1	936	A	N3-C4-C5	-10.63	119.36	126.80
1	16S1	595	A	C5-C6-N6	10.63	132.20	123.70
22	23S1	149	A	N7-C8-N9	-10.63	108.48	113.80
22	23S1	1496	A	N7-C8-N9	-10.63	108.48	113.80
1	16S1	937	A	C5-C6-N6	10.63	132.20	123.70
22	23S1	1028	A	N3-C4-C5	-10.63	119.36	126.80
22	23S1	1847	A	N3-C4-C5	-10.63	119.36	126.80
22	23S1	255	A	N7-C8-N9	-10.62	108.49	113.80
22	23S1	1632	A	N7-C8-N9	-10.62	108.49	113.80
1	16S1	1080	A	C5-C6-N6	10.62	132.20	123.70
1	16S1	1374	A	N3-C4-C5	-10.62	119.36	126.80
22	23S1	1664	A	N7-C8-N9	-10.62	108.49	113.80
22	23S1	348	A	C5-C6-N6	10.62	132.20	123.70
22	23S1	391	A	C5-C6-N6	10.62	132.20	123.70
23	05S1	119	A	N3-C4-C5	-10.62	119.36	126.80
22	23S1	644	A	C5-C6-N6	10.62	132.20	123.70
22	23S1	1420	A	C5-C6-N6	10.62	132.20	123.70
22	23S1	1535	A	N7-C8-N9	-10.62	108.49	113.80
22	23S1	1998	A	N7-C8-N9	-10.62	108.49	113.80
22	23S1	191	A	N3-C4-C5	-10.62	119.37	126.80
1	16S1	10	A	C5-C6-N6	10.62	132.19	123.70
1	16S1	487	A	N3-C4-C5	-10.62	119.37	126.80
22	23S1	742	A	N3-C4-C5	-10.62	119.37	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2665	A	C5-C6-N6	10.62	132.19	123.70
1	16S1	1502	A	N7-C8-N9	-10.62	108.49	113.80
22	23S1	95	A	C5-C6-N6	10.62	132.19	123.70
1	16S1	174	A	N3-C4-C5	-10.62	119.37	126.80
22	23S1	1027	A	N7-C8-N9	-10.62	108.49	113.80
22	23S1	1126	A	N3-C4-C5	-10.62	119.37	126.80
1	16S1	687	A	N7-C8-N9	-10.61	108.49	113.80
22	23S1	1548	A	N3-C4-C5	-10.61	119.37	126.80
22	23S1	2757	A	N3-C4-C5	-10.61	119.37	126.80
22	23S1	1762	A	C5-C6-N6	10.61	132.19	123.70
22	23S1	1803	A	C5-C6-N6	10.61	132.19	123.70
22	23S1	2346	A	C5-C6-N6	10.61	132.19	123.70
55	PTR1	23	A	N7-C8-N9	-10.61	108.49	113.80
1	16S1	907	A	N3-C4-C5	-10.61	119.37	126.80
22	23S1	2287	A	N7-C8-N9	-10.61	108.50	113.80
22	23S1	2639	A	N7-C8-N9	-10.61	108.50	113.80
1	16S1	496	A	C5-C6-N6	10.61	132.18	123.70
22	23S1	1008	A	C5-C6-N6	10.61	132.18	123.70
22	23S1	2809	A	C5-C6-N6	10.61	132.18	123.70
1	16S1	1441	A	C5-C6-N6	10.60	132.18	123.70
22	23S1	2358	A	N7-C8-N9	-10.60	108.50	113.80
23	05S1	58	A	C5-C6-N6	10.60	132.18	123.70
1	16S1	938	A	N3-C4-C5	-10.60	119.38	126.80
22	23S1	899	A	N7-C8-N9	-10.60	108.50	113.80
1	16S1	270	A	N7-C8-N9	-10.60	108.50	113.80
22	23S1	1175	A	N7-C8-N9	-10.60	108.50	113.80
22	23S1	2080	A	C5-C6-N6	10.60	132.18	123.70
22	23S1	2267	A	N7-C8-N9	-10.60	108.50	113.80
22	23S1	2727	A	N3-C4-C5	-10.60	119.38	126.80
23	05S1	104	A	C5-C6-N6	10.60	132.18	123.70
1	16S1	1191	A	C5-C6-N6	10.60	132.18	123.70
22	23S1	5	A	C5-C6-N6	10.60	132.18	123.70
22	23S1	1069	A	C5-C6-N6	10.60	132.18	123.70
22	23S1	1927	A	N3-C4-C5	-10.60	119.38	126.80
1	16S1	448	A	N3-C4-C5	-10.59	119.38	126.80
1	16S1	1152	A	N3-C4-C5	-10.59	119.38	126.80
22	23S1	2097	A	N7-C8-N9	-10.59	108.50	113.80
1	16S1	663	A	N3-C4-C5	-10.59	119.39	126.80
1	16S1	964	A	N7-C8-N9	-10.59	108.50	113.80
22	23S1	155	A	C5-C6-N6	10.59	132.17	123.70
22	23S1	460	A	C5-C6-N6	10.59	132.17	123.70
22	23S1	1175	A	C5-C6-N6	10.59	132.17	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	480	A	C5-C6-N6	10.59	132.17	123.70
1	16S1	1197	A	N3-C4-C5	-10.59	119.39	126.80
1	16S1	1502	A	C5-C6-N6	10.59	132.17	123.70
22	23S1	342	A	C5-C6-N6	10.59	132.17	123.70
22	23S1	849	A	C5-C6-N6	10.59	132.17	123.70
22	23S1	1918	A	N3-C4-C5	-10.59	119.39	126.80
22	23S1	1189	A	N3-C4-C5	-10.59	119.39	126.80
22	23S1	2482	A	C5-C6-N6	10.59	132.17	123.70
1	16S1	263	A	C5-C6-N6	10.58	132.17	123.70
1	16S1	414	A	N3-C4-C5	-10.58	119.39	126.80
22	23S1	2748	A	N7-C8-N9	-10.58	108.51	113.80
23	05S1	59	A	N7-C8-N9	-10.58	108.51	113.80
1	16S1	712	A	N3-C4-C5	-10.58	119.39	126.80
22	23S1	1698	A	N7-C8-N9	-10.58	108.51	113.80
1	16S1	621	A	N7-C8-N9	-10.58	108.51	113.80
22	23S1	255	A	N3-C4-C5	-10.58	119.39	126.80
22	23S1	677	A	N7-C8-N9	-10.58	108.51	113.80
22	23S1	909	A	N3-C4-C5	-10.58	119.39	126.80
1	16S1	155	A	N3-C4-C5	-10.58	119.39	126.80
22	23S1	430	A	N3-C4-C5	-10.58	119.40	126.80
22	23S1	990	A	N7-C8-N9	-10.58	108.51	113.80
22	23S1	1586	A	N3-C4-C5	-10.58	119.40	126.80
1	16S1	32	A	N7-C8-N9	-10.58	108.51	113.80
1	16S1	819	A	N3-C4-C5	-10.58	119.40	126.80
22	23S1	2077	A	N7-C8-N9	-10.58	108.51	113.80
22	23S1	2097	A	C5-C6-N6	10.58	132.16	123.70
22	23S1	1641	A	N7-C8-N9	-10.57	108.51	113.80
1	16S1	579	A	C5-C6-N6	10.57	132.16	123.70
1	16S1	975	A	N7-C8-N9	-10.57	108.51	113.80
1	16S1	1269	A	N7-C8-N9	-10.57	108.51	113.80
22	23S1	142	A	N7-C8-N9	-10.57	108.51	113.80
22	23S1	1496	A	C5-C6-N6	10.57	132.16	123.70
22	23S1	2013	A	N3-C4-C5	-10.57	119.40	126.80
22	23S1	2135	A	N7-C8-N9	-10.57	108.52	113.80
22	23S1	633	A	N7-C8-N9	-10.57	108.52	113.80
1	16S1	338	A	C5-C6-N6	10.57	132.15	123.70
22	23S1	602	A	C5-C6-N6	10.57	132.15	123.70
22	23S1	668	A	C5-C6-N6	10.57	132.15	123.70
22	23S1	1029	A	N3-C4-C5	-10.57	119.40	126.80
22	23S1	2062	A	N7-C8-N9	-10.57	108.52	113.80
22	23S1	2602	A	C5-C6-N6	10.57	132.15	123.70
22	23S1	1580	A	C5-C6-N6	10.56	132.15	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1650	A	N7-C8-N9	-10.56	108.52	113.80
22	23S1	1960	A	C5-C6-N6	10.56	132.15	123.70
22	23S1	2037	A	N3-C4-C5	-10.56	119.41	126.80
1	16S1	712	A	N7-C8-N9	-10.56	108.52	113.80
1	16S1	1012	A	N3-C4-C5	-10.56	119.41	126.80
1	16S1	1257	A	C5-C6-N6	10.56	132.15	123.70
22	23S1	2868	A	N3-C4-C5	-10.56	119.41	126.80
22	23S1	1784	A	C5-C6-N6	10.56	132.15	123.70
1	16S1	382	A	N7-C8-N9	-10.56	108.52	113.80
1	16S1	460	A	N7-C8-N9	-10.56	108.52	113.80
1	16S1	1229	A	C5-C6-N6	10.55	132.14	123.70
22	23S1	466	A	C5-C6-N6	10.56	132.15	123.70
22	23S1	910	A	N3-C4-C5	-10.56	119.41	126.80
22	23S1	2335	A	N3-C4-C5	-10.55	119.41	126.80
22	23S1	2829	A	C5-C6-N6	10.56	132.15	123.70
22	23S1	1866	A	N7-C8-N9	-10.55	108.52	113.80
22	23S1	1276	A	N3-C4-C5	-10.55	119.41	126.80
1	16S1	71	A	C5-C6-N6	10.55	132.14	123.70
1	16S1	609	A	C5-C6-N6	10.55	132.14	123.70
22	23S1	739	A	C5-C6-N6	10.55	132.14	123.70
1	16S1	878	A	C5-C6-N6	10.55	132.14	123.70
22	23S1	1328	A	N7-C8-N9	-10.55	108.53	113.80
22	23S1	1553	A	N3-C4-C5	-10.55	119.42	126.80
22	23S1	2887	A	N7-C8-N9	-10.55	108.53	113.80
1	16S1	1350	A	C5-C6-N6	10.54	132.14	123.70
22	23S1	299	A	N7-C8-N9	-10.55	108.53	113.80
22	23S1	1365	A	N7-C8-N9	-10.54	108.53	113.80
22	23S1	1689	A	N7-C8-N9	-10.55	108.53	113.80
1	16S1	814	A	N3-C4-C5	-10.54	119.42	126.80
22	23S1	1088	A	C5-C6-N6	10.54	132.13	123.70
22	23S1	1759	A	C5-C6-N6	10.54	132.13	123.70
23	05S1	29	A	N3-C4-C5	-10.54	119.42	126.80
1	16S1	246	A	C5-C6-N6	10.54	132.13	123.70
1	16S1	72	A	N7-C8-N9	-10.54	108.53	113.80
1	16S1	681	A	N3-C4-C5	-10.54	119.42	126.80
1	16S1	872	A	C5-C6-N6	10.54	132.13	123.70
22	23S1	95	A	N7-C8-N9	-10.54	108.53	113.80
55	PTR1	38	A	N7-C8-N9	-10.54	108.53	113.80
1	16S1	545	C	C6-N1-C2	-10.54	116.09	120.30
22	23S1	49	A	N3-C4-C5	-10.54	119.42	126.80
1	16S1	205	A	C5-C6-N6	10.53	132.13	123.70
1	16S1	553	A	C5-C6-N6	10.54	132.13	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	629	A	N7-C8-N9	-10.54	108.53	113.80
22	23S1	522	A	N3-C4-C5	-10.54	119.42	126.80
22	23S1	1307	A	C5-C6-N6	10.54	132.13	123.70
22	23S1	2205	A	C5-C6-N6	10.54	132.13	123.70
22	23S1	270	A	C5-C6-N6	10.53	132.13	123.70
22	23S1	1953	A	N7-C8-N9	-10.54	108.53	113.80
22	23S1	2077	A	N3-C4-C5	-10.54	119.42	126.80
22	23S1	2268	A	C5-C6-N6	10.53	132.13	123.70
22	23S1	480	A	N3-C4-C5	-10.53	119.43	126.80
1	16S1	435	A	C5-C6-N6	10.53	132.12	123.70
1	16S1	681	A	C5-C6-N6	10.53	132.12	123.70
1	16S1	1394	A	C5-C6-N6	10.53	132.12	123.70
22	23S1	1552	A	C5-C6-N6	10.53	132.12	123.70
22	23S1	1871	A	N3-C4-C5	-10.53	119.43	126.80
22	23S1	2598	A	N7-C8-N9	-10.53	108.53	113.80
22	23S1	2778	A	C5-C6-N6	10.53	132.12	123.70
1	16S1	523	A	C5-C6-N6	10.53	132.12	123.70
22	23S1	866	A	C5-C6-N6	10.53	132.12	123.70
22	23S1	2823	A	N7-C8-N9	-10.53	108.54	113.80
1	16S1	706	A	N7-C8-N9	-10.53	108.54	113.80
1	16S1	1274	A	N7-C8-N9	-10.53	108.54	113.80
22	23S1	1549	A	N3-C4-C5	-10.53	119.43	126.80
22	23S1	2171	A	N7-C8-N9	-10.53	108.54	113.80
22	23S1	2183	A	C5-C6-N6	10.53	132.12	123.70
1	16S1	282	A	N7-C8-N9	-10.52	108.54	113.80
23	05S1	53	A	C5-C6-N6	10.52	132.12	123.70
22	23S1	1384	A	N7-C8-N9	-10.52	108.54	113.80
1	16S1	430	A	N3-C4-C5	-10.52	119.44	126.80
22	23S1	1654	A	N7-C8-N9	-10.52	108.54	113.80
1	16S1	116	A	N7-C8-N9	-10.52	108.54	113.80
22	23S1	743	A	N3-C4-C5	-10.52	119.44	126.80
1	16S1	655	A	N3-C4-C5	-10.52	119.44	126.80
1	16S1	780	A	C5-C6-N6	10.52	132.11	123.70
1	16S1	1110	A	C5-C6-N6	10.52	132.11	123.70
22	23S1	782	A	N3-C4-C5	-10.52	119.44	126.80
1	16S1	1102	A	N7-C8-N9	-10.51	108.54	113.80
22	23S1	1503	A	N3-C4-C5	-10.51	119.44	126.80
22	23S1	182	A	N3-C4-C5	-10.51	119.44	126.80
22	23S1	345	A	N3-C4-C5	-10.51	119.44	126.80
55	PTR1	14	A	C5-N7-C8	10.51	109.15	103.90
1	16S1	539	A	N3-C4-C5	-10.51	119.44	126.80
22	23S1	320	A	C5-N7-C8	10.51	109.15	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1333	A	N3-C4-C5	-10.51	119.45	126.80
22	23S1	384	A	N7-C8-N9	-10.51	108.55	113.80
22	23S1	2799	A	N7-C8-N9	-10.51	108.55	113.80
1	16S1	101	A	N3-C4-C5	-10.50	119.45	126.80
1	16S1	790	A	N3-C4-C5	-10.50	119.45	126.80
1	16S1	1318	A	C5-C6-N6	10.50	132.10	123.70
22	23S1	44	A	N3-C4-C5	-10.50	119.45	126.80
22	23S1	1365	A	N3-C4-C5	-10.50	119.45	126.80
1	16S1	648	A	C5-C6-N6	10.50	132.10	123.70
1	16S1	1254	A	C5-C6-N6	10.50	132.10	123.70
22	23S1	6	A	C5-C6-N6	10.50	132.10	123.70
22	23S1	1805	A	N3-C4-C5	-10.50	119.45	126.80
1	16S1	373	A	N3-C4-C5	-10.50	119.45	126.80
22	23S1	896	A	N7-C8-N9	-10.50	108.55	113.80
22	23S1	1014	A	N3-C4-C5	-10.50	119.45	126.80
22	23S1	1551	A	N3-C4-C5	-10.50	119.45	126.80
22	23S1	1009	A	C5-C6-N6	10.50	132.10	123.70
1	16S1	1044	A	N3-C4-C5	-10.50	119.45	126.80
1	16S1	1430	A	C5-C6-N6	10.50	132.10	123.70
22	23S1	1054	A	N3-C4-C5	-10.50	119.45	126.80
1	16S1	994	A	C5-C6-N6	10.49	132.10	123.70
1	16S1	1252	A	N3-C4-C5	-10.49	119.45	126.80
22	23S1	505	A	C5-C6-N6	10.49	132.10	123.70
1	16S1	959	A	N3-C4-C5	-10.49	119.45	126.80
22	23S1	1413	A	N7-C8-N9	-10.49	108.55	113.80
22	23S1	199	A	N7-C8-N9	-10.49	108.56	113.80
22	23S1	241	A	N7-C8-N9	-10.49	108.56	113.80
22	23S1	742	A	N7-C8-N9	-10.49	108.56	113.80
22	23S1	2019	A	N7-C8-N9	-10.49	108.56	113.80
22	23S1	2184	A	N7-C8-N9	-10.49	108.56	113.80
1	16S1	1044	A	N7-C8-N9	-10.49	108.56	113.80
1	16S1	1130	A	C5-C6-N6	10.49	132.09	123.70
22	23S1	727	A	N7-C8-N9	-10.49	108.56	113.80
22	23S1	943	A	N3-C4-C5	-10.49	119.46	126.80
22	23S1	2425	A	C5-C6-N6	10.49	132.09	123.70
1	16S1	397	A	N7-C8-N9	-10.48	108.56	113.80
22	23S1	1952	A	N7-C8-N9	-10.48	108.56	113.80
1	16S1	336	A	N7-C8-N9	-10.48	108.56	113.80
22	23S1	877	A	N7-C8-N9	-10.48	108.56	113.80
22	23S1	2284	A	C5-C6-N6	10.48	132.09	123.70
22	23S1	1847	A	C5-C6-N6	10.48	132.08	123.70
22	23S1	1730	C	N1-C2-O2	10.48	125.19	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	167	A	C5-C6-N6	10.47	132.08	123.70
22	23S1	477	A	N3-C4-C5	-10.47	119.47	126.80
22	23S1	1858	A	N3-C4-C5	-10.47	119.47	126.80
22	23S1	447	A	C5-C6-N6	10.47	132.08	123.70
22	23S1	2886	A	N7-C8-N9	-10.47	108.56	113.80
22	23S1	675	A	N3-C4-C5	-10.47	119.47	126.80
1	16S1	59	A	N3-C4-C5	-10.46	119.48	126.80
1	16S1	1042	A	C5-C6-N6	10.46	132.07	123.70
1	16S1	205	A	N3-C4-C5	-10.46	119.48	126.80
1	16S1	263	A	N7-C8-N9	-10.46	108.57	113.80
1	16S1	696	A	N3-C4-C5	-10.46	119.48	126.80
22	23S1	626	A	N7-C8-N9	-10.46	108.57	113.80
22	23S1	1354	A	N7-C8-N9	-10.46	108.57	113.80
23	05S1	57	A	N7-C8-N9	-10.46	108.57	113.80
22	23S1	1641	A	N3-C4-C5	-10.46	119.48	126.80
22	23S1	1679	A	N7-C8-N9	-10.46	108.57	113.80
1	16S1	371	A	N3-C4-C5	-10.46	119.48	126.80
1	16S1	918	A	N3-C4-C5	-10.46	119.48	126.80
22	23S1	1739	A	N3-C4-C5	-10.46	119.48	126.80
22	23S1	2518	A	C5-C6-N6	10.46	132.06	123.70
1	16S1	363	A	C5-C6-N6	10.45	132.06	123.70
22	23S1	2052	A	C5-C6-N6	10.45	132.06	123.70
23	05S1	99	A	N3-C4-C5	-10.45	119.49	126.80
22	23S1	2826	A	C5-C6-N6	10.45	132.06	123.70
23	05S1	119	A	C5-C6-N6	10.45	132.06	123.70
1	16S1	465	A	N7-C8-N9	-10.44	108.58	113.80
1	16S1	702	A	N7-C8-N9	-10.45	108.58	113.80
22	23S1	49	A	C5-C6-N6	10.45	132.06	123.70
22	23S1	1327	A	N7-C8-N9	-10.45	108.58	113.80
22	23S1	1829	A	N3-C4-C5	-10.45	119.49	126.80
22	23S1	2679	A	N3-C4-C5	-10.44	119.49	126.80
1	16S1	663	A	N7-C8-N9	-10.44	108.58	113.80
1	16S1	1081	A	N3-C4-C5	-10.44	119.49	126.80
1	16S1	1339	A	N7-C8-N9	-10.44	108.58	113.80
1	16S1	1418	A	N3-C4-C5	-10.44	119.49	126.80
1	16S1	900	A	N7-C8-N9	-10.44	108.58	113.80
22	23S1	42	A	C5-C6-N6	10.44	132.05	123.70
22	23S1	430	A	N7-C8-N9	-10.44	108.58	113.80
22	23S1	1871	A	C5-C6-N6	10.44	132.05	123.70
22	23S1	2135	A	N3-C4-C5	-10.44	119.49	126.80
22	23S1	2071	A	N7-C8-N9	-10.44	108.58	113.80
1	16S1	1396	A	N3-C4-C5	-10.44	119.49	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	705	A	N3-C4-C5	-10.44	119.49	126.80
22	23S1	750	A	C5-C6-N6	10.44	132.05	123.70
22	23S1	94	A	N7-C8-N9	-10.44	108.58	113.80
22	23S1	2134	A	C5-C6-N6	10.44	132.05	123.70
22	23S1	5	A	N3-C4-C5	-10.44	119.50	126.80
22	23S1	256	A	C5-C6-N6	10.44	132.05	123.70
22	23S1	928	A	C5-C6-N6	10.43	132.05	123.70
1	16S1	393	A	N3-C4-C5	-10.43	119.50	126.80
1	16S1	1362	A	C5-C6-N6	10.43	132.05	123.70
22	23S1	750	A	N3-C4-C5	-10.43	119.50	126.80
22	23S1	794	A	C5-C6-N6	10.43	132.05	123.70
22	23S1	2322	A	C5-C6-N6	10.43	132.04	123.70
1	16S1	642	A	N3-C4-C5	-10.43	119.50	126.80
1	16S1	1256	A	C5-C6-N6	10.43	132.04	123.70
1	16S1	938	A	C5-C6-N6	10.43	132.04	123.70
1	16S1	1055	A	N3-C4-C5	-10.43	119.50	126.80
22	23S1	1246	A	C5-C6-N6	10.43	132.04	123.70
1	16S1	172	A	N7-C8-N9	-10.43	108.59	113.80
1	16S1	459	A	N3-C4-C5	-10.43	119.50	126.80
22	23S1	1274	A	N7-C8-N9	-10.43	108.59	113.80
22	23S1	1608	A	C5-C6-N6	10.43	132.04	123.70
22	23S1	2873	A	C5-C6-N6	10.43	132.04	123.70
1	16S1	819	A	C5-C6-N6	10.43	132.04	123.70
22	23S1	470	A	C5-C6-N6	10.43	132.04	123.70
22	23S1	492	A	N3-C4-C5	-10.43	119.50	126.80
22	23S1	1916	A	N3-C4-C5	-10.42	119.50	126.80
22	23S1	2665	A	N3-C4-C5	-10.42	119.50	126.80
22	23S1	2748	A	C5-C6-N6	10.42	132.04	123.70
1	16S1	1022	A	N3-C4-C5	-10.42	119.51	126.80
23	05S1	101	A	C5-C6-N1	10.42	122.91	117.70
22	23S1	705	A	N7-C8-N9	-10.42	108.59	113.80
22	23S1	1098	A	C5-C6-N6	10.42	132.03	123.70
1	16S1	704	A	N7-C8-N9	-10.42	108.59	113.80
1	16S1	77	A	N3-C4-C5	-10.42	119.51	126.80
22	23S1	429	A	N3-C4-C5	-10.42	119.51	126.80
22	23S1	1746	A	N7-C8-N9	-10.42	108.59	113.80
22	23S1	1901	A	N3-C4-C5	-10.42	119.51	126.80
1	16S1	196	A	N7-C8-N9	-10.41	108.59	113.80
22	23S1	675	A	N7-C8-N9	-10.41	108.59	113.80
22	23S1	1000	A	N7-C8-N9	-10.41	108.59	113.80
22	23S1	1679	A	C5-C6-N6	10.41	132.03	123.70
55	PTR1	17	U	N3-C2-O2	-10.41	114.91	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	415	A	N3-C4-C5	-10.41	119.51	126.80
22	23S1	514	A	N7-C8-N9	-10.41	108.59	113.80
22	23S1	739	A	N3-C4-C5	-10.41	119.51	126.80
22	23S1	2468	A	C5-C6-N6	10.41	132.03	123.70
22	23S1	2734	A	C5-C6-N6	10.41	132.03	123.70
22	23S1	2850	A	C5-C6-N6	10.41	132.03	123.70
1	16S1	1275	A	C5-C6-N6	10.41	132.03	123.70
22	23S1	1354	A	C5-C6-N6	10.41	132.03	123.70
22	23S1	1848	A	N3-C4-C5	-10.41	119.51	126.80
22	23S1	453	A	C5-C6-N6	10.41	132.03	123.70
22	23S1	2662	A	C4-C5-C6	10.41	122.20	117.00
1	16S1	451	A	C5-C6-N6	10.41	132.03	123.70
1	16S1	1000	A	N3-C4-C5	-10.40	119.52	126.80
1	16S1	1163	A	N7-C8-N9	-10.40	108.60	113.80
1	16S1	336	A	C5-C6-N6	10.40	132.02	123.70
1	16S1	1093	A	C5-C6-N6	10.40	132.02	123.70
22	23S1	203	A	C5-C6-N6	10.40	132.02	123.70
22	23S1	439	A	C5-C6-N6	10.40	132.02	123.70
22	23S1	1070	A	C5-C6-N6	10.40	132.02	123.70
22	23S1	1284	A	N7-C8-N9	-10.40	108.60	113.80
22	23S1	2101	A	N3-C4-C5	-10.40	119.52	126.80
22	23S1	2273	A	C5-C6-N6	10.40	132.02	123.70
22	23S1	2705	A	N7-C8-N9	-10.40	108.60	113.80
1	16S1	189	A	N3-C4-C5	-10.40	119.52	126.80
1	16S1	1229	A	N3-C4-C5	-10.40	119.52	126.80
22	23S1	1301	A	N3-C4-C5	-10.40	119.52	126.80
22	23S1	226	A	N7-C8-N9	-10.40	108.60	113.80
1	16S1	906	A	C5-C6-N6	10.40	132.02	123.70
1	16S1	1357	A	N3-C4-C5	-10.40	119.52	126.80
22	23S1	472	A	N7-C8-N9	-10.40	108.60	113.80
22	23S1	1151	A	N7-C8-N9	-10.40	108.60	113.80
1	16S1	66	A	C5-C6-N6	10.39	132.01	123.70
22	23S1	941	A	N3-C4-C5	-10.39	119.52	126.80
22	23S1	1535	A	N3-C4-C5	-10.39	119.52	126.80
22	23S1	2173	A	N7-C8-N9	-10.39	108.60	113.80
22	23S1	2851	A	C5-C6-N6	10.39	132.02	123.70
23	05S1	59	A	C5-C6-N1	10.39	122.90	117.70
22	23S1	2886	A	N3-C4-C5	-10.39	119.53	126.80
1	16S1	816	A	N3-C4-C5	-10.39	119.53	126.80
22	23S1	2183	A	N7-C8-N9	-10.39	108.60	113.80
1	16S1	1171	A	N3-C4-C5	-10.39	119.53	126.80
22	23S1	918	A	N7-C8-N9	-10.39	108.61	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2031	A	N3-C4-C5	-10.39	119.53	126.80
22	23S1	439	A	N3-C4-C5	-10.39	119.53	126.80
22	23S1	529	A	N7-C8-N9	-10.39	108.61	113.80
1	16S1	546	A	C5-C6-N6	10.39	132.01	123.70
22	23S1	1938	A	C5-C6-N6	10.38	132.01	123.70
22	23S1	2879	A	N3-C4-C5	-10.38	119.53	126.80
1	16S1	72	A	C5-C6-N6	10.38	132.00	123.70
22	23S1	219	A	N3-C4-C5	-10.38	119.53	126.80
22	23S1	1808	A	C5-C6-N6	10.38	132.00	123.70
22	23S1	2090	A	C5-C6-N6	10.38	132.00	123.70
22	23S1	2434	A	N7-C8-N9	-10.38	108.61	113.80
22	23S1	1490	A	N7-C8-N9	-10.38	108.61	113.80
23	05S1	109	A	C5-C6-N6	10.38	132.00	123.70
1	16S1	1151	A	N3-C4-C5	-10.38	119.54	126.80
22	23S1	2366	A	N7-C8-N9	-10.38	108.61	113.80
22	23S1	2810	A	N7-C8-N9	-10.38	108.61	113.80
22	23S1	1650	A	C5-C6-N6	10.37	132.00	123.70
22	23S1	2014	A	N3-C4-C5	-10.38	119.54	126.80
23	05S1	99	A	N7-C8-N9	-10.38	108.61	113.80
1	16S1	19	A	N3-C4-C5	-10.37	119.54	126.80
22	23S1	56	A	N3-C4-C5	-10.37	119.54	126.80
22	23S1	191	A	C5-C6-N6	10.37	132.00	123.70
22	23S1	877	A	C5-C6-N6	10.37	132.00	123.70
22	23S1	1264	A	N7-C8-N9	-10.37	108.61	113.80
22	23S1	1757	A	N7-C8-N9	-10.37	108.61	113.80
23	05S1	108	A	C5-C6-N6	10.37	132.00	123.70
22	23S1	1700	A	N3-C4-C5	-10.37	119.54	126.80
22	23S1	2170	A	N3-C4-C5	-10.37	119.54	126.80
22	23S1	582	A	N7-C8-N9	-10.37	108.62	113.80
22	23S1	1265	A	N3-C4-C5	-10.37	119.54	126.80
22	23S1	2381	A	C5-C6-N6	10.37	131.99	123.70
1	16S1	1375	A	N3-C4-C5	-10.37	119.54	126.80
22	23S1	2899	A	N3-C4-C5	-10.37	119.54	126.80
1	16S1	55	A	C5-N7-C8	10.36	109.08	103.90
22	23S1	1260	A	N7-C8-N9	-10.36	108.62	113.80
1	16S1	1492	A	N3-C4-C5	-10.36	119.55	126.80
22	23S1	2792	A	N3-C4-C5	-10.36	119.55	126.80
1	16S1	1261	A	C5-C6-N6	10.36	131.99	123.70
22	23S1	996	A	N3-C4-C5	-10.36	119.55	126.80
22	23S1	1084	A	N3-C4-C5	-10.36	119.55	126.80
22	23S1	1336	A	N3-C4-C5	-10.36	119.55	126.80
22	23S1	1392	A	N7-C8-N9	-10.36	108.62	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1191	A	N7-C8-N9	-10.35	108.62	113.80
22	23S1	160	A	N7-C8-N9	-10.35	108.62	113.80
22	23S1	1632	A	N3-C4-C5	-10.35	119.55	126.80
55	PTR1	3	A	C5-C6-N6	10.35	131.98	123.70
22	23S1	1901	A	C5-C6-N6	10.35	131.98	123.70
1	16S1	1428	A	N3-C4-C5	-10.35	119.56	126.80
1	16S1	174	A	C5-C6-N6	10.35	131.98	123.70
1	16S1	629	A	N3-C4-C5	-10.35	119.56	126.80
22	23S1	1431	A	N3-C4-C5	-10.35	119.56	126.80
22	23S1	1749	A	N3-C4-C5	-10.35	119.56	126.80
22	23S1	2335	A	N7-C8-N9	-10.35	108.62	113.80
1	16S1	262	A	C5-C6-N6	10.35	131.98	123.70
22	23S1	190	A	N7-C8-N9	-10.35	108.63	113.80
22	23S1	1711	A	N3-C4-C5	-10.35	119.56	126.80
1	16S1	452	A	N7-C8-N9	-10.35	108.63	113.80
1	16S1	695	A	N3-C4-C5	-10.35	119.56	126.80
1	16S1	1130	A	N7-C8-N9	-10.35	108.63	113.80
22	23S1	203	A	N3-C4-C5	-10.35	119.56	126.80
22	23S1	1746	A	C5-C6-N6	10.35	131.98	123.70
22	23S1	2879	A	C5-C6-N6	10.35	131.98	123.70
1	16S1	363	A	N7-C8-N9	-10.34	108.63	113.80
22	23S1	917	A	N3-C4-C5	-10.34	119.56	126.80
22	23S1	2199	A	N7-C8-N9	-10.34	108.63	113.80
1	16S1	608	A	N3-C4-C5	-10.34	119.56	126.80
1	16S1	784	A	C5-C6-N6	10.34	131.97	123.70
22	23S1	504	A	C6-N1-C2	10.34	124.81	118.60
1	16S1	559	A	N3-C4-C5	-10.34	119.56	126.80
1	16S1	1431	A	N3-C4-C5	-10.34	119.56	126.80
22	23S1	1048	A	N3-C4-C5	-10.34	119.56	126.80
22	23S1	1916	A	C5-C6-N6	10.34	131.97	123.70
22	23S1	1966	A	C5-C6-N6	10.34	131.97	123.70
22	23S1	1614	A	C5-C6-N6	10.34	131.97	123.70
23	05S1	57	A	C5-C6-N6	10.34	131.97	123.70
1	16S1	901	A	C4-C5-C6	10.33	122.17	117.00
1	16S1	1005	A	C5-C6-N6	10.33	131.97	123.70
22	23S1	909	A	N7-C8-N9	-10.33	108.63	113.80
1	16S1	1350	A	N7-C8-N9	-10.33	108.63	113.80
22	23S1	49	A	N7-C8-N9	-10.33	108.63	113.80
22	23S1	2163	A	N3-C4-C5	-10.33	119.57	126.80
1	16S1	1019	A	N3-C4-C5	-10.33	119.57	126.80
1	16S1	1197	A	C5-C6-N6	10.33	131.96	123.70
1	16S1	1375	A	C5-C6-N6	10.33	131.97	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2418	A	C5-C6-N6	10.33	131.97	123.70
22	23S1	94	A	C5-C6-N6	10.33	131.96	123.70
22	23S1	391	A	N3-C4-C5	-10.33	119.57	126.80
22	23S1	1302	A	C5-C6-N6	10.33	131.96	123.70
22	23S1	1789	A	N7-C8-N9	-10.33	108.64	113.80
22	23S1	2212	A	N3-C4-C5	-10.33	119.57	126.80
1	16S1	130	A	C5-C6-N6	10.32	131.96	123.70
1	16S1	560	A	N3-C4-C5	-10.32	119.57	126.80
1	16S1	609	A	N7-C8-N9	-10.32	108.64	113.80
1	16S1	630	A	N7-C8-N9	-10.32	108.64	113.80
1	16S1	1102	A	N3-C4-C5	-10.32	119.57	126.80
22	23S1	152	A	N3-C4-C5	-10.32	119.57	126.80
22	23S1	1321	A	C5-C6-N6	10.32	131.96	123.70
22	23S1	218	A	N3-C4-C5	-10.32	119.58	126.80
22	23S1	244	A	N3-C4-C5	-10.32	119.57	126.80
22	23S1	218	A	N7-C8-N9	-10.32	108.64	113.80
22	23S1	227	A	C5-C6-N6	10.32	131.96	123.70
22	23S1	1650	A	N3-C4-C5	-10.32	119.58	126.80
22	23S1	2080	A	N3-C4-C5	-10.32	119.58	126.80
22	23S1	2097	A	N3-C4-C5	-10.32	119.58	126.80
1	16S1	412	A	N7-C8-N9	-10.32	108.64	113.80
22	23S1	176	A	N3-C4-C5	-10.32	119.58	126.80
22	23S1	972	A	N3-C4-C5	-10.32	119.58	126.80
1	16S1	968	A	C5-C6-N6	10.31	131.95	123.70
1	16S1	493	A	N7-C8-N9	-10.31	108.64	113.80
1	16S1	600	A	C5-C6-N6	10.31	131.95	123.70
22	23S1	975	A	C5-C6-N6	10.31	131.95	123.70
1	16S1	860	A	C5-N7-C8	10.31	109.06	103.90
22	23S1	849	A	N3-C4-C5	-10.31	119.58	126.80
22	23S1	1127	A	N7-C8-N9	-10.31	108.64	113.80
1	16S1	559	A	N7-C8-N9	-10.31	108.65	113.80
1	16S1	1465	A	N3-C4-C5	-10.31	119.58	126.80
22	23S1	56	A	C5-C6-N6	10.31	131.95	123.70
1	16S1	1476	A	N3-C4-C5	-10.30	119.59	126.80
22	23S1	609	A	N7-C8-N9	-10.30	108.65	113.80
22	23S1	74	A	N7-C8-N9	-10.30	108.65	113.80
22	23S1	14	A	N7-C8-N9	-10.30	108.65	113.80
22	23S1	614	A	C5-C6-N6	10.30	131.94	123.70
22	23S1	1664	A	C5-C6-N6	10.30	131.94	123.70
22	23S1	2531	A	C5-C6-N6	10.30	131.94	123.70
22	23S1	1854	A	N3-C4-C5	-10.29	119.59	126.80
22	23S1	2119	A	C5-N7-C8	10.29	109.05	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2560	A	N3-C4-C5	-10.29	119.59	126.80
22	23S1	820	A	N7-C8-N9	-10.29	108.65	113.80
22	23S1	2459	A	N3-C4-C5	-10.29	119.59	126.80
22	23S1	156	A	N3-C4-C5	-10.29	119.60	126.80
22	23S1	1773	A	N3-C4-C5	-10.29	119.60	126.80
22	23S1	1912	A	C5-N7-C8	10.29	109.05	103.90
22	23S1	2873	A	N7-C8-N9	-10.29	108.65	113.80
1	16S1	630	A	C5-C6-N6	10.29	131.93	123.70
22	23S1	2247	A	C5-C6-N6	10.29	131.93	123.70
1	16S1	718	A	C5-C6-N6	10.29	131.93	123.70
22	23S1	613	A	N7-C8-N9	-10.29	108.66	113.80
1	16S1	1014	A	C5-C6-N6	10.28	131.93	123.70
22	23S1	2108	A	N3-C4-C5	-10.28	119.60	126.80
1	16S1	109	A	C5-C6-N6	10.28	131.92	123.70
22	23S1	482	A	N7-C8-N9	-10.28	108.66	113.80
1	16S1	478	A	N7-C8-N9	-10.28	108.66	113.80
22	23S1	2020	A	C5-C6-N6	10.28	131.92	123.70
22	23S1	2741	A	C5-C6-N6	10.28	131.92	123.70
1	16S1	845	A	N3-C4-C5	-10.28	119.61	126.80
23	05S1	73	A	C5-C6-N6	10.28	131.92	123.70
1	16S1	1339	A	N3-C4-C5	-10.28	119.61	126.80
1	16S1	338	A	N7-C8-N9	-10.27	108.66	113.80
1	16S1	1246	A	C5-C6-N6	10.27	131.92	123.70
22	23S1	13	A	N3-C4-C5	-10.27	119.61	126.80
22	23S1	1260	A	C5-C6-N6	10.27	131.92	123.70
1	16S1	1151	A	C5-C6-N6	10.27	131.91	123.70
22	23S1	1085	A	C5-C6-N6	10.27	131.92	123.70
22	23S1	2126	A	N3-C4-C5	-10.27	119.61	126.80
22	23S1	2199	A	N3-C4-C5	-10.27	119.61	126.80
1	16S1	1513	A	N3-C4-C5	-10.27	119.61	126.80
1	16S1	563	A	N7-C8-N9	-10.27	108.67	113.80
22	23S1	182	A	C5-C6-N6	10.27	131.91	123.70
22	23S1	472	A	C5-C6-N6	10.27	131.91	123.70
22	23S1	1504	A	C5-C6-N6	10.27	131.91	123.70
1	16S1	1410	A	N3-C4-C5	-10.26	119.62	126.80
1	16S1	72	A	N3-C4-C5	-10.26	119.62	126.80
22	23S1	2042	A	C5-C6-N6	10.26	131.91	123.70
22	23S1	2634	A	N3-C4-C5	-10.26	119.62	126.80
22	23S1	1262	A	N3-C4-C5	-10.26	119.62	126.80
1	16S1	816	A	N7-C8-N9	-10.26	108.67	113.80
1	16S1	192	A	C5-C6-N6	10.25	131.90	123.70
22	23S1	1590	A	N3-C4-C5	-10.25	119.62	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1787	A	C5-C6-N6	10.25	131.90	123.70
22	23S1	2799	A	N3-C4-C5	-10.25	119.62	126.80
1	16S1	129	A	C5-C6-N6	10.25	131.90	123.70
22	23S1	1677	A	N7-C8-N9	-10.25	108.67	113.80
22	23S1	2614	A	N7-C8-N9	-10.25	108.67	113.80
22	23S1	144	A	N3-C4-C5	-10.25	119.62	126.80
22	23S1	626	A	C5-C6-N6	10.25	131.90	123.70
22	23S1	1085	A	N3-C4-C5	-10.25	119.63	126.80
22	23S1	1794	A	N3-C4-C5	-10.25	119.62	126.80
22	23S1	1848	A	C5-C6-N6	10.25	131.90	123.70
1	16S1	366	A	C5-C6-N6	10.25	131.90	123.70
22	23S1	1230	A	N3-C4-C5	-10.25	119.63	126.80
22	23S1	2059	A	C5-C6-N6	10.25	131.90	123.70
55	PTR1	58	A	N3-C4-C5	-10.25	119.63	126.80
1	16S1	432	A	N3-C4-C5	-10.24	119.63	126.80
1	16S1	974	A	C5-C6-N6	10.24	131.90	123.70
22	23S1	1301	A	C5-C6-N6	10.24	131.90	123.70
22	23S1	2054	A	N3-C4-C5	-10.24	119.63	126.80
1	16S1	28	A	N3-C4-C5	-10.24	119.63	126.80
1	16S1	223	A	C5-C6-N6	10.24	131.89	123.70
1	16S1	1324	A	N3-C4-C5	-10.24	119.63	126.80
22	23S1	2071	A	N3-C4-C5	-10.24	119.63	126.80
22	23S1	2003	A	C5-C6-N6	10.24	131.89	123.70
22	23S1	2268	A	N7-C8-N9	-10.24	108.68	113.80
22	23S1	2273	A	N7-C8-N9	-10.24	108.68	113.80
1	16S1	864	A	N3-C4-C5	-10.24	119.63	126.80
1	16S1	675	A	C5-C6-N6	10.24	131.89	123.70
1	16S1	1157	A	C5-C6-N6	10.24	131.89	123.70
22	23S1	582	A	N3-C4-C5	-10.24	119.63	126.80
22	23S1	2700	A	N3-C4-C5	-10.24	119.63	126.80
1	16S1	1176	A	N3-C4-C5	-10.24	119.63	126.80
22	23S1	2163	A	N7-C8-N9	-10.24	108.68	113.80
22	23S1	21	A	N3-C4-C5	-10.24	119.64	126.80
22	23S1	6	A	N3-C4-C5	-10.23	119.64	126.80
22	23S1	947	A	C5-C6-N6	10.23	131.89	123.70
22	23S1	1665	A	C5-C6-N6	10.23	131.89	123.70
22	23S1	1744	A	N7-C8-N9	-10.23	108.68	113.80
1	16S1	28	A	N7-C8-N9	-10.23	108.68	113.80
1	16S1	777	A	N3-C4-C5	-10.23	119.64	126.80
22	23S1	900	A	N3-C4-C5	-10.23	119.64	126.80
22	23S1	2564	A	N3-C4-C5	-10.23	119.64	126.80
1	16S1	1176	A	C5-C6-N6	10.23	131.88	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1368	A	C5-C6-N6	10.23	131.88	123.70
22	23S1	2070	A	N3-C4-C5	-10.23	119.64	126.80
22	23S1	1276	A	C5-C6-N6	10.23	131.88	123.70
22	23S1	1746	A	N3-C4-C5	-10.22	119.64	126.80
22	23S1	2328	A	C5-C6-N6	10.22	131.88	123.70
1	16S1	1363	A	C5-C6-N6	10.22	131.88	123.70
1	16S1	1483	A	C5-C6-N6	10.22	131.88	123.70
22	23S1	13	A	N7-C8-N9	-10.22	108.69	113.80
22	23S1	2893	A	C5-C6-N6	10.22	131.88	123.70
1	16S1	502	A	N7-C8-N9	-10.22	108.69	113.80
22	23S1	309	A	N7-C8-N9	-10.22	108.69	113.80
22	23S1	722	A	N3-C4-C5	-10.22	119.65	126.80
22	23S1	2158	A	C5-C6-N6	10.22	131.88	123.70
1	16S1	622	A	N7-C8-N9	-10.22	108.69	113.80
22	23S1	479	A	C5-C6-N6	10.22	131.87	123.70
22	23S1	2547	A	N3-C4-C5	-10.22	119.65	126.80
1	16S1	306	A	N3-C4-C5	-10.21	119.65	126.80
1	16S1	441	A	N3-C4-C5	-10.21	119.65	126.80
22	23S1	751	A	N7-C8-N9	-10.21	108.69	113.80
1	16S1	977	A	C5-C6-N6	10.21	131.87	123.70
22	23S1	781	A	N3-C4-C5	-10.21	119.65	126.80
22	23S1	1040	A	C5-C6-N6	10.21	131.87	123.70
1	16S1	673	A	N7-C8-N9	-10.21	108.70	113.80
22	23S1	2090	A	N3-C4-C5	-10.21	119.66	126.80
22	23S1	2547	A	N7-C8-N9	-10.21	108.70	113.80
22	23S1	2425	A	N3-C4-C5	-10.20	119.66	126.80
1	16S1	189	A	C5-C6-N6	10.20	131.86	123.70
1	16S1	782	A	N3-C4-C5	-10.20	119.66	126.80
1	16S1	1350	A	N3-C4-C5	-10.20	119.66	126.80
22	23S1	861	A	C5-C6-N6	10.20	131.86	123.70
22	23S1	1609	A	N3-C4-C5	-10.20	119.66	126.80
22	23S1	2439	A	C5-C6-N6	10.20	131.86	123.70
22	23S1	2541	A	N3-C4-C5	-10.20	119.66	126.80
22	23S1	172	A	C5-C6-N6	10.20	131.86	123.70
22	23S1	197	A	N3-C4-C5	-10.20	119.66	126.80
22	23S1	693	A	N3-C4-C5	-10.20	119.66	126.80
22	23S1	975	A	N7-C8-N9	-10.20	108.70	113.80
22	23S1	1040	A	N3-C4-C5	-10.20	119.66	126.80
1	16S1	236	A	N3-C4-C5	-10.20	119.66	126.80
1	16S1	363	A	N3-C4-C5	-10.19	119.66	126.80
55	PTR1	69	A	N3-C4-C5	-10.19	119.66	126.80
1	16S1	10	A	N3-C4-C5	-10.19	119.67	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2037	A	N7-C8-N9	-10.19	108.70	113.80
22	23S1	346	A	N3-C4-C5	-10.19	119.67	126.80
22	23S1	255	A	C5-C6-N6	10.19	131.85	123.70
1	16S1	466	A	N3-C4-C5	-10.19	119.67	126.80
1	16S1	819	A	N7-C8-N9	-10.19	108.70	113.80
1	16S1	1130	A	N3-C4-C5	-10.19	119.67	126.80
22	23S1	2154	A	N3-C4-C5	-10.19	119.67	126.80
22	23S1	2377	A	C5-C6-N6	10.19	131.85	123.70
22	23S1	2482	A	N7-C8-N9	-10.19	108.71	113.80
22	23S1	1373	A	N3-C4-C5	-10.18	119.67	126.80
22	23S1	1598	A	N3-C4-C5	-10.18	119.67	126.80
1	16S1	908	A	N3-C4-C5	-10.18	119.67	126.80
1	16S1	344	A	C5-C6-N6	10.18	131.84	123.70
22	23S1	2757	A	N7-C8-N9	-10.18	108.71	113.80
1	16S1	621	A	C5-C6-N6	10.18	131.84	123.70
22	23S1	1815	A	N7-C8-N9	-10.18	108.71	113.80
23	05S1	101	A	N3-C4-N9	10.18	135.54	127.40
1	16S1	28	A	C5-C6-N6	10.18	131.84	123.70
22	23S1	2019	A	N3-C4-C5	-10.18	119.68	126.80
22	23S1	1085	A	N7-C8-N9	-10.18	108.71	113.80
22	23S1	1327	A	C5-C6-N6	10.18	131.84	123.70
55	PTR1	58	A	C5-C6-N6	10.18	131.84	123.70
22	23S1	2418	A	N3-C4-C5	-10.17	119.68	126.80
1	16S1	1019	A	C5-C6-N6	10.17	131.84	123.70
22	23S1	1735	A	C5-C6-N6	10.17	131.84	123.70
22	23S1	1900	A	C5-C6-N6	10.17	131.84	123.70
22	23S1	2727	A	C5-C6-N6	10.17	131.84	123.70
1	16S1	1288	A	N3-C4-C5	-10.17	119.68	126.80
1	16S1	1318	A	N3-C4-C5	-10.17	119.68	126.80
1	16S1	1483	A	N7-C8-N9	-10.17	108.71	113.80
22	23S1	1103	A	C5-C6-N6	10.17	131.84	123.70
23	05S1	66	A	C5-C6-N6	10.17	131.84	123.70
23	05S1	115	A	C5-C6-N6	10.17	131.84	123.70
22	23S1	348	A	N3-C4-C5	-10.17	119.68	126.80
22	23S1	666	A	C5-C6-N6	10.17	131.83	123.70
22	23S1	909	A	C5-C6-N6	10.17	131.83	123.70
22	23S1	727	A	C5-C6-N6	10.16	131.83	123.70
22	23S1	1912	A	N3-C4-C5	-10.16	119.69	126.80
22	23S1	95	A	N3-C4-C5	-10.16	119.69	126.80
22	23S1	1597	A	N3-C4-C5	-10.16	119.69	126.80
22	23S1	2886	A	C5-C6-N6	10.16	131.83	123.70
1	16S1	55	A	C5-C6-N6	10.16	131.83	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2872	A	C5-N7-C8	10.16	108.98	103.90
1	16S1	1288	A	C5-C6-N6	10.16	131.82	123.70
22	23S1	980	A	N7-C8-N9	-10.16	108.72	113.80
22	23S1	1469	A	C5-C6-N6	10.16	131.83	123.70
22	23S1	1626	A	C5-C6-N6	10.16	131.82	123.70
22	23S1	2725	A	N3-C4-C5	-10.16	119.69	126.80
1	16S1	116	A	N3-C4-C5	-10.15	119.69	126.80
22	23S1	1532	A	N3-C4-C5	-10.15	119.69	126.80
22	23S1	131	A	N7-C8-N9	-10.15	108.72	113.80
22	23S1	1544	A	N7-C8-N9	-10.15	108.72	113.80
1	16S1	250	A	C5-C6-N6	10.15	131.82	123.70
1	16S1	1508	A	N7-C8-N9	-10.15	108.72	113.80
1	16S1	435	A	N3-C4-C5	-10.15	119.70	126.80
1	16S1	608	A	C5-C6-N6	10.15	131.82	123.70
1	16S1	777	A	N7-C8-N9	-10.15	108.73	113.80
22	23S1	1672	A	C5-C6-N6	10.15	131.82	123.70
22	23S1	2476	A	N3-C4-C5	-10.15	119.70	126.80
23	05S1	50	A	N3-C4-C5	-10.15	119.70	126.80
22	23S1	2813	A	N7-C8-N9	-10.15	108.73	113.80
1	16S1	629	A	C5-C6-N6	10.14	131.82	123.70
1	16S1	635	A	C5-C6-N6	10.14	131.81	123.70
1	16S1	655	A	C5-C6-N6	10.14	131.81	123.70
22	23S1	2059	A	N3-C4-C5	-10.14	119.70	126.80
22	23S1	2392	A	N7-C8-N9	-10.14	108.73	113.80
23	05S1	94	A	N3-C4-C5	-10.14	119.70	126.80
22	23S1	1549	A	C5-C6-N6	10.14	131.81	123.70
22	23S1	2733	A	N3-C4-C5	-10.14	119.70	126.80
1	16S1	1483	A	N3-C4-C5	-10.14	119.70	126.80
22	23S1	1262	A	N7-C8-N9	-10.14	108.73	113.80
22	23S1	2721	A	C5-C6-N6	10.14	131.81	123.70
1	16S1	320	A	N3-C4-C5	-10.13	119.71	126.80
1	16S1	327	A	C5-C6-N6	10.13	131.81	123.70
1	16S1	553	A	N3-C4-C5	-10.13	119.71	126.80
1	16S1	1080	A	N7-C8-N9	-10.13	108.73	113.80
1	16S1	1170	A	C4-C5-C6	10.13	122.07	117.00
1	16S1	1271	A	N3-C4-C5	-10.13	119.70	126.80
22	23S1	945	A	N7-C8-N9	-10.13	108.73	113.80
55	PTR1	42	A	N3-C4-C5	-10.13	119.71	126.80
1	16S1	1082	A	N3-C4-C5	-10.13	119.71	126.80
22	23S1	478	A	N7-C8-N9	-10.13	108.73	113.80
22	23S1	1603	A	N3-C4-C5	-10.13	119.71	126.80
22	23S1	608	A	C5-C6-N6	10.13	131.80	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1142	A	C5-C6-N6	10.13	131.81	123.70
22	23S1	1637	A	N3-C4-C5	-10.13	119.71	126.80
22	23S1	849	A	N7-C8-N9	-10.13	108.74	113.80
22	23S1	943	A	C5-C6-N6	10.13	131.80	123.70
22	23S1	1913	A	C5-C6-N6	10.13	131.80	123.70
22	23S1	718	A	N3-C4-C5	-10.13	119.71	126.80
22	23S1	1354	A	N3-C4-C5	-10.13	119.71	126.80
1	16S1	373	A	C5-C6-N6	10.12	131.80	123.70
22	23S1	2879	A	N7-C8-N9	-10.12	108.74	113.80
1	16S1	282	A	N3-C4-C5	-10.12	119.72	126.80
1	16S1	609	A	N3-C4-C5	-10.12	119.72	126.80
22	23S1	920	A	N3-C4-C5	-10.12	119.72	126.80
22	23S1	2850	A	N3-C4-C5	-10.12	119.72	126.80
1	16S1	383	A	N3-C4-N9	10.11	135.49	127.40
1	16S1	1155	A	C5-C6-N6	10.12	131.79	123.70
22	23S1	996	A	C5-C6-N6	10.12	131.79	123.70
22	23S1	2635	A	N3-C4-C5	-10.12	119.72	126.80
1	16S1	44	A	N3-C4-C5	-10.11	119.72	126.80
22	23S1	1230	A	C5-C6-N6	10.11	131.79	123.70
22	23S1	602	A	N3-C4-C5	-10.11	119.72	126.80
22	23S1	1937	A	N3-C4-C5	-10.11	119.72	126.80
22	23S1	2736	A	N3-C4-C5	-10.11	119.72	126.80
1	16S1	181	A	N3-C4-C5	-10.11	119.72	126.80
22	23S1	2317	A	N3-C4-C5	-10.11	119.72	126.80
22	23S1	2386	A	N3-C4-C5	-10.11	119.72	126.80
1	16S1	694	A	N3-C4-C5	-10.11	119.72	126.80
22	23S1	693	A	C5-C6-N6	10.11	131.78	123.70
22	23S1	1745	A	N3-C4-C5	-10.11	119.73	126.80
1	16S1	456	A	C5-C6-N6	10.10	131.78	123.70
22	23S1	176	A	C5-C6-N6	10.10	131.78	123.70
22	23S1	1237	A	C5-C6-N6	10.10	131.78	123.70
22	23S1	282	A	C5-C6-N6	10.10	131.78	123.70
1	16S1	139	A	C5-C6-N6	10.10	131.78	123.70
1	16S1	1146	A	N3-C4-C5	-10.10	119.73	126.80
22	23S1	1301	A	N7-C8-N9	-10.10	108.75	113.80
22	23S1	2518	A	N7-C8-N9	-10.10	108.75	113.80
1	16S1	81	A	N7-C8-N9	-10.10	108.75	113.80
22	23S1	980	A	N3-C4-C5	-10.10	119.73	126.80
22	23S1	2837	A	N3-C4-C5	-10.10	119.73	126.80
1	16S1	456	A	N3-C4-C5	-10.09	119.73	126.80
1	16S1	878	A	N3-C4-C5	-10.09	119.73	126.80
22	23S1	514	A	N3-C4-C5	-10.09	119.73	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1496	A	N3-C4-C5	-10.09	119.73	126.80
22	23S1	1853	A	N3-C4-C5	-10.09	119.74	126.80
22	23S1	1916	A	N7-C8-N9	-10.09	108.75	113.80
22	23S1	1819	A	N3-C4-C5	-10.09	119.74	126.80
1	16S1	1429	A	N3-C4-C5	-10.09	119.74	126.80
22	23S1	146	A	N3-C4-C5	-10.09	119.74	126.80
22	23S1	2327	A	N7-C8-N9	-10.09	108.75	113.80
22	23S1	2482	A	N3-C4-C5	-10.09	119.74	126.80
22	23S1	2900	A	N3-C4-C5	-10.09	119.74	126.80
22	23S1	753	A	C5-C6-N6	10.09	131.77	123.70
22	23S1	1689	A	N3-C4-C5	-10.09	119.74	126.80
22	23S1	1144	A	N3-C4-C5	-10.09	119.74	126.80
23	05S1	59	A	N3-C4-N9	10.09	135.47	127.40
1	16S1	161	A	N3-C4-C5	-10.09	119.74	126.80
1	16S1	263	A	N3-C4-C5	-10.09	119.74	126.80
1	16S1	767	A	N3-C4-C5	-10.09	119.74	126.80
1	16S1	1250	A	N3-C4-C5	-10.09	119.74	126.80
22	23S1	1433	A	C5-C6-N6	10.09	131.77	123.70
22	23S1	2530	A	N3-C4-C5	-10.09	119.74	126.80
22	23S1	2813	A	C5-C6-N6	10.09	131.77	123.70
1	16S1	1332	A	N3-C4-C5	-10.08	119.74	126.80
22	23S1	19	A	N3-C4-C5	-10.08	119.74	126.80
22	23S1	2392	A	N3-C4-C5	-10.08	119.74	126.80
1	16S1	288	A	N3-C4-C5	-10.08	119.75	126.80
22	23S1	574	A	N3-C4-C5	-10.08	119.75	126.80
22	23S1	2268	A	N3-C4-C5	-10.08	119.74	126.80
1	16S1	1021	A	N3-C4-C5	-10.08	119.75	126.80
1	16S1	1236	A	N3-C4-C5	-10.08	119.75	126.80
1	16S1	1465	A	C5-C6-N6	10.07	131.76	123.70
22	23S1	412	A	C5-C6-N6	10.07	131.76	123.70
22	23S1	1502	A	N3-C4-C5	-10.07	119.75	126.80
1	16S1	397	A	N3-C4-N9	10.07	135.46	127.40
1	16S1	1036	A	N7-C8-N9	-10.07	108.76	113.80
22	23S1	1373	A	C5-C6-N6	10.07	131.76	123.70
1	16S1	784	A	N3-C4-C5	-10.07	119.75	126.80
22	23S1	1470	A	C5-C6-N6	10.07	131.76	123.70
22	23S1	1580	A	N3-C4-C5	-10.07	119.75	126.80
22	23S1	1802	A	C5-C6-N6	10.07	131.76	123.70
22	23S1	2311	A	N3-C4-C5	-10.07	119.75	126.80
22	23S1	2706	A	N7-C8-N9	-10.07	108.76	113.80
1	16S1	523	A	N3-C4-C5	-10.07	119.75	126.80
1	16S1	574	A	N7-C8-N9	-10.07	108.77	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	64	A	C5-C6-N6	10.07	131.75	123.70
22	23S1	309	A	N3-C4-C5	-10.07	119.75	126.80
22	23S1	477	A	N7-C8-N9	-10.07	108.77	113.80
1	16S1	1225	A	N7-C8-N9	-10.06	108.77	113.80
22	23S1	478	A	N3-C4-C5	-10.06	119.76	126.80
22	23S1	503	A	C5-C6-N6	10.06	131.75	123.70
22	23S1	1713	A	C5-C6-N6	10.06	131.75	123.70
22	23S1	471	A	C5-C6-N6	10.06	131.75	123.70
22	23S1	422	A	N3-C4-C5	-10.06	119.76	126.80
22	23S1	1054	A	N7-C8-N9	-10.06	108.77	113.80
22	23S1	2476	A	C5-C6-N6	10.06	131.75	123.70
1	16S1	253	A	N3-C4-C5	-10.05	119.76	126.80
1	16S1	935	A	N3-C4-C5	-10.06	119.76	126.80
1	16S1	1158	C	C2-N1-C1'	10.05	129.86	118.80
22	23S1	149	A	N3-C4-C5	-10.05	119.76	126.80
22	23S1	2134	A	N3-C4-C5	-10.05	119.76	126.80
22	23S1	742	A	C5-C6-N6	10.05	131.74	123.70
22	23S1	1593	A	N3-C4-C5	-10.05	119.76	126.80
22	23S1	2407	A	C5-C6-N6	10.05	131.74	123.70
1	16S1	807	A	N3-C4-C5	-10.05	119.77	126.80
22	23S1	432	A	N3-C4-C5	-10.05	119.76	126.80
22	23S1	1665	A	N3-C4-C5	-10.05	119.76	126.80
22	23S1	52	A	C5-C6-N6	10.05	131.74	123.70
22	23S1	646	U	O4'-C1'-N1	10.05	116.24	108.20
22	23S1	756	A	C5-C6-N6	10.05	131.74	123.70
22	23S1	1089	A	C5-C6-N6	10.05	131.74	123.70
22	23S1	374	A	C5-C6-N6	10.05	131.74	123.70
22	23S1	2450	A	N7-C8-N9	-10.05	108.78	113.80
22	23S1	764	A	N7-C8-N9	-10.05	108.78	113.80
1	16S1	749	A	C5-C6-N6	10.04	131.74	123.70
22	23S1	793	A	N3-C4-C5	-10.04	119.77	126.80
22	23S1	1393	A	N7-C8-N9	-10.04	108.78	113.80
22	23S1	2711	A	N3-C4-C5	-10.04	119.77	126.80
22	23S1	2872	A	C4-C5-N7	-10.04	105.68	110.70
22	23S1	38	A	N3-C4-C5	-10.04	119.77	126.80
1	16S1	238	A	N3-C4-C5	-10.04	119.77	126.80
1	16S1	1508	A	N3-C4-C5	-10.04	119.77	126.80
22	23S1	960	A	C4-C5-C6	10.04	122.02	117.00
1	16S1	228	A	N3-C4-C5	-10.03	119.78	126.80
1	16S1	1311	A	C5-C6-N6	10.03	131.73	123.70
22	23S1	1147	A	C5-C6-N6	10.04	131.73	123.70
22	23S1	933	A	N7-C8-N9	-10.03	108.78	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1429	A	C5-C6-N6	10.03	131.72	123.70
22	23S1	730	A	N7-C8-N9	-10.03	108.78	113.80
22	23S1	1328	A	N3-C4-C5	-10.03	119.78	126.80
55	PTR1	17	U	C5-C6-N1	-10.03	117.68	122.70
22	23S1	1470	A	N7-C8-N9	-10.03	108.79	113.80
22	23S1	2314	A	N3-C4-C5	-10.03	119.78	126.80
22	23S1	1762	A	N3-C4-C5	-10.03	119.78	126.80
22	23S1	2003	A	N3-C4-C5	-10.03	119.78	126.80
22	23S1	2314	A	C5-C6-N6	10.02	131.72	123.70
22	23S1	2461	A	C5-C6-N6	10.02	131.72	123.70
55	PTR1	42	A	C5-C6-N6	10.02	131.72	123.70
1	16S1	908	A	C5-C6-N6	10.02	131.72	123.70
1	16S1	1306	A	N3-C4-C5	-10.02	119.79	126.80
22	23S1	936	A	C5-C6-N6	10.02	131.71	123.70
22	23S1	1027	A	C5-C6-N6	10.02	131.71	123.70
1	16S1	1044	A	C5-C6-N6	10.01	131.71	123.70
22	23S1	1872	A	C4-C5-C6	10.01	122.01	117.00
22	23S1	52	A	N3-C4-C5	-10.01	119.79	126.80
22	23S1	470	A	N7-C8-N9	-10.01	108.79	113.80
22	23S1	960	A	N7-C8-N9	-10.01	108.79	113.80
22	23S1	1073	A	N3-C4-C5	-10.01	119.79	126.80
1	16S1	313	A	N3-C4-C5	-10.01	119.79	126.80
1	16S1	1319	A	N7-C8-N9	-10.01	108.80	113.80
22	23S1	231	A	N3-C4-C5	-10.01	119.79	126.80
22	23S1	2366	A	C5-C6-N6	10.01	131.71	123.70
22	23S1	2412	A	N3-C4-C5	-10.01	119.79	126.80
1	16S1	1191	A	N3-C4-C5	-10.01	119.80	126.80
1	16S1	958	A	N3-C4-C5	-10.01	119.80	126.80
22	23S1	503	A	N7-C8-N9	-10.01	108.80	113.80
22	23S1	2278	A	N3-C4-C5	-10.01	119.80	126.80
1	16S1	539	A	C5-C6-N6	10.00	131.70	123.70
22	23S1	631	A	N3-C4-C5	-10.00	119.80	126.80
22	23S1	1889	A	N3-C4-C5	-10.00	119.80	126.80
22	23S1	1253	A	N7-C8-N9	-10.00	108.80	113.80
22	23S1	2468	A	N3-C4-C5	-10.00	119.80	126.80
1	16S1	937	A	N3-C4-C5	-10.00	119.80	126.80
22	23S1	608	A	N3-C4-C5	-10.00	119.80	126.80
22	23S1	833	A	C5-C6-N6	10.00	131.70	123.70
22	23S1	1505	A	N3-C4-C5	-10.00	119.80	126.80
22	23S1	2821	A	C5-C6-N6	10.00	131.70	123.70
22	23S1	927	A	N3-C4-C5	-9.99	119.80	126.80
1	16S1	66	A	N3-C4-C5	-9.99	119.81	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2471	A	C5-C6-N6	9.99	131.69	123.70
1	16S1	389	A	N7-C8-N9	-9.99	108.81	113.80
1	16S1	964	A	N3-C4-C5	-9.99	119.81	126.80
22	23S1	1274	A	N3-C4-C5	-9.99	119.81	126.80
22	23S1	1477	A	N3-C4-C5	-9.99	119.81	126.80
22	23S1	1978	A	C5-C6-N6	9.99	131.69	123.70
1	16S1	1311	A	N3-C4-C5	-9.99	119.81	126.80
1	16S1	33	A	N7-C8-N9	-9.99	108.81	113.80
22	23S1	63	A	C5-C6-N6	9.99	131.69	123.70
22	23S1	89	A	N3-C4-C5	-9.99	119.81	126.80
22	23S1	1244	A	N3-C4-C5	-9.99	119.81	126.80
1	16S1	1368	A	N3-C4-C5	-9.98	119.81	126.80
22	23S1	89	A	C5-C6-N6	9.98	131.69	123.70
22	23S1	256	A	N3-C4-C5	-9.98	119.81	126.80
22	23S1	1284	A	N3-C4-C5	-9.98	119.81	126.80
22	23S1	1439	A	N3-C4-C5	-9.98	119.81	126.80
22	23S1	1504	A	N3-C4-C5	-9.98	119.81	126.80
55	PTR1	21	A	N7-C8-N9	-9.98	108.81	113.80
22	23S1	415	A	N3-C4-C5	-9.98	119.81	126.80
1	16S1	1014	A	N3-C4-C5	-9.98	119.81	126.80
1	16S1	1340	A	N3-C4-C5	-9.98	119.81	126.80
22	23S1	2014	A	C5-C6-N6	9.98	131.68	123.70
22	23S1	2184	A	N3-C4-C5	-9.98	119.81	126.80
22	23S1	2868	A	N7-C8-N9	-9.98	108.81	113.80
1	16S1	1238	A	N3-C4-C5	-9.97	119.82	126.80
22	23S1	1553	A	C5-C6-N6	9.97	131.68	123.70
22	23S1	1735	A	N3-C4-C5	-9.97	119.82	126.80
22	23S1	2094	A	N3-C4-C5	-9.97	119.82	126.80
1	16S1	482	A	N3-C4-C5	-9.97	119.82	126.80
1	16S1	371	A	C5-C6-N6	9.97	131.68	123.70
1	16S1	873	A	C5-C6-N6	9.97	131.68	123.70
22	23S1	892	A	N7-C8-N9	-9.97	108.81	113.80
22	23S1	1268	A	N3-C4-C5	-9.97	119.82	126.80
1	16S1	309	A	N3-C4-C5	-9.97	119.82	126.80
22	23S1	2471	A	N3-C4-C5	-9.97	119.82	126.80
22	23S1	222	A	N3-C4-C5	-9.96	119.82	126.80
22	23S1	300	A	N7-C8-N9	-9.96	108.82	113.80
22	23S1	980	A	C5-C6-N6	9.96	131.67	123.70
22	23S1	1676	A	C5-C6-N6	9.96	131.67	123.70
1	16S1	262	A	N3-C4-C5	-9.96	119.83	126.80
22	23S1	492	A	N7-C8-N9	-9.96	108.82	113.80
22	23S1	1596	A	N3-C4-C5	-9.96	119.83	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	78	A	N7-C8-N9	-9.96	108.82	113.80
1	16S1	715	A	C5-C6-N6	9.96	131.67	123.70
1	16S1	1055	A	C5-C6-N6	9.96	131.66	123.70
1	16S1	1433	A	N3-C4-C5	-9.96	119.83	126.80
1	16S1	1507	A	N3-C4-C5	-9.96	119.83	126.80
22	23S1	1802	A	N7-C8-N9	-9.96	108.82	113.80
22	23S1	699	A	N7-C8-N9	-9.96	108.82	113.80
22	23S1	2033	A	N3-C4-C5	-9.96	119.83	126.80
22	23S1	586	A	N7-C8-N9	-9.96	108.82	113.80
1	16S1	98	A	N7-C8-N9	-9.95	108.82	113.80
22	23S1	428	A	C5-C6-N6	9.95	131.66	123.70
22	23S1	1705	A	C5-C6-N6	9.95	131.66	123.70
22	23S1	2829	A	N3-C4-C5	-9.95	119.83	126.80
23	05S1	50	A	C5-C6-N6	9.95	131.66	123.70
1	16S1	630	A	N3-C4-C5	-9.95	119.83	126.80
22	23S1	990	A	N3-C4-C5	-9.95	119.83	126.80
23	05S1	78	A	N3-C4-C5	-9.95	119.83	126.80
22	23S1	233	A	N3-C4-C5	-9.95	119.84	126.80
1	16S1	325	A	N3-C4-C5	-9.95	119.84	126.80
1	16S1	1093	A	N3-C4-C5	-9.94	119.84	126.80
1	16S1	1155	A	N3-C4-C5	-9.95	119.84	126.80
1	16S1	1288	A	N7-C8-N9	-9.94	108.83	113.80
22	23S1	324	A	N3-C4-C5	-9.95	119.84	126.80
22	23S1	1528	A	N7-C8-N9	-9.94	108.83	113.80
23	05S1	57	A	N3-C4-C5	-9.94	119.84	126.80
22	23S1	1508	A	N7-C8-N9	-9.94	108.83	113.80
22	23S1	1572	A	C5-C6-N6	9.94	131.65	123.70
22	23S1	480	A	N7-C8-N9	-9.94	108.83	113.80
22	23S1	2531	A	N3-C4-C5	-9.94	119.84	126.80
1	16S1	635	A	N3-C4-C5	-9.94	119.84	126.80
1	16S1	1167	A	C5-C6-N6	9.94	131.65	123.70
22	23S1	2634	A	C5-C6-N6	9.94	131.65	123.70
1	16S1	329	A	C5-C6-N6	9.93	131.65	123.70
1	16S1	909	A	N3-C4-C5	-9.93	119.85	126.80
22	23S1	670	A	N3-C4-C5	-9.93	119.85	126.80
22	23S1	975	A	N3-C4-C5	-9.93	119.85	126.80
22	23S1	1057	A	C5-C6-N6	9.93	131.65	123.70
22	23S1	2094	A	C5-C6-N6	9.93	131.65	123.70
22	23S1	2761	A	C5-C6-N6	9.93	131.65	123.70
1	16S1	532	A	N3-C4-C5	-9.93	119.85	126.80
1	16S1	1246	A	N3-C4-C5	-9.93	119.85	126.80
1	16S1	1299	A	C5-C6-N6	9.93	131.64	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	251	A	C4-C5-C6	9.93	121.97	117.00
22	23S1	2052	A	N3-C4-C5	-9.93	119.85	126.80
22	23S1	637	A	N3-C4-C5	-9.93	119.85	126.80
1	16S1	496	A	N3-C4-C5	-9.93	119.85	126.80
1	16S1	780	A	N7-C8-N9	-9.93	108.84	113.80
22	23S1	2778	A	N3-C4-C5	-9.93	119.85	126.80
1	16S1	946	A	N3-C4-C5	-9.92	119.85	126.80
1	16S1	1110	A	N7-C8-N9	-9.92	108.84	113.80
22	23S1	1470	A	N3-C4-C5	-9.92	119.85	126.80
22	23S1	2435	A	N3-C4-C5	-9.92	119.85	126.80
22	23S1	429	A	N7-C8-N9	-9.92	108.84	113.80
22	23S1	482	A	C4-C5-C6	9.92	121.96	117.00
22	23S1	789	A	N3-C4-C5	-9.92	119.85	126.80
22	23S1	2439	A	N3-C4-C5	-9.92	119.86	126.80
1	16S1	747	A	N3-C4-C5	-9.92	119.86	126.80
22	23S1	155	A	N3-C4-C5	-9.92	119.86	126.80
1	16S1	892	A	N3-C4-C5	-9.92	119.86	126.80
22	23S1	1572	A	N3-C4-C5	-9.92	119.86	126.80
1	16S1	1363	A	N7-C8-N9	-9.92	108.84	113.80
22	23S1	111	A	N3-C4-C5	-9.92	119.86	126.80
22	23S1	1789	A	N3-C4-C5	-9.92	119.86	126.80
22	23S1	2813	A	N3-C4-C5	-9.92	119.86	126.80
1	16S1	1180	A	N3-C4-C5	-9.91	119.86	126.80
22	23S1	1307	A	N3-C4-C5	-9.91	119.86	126.80
22	23S1	1626	A	N3-C4-C5	-9.91	119.86	126.80
1	16S1	794	A	N3-C4-C5	-9.91	119.86	126.80
22	23S1	146	A	C5-C6-N6	9.91	131.63	123.70
22	23S1	1327	A	N3-C4-C5	-9.91	119.86	126.80
22	23S1	1029	A	C5-C6-N6	9.91	131.63	123.70
22	23S1	1755	A	N3-C4-C5	-9.91	119.86	126.80
22	23S1	1885	A	N3-C4-C5	-9.91	119.86	126.80
23	05S1	104	A	N3-C4-C5	-9.91	119.86	126.80
23	05S1	109	A	N3-C4-C5	-9.91	119.86	126.80
1	16S1	430	A	C5-C6-N6	9.91	131.63	123.70
22	23S1	172	A	N3-C4-C5	-9.91	119.86	126.80
22	23S1	541	A	N3-C4-C5	-9.91	119.86	126.80
22	23S1	920	A	C5-C6-N6	9.91	131.62	123.70
22	23S1	933	A	C5-C6-N6	9.91	131.62	123.70
22	23S1	1970	A	O5'-P-OP1	-9.91	96.78	105.70
1	16S1	1251	A	N3-C4-C5	-9.90	119.87	126.80
1	16S1	648	A	N3-C4-C5	-9.90	119.87	126.80
22	23S1	1780	A	N3-C4-C5	-9.90	119.87	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	349	A	C5-C6-N6	9.90	131.62	123.70
1	16S1	546	A	N3-C4-C5	-9.90	119.87	126.80
22	23S1	374	A	N3-C4-C5	-9.90	119.87	126.80
22	23S1	492	A	C5-C6-N6	9.90	131.62	123.70
22	23S1	896	A	N3-C4-C5	-9.90	119.87	126.80
22	23S1	1932	A	N7-C8-N9	-9.90	108.85	113.80
22	23S1	2170	A	C5-N7-C8	9.90	108.85	103.90
1	16S1	279	A	N7-C8-N9	-9.90	108.85	113.80
1	16S1	461	A	C5-C6-N6	9.90	131.62	123.70
1	16S1	1318	A	N7-C8-N9	-9.90	108.85	113.80
1	16S1	496	A	N7-C8-N9	-9.89	108.85	113.80
1	16S1	977	A	N7-C8-N9	-9.89	108.85	113.80
55	PTR1	59	A	N3-C4-C5	-9.89	119.87	126.80
1	16S1	1256	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	802	A	N3-C4-C5	-9.89	119.88	126.80
1	16S1	315	A	C5-C6-N6	9.89	131.61	123.70
1	16S1	815	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	217	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	42	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	1111	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	1717	A	C5-C6-N6	9.89	131.61	123.70
22	23S1	1932	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	2758	A	N3-C4-C5	-9.89	119.88	126.80
1	16S1	1274	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	592	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	794	A	N7-C8-N9	-9.89	108.86	113.80
22	23S1	472	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	945	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	2225	A	N3-C4-C5	-9.89	119.88	126.80
22	23S1	216	A	N3-C4-C5	-9.88	119.88	126.80
22	23S1	654	A	N7-C8-N9	-9.88	108.86	113.80
1	16S1	33	A	C5-C6-N6	9.88	131.61	123.70
1	16S1	974	A	N3-C4-C5	-9.88	119.88	126.80
22	23S1	1655	A	N3-C4-C5	-9.88	119.88	126.80
22	23S1	1070	A	N3-C4-C5	-9.88	119.88	126.80
22	23S1	2826	A	N3-C4-C5	-9.88	119.88	126.80
22	23S1	2247	A	N3-C4-C5	-9.88	119.89	126.80
22	23S1	609	A	N3-C4-C5	-9.88	119.89	126.80
1	16S1	149	A	N3-C4-C5	-9.87	119.89	126.80
22	23S1	878	A	N3-C4-C5	-9.88	119.89	126.80
22	23S1	959	A	N7-C8-N9	-9.87	108.86	113.80
22	23S1	1014	A	C5-C6-N6	9.88	131.60	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2670	A	N3-C4-C5	-9.88	119.89	126.80
1	16S1	1480	A	N3-C4-C5	-9.87	119.89	126.80
22	23S1	2835	A	N3-C4-C5	-9.87	119.89	126.80
1	16S1	676	A	N3-C4-C5	-9.87	119.89	126.80
22	23S1	1090	A	N3-C4-C5	-9.87	119.89	126.80
22	23S1	1690	A	N3-C4-C5	-9.87	119.89	126.80
22	23S1	1698	A	N3-C4-C5	-9.87	119.89	126.80
22	23S1	2377	A	N3-C4-C5	-9.87	119.89	126.80
22	23S1	2856	A	N3-C4-C5	-9.87	119.89	126.80
22	23S1	1431	A	C5-C6-N6	9.87	131.59	123.70
22	23S1	1654	A	N3-C4-C5	-9.87	119.89	126.80
1	16S1	1014	A	N7-C8-N9	-9.86	108.87	113.80
22	23S1	721	A	N3-C4-C5	-9.86	119.89	126.80
22	23S1	911	A	C5-C6-N6	9.86	131.59	123.70
22	23S1	1147	A	N3-C4-C5	-9.86	119.90	126.80
22	23S1	1571	A	N7-C8-N9	-9.86	108.87	113.80
22	23S1	1786	A	N3-C4-C5	-9.86	119.90	126.80
22	23S1	1010	A	N7-C8-N9	-9.86	108.87	113.80
1	16S1	906	A	N3-C4-C5	-9.86	119.90	126.80
22	23S1	126	A	N3-C4-C5	-9.86	119.90	126.80
1	16S1	364	A	N3-C4-C5	-9.86	119.90	126.80
55	PTR1	9	A	C5-C6-N6	9.86	131.59	123.70
22	23S1	1143	A	N3-C4-C5	-9.85	119.90	126.80
22	23S1	1937	A	C5-N7-C8	9.85	108.83	103.90
22	23S1	1095	A	N3-C4-C5	-9.85	119.90	126.80
22	23S1	1635	A	N3-C4-C5	-9.85	119.90	126.80
22	23S1	1745	A	N7-C8-N9	-9.85	108.87	113.80
23	05S1	73	A	N7-C8-N9	-9.85	108.88	113.80
1	16S1	274	A	C5-C6-N6	9.85	131.58	123.70
1	16S1	780	A	N3-C4-C5	-9.85	119.91	126.80
22	23S1	207	A	C5-C6-N6	9.85	131.58	123.70
22	23S1	1705	A	N3-C4-C5	-9.85	119.91	126.80
22	23S1	2278	A	C5-C6-N6	9.85	131.58	123.70
1	16S1	907	A	C5-C6-N6	9.84	131.57	123.70
1	16S1	1102	A	C5-C6-N6	9.84	131.57	123.70
22	23S1	199	A	N3-C4-C5	-9.84	119.91	126.80
22	23S1	371	A	N3-C4-C5	-9.84	119.91	126.80
22	23S1	1260	A	N3-C4-C5	-9.84	119.91	126.80
22	23S1	1579	A	N3-C4-C5	-9.84	119.91	126.80
22	23S1	1987	A	C5-C6-N6	9.84	131.57	123.70
22	23S1	2227	A	N3-C4-C5	-9.84	119.91	126.80
22	23S1	735	A	N3-C4-C5	-9.84	119.91	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	863	A	N7-C8-N9	-9.84	108.88	113.80
22	23S1	911	A	N3-C4-C5	-9.84	119.91	126.80
22	23S1	1050	A	N3-C4-C5	-9.84	119.91	126.80
22	23S1	173	A	N3-C4-C5	-9.83	119.92	126.80
22	23S1	167	A	C5-C6-N6	9.83	131.56	123.70
22	23S1	2183	A	N3-C4-C5	-9.83	119.92	126.80
22	23S1	1151	A	N3-C4-C5	-9.83	119.92	126.80
22	23S1	1477	A	C5-C6-N6	9.83	131.56	123.70
22	23S1	384	A	N3-C4-C5	-9.82	119.92	126.80
1	16S1	749	A	N3-C4-C5	-9.82	119.92	126.80
22	23S1	1420	A	N3-C4-C5	-9.82	119.92	126.80
22	23S1	2614	A	C5-C6-N6	9.82	131.56	123.70
1	16S1	327	A	N3-C4-C5	-9.82	119.93	126.80
1	16S1	1219	A	N7-C8-N9	-9.82	108.89	113.80
1	16S1	600	A	N3-C4-C5	-9.82	119.93	126.80
22	23S1	1089	A	N3-C4-C5	-9.82	119.93	126.80
22	23S1	2434	A	N3-C4-C5	-9.82	119.93	126.80
55	PTR1	3	A	N3-C4-C5	-9.82	119.93	126.80
1	16S1	98	A	C5-C6-N6	9.82	131.55	123.70
22	23S1	453	A	N3-C4-C5	-9.82	119.93	126.80
22	23S1	614	A	N3-C4-C5	-9.82	119.93	126.80
1	16S1	1	A	N3-C4-C5	-9.81	119.93	126.80
22	23S1	661	A	C5-C6-N6	9.81	131.55	123.70
22	23S1	866	A	N3-C4-C5	-9.81	119.93	126.80
22	23S1	1433	A	N3-C4-C5	-9.81	119.93	126.80
1	16S1	253	A	C5-C6-N6	9.81	131.55	123.70
22	23S1	2346	A	N3-C4-C5	-9.81	119.93	126.80
1	16S1	171	A	N3-C4-C5	-9.81	119.93	126.80
22	23S1	1067	A	N3-C4-C5	-9.81	119.93	126.80
22	23S1	1960	A	N3-C4-C5	-9.81	119.94	126.80
22	23S1	2868	A	C5-C6-N6	9.81	131.55	123.70
22	23S1	1609	A	C5-C6-N6	9.80	131.54	123.70
22	23S1	2340	A	N3-C4-C5	-9.81	119.94	126.80
23	05S1	15	A	N3-C4-C5	-9.80	119.94	126.80
22	23S1	2270	A	N3-C4-C5	-9.80	119.94	126.80
1	16S1	349	A	N3-C4-C5	-9.80	119.94	126.80
22	23S1	984	A	N7-C8-N9	-9.80	108.90	113.80
1	16S1	1437	A	C5-C6-N6	9.80	131.54	123.70
22	23S1	715	A	N3-C4-C5	-9.80	119.94	126.80
22	23S1	1630	A	N3-C4-C5	-9.80	119.94	126.80
22	23S1	2600	A	N3-C4-C5	-9.80	119.94	126.80
1	16S1	459	A	C5-C6-N6	9.79	131.54	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	401	A	N3-C4-C5	-9.80	119.94	126.80
22	23S1	422	A	N7-C8-N9	-9.80	108.90	113.80
22	23S1	1549	A	N7-C8-N9	-9.79	108.90	113.80
22	23S1	2407	A	N7-C8-N9	-9.80	108.90	113.80
22	23S1	727	A	N3-C4-C5	-9.79	119.95	126.80
22	23S1	2297	A	N3-C4-C5	-9.79	119.95	126.80
1	16S1	1236	A	C5-C6-N6	9.79	131.53	123.70
22	23S1	947	A	N3-C4-C5	-9.79	119.95	126.80
22	23S1	1144	A	C5-C6-N6	9.79	131.53	123.70
23	05S1	45	A	N3-C4-C5	-9.79	119.95	126.80
1	16S1	482	A	N7-C8-N9	-9.78	108.91	113.80
22	23S1	1264	A	N3-C4-C5	-9.78	119.95	126.80
22	23S1	1969	A	C5-C6-N6	9.78	131.53	123.70
1	16S1	33	A	N3-C4-C5	-9.78	119.95	126.80
22	23S1	142	A	C5-C6-N6	9.78	131.52	123.70
22	23S1	743	A	C5-C6-N6	9.78	131.53	123.70
22	23S1	1413	A	N3-C4-C5	-9.78	119.95	126.80
22	23S1	1919	A	N3-C4-C5	-9.78	119.95	126.80
22	23S1	2058	A	N3-C4-C5	-9.78	119.95	126.80
22	23S1	590	A	N3-C4-C5	-9.78	119.95	126.80
22	23S1	1593	A	C5-C6-N6	9.78	131.52	123.70
22	23S1	2406	A	N3-C4-C5	-9.78	119.95	126.80
22	23S1	2705	A	N3-C4-C5	-9.78	119.95	126.80
22	23S1	632	A	N3-C4-C5	-9.78	119.96	126.80
1	16S1	1105	A	C5-C6-N6	9.77	131.52	123.70
22	23S1	2366	A	N3-C4-C5	-9.77	119.96	126.80
22	23S1	761	A	N7-C8-N9	-9.77	108.91	113.80
22	23S1	972	A	N7-C8-N9	-9.77	108.91	113.80
22	23S1	1169	A	N3-C4-C5	-9.77	119.96	126.80
22	23S1	2188	U	OP2-P-O3'	-9.77	83.70	105.20
1	16S1	1275	A	N3-C4-C5	-9.77	119.96	126.80
22	23S1	1165	A	N3-C4-C5	-9.77	119.96	126.80
22	23S1	382	A	C5-C6-N6	9.77	131.51	123.70
22	23S1	1679	A	N3-C4-C5	-9.77	119.97	126.80
1	16S1	1306	A	C5-C6-N6	9.76	131.51	123.70
22	23S1	716	A	N3-C4-C5	-9.76	119.97	126.80
22	23S1	861	A	N3-C4-C5	-9.76	119.97	126.80
22	23S1	1269	A	N7-C8-N9	-9.76	108.92	113.80
22	23S1	1970	A	N3-C4-C5	-9.76	119.97	126.80
22	23S1	270	A	N3-C4-C5	-9.76	119.97	126.80
22	23S1	512	G	O4'-C1'-N9	9.76	116.01	108.20
22	23S1	1640	A	N3-C4-C5	-9.76	119.97	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1676	A	N3-C4-C5	-9.76	119.97	126.80
22	23S1	1978	A	N3-C4-C5	-9.76	119.97	126.80
22	23S1	2322	A	N3-C4-C5	-9.76	119.97	126.80
22	23S1	2426	A	C5-C6-N6	9.76	131.51	123.70
22	23S1	1169	A	C5-C6-N6	9.76	131.50	123.70
22	23S1	2899	A	C5-C6-N6	9.76	131.51	123.70
1	16S1	1035	A	N3-C4-C5	-9.75	119.97	126.80
22	23S1	460	A	N3-C4-C5	-9.75	119.97	126.80
22	23S1	340	A	N3-C4-C5	-9.75	119.97	126.80
22	23S1	722	A	C5-C6-N6	9.75	131.50	123.70
22	23S1	1552	A	N3-C4-C5	-9.75	119.98	126.80
22	23S1	1953	A	N3-C4-C5	-9.75	119.98	126.80
22	23S1	2381	A	N3-C4-C5	-9.75	119.97	126.80
22	23S1	739	A	N7-C8-N9	-9.75	108.93	113.80
22	23S1	1308	A	N3-C4-C5	-9.75	119.98	126.80
22	23S1	572	A	N7-C8-N9	-9.74	108.93	113.80
1	16S1	1105	A	N3-C4-C5	-9.74	119.98	126.80
1	16S1	1357	A	C5-C6-N6	9.74	131.49	123.70
1	16S1	179	A	N3-C4-C5	-9.74	119.98	126.80
22	23S1	2679	A	C5-C6-N6	9.74	131.49	123.70
1	16S1	499	A	N3-C4-C5	-9.73	119.99	126.80
22	23S1	1591	A	C5-C6-N6	9.73	131.49	123.70
1	16S1	753	A	N3-C4-C5	-9.73	119.99	126.80
1	16S1	1289	A	N3-C4-C5	-9.73	119.99	126.80
22	23S1	483	A	N3-C4-C5	-9.73	119.99	126.80
22	23S1	556	A	N3-C4-C5	-9.73	119.99	126.80
22	23S1	1508	A	C5-C6-N6	9.73	131.48	123.70
22	23S1	1717	A	N3-C4-C5	-9.73	119.99	126.80
1	16S1	1016	A	N3-C4-C5	-9.72	119.99	126.80
22	23S1	1098	A	N7-C8-N9	-9.72	108.94	113.80
22	23S1	2675	A	N3-C4-C5	-9.72	119.99	126.80
1	16S1	51	A	N3-C4-C5	-9.72	120.00	126.80
1	16S1	1042	A	N3-C4-C5	-9.72	120.00	126.80
22	23S1	347	A	N3-C4-C5	-9.72	120.00	126.80
1	16S1	167	A	N3-C4-C5	-9.72	120.00	126.80
1	16S1	1502	A	N3-C4-C5	-9.72	120.00	126.80
22	23S1	64	A	N3-C4-C5	-9.72	120.00	126.80
1	16S1	781	A	N3-C4-C5	-9.72	120.00	126.80
1	16S1	1271	A	C5-C6-N6	9.72	131.47	123.70
22	23S1	428	A	N3-C4-C5	-9.71	120.00	126.80
1	16S1	706	A	C5-C6-N6	9.71	131.47	123.70
1	16S1	1495	U	N3-C2-O2	-9.71	115.40	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	213	A	N3-C4-C5	-9.71	120.00	126.80
22	23S1	454	A	N3-C4-C5	-9.71	120.00	126.80
22	23S1	833	A	N3-C4-C5	-9.71	120.00	126.80
22	23S1	845	A	N7-C8-N9	-9.71	108.94	113.80
22	23S1	207	A	N3-C4-C5	-9.71	120.00	126.80
22	23S1	505	A	N3-C4-C5	-9.71	120.00	126.80
22	23S1	616	A	N3-C4-C5	-9.71	120.00	126.80
22	23S1	699	A	N3-C4-C5	-9.71	120.00	126.80
22	23S1	1244	A	C5-C6-N6	9.70	131.46	123.70
22	23S1	925	A	N3-C4-C5	-9.70	120.01	126.80
22	23S1	1701	A	N3-C4-C5	-9.70	120.01	126.80
1	16S1	130	A	N3-C4-C5	-9.70	120.01	126.80
22	23S1	2298	A	N3-C4-C5	-9.70	120.01	126.80
1	16S1	1531	A	N3-C4-C5	-9.70	120.01	126.80
22	23S1	2147	A	N3-C4-C5	-9.70	120.01	126.80
22	23S1	2577	A	N3-C4-C5	-9.70	120.01	126.80
22	23S1	2823	A	N3-C4-C5	-9.70	120.01	126.80
1	16S1	461	A	N3-C4-C5	-9.70	120.01	126.80
55	PTR1	21	A	N3-C4-C5	-9.69	120.01	126.80
1	16S1	1111	A	N3-C4-C5	-9.69	120.02	126.80
22	23S1	1508	A	N3-C4-C5	-9.69	120.02	126.80
1	16S1	152	A	N7-C8-N9	-9.69	108.95	113.80
1	16S1	468	A	N3-C4-C5	-9.69	120.02	126.80
1	16S1	533	A	C5-C6-N6	9.69	131.45	123.70
22	23S1	104	A	N3-C4-C5	-9.69	120.02	126.80
22	23S1	1603	A	C5-C6-N6	9.69	131.45	123.70
22	23S1	2513	A	N7-C8-N9	-9.69	108.95	113.80
23	05S1	53	A	N3-C4-C5	-9.69	120.02	126.80
22	23S1	1801	A	N3-C4-C5	-9.69	120.02	126.80
1	16S1	60	A	N3-C4-C5	-9.68	120.02	126.80
1	16S1	1117	A	C5-C6-N6	9.68	131.45	123.70
22	23S1	730	A	C5-C6-N6	9.68	131.45	123.70
1	16S1	53	A	C5-C6-N6	9.68	131.44	123.70
22	23S1	63	A	N3-C4-C5	-9.68	120.02	126.80
22	23S1	342	A	N3-C4-C5	-9.68	120.02	126.80
22	23S1	1021	A	N7-C8-N9	-9.68	108.96	113.80
22	23S1	1987	A	N3-C4-C5	-9.68	120.02	126.80
22	23S1	2453	A	N7-C8-N9	-9.68	108.96	113.80
1	16S1	66	A	N7-C8-N9	-9.68	108.96	113.80
22	23S1	1757	A	N3-C4-C5	-9.68	120.03	126.80
1	16S1	1196	A	N3-C4-C5	-9.68	120.03	126.80
22	23S1	1126	A	N7-C8-N9	-9.68	108.96	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2266	A	N3-C4-C5	-9.68	120.03	126.80
1	16S1	250	A	N3-C4-C5	-9.67	120.03	126.80
1	16S1	51	A	C5-N7-C8	9.67	108.74	103.90
22	23S1	101	A	C5-C6-N6	9.67	131.44	123.70
22	23S1	2171	A	N3-C4-C5	-9.67	120.03	126.80
1	16S1	129	A	N3-C4-C5	-9.67	120.03	126.80
22	23S1	979	A	N3-C4-C5	-9.67	120.03	126.80
22	23S1	1247	A	N3-C4-C5	-9.67	120.03	126.80
22	23S1	1525	A	N3-C4-C5	-9.67	120.03	126.80
22	23S1	1591	A	N3-C4-C5	-9.67	120.03	126.80
1	16S1	329	A	N3-C4-C5	-9.66	120.03	126.80
22	23S1	311	A	N3-C4-C5	-9.66	120.04	126.80
1	16S1	195	A	N7-C8-N9	-9.66	108.97	113.80
22	23S1	1265	A	N7-C8-N9	-9.66	108.97	113.80
22	23S1	83	A	N3-C4-C5	-9.66	120.04	126.80
22	23S1	508	A	N3-C4-C5	-9.66	120.04	126.80
22	23S1	1367	A	N3-C4-C5	-9.66	120.04	126.80
1	16S1	1005	A	N3-C4-C5	-9.66	120.04	126.80
22	23S1	300	A	N3-C4-C5	-9.66	120.04	126.80
22	23S1	2176	A	N3-C4-C5	-9.65	120.04	126.80
1	16S1	596	A	N3-C4-C5	-9.65	120.04	126.80
1	16S1	996	A	N3-C4-C5	-9.65	120.04	126.80
22	23S1	1080	A	C5-C6-N6	9.65	131.42	123.70
22	23S1	1672	A	N3-C4-C5	-9.65	120.05	126.80
1	16S1	1492	A	N7-C8-N9	-9.65	108.97	113.80
1	16S1	452	A	C5-C6-N6	9.64	131.41	123.70
1	16S1	889	A	N3-C4-C5	-9.64	120.05	126.80
22	23S1	125	A	N3-C4-C5	-9.64	120.05	126.80
22	23S1	1342	A	N3-C4-C5	-9.64	120.05	126.80
22	23S1	1977	A	N3-C4-C5	-9.64	120.05	126.80
22	23S1	1214	A	N3-C4-C5	-9.64	120.05	126.80
22	23S1	666	A	N3-C4-C5	-9.64	120.05	126.80
22	23S1	2632	A	N3-C4-C5	-9.64	120.05	126.80
22	23S1	1453	A	N3-C4-C5	-9.64	120.06	126.80
22	23S1	2534	A	N3-C4-C5	-9.64	120.06	126.80
22	23S1	1384	A	N3-C4-C5	-9.63	120.06	126.80
22	23S1	1809	A	N7-C8-N9	-9.63	108.98	113.80
22	23S1	2386	A	C5-C6-N6	9.63	131.41	123.70
22	23S1	2810	A	N3-C4-C5	-9.63	120.06	126.80
1	16S1	192	A	N3-C4-C5	-9.63	120.06	126.80
22	23S1	466	A	N7-C8-N9	-9.63	108.98	113.80
22	23S1	522	A	C5-C6-N6	9.63	131.41	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1150	A	N3-C4-C5	-9.63	120.06	126.80
22	23S1	412	A	N3-C4-C5	-9.62	120.06	126.80
22	23S1	844	A	C5-C6-N6	9.63	131.40	123.70
1	16S1	535	A	N3-C4-C5	-9.62	120.06	126.80
1	16S1	1110	A	N3-C4-C5	-9.62	120.06	126.80
22	23S1	181	A	N3-C4-C5	-9.62	120.06	126.80
22	23S1	226	A	N3-C4-C5	-9.62	120.06	126.80
22	23S1	2516	A	C5-C6-N6	9.62	131.40	123.70
1	16S1	1261	A	N3-C4-C5	-9.62	120.07	126.80
1	16S1	1329	A	N3-C4-C5	-9.62	120.07	126.80
22	23S1	1913	A	N3-C4-C5	-9.62	120.07	126.80
1	16S1	718	A	N7-C8-N9	-9.61	108.99	113.80
1	16S1	759	A	N3-C4-C5	-9.62	120.07	126.80
22	23S1	501	A	N3-C4-C5	-9.62	120.07	126.80
22	23S1	1745	A	C5-C6-N6	9.61	131.39	123.70
1	16S1	790	A	C5-C6-N6	9.61	131.39	123.70
1	16S1	1456	A	N3-C4-C5	-9.61	120.07	126.80
22	23S1	661	A	N3-C4-C5	-9.61	120.07	126.80
1	16S1	321	A	N3-C4-C5	-9.61	120.07	126.80
1	16S1	520	A	N3-C4-C5	-9.61	120.07	126.80
22	23S1	633	A	C5-C6-N6	9.61	131.39	123.70
22	23S1	2135	A	C5-C6-N6	9.61	131.39	123.70
1	16S1	139	A	N3-C4-C5	-9.61	120.08	126.80
1	16S1	1357	A	N7-C8-N9	-9.61	109.00	113.80
22	23S1	477	A	C5-C6-N6	9.61	131.38	123.70
22	23S1	1739	A	C5-C6-N6	9.61	131.38	123.70
22	23S1	2119	A	N3-C4-C5	-9.60	120.08	126.80
22	23S1	2352	A	N7-C8-N9	-9.60	109.00	113.80
22	23S1	2893	A	N3-C4-C5	-9.60	120.08	126.80
22	23S1	1336	A	C5-C6-N6	9.60	131.38	123.70
22	23S1	2205	A	N3-C4-C5	-9.60	120.08	126.80
22	23S1	142	A	N3-C4-C5	-9.60	120.08	126.80
22	23S1	2851	A	N3-C4-C5	-9.60	120.08	126.80
1	16S1	315	A	N3-C4-C5	-9.60	120.08	126.80
22	23S1	1027	A	N3-C4-C5	-9.59	120.08	126.80
22	23S1	2516	A	N3-C4-C5	-9.59	120.08	126.80
23	05S1	101	A	C4-C5-C6	9.59	121.80	117.00
22	23S1	2388	A	N3-C4-C5	-9.59	120.09	126.80
55	PTR1	26	A	N3-C4-C5	-9.59	120.09	126.80
1	16S1	466	A	N7-C8-N9	-9.59	109.01	113.80
1	16S1	1507	A	C5-C6-N6	9.59	131.37	123.70
22	23S1	2766	A	N3-C4-N9	9.59	135.07	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	05S1	34	A	N3-C4-C5	-9.59	120.09	126.80
23	05S1	59	A	C4-C5-C6	9.59	121.79	117.00
22	23S1	262	A	N3-C4-C5	-9.59	120.09	126.80
1	16S1	768	A	N3-C4-C5	-9.59	120.09	126.80
22	23S1	529	A	N3-C4-C5	-9.59	120.09	126.80
1	16S1	864	A	N7-C8-N9	-9.59	109.01	113.80
22	23S1	152	A	C5-C6-N6	9.59	131.37	123.70
23	05S1	108	A	N3-C4-C5	-9.59	120.09	126.80
22	23S1	1347	A	N3-C4-C5	-9.58	120.09	126.80
23	05S1	94	A	C5-C6-N6	9.58	131.36	123.70
1	16S1	1503	A	N3-C4-C5	-9.58	120.09	126.80
22	23S1	2675	A	C5-C6-N6	9.58	131.36	123.70
22	23S1	279	A	N3-C4-C5	-9.58	120.10	126.80
1	16S1	77	A	N7-C8-N9	-9.57	109.01	113.80
22	23S1	928	A	N3-C4-C5	-9.57	120.10	126.80
1	16S1	1362	A	N3-C4-C5	-9.57	120.10	126.80
1	16S1	968	A	N3-C4-C5	-9.57	120.10	126.80
1	16S1	1227	A	C5-C6-N6	9.57	131.35	123.70
22	23S1	1791	A	N3-C4-C5	-9.57	120.10	126.80
1	16S1	441	A	C5-C6-N6	9.56	131.35	123.70
22	23S1	131	A	C5-C6-N6	9.56	131.35	123.70
22	23S1	156	A	C5-C6-N6	9.56	131.35	123.70
22	23S1	471	A	N3-C4-C5	-9.56	120.11	126.80
22	23S1	804	A	N3-C4-C5	-9.56	120.11	126.80
22	23S1	575	A	N3-C4-C5	-9.56	120.11	126.80
23	05S1	39	A	N3-C4-C5	-9.56	120.11	126.80
22	23S1	1969	A	N3-C4-C5	-9.56	120.11	126.80
22	23S1	2882	A	N3-C4-C5	-9.56	120.11	126.80
1	16S1	873	A	N3-C4-C5	-9.56	120.11	126.80
22	23S1	1876	A	N3-C4-C5	-9.55	120.11	126.80
1	16S1	1257	A	N3-C4-C5	-9.55	120.11	126.80
22	23S1	2660	A	N3-C4-C5	-9.55	120.11	126.80
22	23S1	2411	A	N3-C4-C5	-9.55	120.11	126.80
1	16S1	236	A	C5-C6-N6	9.55	131.34	123.70
1	16S1	336	A	N3-C4-C5	-9.55	120.12	126.80
1	16S1	451	A	N3-C4-C5	-9.55	120.12	126.80
22	23S1	2158	A	N3-C4-C5	-9.55	120.12	126.80
1	16S1	1254	A	N3-C4-C5	-9.55	120.12	126.80
1	16S1	143	A	N3-C4-C5	-9.54	120.12	126.80
1	16S1	1252	A	C5-C6-N6	9.54	131.33	123.70
1	16S1	1434	A	N3-C4-C5	-9.54	120.12	126.80
22	23S1	21	A	C5-C6-N6	9.54	131.33	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	844	A	N3-C4-C5	-9.54	120.12	126.80
22	23S1	1866	A	C5-C6-N6	9.54	131.33	123.70
22	23S1	706	A	N3-C4-C5	-9.54	120.12	126.80
22	23S1	1008	A	N3-C4-C5	-9.54	120.12	126.80
1	16S1	694	A	C5-N7-C8	9.54	108.67	103.90
1	16S1	831	A	N3-C4-C5	-9.54	120.12	126.80
22	23S1	1029	A	N7-C8-N9	-9.53	109.03	113.80
55	PTR1	38	A	N3-C4-C5	-9.54	120.12	126.80
22	23S1	685	A	N3-C4-C5	-9.53	120.13	126.80
22	23S1	2565	A	N3-C4-C5	-9.53	120.13	126.80
1	16S1	946	A	C5-C6-N6	9.53	131.32	123.70
22	23S1	1304	A	N3-C4-C5	-9.53	120.13	126.80
22	23S1	1528	A	C4-C5-C6	9.53	121.77	117.00
23	05S1	115	A	N3-C4-C5	-9.53	120.13	126.80
1	16S1	101	A	C5-C6-N6	9.53	131.32	123.70
1	16S1	1117	A	N3-C4-C5	-9.53	120.13	126.80
22	23S1	743	A	N7-C8-N9	-9.53	109.04	113.80
23	05S1	52	A	N3-C4-C5	-9.53	120.13	126.80
22	23S1	905	A	N3-C4-C5	-9.53	120.13	126.80
1	16S1	1012	A	C5-C6-N6	9.52	131.32	123.70
22	23S1	1287	A	N3-C4-C5	-9.52	120.13	126.80
1	16S1	649	A	N3-C4-C5	-9.52	120.14	126.80
22	23S1	322	A	N3-C4-C5	-9.52	120.14	126.80
22	23S1	2856	A	C5-C6-N6	9.52	131.31	123.70
22	23S1	344	A	N3-C4-C5	-9.51	120.14	126.80
22	23S1	2108	A	N7-C8-N9	-9.51	109.04	113.80
22	23S1	502	A	N3-C4-C5	-9.51	120.14	126.80
1	16S1	782	A	C5-N7-C8	9.51	108.65	103.90
1	16S1	919	A	N7-C8-N9	-9.51	109.05	113.80
22	23S1	1054	A	C5-C6-N6	9.51	131.31	123.70
22	23S1	2376	A	N3-C4-C5	-9.51	120.15	126.80
1	16S1	374	A	N3-C4-C5	-9.50	120.15	126.80
1	16S1	787	A	N3-C4-C5	-9.50	120.15	126.80
22	23S1	1387	A	C5-C6-N6	9.50	131.30	123.70
1	16S1	26	A	C5-C6-N6	9.50	131.30	123.70
22	23S1	1877	A	N3-C4-C5	-9.50	120.15	126.80
1	16S1	792	A	N3-C4-C5	-9.50	120.15	126.80
22	23S1	165	A	N3-C4-C5	-9.50	120.15	126.80
1	16S1	1493	A	N3-C4-C5	-9.49	120.16	126.80
22	23S1	574	A	C5-C6-N6	9.49	131.29	123.70
22	23S1	973	A	N3-C4-C5	-9.49	120.16	126.80
22	23S1	1151	A	C5-C6-N6	9.49	131.29	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1383	A	N3-C4-C5	-9.49	120.16	126.80
1	16S1	1299	A	N7-C8-N9	-9.49	109.06	113.80
1	16S1	802	A	N3-C4-C5	-9.49	120.16	126.80
1	16S1	1080	A	N3-C4-C5	-9.49	120.16	126.80
1	16S1	1339	A	C5-C6-N6	9.49	131.29	123.70
22	23S1	673	C	C2-N3-C4	-9.49	115.16	119.90
1	16S1	338	A	N3-C4-C5	-9.48	120.16	126.80
1	16S1	1324	A	N7-C8-N9	-9.48	109.06	113.80
22	23S1	1096	A	N3-C4-C5	-9.47	120.17	126.80
22	23S1	1566	A	N3-C4-C5	-9.47	120.17	126.80
1	16S1	274	A	N3-C4-C5	-9.47	120.17	126.80
22	23S1	1143	A	C5-C6-N6	9.47	131.28	123.70
22	23S1	501	A	N7-C8-N9	-9.47	109.06	113.80
22	23S1	1285	A	N3-C4-C5	-9.47	120.17	126.80
22	23S1	227	A	N3-C4-C5	-9.47	120.17	126.80
22	23S1	734	A	N3-C4-C5	-9.46	120.17	126.80
1	16S1	1269	A	N3-C4-C5	-9.46	120.18	126.80
22	23S1	2753	A	N3-C4-C5	-9.46	120.18	126.80
22	23S1	877	A	N3-C4-C5	-9.46	120.18	126.80
1	16S1	366	A	N3-C4-C5	-9.45	120.18	126.80
22	23S1	2267	A	C5-C6-N6	9.46	131.26	123.70
22	23S1	2432	A	N3-C4-C5	-9.46	120.18	126.80
22	23S1	1189	A	C5-C6-N6	9.45	131.26	123.70
22	23S1	1772	A	N3-C4-C5	-9.45	120.18	126.80
1	16S1	969	A	N3-C4-C5	-9.45	120.19	126.80
22	23S1	820	A	C5-C6-N6	9.45	131.26	123.70
22	23S1	2297	A	C5-N7-C8	9.45	108.62	103.90
23	05S1	58	A	N3-C4-C5	-9.45	120.19	126.80
22	23S1	173	A	C5-C6-N6	9.45	131.26	123.70
22	23S1	2154	A	C5-C6-N6	9.45	131.26	123.70
22	23S1	2497	A	N7-C8-N9	-9.45	109.08	113.80
22	23S1	2598	A	N3-C4-C5	-9.45	120.19	126.80
22	23S1	2800	A	C5-C6-N6	9.45	131.26	123.70
55	PTR1	69	A	C5-C6-N6	9.44	131.26	123.70
22	23S1	1308	A	C5-N7-C8	9.44	108.62	103.90
1	16S1	1046	A	C5-C6-N6	9.44	131.25	123.70
22	23S1	1678	A	N3-C4-C5	-9.44	120.19	126.80
22	23S1	2459	A	C5-C6-N6	9.44	131.25	123.70
1	16S1	65	A	N3-C4-C5	-9.44	120.19	126.80
1	16S1	602	A	C5-C6-N6	9.43	131.25	123.70
22	23S1	2700	A	C5-C6-N6	9.43	131.25	123.70
1	16S1	716	A	N7-C8-N9	-9.43	109.08	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1534	A	N3-C4-C5	-9.43	120.20	126.80
22	23S1	845	A	N3-C4-N9	9.43	134.95	127.40
1	16S1	1437	A	N3-C4-C5	-9.43	120.20	126.80
22	23S1	272	A	N3-C4-C5	-9.43	120.20	126.80
22	23S1	1548	A	C5-C6-N6	9.43	131.24	123.70
22	23S1	1900	A	N3-C4-C5	-9.43	120.20	126.80
22	23S1	2054	A	C5-C6-N6	9.43	131.24	123.70
1	16S1	1179	A	N3-C4-C5	-9.43	120.20	126.80
22	23S1	196	A	N7-C8-N9	-9.43	109.09	113.80
1	16S1	1377	A	N3-C4-C5	-9.42	120.20	126.80
22	23S1	918	A	N3-C4-C5	-9.42	120.20	126.80
22	23S1	2333	A	N3-C4-C5	-9.42	120.20	126.80
22	23S1	1039	A	N3-C4-C5	-9.42	120.20	126.80
22	23S1	2005	A	N3-C4-C5	-9.42	120.21	126.80
22	23S1	2340	A	C5-C6-N6	9.42	131.24	123.70
22	23S1	2037	A	C5-C6-N6	9.42	131.23	123.70
1	16S1	825	A	N3-C4-C5	-9.41	120.21	126.80
22	23S1	2682	A	N3-C4-C5	-9.41	120.21	126.80
22	23S1	925	A	C5-C6-N6	9.41	131.23	123.70
22	23S1	14	A	N3-C4-C5	-9.41	120.21	126.80
1	16S1	1446	A	N7-C8-N9	-9.41	109.10	113.80
22	23S1	1155	A	N3-C4-C5	-9.41	120.21	126.80
22	23S1	2281	A	C5-C6-N6	9.41	131.23	123.70
22	23S1	582	A	C5-C6-N6	9.41	131.22	123.70
1	16S1	1324	A	C5-C6-N6	9.40	131.22	123.70
22	23S1	1032	A	N3-C4-C5	-9.40	120.22	126.80
22	23S1	1936	A	C5-C6-N6	9.40	131.22	123.70
22	23S1	2654	A	N3-C4-C5	-9.40	120.22	126.80
1	16S1	120	A	N3-C4-C5	-9.40	120.22	126.80
22	23S1	1966	A	N3-C4-C5	-9.40	120.22	126.80
22	23S1	2748	A	N3-C4-C5	-9.40	120.22	126.80
1	16S1	189	A	N7-C8-N9	-9.39	109.11	113.80
1	16S1	1204	A	N3-C4-C5	-9.39	120.22	126.80
22	23S1	1156	A	N3-C4-C5	-9.39	120.22	126.80
1	16S1	923	A	N7-C8-N9	-9.39	109.11	113.80
22	23S1	1077	A	N3-C4-C5	-9.39	120.23	126.80
1	16S1	95	C	N1-C2-O2	9.39	124.53	118.90
22	23S1	988	A	N3-C4-C5	-9.39	120.23	126.80
22	23S1	2309	A	N3-C4-C5	-9.38	120.23	126.80
22	23S1	2602	A	N3-C4-C5	-9.38	120.23	126.80
22	23S1	1080	A	N3-C4-C5	-9.38	120.24	126.80
22	23S1	2734	A	N3-C4-C5	-9.38	120.24	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1169	A	N3-C4-C5	-9.37	120.24	126.80
22	23S1	2587	A	N3-C4-C5	-9.37	120.24	126.80
1	16S1	502	A	C5-C6-N6	9.37	131.19	123.70
1	16S1	729	A	N3-C4-C5	-9.37	120.24	126.80
22	23S1	1803	A	N7-C8-N9	-9.36	109.12	113.80
1	16S1	563	A	C5-C6-N6	9.36	131.19	123.70
1	16S1	572	A	N3-C4-C5	-9.36	120.25	126.80
1	16S1	1248	A	N3-C4-C5	-9.36	120.25	126.80
22	23S1	2781	A	N7-C8-N9	-9.36	109.12	113.80
22	23S1	1590	A	C5-C6-N6	9.36	131.19	123.70
1	16S1	50	A	N3-C4-C5	-9.35	120.25	126.80
22	23S1	167	A	N3-C4-C5	-9.35	120.25	126.80
22	23S1	1127	A	N3-C4-C5	-9.35	120.25	126.80
1	16S1	1081	A	C5-C6-N6	9.35	131.18	123.70
22	23S1	497	A	N3-C4-C5	-9.35	120.26	126.80
1	16S1	8	A	N3-C4-C5	-9.34	120.26	126.80
1	16S1	80	A	N7-C8-N9	-9.34	109.13	113.80
1	16S1	595	A	N3-C4-C5	-9.34	120.26	126.80
22	23S1	1028	A	C5-C6-N6	9.34	131.18	123.70
22	23S1	1532	A	C5-C6-N6	9.34	131.17	123.70
22	23S1	1608	A	N7-C8-N9	-9.34	109.13	113.80
22	23S1	2873	A	N3-C4-C5	-9.34	120.26	126.80
22	23S1	1713	A	N3-C4-C5	-9.34	120.26	126.80
22	23S1	1919	A	N7-C8-N9	-9.34	109.13	113.80
22	23S1	2426	A	N3-C4-C5	-9.34	120.26	126.80
1	16S1	554	A	N3-C4-C5	-9.34	120.26	126.80
22	23S1	1711	A	C5-C6-N6	9.34	131.17	123.70
22	23S1	2169	A	C5-N7-C8	9.34	108.57	103.90
22	23S1	2352	A	C5-C6-N6	9.34	131.17	123.70
1	16S1	792	A	C5-N7-C8	9.33	108.57	103.90
1	16S1	26	A	N3-C4-C5	-9.33	120.27	126.80
1	16S1	545	C	C5-C6-N1	9.33	125.67	121.00
22	23S1	479	A	N3-C4-C5	-9.33	120.27	126.80
22	23S1	721	A	C5-C6-N6	9.33	131.16	123.70
22	23S1	2392	A	C5-C6-N6	9.33	131.16	123.70
23	05S1	101	A	N7-C8-N9	-9.33	109.14	113.80
1	16S1	160	A	N3-C4-C5	-9.32	120.28	126.80
22	23S1	423	A	N3-C4-C5	-9.32	120.28	126.80
1	16S1	1430	A	N3-C4-C5	-9.32	120.28	126.80
22	23S1	689	A	C5-C6-N6	9.32	131.15	123.70
1	16S1	1418	A	C5-C6-N6	9.31	131.15	123.70
22	23S1	2721	A	N3-C4-C5	-9.31	120.28	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1700	A	C5-N7-C8	9.31	108.56	103.90
22	23S1	1872	A	C5-C6-N6	9.31	131.15	123.70
22	23S1	1936	A	N7-C8-N9	-9.31	109.14	113.80
22	23S1	2378	A	N3-C4-C5	-9.31	120.28	126.80
1	16S1	270	A	C5-C6-N6	9.31	131.15	123.70
22	23S1	103	A	N3-C4-C5	-9.31	120.28	126.80
22	23S1	2009	A	N3-C4-C5	-9.31	120.28	126.80
1	16S1	161	A	N7-C8-N9	-9.31	109.15	113.80
22	23S1	1773	A	N7-C8-N9	-9.30	109.15	113.80
22	23S1	2358	A	N3-C4-C5	-9.30	120.29	126.80
22	23S1	2750	A	N3-C4-C5	-9.30	120.29	126.80
1	16S1	1252	A	N7-C8-N9	-9.30	109.15	113.80
22	23S1	788	A	N3-C4-C5	-9.30	120.29	126.80
22	23S1	1522	A	N3-C4-C5	-9.30	120.29	126.80
22	23S1	1134	A	N3-C4-C5	-9.30	120.29	126.80
22	23S1	1668	A	N3-C4-C5	-9.30	120.29	126.80
22	23S1	633	A	N3-C4-C5	-9.29	120.29	126.80
1	16S1	7	A	N3-C4-C5	-9.29	120.30	126.80
1	16S1	1188	A	N3-C4-C5	-9.29	120.30	126.80
22	23S1	447	A	N3-C4-C5	-9.29	120.30	126.80
22	23S1	599	A	C5-C6-N6	9.29	131.13	123.70
22	23S1	627	A	N3-C4-C5	-9.29	120.30	126.80
1	16S1	2	A	N7-C8-N9	-9.29	109.16	113.80
1	16S1	1332	A	N7-C8-N9	-9.29	109.16	113.80
22	23S1	2020	A	N3-C4-C5	-9.29	120.30	126.80
22	23S1	2042	A	N3-C4-C5	-9.29	120.30	126.80
1	16S1	1171	A	C5-C6-N6	9.29	131.13	123.70
22	23S1	1677	A	N3-C4-C5	-9.28	120.30	126.80
1	16S1	712	A	C5-C6-N6	9.28	131.12	123.70
22	23S1	1133	A	N3-C4-C5	-9.28	120.31	126.80
22	23S1	1580	A	C5-N7-C8	9.27	108.54	103.90
1	16S1	1280	A	N3-C4-C5	-9.27	120.31	126.80
22	23S1	1598	A	N7-C8-N9	-9.27	109.17	113.80
22	23S1	2430	A	N1-C2-N3	-9.27	124.67	129.30
22	23S1	599	A	N3-C4-C5	-9.27	120.31	126.80
1	16S1	116	A	C5-C6-N6	9.26	131.11	123.70
22	23S1	761	A	N3-C4-C5	-9.26	120.32	126.80
22	23S1	2013	A	C5-N7-C8	9.26	108.53	103.90
22	23S1	2451	A	N3-C4-C5	-9.26	120.32	126.80
22	23S1	2820	A	N3-C4-C5	-9.26	120.32	126.80
22	23S1	626	A	N3-C4-C5	-9.26	120.32	126.80
1	16S1	1000	A	C5-C6-N6	9.26	131.10	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1170	A	C5-N7-C8	9.26	108.53	103.90
1	16S1	344	A	N3-C4-C5	-9.25	120.32	126.80
1	16S1	300	A	N1-C6-N6	-9.25	113.05	118.60
22	23S1	1614	A	N3-C4-C5	-9.25	120.32	126.80
1	16S1	246	A	N3-C4-C5	-9.25	120.32	126.80
1	16S1	1349	A	N3-C4-C5	-9.25	120.33	126.80
22	23S1	1890	A	N3-C4-C5	-9.25	120.33	126.80
22	23S1	2741	A	N3-C4-C5	-9.25	120.33	126.80
22	23S1	1821	A	N3-C4-C5	-9.25	120.33	126.80
1	16S1	533	A	C5-N7-C8	9.24	108.52	103.90
22	23S1	1634	A	N3-C4-C5	-9.24	120.33	126.80
1	16S1	119	A	N3-C4-C5	-9.24	120.33	126.80
1	16S1	949	A	C5-N7-C8	9.24	108.52	103.90
22	23S1	1509	A	N3-C4-C5	-9.24	120.33	126.80
22	23S1	2572	A	C5-N7-C8	9.24	108.52	103.90
1	16S1	1408	A	N3-C4-C5	-9.24	120.33	126.80
22	23S1	752	A	N3-C4-C5	-9.24	120.33	126.80
22	23S1	792	A	N3-C4-C5	-9.24	120.33	126.80
22	23S1	443	A	N3-C4-C5	-9.23	120.34	126.80
1	16S1	1167	A	N3-C4-C5	-9.23	120.34	126.80
1	16S1	411	A	N3-C4-C5	-9.23	120.34	126.80
22	23S1	2478	A	N3-C4-C5	-9.23	120.34	126.80
1	16S1	1319	A	N3-C4-C5	-9.23	120.34	126.80
1	16S1	190	A	N3-C4-N9	9.22	134.78	127.40
22	23S1	1434	A	C5-N7-C8	9.22	108.51	103.90
22	23S1	538	A	N3-C4-C5	-9.22	120.35	126.80
22	23S1	1803	A	N3-C4-C5	-9.21	120.35	126.80
22	23S1	1871	A	C5-N7-C8	9.22	108.51	103.90
23	05S1	59	A	C5-N7-C8	9.21	108.51	103.90
1	16S1	460	A	C5-C6-N6	9.21	131.07	123.70
1	16S1	1500	A	N3-C4-C5	-9.21	120.36	126.80
22	23S1	845	A	C5-C6-N6	9.21	131.07	123.70
22	23S1	1204	A	N3-C4-C5	-9.21	120.36	126.80
1	16S1	983	A	N7-C8-N9	-9.21	109.20	113.80
1	16S1	815	A	C5-N7-C8	9.20	108.50	103.90
22	23S1	1103	A	N3-C4-C5	-9.20	120.36	126.80
1	16S1	131	A	N3-C4-C5	-9.20	120.36	126.80
1	16S1	794	A	C5-N7-C8	9.20	108.50	103.90
22	23S1	1586	A	N7-C8-N9	-9.20	109.20	113.80
22	23S1	2706	A	C5-C6-N6	9.20	131.06	123.70
1	16S1	510	A	N3-C4-C5	-9.19	120.36	126.80
1	16S1	495	A	N3-C4-C5	-9.19	120.37	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	310	A	N3-C4-C5	-9.19	120.36	126.80
22	23S1	1378	A	N3-C4-C5	-9.19	120.36	126.80
22	23S1	1938	A	N3-C4-C5	-9.19	120.37	126.80
1	16S1	1447	A	N3-C4-C5	-9.19	120.37	126.80
22	23S1	294	A	N3-C4-C5	-9.19	120.37	126.80
1	16S1	196	A	N3-C4-C5	-9.19	120.37	126.80
22	23S1	1069	A	N3-C4-C5	-9.19	120.37	126.80
22	23S1	544	C	N1-C2-O2	9.18	124.41	118.90
22	23S1	1046	A	N3-C4-C5	-9.18	120.37	126.80
22	23S1	1194	A	N3-C4-C5	-9.18	120.37	126.80
22	23S1	1787	A	N7-C8-N9	-9.18	109.21	113.80
22	23S1	2614	A	C5-N7-C8	9.18	108.49	103.90
1	16S1	109	A	N3-C4-C5	-9.18	120.38	126.80
22	23S1	415	A	C5-C6-N6	9.18	131.04	123.70
1	16S1	1287	A	N3-C4-C5	-9.18	120.38	126.80
22	23S1	28	A	N3-C4-C5	-9.18	120.38	126.80
22	23S1	1111	A	C5-C6-N6	9.17	131.04	123.70
22	23S1	1241	A	C5-C6-N6	9.17	131.04	123.70
1	16S1	298	A	N3-C4-C5	-9.17	120.38	126.80
22	23S1	1010	A	N3-C4-C5	-9.17	120.38	126.80
22	23S1	2589	A	N3-C4-C5	-9.16	120.39	126.80
22	23S1	1254	A	N3-C4-C5	-9.16	120.39	126.80
22	23S1	1652	A	N3-C4-C5	-9.16	120.39	126.80
22	23S1	2781	A	N3-C4-C5	-9.15	120.39	126.80
22	23S1	2860	A	N3-C4-C5	-9.15	120.39	126.80
22	23S1	1403	A	C5-C6-N6	9.15	131.02	123.70
22	23S1	2015	A	N3-C4-C5	-9.15	120.40	126.80
1	16S1	1158	C	N3-C2-O2	-9.15	115.50	121.90
22	23S1	526	A	N3-C4-C5	-9.15	120.40	126.80
1	16S1	696	A	C5-C6-N6	9.14	131.02	123.70
1	16S1	199	A	C5-C6-N6	9.14	131.01	123.70
22	23S1	1088	A	C5-N7-C8	9.14	108.47	103.90
22	23S1	1213	A	C5-C6-N6	9.14	131.01	123.70
22	23S1	2051	A	N7-C8-N9	-9.14	109.23	113.80
1	16S1	1418	A	N7-C8-N9	-9.14	109.23	113.80
1	16S1	743	A	C5-C6-N6	9.14	131.01	123.70
22	23S1	532	A	C5-N7-C8	9.13	108.47	103.90
22	23S1	282	A	N3-C4-C5	-9.13	120.41	126.80
1	16S1	1152	A	C5-C6-N6	9.13	131.00	123.70
1	16S1	1227	A	N3-C4-C5	-9.12	120.41	126.80
1	16S1	1441	A	N3-C4-C5	-9.12	120.41	126.80
22	23S1	2639	A	N3-C4-C5	-9.12	120.41	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	915	A	N3-C4-C5	-9.12	120.42	126.80
22	23S1	833	A	N7-C8-N9	-9.12	109.24	113.80
22	23S1	2814	A	N3-C4-C5	-9.12	120.42	126.80
22	23S1	2284	A	N7-C8-N9	-9.12	109.24	113.80
1	16S1	547	A	N3-C4-C5	-9.11	120.42	126.80
22	23S1	2088	A	C5-C6-N6	9.12	130.99	123.70
22	23S1	2800	A	N3-C4-C5	-9.11	120.42	126.80
22	23S1	943	A	N7-C8-N9	-9.11	109.25	113.80
22	23S1	1434	A	N9-C4-C5	9.11	109.44	105.80
1	16S1	520	A	C5-N7-C8	9.11	108.45	103.90
22	23S1	2095	A	N3-C4-C5	-9.11	120.43	126.80
22	23S1	2726	A	N3-C4-C5	-9.10	120.43	126.80
55	PTR1	9	A	N3-C4-C5	-9.10	120.43	126.80
1	16S1	935	A	C5-C6-N6	9.10	130.98	123.70
1	16S1	574	A	N3-C4-C5	-9.09	120.44	126.80
1	16S1	1396	A	C5-C6-N6	9.09	130.97	123.70
22	23S1	983	A	N3-C4-C5	-9.09	120.44	126.80
22	23S1	1226	A	N3-C4-C5	-9.09	120.44	126.80
22	23S1	1494	A	N3-C4-C5	-9.09	120.44	126.80
22	23S1	2082	A	C5-C6-N6	9.09	130.97	123.70
22	23S1	272	A	C5-C6-N6	9.09	130.97	123.70
22	23S1	1616	A	N3-C4-C5	-9.09	120.44	126.80
1	16S1	498	A	N3-C4-N9	9.08	134.66	127.40
1	16S1	489	C	C2-N1-C1'	9.07	128.78	118.80
1	16S1	356	A	C5-C6-N6	9.07	130.95	123.70
22	23S1	2542	A	C5-N7-C8	9.07	108.43	103.90
1	16S1	499	A	C5-C6-N6	9.06	130.95	123.70
1	16S1	673	A	C5-C6-N6	9.06	130.95	123.70
22	23S1	2450	A	N3-C4-C5	-9.06	120.46	126.80
22	23S1	223	A	N3-C4-C5	-9.06	120.46	126.80
1	16S1	977	A	N3-C4-N9	9.06	134.65	127.40
22	23S1	233	A	C5-C6-N6	9.06	130.95	123.70
22	23S1	1366	A	N3-C4-C5	-9.05	120.46	126.80
55	PTR1	23	A	C5-C6-N6	9.05	130.94	123.70
1	16S1	923	A	C5-C6-N6	9.05	130.94	123.70
22	23S1	1785	A	N3-C4-C5	-9.05	120.47	126.80
1	16S1	900	A	N3-C4-C5	-9.05	120.47	126.80
1	16S1	1213	A	N3-C4-C5	-9.04	120.47	126.80
22	23S1	2469	A	N3-C4-C5	-9.04	120.47	126.80
1	16S1	1216	A	N3-C4-C5	-9.04	120.47	126.80
22	23S1	515	A	N3-C4-C5	-9.03	120.48	126.80
22	23S1	911	A	N7-C8-N9	-9.03	109.28	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1313	U	C2-N1-C1'	9.03	128.54	117.70
22	23S1	332	A	N3-C4-C5	-9.03	120.48	126.80
22	23S1	603	A	N3-C4-C5	-9.03	120.48	126.80
22	23S1	2117	A	N3-C4-C5	-9.03	120.48	126.80
22	23S1	1385	A	N3-C4-C5	-9.02	120.48	126.80
22	23S1	1755	A	C5-N7-C8	9.02	108.41	103.90
22	23S1	2764	A	N3-C4-C5	-9.02	120.48	126.80
22	23S1	2900	A	C5-C6-N6	9.02	130.92	123.70
22	23S1	718	A	C5-N7-C8	9.02	108.41	103.90
1	16S1	1022	A	N7-C8-N9	-9.02	109.29	113.80
22	23S1	1286	A	N3-C4-C5	-9.02	120.49	126.80
22	23S1	1393	A	N3-C4-C5	-9.02	120.49	126.80
22	23S1	1669	A	N7-C8-N9	-9.01	109.29	113.80
1	16S1	1275	A	C5-N7-C8	9.01	108.41	103.90
1	16S1	411	A	C5-C6-N6	9.01	130.91	123.70
22	23S1	368	A	N3-C4-C5	-9.01	120.50	126.80
22	23S1	466	A	N3-C4-C5	-9.01	120.50	126.80
1	16S1	715	A	N3-C4-C5	-9.00	120.50	126.80
1	16S1	353	A	N3-C4-C5	-9.00	120.50	126.80
1	16S1	1499	A	C5-N7-C8	9.00	108.40	103.90
22	23S1	10	A	N3-C4-C5	-9.00	120.50	126.80
22	23S1	1783	A	N3-C4-C5	-9.00	120.50	126.80
22	23S1	792	A	C5-N7-C8	9.00	108.40	103.90
22	23S1	819	A	C5-C6-N6	9.00	130.90	123.70
22	23S1	751	A	N3-C4-C5	-9.00	120.50	126.80
1	16S1	155	A	C5-C6-N6	8.99	130.90	123.70
22	23S1	1096	A	C5-N7-C8	8.99	108.40	103.90
22	23S1	1434	A	N3-C4-C5	-8.99	120.51	126.80
22	23S1	2662	A	C5-C6-N6	8.99	130.89	123.70
22	23S1	53	A	N3-C4-C5	-8.98	120.51	126.80
22	23S1	91	A	N3-C4-C5	-8.98	120.52	126.80
1	16S1	151	A	C5-N7-C8	8.98	108.39	103.90
1	16S1	978	A	N3-C4-C5	-8.98	120.52	126.80
1	16S1	197	A	N3-C4-C5	-8.98	120.52	126.80
22	23S1	454	A	C5-N7-C8	8.98	108.39	103.90
22	23S1	2101	A	C5-N7-C8	8.98	108.39	103.90
22	23S1	2670	A	C5-C6-N6	8.98	130.88	123.70
22	23S1	621	A	N3-C4-C5	-8.97	120.52	126.80
22	23S1	783	A	N3-C4-N9	8.97	134.58	127.40
22	23S1	1322	A	N3-C4-C5	-8.97	120.52	126.80
22	23S1	1583	A	N3-C4-C5	-8.97	120.52	126.80
22	23S1	1970	A	C5-C6-N6	8.97	130.88	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	554	A	C5-N7-C8	8.97	108.38	103.90
1	16S1	766	A	N3-C4-C5	-8.96	120.53	126.80
22	23S1	2776	A	N3-C4-C5	-8.97	120.52	126.80
1	16S1	663	A	C5-C6-N6	8.96	130.87	123.70
23	05S1	66	A	N3-C4-C5	-8.96	120.53	126.80
1	16S1	498	A	C5-C6-N6	8.96	130.87	123.70
1	16S1	493	A	N3-C4-C5	-8.96	120.53	126.80
22	23S1	705	A	C5-C6-N6	8.96	130.86	123.70
22	23S1	203	A	N7-C8-N9	-8.95	109.32	113.80
1	16S1	77	A	C5-C6-N6	8.95	130.86	123.70
22	23S1	2765	A	N7-C8-N9	-8.95	109.33	113.80
22	23S1	825	A	C5-N7-C8	8.95	108.37	103.90
22	23S1	2117	A	C5-N7-C8	8.95	108.37	103.90
22	23S1	354	A	N3-C4-C5	-8.94	120.54	126.80
22	23S1	144	A	C5-C6-N6	8.94	130.85	123.70
22	23S1	1495	A	N3-C4-C5	-8.94	120.54	126.80
1	16S1	1163	A	C5-C6-N6	8.93	130.84	123.70
22	23S1	1469	A	C5-N7-C8	8.93	108.36	103.90
22	23S1	2336	A	N3-C4-C5	-8.93	120.55	126.80
22	23S1	1213	A	C5-N7-C8	8.92	108.36	103.90
22	23S1	2274	A	N3-C4-C5	-8.92	120.55	126.80
22	23S1	1998	A	C5-N7-C8	8.92	108.36	103.90
22	23S1	2433	A	C5-N7-C8	8.92	108.36	103.90
22	23S1	2821	A	N3-C4-C5	-8.92	120.56	126.80
1	16S1	71	A	N3-C4-C5	-8.92	120.56	126.80
22	23S1	2792	A	C5-C6-N6	8.92	130.83	123.70
22	23S1	1021	A	N3-C4-N9	8.91	134.53	127.40
22	23S1	2542	A	N3-C4-C5	-8.91	120.56	126.80
55	PTR1	73	A	N3-C4-C5	-8.91	120.56	126.80
22	23S1	2147	A	N7-C8-N9	-8.91	109.34	113.80
22	23S1	2451	A	N9-C4-C5	8.91	109.36	105.80
22	23S1	513	A	N7-C8-N9	-8.91	109.35	113.80
1	16S1	243	A	N3-C4-C5	-8.91	120.56	126.80
22	23S1	1730	C	C2-N1-C1'	8.91	128.60	118.80
1	16S1	487	A	C5-N7-C8	8.91	108.35	103.90
22	23S1	402	A	N3-C4-C5	-8.91	120.57	126.80
22	23S1	1285	A	C5-N7-C8	8.90	108.35	103.90
22	23S1	2388	A	C5-N7-C8	8.90	108.35	103.90
1	16S1	702	A	N3-C4-C5	-8.90	120.57	126.80
22	23S1	655	A	N3-C4-C5	-8.89	120.57	126.80
22	23S1	352	A	N3-C4-C5	-8.89	120.58	126.80
22	23S1	1129	A	N3-C4-C5	-8.89	120.58	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2274	A	N7-C8-N9	-8.88	109.36	113.80
22	23S1	2749	A	N3-C4-C5	-8.88	120.58	126.80
1	16S1	303	A	N3-C4-C5	-8.88	120.58	126.80
1	16S1	1285	A	N3-C4-C5	-8.88	120.58	126.80
22	23S1	2572	A	N3-C4-C5	-8.88	120.58	126.80
1	16S1	1219	A	C5-C6-N6	8.87	130.80	123.70
1	16S1	279	A	N3-C4-C5	-8.87	120.59	126.80
22	23S1	676	A	N3-C4-C5	-8.87	120.59	126.80
22	23S1	752	A	C5-N7-C8	8.87	108.33	103.90
22	23S1	241	A	N3-C4-C5	-8.87	120.59	126.80
22	23S1	1057	A	N3-C4-C5	-8.87	120.59	126.80
22	23S1	1854	A	N7-C8-N9	-8.87	109.37	113.80
22	23S1	2632	A	C5-N7-C8	8.87	108.33	103.90
22	23S1	905	A	C5-N7-C8	8.86	108.33	103.90
22	23S1	1050	A	C5-N7-C8	8.86	108.33	103.90
22	23S1	2766	A	N7-C8-N9	-8.86	109.37	113.80
22	23S1	118	A	N3-C4-C5	-8.86	120.60	126.80
1	16S1	182	A	N3-C4-C5	-8.86	120.60	126.80
1	16S1	1201	A	C5-N7-C8	8.86	108.33	103.90
22	23S1	127	A	N3-C4-C5	-8.86	120.60	126.80
22	23S1	2270	A	C5-N7-C8	8.86	108.33	103.90
22	23S1	12	U	N1-C2-O2	8.85	129.00	122.80
22	23S1	2070	A	C5-N7-C8	8.85	108.33	103.90
1	16S1	74	A	N3-C4-C5	-8.85	120.61	126.80
1	16S1	181	A	C5-C6-N6	8.85	130.78	123.70
1	16S1	583	A	N3-C4-C5	-8.85	120.61	126.80
22	23S1	1901	A	N7-C8-N9	-8.85	109.38	113.80
22	23S1	422	A	C5-C6-N6	8.85	130.78	123.70
22	23S1	668	A	N3-C4-C5	-8.85	120.61	126.80
1	16S1	3	A	N3-C4-C5	-8.84	120.61	126.80
22	23S1	764	A	N3-C4-C5	-8.84	120.61	126.80
1	16S1	675	A	N3-C4-C5	-8.84	120.61	126.80
1	16S1	1503	A	C5-N7-C8	8.84	108.32	103.90
22	23S1	563	A	C5-N7-C8	8.84	108.32	103.90
55	PTR1	14	A	C4-C5-C6	8.84	121.42	117.00
22	23S1	2077	A	C5-C6-N6	8.83	130.76	123.70
22	23S1	1395	A	N3-C4-C5	-8.83	120.62	126.80
22	23S1	1226	A	N7-C8-N9	-8.82	109.39	113.80
23	05S1	29	A	C5-N7-C8	8.82	108.31	103.90
55	PTR1	58	A	C5-N7-C8	8.82	108.31	103.90
1	16S1	1201	A	C5-C6-N1	8.82	122.11	117.70
1	16S1	687	A	N3-C4-C5	-8.82	120.63	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	373	A	C5-N7-C8	8.81	108.31	103.90
22	23S1	1427	A	N3-C4-C5	-8.81	120.63	126.80
22	23S1	1815	A	N3-C4-C5	-8.80	120.64	126.80
1	16S1	152	A	N3-C4-C5	-8.80	120.64	126.80
22	23S1	2657	A	N3-C4-C5	-8.80	120.64	126.80
22	23S1	829	A	N3-C4-C5	-8.79	120.64	126.80
1	16S1	195	A	N3-C4-C5	-8.79	120.65	126.80
22	23S1	693	A	C5-N7-C8	8.78	108.29	103.90
22	23S1	1302	A	N3-C4-C5	-8.78	120.66	126.80
1	16S1	408	A	C5-N7-C8	8.77	108.29	103.90
1	16S1	1398	A	N3-C4-C5	-8.77	120.66	126.80
22	23S1	2288	A	N3-C4-C5	-8.77	120.66	126.80
1	16S1	309	A	C5-N7-C8	8.77	108.28	103.90
22	23S1	265	A	N3-C4-C5	-8.77	120.66	126.80
1	16S1	190	A	N7-C8-N9	-8.76	109.42	113.80
1	16S1	451	A	C5-N7-C8	8.76	108.28	103.90
22	23S1	2031	A	C5-N7-C8	8.76	108.28	103.90
22	23S1	644	A	C4-C5-C6	8.76	121.38	117.00
1	16S1	1394	A	N3-C4-C5	-8.76	120.67	126.80
22	23S1	2765	A	N3-C4-N9	8.76	134.40	127.40
1	16S1	1531	A	N7-C8-N9	-8.75	109.42	113.80
22	23S1	749	A	N3-C4-C5	-8.74	120.68	126.80
1	16S1	1239	A	C5-N7-C8	8.74	108.27	103.90
22	23S1	863	A	C5-C6-N6	8.74	130.69	123.70
1	16S1	665	A	N3-C4-C5	-8.74	120.68	126.80
1	16S1	1508	A	C5-C6-N6	8.74	130.69	123.70
22	23S1	716	A	C5-N7-C8	8.74	108.27	103.90
22	23S1	1569	A	N3-C4-C5	-8.74	120.68	126.80
22	23S1	1937	A	N9-C4-C5	8.74	109.30	105.80
22	23S1	2114	A	N3-C4-N9	8.74	134.39	127.40
22	23S1	1570	A	N3-C4-C5	-8.73	120.69	126.80
22	23S1	2469	A	C5-C6-N6	8.73	130.69	123.70
22	23S1	1847	A	N7-C8-N9	-8.73	109.43	113.80
22	23S1	2189	U	C5-C6-N1	8.73	127.06	122.70
1	16S1	300	A	N3-C4-N9	8.73	134.38	127.40
1	16S1	572	A	C5-N7-C8	8.71	108.26	103.90
1	16S1	74	A	C5-N7-C8	8.71	108.25	103.90
1	16S1	478	A	C5-N7-C8	8.71	108.25	103.90
1	16S1	520	A	N9-C4-C5	8.70	109.28	105.80
22	23S1	362	A	N3-C4-N9	8.70	134.36	127.40
22	23S1	2369	A	C5-C6-N6	8.70	130.66	123.70
22	23S1	1669	A	N3-C4-N9	8.70	134.36	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1001	A	N3-C4-C5	-8.69	120.72	126.80
22	23S1	1253	A	N3-C4-C5	-8.69	120.72	126.80
55	PTR1	51	A	C5-N7-C8	8.69	108.25	103.90
22	23S1	1247	A	C5-N7-C8	8.69	108.24	103.90
1	16S1	1346	A	N3-C4-C5	-8.68	120.72	126.80
22	23S1	1829	A	C5-N7-C8	8.68	108.24	103.90
1	16S1	913	A	N3-C4-C5	-8.68	120.72	126.80
22	23S1	1545	A	N3-C4-C5	-8.68	120.72	126.80
22	23S1	2298	A	C5-N7-C8	8.68	108.24	103.90
1	16S1	563	A	N3-C4-N9	8.68	134.34	127.40
1	16S1	411	A	C5-N7-C8	8.67	108.24	103.90
22	23S1	643	A	N3-C4-C5	-8.67	120.73	126.80
22	23S1	547	A	N3-C4-C5	-8.67	120.73	126.80
55	PTR1	38	A	C5-C6-N6	8.67	130.63	123.70
1	16S1	865	A	N7-C8-N9	-8.67	109.47	113.80
22	23S1	616	A	C5-N7-C8	8.67	108.23	103.90
22	23S1	2163	A	O5'-P-OP1	-8.67	97.90	105.70
1	16S1	1046	A	C5-N7-C8	8.66	108.23	103.90
22	23S1	1630	A	C5-N7-C8	8.66	108.23	103.90
22	23S1	800	A	C5-N7-C8	8.66	108.23	103.90
22	23S1	2211	A	N3-C4-C5	-8.66	120.74	126.80
22	23S1	1237	A	N3-C4-C5	-8.66	120.74	126.80
1	16S1	223	A	C5-N7-C8	8.65	108.23	103.90
1	16S1	1360	A	C5-N7-C8	8.65	108.23	103.90
22	23S1	1610	A	N3-C4-C5	-8.65	120.74	126.80
1	16S1	1101	A	N3-C4-C5	-8.65	120.75	126.80
22	23S1	1353	A	C5-N7-C8	8.65	108.22	103.90
1	16S1	1413	A	N3-C4-C5	-8.64	120.75	126.80
22	23S1	807	U	C2-N3-C4	-8.64	121.82	127.00
22	23S1	2451	A	C5-C6-N1	8.64	122.02	117.70
1	16S1	172	A	N3-C4-C5	-8.63	120.76	126.80
1	16S1	32	A	C5-C6-N6	8.63	130.60	123.70
1	16S1	1329	A	C5-N7-C8	8.63	108.22	103.90
22	23S1	73	A	N3-C4-C5	-8.63	120.76	126.80
22	23S1	191	A	C5-N7-C8	8.63	108.22	103.90
22	23S1	204	A	N3-C4-C5	-8.63	120.76	126.80
1	16S1	509	A	C5-N7-C8	8.63	108.21	103.90
1	16S1	607	A	N3-C4-C5	-8.63	120.76	126.80
22	23S1	1791	A	N7-C8-N9	-8.63	109.48	113.80
22	23S1	547	A	C5-N7-C8	8.62	108.21	103.90
22	23S1	900	A	C5-N7-C8	8.62	108.21	103.90
1	16S1	1145	A	N3-C4-C5	-8.62	120.77	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1032	A	C5-N7-C8	8.62	108.21	103.90
23	05S1	75	G	C6-N1-C2	-8.62	119.93	125.10
1	16S1	845	A	C5-N7-C8	8.61	108.21	103.90
1	16S1	179	A	C5-N7-C8	8.61	108.20	103.90
1	16S1	1428	A	C5-N7-C8	8.60	108.20	103.90
1	16S1	975	A	N3-C4-C5	-8.60	120.78	126.80
22	23S1	2711	A	C5-N7-C8	8.60	108.20	103.90
55	PTR1	76	A	C8-N9-C4	8.60	109.24	105.80
22	23S1	2577	A	C5-N7-C8	8.59	108.20	103.90
1	16S1	459	A	C5-N7-C8	8.59	108.20	103.90
22	23S1	1676	A	N7-C8-N9	-8.59	109.50	113.80
22	23S1	2311	A	C5-N7-C8	8.59	108.20	103.90
22	23S1	2412	A	C5-N7-C8	8.59	108.19	103.90
22	23S1	1515	A	N3-C4-C5	-8.58	120.79	126.80
1	16S1	1213	A	C5-N7-C8	8.58	108.19	103.90
22	23S1	204	A	C5-N7-C8	8.56	108.18	103.90
22	23S1	2850	A	C5-N7-C8	8.56	108.18	103.90
22	23S1	2740	A	C5-N7-C8	8.56	108.18	103.90
22	23S1	1439	A	C5-N7-C8	8.56	108.18	103.90
1	16S1	19	A	C5-N7-C8	8.56	108.18	103.90
22	23S1	101	A	N3-C4-N9	8.56	134.25	127.40
22	23S1	1785	A	N7-C8-N9	-8.56	109.52	113.80
22	23S1	2887	A	C5-N7-C8	8.56	108.18	103.90
22	23S1	382	A	C5-N7-C8	8.55	108.18	103.90
1	16S1	919	A	N3-C4-C5	-8.55	120.81	126.80
22	23S1	1571	A	C4-C5-C6	8.55	121.28	117.00
22	23S1	38	A	C5-N7-C8	8.55	108.17	103.90
22	23S1	443	A	C5-N7-C8	8.55	108.17	103.90
22	23S1	750	A	C5-N7-C8	8.54	108.17	103.90
1	16S1	432	A	C5-N7-C8	8.54	108.17	103.90
1	16S1	8	A	C5-N7-C8	8.54	108.17	103.90
1	16S1	1480	A	C5-N7-C8	8.53	108.17	103.90
22	23S1	1821	A	C5-N7-C8	8.53	108.17	103.90
1	16S1	728	A	C5-N7-C8	8.53	108.17	103.90
22	23S1	2872	A	N3-C4-C5	-8.52	120.83	126.80
1	16S1	49	U	C5-C4-O4	8.52	131.01	125.90
22	23S1	538	A	C5-N7-C8	8.52	108.16	103.90
1	16S1	499	A	C5-N7-C8	8.52	108.16	103.90
22	23S1	917	A	C5-N7-C8	8.52	108.16	103.90
22	23S1	2738	A	N3-C4-C5	-8.51	120.84	126.80
22	23S1	1503	A	C5-N7-C8	8.51	108.16	103.90
1	16S1	1225	A	N3-C4-N9	8.51	134.21	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	PTR1	59	A	C5-N7-C8	8.50	108.15	103.90
22	23S1	800	A	N3-C4-C5	-8.50	120.85	126.80
22	23S1	2809	A	C5-N7-C8	8.50	108.15	103.90
1	16S1	781	A	C5-N7-C8	8.50	108.15	103.90
22	23S1	1889	A	C5-N7-C8	8.50	108.15	103.90
22	23S1	1981	A	N3-C4-C5	-8.50	120.85	126.80
1	16S1	16	A	N3-C4-C5	-8.49	120.86	126.80
1	16S1	151	A	N9-C4-C5	8.49	109.20	105.80
22	23S1	1359	A	N3-C4-C5	-8.49	120.86	126.80
22	23S1	878	A	C5-N7-C8	8.49	108.14	103.90
22	23S1	1730	C	N3-C2-O2	-8.49	115.96	121.90
22	23S1	1551	A	C5-N7-C8	8.48	108.14	103.90
1	16S1	1004	A	C4-C5-N7	-8.48	106.46	110.70
22	23S1	2448	A	N3-C4-C5	-8.47	120.87	126.80
22	23S1	119	A	N3-C4-C5	-8.47	120.87	126.80
1	16S1	784	A	C5-N7-C8	8.47	108.14	103.90
22	23S1	1571	A	C5-C6-N6	8.47	130.48	123.70
22	23S1	1021	A	C5-N7-C8	8.47	108.13	103.90
1	16S1	397	A	C4-C5-C6	8.46	121.23	117.00
22	23S1	1276	A	C5-N7-C8	8.46	108.13	103.90
22	23S1	2369	A	N7-C8-N9	-8.46	109.57	113.80
1	16S1	746	A	C5-C6-N6	8.45	130.46	123.70
22	23S1	2883	A	C5-N7-C8	8.45	108.12	103.90
1	16S1	1375	A	C5-N7-C8	8.45	108.12	103.90
22	23S1	689	A	C5-N7-C8	8.45	108.12	103.90
22	23S1	1722	A	C4-C5-C6	8.44	121.22	117.00
55	PTR1	51	A	N3-C4-C5	-8.44	120.89	126.80
1	16S1	635	A	C5-N7-C8	8.44	108.12	103.90
1	16S1	996	A	C5-N7-C8	8.44	108.12	103.90
22	23S1	513	A	C4-C5-C6	8.43	121.22	117.00
22	23S1	101	A	C4-C5-C6	8.43	121.22	117.00
1	16S1	704	A	N3-C4-C5	-8.43	120.90	126.80
22	23S1	984	A	N3-C4-N9	8.43	134.14	127.40
22	23S1	2761	A	C5-N7-C8	8.43	108.11	103.90
22	23S1	2826	A	C5-N7-C8	8.43	108.11	103.90
22	23S1	1819	A	C5-N7-C8	8.42	108.11	103.90
1	16S1	383	A	N7-C8-N9	-8.41	109.59	113.80
1	16S1	560	A	C5-N7-C8	8.41	108.11	103.90
22	23S1	1046	A	C5-N7-C8	8.41	108.11	103.90
1	16S1	1216	A	C5-N7-C8	8.41	108.11	103.90
22	23S1	278	A	N7-C8-N9	-8.41	109.59	113.80
22	23S1	2241	A	C5-N7-C8	8.41	108.11	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	120	A	C5-N7-C8	8.41	108.11	103.90
1	16S1	1151	A	C5-N7-C8	8.41	108.11	103.90
1	16S1	1152	A	N7-C8-N9	-8.41	109.59	113.80
22	23S1	819	A	C5-N7-C8	8.41	108.11	103.90
22	23S1	1783	A	C5-N7-C8	8.41	108.11	103.90
22	23S1	262	A	C5-N7-C8	8.41	108.10	103.90
22	23S1	2439	A	C5-N7-C8	8.40	108.10	103.90
22	23S1	2726	A	C5-N7-C8	8.40	108.10	103.90
23	05S1	34	A	C5-N7-C8	8.40	108.10	103.90
22	23S1	1784	A	N3-C4-C5	-8.40	120.92	126.80
1	16S1	1067	A	C5-N7-C8	8.39	108.10	103.90
1	16S1	1250	A	C5-N7-C8	8.39	108.09	103.90
22	23S1	2198	A	N3-C4-C5	-8.39	120.93	126.80
1	16S1	44	A	C5-N7-C8	8.39	108.09	103.90
22	23S1	1205	A	N3-C4-C5	-8.39	120.93	126.80
22	23S1	1378	A	C5-N7-C8	8.39	108.09	103.90
23	05S1	45	A	C5-C6-N6	8.39	130.41	123.70
23	05S1	104	A	C5-N7-C8	8.39	108.09	103.90
22	23S1	101	A	C5-N7-C8	8.38	108.09	103.90
22	23S1	222	A	C5-N7-C8	8.38	108.09	103.90
22	23S1	1652	A	C5-N7-C8	8.38	108.09	103.90
22	23S1	165	A	C5-N7-C8	8.38	108.09	103.90
22	23S1	586	A	N3-C4-C5	-8.38	120.93	126.80
22	23S1	973	A	N7-C8-N9	-8.38	109.61	113.80
22	23S1	2227	A	C5-N7-C8	8.38	108.09	103.90
22	23S1	1069	A	C5-N7-C8	8.38	108.09	103.90
22	23S1	2776	A	C5-N7-C8	8.38	108.09	103.90
22	23S1	2564	A	C5-N7-C8	8.38	108.09	103.90
1	16S1	10	A	C5-N7-C8	8.37	108.09	103.90
22	23S1	1928	A	C5-N7-C8	8.38	108.09	103.90
1	16S1	431	A	N9-C4-C5	8.37	109.15	105.80
22	23S1	981	A	N3-C4-C5	-8.37	120.94	126.80
22	23S1	104	A	C5-N7-C8	8.37	108.09	103.90
22	23S1	2882	A	C5-N7-C8	8.37	108.08	103.90
22	23S1	2447	G	C6-N1-C2	-8.37	120.08	125.10
1	16S1	1101	A	C5-N7-C8	8.37	108.08	103.90
22	23S1	354	A	C5-N7-C8	8.36	108.08	103.90
22	23S1	1287	A	C5-N7-C8	8.36	108.08	103.90
1	16S1	640	A	C5-N7-C8	8.36	108.08	103.90
22	23S1	2003	A	C5-N7-C8	8.36	108.08	103.90
22	23S1	2014	A	C5-N7-C8	8.36	108.08	103.90
22	23S1	2736	A	C5-N7-C8	8.36	108.08	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	12	U	C2-N1-C1'	8.36	127.73	117.70
1	16S1	274	A	C5-N7-C8	8.36	108.08	103.90
1	16S1	1225	A	C5-N7-C8	8.36	108.08	103.90
1	16S1	468	A	C5-N7-C8	8.35	108.08	103.90
1	16S1	648	A	C5-N7-C8	8.35	108.08	103.90
22	23S1	2682	A	C5-N7-C8	8.35	108.08	103.90
22	23S1	1597	A	C5-N7-C8	8.35	108.08	103.90
22	23S1	866	A	C5-N7-C8	8.35	108.07	103.90
22	23S1	1808	A	N3-C4-C5	-8.35	120.96	126.80
22	23S1	821	A	N3-C4-C5	-8.35	120.96	126.80
1	16S1	1251	A	C5-N7-C8	8.35	108.07	103.90
22	23S1	984	A	C5-N7-C8	8.35	108.07	103.90
22	23S1	2725	A	C5-C6-N6	8.35	130.38	123.70
22	23S1	2590	A	N3-C4-C5	-8.34	120.96	126.80
22	23S1	19	A	C5-N7-C8	8.34	108.07	103.90
22	23S1	933	A	N3-C4-N9	8.34	134.07	127.40
22	23S1	2665	A	C5-N7-C8	8.33	108.07	103.90
1	16S1	533	A	N3-C4-N9	8.33	134.07	127.40
22	23S1	1272	A	N3-C4-C5	-8.33	120.97	126.80
22	23S1	2173	A	N3-C4-N9	8.33	134.06	127.40
1	16S1	498	A	C5-N7-C8	8.32	108.06	103.90
22	23S1	196	A	C5-N7-C8	8.32	108.06	103.90
22	23S1	1566	A	C5-N7-C8	8.32	108.06	103.90
22	23S1	1810	A	N3-C4-N9	8.32	134.06	127.40
22	23S1	677	A	C5-C6-N6	8.32	130.36	123.70
1	16S1	495	A	C5-N7-C8	8.32	108.06	103.90
22	23S1	1722	A	C5-C6-N6	8.31	130.35	123.70
22	23S1	1241	A	C4-C5-C6	8.31	121.16	117.00
22	23S1	2887	A	N9-C4-C5	8.31	109.12	105.80
1	16S1	60	A	C5-N7-C8	8.31	108.06	103.90
22	23S1	2560	A	C5-N7-C8	8.31	108.05	103.90
1	16S1	197	A	C5-N7-C8	8.30	108.05	103.90
1	16S1	1410	A	C5-N7-C8	8.30	108.05	103.90
22	23S1	103	A	C5-N7-C8	8.30	108.05	103.90
22	23S1	1664	A	C5-N7-C8	8.30	108.05	103.90
22	23S1	1754	A	N3-C4-C5	-8.30	120.99	126.80
22	23S1	2328	A	N7-C8-N9	-8.30	109.65	113.80
22	23S1	2883	A	N3-C4-C5	-8.30	120.99	126.80
22	23S1	1342	A	C5-N7-C8	8.29	108.05	103.90
22	23S1	1509	A	C5-N7-C8	8.30	108.05	103.90
22	23S1	2837	A	C5-N7-C8	8.29	108.05	103.90
22	23S1	181	A	C5-N7-C8	8.29	108.05	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	804	A	C5-N7-C8	8.29	108.04	103.90
23	05S1	101	A	C5-N7-C8	8.29	108.04	103.90
22	23S1	2565	A	C5-N7-C8	8.29	108.04	103.90
22	23S1	482	A	N3-C4-N9	8.28	134.03	127.40
22	23S1	1502	A	C5-N7-C8	8.28	108.04	103.90
22	23S1	2602	A	C5-N7-C8	8.28	108.04	103.90
1	16S1	1513	A	C5-N7-C8	8.28	108.04	103.90
22	23S1	1009	A	C5-N7-C8	8.28	108.04	103.90
22	23S1	371	A	C5-N7-C8	8.28	108.04	103.90
22	23S1	1848	A	N7-C8-N9	-8.27	109.66	113.80
22	23S1	1420	A	C5-N7-C8	8.27	108.03	103.90
1	16S1	1093	A	C5-N7-C8	8.27	108.03	103.90
1	16S1	1180	A	C5-N7-C8	8.27	108.03	103.90
22	23S1	71	A	C5-N7-C8	8.27	108.03	103.90
22	23S1	1073	A	C5-N7-C8	8.27	108.03	103.90
22	23S1	1133	A	C5-N7-C8	8.27	108.03	103.90
22	23S1	1928	A	N3-C4-C5	-8.27	121.01	126.80
22	23S1	2273	A	C5-N7-C8	8.27	108.03	103.90
1	16S1	149	A	C5-N7-C8	8.27	108.03	103.90
1	16S1	681	A	C5-N7-C8	8.27	108.03	103.90
22	23S1	532	A	N3-C4-N9	8.26	134.01	127.40
22	23S1	1385	A	C5-N7-C8	8.26	108.03	103.90
22	23S1	412	A	C5-N7-C8	8.26	108.03	103.90
22	23S1	2205	A	C5-N7-C8	8.26	108.03	103.90
1	16S1	162	A	N3-C4-N9	8.26	134.01	127.40
1	16S1	320	A	C5-N7-C8	8.26	108.03	103.90
22	23S1	42	A	C5-N7-C8	8.26	108.03	103.90
22	23S1	756	A	C5-N7-C8	8.26	108.03	103.90
22	23S1	2317	A	C5-N7-C8	8.26	108.03	103.90
1	16S1	1333	A	C5-N7-C8	8.26	108.03	103.90
22	23S1	483	A	C5-N7-C8	8.26	108.03	103.90
22	23S1	1029	A	C4-C5-C6	8.26	121.13	117.00
22	23S1	322	A	C5-N7-C8	8.25	108.03	103.90
22	23S1	1095	A	C5-N7-C8	8.25	108.03	103.90
22	23S1	1749	A	C5-N7-C8	8.25	108.03	103.90
22	23S1	1853	A	C5-N7-C8	8.25	108.03	103.90
1	16S1	914	A	N3-C4-C5	-8.25	121.03	126.80
22	23S1	352	A	C5-N7-C8	8.25	108.02	103.90
22	23S1	783	A	C5-N7-C8	8.25	108.02	103.90
22	23S1	2095	A	C5-N7-C8	8.25	108.02	103.90
22	23S1	457	A	N3-C4-C5	-8.24	121.03	126.80
22	23S1	753	A	C5-N7-C8	8.24	108.02	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1201	A	N3-C4-N9	8.24	134.00	127.40
23	05S1	78	A	C5-N7-C8	8.24	108.02	103.90
22	23S1	1802	A	C4-C5-C6	8.24	121.12	117.00
22	23S1	2094	A	C5-N7-C8	8.24	108.02	103.90
22	23S1	2435	A	C5-N7-C8	8.24	108.02	103.90
1	16S1	53	A	C5-N7-C8	8.23	108.02	103.90
22	23S1	960	A	N3-C4-N9	8.23	133.99	127.40
22	23S1	507	A	N3-C4-C5	-8.23	121.04	126.80
1	16S1	131	A	C5-N7-C8	8.23	108.02	103.90
1	16S1	171	A	C5-N7-C8	8.23	108.01	103.90
22	23S1	1805	A	C5-N7-C8	8.23	108.01	103.90
1	16S1	246	A	C5-N7-C8	8.22	108.01	103.90
22	23S1	2461	A	C5-N7-C8	8.22	108.01	103.90
22	23S1	89	A	C5-N7-C8	8.22	108.01	103.90
22	23S1	1876	A	C5-N7-C8	8.22	108.01	103.90
22	23S1	279	A	C5-N7-C8	8.21	108.01	103.90
1	16S1	767	A	C5-N7-C8	8.21	108.01	103.90
1	16S1	1197	A	C5-N7-C8	8.21	108.01	103.90
22	23S1	670	A	C5-N7-C8	8.21	108.01	103.90
22	23S1	960	A	C5-N7-C8	8.21	108.00	103.90
22	23S1	1230	A	C5-N7-C8	8.21	108.00	103.90
22	23S1	2142	A	N3-C4-N9	8.21	133.97	127.40
22	23S1	1272	A	C8-N9-C4	8.20	109.08	105.80
22	23S1	1913	A	C5-N7-C8	8.20	108.00	103.90
22	23S1	2191	A	N7-C8-N9	-8.20	109.70	113.80
22	23S1	310	A	C5-N7-C8	8.20	108.00	103.90
22	23S1	1048	A	C5-N7-C8	8.20	108.00	103.90
1	16S1	167	A	C5-N7-C8	8.20	108.00	103.90
22	23S1	528	A	C5-N7-C8	8.20	108.00	103.90
22	23S1	1084	A	C5-N7-C8	8.19	108.00	103.90
1	16S1	411	A	C8-N9-C4	8.19	109.08	105.80
22	23S1	2453	A	C5-N7-C8	8.18	107.99	103.90
1	16S1	994	A	C5-N7-C8	8.18	107.99	103.90
22	23S1	1669	A	C5-N7-C8	8.18	107.99	103.90
1	16S1	199	A	C5-N7-C8	8.18	107.99	103.90
22	23S1	1067	A	C5-N7-C8	8.18	107.99	103.90
22	23S1	213	A	C5-N7-C8	8.18	107.99	103.90
22	23S1	460	A	C5-N7-C8	8.17	107.99	103.90
1	16S1	759	A	C5-N7-C8	8.17	107.99	103.90
1	16S1	1340	A	C5-N7-C8	8.17	107.99	103.90
22	23S1	782	A	C5-N7-C8	8.17	107.99	103.90
1	16S1	1311	A	C5-N7-C8	8.17	107.98	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	908	A	C5-N7-C8	8.16	107.98	103.90
1	16S1	356	A	C5-N7-C8	8.16	107.98	103.90
1	16S1	1055	A	C5-N7-C8	8.16	107.98	103.90
22	23S1	161	A	N3-C4-C5	-8.16	121.08	126.80
22	23S1	2212	A	C5-N7-C8	8.16	107.98	103.90
22	23S1	1937	A	C4-C5-N7	-8.16	106.62	110.70
22	23S1	2176	A	N7-C8-N9	-8.16	109.72	113.80
1	16S1	533	A	C4-C5-C6	8.16	121.08	117.00
1	16S1	1005	A	C5-N7-C8	8.16	107.98	103.90
1	16S1	1377	A	C5-N7-C8	8.16	107.98	103.90
22	23S1	1634	A	C5-N7-C8	8.16	107.98	103.90
22	23S1	1858	A	C5-N7-C8	8.16	107.98	103.90
1	16S1	155	A	C5-N7-C8	8.15	107.98	103.90
22	23S1	637	A	C5-N7-C8	8.15	107.98	103.90
22	23S1	2758	A	C5-N7-C8	8.15	107.98	103.90
1	16S1	51	A	C4-C5-C6	8.15	121.08	117.00
1	16S1	1229	A	C5-N7-C8	8.15	107.98	103.90
1	16S1	1257	A	C5-N7-C8	8.15	107.97	103.90
1	16S1	729	A	C5-N7-C8	8.15	107.97	103.90
22	23S1	1690	A	C5-N7-C8	8.15	107.97	103.90
22	23S1	2378	A	C5-N7-C8	8.15	107.97	103.90
22	23S1	783	A	N7-C8-N9	-8.14	109.73	113.80
1	16S1	478	A	N3-C4-N9	8.14	133.91	127.40
1	16S1	1105	A	C5-N7-C8	8.14	107.97	103.90
22	23S1	2060	A	N3-C4-C5	-8.14	121.10	126.80
1	16S1	1067	A	N3-C4-C5	-8.14	121.11	126.80
22	23S1	2033	A	C5-N7-C8	8.14	107.97	103.90
22	23S1	2082	A	C5-N7-C8	8.13	107.97	103.90
1	16S1	238	A	C5-N7-C8	8.13	107.97	103.90
1	16S1	1170	A	N3-C4-N9	8.13	133.91	127.40
1	16S1	1408	A	C5-N7-C8	8.13	107.97	103.90
22	23S1	1772	A	C5-N7-C8	8.13	107.97	103.90
22	23S1	2600	A	C5-N7-C8	8.13	107.97	103.90
22	23S1	5	A	C5-N7-C8	8.13	107.96	103.90
22	23S1	52	A	C5-N7-C8	8.13	107.96	103.90
22	23S1	251	A	C5-C6-N6	8.13	130.20	123.70
22	23S1	613	A	C5-N7-C8	8.13	107.96	103.90
22	23S1	910	A	C5-N7-C8	8.13	107.96	103.90
22	23S1	1419	A	N3-C4-C5	-8.13	121.11	126.80
22	23S1	1722	A	C5-N7-C8	8.13	107.96	103.90
1	16S1	80	A	C5-N7-C8	8.13	107.96	103.90
1	16S1	676	A	C5-N7-C8	8.12	107.96	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1456	A	C5-N7-C8	8.12	107.96	103.90
22	23S1	2820	A	C5-N7-C8	8.12	107.96	103.90
1	16S1	349	A	C5-N7-C8	8.12	107.96	103.90
1	16S1	274	A	C8-N9-C4	8.12	109.05	105.80
22	23S1	1098	A	C4-C5-C6	8.12	121.06	117.00
22	23S1	1669	A	C4-C5-C6	8.12	121.06	117.00
23	05S1	46	A	N3-C4-C5	-8.12	121.12	126.80
22	23S1	172	A	C5-N7-C8	8.12	107.96	103.90
22	23S1	1854	A	C5-C6-N6	8.12	130.19	123.70
22	23S1	522	A	C5-N7-C8	8.11	107.96	103.90
22	23S1	2821	A	C5-N7-C8	8.12	107.96	103.90
22	23S1	1668	A	C5-N7-C8	8.11	107.96	103.90
1	16S1	959	A	N7-C8-N9	-8.11	109.75	113.80
22	23S1	1304	A	C5-N7-C8	8.11	107.95	103.90
23	05S1	115	A	C5-N7-C8	8.11	107.95	103.90
1	16S1	915	A	C5-N7-C8	8.11	107.95	103.90
22	23S1	1453	A	C5-N7-C8	8.11	107.95	103.90
22	23S1	480	A	C5-N7-C8	8.10	107.95	103.90
22	23S1	2733	A	C5-N7-C8	8.10	107.95	103.90
22	23S1	278	A	N3-C4-N9	8.10	133.88	127.40
22	23S1	1504	A	C5-N7-C8	8.10	107.95	103.90
1	16S1	431	A	C5-N7-C8	8.10	107.95	103.90
1	16S1	958	A	C5-N7-C8	8.10	107.95	103.90
22	23S1	471	A	C5-N7-C8	8.10	107.95	103.90
22	23S1	1637	A	C5-N7-C8	8.10	107.95	103.90
22	23S1	1241	A	C5-N7-C8	8.09	107.95	103.90
22	23S1	1494	A	C5-N7-C8	8.09	107.95	103.90
22	23S1	497	A	C5-N7-C8	8.09	107.95	103.90
22	23S1	1039	A	C5-N7-C8	8.09	107.95	103.90
22	23S1	2518	A	N3-C4-N9	8.09	133.87	127.40
22	23S1	2314	A	C5-N7-C8	8.09	107.94	103.90
1	16S1	1248	A	C5-N7-C8	8.09	107.94	103.90
22	23S1	391	A	C5-N7-C8	8.09	107.94	103.90
22	23S1	2225	A	C5-N7-C8	8.09	107.94	103.90
22	23S1	1885	A	C5-N7-C8	8.08	107.94	103.90
29	L091	122	LEU	CA-CB-CG	8.08	133.89	115.30
22	23S1	1981	A	C5-N7-C8	8.08	107.94	103.90
22	23S1	1583	A	C5-N7-C8	8.08	107.94	103.90
22	23S1	1789	A	C5-N7-C8	8.08	107.94	103.90
22	23S1	2425	A	C5-N7-C8	8.08	107.94	103.90
22	23S1	449	A	C5-N7-C8	8.08	107.94	103.90
22	23S1	270	A	C5-N7-C8	8.07	107.94	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2005	A	C5-N7-C8	8.07	107.94	103.90
22	23S1	2134	A	C5-N7-C8	8.07	107.94	103.90
1	16S1	374	A	C5-N7-C8	8.07	107.94	103.90
22	23S1	432	A	C5-N7-C8	8.07	107.94	103.90
1	16S1	909	A	C5-N7-C8	8.07	107.93	103.90
1	16S1	918	A	C5-N7-C8	8.07	107.93	103.90
23	05S1	39	A	C5-N7-C8	8.07	107.93	103.90
22	23S1	936	A	C5-N7-C8	8.06	107.93	103.90
23	05S1	119	A	C5-N7-C8	8.06	107.93	103.90
1	16S1	1239	A	N3-C4-C5	-8.06	121.16	126.80
1	16S1	430	A	C5-N7-C8	8.06	107.93	103.90
1	16S1	243	A	C5-N7-C8	8.06	107.93	103.90
22	23S1	1307	A	C5-N7-C8	8.06	107.93	103.90
1	16S1	696	A	N7-C8-N9	-8.06	109.77	113.80
22	23S1	1088	A	C4-C5-C6	8.06	121.03	117.00
1	16S1	860	A	C4-C5-C6	8.05	121.03	117.00
22	23S1	347	A	C5-N7-C8	8.05	107.93	103.90
1	16S1	600	A	C5-N7-C8	8.05	107.93	103.90
22	23S1	1367	A	C5-N7-C8	8.05	107.93	103.90
22	23S1	1553	A	C5-N7-C8	8.05	107.93	103.90
1	16S1	768	A	C5-N7-C8	8.05	107.92	103.90
22	23S1	1739	A	N7-C8-N9	-8.05	109.78	113.80
1	16S1	1493	A	C5-N7-C8	8.05	107.92	103.90
22	23S1	44	A	C5-N7-C8	8.05	107.92	103.90
22	23S1	1802	A	C5-N7-C8	8.05	107.92	103.90
22	23S1	1759	A	C5-N7-C8	8.04	107.92	103.90
22	23S1	2764	A	C5-N7-C8	8.04	107.92	103.90
22	23S1	2835	A	C5-N7-C8	8.05	107.92	103.90
1	16S1	431	A	N3-C4-C5	-8.04	121.17	126.80
1	16S1	1468	A	C5-C6-N6	8.04	130.13	123.70
22	23S1	345	A	C5-N7-C8	8.04	107.92	103.90
22	23S1	111	A	C5-N7-C8	8.04	107.92	103.90
23	05S1	58	A	C5-N7-C8	8.04	107.92	103.90
22	23S1	1794	A	C5-N7-C8	8.04	107.92	103.90
1	16S1	1019	A	C5-N7-C8	8.04	107.92	103.90
22	23S1	507	A	N7-C8-N9	-8.04	109.78	113.80
22	23S1	627	A	C5-N7-C8	8.03	107.92	103.90
22	23S1	404	A	N3-C4-C5	-8.03	121.18	126.80
1	16S1	831	A	C5-N7-C8	8.03	107.92	103.90
22	23S1	278	A	C4-C5-C6	8.03	121.01	117.00
22	23S1	430	A	C5-N7-C8	8.03	107.92	103.90
22	23S1	734	A	C5-N7-C8	8.03	107.92	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	781	A	C5-N7-C8	8.03	107.91	103.90
1	16S1	695	A	C5-N7-C8	8.03	107.91	103.90
22	23S1	190	A	C5-N7-C8	8.03	107.91	103.90
22	23S1	1194	A	C5-N7-C8	8.03	107.91	103.90
22	23S1	1147	A	C5-N7-C8	8.02	107.91	103.90
22	23S1	1872	A	N3-C4-N9	8.02	133.82	127.40
22	23S1	1960	A	C5-N7-C8	8.02	107.91	103.90
22	23S1	2267	A	N3-C4-N9	8.02	133.82	127.40
22	23S1	1434	A	C4-C5-N7	-8.02	106.69	110.70
22	23S1	1640	A	C5-N7-C8	8.02	107.91	103.90
22	23S1	2430	A	N3-C4-C5	-8.02	121.19	126.80
22	23S1	1111	A	C5-N7-C8	8.01	107.91	103.90
1	16S1	55	A	C4-C5-C6	8.01	121.01	117.00
22	23S1	1246	A	C5-N7-C8	8.01	107.91	103.90
1	16S1	489	C	N1-C2-O2	8.01	123.71	118.90
1	16S1	825	A	C5-N7-C8	8.01	107.91	103.90
1	16S1	1035	A	C5-N7-C8	8.01	107.90	103.90
22	23S1	311	A	C5-N7-C8	8.01	107.90	103.90
1	16S1	1246	A	C5-N7-C8	8.00	107.90	103.90
22	23S1	2727	A	C5-N7-C8	8.00	107.90	103.90
22	23S1	820	A	C5-N7-C8	8.00	107.90	103.90
22	23S1	1596	A	C5-N7-C8	8.00	107.90	103.90
1	16S1	596	A	C5-N7-C8	8.00	107.90	103.90
20	S201	86	LEU	CA-CB-CG	7.99	133.69	115.30
22	23S1	1090	A	C5-N7-C8	7.99	107.90	103.90
22	23S1	1505	A	C5-N7-C8	7.99	107.90	103.90
22	23S1	2646	C	C6-N1-C2	-7.99	117.10	120.30
1	16S1	892	A	C5-N7-C8	7.99	107.90	103.90
1	16S1	441	A	C5-N7-C8	7.99	107.90	103.90
1	16S1	489	C	N3-C2-O2	-7.99	116.31	121.90
1	16S1	969	A	C5-N7-C8	7.99	107.90	103.90
22	23S1	793	A	C5-N7-C8	7.99	107.89	103.90
22	23S1	1890	A	C5-N7-C8	7.99	107.89	103.90
22	23S1	2590	A	C5-N7-C8	7.99	107.90	103.90
22	23S1	2766	A	C5-C6-N6	7.99	130.09	123.70
1	16S1	642	A	C5-N7-C8	7.99	107.89	103.90
1	16S1	743	A	C5-N7-C8	7.99	107.89	103.90
22	23S1	161	A	C5-N7-C8	7.99	107.89	103.90
22	23S1	2060	A	C5-N7-C8	7.99	107.89	103.90
55	PTR1	73	A	C5-N7-C8	7.99	107.89	103.90
22	23S1	320	A	C4-C5-N7	-7.99	106.71	110.70
22	23S1	1040	A	C5-N7-C8	7.99	107.89	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1189	A	C5-N7-C8	7.98	107.89	103.90
1	16S1	366	A	C5-N7-C8	7.98	107.89	103.90
1	16S1	371	A	C5-N7-C8	7.98	107.89	103.90
1	16S1	1196	A	C5-N7-C8	7.98	107.89	103.90
22	23S1	979	A	C5-N7-C8	7.98	107.89	103.90
22	23S1	1336	A	C5-N7-C8	7.98	107.89	103.90
22	23S1	2530	A	C5-N7-C8	7.98	107.89	103.90
22	23S1	1070	A	C5-N7-C8	7.98	107.89	103.90
22	23S1	655	A	C5-N7-C8	7.98	107.89	103.90
22	23S1	1936	A	N3-C4-N9	7.98	133.78	127.40
1	16S1	1170	A	C5-C6-N6	7.97	130.08	123.70
22	23S1	1000	A	C5-N7-C8	7.97	107.89	103.90
22	23S1	1086	A	C5-N7-C8	7.97	107.89	103.90
22	23S1	2158	A	C5-N7-C8	7.97	107.89	103.90
1	16S1	364	A	C5-N7-C8	7.97	107.88	103.90
22	23S1	861	A	C5-N7-C8	7.97	107.88	103.90
1	16S1	579	A	C5-N7-C8	7.97	107.88	103.90
1	16S1	807	A	C5-N7-C8	7.97	107.88	103.90
22	23S1	492	A	C4-C5-C6	7.97	120.98	117.00
22	23S1	2778	A	C5-N7-C8	7.97	107.88	103.90
1	16S1	1271	A	C5-N7-C8	7.96	107.88	103.90
1	16S1	1441	A	C5-N7-C8	7.96	107.88	103.90
22	23S1	1392	A	C5-N7-C8	7.96	107.88	103.90
1	16S1	415	A	C5-N7-C8	7.96	107.88	103.90
22	23S1	1936	A	C4-C5-C6	7.96	120.98	117.00
22	23S1	182	A	C5-N7-C8	7.96	107.88	103.90
22	23S1	2335	A	C5-N7-C8	7.96	107.88	103.90
22	23S1	1490	A	N3-C4-N9	7.96	133.77	127.40
1	16S1	228	A	C5-N7-C8	7.96	107.88	103.90
22	23S1	2534	A	C5-N7-C8	7.96	107.88	103.90
1	16S1	938	A	C5-N7-C8	7.95	107.88	103.90
22	23S1	508	A	C5-N7-C8	7.95	107.87	103.90
22	23S1	1088	A	N3-C4-N9	7.95	133.76	127.40
1	16S1	1299	A	N3-C4-N9	7.95	133.76	127.40
22	23S1	819	A	C4-C5-C6	7.95	120.97	117.00
22	23S1	1635	A	C5-N7-C8	7.95	107.87	103.90
22	23S1	2406	A	C5-N7-C8	7.94	107.87	103.90
22	23S1	1272	A	C5-N7-C8	7.94	107.87	103.90
22	23S1	2088	A	C5-N7-C8	7.94	107.87	103.90
22	23S1	2322	A	C5-N7-C8	7.94	107.87	103.90
22	23S1	330	A	C5-N7-C8	7.94	107.87	103.90
22	23S1	2750	A	C5-N7-C8	7.94	107.87	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1368	A	C5-N7-C8	7.94	107.87	103.90
22	23S1	160	A	C5-N7-C8	7.94	107.87	103.90
22	23S1	513	A	C5-C6-N6	7.94	130.05	123.70
22	23S1	749	A	C5-N7-C8	7.94	107.87	103.90
22	23S1	820	A	C4-C5-C6	7.94	120.97	117.00
22	23S1	1525	A	C5-N7-C8	7.94	107.87	103.90
29	L091	54	LEU	CA-CB-CG	7.94	133.56	115.30
22	23S1	1021	A	C4-C5-C6	7.93	120.97	117.00
22	23S1	2042	A	C5-N7-C8	7.93	107.87	103.90
55	PTR1	26	A	C5-N7-C8	7.93	107.87	103.90
1	16S1	162	A	N7-C8-N9	-7.93	109.83	113.80
22	23S1	1579	A	C5-N7-C8	7.93	107.87	103.90
22	23S1	479	A	C5-N7-C8	7.93	107.86	103.90
22	23S1	789	A	C5-N7-C8	7.93	107.86	103.90
22	23S1	505	A	C5-N7-C8	7.93	107.86	103.90
22	23S1	608	A	C5-N7-C8	7.93	107.86	103.90
22	23S1	715	A	C5-N7-C8	7.93	107.86	103.90
22	23S1	1268	A	C5-N7-C8	7.93	107.86	103.90
22	23S1	1347	A	C5-N7-C8	7.93	107.86	103.90
22	23S1	439	A	C5-N7-C8	7.92	107.86	103.90
1	16S1	192	A	C5-N7-C8	7.92	107.86	103.90
22	23S1	632	A	C5-N7-C8	7.92	107.86	103.90
22	23S1	1689	A	C5-N7-C8	7.92	107.86	103.90
22	23S1	197	A	C5-N7-C8	7.92	107.86	103.90
22	23S1	802	A	C5-N7-C8	7.92	107.86	103.90
22	23S1	1572	A	C5-N7-C8	7.92	107.86	103.90
22	23S1	2171	A	C5-C6-N6	7.92	130.03	123.70
22	23S1	541	A	C5-N7-C8	7.92	107.86	103.90
22	23S1	1927	A	C5-N7-C8	7.92	107.86	103.90
22	23S1	2468	A	C5-N7-C8	7.92	107.86	103.90
1	16S1	81	A	C5-N7-C8	7.92	107.86	103.90
1	16S1	325	A	C5-N7-C8	7.92	107.86	103.90
1	16S1	547	A	C5-N7-C8	7.92	107.86	103.90
1	16S1	907	A	C5-N7-C8	7.91	107.86	103.90
1	16S1	205	A	C5-N7-C8	7.91	107.86	103.90
22	23S1	167	A	C5-N7-C8	7.91	107.86	103.90
22	23S1	735	A	C5-N7-C8	7.91	107.86	103.90
22	23S1	2381	A	C5-N7-C8	7.91	107.86	103.90
1	16S1	553	A	C5-N7-C8	7.91	107.85	103.90
22	23S1	324	A	C5-C6-N6	7.91	130.03	123.70
22	23S1	1366	A	C5-N7-C8	7.91	107.85	103.90
1	16S1	435	A	C5-N7-C8	7.91	107.85	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1012	A	C5-N7-C8	7.91	107.85	103.90
1	16S1	1256	A	C5-N7-C8	7.91	107.85	103.90
22	23S1	1528	A	C5-N7-C8	7.91	107.85	103.90
22	23S1	1665	A	C5-N7-C8	7.91	107.85	103.90
55	PTR1	17	U	N1-C2-O2	7.91	128.33	122.80
22	23S1	21	A	C5-N7-C8	7.90	107.85	103.90
1	16S1	1431	A	C5-N7-C8	7.90	107.85	103.90
22	23S1	502	A	C5-N7-C8	7.90	107.85	103.90
1	16S1	412	A	N3-C4-C5	-7.90	121.27	126.80
22	23S1	1213	A	C4-C5-C6	7.90	120.95	117.00
1	16S1	389	A	N3-C4-N9	7.90	133.72	127.40
1	16S1	946	A	C5-N7-C8	7.90	107.85	103.90
22	23S1	256	A	C5-N7-C8	7.89	107.85	103.90
22	23S1	1528	A	C5-C6-N6	7.89	130.01	123.70
1	16S1	263	A	C5-N7-C8	7.89	107.84	103.90
1	16S1	393	A	C5-N7-C8	7.89	107.85	103.90
22	23S1	6	A	C5-N7-C8	7.89	107.85	103.90
22	23S1	2126	A	C5-N7-C8	7.89	107.85	103.90
1	16S1	383	A	N1-C6-N6	-7.89	113.87	118.60
1	16S1	878	A	C5-N7-C8	7.89	107.84	103.90
22	23S1	2572	A	C8-N9-C4	7.89	108.95	105.80
1	16S1	298	A	C5-N7-C8	7.89	107.84	103.90
1	16S1	1534	A	C5-N7-C8	7.89	107.84	103.90
22	23S1	2287	A	N3-C4-N9	7.89	133.71	127.40
1	16S1	95	C	N3-C2-O2	-7.88	116.38	121.90
1	16S1	1000	A	C5-N7-C8	7.88	107.84	103.90
1	16S1	1213	A	N9-C4-C5	7.88	108.95	105.80
22	23S1	556	A	C5-N7-C8	7.88	107.84	103.90
22	23S1	1786	A	C5-N7-C8	7.88	107.84	103.90
1	16S1	1465	A	C5-N7-C8	7.88	107.84	103.90
22	23S1	1098	A	C5-N7-C8	7.88	107.84	103.90
22	23S1	1490	A	C5-N7-C8	7.88	107.84	103.90
1	16S1	1349	A	C5-N7-C8	7.88	107.84	103.90
22	23S1	447	A	C5-N7-C8	7.88	107.84	103.90
22	23S1	453	A	C5-N7-C8	7.88	107.84	103.90
1	16S1	1287	A	C5-N7-C8	7.88	107.84	103.90
22	23S1	217	A	C5-N7-C8	7.88	107.84	103.90
55	PTR1	42	A	C5-N7-C8	7.88	107.84	103.90
1	16S1	465	A	C5-N7-C8	7.88	107.84	103.90
22	23S1	2566	A	N3-C4-C5	-7.88	121.29	126.80
22	23S1	1591	A	C5-N7-C8	7.87	107.84	103.90
22	23S1	2700	A	C5-N7-C8	7.87	107.84	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	PTR1	17	U	N3-C4-C5	7.87	119.32	114.60
1	16S1	288	A	C5-N7-C8	7.87	107.84	103.90
22	23S1	255	A	C5-N7-C8	7.87	107.83	103.90
22	23S1	1365	A	C5-N7-C8	7.87	107.84	103.90
22	23S1	2062	A	C5-N7-C8	7.87	107.84	103.90
55	PTR1	76	A	N3-C4-C5	-7.87	121.29	126.80
22	23S1	2327	A	C5-N7-C8	7.87	107.83	103.90
1	16S1	321	A	C5-N7-C8	7.87	107.83	103.90
22	23S1	1328	A	C5-N7-C8	7.87	107.83	103.90
22	23S1	1545	A	C5-N7-C8	7.87	107.83	103.90
1	16S1	901	A	C5-C6-N6	7.86	129.99	123.70
22	23S1	1641	A	C5-N7-C8	7.86	107.83	103.90
22	23S1	2135	A	C5-N7-C8	7.86	107.83	103.90
1	16S1	389	A	C5-N7-C8	7.86	107.83	103.90
1	16S1	1418	A	C4-C5-C6	7.86	120.93	117.00
22	23S1	2071	A	C5-N7-C8	7.86	107.83	103.90
23	05S1	50	A	C5-N7-C8	7.85	107.83	103.90
22	23S1	2471	A	C5-N7-C8	7.85	107.83	103.90
1	16S1	313	A	C5-N7-C8	7.85	107.83	103.90
22	23S1	677	A	N3-C4-N9	7.85	133.68	127.40
1	16S1	1042	A	C5-N7-C8	7.85	107.83	103.90
22	23S1	983	A	C5-N7-C8	7.85	107.82	103.90
22	23S1	821	A	C5-N7-C8	7.85	107.82	103.90
22	23S1	1144	A	C5-N7-C8	7.85	107.82	103.90
22	23S1	2829	A	C5-N7-C8	7.85	107.82	103.90
1	16S1	16	A	C5-N7-C8	7.84	107.82	103.90
22	23S1	125	A	C5-N7-C8	7.84	107.82	103.90
22	23S1	2059	A	C5-N7-C8	7.84	107.82	103.90
1	16S1	1146	A	C5-N7-C8	7.84	107.82	103.90
1	16S1	901	A	N3-C4-N9	7.84	133.67	127.40
22	23S1	646	U	C5-C6-N1	-7.84	118.78	122.70
1	16S1	1289	A	C5-N7-C8	7.84	107.82	103.90
30	L311	32	LEU	CB-CG-CD2	-7.84	97.68	111.00
1	16S1	139	A	C5-N7-C8	7.83	107.82	103.90
1	16S1	978	A	C5-N7-C8	7.83	107.82	103.90
1	16S1	1157	A	C5-N7-C8	7.83	107.82	103.90
22	23S1	346	A	C5-N7-C8	7.83	107.82	103.90
22	23S1	1156	A	C5-N7-C8	7.83	107.82	103.90
1	16S1	397	A	C5-N7-C8	7.83	107.82	103.90
1	16S1	983	A	N3-C4-N9	7.83	133.67	127.40
22	23S1	609	A	C5-N7-C8	7.83	107.82	103.90
22	23S1	668	A	C5-N7-C8	7.83	107.82	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2792	A	C5-N7-C8	7.83	107.81	103.90
22	23S1	1387	A	C5-N7-C8	7.83	107.81	103.90
22	23S1	1918	A	C5-N7-C8	7.83	107.81	103.90
22	23S1	348	A	C5-N7-C8	7.83	107.81	103.90
22	23S1	592	A	C5-N7-C8	7.82	107.81	103.90
22	23S1	675	A	C5-N7-C8	7.82	107.81	103.90
22	23S1	2054	A	C5-N7-C8	7.82	107.81	103.90
22	23S1	2799	A	N3-C4-N9	7.82	133.66	127.40
22	23S1	829	A	C5-N7-C8	7.82	107.81	103.90
22	23S1	896	A	C5-N7-C8	7.82	107.81	103.90
1	16S1	1021	A	C5-N7-C8	7.82	107.81	103.90
1	16S1	1483	A	C5-N7-C8	7.82	107.81	103.90
22	23S1	342	A	C5-N7-C8	7.82	107.81	103.90
22	23S1	2352	A	C4-C5-C6	7.82	120.91	117.00
1	16S1	906	A	C5-N7-C8	7.82	107.81	103.90
22	23S1	644	A	N3-C4-N9	7.82	133.65	127.40
22	23S1	2851	A	C5-N7-C8	7.82	107.81	103.90
1	16S1	1092	A	N3-C4-C5	-7.81	121.33	126.80
1	16S1	1447	A	C5-N7-C8	7.81	107.81	103.90
22	23S1	1089	A	C5-N7-C8	7.81	107.81	103.90
22	23S1	1672	A	C5-N7-C8	7.81	107.81	103.90
22	23S1	2766	A	C4-C5-C6	7.81	120.91	117.00
22	23S1	1866	A	C5-N7-C8	7.81	107.81	103.90
22	23S1	1969	A	C5-N7-C8	7.81	107.81	103.90
1	16S1	353	A	C5-N7-C8	7.81	107.81	103.90
22	23S1	195	A	N3-C4-C5	-7.81	121.33	126.80
22	23S1	788	A	C5-N7-C8	7.81	107.81	103.90
1	16S1	382	A	C5-N7-C8	7.81	107.80	103.90
1	16S1	873	A	C5-N7-C8	7.81	107.80	103.90
22	23S1	2418	A	C5-N7-C8	7.81	107.80	103.90
1	16S1	1374	A	C5-N7-C8	7.80	107.80	103.90
22	23S1	2077	A	C5-N7-C8	7.80	107.80	103.90
23	05S1	101	A	C5-C6-N6	7.80	129.94	123.70
22	23S1	231	A	C5-N7-C8	7.80	107.80	103.90
22	23S1	340	A	C5-N7-C8	7.80	107.80	103.90
22	23S1	1548	A	C5-N7-C8	7.80	107.80	103.90
22	23S1	1532	A	C5-N7-C8	7.80	107.80	103.90
22	23S1	49	A	C5-N7-C8	7.79	107.80	103.90
22	23S1	2281	A	C5-N7-C8	7.79	107.80	103.90
1	16S1	1236	A	C5-N7-C8	7.79	107.80	103.90
22	23S1	1014	A	C5-N7-C8	7.79	107.80	103.90
1	16S1	935	A	C5-N7-C8	7.79	107.80	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1155	A	C5-N7-C8	7.79	107.80	103.90
22	23S1	1528	A	N3-C4-N9	7.79	133.63	127.40
22	23S1	947	A	C5-N7-C8	7.79	107.80	103.90
1	16S1	1254	A	C5-N7-C8	7.79	107.79	103.90
1	16S1	174	A	C5-N7-C8	7.79	107.79	103.90
1	16S1	431	A	C6-N1-C2	7.79	123.27	118.60
1	16S1	1396	A	C5-N7-C8	7.78	107.79	103.90
1	16S1	1158	C	C6-N1-C2	-7.78	117.19	120.30
22	23S1	1244	A	C5-N7-C8	7.78	107.79	103.90
22	23S1	2679	A	C5-N7-C8	7.78	107.79	103.90
1	16S1	802	A	C5-N7-C8	7.78	107.79	103.90
22	23S1	2675	A	C5-N7-C8	7.78	107.79	103.90
22	23S1	1655	A	C5-N7-C8	7.78	107.79	103.90
1	16S1	160	A	C5-N7-C8	7.78	107.79	103.90
1	16S1	520	A	C4-C5-N7	-7.77	106.81	110.70
22	23S1	1735	A	C5-N7-C8	7.77	107.79	103.90
1	16S1	1413	A	C5-N7-C8	7.77	107.78	103.90
22	23S1	492	A	C5-N7-C8	7.77	107.78	103.90
22	23S1	1431	A	C5-N7-C8	7.77	107.78	103.90
55	PTR1	20	U	N3-C2-O2	-7.77	116.76	122.20
1	16S1	706	A	C5-N7-C8	7.77	107.78	103.90
22	23S1	2634	A	C5-N7-C8	7.77	107.78	103.90
22	23S1	146	A	C5-N7-C8	7.76	107.78	103.90
22	23S1	251	A	N3-C4-N9	7.76	133.61	127.40
22	23S1	1103	A	C5-N7-C8	7.76	107.78	103.90
48	L321	40	ARG	NE-CZ-NH1	7.76	124.18	120.30
22	23S1	131	A	N3-C4-N9	7.76	133.61	127.40
1	16S1	814	A	C5-N7-C8	7.76	107.78	103.90
1	16S1	746	A	C5-N7-C8	7.76	107.78	103.90
22	23S1	899	A	C5-N7-C8	7.76	107.78	103.90
22	23S1	2090	A	C5-N7-C8	7.76	107.78	103.90
1	16S1	649	A	C5-N7-C8	7.76	107.78	103.90
22	23S1	1987	A	C5-N7-C8	7.76	107.78	103.90
22	23S1	2541	A	C5-N7-C8	7.76	107.78	103.90
22	23S1	2670	A	C5-N7-C8	7.76	107.78	103.90
1	16S1	655	A	C5-N7-C8	7.75	107.78	103.90
1	16S1	746	A	N3-C4-N9	7.75	133.60	127.40
1	16S1	1227	A	N7-C8-N9	-7.75	109.92	113.80
22	23S1	513	A	N3-C4-N9	7.75	133.60	127.40
22	23S1	2173	A	C5-N7-C8	7.75	107.78	103.90
22	23S1	2278	A	C5-N7-C8	7.75	107.78	103.90
22	23S1	2738	A	C5-N7-C8	7.75	107.78	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	PTR1	9	A	C5-N7-C8	7.75	107.78	103.90
1	16S1	3	A	C5-N7-C8	7.75	107.77	103.90
22	23S1	344	A	C5-N7-C8	7.75	107.77	103.90
22	23S1	661	A	C5-N7-C8	7.75	107.77	103.90
22	23S1	1395	A	C5-N7-C8	7.75	107.77	103.90
1	16S1	1468	A	C4-C5-C6	7.75	120.87	117.00
22	23S1	1275	A	N3-C4-C5	-7.75	121.38	126.80
22	23S1	374	A	C5-N7-C8	7.74	107.77	103.90
1	16S1	478	A	C4-C5-C6	7.74	120.87	117.00
1	16S1	860	A	C4-C5-N7	-7.74	106.83	110.70
1	16S1	573	A	C5-N7-C8	7.74	107.77	103.90
22	23S1	196	A	N3-C4-N9	7.74	133.59	127.40
22	23S1	1354	A	C5-N7-C8	7.74	107.77	103.90
1	16S1	1433	A	C5-N7-C8	7.73	107.77	103.90
22	23S1	2009	A	C5-N7-C8	7.73	107.77	103.90
1	16S1	622	A	N3-C4-C5	-7.73	121.39	126.80
1	16S1	747	A	C5-N7-C8	7.73	107.77	103.90
22	23S1	152	A	C5-N7-C8	7.73	107.77	103.90
22	23S1	1269	A	C5-N7-C8	7.73	107.77	103.90
23	05S1	15	A	C5-N7-C8	7.73	107.77	103.90
22	23S1	368	A	C5-N7-C8	7.73	107.76	103.90
22	23S1	2058	A	C5-N7-C8	7.73	107.76	103.90
1	16S1	502	A	C5-N7-C8	7.72	107.76	103.90
1	16S1	554	A	N9-C4-C5	7.72	108.89	105.80
22	23S1	2753	A	C5-N7-C8	7.72	107.76	103.90
1	16S1	1	A	C5-N7-C8	7.72	107.76	103.90
1	16S1	143	A	C5-N7-C8	7.72	107.76	103.90
22	23S1	1142	A	C5-N7-C8	7.72	107.76	103.90
22	23S1	457	A	C5-N7-C8	7.72	107.76	103.90
22	23S1	2268	A	C5-N7-C8	7.72	107.76	103.90
22	23S1	2333	A	C5-N7-C8	7.72	107.76	103.90
1	16S1	532	A	C5-N7-C8	7.71	107.76	103.90
1	16S1	1082	A	C5-N7-C8	7.71	107.76	103.90
22	23S1	155	A	C5-N7-C8	7.71	107.76	103.90
22	23S1	2432	A	C5-N7-C8	7.71	107.76	103.90
22	23S1	2449	U	N3-C2-O2	-7.71	116.80	122.20
23	05S1	108	A	C5-N7-C8	7.71	107.76	103.90
22	23S1	2358	A	C5-N7-C8	7.71	107.76	103.90
55	PTR1	3	A	C5-N7-C8	7.71	107.76	103.90
22	23S1	299	A	C5-N7-C8	7.71	107.76	103.90
22	23S1	64	A	C5-N7-C8	7.71	107.75	103.90
22	23S1	384	A	C5-N7-C8	7.71	107.75	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2211	A	C5-N7-C8	7.71	107.75	103.90
1	16S1	414	A	C5-N7-C8	7.70	107.75	103.90
22	23S1	1609	A	C5-N7-C8	7.70	107.75	103.90
22	23S1	1780	A	C5-N7-C8	7.70	107.75	103.90
22	23S1	2287	A	C5-N7-C8	7.70	107.75	103.90
22	23S1	2430	A	N9-C4-C5	7.70	108.88	105.80
1	16S1	1172	C	N1-C2-O2	7.70	123.52	118.90
22	23S1	149	A	C5-N7-C8	7.70	107.75	103.90
22	23S1	195	A	N7-C8-N9	-7.70	109.95	113.80
1	16S1	749	A	C5-N7-C8	7.70	107.75	103.90
1	16S1	1176	A	C5-N7-C8	7.70	107.75	103.90
22	23S1	94	A	C5-N7-C8	7.70	107.75	103.90
22	23S1	2657	A	C5-N7-C8	7.70	107.75	103.90
1	16S1	461	A	C5-N7-C8	7.69	107.75	103.90
1	16S1	696	A	C4-C5-C6	7.69	120.85	117.00
22	23S1	2734	A	C5-N7-C8	7.69	107.75	103.90
1	16S1	1081	A	C5-N7-C8	7.69	107.75	103.90
22	23S1	1165	A	C5-N7-C8	7.69	107.75	103.90
22	23S1	1632	A	C5-N7-C8	7.69	107.75	103.90
22	23S1	676	A	C5-N7-C8	7.69	107.74	103.90
23	05S1	59	A	C5-C6-N6	7.69	129.85	123.70
22	23S1	320	A	C6-N1-C2	7.69	123.21	118.60
1	16S1	327	A	C5-N7-C8	7.68	107.74	103.90
1	16S1	59	A	C5-N7-C8	7.68	107.74	103.90
1	16S1	71	A	C5-N7-C8	7.68	107.74	103.90
1	16S1	746	A	C4-C5-C6	7.68	120.84	117.00
1	16S1	1346	A	C5-N7-C8	7.68	107.74	103.90
1	16S1	448	A	C5-N7-C8	7.68	107.74	103.90
22	23S1	1155	A	C5-N7-C8	7.68	107.74	103.90
22	23S1	1373	A	C5-N7-C8	7.68	107.74	103.90
1	16S1	270	A	C5-N7-C8	7.68	107.74	103.90
22	23S1	742	A	C5-N7-C8	7.68	107.74	103.90
22	23S1	892	A	C5-N7-C8	7.68	107.74	103.90
22	23S1	1321	A	C5-N7-C8	7.68	107.74	103.90
1	16S1	1239	A	C8-N9-C4	7.68	108.87	105.80
22	23S1	156	A	C5-N7-C8	7.68	107.74	103.90
22	23S1	2247	A	C5-N7-C8	7.68	107.74	103.90
22	23S1	1322	A	C5-N7-C8	7.67	107.74	103.90
22	23S1	2459	A	C5-N7-C8	7.67	107.74	103.90
1	16S1	397	A	C5-C6-N6	7.67	129.84	123.70
22	23S1	2020	A	C5-N7-C8	7.67	107.74	103.90
22	23S1	216	A	C5-N7-C8	7.67	107.73	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	960	A	C5-C6-N6	7.67	129.84	123.70
2	S021	137	ARG	NE-CZ-NH1	-7.67	116.47	120.30
22	23S1	218	A	C5-N7-C8	7.67	107.73	103.90
22	23S1	927	A	C5-N7-C8	7.67	107.73	103.90
1	16S1	1150	A	C5-N7-C8	7.66	107.73	103.90
22	23S1	547	A	C8-N9-C4	7.66	108.86	105.80
22	23S1	794	A	C5-N7-C8	7.66	107.73	103.90
22	23S1	959	A	C5-N7-C8	7.66	107.73	103.90
1	16S1	1274	A	C5-N7-C8	7.65	107.73	103.90
22	23S1	1705	A	C5-N7-C8	7.65	107.73	103.90
22	23S1	1593	A	C5-N7-C8	7.65	107.72	103.90
1	16S1	974	A	C5-N7-C8	7.64	107.72	103.90
22	23S1	1001	A	C5-N7-C8	7.64	107.72	103.90
22	23S1	2062	A	N3-C4-N9	7.64	133.51	127.40
23	05S1	46	A	C5-N7-C8	7.64	107.72	103.90
22	23S1	590	A	C5-N7-C8	7.64	107.72	103.90
22	23S1	2019	A	C5-N7-C8	7.64	107.72	103.90
1	16S1	1111	A	C5-N7-C8	7.64	107.72	103.90
55	PTR1	69	A	C5-N7-C8	7.64	107.72	103.90
1	16S1	523	A	C5-N7-C8	7.63	107.72	103.90
22	23S1	402	A	C5-N7-C8	7.63	107.72	103.90
22	23S1	2080	A	C5-N7-C8	7.63	107.72	103.90
22	23S1	1313	U	N1-C2-O2	7.63	128.14	122.80
22	23S1	2376	A	C5-N7-C8	7.63	107.72	103.90
22	23S1	2660	A	C5-N7-C8	7.63	107.72	103.90
1	16S1	1500	A	C5-N7-C8	7.63	107.71	103.90
22	23S1	74	A	C5-N7-C8	7.63	107.71	103.90
22	23S1	401	A	C5-N7-C8	7.63	107.71	103.90
22	23S1	2189	U	N1-C2-O2	7.63	128.14	122.80
1	16S1	1145	A	C5-N7-C8	7.62	107.71	103.90
22	23S1	244	A	C5-N7-C8	7.62	107.71	103.90
1	16S1	456	A	C5-N7-C8	7.62	107.71	103.90
22	23S1	544	C	C2-N1-C1'	7.62	127.19	118.80
1	16S1	608	A	C5-N7-C8	7.62	107.71	103.90
22	23S1	2598	A	C5-N7-C8	7.62	107.71	103.90
22	23S1	1938	A	C5-N7-C8	7.62	107.71	103.90
22	23S1	783	A	C4-C5-C6	7.62	120.81	117.00
22	23S1	1711	A	C5-N7-C8	7.62	107.71	103.90
1	16S1	753	A	C5-N7-C8	7.61	107.71	103.90
1	16S1	1434	A	C5-N7-C8	7.61	107.71	103.90
22	23S1	2154	A	C5-N7-C8	7.61	107.71	103.90
1	16S1	673	A	N3-C4-N9	7.61	133.49	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	675	A	C5-N7-C8	7.61	107.70	103.90
1	16S1	937	A	C5-N7-C8	7.61	107.70	103.90
22	23S1	1535	A	C5-N7-C8	7.61	107.70	103.90
1	16S1	119	A	C5-N7-C8	7.60	107.70	103.90
1	16S1	1476	A	C5-N7-C8	7.60	107.70	103.90
22	23S1	176	A	C5-N7-C8	7.60	107.70	103.90
1	16S1	1016	A	C5-N7-C8	7.60	107.70	103.90
1	16S1	1219	A	N3-C4-N9	7.60	133.48	127.40
1	16S1	1468	A	C5-N7-C8	7.60	107.70	103.90
22	23S1	482	A	C5-N7-C8	7.60	107.70	103.90
1	16S1	1339	A	C5-N7-C8	7.60	107.70	103.90
55	PTR1	51	A	N9-C4-C5	7.60	108.84	105.80
23	05S1	109	A	C5-N7-C8	7.59	107.70	103.90
1	16S1	1046	A	N3-C4-N9	7.59	133.47	127.40
22	23S1	1262	A	C5-N7-C8	7.59	107.70	103.90
1	16S1	1188	A	C5-N7-C8	7.59	107.69	103.90
22	23S1	2199	A	C5-N7-C8	7.59	107.69	103.90
22	23S1	996	A	C5-N7-C8	7.59	107.69	103.90
22	23S1	1953	A	C5-N7-C8	7.59	107.69	103.90
1	16S1	65	A	C5-N7-C8	7.58	107.69	103.90
22	23S1	1086	A	N3-C4-N9	7.58	133.47	127.40
1	16S1	994	A	N3-C4-N9	7.58	133.47	127.40
1	16S1	1102	A	C5-N7-C8	7.58	107.69	103.90
1	16S1	430	A	C4-C5-C6	7.58	120.79	117.00
1	16S1	1204	A	C5-N7-C8	7.58	107.69	103.90
22	23S1	1241	A	N3-C4-N9	7.58	133.46	127.40
22	23S1	1801	A	C5-N7-C8	7.58	107.69	103.90
22	23S1	574	A	C5-N7-C8	7.58	107.69	103.90
22	23S1	95	A	C5-N7-C8	7.58	107.69	103.90
22	23S1	1614	A	C5-N7-C8	7.58	107.69	103.90
22	23S1	1678	A	C5-N7-C8	7.58	107.69	103.90
22	23S1	2587	A	C5-N7-C8	7.58	107.69	103.90
1	16S1	609	A	C5-N7-C8	7.57	107.69	103.90
22	23S1	613	A	N3-C4-N9	7.57	133.46	127.40
22	23S1	2635	A	C5-N7-C8	7.57	107.69	103.90
55	PTR1	14	A	N3-C4-N9	7.57	133.46	127.40
22	23S1	127	A	C5-N7-C8	7.57	107.68	103.90
22	23S1	819	A	N3-C4-N9	7.57	133.45	127.40
22	23S1	1403	A	C5-N7-C8	7.57	107.68	103.90
22	23S1	2328	A	C4-C5-C6	7.57	120.78	117.00
22	23S1	2883	A	C8-N9-C4	7.57	108.83	105.80
22	23S1	83	A	C5-N7-C8	7.57	107.68	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	706	A	C5-N7-C8	7.56	107.68	103.90
22	23S1	1871	A	C4-C5-C6	7.56	120.78	117.00
22	23S1	429	A	C5-N7-C8	7.56	107.68	103.90
22	23S1	515	A	C5-N7-C8	7.56	107.68	103.90
22	23S1	990	A	C5-N7-C8	7.56	107.68	103.90
22	23S1	1129	A	C5-N7-C8	7.56	107.68	103.90
22	23S1	2430	A	C4-C5-C6	7.56	120.78	117.00
22	23S1	2662	A	N3-C4-N9	7.56	133.45	127.40
1	16S1	303	A	C5-N7-C8	7.55	107.68	103.90
22	23S1	1274	A	C5-N7-C8	7.55	107.68	103.90
22	23S1	1899	A	N7-C8-N9	-7.55	110.02	113.80
22	23S1	470	A	C4-C5-C6	7.55	120.78	117.00
22	23S1	863	A	N3-C4-N9	7.55	133.44	127.40
22	23S1	2309	A	C5-N7-C8	7.55	107.68	103.90
1	16S1	621	A	C5-N7-C8	7.55	107.67	103.90
22	23S1	2411	A	C5-N7-C8	7.55	107.67	103.90
1	16S1	1092	A	C5-N7-C8	7.55	107.67	103.90
22	23S1	920	A	C5-N7-C8	7.55	107.67	103.90
22	23S1	2614	A	C4-C5-C6	7.55	120.77	117.00
23	05S1	94	A	C5-N7-C8	7.55	107.67	103.90
22	23S1	2814	A	C5-N7-C8	7.54	107.67	103.90
55	PTR1	62	C	N1-C2-O2	7.54	123.43	118.90
1	16S1	1201	A	C4-C5-C6	7.54	120.77	117.00
1	16S1	1179	A	C5-N7-C8	7.54	107.67	103.90
22	23S1	572	A	C5-N7-C8	7.54	107.67	103.90
1	16S1	329	A	C5-N7-C8	7.54	107.67	103.90
1	16S1	1468	A	N3-C4-N9	7.54	133.43	127.40
1	16S1	499	A	C4-C5-C6	7.54	120.77	117.00
22	23S1	981	A	C5-N7-C8	7.54	107.67	103.90
22	23S1	1205	A	C5-N7-C8	7.54	107.67	103.90
1	16S1	477	C	N1-C2-O2	7.53	123.42	118.90
22	23S1	1495	A	C5-N7-C8	7.53	107.67	103.90
1	16S1	629	A	C5-N7-C8	7.53	107.67	103.90
22	23S1	941	A	C5-N7-C8	7.53	107.67	103.90
1	16S1	306	A	C5-N7-C8	7.53	107.67	103.90
22	23S1	1977	A	C5-N7-C8	7.53	107.67	103.90
23	05S1	99	A	C5-N7-C8	7.53	107.66	103.90
1	16S1	510	A	C5-N7-C8	7.53	107.66	103.90
1	16S1	923	A	C4-C5-C6	7.53	120.76	117.00
22	23S1	227	A	C5-N7-C8	7.53	107.66	103.90
22	23S1	933	A	C5-N7-C8	7.53	107.66	103.90
22	23S1	794	A	N3-C4-N9	7.53	133.42	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1762	A	C5-N7-C8	7.53	107.66	103.90
22	23S1	972	A	C5-N7-C8	7.52	107.66	103.90
22	23S1	2810	A	C5-N7-C8	7.52	107.66	103.90
1	16S1	1044	A	C5-N7-C8	7.52	107.66	103.90
22	23S1	1744	A	C5-N7-C8	7.52	107.66	103.90
22	23S1	2015	A	C5-N7-C8	7.52	107.66	103.90
22	23S1	575	A	C5-N7-C8	7.52	107.66	103.90
22	23S1	1730	C	C6-N1-C2	-7.52	117.29	120.30
22	23S1	362	A	C4-C5-C6	7.51	120.76	117.00
22	23S1	1952	A	C5-N7-C8	7.51	107.66	103.90
23	05S1	53	A	C5-N7-C8	7.51	107.66	103.90
22	23S1	2823	A	C5-N7-C8	7.51	107.66	103.90
1	16S1	535	A	C5-N7-C8	7.51	107.66	103.90
22	23S1	1570	A	C5-N7-C8	7.51	107.66	103.90
22	23S1	1175	A	C5-N7-C8	7.51	107.66	103.90
22	23S1	2377	A	C5-N7-C8	7.51	107.65	103.90
22	23S1	2765	A	C4-C5-C6	7.51	120.75	117.00
1	16S1	1363	A	N3-C4-N9	7.51	133.41	127.40
1	16S1	262	A	C5-N7-C8	7.51	107.65	103.90
22	23S1	470	A	C5-N7-C8	7.51	107.65	103.90
22	23S1	1214	A	C5-N7-C8	7.50	107.65	103.90
22	23S1	1626	A	C5-N7-C8	7.50	107.65	103.90
22	23S1	1739	A	C4-C5-C6	7.50	120.75	117.00
1	16S1	1363	A	C5-N7-C8	7.50	107.65	103.90
22	23S1	2082	A	N3-C4-N9	7.50	133.40	127.40
22	23S1	423	A	C5-N7-C8	7.50	107.65	103.90
1	16S1	130	A	C5-N7-C8	7.50	107.65	103.90
1	16S1	363	A	C5-N7-C8	7.50	107.65	103.90
22	23S1	480	A	C4-C5-C6	7.50	120.75	117.00
22	23S1	602	A	C5-N7-C8	7.50	107.65	103.90
22	23S1	2273	A	N3-C4-N9	7.50	133.40	127.40
1	16S1	55	A	N3-C4-N9	7.50	133.40	127.40
22	23S1	621	A	C5-N7-C8	7.50	107.65	103.90
1	16S1	356	A	N3-C4-N9	7.49	133.40	127.40
1	16S1	1350	A	C5-N7-C8	7.49	107.65	103.90
22	23S1	428	A	C5-N7-C8	7.49	107.64	103.90
22	23S1	685	A	C5-N7-C8	7.49	107.64	103.90
22	23S1	1175	A	N3-C4-N9	7.49	133.39	127.40
22	23S1	2352	A	C5-N7-C8	7.49	107.64	103.90
22	23S1	1654	A	C5-N7-C8	7.49	107.64	103.90
22	23S1	2478	A	C5-N7-C8	7.49	107.64	103.90
22	23S1	56	A	C5-N7-C8	7.48	107.64	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1477	A	C5-N7-C8	7.48	107.64	103.90
22	23S1	1787	A	N3-C4-N9	7.48	133.39	127.40
22	23S1	1978	A	C5-N7-C8	7.48	107.64	103.90
22	23S1	219	A	C5-N7-C8	7.48	107.64	103.90
22	23S1	1057	A	C5-N7-C8	7.48	107.64	103.90
22	23S1	2547	A	C5-N7-C8	7.48	107.64	103.90
22	23S1	1900	A	C5-N7-C8	7.48	107.64	103.90
1	16S1	109	A	C5-N7-C8	7.48	107.64	103.90
1	16S1	968	A	C5-N7-C8	7.48	107.64	103.90
22	23S1	2589	A	C5-N7-C8	7.48	107.64	103.90
1	16S1	32	A	N3-C4-N9	7.47	133.38	127.40
22	23S1	1433	A	C5-N7-C8	7.47	107.64	103.90
1	16S1	373	A	N3-C4-N9	7.47	133.38	127.40
1	16S1	546	A	C5-N7-C8	7.47	107.63	103.90
22	23S1	1029	A	C5-N7-C8	7.47	107.64	103.90
22	23S1	845	A	C5-N7-C8	7.47	107.63	103.90
22	23S1	1142	A	N3-C4-N9	7.47	133.38	127.40
22	23S1	1722	A	N3-C4-N9	7.47	133.38	127.40
1	16S1	412	A	N9-C4-C5	7.47	108.79	105.80
1	16S1	465	A	N3-C4-N9	7.47	133.37	127.40
22	23S1	705	A	C5-N7-C8	7.47	107.63	103.90
22	23S1	599	A	C5-N7-C8	7.46	107.63	103.90
22	23S1	1877	A	C5-N7-C8	7.46	107.63	103.90
22	23S1	1899	A	C4-C5-C6	7.46	120.73	117.00
22	23S1	1552	A	C5-N7-C8	7.46	107.63	103.90
22	23S1	2170	A	C4-C5-C6	7.46	120.73	117.00
22	23S1	2340	A	C5-N7-C8	7.46	107.63	103.90
1	16S1	923	A	N3-C4-N9	7.46	133.37	127.40
1	16S1	7	A	C5-N7-C8	7.46	107.63	103.90
22	23S1	2184	A	C5-N7-C8	7.46	107.63	103.90
22	23S1	2434	A	C5-N7-C8	7.46	107.63	103.90
1	16S1	253	A	C5-N7-C8	7.45	107.63	103.90
22	23S1	2191	A	C4-C5-C6	7.45	120.73	117.00
1	16S1	790	A	C5-N7-C8	7.45	107.63	103.90
1	16S1	718	A	N3-C4-N9	7.45	133.36	127.40
22	23S1	144	A	C5-N7-C8	7.45	107.63	103.90
22	23S1	1383	A	C5-N7-C8	7.45	107.62	103.90
1	16S1	563	A	C5-N7-C8	7.45	107.62	103.90
1	16S1	1036	A	C5-N7-C8	7.45	107.62	103.90
22	23S1	52	A	C4-C5-C6	7.45	120.72	117.00
22	23S1	2077	A	C4-C5-C6	7.45	120.72	117.00
23	05S1	73	A	N3-C4-N9	7.45	133.36	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	945	A	C5-N7-C8	7.45	107.62	103.90
22	23S1	1314	C	C6-N1-C2	-7.45	117.32	120.30
22	23S1	1650	A	C5-N7-C8	7.45	107.62	103.90
22	23S1	2426	A	C5-N7-C8	7.45	107.62	103.90
1	16S1	865	A	C4-C5-C6	7.44	120.72	117.00
1	16S1	819	A	C5-N7-C8	7.44	107.62	103.90
1	16S1	466	A	C5-N7-C8	7.44	107.62	103.90
22	23S1	1698	A	C5-N7-C8	7.44	107.62	103.90
22	23S1	332	A	C5-N7-C8	7.44	107.62	103.90
1	16S1	872	A	N7-C8-N9	-7.44	110.08	113.80
22	23S1	265	A	C5-N7-C8	7.44	107.62	103.90
22	23S1	631	A	C5-N7-C8	7.44	107.62	103.90
22	23S1	1544	A	C5-N7-C8	7.44	107.62	103.90
22	23S1	1603	A	C5-N7-C8	7.43	107.62	103.90
22	23S1	1746	A	C5-N7-C8	7.43	107.62	103.90
1	16S1	602	A	C5-N7-C8	7.43	107.61	103.90
22	23S1	2542	A	N9-C4-C5	7.43	108.77	105.80
22	23S1	2142	A	C5-N7-C8	7.43	107.61	103.90
22	23S1	2856	A	C5-N7-C8	7.43	107.61	103.90
22	23S1	2654	A	C5-N7-C8	7.42	107.61	103.90
1	16S1	1004	A	N3-C4-N9	7.42	133.34	127.40
22	23S1	933	A	C4-C5-C6	7.42	120.71	117.00
22	23S1	2765	A	C5-N7-C8	7.42	107.61	103.90
22	23S1	1054	A	C5-N7-C8	7.42	107.61	103.90
22	23S1	1469	A	C4-C5-C6	7.42	120.71	117.00
1	16S1	383	A	C6-C5-N7	-7.42	127.11	132.30
22	23S1	294	A	C5-N7-C8	7.42	107.61	103.90
1	16S1	80	A	C4-C5-C6	7.41	120.71	117.00
22	23S1	1496	A	C5-N7-C8	7.41	107.61	103.90
22	23S1	1302	A	C5-N7-C8	7.41	107.61	103.90
22	23S1	1854	A	C4-C5-C6	7.41	120.71	117.00
1	16S1	50	A	C5-N7-C8	7.41	107.61	103.90
1	16S1	452	A	N3-C4-N9	7.41	133.33	127.40
22	23S1	2108	A	C5-N7-C8	7.41	107.61	103.90
22	23S1	2899	A	C5-N7-C8	7.41	107.61	103.90
22	23S1	2198	A	C5-N7-C8	7.41	107.60	103.90
22	23S1	654	A	N3-C4-N9	7.41	133.33	127.40
22	23S1	705	A	C4-C5-C6	7.41	120.70	117.00
1	16S1	1152	A	C4-C5-C6	7.41	120.70	117.00
22	23S1	988	A	C5-N7-C8	7.40	107.60	103.90
22	23S1	1169	A	C5-N7-C8	7.40	107.60	103.90
1	16S1	901	A	N7-C8-N9	-7.40	110.10	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	907	A	C4-C5-C6	7.40	120.70	117.00
22	23S1	845	A	C5-C6-N1	7.40	121.40	117.70
22	23S1	2476	A	C5-N7-C8	7.40	107.60	103.90
22	23S1	2142	A	C4-C5-C6	7.40	120.70	117.00
22	23S1	2163	A	C5-N7-C8	7.40	107.60	103.90
22	23S1	2097	A	C5-N7-C8	7.39	107.60	103.90
22	23S1	2346	A	C5-N7-C8	7.39	107.60	103.90
1	16S1	431	A	C4-C5-N7	-7.39	107.01	110.70
1	16S1	199	A	N3-C4-N9	7.39	133.31	127.40
22	23S1	503	A	C5-N7-C8	7.38	107.59	103.90
22	23S1	526	A	C5-N7-C8	7.38	107.59	103.90
22	23S1	1008	A	C5-N7-C8	7.38	107.59	103.90
22	23S1	2516	A	C5-N7-C8	7.38	107.59	103.90
22	23S1	722	A	C5-N7-C8	7.38	107.59	103.90
22	23S1	1264	A	C5-N7-C8	7.38	107.59	103.90
22	23S1	1275	A	C8-N9-C4	7.38	108.75	105.80
22	23S1	1866	A	C4-C5-C6	7.38	120.69	117.00
22	23S1	2860	A	C5-N7-C8	7.38	107.59	103.90
22	23S1	2879	A	C5-N7-C8	7.38	107.59	103.90
1	16S1	8	A	C8-N9-C4	7.38	108.75	105.80
22	23S1	2893	A	C5-N7-C8	7.37	107.59	103.90
1	16S1	533	A	C5-C6-N1	7.37	121.39	117.70
22	23S1	654	A	C5-N7-C8	7.37	107.58	103.90
1	16S1	539	A	C5-N7-C8	7.37	107.58	103.90
1	16S1	1046	A	C4-C5-C6	7.37	120.68	117.00
22	23S1	1134	A	C5-N7-C8	7.37	107.58	103.90
22	23S1	2449	U	N3-C4-C5	7.36	119.02	114.60
22	23S1	1970	A	N3-C4-N9	7.36	133.29	127.40
1	16S1	181	A	C5-N7-C8	7.36	107.58	103.90
1	16S1	344	A	C5-N7-C8	7.36	107.58	103.90
1	16S1	460	A	C5-N7-C8	7.36	107.58	103.90
1	16S1	889	A	C5-N7-C8	7.36	107.58	103.90
22	23S1	892	A	N3-C4-N9	7.36	133.29	127.40
22	23S1	126	A	C5-N7-C8	7.36	107.58	103.90
22	23S1	1970	A	C8-N9-C4	7.36	108.74	105.80
22	23S1	721	A	C5-N7-C8	7.36	107.58	103.90
22	23S1	877	A	C5-N7-C8	7.35	107.58	103.90
1	16S1	673	A	C5-N7-C8	7.35	107.58	103.90
22	23S1	2111	U	N1-C2-O2	7.35	127.95	122.80
1	16S1	913	A	C5-N7-C8	7.35	107.58	103.90
22	23S1	2513	A	C5-N7-C8	7.35	107.57	103.90
1	16S1	182	A	C5-N7-C8	7.35	107.57	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1130	A	C5-N7-C8	7.35	107.57	103.90
22	23S1	84	A	C8-N9-C4	7.35	108.74	105.80
22	23S1	2433	A	C4-C5-C6	7.34	120.67	117.00
1	16S1	1503	A	C8-N9-C4	7.34	108.74	105.80
22	23S1	1553	A	C4-C5-C6	7.34	120.67	117.00
22	23S1	207	A	C5-N7-C8	7.34	107.57	103.90
22	23S1	53	A	C5-N7-C8	7.34	107.57	103.90
22	23S1	2412	A	C4-C5-C6	7.34	120.67	117.00
22	23S1	2705	A	C5-N7-C8	7.34	107.57	103.90
1	16S1	101	A	C5-N7-C8	7.34	107.57	103.90
22	23S1	13	A	C5-N7-C8	7.34	107.57	103.90
22	23S1	1143	A	C5-N7-C8	7.34	107.57	103.90
22	23S1	272	A	C5-N7-C8	7.33	107.57	103.90
1	16S1	977	A	C4-C5-C6	7.33	120.67	117.00
55	PTR1	20	U	N3-C4-C5	7.33	119.00	114.60
1	16S1	1046	A	C5-C6-N1	7.33	121.36	117.70
1	16S1	1117	A	C5-N7-C8	7.33	107.56	103.90
1	16S1	787	A	C5-N7-C8	7.33	107.56	103.90
1	16S1	1227	A	C4-C5-C6	7.33	120.66	117.00
22	23S1	282	A	C5-N7-C8	7.32	107.56	103.90
1	16S1	190	A	C5-N7-C8	7.32	107.56	103.90
1	16S1	777	A	C5-N7-C8	7.32	107.56	103.90
22	23S1	2757	A	N3-C4-N9	7.32	133.26	127.40
1	16S1	28	A	C5-N7-C8	7.32	107.56	103.90
1	16S1	77	A	N3-C4-N9	7.32	133.25	127.40
22	23S1	1077	A	C5-N7-C8	7.32	107.56	103.90
22	23S1	1569	A	C5-N7-C8	7.32	107.56	103.90
22	23S1	2135	A	C4-C5-C6	7.32	120.66	117.00
22	23S1	666	A	C5-N7-C8	7.32	107.56	103.90
1	16S1	452	A	C5-N7-C8	7.31	107.56	103.90
22	23S1	2198	A	C8-N9-C4	7.31	108.72	105.80
22	23S1	2426	A	C8-N9-C4	7.31	108.72	105.80
22	23S1	160	A	N9-C4-C5	7.31	108.72	105.80
22	23S1	572	A	C4-C5-C6	7.31	120.65	117.00
22	23S1	1275	A	C5-N7-C8	7.31	107.55	103.90
1	16S1	1375	A	C4-C5-C6	7.31	120.65	117.00
22	23S1	603	A	C5-N7-C8	7.31	107.55	103.90
1	16S1	151	A	C4-C5-N7	-7.30	107.05	110.70
1	16S1	595	A	C5-N7-C8	7.30	107.55	103.90
22	23S1	928	A	C5-N7-C8	7.30	107.55	103.90
22	23S1	2183	A	C5-N7-C8	7.30	107.55	103.90
1	16S1	977	A	C5-N7-C8	7.30	107.55	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	315	A	C5-N7-C8	7.30	107.55	103.90
1	16S1	1507	A	C5-N7-C8	7.30	107.55	103.90
22	23S1	1900	A	C8-N9-C4	7.30	108.72	105.80
22	23S1	1916	A	C5-N7-C8	7.30	107.55	103.90
1	16S1	32	A	C5-N7-C8	7.29	107.55	103.90
22	23S1	320	A	N9-C4-C5	7.29	108.72	105.80
1	16S1	1394	A	C5-N7-C8	7.29	107.55	103.90
22	23S1	1616	A	C5-N7-C8	7.29	107.55	103.90
1	16S1	499	A	C8-N9-C4	7.29	108.72	105.80
22	23S1	2077	A	N3-C4-N9	7.29	133.23	127.40
1	16S1	559	A	C5-N7-C8	7.29	107.54	103.90
1	16S1	673	A	C4-C5-C6	7.29	120.64	117.00
1	16S1	1171	A	N3-C4-N9	7.29	133.23	127.40
22	23S1	2518	A	C5-N7-C8	7.29	107.54	103.90
22	23S1	1809	A	C5-N7-C8	7.29	107.54	103.90
1	16S1	1219	A	C4-C5-C6	7.28	120.64	117.00
22	23S1	2386	A	C5-N7-C8	7.28	107.54	103.90
22	23S1	2565	A	C4-C5-C6	7.28	120.64	117.00
22	23S1	1470	A	C5-N7-C8	7.28	107.54	103.90
22	23S1	472	A	C5-N7-C8	7.28	107.54	103.90
1	16S1	1171	A	C5-N7-C8	7.28	107.54	103.90
1	16S1	1261	A	C5-N7-C8	7.28	107.54	103.90
22	23S1	2114	A	C4-C5-C6	7.28	120.64	117.00
22	23S1	677	A	C5-N7-C8	7.28	107.54	103.90
22	23S1	730	A	C5-N7-C8	7.28	107.54	103.90
22	23S1	984	A	C4-C5-C6	7.28	120.64	117.00
22	23S1	1701	A	C5-N7-C8	7.28	107.54	103.90
22	23S1	1717	A	C5-N7-C8	7.27	107.54	103.90
1	16S1	1163	A	C5-N7-C8	7.27	107.54	103.90
1	16S1	1004	A	C4-C5-C6	7.27	120.64	117.00
1	16S1	743	A	N3-C4-N9	7.27	133.22	127.40
1	16S1	1157	A	N3-C4-N9	7.27	133.22	127.40
1	16S1	236	A	C5-N7-C8	7.27	107.53	103.90
22	23S1	223	A	C5-N7-C8	7.27	107.53	103.90
22	23S1	1286	A	C5-N7-C8	7.26	107.53	103.90
1	16S1	1430	A	C5-N7-C8	7.26	107.53	103.90
22	23S1	1085	A	C5-N7-C8	7.26	107.53	103.90
1	16S1	162	A	C5-C6-N6	7.26	129.51	123.70
22	23S1	73	A	C5-N7-C8	7.26	107.53	103.90
1	16S1	663	A	C5-N7-C8	7.26	107.53	103.90
1	16S1	1483	A	C4-C5-C6	7.26	120.63	117.00
22	23S1	299	A	N9-C4-C5	7.26	108.70	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1773	A	C5-N7-C8	7.26	107.53	103.90
1	16S1	98	A	C5-N7-C8	7.25	107.53	103.90
22	23S1	2614	A	N9-C4-C5	7.25	108.70	105.80
22	23S1	2799	A	C5-C6-N6	7.25	129.50	123.70
22	23S1	1010	A	C5-N7-C8	7.25	107.53	103.90
22	23S1	2088	A	N3-C4-N9	7.25	133.20	127.40
23	05S1	52	A	C5-N7-C8	7.25	107.53	103.90
1	16S1	365	U	N3-C2-O2	-7.25	117.12	122.20
1	16S1	1285	A	C5-N7-C8	7.25	107.53	103.90
22	23S1	118	A	C5-N7-C8	7.25	107.53	103.90
22	23S1	614	A	C5-N7-C8	7.25	107.53	103.90
22	23S1	909	A	C5-N7-C8	7.25	107.53	103.90
22	23S1	1571	A	C5-N7-C8	7.25	107.53	103.90
22	23S1	2800	A	C5-N7-C8	7.25	107.53	103.90
22	23S1	1314	C	N1-C2-O2	7.25	123.25	118.90
22	23S1	844	A	C5-N7-C8	7.25	107.52	103.90
22	23S1	2461	A	N3-C4-N9	7.25	133.20	127.40
1	16S1	129	A	C5-N7-C8	7.25	107.52	103.90
22	23S1	2288	A	C5-N7-C8	7.25	107.52	103.90
22	23S1	821	A	N9-C4-C5	7.24	108.70	105.80
22	23S1	2082	A	C4-C5-C6	7.24	120.62	117.00
22	23S1	1265	A	C5-N7-C8	7.24	107.52	103.90
22	23S1	529	A	C5-N7-C8	7.24	107.52	103.90
1	16S1	1238	A	C5-N7-C8	7.23	107.52	103.90
22	23S1	1821	A	N9-C4-C5	7.23	108.69	105.80
22	23S1	470	A	N3-C4-N9	7.23	133.18	127.40
22	23S1	1313	U	N3-C2-O2	-7.23	117.14	122.20
1	16S1	77	A	C4-C5-C6	7.23	120.61	117.00
1	16S1	1362	A	C5-N7-C8	7.23	107.51	103.90
23	05S1	57	A	C5-N7-C8	7.22	107.51	103.90
1	16S1	1163	A	N3-C4-N9	7.22	133.18	127.40
22	23S1	1387	A	N3-C4-N9	7.22	133.18	127.40
22	23S1	2173	A	C5-C6-N1	7.22	121.31	117.70
22	23S1	2448	A	C5-N7-C8	7.22	107.51	103.90
22	23S1	1213	A	N3-C4-N9	7.22	133.17	127.40
22	23S1	1353	A	N9-C4-C5	7.22	108.69	105.80
22	23S1	1403	A	N3-C4-N9	7.22	133.17	127.40
22	23S1	2757	A	C5-N7-C8	7.22	107.51	103.90
22	23S1	1571	A	N3-C4-N9	7.21	133.17	127.40
22	23S1	2482	A	C5-N7-C8	7.21	107.51	103.90
1	16S1	365	U	C5-C4-O4	7.21	130.23	125.90
1	16S1	579	A	N3-C4-N9	7.21	133.17	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1269	A	C5-N7-C8	7.21	107.50	103.90
22	23S1	1544	A	N9-C4-C5	7.21	108.68	105.80
22	23S1	2453	A	N9-C4-C5	7.21	108.68	105.80
1	16S1	49	U	N3-C4-O4	-7.21	114.36	119.40
22	23S1	1127	A	C5-N7-C8	7.21	107.50	103.90
22	23S1	2111	U	C2-N1-C1'	7.21	126.35	117.70
1	16S1	716	A	C5-N7-C8	7.20	107.50	103.90
22	23S1	1254	A	C5-N7-C8	7.20	107.50	103.90
22	23S1	1413	A	C5-N7-C8	7.20	107.50	103.90
22	23S1	278	A	C5-N7-C8	7.20	107.50	103.90
22	23S1	2037	A	C5-N7-C8	7.20	107.50	103.90
22	23S1	2051	A	C5-N7-C8	7.20	107.50	103.90
22	23S1	2052	A	C5-N7-C8	7.20	107.50	103.90
22	23S1	2287	A	C4-C5-C6	7.20	120.60	117.00
22	23S1	2886	A	C5-N7-C8	7.20	107.50	103.90
1	16S1	282	A	C5-N7-C8	7.20	107.50	103.90
1	16S1	498	A	C4-C5-C6	7.20	120.60	117.00
22	23S1	1522	A	C5-N7-C8	7.20	107.50	103.90
22	23S1	1590	A	C5-N7-C8	7.20	107.50	103.90
1	16S1	715	A	C5-N7-C8	7.20	107.50	103.90
22	23S1	131	A	C5-N7-C8	7.20	107.50	103.90
22	23S1	794	A	C4-C5-C6	7.20	120.60	117.00
1	16S1	412	A	C5-C6-N1	7.19	121.30	117.70
22	23S1	849	A	C5-N7-C8	7.19	107.50	103.90
22	23S1	582	A	C5-N7-C8	7.19	107.50	103.90
22	23S1	1677	A	C5-N7-C8	7.19	107.50	103.90
22	23S1	1664	A	C4-C5-C6	7.19	120.59	117.00
22	23S1	2336	A	C5-N7-C8	7.19	107.49	103.90
1	16S1	1429	A	C5-N7-C8	7.19	107.49	103.90
22	23S1	820	A	N3-C4-N9	7.19	133.15	127.40
22	23S1	477	A	C5-N7-C8	7.19	107.49	103.90
22	23S1	482	A	C5-C6-N6	7.19	129.45	123.70
22	23S1	2119	A	C8-N9-C4	7.19	108.67	105.80
22	23S1	1679	A	C5-N7-C8	7.18	107.49	103.90
22	23S1	2721	A	C5-N7-C8	7.18	107.49	103.90
1	16S1	816	A	C5-N7-C8	7.18	107.49	103.90
22	23S1	1848	A	C4-C5-C6	7.17	120.59	117.00
22	23S1	2033	A	N9-C4-C5	7.17	108.67	105.80
22	23S1	2169	A	C4-C5-C6	7.17	120.58	117.00
24	L021	130	LEU	CA-CB-CG	7.17	131.79	115.30
1	16S1	2	A	C5-N7-C8	7.17	107.48	103.90
1	16S1	365	U	N1-C2-O2	7.17	127.82	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	630	A	C5-N7-C8	7.17	107.48	103.90
1	16S1	1213	A	C4-C5-N7	-7.17	107.12	110.70
1	16S1	451	A	C8-N9-C4	7.16	108.67	105.80
1	16S1	914	A	C5-N7-C8	7.16	107.48	103.90
22	23S1	119	A	C5-N7-C8	7.16	107.48	103.90
22	23S1	1098	A	N3-C4-N9	7.16	133.13	127.40
22	23S1	2267	A	C5-N7-C8	7.16	107.48	103.90
22	23S1	2741	A	C5-N7-C8	7.16	107.48	103.90
1	16S1	32	A	C4-C5-C6	7.16	120.58	117.00
22	23S1	1284	A	C5-N7-C8	7.16	107.48	103.90
22	23S1	1802	A	N3-C4-N9	7.16	133.13	127.40
1	16S1	197	A	C8-N9-C4	7.16	108.66	105.80
22	23S1	1189	A	N3-C4-N9	7.16	133.13	127.40
22	23S1	1301	A	C5-N7-C8	7.16	107.48	103.90
1	16S1	250	A	C5-N7-C8	7.16	107.48	103.90
22	23S1	2706	A	C5-N7-C8	7.16	107.48	103.90
22	23S1	1970	A	C4-C5-C6	7.15	120.58	117.00
1	16S1	712	A	C5-N7-C8	7.15	107.48	103.90
1	16S1	1169	A	C5-N7-C8	7.15	107.48	103.90
22	23S1	119	A	N9-C4-C5	7.15	108.66	105.80
22	23S1	792	A	C8-N9-C4	7.15	108.66	105.80
22	23S1	1580	A	C4-C5-C6	7.15	120.57	117.00
22	23S1	2273	A	C4-C5-C6	7.15	120.57	117.00
22	23S1	1080	A	C5-N7-C8	7.14	107.47	103.90
55	PTR1	9	A	C8-N9-C4	7.14	108.66	105.80
22	23S1	1237	A	C5-N7-C8	7.14	107.47	103.90
22	23S1	1548	A	N3-C4-N9	7.14	133.11	127.40
1	16S1	389	A	C5-C6-N1	7.14	121.27	117.70
1	16S1	336	A	C5-N7-C8	7.14	107.47	103.90
1	16S1	1339	A	C4-C5-C6	7.14	120.57	117.00
1	16S1	1306	A	C5-N7-C8	7.13	107.47	103.90
1	16S1	16	A	C8-N9-C4	7.13	108.65	105.80
1	16S1	964	A	C5-N7-C8	7.13	107.47	103.90
22	23S1	195	A	N9-C4-C5	7.13	108.65	105.80
22	23S1	1020	A	N3-C4-C5	-7.13	121.81	126.80
1	16S1	1022	A	C5-N7-C8	7.13	107.47	103.90
1	16S1	1508	A	C5-N7-C8	7.13	107.47	103.90
1	16S1	98	A	C4-C5-C6	7.13	120.56	117.00
1	16S1	1299	A	C4-C5-C6	7.12	120.56	117.00
22	23S1	255	A	N3-C4-N9	7.12	133.10	127.40
22	23S1	643	A	C5-N7-C8	7.12	107.46	103.90
22	23S1	739	A	C5-N7-C8	7.12	107.46	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2328	A	N3-C4-N9	7.12	133.10	127.40
1	16S1	907	A	N3-C4-N9	7.12	133.10	127.40
22	23S1	2531	A	C5-N7-C8	7.12	107.46	103.90
1	16S1	563	A	C4-C5-C6	7.12	120.56	117.00
22	23S1	330	A	N3-C4-N9	7.12	133.09	127.40
1	16S1	1437	A	C5-N7-C8	7.11	107.46	103.90
22	23S1	199	A	C5-N7-C8	7.11	107.46	103.90
22	23S1	572	A	N3-C4-N9	7.11	133.09	127.40
22	23S1	10	A	C5-N7-C8	7.11	107.46	103.90
1	16S1	459	A	N3-C4-N9	7.11	133.09	127.40
1	16S1	502	A	C4-C5-C6	7.11	120.56	117.00
1	16S1	994	A	C4-C5-C6	7.11	120.56	117.00
22	23S1	226	A	C5-N7-C8	7.11	107.45	103.90
22	23S1	2388	A	C8-N9-C4	7.11	108.64	105.80
22	23S1	1969	A	C4-C5-C6	7.11	120.56	117.00
22	23S1	2753	A	N9-C4-C5	7.11	108.64	105.80
1	16S1	78	A	C5-N7-C8	7.11	107.45	103.90
22	23S1	689	A	C5-C6-N1	7.11	121.25	117.70
22	23S1	2879	A	N3-C4-N9	7.11	133.09	127.40
1	16S1	383	A	C5-N7-C8	7.11	107.45	103.90
1	16S1	1201	A	C5-C6-N6	7.11	129.38	123.70
22	23S1	233	A	C5-N7-C8	7.11	107.45	103.90
22	23S1	457	A	C8-N9-C4	7.11	108.64	105.80
1	16S1	51	A	C8-N9-C4	7.10	108.64	105.80
1	16S1	1492	A	C5-N7-C8	7.10	107.45	103.90
22	23S1	2447	G	C5-C6-N1	7.10	115.05	111.50
22	23S1	91	A	C5-N7-C8	7.10	107.45	103.90
22	23S1	1029	A	N3-C4-N9	7.10	133.08	127.40
22	23S1	2453	A	C4-C5-C6	7.10	120.55	117.00
22	23S1	2602	A	C8-N9-C4	7.10	108.64	105.80
22	23S1	84	A	C5-N7-C8	7.10	107.45	103.90
55	PTR1	76	A	C5-N7-C8	7.10	107.45	103.90
1	16S1	502	A	N3-C4-N9	7.10	133.08	127.40
22	23S1	668	A	C8-N9-C4	7.10	108.64	105.80
22	23S1	2284	A	C5-N7-C8	7.09	107.45	103.90
1	16S1	860	A	N9-C4-C5	7.09	108.64	105.80
22	23S1	532	A	C4-C5-C6	7.09	120.55	117.00
22	23S1	689	A	N3-C4-N9	7.09	133.07	127.40
22	23S1	1966	A	C5-N7-C8	7.09	107.45	103.90
22	23S1	2267	A	C5-C6-N1	7.09	121.25	117.70
22	23S1	2727	A	N3-C4-N9	7.09	133.07	127.40
1	16S1	373	A	C4-C5-C6	7.09	120.54	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	900	A	C5-N7-C8	7.09	107.44	103.90
1	16S1	1080	A	C5-N7-C8	7.09	107.44	103.90
22	23S1	845	A	C4-C5-C6	7.09	120.54	117.00
22	23S1	863	A	C4-C5-C6	7.09	120.54	117.00
22	23S1	1359	A	C5-N7-C8	7.09	107.44	103.90
1	16S1	814	A	N3-C4-N9	7.08	133.07	127.40
22	23S1	221	A	C8-N9-C4	7.08	108.63	105.80
22	23S1	2335	A	C4-C5-C6	7.08	120.54	117.00
1	16S1	199	A	C4-C5-C6	7.08	120.54	117.00
22	23S1	1969	A	C8-N9-C4	7.08	108.63	105.80
1	16S1	718	A	C5-N7-C8	7.07	107.44	103.90
22	23S1	1713	A	C5-N7-C8	7.07	107.44	103.90
22	23S1	918	A	C5-N7-C8	7.07	107.44	103.90
1	16S1	72	A	C5-N7-C8	7.07	107.44	103.90
22	23S1	1111	A	C4-C5-C6	7.07	120.53	117.00
1	16S1	728	A	N9-C4-C5	7.07	108.63	105.80
22	23S1	415	A	C5-N7-C8	7.07	107.43	103.90
22	23S1	1553	A	N3-C4-N9	7.07	133.06	127.40
1	16S1	1014	A	C5-N7-C8	7.07	107.43	103.90
1	16S1	1167	A	C5-N7-C8	7.07	107.43	103.90
1	16S1	872	A	N3-C4-N9	7.06	133.05	127.40
22	23S1	925	A	C5-N7-C8	7.06	107.43	103.90
22	23S1	1427	A	C5-N7-C8	7.06	107.43	103.90
1	16S1	487	A	C4-C5-C6	7.06	120.53	117.00
1	16S1	706	A	C4-C5-C6	7.06	120.53	117.00
22	23S1	1020	A	C8-N9-C4	7.06	108.62	105.80
22	23S1	1204	A	C5-N7-C8	7.06	107.43	103.90
22	23S1	477	A	C4-C5-C6	7.06	120.53	117.00
22	23S1	1020	A	C5-N7-C8	7.06	107.43	103.90
22	23S1	1260	A	C5-N7-C8	7.06	107.43	103.90
22	23S1	1387	A	C4-C5-C6	7.06	120.53	117.00
22	23S1	1641	A	C4-C5-C6	7.05	120.53	117.00
22	23S1	1670	C	O5'-P-OP2	-7.05	99.35	105.70
22	23S1	2281	A	C5-C6-N1	7.05	121.23	117.70
22	23S1	2566	A	C5-N7-C8	7.05	107.43	103.90
22	23S1	309	A	C5-N7-C8	7.05	107.42	103.90
22	23S1	2369	A	C4-C5-C6	7.05	120.53	117.00
22	23S1	2392	A	N3-C4-N9	7.05	133.04	127.40
1	16S1	1502	A	C5-N7-C8	7.05	107.42	103.90
22	23S1	1069	A	C8-N9-C4	7.05	108.62	105.80
22	23S1	1754	A	C5-N7-C8	7.05	107.42	103.90
22	23S1	574	A	N3-C4-N9	7.05	133.04	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1269	A	C4-C5-C6	7.05	120.52	117.00
22	23S1	492	A	N3-C4-N9	7.05	133.04	127.40
22	23S1	829	A	C8-N9-C4	7.05	108.62	105.80
1	16S1	1398	A	C5-N7-C8	7.04	107.42	103.90
22	23S1	324	A	N3-C4-N9	7.04	133.03	127.40
22	23S1	750	A	N3-C4-N9	7.04	133.03	127.40
1	16S1	338	A	C5-N7-C8	7.04	107.42	103.90
1	16S1	1055	A	C4-C5-C6	7.04	120.52	117.00
1	16S1	116	A	N3-C4-N9	7.04	133.03	127.40
1	16S1	554	A	C4-C5-N7	-7.04	107.18	110.70
55	PTR1	23	A	C5-N7-C8	7.04	107.42	103.90
22	23S1	1028	A	C5-C6-N1	7.03	121.22	117.70
22	23S1	1953	A	C4-C5-C6	7.03	120.52	117.00
22	23S1	241	A	C5-N7-C8	7.03	107.42	103.90
22	23S1	2887	A	N3-C4-N9	7.03	133.03	127.40
1	16S1	80	A	N3-C4-N9	7.03	133.02	127.40
22	23S1	705	A	N3-C4-N9	7.03	133.02	127.40
22	23S1	1392	A	N9-C4-C5	7.03	108.61	105.80
22	23S1	1583	A	C8-N9-C4	7.03	108.61	105.80
1	16S1	780	A	C5-N7-C8	7.03	107.41	103.90
1	16S1	499	A	N3-C4-N9	7.03	133.02	127.40
22	23S1	251	A	N7-C8-N9	-7.02	110.29	113.80
22	23S1	2114	A	N7-C8-N9	-7.02	110.29	113.80
22	23S1	2188	U	O3'-P-O5'	7.02	117.35	104.00
22	23S1	2369	A	N3-C4-N9	7.02	133.02	127.40
55	PTR1	21	A	C5-N7-C8	7.02	107.41	103.90
1	16S1	1036	A	C4-C5-C6	7.02	120.51	117.00
22	23S1	1000	A	N9-C4-C5	7.02	108.61	105.80
22	23S1	1586	A	C4-C5-C6	7.02	120.51	117.00
22	23S1	2497	A	C5-N7-C8	7.02	107.41	103.90
22	23S1	382	A	C4-C5-C6	7.02	120.51	117.00
22	23S1	1744	A	N3-C4-N9	7.02	133.01	127.40
22	23S1	14	A	C5-N7-C8	7.01	107.41	103.90
1	16S1	1357	A	N3-C4-N9	7.01	133.01	127.40
22	23S1	63	A	C5-N7-C8	7.01	107.41	103.90
22	23S1	2119	A	C4-C5-N7	-7.01	107.19	110.70
22	23S1	2288	A	C8-N9-C4	7.01	108.61	105.80
22	23S1	2366	A	C5-N7-C8	7.01	107.41	103.90
22	23S1	1570	A	N9-C4-C5	7.01	108.60	105.80
22	23S1	2868	A	C5-N7-C8	7.01	107.41	103.90
22	23S1	173	A	C5-N7-C8	7.01	107.41	103.90
22	23S1	477	A	N3-C4-N9	7.01	133.01	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	699	A	C5-N7-C8	7.01	107.40	103.90
22	23S1	1920	C	C6-N1-C2	-7.01	117.50	120.30
22	23S1	2430	A	N7-C8-N9	-7.01	110.30	113.80
22	23S1	2899	A	N3-C4-N9	7.00	133.00	127.40
22	23S1	2051	A	C4-C5-C6	7.00	120.50	117.00
22	23S1	2281	A	N3-C4-N9	7.00	133.00	127.40
22	23S1	528	A	N3-C4-N9	7.00	133.00	127.40
22	23S1	1321	A	N3-C4-N9	7.00	133.00	127.40
1	16S1	1219	A	C5-N7-C8	7.00	107.40	103.90
22	23S1	1384	A	C5-N7-C8	7.00	107.40	103.90
1	16S1	300	A	C6-C5-N7	-7.00	127.40	132.30
1	16S1	1171	A	C4-C5-C6	7.00	120.50	117.00
22	23S1	677	A	C4-C5-C6	7.00	120.50	117.00
22	23S1	1143	A	N3-C4-N9	7.00	133.00	127.40
22	23S1	2266	A	C5-N7-C8	7.00	107.40	103.90
1	16S1	356	A	C4-C5-C6	7.00	120.50	117.00
1	16S1	687	A	C5-N7-C8	7.00	107.40	103.90
22	23S1	382	A	N3-C4-N9	7.00	133.00	127.40
22	23S1	574	A	C8-N9-C4	6.99	108.60	105.80
22	23S1	863	A	C5-N7-C8	6.99	107.40	103.90
22	23S1	1328	A	N9-C4-C5	6.99	108.60	105.80
22	23S1	2868	A	N3-C4-N9	6.99	133.00	127.40
1	16S1	415	A	C4-C5-C6	6.99	120.50	117.00
1	16S1	1446	A	C5-N7-C8	6.99	107.39	103.90
22	23S1	2101	A	N9-C4-C5	6.99	108.60	105.80
22	23S1	1276	A	C4-C5-C6	6.99	120.49	117.00
1	16S1	607	A	C5-N7-C8	6.99	107.39	103.90
22	23S1	422	A	N3-C4-N9	6.99	132.99	127.40
22	23S1	1027	A	C5-N7-C8	6.99	107.39	103.90
22	23S1	1126	A	C5-N7-C8	6.99	107.39	103.90
22	23S1	1759	A	N3-C4-N9	6.99	132.99	127.40
1	16S1	116	A	C4-C5-C6	6.98	120.49	117.00
1	16S1	270	A	C4-C5-C6	6.98	120.49	117.00
1	16S1	790	A	N3-C4-N9	6.98	132.99	127.40
22	23S1	391	A	N3-C4-N9	6.98	132.99	127.40
22	23S1	743	A	C5-N7-C8	6.98	107.39	103.90
22	23S1	2542	A	C4-C5-N7	-6.98	107.21	110.70
1	16S1	983	A	C4-C5-C6	6.98	120.49	117.00
22	23S1	478	A	C5-N7-C8	6.98	107.39	103.90
1	16S1	98	A	N3-C4-N9	6.98	132.98	127.40
22	23S1	1664	A	N3-C4-N9	6.98	132.98	127.40
22	23S1	2706	A	N3-C4-N9	6.98	132.98	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	191	A	C4-C5-C6	6.97	120.49	117.00
22	23S1	196	A	C4-C5-C6	6.97	120.49	117.00
22	23S1	727	A	C5-N7-C8	6.97	107.39	103.90
22	23S1	1314	C	C2-N1-C1'	6.97	126.47	118.80
1	16S1	1081	A	N3-C4-N9	6.97	132.98	127.40
22	23S1	1143	A	C4-C5-C6	6.97	120.49	117.00
22	23S1	2268	A	C4-C5-C6	6.97	120.48	117.00
22	23S1	1586	A	C5-N7-C8	6.97	107.39	103.90
1	16S1	1318	A	C5-N7-C8	6.97	107.38	103.90
22	23S1	1969	A	N3-C4-N9	6.97	132.97	127.40
22	23S1	2352	A	N3-C4-N9	6.97	132.97	127.40
1	16S1	466	A	N9-C4-C5	6.96	108.59	105.80
22	23S1	2740	A	N9-C4-C5	6.96	108.59	105.80
22	23S1	49	A	N3-C4-N9	6.96	132.97	127.40
22	23S1	2037	A	N3-C4-N9	6.96	132.97	127.40
22	23S1	544	C	N3-C2-O2	-6.96	117.03	121.90
22	23S1	2873	A	C5-N7-C8	6.96	107.38	103.90
1	16S1	161	A	C5-N7-C8	6.96	107.38	103.90
22	23S1	514	A	C5-N7-C8	6.96	107.38	103.90
22	23S1	2439	A	C4-C5-C6	6.96	120.48	117.00
22	23S1	2900	A	C5-N7-C8	6.96	107.38	103.90
1	16S1	864	A	C5-N7-C8	6.96	107.38	103.90
22	23S1	1057	A	C8-N9-C4	6.96	108.58	105.80
1	16S1	621	A	N3-C4-N9	6.95	132.96	127.40
1	16S1	1396	A	N3-C4-N9	6.95	132.96	127.40
22	23S1	1854	A	N3-C4-N9	6.95	132.96	127.40
1	16S1	712	A	N3-C4-N9	6.95	132.96	127.40
1	16S1	923	A	C5-N7-C8	6.95	107.38	103.90
1	16S1	1280	A	C5-N7-C8	6.95	107.38	103.90
22	23S1	1609	A	C4-C5-C6	6.95	120.47	117.00
1	16S1	1418	A	N3-C4-N9	6.94	132.95	127.40
22	23S1	718	A	C4-C5-C6	6.94	120.47	117.00
22	23S1	2212	A	N9-C4-C5	6.94	108.58	105.80
1	16S1	908	A	C4-C5-C6	6.94	120.47	117.00
22	23S1	503	A	N3-C4-N9	6.94	132.95	127.40
22	23S1	94	A	N3-C4-N9	6.94	132.95	127.40
1	16S1	694	A	C4-C5-C6	6.94	120.47	117.00
22	23S1	2054	A	N3-C4-N9	6.94	132.95	127.40
1	16S1	101	A	N3-C4-N9	6.93	132.95	127.40
22	23S1	1912	A	C4-C5-C6	6.93	120.47	117.00
22	23S1	2014	A	N3-C4-N9	6.93	132.95	127.40
1	16S1	718	A	C4-C5-C6	6.93	120.47	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	633	A	C5-N7-C8	6.93	107.37	103.90
22	23S1	1028	A	N3-C4-N9	6.93	132.94	127.40
22	23S1	1085	A	C4-C5-C6	6.93	120.47	117.00
22	23S1	1419	A	C8-N9-C4	6.93	108.57	105.80
22	23S1	2813	A	C5-N7-C8	6.93	107.37	103.90
1	16S1	983	A	C5-N7-C8	6.93	107.36	103.90
22	23S1	1548	A	C4-C5-C6	6.93	120.46	117.00
1	16S1	53	A	N3-C4-N9	6.93	132.94	127.40
1	16S1	1157	A	C4-C5-C6	6.93	120.46	117.00
22	23S1	28	A	C5-N7-C8	6.93	107.36	103.90
22	23S1	1755	A	N9-C4-C5	6.92	108.57	105.80
22	23S1	2014	A	C4-C5-C6	6.92	120.46	117.00
22	23S1	2311	A	N9-C4-C5	6.92	108.57	105.80
1	16S1	949	A	C4-C5-C6	6.92	120.46	117.00
22	23S1	730	A	N3-C4-N9	6.92	132.94	127.40
22	23S1	1808	A	C5-N7-C8	6.92	107.36	103.90
1	16S1	754	C	C2-N1-C1'	6.92	126.41	118.80
1	16S1	1022	A	C4-C5-C6	6.92	120.46	117.00
22	23S1	1866	A	N3-C4-N9	6.92	132.94	127.40
22	23S1	2392	A	C4-C5-C6	6.92	120.46	117.00
22	23S1	2868	A	C4-C5-C6	6.92	120.46	117.00
22	23S1	627	A	C8-N9-C4	6.91	108.57	105.80
22	23S1	1312	U	C5-C4-O4	6.91	130.05	125.90
22	23S1	2469	A	C8-N9-C4	6.91	108.56	105.80
1	16S1	181	A	N3-C4-N9	6.91	132.93	127.40
22	23S1	1085	A	N3-C4-N9	6.91	132.93	127.40
22	23S1	1912	A	C8-N9-C4	6.91	108.56	105.80
22	23S1	599	A	C8-N9-C4	6.91	108.56	105.80
22	23S1	1549	A	C5-N7-C8	6.91	107.35	103.90
22	23S1	742	A	N3-C4-N9	6.90	132.92	127.40
1	16S1	702	A	C5-N7-C8	6.90	107.35	103.90
23	05S1	73	A	C5-N7-C8	6.90	107.35	103.90
22	23S1	479	A	C8-N9-C4	6.90	108.56	105.80
22	23S1	2171	A	N3-C4-N9	6.90	132.92	127.40
22	23S1	849	A	C4-C5-C6	6.90	120.45	117.00
1	16S1	746	A	C5-C6-N1	6.89	121.15	117.70
1	16S1	270	A	N3-C4-N9	6.89	132.91	127.40
1	16S1	496	A	N3-C4-N9	6.89	132.91	127.40
1	16S1	865	A	C5-N7-C8	6.89	107.34	103.90
22	23S1	2706	A	C4-C5-C6	6.89	120.44	117.00
22	23S1	2135	A	N3-C4-N9	6.89	132.91	127.40
55	PTR1	23	A	C5-C6-N1	6.89	121.14	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	155	A	N3-C4-N9	6.89	132.91	127.40
1	16S1	408	A	C4-C5-C6	6.89	120.44	117.00
22	23S1	2439	A	C8-N9-C4	6.88	108.55	105.80
22	23S1	221	A	N3-C4-C5	-6.88	121.98	126.80
22	23S1	2614	A	N3-C4-N9	6.88	132.91	127.40
1	16S1	88	U	N3-C2-O2	-6.88	117.38	122.20
22	23S1	2459	A	N3-C4-N9	6.88	132.91	127.40
1	16S1	706	A	N3-C4-N9	6.88	132.90	127.40
22	23S1	1111	A	C8-N9-C4	6.88	108.55	105.80
1	16S1	1197	A	C4-C5-C6	6.88	120.44	117.00
1	16S1	1333	A	N9-C4-C5	6.88	108.55	105.80
22	23S1	203	A	C5-N7-C8	6.88	107.34	103.90
22	23S1	190	A	C4-C5-C6	6.88	120.44	117.00
22	23S1	1970	A	C5-N7-C8	6.88	107.34	103.90
22	23S1	2451	A	N7-C8-N9	-6.88	110.36	113.80
1	16S1	448	A	N3-C4-N9	6.87	132.90	127.40
22	23S1	131	A	C4-C5-C6	6.87	120.44	117.00
22	23S1	2799	A	C4-C5-C6	6.87	120.44	117.00
22	23S1	996	A	N3-C4-N9	6.87	132.90	127.40
1	16S1	1374	A	N3-C4-N9	6.87	132.90	127.40
1	16S1	81	A	C4-C5-C6	6.87	120.43	117.00
1	16S1	663	A	C4-C5-C6	6.87	120.43	117.00
22	23S1	730	A	C4-C5-C6	6.87	120.43	117.00
22	23S1	2761	A	N3-C4-N9	6.87	132.89	127.40
22	23S1	2158	A	C8-N9-C4	6.86	108.55	105.80
22	23S1	1871	A	N3-C4-N9	6.86	132.89	127.40
22	23S1	2564	A	N9-C4-C5	6.86	108.54	105.80
1	16S1	1441	A	C8-N9-C4	6.86	108.54	105.80
22	23S1	1744	A	C4-C5-C6	6.86	120.43	117.00
22	23S1	2748	A	C5-N7-C8	6.86	107.33	103.90
22	23S1	233	A	N3-C4-N9	6.86	132.88	127.40
22	23S1	255	A	C4-C5-C6	6.86	120.43	117.00
1	16S1	397	A	C5-C6-N1	6.85	121.13	117.70
1	16S1	1152	A	N3-C4-N9	6.85	132.88	127.40
22	23S1	2191	A	N3-C4-N9	6.85	132.88	127.40
1	16S1	116	A	C5-N7-C8	6.85	107.33	103.90
22	23S1	1745	A	C4-C5-C6	6.85	120.43	117.00
22	23S1	2108	A	C4-C5-C6	6.85	120.43	117.00
1	16S1	489	C	C6-N1-C2	-6.85	117.56	120.30
1	16S1	155	A	C4-C5-C6	6.85	120.42	117.00
1	16S1	663	A	N3-C4-N9	6.85	132.88	127.40
22	23S1	454	A	N9-C4-C5	6.85	108.54	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	582	A	N3-C4-N9	6.85	132.88	127.40
1	16S1	602	A	N3-C4-N9	6.85	132.88	127.40
1	16S1	393	A	N3-C4-N9	6.84	132.88	127.40
22	23S1	2284	A	C4-C5-C6	6.84	120.42	117.00
55	PTR1	23	A	N3-C4-N9	6.84	132.88	127.40
1	16S1	205	A	C4-C5-C6	6.84	120.42	117.00
1	16S1	539	A	N3-C4-N9	6.84	132.87	127.40
22	23S1	2051	A	N3-C4-N9	6.84	132.87	127.40
22	23S1	2101	A	C4-C5-N7	-6.84	107.28	110.70
22	23S1	2614	A	C4-C5-N7	-6.84	107.28	110.70
1	16S1	1000	A	N3-C4-N9	6.84	132.87	127.40
22	23S1	1054	A	C4-C5-C6	6.84	120.42	117.00
22	23S1	324	A	C5-N7-C8	6.84	107.32	103.90
22	23S1	2088	A	C4-C5-C6	6.84	120.42	117.00
55	PTR1	51	A	C4-C5-N7	-6.84	107.28	110.70
1	16S1	66	A	C5-N7-C8	6.83	107.32	103.90
22	23S1	94	A	C4-C5-C6	6.83	120.42	117.00
22	23S1	1009	A	N3-C4-N9	6.83	132.87	127.40
22	23S1	1419	A	C5-N7-C8	6.83	107.32	103.90
22	23S1	1515	A	N9-C4-C5	6.83	108.53	105.80
1	16S1	1172	C	C2-N1-C1'	6.83	126.32	118.80
22	23S1	49	A	C4-C5-C6	6.83	120.42	117.00
22	23S1	1858	A	N3-C4-N9	6.83	132.87	127.40
1	16S1	1197	A	N3-C4-N9	6.83	132.87	127.40
22	23S1	2700	A	N3-C4-N9	6.83	132.87	127.40
22	23S1	756	A	N3-C4-N9	6.83	132.86	127.40
1	16S1	845	A	N9-C4-C5	6.83	108.53	105.80
22	23S1	142	A	C5-N7-C8	6.83	107.31	103.90
22	23S1	503	A	C4-C5-C6	6.83	120.41	117.00
1	16S1	151	A	C5-C6-N1	6.83	121.11	117.70
1	16S1	1319	A	C5-N7-C8	6.83	107.31	103.90
22	23S1	1189	A	C4-C5-C6	6.83	120.41	117.00
22	23S1	2879	A	C4-C5-C6	6.83	120.41	117.00
1	16S1	439	U	C2-N3-C4	-6.82	122.91	127.00
1	16S1	441	A	N3-C4-N9	6.82	132.86	127.40
1	16S1	1191	A	C5-N7-C8	6.82	107.31	103.90
22	23S1	945	A	N9-C4-C5	6.82	108.53	105.80
1	16S1	189	A	C5-N7-C8	6.82	107.31	103.90
22	23S1	1403	A	C4-C5-C6	6.82	120.41	117.00
22	23S1	1927	A	N9-C4-C5	6.82	108.53	105.80
1	16S1	792	A	C8-N9-C4	6.82	108.53	105.80
1	16S1	1350	A	C4-C5-C6	6.82	120.41	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	422	A	C4-C5-C6	6.82	120.41	117.00
22	23S1	1111	A	N3-C4-N9	6.82	132.85	127.40
22	23S1	1431	A	N3-C4-N9	6.82	132.85	127.40
22	23S1	1757	A	C5-N7-C8	6.82	107.31	103.90
22	23S1	2327	A	C4-C5-C6	6.82	120.41	117.00
22	23S1	959	A	N3-C4-N9	6.82	132.85	127.40
22	23S1	2461	A	C5-C6-N1	6.82	121.11	117.70
22	23S1	2639	A	C5-N7-C8	6.82	107.31	103.90
22	23S1	2054	A	C5-C6-N1	6.81	121.11	117.70
1	16S1	1130	A	C4-C5-C6	6.81	120.41	117.00
22	23S1	191	A	N3-C4-N9	6.81	132.85	127.40
22	23S1	1308	A	C4-C5-N7	-6.81	107.29	110.70
22	23S1	2059	A	N3-C4-N9	6.81	132.85	127.40
1	16S1	574	A	C5-N7-C8	6.81	107.31	103.90
1	16S1	1110	A	C5-N7-C8	6.81	107.30	103.90
22	23S1	2449	U	C5-C4-O4	-6.81	121.82	125.90
22	23S1	936	A	N3-C4-N9	6.81	132.84	127.40
1	16S1	430	A	N3-C4-N9	6.80	132.84	127.40
22	23S1	1021	A	C5-C6-N1	6.80	121.10	117.70
1	16S1	790	A	C4-C5-C6	6.80	120.40	117.00
22	23S1	1549	A	N3-C4-N9	6.80	132.84	127.40
55	PTR1	58	A	N3-C4-N9	6.80	132.84	127.40
1	16S1	1418	A	C5-N7-C8	6.80	107.30	103.90
1	16S1	1508	A	C4-C5-C6	6.80	120.40	117.00
1	16S1	71	A	C8-N9-C4	6.80	108.52	105.80
22	23S1	2407	A	C5-N7-C8	6.80	107.30	103.90
22	23S1	354	A	N9-C4-C5	6.80	108.52	105.80
1	16S1	162	A	C5-N7-C8	6.79	107.30	103.90
22	23S1	2407	A	N3-C4-N9	6.79	132.84	127.40
1	16S1	172	A	C5-N7-C8	6.79	107.30	103.90
22	23S1	644	A	C4-C5-N7	-6.79	107.30	110.70
22	23S1	1739	A	N3-C4-N9	6.79	132.83	127.40
22	23S1	1028	A	C5-N7-C8	6.79	107.29	103.90
1	16S1	743	A	C4-C5-C6	6.79	120.39	117.00
1	16S1	1363	A	C4-C5-C6	6.79	120.39	117.00
22	23S1	300	A	C5-N7-C8	6.79	107.29	103.90
1	16S1	1306	A	N3-C4-N9	6.78	132.83	127.40
22	23S1	2459	A	C4-C5-C6	6.78	120.39	117.00
22	23S1	1872	A	N7-C8-N9	-6.78	110.41	113.80
22	23S1	753	A	N3-C4-N9	6.78	132.82	127.40
22	23S1	2749	A	C5-N7-C8	6.78	107.29	103.90
22	23S1	1246	A	N3-C4-N9	6.78	132.82	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1515	A	C5-N7-C8	6.78	107.29	103.90
1	16S1	640	A	N9-C4-C5	6.77	108.51	105.80
1	16S1	873	A	N3-C4-N9	6.77	132.82	127.40
22	23S1	71	A	N3-C4-N9	6.77	132.82	127.40
22	23S1	152	A	N3-C4-N9	6.77	132.81	127.40
22	23S1	1393	A	C5-N7-C8	6.77	107.28	103.90
22	23S1	2725	A	C5-N7-C8	6.77	107.28	103.90
1	16S1	559	A	N3-C4-N9	6.76	132.81	127.40
1	16S1	946	A	N3-C4-N9	6.76	132.81	127.40
1	16S1	1357	A	C4-C5-C6	6.76	120.38	117.00
22	23S1	1616	A	C8-N9-C4	6.76	108.51	105.80
1	16S1	2	A	N3-C4-N9	6.76	132.81	127.40
1	16S1	959	A	C4-C5-C6	6.76	120.38	117.00
1	16S1	1102	A	C4-C5-C6	6.76	120.38	117.00
22	23S1	1936	A	C5-N7-C8	6.76	107.28	103.90
1	16S1	223	A	N3-C4-N9	6.76	132.81	127.40
1	16S1	1102	A	N3-C4-N9	6.76	132.81	127.40
22	23S1	167	A	C8-N9-C4	6.76	108.50	105.80
22	23S1	2800	A	C8-N9-C4	6.76	108.50	105.80
23	05S1	45	A	N3-C4-N9	6.76	132.81	127.40
1	16S1	559	A	C4-C5-C6	6.76	120.38	117.00
1	16S1	1375	A	N3-C4-N9	6.76	132.81	127.40
22	23S1	2725	A	N3-C4-N9	6.75	132.80	127.40
22	23S1	1987	A	C8-N9-C4	6.75	108.50	105.80
22	23S1	2679	A	N3-C4-N9	6.75	132.80	127.40
1	16S1	493	A	C5-N7-C8	6.75	107.28	103.90
22	23S1	980	A	N3-C4-N9	6.75	132.80	127.40
55	PTR1	73	A	C8-N9-C4	6.75	108.50	105.80
1	16S1	754	C	N1-C2-O2	6.75	122.95	118.90
22	23S1	1327	A	C5-N7-C8	6.75	107.28	103.90
22	23S1	1608	A	C5-N7-C8	6.75	107.28	103.90
1	16S1	189	A	C4-C5-C6	6.75	120.37	117.00
22	23S1	1301	A	N3-C4-N9	6.75	132.80	127.40
1	16S1	1508	A	N3-C4-N9	6.75	132.80	127.40
22	23S1	2665	A	C4-C5-C6	6.75	120.37	117.00
1	16S1	329	A	C4-C5-C6	6.75	120.37	117.00
1	16S1	1271	A	C8-N9-C4	6.74	108.50	105.80
22	23S1	204	A	C8-N9-C4	6.74	108.50	105.80
22	23S1	362	A	C5-C6-N1	6.74	121.07	117.70
22	23S1	677	A	C5-C6-N1	6.74	121.07	117.70
22	23S1	1469	A	N3-C4-N9	6.74	132.79	127.40
22	23S1	1609	A	N3-C4-N9	6.74	132.79	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	978	A	N9-C4-C5	6.74	108.50	105.80
22	23S1	751	A	C5-N7-C8	6.74	107.27	103.90
22	23S1	943	A	C4-C5-C6	6.74	120.37	117.00
1	16S1	482	A	C5-N7-C8	6.74	107.27	103.90
22	23S1	1603	A	N3-C4-N9	6.74	132.79	127.40
22	23S1	2163	A	N3-C4-N9	6.73	132.79	127.40
22	23S1	2900	A	C4-C5-C6	6.73	120.37	117.00
22	23S1	655	A	C8-N9-C4	6.73	108.49	105.80
22	23S1	1809	A	N3-C4-N9	6.73	132.78	127.40
22	23S1	2241	A	N3-C4-N9	6.73	132.78	127.40
1	16S1	349	A	C8-N9-C4	6.73	108.49	105.80
22	23S1	1630	A	N9-C4-C5	6.73	108.49	105.80
1	16S1	642	A	C4-C5-C6	6.72	120.36	117.00
22	23S1	1126	A	N3-C4-N9	6.72	132.78	127.40
22	23S1	1745	A	N3-C4-N9	6.72	132.78	127.40
1	16S1	609	A	C4-C5-C6	6.72	120.36	117.00
22	23S1	1237	A	C8-N9-C4	6.72	108.49	105.80
22	23S1	2461	A	C4-C5-C6	6.72	120.36	117.00
22	23S1	21	A	N3-C4-N9	6.72	132.78	127.40
22	23S1	2189	U	N3-C2-O2	-6.72	117.50	122.20
30	L311	56	ARG	NE-CZ-NH2	6.72	123.66	120.30
22	23S1	1276	A	N3-C4-N9	6.72	132.77	127.40
22	23S1	1598	A	C5-N7-C8	6.72	107.26	103.90
22	23S1	2392	A	C5-N7-C8	6.72	107.26	103.90
1	16S1	716	A	N3-C4-N9	6.71	132.77	127.40
1	16S1	579	A	C4-C5-C6	6.71	120.36	117.00
22	23S1	52	A	N3-C4-N9	6.71	132.77	127.40
1	16S1	236	A	C4-C5-C6	6.71	120.36	117.00
1	16S1	622	A	N9-C4-C5	6.71	108.48	105.80
22	23S1	943	A	N3-C4-N9	6.71	132.77	127.40
1	16S1	59	A	N3-C4-N9	6.71	132.77	127.40
1	16S1	1499	A	N3-C4-N9	6.71	132.77	127.40
22	23S1	504	A	C5-N7-C8	6.71	107.25	103.90
22	23S1	563	A	N3-C4-N9	6.71	132.77	127.40
22	23S1	1932	A	C5-N7-C8	6.71	107.25	103.90
1	16S1	174	A	N3-C4-N9	6.71	132.76	127.40
1	16S1	873	A	C4-C5-C6	6.71	120.35	117.00
22	23S1	1711	A	N3-C4-N9	6.71	132.77	127.40
22	23S1	2142	A	C5-C6-N6	6.71	129.06	123.70
22	23S1	1590	A	N3-C4-N9	6.70	132.76	127.40
22	23S1	1847	A	C4-C5-C6	6.70	120.35	117.00
1	16S1	865	A	N3-C4-N9	6.70	132.76	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	454	A	C4-C5-N7	-6.70	107.35	110.70
22	23S1	522	A	N3-C4-N9	6.70	132.76	127.40
1	16S1	949	A	N3-C4-N9	6.70	132.76	127.40
1	16S1	1285	A	C8-N9-C4	6.70	108.48	105.80
22	23S1	1508	A	C5-N7-C8	6.70	107.25	103.90
22	23S1	1572	A	C4-C5-C6	6.70	120.35	117.00
22	23S1	2598	A	C4-C5-C6	6.70	120.35	117.00
1	16S1	72	A	N3-C4-N9	6.70	132.76	127.40
1	16S1	33	A	C5-N7-C8	6.70	107.25	103.90
22	23S1	943	A	C5-N7-C8	6.70	107.25	103.90
22	23S1	975	A	C5-N7-C8	6.70	107.25	103.90
22	23S1	1755	A	C4-C5-N7	-6.70	107.35	110.70
22	23S1	1321	A	C4-C5-C6	6.69	120.35	117.00
22	23S1	2170	A	N3-C4-N9	6.69	132.75	127.40
22	23S1	2469	A	C5-C6-N1	6.69	121.05	117.70
22	23S1	1373	A	C4-C5-C6	6.69	120.34	117.00
1	16S1	1396	A	C4-C5-C6	6.69	120.34	117.00
22	23S1	1586	A	N9-C4-C5	6.69	108.47	105.80
22	23S1	415	A	N3-C4-N9	6.68	132.75	127.40
23	05S1	119	A	C4-C5-C6	6.68	120.34	117.00
1	16S1	1252	A	C5-N7-C8	6.68	107.24	103.90
22	23S1	374	A	N3-C4-N9	6.68	132.75	127.40
22	23S1	980	A	C5-N7-C8	6.68	107.24	103.90
1	16S1	1288	A	C5-N7-C8	6.68	107.24	103.90
1	16S1	573	A	N3-C4-N9	6.68	132.74	127.40
1	16S1	1036	A	N3-C4-N9	6.68	132.74	127.40
1	16S1	1271	A	N3-C4-N9	6.68	132.74	127.40
22	23S1	693	A	N3-C4-N9	6.68	132.74	127.40
22	23S1	2900	A	N3-C4-N9	6.68	132.74	127.40
22	23S1	1535	A	N3-C4-N9	6.68	132.74	127.40
22	23S1	1610	A	C5-N7-C8	6.68	107.24	103.90
1	16S1	913	A	C8-N9-C4	6.67	108.47	105.80
22	23S1	1470	A	C4-C5-C6	6.67	120.34	117.00
22	23S1	2241	A	C4-C5-C6	6.67	120.34	117.00
22	23S1	1901	A	N3-C4-N9	6.67	132.74	127.40
22	23S1	2761	A	C5-C6-N1	6.67	121.04	117.70
22	23S1	2518	A	C4-C5-C6	6.67	120.34	117.00
23	05S1	73	A	C4-C5-C6	6.67	120.33	117.00
22	23S1	404	A	C5-N7-C8	6.67	107.23	103.90
1	16S1	1012	A	N3-C4-N9	6.67	132.74	127.40
1	16S1	1163	A	C4-C5-C6	6.67	120.33	117.00
22	23S1	1608	A	N3-C4-N9	6.67	132.74	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1952	A	N3-C4-N9	6.67	132.73	127.40
22	23S1	1336	A	N3-C4-N9	6.67	132.73	127.40
22	23S1	1900	A	N3-C4-N9	6.67	132.73	127.40
22	23S1	2433	A	N3-C4-N9	6.67	132.73	127.40
22	23S1	2439	A	N3-C4-N9	6.67	132.73	127.40
1	16S1	196	A	C5-N7-C8	6.67	107.23	103.90
22	23S1	10	A	C5-C6-N1	6.67	121.03	117.70
22	23S1	1048	A	C4-C5-C6	6.67	120.33	117.00
23	05S1	99	A	N3-C4-N9	6.67	132.73	127.40
1	16S1	2	A	N9-C4-C5	6.66	108.47	105.80
22	23S1	203	A	C4-C5-C6	6.66	120.33	117.00
22	23S1	2792	A	C4-C5-C6	6.66	120.33	117.00
1	16S1	1081	A	C4-C5-C6	6.66	120.33	117.00
1	16S1	1261	A	C8-N9-C4	6.66	108.47	105.80
22	23S1	1549	A	C4-C5-C6	6.66	120.33	117.00
1	16S1	946	A	C8-N9-C4	6.66	108.47	105.80
1	16S1	1092	A	C8-N9-C4	6.66	108.46	105.80
22	23S1	2665	A	N3-C4-N9	6.66	132.73	127.40
22	23S1	2886	A	N3-C4-N9	6.66	132.73	127.40
22	23S1	2887	A	C4-C5-N7	-6.66	107.37	110.70
22	23S1	1151	A	C5-N7-C8	6.66	107.23	103.90
22	23S1	2284	A	N3-C4-N9	6.66	132.73	127.40
22	23S1	2482	A	C4-C5-C6	6.66	120.33	117.00
22	23S1	2297	A	C4-C5-N7	-6.66	107.37	110.70
23	05S1	45	A	C5-N7-C8	6.66	107.23	103.90
22	23S1	2426	A	N3-C4-N9	6.65	132.72	127.40
1	16S1	313	A	N9-C4-C5	6.65	108.46	105.80
22	23S1	449	A	N3-C4-N9	6.65	132.72	127.40
22	23S1	522	A	C4-C5-C6	6.65	120.33	117.00
22	23S1	2147	A	N9-C4-C5	6.65	108.46	105.80
1	16S1	236	A	N3-C4-N9	6.65	132.72	127.40
1	16S1	780	A	C4-C5-C6	6.64	120.32	117.00
1	16S1	373	A	C8-N9-C4	6.64	108.46	105.80
1	16S1	1324	A	C5-N7-C8	6.64	107.22	103.90
22	23S1	144	A	N3-C4-N9	6.64	132.71	127.40
22	23S1	1713	A	C8-N9-C4	6.64	108.46	105.80
1	16S1	199	A	C5-C6-N1	6.64	121.02	117.70
22	23S1	84	A	C6-N1-C2	6.64	122.58	118.60
22	23S1	626	A	C5-N7-C8	6.64	107.22	103.90
22	23S1	1532	A	N3-C4-N9	6.64	132.71	127.40
22	23S1	1918	A	N3-C4-N9	6.64	132.71	127.40
1	16S1	161	A	C4-C5-C6	6.64	120.32	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1126	A	C4-C5-C6	6.64	120.32	117.00
1	16S1	460	A	N3-C4-N9	6.63	132.71	127.40
1	16S1	509	A	N3-C4-N9	6.63	132.71	127.40
22	23S1	1774	C	C6-N1-C2	-6.63	117.65	120.30
22	23S1	1899	A	N9-C4-C5	6.63	108.45	105.80
22	23S1	1987	A	N3-C4-N9	6.63	132.71	127.40
23	05S1	57	A	C4-C5-C6	6.63	120.32	117.00
55	PTR1	58	A	C4-C5-C6	6.63	120.32	117.00
55	PTR1	69	A	N3-C4-N9	6.63	132.71	127.40
1	16S1	1299	A	C5-N7-C8	6.63	107.22	103.90
22	23S1	1385	A	C8-N9-C4	6.63	108.45	105.80
22	23S1	782	A	N3-C4-N9	6.63	132.71	127.40
1	16S1	454	G	N3-C4-N9	6.63	129.98	126.00
22	23S1	1787	A	C5-N7-C8	6.63	107.21	103.90
55	PTR1	58	A	C8-N9-C4	6.63	108.45	105.80
1	16S1	695	A	C4-C5-C6	6.63	120.31	117.00
1	16S1	873	A	C8-N9-C4	6.63	108.45	105.80
22	23S1	586	A	C5-N7-C8	6.62	107.21	103.90
22	23S1	727	A	N3-C4-N9	6.62	132.70	127.40
1	16S1	223	A	C4-C5-C6	6.62	120.31	117.00
22	23S1	513	A	C5-N7-C8	6.62	107.21	103.90
22	23S1	721	A	N3-C4-N9	6.62	132.69	127.40
22	23S1	2142	A	C5-C6-N1	6.62	121.01	117.70
1	16S1	1492	A	C4-C5-C6	6.61	120.31	117.00
22	23S1	1490	A	C4-C5-C6	6.61	120.31	117.00
1	16S1	655	A	C4-C5-C6	6.61	120.31	117.00
1	16S1	1101	A	N9-C4-C5	6.61	108.44	105.80
22	23S1	941	A	N3-C4-N9	6.61	132.69	127.40
22	23S1	1590	A	C4-C5-C6	6.61	120.31	117.00
1	16S1	382	A	N3-C4-N9	6.61	132.69	127.40
1	16S1	1005	A	C8-N9-C4	6.61	108.44	105.80
1	16S1	1252	A	C4-C5-C6	6.61	120.30	117.00
22	23S1	2425	A	N3-C4-N9	6.60	132.68	127.40
22	23S1	2199	A	N3-C4-N9	6.60	132.68	127.40
55	PTR1	17	U	C5-C4-O4	-6.60	121.94	125.90
1	16S1	1374	A	C4-C5-C6	6.60	120.30	117.00
22	23S1	1048	A	N3-C4-N9	6.60	132.68	127.40
1	16S1	26	A	C5-C6-N1	6.60	121.00	117.70
1	16S1	1236	A	N3-C4-N9	6.60	132.68	127.40
22	23S1	1700	A	N3-C4-N9	6.60	132.68	127.40
22	23S1	2189	U	C6-N1-C2	-6.60	117.04	121.00
1	16S1	712	A	C5-C6-N1	6.60	121.00	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1054	A	N3-C4-N9	6.60	132.68	127.40
22	23S1	1784	A	C8-N9-C4	6.60	108.44	105.80
22	23S1	2060	A	C8-N9-C4	6.60	108.44	105.80
22	23S1	1046	A	C8-N9-C4	6.60	108.44	105.80
1	16S1	704	A	C5-N7-C8	6.59	107.20	103.90
22	23S1	2646	C	C5-C6-N1	6.59	124.30	121.00
22	23S1	2425	A	C4-C5-C6	6.59	120.30	117.00
22	23S1	2809	A	N3-C4-N9	6.59	132.67	127.40
22	23S1	190	A	N3-C4-N9	6.59	132.67	127.40
22	23S1	2278	A	N3-C4-N9	6.59	132.67	127.40
1	16S1	1446	A	N3-C4-N9	6.59	132.67	127.40
1	16S1	66	A	C4-C5-C6	6.59	120.29	117.00
22	23S1	538	A	C8-N9-C4	6.59	108.43	105.80
22	23S1	2019	A	N3-C4-N9	6.59	132.67	127.40
22	23S1	2513	A	N3-C4-N9	6.59	132.67	127.40
22	23S1	144	A	C4-C5-C6	6.58	120.29	117.00
22	23S1	2434	A	N9-C4-C5	6.58	108.43	105.80
22	23S1	2792	A	N3-C4-N9	6.58	132.67	127.40
1	16S1	466	A	C4-C5-C6	6.58	120.29	117.00
1	16S1	794	A	N3-C4-N9	6.58	132.66	127.40
22	23S1	2327	A	N3-C4-N9	6.58	132.66	127.40
22	23S1	5	A	C4-C5-C6	6.58	120.29	117.00
22	23S1	1014	A	N3-C4-N9	6.58	132.66	127.40
22	23S1	2163	A	C4-C5-C6	6.58	120.29	117.00
1	16S1	53	A	C4-C5-C6	6.57	120.29	117.00
1	16S1	546	A	N3-C4-N9	6.57	132.66	127.40
22	23S1	256	A	C4-C5-C6	6.57	120.29	117.00
1	16S1	716	A	N9-C4-C5	6.57	108.43	105.80
23	05S1	29	A	N9-C4-C5	6.57	108.43	105.80
22	23S1	2388	A	N3-C4-N9	6.57	132.66	127.40
1	16S1	1324	A	C4-C5-C6	6.57	120.28	117.00
22	23S1	936	A	C4-C5-C6	6.57	120.28	117.00
22	23S1	1998	A	N3-C4-N9	6.57	132.65	127.40
1	16S1	816	A	N3-C4-N9	6.56	132.65	127.40
1	16S1	74	A	N9-C4-C5	6.56	108.42	105.80
22	23S1	1916	A	N3-C4-N9	6.56	132.65	127.40
22	23S1	2757	A	C4-C5-C6	6.56	120.28	117.00
1	16S1	408	A	N3-C4-N9	6.56	132.65	127.40
1	16S1	1158	C	C6-N1-C1'	-6.56	112.93	120.80
22	23S1	2497	A	N3-C4-N9	6.56	132.65	127.40
1	16S1	642	A	N3-C4-N9	6.56	132.65	127.40
1	16S1	1275	A	C8-N9-C4	6.56	108.42	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	146	A	N3-C4-N9	6.56	132.65	127.40
22	23S1	2614	A	C5-C6-N1	6.56	120.98	117.70
1	16S1	766	A	C5-N7-C8	6.56	107.18	103.90
22	23S1	2418	A	N3-C4-N9	6.56	132.65	127.40
22	23S1	1142	A	C5-C6-N1	6.55	120.98	117.70
22	23S1	2850	A	C4-C5-C6	6.55	120.28	117.00
1	16S1	353	A	C8-N9-C4	6.55	108.42	105.80
1	16S1	696	A	N3-C4-N9	6.55	132.64	127.40
22	23S1	528	A	C4-C5-C6	6.55	120.28	117.00
1	16S1	975	A	C5-N7-C8	6.55	107.18	103.90
22	23S1	443	A	C8-N9-C4	6.55	108.42	105.80
22	23S1	2636	C	N1-C2-O2	6.55	122.83	118.90
23	05S1	75	G	N3-C4-C5	-6.55	125.32	128.60
42	L241	52	LEU	CA-CB-CG	6.55	130.37	115.30
1	16S1	174	A	C4-C5-C6	6.55	120.28	117.00
22	23S1	899	A	N3-C4-N9	6.55	132.64	127.40
22	23S1	1214	A	C5-C6-N1	6.55	120.97	117.70
22	23S1	1630	A	C4-C5-N7	-6.55	107.42	110.70
22	23S1	1981	A	N9-C4-C5	6.55	108.42	105.80
22	23S1	2176	A	C4-C5-C6	6.55	120.27	117.00
1	16S1	432	A	C4-C5-C6	6.55	120.27	117.00
22	23S1	975	A	N3-C4-N9	6.55	132.64	127.40
22	23S1	2497	A	C4-C5-C6	6.55	120.27	117.00
1	16S1	51	A	N3-C4-N9	6.54	132.64	127.40
1	16S1	55	A	C4-C5-N7	-6.54	107.43	110.70
22	23S1	95	A	C4-C5-C6	6.54	120.27	117.00
1	16S1	794	A	C4-C5-C6	6.54	120.27	117.00
22	23S1	502	A	N9-C4-C5	6.54	108.42	105.80
22	23S1	2340	A	N3-C4-N9	6.54	132.63	127.40
1	16S1	344	A	C8-N9-C4	6.54	108.42	105.80
22	23S1	2134	A	N3-C4-N9	6.54	132.63	127.40
22	23S1	2335	A	N3-C4-N9	6.54	132.63	127.40
1	16S1	1429	A	N3-C4-N9	6.54	132.63	127.40
22	23S1	1214	A	N9-C4-C5	6.54	108.42	105.80
1	16S1	649	A	N9-C4-C5	6.54	108.41	105.80
1	16S1	819	A	C4-C5-C6	6.54	120.27	117.00
22	23S1	2469	A	C5-N7-C8	6.54	107.17	103.90
1	16S1	1349	A	C8-N9-C4	6.53	108.41	105.80
22	23S1	1308	A	N9-C4-C5	6.53	108.41	105.80
22	23S1	1819	A	N3-C4-N9	6.53	132.63	127.40
22	23S1	654	A	C4-C5-C6	6.53	120.27	117.00
1	16S1	414	A	N3-C4-N9	6.53	132.62	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1225	A	C4-C5-C6	6.53	120.27	117.00
23	05S1	94	A	N3-C4-N9	6.53	132.62	127.40
1	16S1	935	A	N3-C4-N9	6.53	132.62	127.40
1	16S1	1227	A	N9-C4-C5	6.53	108.41	105.80
22	23S1	330	A	C4-C5-C6	6.53	120.26	117.00
22	23S1	2354	C	C6-N1-C2	-6.53	117.69	120.30
1	16S1	205	A	N3-C4-N9	6.53	132.62	127.40
1	16S1	1021	A	N3-C4-N9	6.53	132.62	127.40
1	16S1	1360	A	N9-C4-C5	6.53	108.41	105.80
22	23S1	1608	A	C4-C5-C6	6.53	120.26	117.00
22	23S1	1912	A	N3-C4-N9	6.53	132.62	127.40
22	23S1	2860	A	C4-C5-C6	6.53	120.26	117.00
1	16S1	539	A	C4-C5-C6	6.52	120.26	117.00
1	16S1	1055	A	N3-C4-N9	6.52	132.62	127.40
22	23S1	56	A	N3-C4-N9	6.52	132.62	127.40
1	16S1	1357	A	C5-N7-C8	6.52	107.16	103.90
1	16S1	608	A	N3-C4-N9	6.52	132.61	127.40
1	16S1	26	A	C5-N7-C8	6.52	107.16	103.90
22	23S1	5	A	N3-C4-N9	6.52	132.61	127.40
22	23S1	44	A	C4-C5-C6	6.51	120.26	117.00
1	16S1	572	A	C8-N9-C4	6.51	108.41	105.80
55	PTR1	38	A	C5-N7-C8	6.51	107.16	103.90
1	16S1	1093	A	C4-C5-C6	6.51	120.26	117.00
22	23S1	1089	A	C4-C5-C6	6.51	120.25	117.00
22	23S1	2117	A	C8-N9-C4	6.51	108.41	105.80
23	05S1	66	A	C5-N7-C8	6.51	107.16	103.90
22	23S1	722	A	C4-C5-C6	6.51	120.25	117.00
22	23S1	2171	A	C5-N7-C8	6.51	107.16	103.90
1	16S1	1332	A	C4-C5-C6	6.51	120.25	117.00
22	23S1	2634	A	C4-C5-C6	6.51	120.25	117.00
22	23S1	1853	A	N9-C4-C5	6.50	108.40	105.80
22	23S1	84	A	N3-C4-C5	-6.50	122.25	126.80
22	23S1	198	C	C6-N1-C2	-6.50	117.70	120.30
22	23S1	218	A	C4-C5-C6	6.50	120.25	117.00
22	23S1	422	A	C5-N7-C8	6.50	107.15	103.90
22	23S1	1419	A	C5-C6-N1	6.50	120.95	117.70
1	16S1	487	A	N3-C4-N9	6.50	132.60	127.40
22	23S1	2070	A	N9-C4-C5	6.49	108.40	105.80
22	23S1	2171	A	C4-C5-C6	6.49	120.25	117.00
1	16S1	1145	A	C8-N9-C4	6.49	108.40	105.80
22	23S1	1373	A	N3-C4-N9	6.49	132.59	127.40
22	23S1	2822	G	N9-C4-C5	-6.49	102.80	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	819	A	N3-C4-N9	6.49	132.59	127.40
1	16S1	978	A	C4-C5-N7	-6.49	107.46	110.70
22	23S1	233	A	C8-N9-C4	6.49	108.40	105.80
22	23S1	959	A	C4-C5-C6	6.49	120.24	117.00
22	23S1	1626	A	N3-C4-N9	6.49	132.59	127.40
22	23S1	1650	A	N3-C4-N9	6.49	132.59	127.40
22	23S1	1689	A	C4-C5-C6	6.49	120.24	117.00
22	23S1	2042	A	C8-N9-C4	6.49	108.40	105.80
22	23S1	2813	A	C4-C5-C6	6.49	120.24	117.00
22	23S1	722	A	N3-C4-N9	6.49	132.59	127.40
22	23S1	911	A	C4-C5-C6	6.49	120.24	117.00
22	23S1	1477	A	N3-C4-N9	6.49	132.59	127.40
1	16S1	573	A	C4-C5-C6	6.49	120.24	117.00
1	16S1	1465	A	N3-C4-N9	6.49	132.59	127.40
22	23S1	750	A	C8-N9-C4	6.49	108.39	105.80
22	23S1	909	A	N3-C4-N9	6.49	132.59	127.40
22	23S1	1269	A	N3-C4-N9	6.49	132.59	127.40
22	23S1	1916	A	C4-C5-C6	6.49	120.24	117.00
22	23S1	466	A	C5-N7-C8	6.48	107.14	103.90
22	23S1	2059	A	C4-C5-C6	6.48	120.24	117.00
22	23S1	430	A	C4-C5-C6	6.48	120.24	117.00
22	23S1	1535	A	C4-C5-C6	6.48	120.24	117.00
22	23S1	2776	A	C8-N9-C4	6.48	108.39	105.80
22	23S1	2781	A	C5-N7-C8	6.48	107.14	103.90
1	16S1	179	A	N9-C4-C5	6.48	108.39	105.80
1	16S1	665	A	C5-N7-C8	6.48	107.14	103.90
1	16S1	1447	A	C8-N9-C4	6.48	108.39	105.80
22	23S1	1773	A	C4-C5-C6	6.48	120.24	117.00
22	23S1	2114	A	C5-C6-N1	6.48	120.94	117.70
1	16S1	1067	A	C8-N9-C4	6.48	108.39	105.80
22	23S1	472	A	C4-C5-C6	6.48	120.24	117.00
22	23S1	2448	A	N9-C4-C5	6.48	108.39	105.80
22	23S1	2531	A	N3-C4-N9	6.48	132.58	127.40
23	05S1	45	A	C5-C6-N1	6.48	120.94	117.70
22	23S1	156	A	N3-C4-N9	6.47	132.58	127.40
1	16S1	482	A	C4-C5-C6	6.47	120.24	117.00
22	23S1	1593	A	N3-C4-N9	6.47	132.58	127.40
22	23S1	1821	A	C4-C5-N7	-6.47	107.46	110.70
1	16S1	1428	A	N9-C4-C5	6.47	108.39	105.80
22	23S1	1244	A	N3-C4-N9	6.47	132.58	127.40
22	23S1	1899	A	N3-C4-N9	6.47	132.57	127.40
1	16S1	919	A	C5-N7-C8	6.47	107.13	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	152	A	C4-C5-C6	6.47	120.23	117.00
22	23S1	1420	A	C8-N9-C4	6.47	108.39	105.80
22	23S1	2169	A	N3-C4-N9	6.47	132.57	127.40
22	23S1	2407	A	C4-C5-C6	6.47	120.23	117.00
1	16S1	366	A	C8-N9-C4	6.46	108.39	105.80
1	16S1	441	A	C4-C5-C6	6.46	120.23	117.00
22	23S1	764	A	C5-N7-C8	6.46	107.13	103.90
22	23S1	2899	A	C4-C5-C6	6.46	120.23	117.00
22	23S1	1810	A	C5-C6-N6	6.46	128.87	123.70
22	23S1	2850	A	N3-C4-N9	6.46	132.57	127.40
1	16S1	253	A	C4-C5-C6	6.46	120.23	117.00
1	16S1	1146	A	N3-C4-N9	6.46	132.57	127.40
22	23S1	2670	A	C8-N9-C4	6.46	108.39	105.80
1	16S1	655	A	N3-C4-N9	6.46	132.57	127.40
22	23S1	800	A	C4-C5-N7	-6.46	107.47	110.70
22	23S1	2033	A	C4-C5-N7	-6.46	107.47	110.70
22	23S1	74	A	N3-C4-N9	6.45	132.56	127.40
22	23S1	244	A	N3-C4-N9	6.45	132.56	127.40
22	23S1	2199	A	C4-C5-C6	6.45	120.22	117.00
22	23S1	1676	A	C4-C5-C6	6.45	120.22	117.00
23	05S1	29	A	C4-C5-N7	-6.45	107.48	110.70
22	23S1	346	A	N3-C4-N9	6.45	132.56	127.40
22	23S1	1073	A	C4-C5-C6	6.45	120.22	117.00
22	23S1	1230	A	C4-C5-C6	6.45	120.22	117.00
22	23S1	1745	A	C5-N7-C8	6.45	107.12	103.90
1	16S1	695	A	N3-C4-N9	6.44	132.55	127.40
1	16S1	1044	A	N3-C4-N9	6.44	132.55	127.40
1	16S1	1339	A	N3-C4-N9	6.44	132.55	127.40
22	23S1	574	A	C4-C5-C6	6.44	120.22	117.00
22	23S1	1089	A	N3-C4-N9	6.44	132.55	127.40
22	23S1	1644	C	N1-C2-O2	6.44	122.77	118.90
22	23S1	1919	A	N3-C4-N9	6.44	132.55	127.40
22	23S1	2670	A	N3-C4-N9	6.44	132.55	127.40
1	16S1	452	A	C5-C6-N1	6.44	120.92	117.70
1	16S1	629	A	N3-C4-N9	6.44	132.55	127.40
22	23S1	182	A	N3-C4-N9	6.44	132.55	127.40
22	23S1	1155	A	N9-C4-C5	6.44	108.38	105.80
22	23S1	1784	A	C5-N7-C8	6.44	107.12	103.90
22	23S1	1084	A	N3-C4-N9	6.44	132.55	127.40
1	16S1	1151	A	N3-C4-N9	6.44	132.55	127.40
22	23S1	1805	A	N9-C4-C5	6.44	108.38	105.80
1	16S1	195	A	N9-C4-C5	6.43	108.37	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	618	C	N1-C2-O2	6.43	122.76	118.90
1	16S1	767	A	C4-C5-C6	6.43	120.22	117.00
1	16S1	1163	A	C5-C6-N1	6.43	120.92	117.70
1	16S1	1513	A	N3-C4-N9	6.43	132.54	127.40
22	23S1	1597	A	N9-C4-C5	6.43	108.37	105.80
22	23S1	449	A	N9-C4-C5	6.43	108.37	105.80
22	23S1	1353	A	C4-C5-N7	-6.43	107.48	110.70
22	23S1	2386	A	N3-C4-N9	6.43	132.54	127.40
1	16S1	629	A	C4-C5-C6	6.43	120.21	117.00
1	16S1	1256	A	N3-C4-N9	6.43	132.54	127.40
1	16S1	363	A	N3-C4-N9	6.43	132.54	127.40
22	23S1	2095	A	N9-C4-C5	6.43	108.37	105.80
1	16S1	120	A	C8-N9-C4	6.42	108.37	105.80
1	16S1	263	A	C4-C5-C6	6.42	120.21	117.00
1	16S1	1012	A	C4-C5-C6	6.42	120.21	117.00
1	16S1	1250	A	N9-C4-C5	6.42	108.37	105.80
1	16S1	1251	A	N9-C4-C5	6.42	108.37	105.80
1	16S1	1299	A	C5-C6-N1	6.42	120.91	117.70
22	23S1	734	A	C8-N9-C4	6.42	108.37	105.80
22	23S1	1307	A	N3-C4-N9	6.42	132.54	127.40
22	23S1	2097	A	N3-C4-N9	6.42	132.54	127.40
22	23S1	2530	A	C4-C5-C6	6.42	120.21	117.00
1	16S1	66	A	N3-C4-N9	6.42	132.54	127.40
22	23S1	1978	A	N3-C4-N9	6.42	132.54	127.40
1	16S1	938	A	N3-C4-N9	6.42	132.54	127.40
1	16S1	1022	A	N9-C4-C5	6.42	108.37	105.80
1	16S1	1093	A	N3-C4-N9	6.42	132.54	127.40
1	16S1	1368	A	N3-C4-N9	6.42	132.54	127.40
22	23S1	1383	A	N9-C4-C5	6.42	108.37	105.80
22	23S1	529	A	N9-C4-C5	6.42	108.37	105.80
22	23S1	782	A	C4-C5-C6	6.42	120.21	117.00
22	23S1	1847	A	C5-N7-C8	6.42	107.11	103.90
22	23S1	2386	A	C5-C6-N1	6.42	120.91	117.70
22	23S1	2468	A	N3-C4-N9	6.42	132.54	127.40
1	16S1	1110	A	C4-C5-C6	6.42	120.21	117.00
22	23S1	1998	A	N9-C4-C5	6.42	108.37	105.80
22	23S1	1872	A	C5-N7-C8	6.42	107.11	103.90
1	16S1	211	G	N3-C4-N9	6.42	129.85	126.00
3	S031	34	ASP	CB-CG-OD1	6.41	124.07	118.30
1	16S1	181	A	C4-C5-C6	6.41	120.21	117.00
1	16S1	1465	A	C4-C5-C6	6.41	120.20	117.00
1	16S1	74	A	C4-C5-N7	-6.41	107.50	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	609	A	C4-C5-C6	6.41	120.20	117.00
22	23S1	1230	A	N3-C4-N9	6.41	132.53	127.40
22	23S1	2634	A	N3-C4-N9	6.41	132.53	127.40
55	PTR1	62	C	C2-N1-C1'	6.41	125.85	118.80
1	16S1	935	A	C8-N9-C4	6.41	108.36	105.80
22	23S1	2476	A	N3-C4-N9	6.41	132.52	127.40
22	23S1	1129	A	C8-N9-C4	6.40	108.36	105.80
22	23S1	1998	A	C4-C5-C6	6.40	120.20	117.00
1	16S1	1531	A	C4-C5-C6	6.40	120.20	117.00
22	23S1	849	A	N3-C4-N9	6.40	132.52	127.40
1	16S1	681	A	N3-C4-N9	6.40	132.52	127.40
1	16S1	743	A	C5-C6-N1	6.40	120.90	117.70
1	16S1	816	A	C4-C5-C6	6.40	120.20	117.00
1	16S1	1000	A	C4-C5-C6	6.40	120.20	117.00
22	23S1	1336	A	C4-C5-C6	6.40	120.20	117.00
22	23S1	1632	A	N9-C4-C5	6.40	108.36	105.80
22	23S1	910	A	N3-C4-N9	6.40	132.52	127.40
22	23S1	1005	C	C6-N1-C2	-6.40	117.74	120.30
29	L091	122	LEU	CB-CG-CD1	6.40	121.88	111.00
22	23S1	173	A	N3-C4-N9	6.40	132.52	127.40
22	23S1	1509	A	C8-N9-C4	6.40	108.36	105.80
22	23S1	1672	A	N3-C4-N9	6.40	132.52	127.40
22	23S1	2297	A	C4-C5-C6	6.40	120.20	117.00
55	PTR1	42	A	N3-C4-N9	6.40	132.52	127.40
1	16S1	1503	A	C4-C5-C6	6.40	120.20	117.00
22	23S1	1569	A	C8-N9-C4	6.40	108.36	105.80
1	16S1	1324	A	N3-C4-N9	6.39	132.52	127.40
22	23S1	439	A	N3-C4-N9	6.39	132.51	127.40
22	23S1	2670	A	C4-C5-C6	6.39	120.20	117.00
1	16S1	371	A	N3-C4-N9	6.39	132.51	127.40
1	16S1	451	A	N3-C4-N9	6.39	132.51	127.40
1	16S1	465	A	C5-C6-N1	6.39	120.90	117.70
1	16S1	1340	A	N3-C4-N9	6.39	132.51	127.40
22	23S1	781	A	N3-C4-N9	6.39	132.51	127.40
55	PTR1	21	A	C4-C5-C6	6.39	120.20	117.00
23	05S1	45	A	C8-N9-C4	6.39	108.36	105.80
1	16S1	78	A	N3-C4-N9	6.39	132.51	127.40
22	23S1	743	A	N3-C4-N9	6.39	132.51	127.40
22	23S1	2003	A	N3-C4-N9	6.39	132.51	127.40
1	16S1	754	C	N3-C2-O2	-6.39	117.43	121.90
22	23S1	2062	A	C4-C5-C6	6.39	120.19	117.00
22	23S1	2328	A	C5-N7-C8	6.39	107.09	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	324	A	C4-C5-C6	6.39	120.19	117.00
22	23S1	602	A	N3-C4-N9	6.39	132.51	127.40
22	23S1	2126	A	C4-C5-C6	6.39	120.19	117.00
22	23S1	2778	A	C4-C5-C6	6.39	120.19	117.00
22	23S1	1730	C	C5-C6-N1	6.38	124.19	121.00
22	23S1	2013	A	N3-C4-N9	6.38	132.51	127.40
22	23S1	2366	A	N3-C4-N9	6.38	132.51	127.40
1	16S1	1014	A	C4-C5-C6	6.38	120.19	117.00
22	23S1	1773	A	N9-C4-C5	6.38	108.35	105.80
1	16S1	81	A	N9-C4-C5	6.38	108.35	105.80
22	23S1	439	A	C4-C5-C6	6.38	120.19	117.00
22	23S1	1551	A	N3-C4-N9	6.38	132.50	127.40
22	23S1	2723	C	C6-N1-C2	-6.38	117.75	120.30
1	16S1	722	G	N3-C4-C5	-6.38	125.41	128.60
22	23S1	324	A	C8-N9-C4	6.38	108.35	105.80
22	23S1	643	A	C8-N9-C4	6.38	108.35	105.80
22	23S1	947	A	N3-C4-N9	6.38	132.50	127.40
1	16S1	1257	A	C8-N9-C4	6.38	108.35	105.80
22	23S1	2080	A	N3-C4-N9	6.38	132.50	127.40
1	16S1	523	A	C4-C5-C6	6.38	120.19	117.00
22	23S1	449	A	C4-C5-C6	6.38	120.19	117.00
22	23S1	1503	A	C4-C5-C6	6.38	120.19	117.00
22	23S1	1641	A	N3-C4-N9	6.38	132.50	127.40
23	05S1	50	A	N3-C4-N9	6.38	132.50	127.40
1	16S1	325	A	C4-C5-C6	6.37	120.19	117.00
1	16S1	1394	A	C8-N9-C4	6.37	108.35	105.80
22	23S1	608	A	N3-C4-N9	6.37	132.50	127.40
22	23S1	788	A	C8-N9-C4	6.37	108.35	105.80
22	23S1	1655	A	N3-C4-N9	6.37	132.50	127.40
22	23S1	2358	A	N9-C4-C5	6.37	108.35	105.80
22	23S1	265	A	C8-N9-C4	6.37	108.35	105.80
22	23S1	1572	A	N3-C4-N9	6.37	132.50	127.40
1	16S1	253	A	N3-C4-N9	6.37	132.49	127.40
1	16S1	503	C	C5-C6-N1	6.37	124.18	121.00
1	16S1	878	A	C4-C5-C6	6.37	120.19	117.00
22	23S1	2031	A	N3-C4-N9	6.37	132.50	127.40
22	23S1	2158	A	N3-C4-N9	6.37	132.50	127.40
1	16S1	33	A	N3-C4-N9	6.37	132.49	127.40
22	23S1	781	A	C4-C5-C6	6.37	120.18	117.00
22	23S1	1829	A	N3-C4-N9	6.37	132.49	127.40
55	PTR1	38	A	N3-C4-N9	6.37	132.49	127.40
22	23S1	1746	A	C4-C5-C6	6.36	120.18	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1912	A	C4-C5-N7	-6.36	107.52	110.70
22	23S1	345	A	N9-C4-C5	6.36	108.34	105.80
22	23S1	1000	A	N3-C4-N9	6.36	132.49	127.40
1	16S1	1332	A	C5-N7-C8	6.36	107.08	103.90
22	23S1	1244	A	C4-C5-C6	6.36	120.18	117.00
22	23S1	1495	A	N9-C4-C5	6.36	108.34	105.80
22	23S1	1791	A	C5-N7-C8	6.36	107.08	103.90
55	PTR1	14	A	C4-C5-N7	-6.36	107.52	110.70
1	16S1	1503	A	N3-C4-N9	6.36	132.49	127.40
22	23S1	917	A	N3-C4-N9	6.36	132.49	127.40
1	16S1	78	A	C5-C6-N1	6.36	120.88	117.70
1	16S1	1318	A	C4-C5-C6	6.36	120.18	117.00
22	23S1	1532	A	C4-C5-C6	6.36	120.18	117.00
1	16S1	777	A	C4-C5-C6	6.36	120.18	117.00
22	23S1	125	A	C8-N9-C4	6.36	108.34	105.80
22	23S1	2111	U	N3-C2-O2	-6.36	117.75	122.20
22	23S1	909	A	C5-C6-N1	6.35	120.88	117.70
22	23S1	2090	A	N3-C4-N9	6.35	132.48	127.40
22	23S1	743	A	C4-C5-C6	6.35	120.18	117.00
22	23S1	800	A	C8-N9-C4	6.35	108.34	105.80
22	23S1	1913	A	C8-N9-C4	6.35	108.34	105.80
22	23S1	2388	A	C4-C5-C6	6.35	120.18	117.00
1	16S1	109	A	C8-N9-C4	6.35	108.34	105.80
1	16S1	1256	A	C8-N9-C4	6.35	108.34	105.80
22	23S1	471	A	N3-C4-N9	6.35	132.48	127.40
22	23S1	1803	A	C5-N7-C8	6.35	107.08	103.90
22	23S1	2205	A	C8-N9-C4	6.35	108.34	105.80
1	16S1	974	A	N3-C4-N9	6.35	132.48	127.40
22	23S1	990	A	N9-C4-C5	6.35	108.34	105.80
22	23S1	2810	A	C4-C5-C6	6.35	120.17	117.00
1	16S1	243	A	N9-C4-C5	6.34	108.34	105.80
1	16S1	452	A	C4-C5-C6	6.34	120.17	117.00
1	16S1	1004	A	N9-C4-C5	6.34	108.34	105.80
1	16S1	1274	A	N9-C4-C5	6.34	108.34	105.80
22	23S1	2321	U	N3-C2-O2	-6.34	117.76	122.20
1	16S1	460	A	C4-C5-C6	6.34	120.17	117.00
1	16S1	1167	A	C8-N9-C4	6.34	108.34	105.80
22	23S1	2154	A	N3-C4-N9	6.34	132.47	127.40
1	16S1	182	A	C8-N9-C4	6.34	108.34	105.80
1	16S1	274	A	C5-C6-N1	6.34	120.87	117.70
22	23S1	156	A	C4-C5-C6	6.34	120.17	117.00
1	16S1	602	A	C4-C5-C6	6.34	120.17	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	872	A	C4-C5-C6	6.34	120.17	117.00
1	16S1	1146	A	C4-C5-C6	6.34	120.17	117.00
1	16S1	1261	A	N3-C4-N9	6.34	132.47	127.40
22	23S1	1544	A	C5-C6-N1	6.34	120.87	117.70
22	23S1	1815	A	C5-N7-C8	6.34	107.07	103.90
1	16S1	1216	A	N9-C4-C5	6.34	108.33	105.80
22	23S1	203	A	N3-C4-N9	6.34	132.47	127.40
22	23S1	415	A	C4-C5-C6	6.34	120.17	117.00
22	23S1	2758	A	N9-C4-C5	6.34	108.33	105.80
23	05S1	75	G	C5-C6-N1	6.34	114.67	111.50
22	23S1	1314	C	C5-C6-N1	6.33	124.17	121.00
55	PTR1	3	A	N3-C4-N9	6.33	132.47	127.40
1	16S1	782	A	C8-N9-C4	6.33	108.33	105.80
1	16S1	784	A	N3-C4-N9	6.33	132.47	127.40
22	23S1	478	A	N3-C4-N9	6.33	132.47	127.40
1	16S1	393	A	C4-C5-C6	6.33	120.17	117.00
22	23S1	1247	A	C8-N9-C4	6.33	108.33	105.80
22	23S1	2014	A	C8-N9-C4	6.33	108.33	105.80
22	23S1	2727	A	C4-C5-C6	6.33	120.17	117.00
23	05S1	119	A	N3-C4-N9	6.33	132.47	127.40
55	PTR1	59	A	N9-C4-C5	6.33	108.33	105.80
1	16S1	459	A	C4-C5-C6	6.33	120.17	117.00
1	16S1	498	A	C6-N1-C2	-6.33	114.80	118.60
1	16S1	1329	A	N9-C4-C5	6.33	108.33	105.80
22	23S1	2750	A	C8-N9-C4	6.33	108.33	105.80
1	16S1	363	A	C4-C5-C6	6.33	120.16	117.00
1	16S1	782	A	C4-C5-N7	-6.33	107.53	110.70
1	16S1	908	A	N3-C4-N9	6.33	132.46	127.40
22	23S1	362	A	C8-N9-C4	6.33	108.33	105.80
22	23S1	1365	A	N3-C4-N9	6.33	132.46	127.40
22	23S1	2176	A	N9-C4-C5	6.33	108.33	105.80
22	23S1	2705	A	C4-C5-C6	6.33	120.16	117.00
22	23S1	256	A	N3-C4-N9	6.33	132.46	127.40
22	23S1	514	A	C5-C6-N1	6.33	120.86	117.70
1	16S1	441	A	C8-N9-C4	6.33	108.33	105.80
22	23S1	693	A	C8-N9-C4	6.33	108.33	105.80
22	23S1	1890	A	N9-C4-C5	6.33	108.33	105.80
23	05S1	59	A	C6-N1-C2	-6.33	114.81	118.60
1	16S1	722	G	N3-C4-N9	6.32	129.79	126.00
22	23S1	412	A	C8-N9-C4	6.32	108.33	105.80
22	23S1	996	A	C4-C5-C6	6.32	120.16	117.00
1	16S1	303	A	N9-C4-C5	6.32	108.33	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2266	A	N3-C4-N9	6.32	132.46	127.40
22	23S1	2482	A	N3-C4-N9	6.32	132.46	127.40
1	16S1	536	C	C6-N1-C2	-6.32	117.77	120.30
1	16S1	1507	A	C4-C5-C6	6.32	120.16	117.00
22	23S1	866	A	C8-N9-C4	6.32	108.33	105.80
22	23S1	613	A	C4-C5-C6	6.32	120.16	117.00
22	23S1	1103	A	C4-C5-C6	6.32	120.16	117.00
22	23S1	1938	A	C8-N9-C4	6.32	108.33	105.80
22	23S1	2070	A	C4-C5-N7	-6.32	107.54	110.70
22	23S1	391	A	C4-C5-C6	6.32	120.16	117.00
22	23S1	480	A	N3-C4-N9	6.32	132.45	127.40
22	23S1	1020	A	C6-N1-C2	6.32	122.39	118.60
22	23S1	1749	A	N9-C4-C5	6.32	108.33	105.80
1	16S1	189	A	N3-C4-N9	6.31	132.45	127.40
22	23S1	182	A	C4-C5-C6	6.31	120.16	117.00
22	23S1	354	A	C4-C5-N7	-6.31	107.54	110.70
22	23S1	505	A	C4-C5-C6	6.31	120.16	117.00
22	23S1	2778	A	N3-C4-N9	6.31	132.45	127.40
1	16S1	959	A	C5-N7-C8	6.31	107.06	103.90
1	16S1	1191	A	N3-C4-N9	6.31	132.45	127.40
22	23S1	1780	A	N3-C4-N9	6.31	132.45	127.40
22	23S1	2856	A	N3-C4-N9	6.31	132.45	127.40
1	16S1	382	A	C4-C5-C6	6.31	120.16	117.00
1	16S1	602	A	C5-C6-N1	6.31	120.86	117.70
22	23S1	1470	A	N3-C4-N9	6.31	132.45	127.40
22	23S1	1144	A	N3-C4-N9	6.31	132.45	127.40
22	23S1	2590	A	C8-N9-C4	6.31	108.32	105.80
1	16S1	250	A	C4-C5-C6	6.31	120.15	117.00
1	16S1	429	U	O4'-C1'-N1	6.31	113.25	108.20
1	16S1	609	A	N3-C4-N9	6.31	132.44	127.40
22	23S1	310	A	C8-N9-C4	6.31	108.32	105.80
22	23S1	370	G	O4'-C1'-N9	-6.31	103.16	108.20
22	23S1	2191	A	C5-N7-C8	6.31	107.05	103.90
22	23S1	56	A	C4-C5-C6	6.31	120.15	117.00
22	23S1	1899	A	C5-N7-C8	6.31	107.05	103.90
1	16S1	28	A	C4-C5-C6	6.30	120.15	117.00
22	23S1	2170	A	C8-N9-C4	6.30	108.32	105.80
22	23S1	2733	A	N3-C4-N9	6.30	132.44	127.40
1	16S1	583	A	C5-N7-C8	6.30	107.05	103.90
1	16S1	635	A	N3-C4-N9	6.30	132.44	127.40
22	23S1	466	A	C4-C5-C6	6.30	120.15	117.00
1	16S1	246	A	C8-N9-C4	6.30	108.32	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	454	G	N3-C2-N2	6.30	124.31	119.90
22	23S1	1027	A	C4-C5-C6	6.30	120.15	117.00
22	23S1	2003	A	C5-C6-N1	6.30	120.85	117.70
22	23S1	2587	A	C4-C5-C6	6.30	120.15	117.00
1	16S1	60	A	C4-C5-C6	6.30	120.15	117.00
22	23S1	1679	A	C4-C5-C6	6.30	120.15	117.00
1	16S1	327	A	C4-C5-C6	6.30	120.15	117.00
1	16S1	482	A	N3-C4-N9	6.30	132.44	127.40
22	23S1	716	A	C4-C5-C6	6.30	120.15	117.00
22	23S1	735	A	N3-C4-N9	6.30	132.44	127.40
22	23S1	2761	A	C4-C5-C6	6.30	120.15	117.00
22	23S1	2893	A	N3-C4-N9	6.30	132.44	127.40
1	16S1	309	A	C8-N9-C4	6.29	108.32	105.80
22	23S1	825	A	N3-C4-N9	6.29	132.44	127.40
22	23S1	1515	A	C5-C6-N1	6.29	120.85	117.70
1	16S1	1531	A	C5-N7-C8	6.29	107.05	103.90
22	23S1	1084	A	C4-C5-C6	6.29	120.15	117.00
22	23S1	1285	A	C4-C5-N7	-6.29	107.55	110.70
22	23S1	1603	A	C4-C5-C6	6.29	120.14	117.00
22	23S1	2887	A	C5-C6-N1	6.29	120.85	117.70
55	PTR1	62	C	N3-C2-O2	-6.29	117.50	121.90
1	16S1	1332	A	N3-C4-N9	6.29	132.43	127.40
1	16S1	712	A	C4-C5-C6	6.29	120.14	117.00
1	16S1	1507	A	N3-C4-N9	6.29	132.43	127.40
22	23S1	920	A	N3-C4-N9	6.29	132.43	127.40
22	23S1	1713	A	N3-C4-N9	6.29	132.43	127.40
22	23S1	2094	A	N3-C4-N9	6.29	132.43	127.40
22	23S1	197	A	N3-C4-N9	6.29	132.43	127.40
22	23S1	64	A	N3-C4-N9	6.29	132.43	127.40
22	23S1	1307	A	C4-C5-C6	6.29	120.14	117.00
1	16S1	415	A	N3-C4-N9	6.28	132.43	127.40
22	23S1	216	A	N9-C4-C5	6.28	108.31	105.80
22	23S1	877	A	C4-C5-C6	6.28	120.14	117.00
22	23S1	1672	A	C8-N9-C4	6.28	108.31	105.80
22	23S1	10	A	C8-N9-C4	6.28	108.31	105.80
1	16S1	794	A	C8-N9-C4	6.28	108.31	105.80
1	16S1	1350	A	N3-C4-N9	6.28	132.42	127.40
22	23S1	131	A	C5-C6-N1	6.28	120.84	117.70
22	23S1	616	A	C8-N9-C4	6.28	108.31	105.80
22	23S1	1265	A	N3-C4-N9	6.28	132.43	127.40
22	23S1	1665	A	N3-C4-N9	6.28	132.43	127.40
22	23S1	1086	A	C4-C5-C6	6.28	120.14	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	PTR1	56	C	C5-C6-N1	6.28	124.14	121.00
1	16S1	246	A	C4-C5-C6	6.28	120.14	117.00
1	16S1	1176	A	N3-C4-N9	6.28	132.42	127.40
22	23S1	2346	A	C4-C5-C6	6.28	120.14	117.00
23	05S1	115	A	C8-N9-C4	6.28	108.31	105.80
22	23S1	1070	A	N3-C4-N9	6.28	132.42	127.40
22	23S1	2453	A	N3-C4-N9	6.28	132.42	127.40
22	23S1	742	A	C4-C5-C6	6.27	120.14	117.00
1	16S1	1340	A	C4-C5-C6	6.27	120.14	117.00
22	23S1	412	A	N3-C4-N9	6.27	132.42	127.40
22	23S1	1151	A	N3-C4-N9	6.27	132.42	127.40
22	23S1	1204	A	C8-N9-C4	6.27	108.31	105.80
22	23S1	1327	A	N3-C4-N9	6.27	132.42	127.40
22	23S1	1650	A	C4-C5-C6	6.27	120.14	117.00
1	16S1	2	A	C4-C5-C6	6.27	120.14	117.00
1	16S1	171	A	N9-C4-C5	6.27	108.31	105.80
1	16S1	1158	C	C5-C6-N1	6.27	124.14	121.00
22	23S1	721	A	C4-C5-C6	6.27	120.14	117.00
22	23S1	1246	A	C4-C5-C6	6.27	120.14	117.00
1	16S1	509	A	C4-C5-C6	6.27	120.13	117.00
1	16S1	918	A	N9-C4-C5	6.27	108.31	105.80
22	23S1	501	A	C5-N7-C8	6.27	107.03	103.90
22	23S1	753	A	C5-C6-N1	6.27	120.83	117.70
22	23S1	1431	A	C4-C5-C6	6.27	120.13	117.00
22	23S1	2043	C	N1-C2-O2	6.27	122.66	118.90
1	16S1	640	A	C5-C6-N1	6.26	120.83	117.70
1	16S1	1216	A	C8-N9-C4	6.26	108.31	105.80
1	16S1	1363	A	C5-C6-N1	6.26	120.83	117.70
22	23S1	89	A	N3-C4-N9	6.26	132.41	127.40
22	23S1	384	A	C4-C5-C6	6.26	120.13	117.00
22	23S1	1287	A	C8-N9-C4	6.26	108.31	105.80
22	23S1	2247	A	N3-C4-N9	6.26	132.41	127.40
22	23S1	2274	A	C4-C5-C6	6.26	120.13	117.00
22	23S1	2675	A	N3-C4-N9	6.26	132.41	127.40
22	23S1	2799	A	C5-N7-C8	6.26	107.03	103.90
55	PTR1	3	A	C4-C5-C6	6.26	120.13	117.00
1	16S1	460	A	C5-C6-N1	6.26	120.83	117.70
1	16S1	560	A	C4-C5-C6	6.26	120.13	117.00
1	16S1	621	A	C4-C5-C6	6.26	120.13	117.00
22	23S1	116	C	N3-C2-O2	-6.26	117.52	121.90
22	23S1	2662	A	N7-C8-N9	-6.26	110.67	113.80
22	23S1	384	A	N3-C4-N9	6.26	132.41	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1780	A	C4-C5-C6	6.26	120.13	117.00
1	16S1	77	A	C5-N7-C8	6.25	107.03	103.90
1	16S1	33	A	C4-C5-C6	6.25	120.13	117.00
23	05S1	57	A	N3-C4-N9	6.25	132.40	127.40
1	16S1	19	A	N3-C4-N9	6.25	132.40	127.40
1	16S1	459	A	C8-N9-C4	6.25	108.30	105.80
22	23S1	635	C	C6-N1-C2	-6.25	117.80	120.30
1	16S1	648	A	C8-N9-C4	6.25	108.30	105.80
1	16S1	665	A	N9-C4-C5	6.25	108.30	105.80
1	16S1	1252	A	N3-C4-N9	6.25	132.40	127.40
1	16S1	1219	A	C5-C6-N1	6.25	120.82	117.70
22	23S1	761	A	N9-C4-C5	6.25	108.30	105.80
22	23S1	1705	A	N3-C4-N9	6.25	132.40	127.40
22	23S1	1746	A	N3-C4-N9	6.25	132.40	127.40
22	23S1	1801	A	C4-C5-C6	6.25	120.12	117.00
1	16S1	520	A	C4-C5-C6	6.25	120.12	117.00
22	23S1	666	A	N3-C4-N9	6.25	132.40	127.40
22	23S1	911	A	N3-C4-N9	6.25	132.40	127.40
1	16S1	1275	A	N3-C4-N9	6.25	132.40	127.40
1	16S1	496	A	C5-N7-C8	6.24	107.02	103.90
1	16S1	865	A	N9-C4-C5	6.24	108.30	105.80
22	23S1	1810	A	C6-C5-N7	-6.24	127.93	132.30
1	16S1	10	A	N3-C4-N9	6.24	132.39	127.40
1	16S1	946	A	C4-C5-C6	6.24	120.12	117.00
22	23S1	1735	A	N3-C4-N9	6.24	132.39	127.40
22	23S1	1847	A	N3-C4-N9	6.24	132.39	127.40
22	23S1	2052	A	N3-C4-N9	6.24	132.39	127.40
22	23S1	1403	A	C5-C6-N1	6.24	120.82	117.70
1	16S1	74	A	C8-N9-C4	6.24	108.30	105.80
22	23S1	1014	A	C4-C5-C6	6.24	120.12	117.00
22	23S1	1133	A	C4-C5-C6	6.24	120.12	117.00
22	23S1	1919	A	C5-N7-C8	6.24	107.02	103.90
1	16S1	81	A	N3-C4-N9	6.24	132.39	127.40
1	16S1	95	C	C2-N1-C1'	6.24	125.66	118.80
1	16S1	101	A	C4-C5-C6	6.24	120.12	117.00
1	16S1	1360	A	C4-C5-N7	-6.24	107.58	110.70
22	23S1	453	A	C4-C5-C6	6.24	120.12	117.00
22	23S1	483	A	C4-C5-C6	6.24	120.12	117.00
22	23S1	1354	A	N3-C4-N9	6.24	132.39	127.40
22	23S1	1670	C	N1-C2-O2	6.24	122.64	118.90
1	16S1	250	A	N3-C4-N9	6.23	132.39	127.40
1	16S1	1151	A	C4-C5-C6	6.23	120.12	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	349	A	N3-C4-N9	6.23	132.39	127.40
1	16S1	635	A	C8-N9-C4	6.23	108.29	105.80
22	23S1	1566	A	C8-N9-C4	6.23	108.29	105.80
1	16S1	1032	G	N3-C4-C5	-6.23	125.48	128.60
22	23S1	374	A	C8-N9-C4	6.23	108.29	105.80
22	23S1	925	A	N3-C4-N9	6.23	132.38	127.40
1	16S1	414	A	C5-C6-N1	6.23	120.81	117.70
23	05S1	66	A	C4-C5-C6	6.23	120.11	117.00
1	16S1	274	A	N3-C4-N9	6.23	132.38	127.40
22	23S1	2711	A	N3-C4-N9	6.23	132.38	127.40
22	23S1	91	A	C8-N9-C4	6.23	108.29	105.80
22	23S1	756	A	C4-C5-C6	6.23	120.11	117.00
1	16S1	1311	A	N3-C4-N9	6.22	132.38	127.40
1	16S1	1318	A	N3-C4-N9	6.22	132.38	127.40
22	23S1	1503	A	N3-C4-N9	6.22	132.38	127.40
1	16S1	320	A	N9-C4-C5	6.22	108.29	105.80
1	16S1	465	A	C4-C5-C6	6.22	120.11	117.00
22	23S1	1791	A	C4-C5-C6	6.22	120.11	117.00
22	23S1	2142	A	C8-N9-C4	6.22	108.29	105.80
22	23S1	2377	A	N3-C4-N9	6.22	132.38	127.40
22	23S1	282	A	C8-N9-C4	6.22	108.29	105.80
22	23S1	1070	A	C4-C5-C6	6.22	120.11	117.00
22	23S1	1302	A	C8-N9-C4	6.22	108.29	105.80
22	23S1	2052	A	C5-C6-N1	6.22	120.81	117.70
1	16S1	327	A	N3-C4-N9	6.22	132.38	127.40
22	23S1	218	A	N3-C4-N9	6.22	132.38	127.40
22	23S1	460	A	C4-C5-C6	6.22	120.11	117.00
22	23S1	599	A	N3-C4-N9	6.22	132.38	127.40
22	23S1	1700	A	C4-C5-C6	6.22	120.11	117.00
22	23S1	1808	A	C8-N9-C4	6.22	108.29	105.80
22	23S1	2023	C	C6-N1-C2	-6.22	117.81	120.30
22	23S1	917	A	C4-C5-C6	6.22	120.11	117.00
1	16S1	435	A	N3-C4-N9	6.22	132.37	127.40
1	16S1	451	A	C4-C5-C6	6.22	120.11	117.00
1	16S1	968	A	N3-C4-N9	6.22	132.37	127.40
1	16S1	1032	G	C2-N3-C4	6.22	115.01	111.90
22	23S1	1040	A	N3-C4-N9	6.22	132.37	127.40
22	23S1	1395	A	C8-N9-C4	6.22	108.29	105.80
22	23S1	1998	A	C4-C5-N7	-6.22	107.59	110.70
22	23S1	2740	A	C5-C6-N1	6.22	120.81	117.70
49	L331	6	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	16S1	44	A	C4-C5-C6	6.21	120.11	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	681	A	C4-C5-C6	6.21	120.11	117.00
22	23S1	2126	A	N3-C4-N9	6.21	132.37	127.40
1	16S1	959	A	N3-C4-N9	6.21	132.37	127.40
22	23S1	1585	C	C6-N1-C2	-6.21	117.81	120.30
1	16S1	640	A	C4-C5-C6	6.21	120.11	117.00
1	16S1	938	A	C4-C5-C6	6.21	120.11	117.00
1	16S1	1246	A	N3-C4-N9	6.21	132.37	127.40
1	16S1	1360	A	N3-C4-N9	6.21	132.37	127.40
1	16S1	1534	A	N9-C4-C5	6.21	108.28	105.80
22	23S1	1918	A	C4-C5-C6	6.21	120.11	117.00
22	23S1	2154	A	C4-C5-C6	6.21	120.11	117.00
22	23S1	2886	A	C4-C5-C6	6.21	120.11	117.00
1	16S1	1005	A	N3-C4-N9	6.21	132.37	127.40
1	16S1	1288	A	N3-C4-N9	6.21	132.37	127.40
22	23S1	483	A	N3-C4-N9	6.21	132.37	127.40
22	23S1	548	G	N3-C4-N9	6.21	129.72	126.00
22	23S1	1711	A	C4-C5-C6	6.21	120.10	117.00
22	23S1	2171	A	C8-N9-C4	6.21	108.28	105.80
1	16S1	503	C	N1-C2-O2	6.21	122.62	118.90
1	16S1	782	A	N3-C4-N9	6.21	132.37	127.40
22	23S1	111	A	N9-C4-C5	6.21	108.28	105.80
22	23S1	362	A	C5-N7-C8	6.21	107.00	103.90
22	23S1	633	A	N3-C4-N9	6.21	132.37	127.40
22	23S1	2518	A	C5-C6-N1	6.21	120.80	117.70
1	16S1	1410	A	N9-C4-C5	6.21	108.28	105.80
22	23S1	430	A	N3-C4-N9	6.21	132.36	127.40
22	23S1	1591	A	C8-N9-C4	6.20	108.28	105.80
22	23S1	2733	A	C4-C5-C6	6.20	120.10	117.00
22	23S1	2809	A	C4-C5-C6	6.20	120.10	117.00
22	23S1	275	C	C6-N1-C2	-6.20	117.82	120.30
22	23S1	2564	A	C4-C5-N7	-6.20	107.60	110.70
1	16S1	892	A	C4-C5-C6	6.20	120.10	117.00
22	23S1	207	A	N3-C4-N9	6.20	132.36	127.40
22	23S1	244	A	C4-C5-C6	6.20	120.10	117.00
22	23S1	899	A	C4-C5-C6	6.20	120.10	117.00
22	23S1	1810	A	N7-C8-N9	-6.20	110.70	113.80
22	23S1	2851	A	N3-C4-N9	6.20	132.36	127.40
1	16S1	648	A	N3-C4-N9	6.20	132.36	127.40
22	23S1	2476	A	C4-C5-C6	6.20	120.10	117.00
1	16S1	65	A	C8-N9-C4	6.20	108.28	105.80
22	23S1	1169	A	N3-C4-N9	6.20	132.36	127.40
22	23S1	2736	A	N3-C4-N9	6.20	132.36	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1271	A	C4-C5-C6	6.19	120.10	117.00
22	23S1	1920	C	C5-C6-N1	6.19	124.10	121.00
22	23S1	13	A	C4-C5-C6	6.19	120.09	117.00
22	23S1	429	A	N3-C4-N9	6.19	132.35	127.40
1	16S1	782	A	C4-C5-C6	6.19	120.09	117.00
1	16S1	845	A	C4-C5-N7	-6.19	107.61	110.70
1	16S1	1019	A	N3-C4-N9	6.19	132.35	127.40
22	23S1	6	A	N3-C4-N9	6.19	132.35	127.40
23	05S1	34	A	N9-C4-C5	6.19	108.28	105.80
22	23S1	161	A	C8-N9-C4	6.19	108.28	105.80
22	23S1	915	C	N1-C2-O2	6.19	122.61	118.90
22	23S1	1598	A	C4-C5-C6	6.19	120.09	117.00
22	23S1	2003	A	C8-N9-C4	6.19	108.28	105.80
22	23S1	2435	A	C4-C5-C6	6.19	120.09	117.00
22	23S1	2820	A	N9-C4-C5	6.19	108.28	105.80
1	16S1	315	A	N3-C4-N9	6.19	132.35	127.40
1	16S1	1306	A	C8-N9-C4	6.19	108.27	105.80
22	23S1	1328	A	C4-C5-N7	-6.19	107.61	110.70
22	23S1	1848	A	N9-C4-C5	6.19	108.27	105.80
1	16S1	2	A	C5-C6-N1	6.18	120.79	117.70
1	16S1	1333	A	C4-C5-N7	-6.18	107.61	110.70
22	23S1	548	G	C4-N9-C1'	6.18	134.54	126.50
22	23S1	1676	A	N3-C4-N9	6.18	132.35	127.40
22	23S1	2560	A	N3-C4-N9	6.18	132.35	127.40
23	05S1	94	A	C4-C5-C6	6.18	120.09	117.00
1	16S1	228	A	C4-C5-C6	6.18	120.09	117.00
22	23S1	63	A	N3-C4-N9	6.18	132.35	127.40
22	23S1	1014	A	C5-C6-N1	6.18	120.79	117.70
23	05S1	31	C	N1-C2-O2	6.18	122.61	118.90
1	16S1	864	A	C4-C5-C6	6.18	120.09	117.00
22	23S1	2190	G	N7-C8-N9	6.18	116.19	113.10
22	23S1	2572	A	C4-C5-N7	-6.18	107.61	110.70
1	16S1	329	A	N3-C4-N9	6.18	132.34	127.40
1	16S1	1216	A	C4-C5-N7	-6.18	107.61	110.70
22	23S1	161	A	N9-C4-C5	6.18	108.27	105.80
22	23S1	2826	A	N3-C4-N9	6.18	132.34	127.40
1	16S1	139	A	C8-N9-C4	6.18	108.27	105.80
22	23S1	925	A	C8-N9-C4	6.18	108.27	105.80
22	23S1	1096	A	C4-C5-N7	-6.18	107.61	110.70
1	16S1	1155	A	N3-C4-N9	6.17	132.34	127.40
1	16S1	1229	A	N3-C4-N9	6.17	132.34	127.40
22	23S1	675	A	N3-C4-N9	6.17	132.34	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1668	A	N9-C4-C5	6.17	108.27	105.80
22	23S1	2058	A	N3-C4-N9	6.17	132.34	127.40
22	23S1	1717	A	N3-C4-N9	6.17	132.34	127.40
1	16S1	356	A	C5-C6-N1	6.17	120.79	117.70
1	16S1	1042	A	N3-C4-N9	6.17	132.34	127.40
22	23S1	172	A	N3-C4-N9	6.17	132.34	127.40
22	23S1	739	A	N3-C4-N9	6.17	132.34	127.40
22	23S1	788	A	N3-C4-N9	6.17	132.34	127.40
22	23S1	1039	A	N9-C4-C5	6.17	108.27	105.80
22	23S1	2406	A	C4-C5-C6	6.17	120.08	117.00
22	23S1	2513	A	C4-C5-C6	6.17	120.09	117.00
22	23S1	2679	A	C5-C6-N1	6.17	120.79	117.70
23	05S1	53	A	C4-C5-C6	6.17	120.08	117.00
22	23S1	614	A	N3-C4-N9	6.17	132.34	127.40
1	16S1	109	A	C4-C5-C6	6.17	120.08	117.00
22	23S1	718	A	N3-C4-N9	6.17	132.33	127.40
22	23S1	2298	A	C8-N9-C4	6.17	108.27	105.80
1	16S1	968	A	C4-C5-C6	6.17	120.08	117.00
22	23S1	758	C	N3-C2-O2	-6.17	117.58	121.90
22	23S1	1286	A	N9-C4-C5	6.17	108.27	105.80
22	23S1	1551	A	C4-C5-C6	6.17	120.08	117.00
22	23S1	1858	A	C4-C5-C6	6.17	120.08	117.00
22	23S1	251	A	C5-N7-C8	6.17	106.98	103.90
1	16S1	55	A	C8-N9-C4	6.16	108.27	105.80
1	16S1	408	A	C4-C5-N7	-6.16	107.62	110.70
1	16S1	1021	A	C4-C5-C6	6.16	120.08	117.00
22	23S1	149	A	N3-C4-N9	6.16	132.33	127.40
1	16S1	349	A	C4-C5-C6	6.16	120.08	117.00
1	16S1	1433	A	N9-C4-C5	6.16	108.27	105.80
22	23S1	44	A	N3-C4-N9	6.16	132.33	127.40
22	23S1	1749	A	C5-C6-N1	6.16	120.78	117.70
1	16S1	560	A	N3-C4-N9	6.16	132.33	127.40
1	16S1	676	A	C4-C5-C6	6.16	120.08	117.00
1	16S1	784	A	C8-N9-C4	6.16	108.26	105.80
22	23S1	429	A	C4-C5-C6	6.16	120.08	117.00
22	23S1	556	A	N3-C4-N9	6.16	132.33	127.40
22	23S1	1598	A	N3-C4-N9	6.16	132.33	127.40
1	16S1	635	A	C4-C5-C6	6.16	120.08	117.00
22	23S1	1285	A	N9-C4-C5	6.16	108.26	105.80
1	16S1	919	A	N9-C4-C5	6.16	108.26	105.80
1	16S1	1368	A	C8-N9-C4	6.16	108.26	105.80
22	23S1	861	A	N3-C4-N9	6.16	132.33	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2346	A	N3-C4-N9	6.16	132.32	127.40
22	23S1	2377	A	C4-C5-C6	6.16	120.08	117.00
55	PTR1	23	A	C4-C5-C6	6.16	120.08	117.00
22	23S1	1008	A	N3-C4-N9	6.16	132.32	127.40
22	23S1	1689	A	N3-C4-N9	6.16	132.32	127.40
22	23S1	1848	A	C5-N7-C8	6.16	106.98	103.90
22	23S1	2837	A	N3-C4-N9	6.16	132.32	127.40
22	23S1	21	A	C4-C5-C6	6.15	120.08	117.00
22	23S1	160	A	C4-C5-N7	-6.15	107.62	110.70
22	23S1	221	A	C6-N1-C2	6.15	122.29	118.60
1	16S1	630	A	N3-C4-N9	6.15	132.32	127.40
22	23S1	514	A	N3-C4-N9	6.15	132.32	127.40
22	23S1	1762	A	C4-C5-C6	6.15	120.08	117.00
22	23S1	1953	A	N3-C4-N9	6.15	132.32	127.40
1	16S1	298	A	C8-N9-C4	6.15	108.26	105.80
22	23S1	197	A	C4-C5-C6	6.15	120.08	117.00
22	23S1	428	A	C4-C5-C6	6.15	120.08	117.00
22	23S1	825	A	C4-C5-C6	6.15	120.08	117.00
22	23S1	348	A	N3-C4-N9	6.15	132.32	127.40
22	23S1	735	A	C8-N9-C4	6.15	108.26	105.80
22	23S1	1626	A	C4-C5-C6	6.15	120.07	117.00
22	23S1	2560	A	C4-C5-C6	6.15	120.07	117.00
1	16S1	432	A	N3-C4-N9	6.15	132.32	127.40
22	23S1	12	U	C6-N1-C2	-6.15	117.31	121.00
22	23S1	173	A	C4-C5-C6	6.14	120.07	117.00
22	23S1	756	A	C5-C6-N1	6.14	120.77	117.70
22	23S1	911	A	C5-N7-C8	6.14	106.97	103.90
22	23S1	1545	A	N9-C4-C5	6.14	108.26	105.80
22	23S1	1717	A	C4-C5-C6	6.14	120.07	117.00
22	23S1	2450	A	C5-N7-C8	6.14	106.97	103.90
22	23S1	2516	A	N3-C4-N9	6.14	132.32	127.40
1	16S1	53	A	C5-C6-N1	6.14	120.77	117.70
1	16S1	675	A	C8-N9-C4	6.14	108.26	105.80
1	16S1	777	A	N3-C4-N9	6.14	132.31	127.40
22	23S1	294	A	C8-N9-C4	6.14	108.26	105.80
22	23S1	1420	A	N3-C4-N9	6.14	132.31	127.40
22	23S1	2719	G	N9-C4-C5	-6.14	102.94	105.40
23	05S1	29	A	C4-C5-C6	6.14	120.07	117.00
1	16S1	640	A	C4-C5-N7	-6.14	107.63	110.70
22	23S1	1759	A	C4-C5-C6	6.14	120.07	117.00
1	16S1	546	A	C8-N9-C4	6.14	108.25	105.80
22	23S1	1253	A	N9-C4-C5	6.14	108.25	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1978	A	C8-N9-C4	6.14	108.25	105.80
1	16S1	179	A	C4-C5-N7	-6.14	107.63	110.70
1	16S1	949	A	C4-C5-N7	-6.14	107.63	110.70
1	16S1	1201	A	C8-N9-C4	6.14	108.25	105.80
22	23S1	231	A	C5-C6-N1	6.14	120.77	117.70
22	23S1	2169	A	C4-C5-N7	-6.14	107.63	110.70
22	23S1	2322	A	C8-N9-C4	6.14	108.25	105.80
22	23S1	2412	A	N3-C4-N9	6.14	132.31	127.40
1	16S1	288	A	N3-C4-N9	6.13	132.31	127.40
22	23S1	19	A	N3-C4-N9	6.13	132.31	127.40
22	23S1	1637	A	N3-C4-N9	6.13	132.31	127.40
22	23S1	1794	A	N3-C4-N9	6.13	132.31	127.40
22	23S1	1829	A	C4-C5-C6	6.13	120.07	117.00
22	23S1	2227	A	C4-C5-C6	6.13	120.07	117.00
1	16S1	546	A	C4-C5-C6	6.13	120.07	117.00
22	23S1	821	A	C4-C5-N7	-6.13	107.63	110.70
22	23S1	2851	A	C8-N9-C4	6.13	108.25	105.80
1	16S1	152	A	N9-C4-C5	6.13	108.25	105.80
1	16S1	937	A	N3-C4-N9	6.13	132.31	127.40
1	16S1	1340	A	C8-N9-C4	6.13	108.25	105.80
22	23S1	219	A	N3-C4-N9	6.13	132.31	127.40
22	23S1	270	A	N3-C4-N9	6.13	132.31	127.40
22	23S1	401	A	C4-C5-C6	6.13	120.07	117.00
22	23S1	1265	A	C4-C5-C6	6.13	120.07	117.00
22	23S1	2468	A	C8-N9-C4	6.13	108.25	105.80
22	23S1	176	A	N3-C4-N9	6.13	132.30	127.40
22	23S1	1000	A	C5-C6-N1	6.13	120.77	117.70
22	23S1	1287	A	N3-C4-N9	6.13	132.30	127.40
22	23S1	526	A	N9-C4-C5	6.13	108.25	105.80
22	23S1	608	A	C4-C5-C6	6.13	120.06	117.00
22	23S1	699	A	N9-C4-C5	6.13	108.25	105.80
22	23S1	1077	A	N9-C4-C5	6.13	108.25	105.80
22	23S1	1966	A	N3-C4-N9	6.13	132.30	127.40
22	23S1	2080	A	C4-C5-C6	6.13	120.06	117.00
22	23S1	2094	A	C8-N9-C4	6.13	108.25	105.80
22	23S1	2340	A	C8-N9-C4	6.13	108.25	105.80
22	23S1	2736	A	C4-C5-C6	6.13	120.06	117.00
22	23S1	2740	A	N3-C4-N9	6.13	132.30	127.40
1	16S1	238	A	N3-C4-N9	6.13	132.30	127.40
1	16S1	1019	A	C4-C5-C6	6.13	120.06	117.00
1	16S1	1225	A	C5-C6-N1	6.13	120.76	117.70
1	16S1	1289	A	N9-C4-C5	6.13	108.25	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	432	A	N9-C4-C5	6.13	108.25	105.80
22	23S1	563	A	C4-C5-N7	-6.13	107.64	110.70
22	23S1	2471	A	N3-C4-N9	6.13	132.30	127.40
1	16S1	1012	A	C5-C6-N1	6.12	120.76	117.70
22	23S1	176	A	C5-C6-N1	6.12	120.76	117.70
22	23S1	1313	U	C6-N1-C1'	-6.12	112.62	121.20
1	16S1	10	A	C4-C5-C6	6.12	120.06	117.00
1	16S1	728	A	C4-C5-C6	6.12	120.06	117.00
1	16S1	1004	A	C8-N9-C4	6.12	108.25	105.80
55	PTR1	62	C	C6-N1-C2	-6.12	117.85	120.30
1	16S1	73	C	C6-N1-C2	-6.12	117.85	120.30
1	16S1	687	A	C8-N9-C4	6.12	108.25	105.80
1	16S1	858	G	N1-C6-O6	-6.12	116.23	119.90
22	23S1	160	A	N3-C4-N9	6.12	132.30	127.40
22	23S1	227	A	N3-C4-N9	6.12	132.30	127.40
22	23S1	348	A	C4-C5-C6	6.12	120.06	117.00
22	23S1	863	A	C5-C6-N1	6.12	120.76	117.70
22	23S1	1614	A	C4-C5-C6	6.12	120.06	117.00
22	23S1	2108	A	N9-C4-C5	6.12	108.25	105.80
22	23S1	2147	A	C5-N7-C8	6.12	106.96	103.90
22	23S1	2274	A	C5-N7-C8	6.12	106.96	103.90
1	16S1	155	A	C5-C6-N1	6.12	120.76	117.70
1	16S1	1513	A	C4-C5-C6	6.12	120.06	117.00
22	23S1	1654	A	N3-C4-N9	6.12	132.30	127.40
22	23S1	2311	A	C4-C5-N7	-6.12	107.64	110.70
1	16S1	694	A	N3-C4-N9	6.12	132.29	127.40
1	16S1	749	A	N3-C4-N9	6.12	132.29	127.40
1	16S1	1196	A	C8-N9-C4	6.12	108.25	105.80
22	23S1	167	A	N3-C4-N9	6.12	132.29	127.40
22	23S1	453	A	N3-C4-N9	6.12	132.29	127.40
22	23S1	783	A	N9-C4-C5	6.12	108.25	105.80
22	23S1	972	A	C4-C5-C6	6.12	120.06	117.00
22	23S1	2531	A	C4-C5-C6	6.12	120.06	117.00
1	16S1	448	A	C4-C5-C6	6.12	120.06	117.00
1	16S1	1042	A	C4-C5-C6	6.12	120.06	117.00
1	16S1	1360	A	C4-C5-C6	6.12	120.06	117.00
22	23S1	2088	A	C5-C6-N1	6.12	120.76	117.70
22	23S1	2468	A	C4-C5-C6	6.12	120.06	117.00
1	16S1	366	A	N3-C4-N9	6.11	132.29	127.40
22	23S1	1885	A	N3-C4-N9	6.11	132.29	127.40
22	23S1	2013	A	C4-C5-N7	-6.11	107.64	110.70
1	16S1	461	A	C8-N9-C4	6.11	108.25	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2706	A	C5-C6-N1	6.11	120.76	117.70
1	16S1	374	A	C8-N9-C4	6.11	108.24	105.80
1	16S1	1346	A	C8-N9-C4	6.11	108.24	105.80
1	16S1	1431	A	N9-C4-C5	6.11	108.24	105.80
1	16S1	1446	A	C4-C5-C6	6.11	120.06	117.00
22	23S1	1393	A	C4-C5-C6	6.11	120.06	117.00
1	16S1	676	A	N3-C4-N9	6.11	132.29	127.40
1	16S1	1167	A	N3-C4-N9	6.11	132.29	127.40
1	16S1	80	A	N9-C4-C5	6.11	108.24	105.80
1	16S1	167	A	C8-N9-C4	6.11	108.24	105.80
1	16S1	1306	A	C4-C5-C6	6.11	120.05	117.00
1	16S1	1502	A	N3-C4-N9	6.11	132.29	127.40
22	23S1	483	A	C8-N9-C4	6.11	108.24	105.80
1	16S1	7	A	N9-C4-C5	6.11	108.24	105.80
1	16S1	807	A	N9-C4-C5	6.11	108.24	105.80
1	16S1	901	A	C5-N7-C8	6.11	106.95	103.90
22	23S1	233	A	C4-C5-C6	6.11	120.05	117.00
22	23S1	2725	A	C5-C6-N1	6.11	120.75	117.70
1	16S1	1044	A	C5-C6-N1	6.10	120.75	117.70
1	16S1	1476	A	N3-C4-N9	6.10	132.28	127.40
22	23S1	1496	A	N3-C4-N9	6.10	132.28	127.40
22	23S1	2726	A	N9-C4-C5	6.10	108.24	105.80
1	16S1	211	G	C5-C6-O6	-6.10	124.94	128.60
1	16S1	1250	A	C4-C5-N7	-6.10	107.65	110.70
22	23S1	447	A	C8-N9-C4	6.10	108.24	105.80
22	23S1	825	A	C4-C5-N7	-6.10	107.65	110.70
22	23S1	1819	A	C4-C5-C6	6.10	120.05	117.00
1	16S1	309	A	N3-C4-N9	6.10	132.28	127.40
1	16S1	892	A	N3-C4-N9	6.10	132.28	127.40
22	23S1	430	A	N9-C4-C5	6.10	108.24	105.80
22	23S1	866	A	N3-C4-N9	6.10	132.28	127.40
22	23S1	1010	A	C4-C5-C6	6.10	120.05	117.00
22	23S1	1205	A	C8-N9-C4	6.10	108.24	105.80
1	16S1	1229	A	C4-C5-C6	6.10	120.05	117.00
22	23S1	631	A	N3-C4-N9	6.10	132.28	127.40
22	23S1	1505	A	C4-C5-C6	6.10	120.05	117.00
22	23S1	1580	A	N3-C4-N9	6.10	132.28	127.40
22	23S1	2314	A	N3-C4-N9	6.10	132.28	127.40
22	23S1	2810	A	N9-C4-C5	6.10	108.24	105.80
1	16S1	456	A	N3-C4-N9	6.10	132.28	127.40
1	16S1	306	A	N3-C4-N9	6.09	132.28	127.40
22	23S1	95	A	N9-C4-C5	6.09	108.24	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1050	A	C4-C5-C6	6.09	120.05	117.00
22	23S1	1505	A	N9-C4-C5	6.09	108.24	105.80
22	23S1	2700	A	C4-C5-C6	6.09	120.05	117.00
1	16S1	878	A	N3-C4-N9	6.09	132.28	127.40
1	16S1	1236	A	C4-C5-C6	6.09	120.05	117.00
22	23S1	1847	A	N9-C4-C5	6.09	108.24	105.80
1	16S1	608	A	C4-C5-C6	6.09	120.05	117.00
1	16S1	1171	A	C8-N9-C4	6.09	108.24	105.80
22	23S1	614	A	C4-C5-C6	6.09	120.05	117.00
22	23S1	802	A	N3-C4-N9	6.09	132.27	127.40
22	23S1	1009	A	C4-C5-C6	6.09	120.05	117.00
22	23S1	1439	A	C4-C5-C6	6.09	120.05	117.00
22	23S1	2406	A	N3-C4-N9	6.09	132.27	127.40
22	23S1	2632	A	C4-C5-N7	-6.09	107.65	110.70
23	05S1	24	G	C6-N1-C2	-6.09	121.45	125.10
22	23S1	789	A	N3-C4-N9	6.09	132.27	127.40
22	23S1	1089	A	C8-N9-C4	6.09	108.24	105.80
22	23S1	1679	A	N3-C4-N9	6.09	132.27	127.40
22	23S1	1700	A	C8-N9-C4	6.09	108.24	105.80
22	23S1	1801	A	N3-C4-N9	6.09	132.27	127.40
22	23S1	1387	A	C5-C6-N1	6.09	120.74	117.70
22	23S1	1301	A	C4-C5-C6	6.09	120.04	117.00
22	23S1	2547	A	N9-C4-C5	6.09	108.23	105.80
23	05S1	15	A	C4-C5-C6	6.09	120.04	117.00
1	16S1	279	A	C5-N7-C8	6.08	106.94	103.90
22	23S1	300	A	N9-C4-C5	6.08	108.23	105.80
22	23S1	1854	A	C5-N7-C8	6.08	106.94	103.90
1	16S1	28	A	N3-C4-N9	6.08	132.27	127.40
22	23S1	912	C	N1-C2-O2	6.08	122.55	118.90
22	23S1	1504	A	N3-C4-N9	6.08	132.27	127.40
22	23S1	2037	A	C4-C5-C6	6.08	120.04	117.00
22	23S1	2566	A	N9-C4-C5	6.08	108.23	105.80
22	23S1	368	A	N9-C4-C5	6.08	108.23	105.80
22	23S1	371	A	C4-C5-C6	6.08	120.04	117.00
22	23S1	1095	A	N3-C4-N9	6.08	132.27	127.40
22	23S1	1544	A	N3-C4-N9	6.08	132.27	127.40
1	16S1	139	A	N3-C4-N9	6.08	132.26	127.40
1	16S1	1044	A	C4-C5-C6	6.08	120.04	117.00
22	23S1	621	A	N9-C4-C5	6.08	108.23	105.80
1	16S1	306	A	C4-C5-C6	6.08	120.04	117.00
22	23S1	1175	A	C4-C5-C6	6.08	120.04	117.00
22	23S1	1246	A	C5-C6-N1	6.08	120.74	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1596	A	N3-C4-N9	6.08	132.26	127.40
22	23S1	2541	A	N3-C4-N9	6.08	132.26	127.40
22	23S1	1522	A	C5-C6-N1	6.08	120.74	117.70
22	23S1	2530	A	N3-C4-N9	6.08	132.26	127.40
23	05S1	58	A	C4-C5-C6	6.08	120.04	117.00
22	23S1	920	A	C4-C5-C6	6.08	120.04	117.00
22	23S1	1978	A	C4-C5-C6	6.08	120.04	117.00
22	23S1	42	A	N3-C4-N9	6.07	132.26	127.40
22	23S1	632	A	N3-C4-N9	6.07	132.26	127.40
22	23S1	1144	A	C4-C5-C6	6.07	120.04	117.00
1	16S1	1101	A	C4-C5-N7	-6.07	107.66	110.70
22	23S1	1262	A	N3-C4-N9	6.07	132.26	127.40
22	23S1	2013	A	C4-C5-C6	6.07	120.04	117.00
1	16S1	747	A	N9-C4-C5	6.07	108.23	105.80
1	16S1	1080	A	C4-C5-C6	6.07	120.04	117.00
1	16S1	1492	A	N9-C4-C5	6.07	108.23	105.80
22	23S1	142	A	C4-C5-C6	6.07	120.03	117.00
22	23S1	2097	A	C4-C5-C6	6.07	120.04	117.00
23	05S1	50	A	C4-C5-C6	6.07	120.03	117.00
1	16S1	780	A	N3-C4-N9	6.07	132.25	127.40
22	23S1	825	A	N9-C4-C5	6.07	108.23	105.80
22	23S1	2322	A	N3-C4-N9	6.07	132.25	127.40
22	23S1	2471	A	C5-C6-N1	6.07	120.73	117.70
22	23S1	2758	A	C5-C6-N1	6.07	120.73	117.70
22	23S1	972	A	N9-C4-C5	6.07	108.23	105.80
1	16S1	937	A	C4-C5-C6	6.07	120.03	117.00
22	23S1	2851	A	C4-C5-C6	6.06	120.03	117.00
1	16S1	553	A	C5-C6-N1	6.06	120.73	117.70
1	16S1	747	A	C4-C5-C6	6.06	120.03	117.00
1	16S1	1428	A	C4-C5-N7	-6.06	107.67	110.70
22	23S1	1960	A	C8-N9-C4	6.06	108.22	105.80
22	23S1	2753	A	C4-C5-N7	-6.06	107.67	110.70
22	23S1	2117	A	C4-C5-C6	6.06	120.03	117.00
1	16S1	131	A	N9-C4-C5	6.06	108.22	105.80
22	23S1	320	A	N3-C4-N9	6.06	132.25	127.40
22	23S1	1260	A	N3-C4-N9	6.06	132.25	127.40
22	23S1	1354	A	C4-C5-C6	6.06	120.03	117.00
22	23S1	1634	A	C8-N9-C4	6.06	108.22	105.80
1	16S1	1117	A	N3-C4-N9	6.06	132.25	127.40
22	23S1	472	A	N3-C4-N9	6.06	132.25	127.40
22	23S1	1365	A	C4-C5-C6	6.06	120.03	117.00
22	23S1	2577	A	C4-C5-C6	6.06	120.03	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	968	A	C8-N9-C4	6.06	108.22	105.80
22	23S1	6	A	C4-C5-C6	6.06	120.03	117.00
22	23S1	44	A	N9-C4-C5	6.06	108.22	105.80
1	16S1	172	A	N9-C4-C5	6.05	108.22	105.80
22	23S1	1502	A	N9-C4-C5	6.05	108.22	105.80
1	16S1	1499	A	C4-C5-C6	6.05	120.03	117.00
2	S021	126	PHE	CB-CG-CD1	6.05	125.04	120.80
22	23S1	750	A	C4-C5-C6	6.05	120.03	117.00
22	23S1	2660	A	N9-C4-C5	6.05	108.22	105.80
1	16S1	1082	A	N3-C4-N9	6.05	132.24	127.40
22	23S1	1829	A	C4-C5-N7	-6.05	107.67	110.70
1	16S1	288	A	C4-C5-C6	6.05	120.03	117.00
1	16S1	673	A	C5-C6-N1	6.05	120.72	117.70
22	23S1	753	A	C4-C5-C6	6.05	120.03	117.00
22	23S1	1274	A	C4-C5-C6	6.05	120.03	117.00
1	16S1	831	A	C8-N9-C4	6.05	108.22	105.80
22	23S1	38	A	C4-C5-C6	6.05	120.02	117.00
22	23S1	1204	A	C5-C6-N1	6.05	120.72	117.70
22	23S1	1819	A	C8-N9-C4	6.05	108.22	105.80
23	05S1	104	A	N3-C4-N9	6.05	132.24	127.40
22	23S1	404	A	C8-N9-C4	6.05	108.22	105.80
22	23S1	1226	A	C5-N7-C8	6.05	106.92	103.90
22	23S1	1268	A	C4-C5-C6	6.05	120.02	117.00
22	23S1	1433	A	N3-C4-N9	6.05	132.24	127.40
1	16S1	1254	A	N3-C4-N9	6.04	132.24	127.40
22	23S1	142	A	N3-C4-N9	6.04	132.24	127.40
22	23S1	1226	A	C4-C5-C6	6.04	120.02	117.00
1	16S1	190	A	C5-C6-N6	6.04	128.53	123.70
22	23S1	800	A	N9-C4-C5	6.04	108.22	105.80
22	23S1	1080	A	C8-N9-C4	6.04	108.22	105.80
22	23S1	1095	A	C8-N9-C4	6.04	108.22	105.80
22	23S1	1205	A	N9-C4-C5	6.04	108.22	105.80
22	23S1	1367	A	C4-C5-C6	6.04	120.02	117.00
22	23S1	2813	A	N3-C4-N9	6.04	132.23	127.40
1	16S1	1117	A	C4-C5-C6	6.04	120.02	117.00
22	23S1	508	A	C4-C5-C6	6.04	120.02	117.00
22	23S1	2471	A	C8-N9-C4	6.04	108.22	105.80
22	23S1	2547	A	C4-C5-C6	6.04	120.02	117.00
23	05S1	46	A	C8-N9-C4	6.04	108.22	105.80
22	23S1	222	A	C8-N9-C4	6.04	108.22	105.80
22	23S1	670	A	N9-C4-C5	6.04	108.22	105.80
22	23S1	1885	A	C4-C5-C6	6.04	120.02	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	60	A	C4-C5-N7	-6.04	107.68	110.70
1	16S1	371	A	C5-C6-N1	6.04	120.72	117.70
1	16S1	1275	A	C4-C5-C6	6.04	120.02	117.00
22	23S1	64	A	C8-N9-C4	6.04	108.22	105.80
22	23S1	941	A	C4-C5-C6	6.04	120.02	117.00
22	23S1	1314	C	N3-C2-O2	-6.04	117.67	121.90
22	23S1	1735	A	C4-C5-C6	6.04	120.02	117.00
1	16S1	900	A	N9-C4-C5	6.04	108.22	105.80
22	23S1	2071	A	N3-C4-N9	6.04	132.23	127.40
22	23S1	2736	A	C8-N9-C4	6.04	108.22	105.80
1	16S1	315	A	C8-N9-C4	6.04	108.22	105.80
22	23S1	2285	C	N1-C2-O2	6.04	122.52	118.90
22	23S1	2725	A	C4-C5-C6	6.04	120.02	117.00
1	16S1	596	A	C4-C5-C6	6.03	120.02	117.00
22	23S1	2070	A	C4-C5-C6	6.03	120.02	117.00
1	16S1	640	A	N3-C4-N9	6.03	132.23	127.40
22	23S1	222	A	N3-C4-N9	6.03	132.23	127.40
22	23S1	1591	A	N3-C4-N9	6.03	132.23	127.40
1	16S1	263	A	N3-C4-N9	6.03	132.22	127.40
1	16S1	864	A	N3-C4-N9	6.03	132.22	127.40
22	23S1	38	A	N9-C4-C5	6.03	108.21	105.80
22	23S1	1027	A	N3-C4-N9	6.03	132.22	127.40
23	05S1	109	A	N3-C4-N9	6.03	132.22	127.40
1	16S1	435	A	C4-C5-C6	6.03	120.02	117.00
22	23S1	428	A	N3-C4-N9	6.03	132.22	127.40
1	16S1	81	A	C4-C5-N7	-6.03	107.69	110.70
1	16S1	389	A	C4-C5-C6	6.03	120.01	117.00
1	16S1	553	A	N3-C4-N9	6.03	132.22	127.40
1	16S1	906	A	N3-C4-N9	6.03	132.22	127.40
1	16S1	1329	A	C4-C5-N7	-6.03	107.69	110.70
22	23S1	71	A	C4-C5-C6	6.03	120.01	117.00
22	23S1	1143	A	C8-N9-C4	6.03	108.21	105.80
23	05S1	101	A	C6-N1-C2	-6.03	114.98	118.60
1	16S1	1437	A	N3-C4-N9	6.03	132.22	127.40
1	16S1	1492	A	N3-C4-N9	6.03	132.22	127.40
22	23S1	471	A	C8-N9-C4	6.03	108.21	105.80
22	23S1	975	A	C4-C5-C6	6.03	120.01	117.00
22	23S1	1783	A	N9-C4-C5	6.03	108.21	105.80
22	23S1	2054	A	C8-N9-C4	6.03	108.21	105.80
22	23S1	2675	A	C8-N9-C4	6.03	108.21	105.80
22	23S1	447	A	C4-C5-C6	6.02	120.01	117.00
1	16S1	600	A	C5-C6-N1	6.02	120.71	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	630	A	C4-C5-C6	6.02	120.01	117.00
22	23S1	221	A	C5-N7-C8	6.02	106.91	103.90
22	23S1	592	A	N3-C4-N9	6.02	132.22	127.40
22	23S1	1821	A	C4-C5-C6	6.02	120.01	117.00
22	23S1	2432	A	C4-C5-C6	6.02	120.01	117.00
22	23S1	2711	A	C4-C5-C6	6.02	120.01	117.00
22	23S1	716	A	N3-C4-N9	6.02	132.22	127.40
22	23S1	1103	A	N3-C4-N9	6.02	132.22	127.40
1	16S1	44	A	C4-C5-N7	-6.02	107.69	110.70
1	16S1	95	C	C6-N1-C2	-6.02	117.89	120.30
1	16S1	1495	U	C2-N1-C1'	6.02	124.92	117.70
22	23S1	116	C	N1-C2-O2	6.02	122.51	118.90
22	23S1	2369	A	C5-N7-C8	6.02	106.91	103.90
1	16S1	26	A	C8-N9-C4	6.02	108.21	105.80
1	16S1	510	A	C4-C5-C6	6.02	120.01	117.00
22	23S1	1504	A	C4-C5-C6	6.02	120.01	117.00
22	23S1	1597	A	C4-C5-C6	6.02	120.01	117.00
22	23S1	582	A	C5-C6-N1	6.02	120.71	117.70
1	16S1	439	U	C2-N1-C1'	6.01	124.92	117.70
1	16S1	974	A	C4-C5-C6	6.01	120.01	117.00
22	23S1	176	A	C4-C5-C6	6.01	120.01	117.00
22	23S1	345	A	N3-C4-N9	6.01	132.21	127.40
22	23S1	1070	A	C8-N9-C4	6.01	108.21	105.80
22	23S1	1848	A	N3-C4-N9	6.01	132.21	127.40
22	23S1	2270	A	N9-C4-C5	6.01	108.21	105.80
55	PTR1	42	A	C4-C5-C6	6.01	120.01	117.00
1	16S1	918	A	N3-C4-N9	6.01	132.21	127.40
1	16S1	996	A	C8-N9-C4	6.01	108.20	105.80
22	23S1	126	A	N3-C4-N9	6.01	132.21	127.40
22	23S1	627	A	N3-C4-N9	6.01	132.21	127.40
22	23S1	13	A	N9-C4-C5	6.01	108.20	105.80
22	23S1	19	A	C4-C5-C6	6.01	120.01	117.00
22	23S1	1096	A	C8-N9-C4	6.01	108.20	105.80
22	23S1	1508	A	N3-C4-N9	6.01	132.21	127.40
22	23S1	1591	A	C5-C6-N1	6.01	120.70	117.70
22	23S1	2721	A	C4-C5-C6	6.01	120.01	117.00
23	05S1	108	A	C8-N9-C4	6.01	108.20	105.80
1	16S1	192	A	C4-C5-C6	6.01	120.00	117.00
1	16S1	532	A	N3-C4-N9	6.01	132.21	127.40
22	23S1	181	A	C8-N9-C4	6.01	108.20	105.80
22	23S1	199	A	N9-C4-C5	6.01	108.20	105.80
22	23S1	1347	A	N9-C4-C5	6.01	108.20	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2278	A	C4-C5-C6	6.01	120.00	117.00
22	23S1	2366	A	C4-C5-C6	6.01	120.00	117.00
22	23S1	155	A	C5-C6-N1	6.01	120.70	117.70
22	23S1	447	A	N3-C4-N9	6.01	132.21	127.40
1	16S1	32	A	C5-C6-N1	6.01	120.70	117.70
1	16S1	78	A	C4-C5-C6	6.01	120.00	117.00
1	16S1	411	A	N3-C4-N9	6.01	132.21	127.40
22	23S1	125	A	N3-C4-N9	6.01	132.21	127.40
22	23S1	1073	A	N3-C4-N9	6.01	132.20	127.40
1	16S1	759	A	C8-N9-C4	6.00	108.20	105.80
1	16S1	1180	A	C4-C5-C6	6.00	120.00	117.00
22	23S1	272	A	N3-C4-N9	6.00	132.20	127.40
22	23S1	391	A	C8-N9-C4	6.00	108.20	105.80
22	23S1	1503	A	C4-C5-N7	-6.00	107.70	110.70
22	23S1	2893	A	C8-N9-C4	6.00	108.20	105.80
1	16S1	149	A	N9-C4-C5	6.00	108.20	105.80
1	16S1	461	A	N3-C4-N9	6.00	132.20	127.40
1	16S1	1480	A	C4-C5-C6	6.00	120.00	117.00
1	16S1	600	A	N3-C4-N9	6.00	132.20	127.40
1	16S1	767	A	N3-C4-N9	6.00	132.20	127.40
1	16S1	1531	A	N3-C4-N9	6.00	132.20	127.40
22	23S1	272	A	C8-N9-C4	6.00	108.20	105.80
22	23S1	661	A	N3-C4-N9	6.00	132.20	127.40
22	23S1	900	A	N9-C4-C5	6.00	108.20	105.80
22	23S1	2134	A	C8-N9-C4	6.00	108.20	105.80
22	23S1	2657	A	C8-N9-C4	6.00	108.20	105.80
22	23S1	324	A	C5-C6-N1	6.00	120.70	117.70
22	23S1	1735	A	C8-N9-C4	6.00	108.20	105.80
1	16S1	26	A	N3-C4-N9	6.00	132.20	127.40
1	16S1	196	A	N9-C4-C5	6.00	108.20	105.80
1	16S1	1105	A	C8-N9-C4	6.00	108.20	105.80
22	23S1	181	A	N3-C4-N9	6.00	132.20	127.40
23	05S1	115	A	N3-C4-N9	6.00	132.20	127.40
1	16S1	19	A	C5-C6-N1	6.00	120.70	117.70
1	16S1	171	A	C5-C6-N1	6.00	120.70	117.70
1	16S1	1483	A	N3-C4-N9	6.00	132.20	127.40
2	S021	137	ARG	NE-CZ-NH2	6.00	123.30	120.30
22	23S1	401	A	N3-C4-N9	6.00	132.20	127.40
22	23S1	793	A	N9-C4-C5	6.00	108.20	105.80
55	PTR1	26	A	C8-N9-C4	6.00	108.20	105.80
55	PTR1	69	A	C5-C6-N1	6.00	120.70	117.70
1	16S1	99	C	C6-N1-C2	-6.00	117.90	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1420	A	C4-C5-C6	6.00	120.00	117.00
22	23S1	1040	A	C4-C5-C6	5.99	120.00	117.00
22	23S1	2268	A	N3-C4-N9	5.99	132.19	127.40
22	23S1	2270	A	C4-C5-C6	5.99	120.00	117.00
1	16S1	1431	A	N3-C4-N9	5.99	132.19	127.40
22	23S1	972	A	N3-C4-N9	5.99	132.19	127.40
22	23S1	2740	A	C4-C5-N7	-5.99	107.70	110.70
1	16S1	60	A	N9-C4-C5	5.99	108.20	105.80
22	23S1	633	A	C4-C5-C6	5.99	120.00	117.00
22	23S1	661	A	C5-C6-N1	5.99	120.69	117.70
22	23S1	2873	A	C4-C5-C6	5.99	120.00	117.00
1	16S1	282	A	N3-C4-N9	5.99	132.19	127.40
1	16S1	408	A	N9-C4-C5	5.99	108.20	105.80
1	16S1	1180	A	N3-C4-N9	5.99	132.19	127.40
1	16S1	1288	A	C4-C5-C6	5.99	120.00	117.00
22	23S1	693	A	C5-C6-N1	5.99	120.69	117.70
22	23S1	1392	A	N3-C4-N9	5.99	132.19	127.40
22	23S1	119	A	C5-C6-N1	5.99	120.69	117.70
22	23S1	1050	A	N3-C4-N9	5.99	132.19	127.40
22	23S1	1952	A	C4-C5-C6	5.99	119.99	117.00
22	23S1	165	A	C4-C5-N7	-5.99	107.71	110.70
22	23S1	231	A	N3-C4-N9	5.99	132.19	127.40
22	23S1	262	A	C8-N9-C4	5.99	108.19	105.80
22	23S1	1803	A	C4-C5-C6	5.99	119.99	117.00
22	23S1	2212	A	C4-C5-N7	-5.99	107.71	110.70
22	23S1	2297	A	C8-N9-C4	5.99	108.19	105.80
22	23S1	2632	A	C8-N9-C4	5.99	108.19	105.80
1	16S1	964	A	N3-C4-N9	5.98	132.19	127.40
22	23S1	167	A	C4-C5-C6	5.98	119.99	117.00
22	23S1	1552	A	N9-C4-C5	5.98	108.19	105.80
22	23S1	2721	A	N3-C4-N9	5.98	132.19	127.40
22	23S1	13	A	N3-C4-N9	5.98	132.19	127.40
22	23S1	309	A	N3-C4-N9	5.98	132.19	127.40
22	23S1	1596	A	C4-C5-C6	5.98	119.99	117.00
22	23S1	1977	A	N3-C4-N9	5.98	132.19	127.40
22	23S1	1998	A	C5-C6-N1	5.98	120.69	117.70
1	16S1	1176	A	C5-C6-N1	5.98	120.69	117.70
22	23S1	501	A	N9-C4-C5	5.98	108.19	105.80
22	23S1	1597	A	C4-C5-N7	-5.98	107.71	110.70
22	23S1	2205	A	C4-C5-C6	5.98	119.99	117.00
23	05S1	59	A	C4-C5-N7	-5.98	107.71	110.70
22	23S1	345	A	C4-C5-C6	5.98	119.99	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1360	A	C5-C6-N1	5.98	120.69	117.70
1	16S1	1410	A	C5-C6-N1	5.98	120.69	117.70
22	23S1	1705	A	C8-N9-C4	5.98	108.19	105.80
22	23S1	2317	A	N3-C4-N9	5.98	132.18	127.40
22	23S1	2433	A	C4-C5-N7	-5.98	107.71	110.70
23	05S1	104	A	C4-C5-C6	5.98	119.99	117.00
1	16S1	1000	A	C5-C6-N1	5.98	120.69	117.70
55	PTR1	38	A	C4-C5-C6	5.98	119.99	117.00
1	16S1	535	A	N3-C4-N9	5.97	132.18	127.40
22	23S1	905	A	C4-C5-N7	-5.97	107.71	110.70
22	23S1	979	A	N9-C4-C5	5.97	108.19	105.80
22	23S1	1805	A	C4-C5-N7	-5.97	107.71	110.70
22	23S1	2809	A	C5-C6-N1	5.97	120.69	117.70
1	16S1	696	A	C5-N7-C8	5.97	106.89	103.90
1	16S1	1028	C	C6-N1-C2	-5.97	117.91	120.30
1	16S1	1476	A	C4-C5-C6	5.97	119.99	117.00
22	23S1	2212	A	C4-C5-C6	5.97	119.99	117.00
1	16S1	815	A	N3-C4-N9	5.97	132.18	127.40
1	16S1	1151	A	C5-C6-N1	5.97	120.69	117.70
22	23S1	508	A	N3-C4-N9	5.97	132.18	127.40
22	23S1	616	A	N3-C4-N9	5.97	132.18	127.40
22	23S1	627	A	C4-C5-C6	5.97	119.98	117.00
22	23S1	794	A	C5-C6-N1	5.97	120.69	117.70
22	23S1	1853	A	C5-C6-N1	5.97	120.69	117.70
22	23S1	2821	A	C4-C5-C6	5.97	119.99	117.00
1	16S1	547	A	C8-N9-C4	5.97	108.19	105.80
1	16S1	728	A	C4-C5-N7	-5.97	107.72	110.70
1	16S1	784	A	C5-C6-N1	5.97	120.69	117.70
1	16S1	1500	A	N9-C4-C5	5.97	108.19	105.80
22	23S1	38	A	C4-C5-N7	-5.97	107.72	110.70
22	23S1	693	A	C4-C5-C6	5.97	119.98	117.00
22	23S1	1805	A	N3-C4-N9	5.97	132.18	127.40
22	23S1	2095	A	C4-C5-N7	-5.97	107.72	110.70
22	23S1	146	A	C5-C6-N1	5.97	120.68	117.70
22	23S1	165	A	C8-N9-C4	5.97	108.19	105.80
22	23S1	352	A	C4-C5-C6	5.97	119.98	117.00
22	23S1	1809	A	C4-C5-C6	5.97	119.98	117.00
1	16S1	1130	A	N3-C4-N9	5.97	132.17	127.40
22	23S1	675	A	N9-C4-C5	5.97	108.19	105.80
22	23S1	1268	A	N3-C4-N9	5.97	132.17	127.40
22	23S1	2734	A	C8-N9-C4	5.97	108.19	105.80
22	23S1	2872	A	C6-N1-C2	5.97	122.18	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	PTR1	59	A	C4-C5-N7	-5.97	107.72	110.70
1	16S1	44	A	N9-C4-C5	5.96	108.19	105.80
1	16S1	262	A	N3-C4-N9	5.96	132.17	127.40
1	16S1	1437	A	C4-C5-C6	5.96	119.98	117.00
22	23S1	1711	A	C5-C6-N1	5.96	120.68	117.70
23	05S1	78	A	N9-C4-C5	5.96	108.19	105.80
1	16S1	935	A	C5-C6-N1	5.96	120.68	117.70
1	16S1	1196	A	N3-C4-N9	5.96	132.17	127.40
22	23S1	213	A	C8-N9-C4	5.96	108.19	105.80
22	23S1	454	A	C4-C5-C6	5.96	119.98	117.00
22	23S1	460	A	N3-C4-N9	5.96	132.17	127.40
1	16S1	1105	A	N3-C4-N9	5.96	132.17	127.40
22	23S1	590	A	N3-C4-N9	5.96	132.17	127.40
22	23S1	1274	A	N9-C4-C5	5.96	108.19	105.80
22	23S1	2170	A	C4-C5-N7	-5.96	107.72	110.70
1	16S1	129	A	N3-C4-N9	5.96	132.17	127.40
22	23S1	538	A	N3-C4-N9	5.96	132.17	127.40
22	23S1	927	A	N3-C4-N9	5.96	132.17	127.40
22	23S1	1147	A	N3-C4-N9	5.96	132.17	127.40
22	23S1	1938	A	N3-C4-N9	5.96	132.17	127.40
22	23S1	2856	A	C4-C5-C6	5.96	119.98	117.00
23	05S1	53	A	N3-C4-N9	5.96	132.17	127.40
1	16S1	456	A	C4-C5-C6	5.96	119.98	117.00
1	16S1	489	C	C6-N1-C1'	-5.96	113.65	120.80
1	16S1	1191	A	C4-C5-C6	5.96	119.98	117.00
1	16S1	1520	C	N1-C2-O2	5.96	122.47	118.90
22	23S1	449	A	C5-C6-N1	5.96	120.68	117.70
22	23S1	1913	A	N3-C4-N9	5.96	132.17	127.40
22	23S1	1966	A	C8-N9-C4	5.96	108.18	105.80
22	23S1	161	A	C4-C5-N7	-5.96	107.72	110.70
22	23S1	616	A	C4-C5-C6	5.96	119.98	117.00
22	23S1	1439	A	N3-C4-N9	5.96	132.17	127.40
22	23S1	2705	A	N9-C4-C5	5.96	108.18	105.80
22	23S1	752	A	N9-C4-C5	5.96	108.18	105.80
22	23S1	2453	A	C4-C5-N7	-5.95	107.72	110.70
1	16S1	72	A	C5-C6-N1	5.95	120.68	117.70
1	16S1	502	A	C5-C6-N1	5.95	120.68	117.70
22	23S1	2662	A	C5-N7-C8	5.95	106.88	103.90
55	PTR1	20	U	C5-C4-O4	-5.95	122.33	125.90
22	23S1	896	A	C4-C5-C6	5.95	119.97	117.00
22	23S1	900	A	N3-C4-N9	5.95	132.16	127.40
22	23S1	925	A	C5-C6-N1	5.95	120.68	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1039	A	C4-C5-C6	5.95	119.98	117.00
22	23S1	1127	A	N9-C4-C5	5.95	108.18	105.80
1	16S1	71	A	C4-C5-C6	5.95	119.97	117.00
1	16S1	78	A	N9-C4-C5	5.95	108.18	105.80
1	16S1	1238	A	N9-C4-C5	5.95	108.18	105.80
1	16S1	1254	A	C4-C5-C6	5.95	119.97	117.00
22	23S1	217	A	C4-C5-C6	5.95	119.97	117.00
22	23S1	2176	A	C5-N7-C8	5.95	106.87	103.90
1	16S1	1410	A	C4-C5-C6	5.95	119.97	117.00
1	16S1	155	A	C8-N9-C4	5.95	108.18	105.80
1	16S1	321	A	C4-C5-C6	5.95	119.97	117.00
1	16S1	914	A	C8-N9-C4	5.95	108.18	105.80
22	23S1	734	A	N3-C4-N9	5.95	132.16	127.40
22	23S1	1366	A	C8-N9-C4	5.95	108.18	105.80
22	23S1	1431	A	C8-N9-C4	5.95	108.18	105.80
22	23S1	2183	A	N3-C4-N9	5.94	132.16	127.40
1	16S1	1269	A	C4-C5-C6	5.94	119.97	117.00
22	23S1	586	A	C4-C5-C6	5.94	119.97	117.00
22	23S1	1503	A	N9-C4-C5	5.94	108.18	105.80
22	23S1	2298	A	N3-C4-N9	5.94	132.16	127.40
22	23S1	2469	A	N3-C4-N9	5.94	132.15	127.40
22	23S1	2781	A	C4-C5-C6	5.94	119.97	117.00
22	23S1	2799	A	C8-N9-C4	5.94	108.18	105.80
1	16S1	753	A	N3-C4-N9	5.94	132.15	127.40
1	16S1	792	A	N3-C4-N9	5.94	132.15	127.40
1	16S1	1251	A	C4-C5-N7	-5.94	107.73	110.70
22	23S1	556	A	C4-C5-C6	5.94	119.97	117.00
22	23S1	844	A	C4-C5-C6	5.94	119.97	117.00
22	23S1	878	A	C4-C5-N7	-5.94	107.73	110.70
22	23S1	1787	A	C4-C5-C6	5.94	119.97	117.00
22	23S1	2205	A	N3-C4-N9	5.94	132.15	127.40
1	16S1	503	C	C6-N1-C2	-5.94	117.92	120.30
22	23S1	2173	A	C4-C5-C6	5.94	119.97	117.00
22	23S1	2565	A	N3-C4-N9	5.94	132.15	127.40
1	16S1	704	A	N9-C4-C5	5.94	108.17	105.80
1	16S1	935	A	C4-C5-C6	5.94	119.97	117.00
1	16S1	1502	A	C4-C5-C6	5.94	119.97	117.00
22	23S1	973	A	N9-C4-C5	5.94	108.17	105.80
22	23S1	2211	A	N9-C4-C5	5.94	108.17	105.80
23	05S1	29	A	N3-C4-N9	5.94	132.15	127.40
1	16S1	468	A	C8-N9-C4	5.93	108.17	105.80
1	16S1	918	A	C4-C5-C6	5.93	119.97	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	959	A	N9-C4-C5	5.93	108.17	105.80
1	16S1	1257	A	N3-C4-N9	5.93	132.15	127.40
22	23S1	563	A	N9-C4-C5	5.93	108.17	105.80
22	23S1	897	C	C6-N1-C2	-5.93	117.93	120.30
22	23S1	1987	A	C4-C5-C6	5.93	119.97	117.00
22	23S1	2418	A	C4-C5-C6	5.93	119.97	117.00
22	23S1	2711	A	C8-N9-C4	5.93	108.17	105.80
55	PTR1	69	A	C4-C5-C6	5.93	119.97	117.00
1	16S1	1152	A	C5-N7-C8	5.93	106.87	103.90
2	S021	129	LEU	CB-CG-CD1	-5.93	100.91	111.00
22	23S1	1050	A	C8-N9-C4	5.93	108.17	105.80
22	23S1	1080	A	N3-C4-N9	5.93	132.15	127.40
22	23S1	1433	A	C4-C5-C6	5.93	119.97	117.00
22	23S1	1960	A	N3-C4-N9	5.93	132.15	127.40
22	23S1	2108	A	N3-C4-N9	5.93	132.15	127.40
22	23S1	2602	A	N3-C4-N9	5.93	132.15	127.40
22	23S1	1165	A	N9-C4-C5	5.93	108.17	105.80
22	23S1	1809	A	C5-C6-N1	5.93	120.67	117.70
22	23S1	2058	A	C4-C5-C6	5.93	119.97	117.00
22	23S1	2541	A	C4-C5-C6	5.93	119.96	117.00
22	23S1	905	A	C8-N9-C4	5.93	108.17	105.80
22	23S1	1762	A	N3-C4-N9	5.93	132.14	127.40
1	16S1	208	U	C5-C4-O4	5.93	129.46	125.90
1	16S1	344	A	C4-C5-C6	5.93	119.96	117.00
1	16S1	1246	A	C8-N9-C4	5.93	108.17	105.80
22	23S1	155	A	N3-C4-N9	5.93	132.14	127.40
22	23S1	1322	A	C8-N9-C4	5.93	108.17	105.80
22	23S1	2184	A	N3-C4-N9	5.93	132.14	127.40
23	05S1	119	A	N9-C4-C5	5.93	108.17	105.80
1	16S1	1155	A	C5-C6-N1	5.92	120.66	117.70
22	23S1	374	A	C4-C5-C6	5.92	119.96	117.00
1	16S1	1429	A	C4-C5-C6	5.92	119.96	117.00
22	23S1	382	A	C5-C6-N1	5.92	120.66	117.70
22	23S1	541	A	N3-C4-N9	5.92	132.14	127.40
22	23S1	689	A	C4-C5-C6	5.92	119.96	117.00
22	23S1	1001	A	N9-C4-C5	5.92	108.17	105.80
1	16S1	845	A	C5-C6-N1	5.92	120.66	117.70
22	23S1	478	A	C4-C5-C6	5.92	119.96	117.00
22	23S1	2434	A	C4-C5-C6	5.92	119.96	117.00
1	16S1	1155	A	C8-N9-C4	5.92	108.17	105.80
22	23S1	807	U	N1-C2-N3	5.92	118.45	114.90
22	23S1	1717	A	C8-N9-C4	5.92	108.17	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	344	A	N3-C4-N9	5.92	132.13	127.40
22	23S1	149	A	C4-C5-C6	5.92	119.96	117.00
22	23S1	575	A	N3-C4-N9	5.92	132.13	127.40
22	23S1	1032	A	C8-N9-C4	5.92	108.17	105.80
22	23S1	1096	A	N9-C4-C5	5.92	108.17	105.80
22	23S1	165	A	N9-C4-C5	5.92	108.17	105.80
22	23S1	739	A	C4-C5-C6	5.92	119.96	117.00
22	23S1	2281	A	C4-C5-C6	5.92	119.96	117.00
22	23S1	2880	C	N1-C2-O2	5.92	122.45	118.90
1	16S1	325	A	N3-C4-N9	5.91	132.13	127.40
1	16S1	411	A	C5-C6-N1	5.91	120.66	117.70
22	23S1	217	A	N3-C4-N9	5.91	132.13	127.40
22	23S1	479	A	N3-C4-N9	5.91	132.13	127.40
22	23S1	666	A	C8-N9-C4	5.91	108.17	105.80
22	23S1	1304	A	N9-C4-C5	5.91	108.17	105.80
25	L031	33	ARG	CD-NE-CZ	5.91	131.88	123.60
1	16S1	977	A	C5-C6-N1	5.91	120.66	117.70
22	23S1	353	C	N1-C2-O2	5.91	122.45	118.90
22	23S1	1586	A	N3-C4-N9	5.91	132.13	127.40
1	16S1	161	A	N3-C4-N9	5.91	132.13	127.40
22	23S1	279	A	C4-C5-C6	5.91	119.95	117.00
22	23S1	1134	A	C8-N9-C4	5.91	108.16	105.80
22	23S1	1247	A	C4-C5-N7	-5.91	107.75	110.70
1	16S1	315	A	C5-C6-N1	5.91	120.65	117.70
1	16S1	364	A	N3-C4-N9	5.91	132.13	127.40
1	16S1	1434	A	N3-C4-N9	5.91	132.13	127.40
22	23S1	344	A	C8-N9-C4	5.91	108.16	105.80
22	23S1	844	A	N3-C4-N9	5.91	132.13	127.40
22	23S1	2635	A	N9-C4-C5	5.91	108.16	105.80
22	23S1	2682	A	C8-N9-C4	5.91	108.16	105.80
1	16S1	872	A	C5-C6-N1	5.91	120.65	117.70
1	16S1	87	C	N1-C2-O2	5.91	122.44	118.90
1	16S1	728	A	N3-C4-N9	5.91	132.12	127.40
1	16S1	1022	A	N3-C4-N9	5.91	132.12	127.40
22	23S1	146	A	C8-N9-C4	5.91	108.16	105.80
22	23S1	371	A	N3-C4-N9	5.91	132.12	127.40
22	23S1	1502	A	C4-C5-N7	-5.91	107.75	110.70
22	23S1	1522	A	C8-N9-C4	5.91	108.16	105.80
22	23S1	2516	A	C5-C6-N1	5.91	120.65	117.70
22	23S1	2738	A	C8-N9-C4	5.91	108.16	105.80
1	16S1	130	A	N3-C4-N9	5.90	132.12	127.40
1	16S1	167	A	N3-C4-N9	5.90	132.12	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	219	A	N9-C4-C5	5.90	108.16	105.80
22	23S1	1670	C	N3-C2-O2	-5.90	117.77	121.90
22	23S1	897	C	C5-C6-N1	5.90	123.95	121.00
22	23S1	1579	A	N3-C4-N9	5.90	132.12	127.40
22	23S1	2800	A	N3-C4-N9	5.90	132.12	127.40
1	16S1	509	A	N9-C4-C5	5.90	108.16	105.80
22	23S1	21	A	C5-C6-N1	5.90	120.65	117.70
22	23S1	2381	A	N3-C4-N9	5.90	132.12	127.40
1	16S1	65	A	N3-C4-N9	5.90	132.12	127.40
1	16S1	523	A	N3-C4-N9	5.90	132.12	127.40
22	23S1	347	A	N9-C4-C5	5.90	108.16	105.80
22	23S1	1749	A	N3-C4-N9	5.90	132.12	127.40
22	23S1	1977	A	C4-C5-C6	5.90	119.95	117.00
22	23S1	2635	A	N3-C4-N9	5.90	132.12	127.40
1	16S1	1130	A	N9-C4-C5	5.90	108.16	105.80
22	23S1	637	A	N3-C4-N9	5.90	132.12	127.40
22	23S1	718	A	C4-C5-N7	-5.90	107.75	110.70
22	23S1	752	A	C4-C5-N7	-5.90	107.75	110.70
22	23S1	1254	A	C8-N9-C4	5.90	108.16	105.80
22	23S1	1757	A	N3-C4-N9	5.90	132.12	127.40
22	23S1	2184	A	C4-C5-C6	5.90	119.95	117.00
1	16S1	766	A	N9-C4-C5	5.89	108.16	105.80
1	16S1	1254	A	C8-N9-C4	5.89	108.16	105.80
1	16S1	1311	A	C8-N9-C4	5.89	108.16	105.80
22	23S1	227	A	C8-N9-C4	5.89	108.16	105.80
22	23S1	346	A	C5-C6-N1	5.89	120.65	117.70
22	23S1	1147	A	C5-C6-N1	5.89	120.65	117.70
22	23S1	2547	A	N3-C4-N9	5.89	132.12	127.40
22	23S1	103	A	C8-N9-C4	5.89	108.16	105.80
22	23S1	156	A	C5-C6-N1	5.89	120.65	117.70
22	23S1	510	C	N1-C2-O2	5.89	122.44	118.90
22	23S1	609	A	N3-C4-N9	5.89	132.12	127.40
22	23S1	793	A	C4-C5-C6	5.89	119.95	117.00
22	23S1	927	A	C4-C5-C6	5.89	119.95	117.00
22	23S1	1508	A	C4-C5-C6	5.89	119.95	117.00
22	23S1	1901	A	C5-N7-C8	5.89	106.85	103.90
22	23S1	2019	A	C4-C5-C6	5.89	119.95	117.00
23	05S1	35	C	N1-C2-O2	5.89	122.44	118.90
1	16S1	109	A	N3-C4-N9	5.89	132.11	127.40
1	16S1	495	A	C8-N9-C4	5.89	108.16	105.80
1	16S1	1434	A	C8-N9-C4	5.89	108.16	105.80
13	S131	46	SER	C-N-CA	5.89	136.43	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	905	A	N9-C4-C5	5.89	108.16	105.80
22	23S1	2758	A	C4-C5-N7	-5.89	107.75	110.70
22	23S1	878	A	N9-C4-C5	5.89	108.16	105.80
22	23S1	1690	A	C4-C5-C6	5.89	119.94	117.00
22	23S1	2006	C	C6-N1-C2	-5.89	117.94	120.30
22	23S1	2309	A	C8-N9-C4	5.89	108.16	105.80
22	23S1	2340	A	C4-C5-C6	5.89	119.94	117.00
1	16S1	815	A	C4-C5-C6	5.89	119.94	117.00
22	23S1	1247	A	C5-C6-N1	5.89	120.64	117.70
22	23S1	125	A	C4-C5-C6	5.89	119.94	117.00
22	23S1	910	A	C4-C5-C6	5.89	119.94	117.00
22	23S1	1169	A	C4-C5-C6	5.89	119.94	117.00
22	23S1	1655	A	C5-C6-N1	5.89	120.64	117.70
22	23S1	2766	A	C5-C6-N1	5.89	120.64	117.70
22	23S1	2893	A	C4-C5-C6	5.89	119.94	117.00
1	16S1	964	A	C4-C5-C6	5.88	119.94	117.00
22	23S1	146	A	C4-C5-C6	5.88	119.94	117.00
22	23S1	219	A	C5-C6-N1	5.88	120.64	117.70
22	23S1	1637	A	C4-C5-C6	5.88	119.94	117.00
22	23S1	503	A	C5-C6-N1	5.88	120.64	117.70
23	05S1	109	A	C4-C5-C6	5.88	119.94	117.00
1	16S1	321	A	N3-C4-N9	5.88	132.10	127.40
1	16S1	815	A	C8-N9-C4	5.88	108.15	105.80
1	16S1	906	A	C4-C5-C6	5.88	119.94	117.00
1	16S1	975	A	C8-N9-C4	5.88	108.15	105.80
22	23S1	299	A	C4-C5-N7	-5.88	107.76	110.70
22	23S1	1307	A	C8-N9-C4	5.88	108.15	105.80
22	23S1	1477	A	C4-C5-C6	5.88	119.94	117.00
22	23S1	2378	A	C4-C5-C6	5.88	119.94	117.00
22	23S1	2679	A	C4-C5-C6	5.88	119.94	117.00
23	05S1	108	A	N3-C4-N9	5.88	132.11	127.40
1	16S1	595	A	C4-C5-C6	5.88	119.94	117.00
1	16S1	938	A	C5-C6-N1	5.88	120.64	117.70
22	23S1	402	A	C8-N9-C4	5.88	108.15	105.80
1	16S1	50	A	C4-C5-C6	5.88	119.94	117.00
1	16S1	715	A	C8-N9-C4	5.88	108.15	105.80
1	16S1	1082	A	C4-C5-C6	5.88	119.94	117.00
1	16S1	1410	A	N3-C4-N9	5.88	132.10	127.40
22	23S1	309	A	C4-C5-C6	5.88	119.94	117.00
22	23S1	1665	A	C4-C5-C6	5.88	119.94	117.00
22	23S1	2792	A	C5-C6-N1	5.88	120.64	117.70
1	16S1	969	A	N9-C4-C5	5.88	108.15	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	676	A	C8-N9-C4	5.88	108.15	105.80
22	23S1	739	A	N9-C4-C5	5.88	108.15	105.80
22	23S1	1327	A	C4-C5-C6	5.88	119.94	117.00
22	23S1	2225	A	N3-C4-N9	5.88	132.10	127.40
1	16S1	366	A	C4-C5-C6	5.88	119.94	117.00
1	16S1	509	A	C4-C5-N7	-5.88	107.76	110.70
1	16S1	807	A	C4-C5-C6	5.88	119.94	117.00
22	23S1	143	C	N1-C2-O2	5.88	122.42	118.90
1	16S1	498	A	N9-C4-C5	5.87	108.15	105.80
1	16S1	1431	A	C5-C6-N1	5.87	120.64	117.70
22	23S1	532	A	C5-C6-N1	5.87	120.64	117.70
22	23S1	750	A	C5-C6-N1	5.87	120.64	117.70
22	23S1	1284	A	N3-C4-N9	5.87	132.10	127.40
22	23S1	2037	A	C5-C6-N1	5.87	120.64	117.70
22	23S1	2534	A	N3-C4-N9	5.87	132.10	127.40
22	23S1	2873	A	N3-C4-N9	5.87	132.10	127.40
1	16S1	461	A	C5-C6-N1	5.87	120.64	117.70
1	16S1	1377	A	C8-N9-C4	5.87	108.15	105.80
1	16S1	1456	A	C4-C5-C6	5.87	119.94	117.00
22	23S1	160	A	C5-C6-N1	5.87	120.64	117.70
22	23S1	340	A	N3-C4-N9	5.87	132.10	127.40
22	23S1	601	C	C6-N1-C2	-5.87	117.95	120.30
22	23S1	1809	A	N9-C4-C5	5.87	108.15	105.80
22	23S1	2766	A	C5-N7-C8	5.87	106.83	103.90
1	16S1	320	A	C4-C5-N7	-5.87	107.77	110.70
22	23S1	74	A	C4-C5-C6	5.87	119.94	117.00
22	23S1	742	A	C5-C6-N1	5.87	120.64	117.70
22	23S1	1090	A	N3-C4-N9	5.87	132.09	127.40
22	23S1	2899	A	C8-N9-C4	5.87	108.15	105.80
1	16S1	1252	A	N9-C4-C5	5.87	108.15	105.80
1	16S1	44	A	N3-C4-N9	5.87	132.09	127.40
1	16S1	179	A	C4-C5-C6	5.87	119.93	117.00
1	16S1	1151	A	C8-N9-C4	5.87	108.15	105.80
22	23S1	752	A	C8-N9-C4	5.87	108.15	105.80
1	16S1	270	A	C5-C6-N1	5.86	120.63	117.70
1	16S1	753	A	C8-N9-C4	5.86	108.14	105.80
1	16S1	814	A	C4-C5-C6	5.86	119.93	117.00
1	16S1	1480	A	N9-C4-C5	5.86	108.14	105.80
22	23S1	980	A	C5-C6-N1	5.86	120.63	117.70
22	23S1	2856	A	C5-C6-N1	5.86	120.63	117.70
23	05S1	15	A	N3-C4-N9	5.86	132.09	127.40
22	23S1	1654	A	C4-C5-C6	5.86	119.93	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1239	A	C4-C5-N7	-5.86	107.77	110.70
22	23S1	1532	A	C8-N9-C4	5.86	108.14	105.80
22	23S1	1632	A	N3-C4-N9	5.86	132.09	127.40
22	23S1	2598	A	N3-C4-N9	5.86	132.09	127.40
22	23S1	1593	A	C4-C5-C6	5.86	119.93	117.00
22	23S1	1927	A	N3-C4-N9	5.86	132.09	127.40
1	16S1	228	A	N3-C4-N9	5.86	132.09	127.40
1	16S1	621	A	C5-C6-N1	5.86	120.63	117.70
22	23S1	510	C	N3-C2-O2	-5.86	117.80	121.90
22	23S1	685	A	N3-C4-N9	5.86	132.09	127.40
22	23S1	896	A	N9-C4-C5	5.86	108.14	105.80
22	23S1	2190	G	C8-N9-C4	-5.86	104.06	106.40
22	23S1	2564	A	C5-C6-N1	5.86	120.63	117.70
22	23S1	2600	A	N3-C4-N9	5.86	132.09	127.40
1	16S1	1105	A	C4-C5-C6	5.86	119.93	117.00
22	23S1	900	A	C4-C5-C6	5.86	119.93	117.00
22	23S1	1677	A	N3-C4-N9	5.86	132.08	127.40
1	16S1	716	A	C5-C6-N1	5.85	120.63	117.70
1	16S1	864	A	N9-C4-C5	5.85	108.14	105.80
1	16S1	1236	A	C8-N9-C4	5.85	108.14	105.80
1	16S1	1229	A	N9-C4-C5	5.85	108.14	105.80
22	23S1	282	A	N3-C4-N9	5.85	132.08	127.40
22	23S1	2418	A	C8-N9-C4	5.85	108.14	105.80
22	23S1	2635	A	C4-C5-C6	5.85	119.93	117.00
1	16S1	595	A	N3-C4-N9	5.85	132.08	127.40
1	16S1	1176	A	C4-C5-C6	5.85	119.92	117.00
22	23S1	792	A	C4-C5-N7	-5.85	107.78	110.70
22	23S1	1635	A	N3-C4-N9	5.85	132.08	127.40
22	23S1	2071	A	N9-C4-C5	5.85	108.14	105.80
22	23S1	2284	A	N9-C4-C5	5.85	108.14	105.80
22	23S1	2426	A	C4-C5-C6	5.85	119.92	117.00
22	23S1	2829	A	N3-C4-N9	5.85	132.08	127.40
55	PTR1	26	A	N3-C4-N9	5.85	132.08	127.40
1	16S1	583	A	C5-C6-N1	5.85	120.62	117.70
1	16S1	1246	A	C4-C5-C6	5.85	119.92	117.00
22	23S1	2799	A	C5-C6-N1	5.85	120.62	117.70
1	16S1	477	C	N3-C2-O2	-5.85	117.81	121.90
1	16S1	958	A	N9-C4-C5	5.85	108.14	105.80
22	23S1	63	A	C8-N9-C4	5.85	108.14	105.80
22	23S1	2459	A	C8-N9-C4	5.85	108.14	105.80
1	16S1	228	A	N9-C4-C5	5.84	108.14	105.80
1	16S1	1014	A	N9-C4-C5	5.84	108.14	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	270	A	C4-C5-C6	5.84	119.92	117.00
22	23S1	429	A	N9-C4-C5	5.84	108.14	105.80
22	23S1	602	A	C8-N9-C4	5.84	108.14	105.80
22	23S1	715	A	N9-C4-C5	5.84	108.14	105.80
22	23S1	1090	A	C4-C5-C6	5.84	119.92	117.00
23	05S1	34	A	C4-C5-N7	-5.84	107.78	110.70
55	PTR1	3	A	C8-N9-C4	5.84	108.14	105.80
1	16S1	181	A	C8-N9-C4	5.84	108.14	105.80
1	16S1	238	A	C4-C5-C6	5.84	119.92	117.00
22	23S1	74	A	N9-C4-C5	5.84	108.14	105.80
22	23S1	95	A	N3-C4-N9	5.84	132.07	127.40
22	23S1	294	A	N3-C4-N9	5.84	132.07	127.40
22	23S1	344	A	N3-C4-N9	5.84	132.07	127.40
22	23S1	2090	A	C4-C5-C6	5.84	119.92	117.00
1	16S1	8	A	N3-C4-N9	5.84	132.07	127.40
1	16S1	600	A	C8-N9-C4	5.84	108.14	105.80
1	16S1	759	A	N3-C4-N9	5.84	132.07	127.40
1	16S1	1430	A	N3-C4-N9	5.84	132.07	127.40
22	23S1	716	A	C8-N9-C4	5.84	108.14	105.80
22	23S1	1889	A	N9-C4-C5	5.84	108.14	105.80
22	23S1	2411	A	N3-C4-N9	5.84	132.07	127.40
22	23S1	2600	A	C4-C5-C6	5.84	119.92	117.00
1	16S1	1238	A	C5-C6-N1	5.84	120.62	117.70
22	23S1	279	A	N3-C4-N9	5.84	132.07	127.40
22	23S1	668	A	N3-C4-N9	5.84	132.07	127.40
22	23S1	965	C	C6-N1-C2	-5.84	117.96	120.30
22	23S1	2071	A	C4-C5-C6	5.84	119.92	117.00
55	PTR1	6	C	N1-C2-O2	5.84	122.40	118.90
1	16S1	192	A	N3-C4-N9	5.84	132.07	127.40
1	16S1	1456	A	N3-C4-N9	5.84	132.07	127.40
22	23S1	2566	A	C8-N9-C4	5.84	108.14	105.80
1	16S1	784	A	C4-C5-C6	5.84	119.92	117.00
22	23S1	352	A	N9-C4-C5	5.84	108.14	105.80
22	23S1	2297	A	N9-C4-C5	5.84	108.13	105.80
22	23S1	2309	A	C4-C5-C6	5.84	119.92	117.00
22	23S1	2478	A	C8-N9-C4	5.84	108.13	105.80
22	23S1	1698	A	N9-C4-C5	5.83	108.13	105.80
22	23S1	1913	A	C4-C5-C6	5.83	119.92	117.00
22	23S1	207	A	C5-C6-N1	5.83	120.62	117.70
22	23S1	563	A	C4-C5-C6	5.83	119.92	117.00
22	23S1	1103	A	C8-N9-C4	5.83	108.13	105.80
22	23S1	1932	A	N9-C4-C5	5.83	108.13	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2309	A	N3-C4-N9	5.83	132.07	127.40
1	16S1	1287	A	C8-N9-C4	5.83	108.13	105.80
1	16S1	1349	A	C5-C6-N1	5.83	120.61	117.70
1	16S1	1368	A	C4-C5-C6	5.83	119.92	117.00
22	23S1	1353	A	C5-C6-N1	5.83	120.62	117.70
22	23S1	1359	A	N9-C4-C5	5.83	108.13	105.80
22	23S1	1901	A	C4-C5-C6	5.83	119.92	117.00
1	16S1	787	A	N3-C4-N9	5.83	132.06	127.40
22	23S1	89	A	C5-C6-N1	5.83	120.61	117.70
22	23S1	172	A	C5-C6-N1	5.83	120.61	117.70
22	23S1	900	A	C4-C5-N7	-5.83	107.78	110.70
22	23S1	2247	A	C4-C5-C6	5.83	119.92	117.00
22	23S1	2435	A	N3-C4-N9	5.83	132.06	127.40
1	16S1	149	A	C4-C5-C6	5.83	119.91	117.00
1	16S1	694	A	C4-C5-N7	-5.83	107.79	110.70
1	16S1	958	A	N3-C4-N9	5.83	132.06	127.40
1	16S1	1271	A	C5-C6-N1	5.83	120.61	117.70
22	23S1	1676	A	C5-N7-C8	5.83	106.81	103.90
22	23S1	1705	A	C4-C5-C6	5.83	119.91	117.00
22	23S1	1853	A	C4-C5-N7	-5.83	107.78	110.70
22	23S1	1889	A	N3-C4-N9	5.83	132.06	127.40
22	23S1	2097	A	C5-C6-N1	5.83	120.61	117.70
1	16S1	143	A	C4-C5-C6	5.83	119.91	117.00
22	23S1	1876	A	C8-N9-C4	5.83	108.13	105.80
22	23S1	2322	A	C4-C5-C6	5.83	119.91	117.00
1	16S1	161	A	N9-C4-C5	5.83	108.13	105.80
1	16S1	1005	A	C4-C5-C6	5.83	119.91	117.00
22	23S1	347	A	C4-C5-C6	5.83	119.91	117.00
22	23S1	1353	A	N3-C4-N9	5.83	132.06	127.40
22	23S1	1794	A	C4-C5-C6	5.83	119.91	117.00
22	23S1	2101	A	C4-C5-C6	5.83	119.91	117.00
55	PTR1	56	C	C6-N1-C2	-5.83	117.97	120.30
1	16S1	487	A	C4-C5-N7	-5.82	107.79	110.70
22	23S1	1264	A	N9-C4-C5	5.82	108.13	105.80
22	23S1	2134	A	C4-C5-C6	5.82	119.91	117.00
22	23S1	2288	A	N3-C4-N9	5.82	132.06	127.40
22	23S1	2826	A	C8-N9-C4	5.82	108.13	105.80
23	05S1	115	A	C4-C5-C6	5.82	119.91	117.00
1	16S1	50	A	N3-C4-N9	5.82	132.06	127.40
1	16S1	1248	A	N9-C4-C5	5.82	108.13	105.80
1	16S1	1476	A	N9-C4-C5	5.82	108.13	105.80
1	16S1	1428	A	N3-C4-N9	5.82	132.06	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	789	A	C8-N9-C4	5.82	108.13	105.80
22	23S1	833	A	N3-C4-N9	5.82	132.06	127.40
22	23S1	1269	A	N9-C4-C5	5.82	108.13	105.80
22	23S1	2887	A	C4-C5-C6	5.82	119.91	117.00
1	16S1	523	A	N9-C4-C5	5.82	108.13	105.80
22	23S1	1783	A	C4-C5-N7	-5.82	107.79	110.70
22	23S1	2225	A	C4-C5-C6	5.82	119.91	117.00
22	23S1	2241	A	N9-C4-C5	5.82	108.13	105.80
22	23S1	2662	A	N9-C4-C5	5.82	108.13	105.80
22	23S1	89	A	C8-N9-C4	5.82	108.13	105.80
22	23S1	861	A	C8-N9-C4	5.82	108.13	105.80
22	23S1	1395	A	N9-C4-C5	5.82	108.13	105.80
22	23S1	1785	A	N9-C4-C5	5.82	108.13	105.80
1	16S1	320	A	C5-C6-N1	5.81	120.61	117.70
1	16S1	71	A	N3-C4-N9	5.81	132.05	127.40
1	16S1	246	A	N3-C4-N9	5.81	132.05	127.40
1	16S1	596	A	N9-C4-C5	5.81	108.12	105.80
1	16S1	1256	A	C4-C5-C6	5.81	119.91	117.00
22	23S1	761	A	C5-C6-N1	5.81	120.61	117.70
22	23S1	1496	A	C4-C5-C6	5.81	119.91	117.00
22	23S1	1690	A	N9-C4-C5	5.81	108.12	105.80
22	23S1	1739	A	C5-N7-C8	5.81	106.81	103.90
22	23S1	1789	A	N3-C4-N9	5.81	132.05	127.40
22	23S1	2270	A	C4-C5-N7	-5.81	107.79	110.70
22	23S1	2418	A	C5-C6-N1	5.81	120.61	117.70
1	16S1	493	A	C4-C5-C6	5.81	119.91	117.00
1	16S1	889	A	C5-C6-N1	5.81	120.61	117.70
22	23S1	1773	A	N3-C4-N9	5.81	132.05	127.40
22	23S1	1928	A	N9-C4-C5	5.81	108.12	105.80
1	16S1	167	A	C5-C6-N1	5.81	120.61	117.70
1	16S1	663	A	C5-C6-N1	5.81	120.60	117.70
1	16S1	1169	A	C4-C5-C6	5.81	119.91	117.00
1	16S1	1433	A	C4-C5-C6	5.81	119.91	117.00
22	23S1	471	A	C4-C5-C6	5.81	119.91	117.00
22	23S1	541	A	C4-C5-C6	5.81	119.91	117.00
22	23S1	1253	A	C5-C6-N1	5.81	120.61	117.70
1	16S1	160	A	C8-N9-C4	5.81	108.12	105.80
1	16S1	749	A	C4-C5-C6	5.81	119.90	117.00
22	23S1	172	A	C4-C5-C6	5.81	119.90	117.00
22	23S1	1502	A	C4-C5-C6	5.81	119.90	117.00
22	23S1	1579	A	C4-C5-C6	5.81	119.90	117.00
22	23S1	2835	A	C4-C5-C6	5.81	119.90	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	PTR1	9	A	C4-C5-C6	5.81	119.90	117.00
1	16S1	909	A	N3-C4-N9	5.81	132.04	127.40
22	23S1	1262	A	N9-C4-C5	5.81	108.12	105.80
22	23S1	1786	A	N3-C4-N9	5.81	132.04	127.40
1	16S1	496	A	C4-C5-C6	5.80	119.90	117.00
1	16S1	1014	A	N3-C4-N9	5.80	132.04	127.40
1	16S1	1229	A	C5-C6-N1	5.80	120.60	117.70
1	16S1	1434	A	C4-C5-C6	5.80	119.90	117.00
22	23S1	64	A	C4-C5-C6	5.80	119.90	117.00
22	23S1	1744	A	C5-C6-N1	5.80	120.60	117.70
22	23S1	299	A	N3-C4-N9	5.80	132.04	127.40
22	23S1	497	A	N9-C4-C5	5.80	108.12	105.80
22	23S1	602	A	C5-C6-N1	5.80	120.60	117.70
22	23S1	1413	A	N3-C4-N9	5.80	132.04	127.40
22	23S1	83	A	N3-C4-N9	5.80	132.04	127.40
22	23S1	1144	A	C8-N9-C4	5.80	108.12	105.80
22	23S1	1439	A	C8-N9-C4	5.80	108.12	105.80
22	23S1	2183	A	C4-C5-C6	5.80	119.90	117.00
22	23S1	2764	A	N9-C4-C5	5.80	108.12	105.80
1	16S1	87	C	C6-N1-C2	-5.80	117.98	120.30
22	23S1	2284	A	C5-C6-N1	5.80	120.60	117.70
1	16S1	1	A	N3-C4-N9	5.80	132.04	127.40
22	23S1	480	A	N9-C4-C5	5.80	108.12	105.80
22	23S1	515	A	C5-C6-N1	5.80	120.60	117.70
22	23S1	699	A	C4-C5-C6	5.80	119.90	117.00
22	23S1	1644	C	N3-C2-O2	-5.80	117.84	121.90
22	23S1	2158	A	C4-C5-C6	5.80	119.90	117.00
1	16S1	1311	A	C4-C5-C6	5.79	119.90	117.00
22	23S1	1151	A	C5-C6-N1	5.79	120.60	117.70
22	23S1	2406	A	C8-N9-C4	5.79	108.12	105.80
1	16S1	432	A	C4-C5-N7	-5.79	107.80	110.70
1	16S1	889	A	N9-C4-C5	5.79	108.12	105.80
22	23S1	176	A	N9-C4-C5	5.79	108.12	105.80
22	23S1	1701	A	C5-C6-N1	5.79	120.60	117.70
22	23S1	2835	A	N3-C4-N9	5.79	132.03	127.40
55	PTR1	21	A	N3-C4-N9	5.79	132.03	127.40
22	23S1	1927	A	C4-C5-N7	-5.79	107.80	110.70
22	23S1	2227	A	N3-C4-N9	5.79	132.03	127.40
22	23S1	2314	A	C5-C6-N1	5.79	120.60	117.70
22	23S1	1385	A	C4-C5-N7	-5.79	107.81	110.70
22	23S1	1635	A	C4-C5-C6	5.79	119.89	117.00
22	23S1	2882	A	N9-C4-C5	5.79	108.12	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	279	A	C4-C5-C6	5.79	119.89	117.00
22	23S1	793	A	N3-C4-N9	5.79	132.03	127.40
22	23S1	892	A	C4-C5-C6	5.79	119.89	117.00
22	23S1	1392	A	C4-C5-N7	-5.79	107.81	110.70
55	PTR1	26	A	C4-C5-C6	5.79	119.89	117.00
22	23S1	603	A	C8-N9-C4	5.79	108.11	105.80
22	23S1	1502	A	N3-C4-N9	5.79	132.03	127.40
22	23S1	2725	A	C8-N9-C4	5.79	108.11	105.80
1	16S1	1042	A	C8-N9-C4	5.79	108.11	105.80
1	16S1	1101	A	C8-N9-C4	5.79	108.11	105.80
22	23S1	2042	A	N3-C4-N9	5.79	132.03	127.40
22	23S1	2411	A	C4-C5-C6	5.79	119.89	117.00
22	23S1	2589	A	N3-C4-N9	5.79	132.03	127.40
22	23S1	2826	A	C4-C5-C6	5.79	119.89	117.00
1	16S1	300	A	N7-C8-N9	-5.78	110.91	113.80
1	16S1	1016	A	N3-C4-N9	5.78	132.03	127.40
22	23S1	749	A	C8-N9-C4	5.78	108.11	105.80
22	23S1	915	C	N3-C2-O2	-5.78	117.85	121.90
22	23S1	1067	A	N9-C4-C5	5.78	108.11	105.80
22	23S1	1453	A	C4-C5-C6	5.78	119.89	117.00
1	16S1	223	A	C5-C6-N1	5.78	120.59	117.70
22	23S1	42	A	C4-C5-C6	5.78	119.89	117.00
22	23S1	661	A	C8-N9-C4	5.78	108.11	105.80
22	23S1	1640	A	N3-C4-N9	5.78	132.03	127.40
22	23S1	1858	A	C8-N9-C4	5.78	108.11	105.80
22	23S1	2327	A	N9-C4-C5	5.78	108.11	105.80
22	23S1	2088	A	C8-N9-C4	5.78	108.11	105.80
22	23S1	2407	A	C5-C6-N1	5.78	120.59	117.70
22	23S1	1367	A	N3-C4-N9	5.78	132.02	127.40
22	23S1	2211	A	C8-N9-C4	5.78	108.11	105.80
1	16S1	80	A	C4-C5-N7	-5.78	107.81	110.70
1	16S1	759	A	C4-C5-C6	5.78	119.89	117.00
1	16S1	1319	A	C4-C5-C6	5.78	119.89	117.00
1	16S1	1257	A	C4-C5-C6	5.77	119.89	117.00
22	23S1	2189	U	C2-N1-C1'	5.77	124.63	117.70
22	23S1	804	A	N9-C4-C5	5.77	108.11	105.80
22	23S1	1494	A	N9-C4-C5	5.77	108.11	105.80
22	23S1	2726	A	C4-C5-N7	-5.77	107.81	110.70
1	16S1	919	A	C4-C5-C6	5.77	119.89	117.00
22	23S1	1342	A	C8-N9-C4	5.77	108.11	105.80
1	16S1	243	A	C4-C5-N7	-5.77	107.81	110.70
1	16S1	309	A	C4-C5-C6	5.77	119.89	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	909	A	N9-C4-C5	5.77	108.11	105.80
22	23S1	190	A	N9-C4-C5	5.77	108.11	105.80
22	23S1	2823	A	N3-C4-N9	5.77	132.01	127.40
1	16S1	655	A	C5-C6-N1	5.77	120.58	117.70
1	16S1	1413	A	C8-N9-C4	5.77	108.11	105.80
22	23S1	38	A	N3-C4-N9	5.77	132.01	127.40
22	23S1	582	A	C4-C5-C6	5.77	119.88	117.00
22	23S1	1858	A	C5-C6-N1	5.77	120.58	117.70
22	23S1	2169	A	N9-C4-C5	5.77	108.11	105.80
1	16S1	918	A	C5-C6-N1	5.77	120.58	117.70
1	16S1	1499	A	C4-C5-N7	-5.77	107.82	110.70
22	23S1	1652	A	N9-C4-C5	5.77	108.11	105.80
22	23S1	2534	A	C4-C5-C6	5.77	119.88	117.00
1	16S1	743	A	C8-N9-C4	5.76	108.11	105.80
1	16S1	1269	A	N9-C4-C5	5.76	108.11	105.80
22	23S1	53	A	C8-N9-C4	5.76	108.11	105.80
22	23S1	1552	A	C4-C5-C6	5.76	119.88	117.00
22	23S1	1877	A	C4-C5-C6	5.76	119.88	117.00
22	23S1	1889	A	C4-C5-N7	-5.76	107.82	110.70
22	23S1	2298	A	C4-C5-C6	5.76	119.88	117.00
22	23S1	1009	A	C5-C6-N1	5.76	120.58	117.70
22	23S1	2094	A	C5-C6-N1	5.76	120.58	117.70
1	16S1	1105	A	C5-C6-N1	5.76	120.58	117.70
1	16S1	1274	A	C4-C5-C6	5.76	119.88	117.00
22	23S1	1009	A	C8-N9-C4	5.76	108.10	105.80
22	23S1	1570	A	C4-C5-N7	-5.76	107.82	110.70
1	16S1	1394	A	C4-C5-C6	5.76	119.88	117.00
22	23S1	213	A	N3-C4-N9	5.76	132.01	127.40
22	23S1	522	A	C5-C6-N1	5.76	120.58	117.70
22	23S1	1274	A	N3-C4-N9	5.76	132.01	127.40
22	23S1	2340	A	C5-C6-N1	5.76	120.58	117.70
22	23S1	2850	A	C8-N9-C4	5.76	108.10	105.80
1	16S1	860	A	N3-C4-N9	5.76	132.01	127.40
1	16S1	1016	A	C4-C5-C6	5.76	119.88	117.00
1	16S1	28	A	N9-C4-C5	5.76	108.10	105.80
22	23S1	1614	A	N3-C4-N9	5.76	132.00	127.40
22	23S1	2727	A	C5-C6-N1	5.76	120.58	117.70
1	16S1	320	A	N3-C4-N9	5.75	132.00	127.40
1	16S1	781	A	N3-C4-N9	5.75	132.00	127.40
1	16S1	1110	A	N3-C4-N9	5.75	132.00	127.40
22	23S1	1385	A	N9-C4-C5	5.75	108.10	105.80
22	23S1	2317	A	C4-C5-C6	5.75	119.88	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2531	A	C8-N9-C4	5.75	108.10	105.80
1	16S1	1188	A	C8-N9-C4	5.75	108.10	105.80
1	16S1	1238	A	N3-C4-N9	5.75	132.00	127.40
1	16S1	1333	A	N3-C4-N9	5.75	132.00	127.40
22	23S1	2150	C	N3-C2-O2	-5.75	117.87	121.90
1	16S1	1456	A	C8-N9-C4	5.75	108.10	105.80
22	23S1	278	A	N9-C4-C5	5.75	108.10	105.80
22	23S1	833	A	C5-N7-C8	5.75	106.78	103.90
22	23S1	981	A	C6-N1-C2	5.75	122.05	118.60
22	23S1	1701	A	N3-C4-N9	5.75	132.00	127.40
22	23S1	2031	A	C4-C5-N7	-5.75	107.82	110.70
22	23S1	270	A	C8-N9-C4	5.75	108.10	105.80
22	23S1	322	A	C8-N9-C4	5.75	108.10	105.80
22	23S1	1095	A	C4-C5-C6	5.75	119.88	117.00
1	16S1	649	A	C4-C5-N7	-5.75	107.83	110.70
1	16S1	1483	A	N9-C4-C5	5.75	108.10	105.80
22	23S1	783	A	C4-C5-N7	-5.75	107.83	110.70
22	23S1	1308	A	C8-N9-C4	5.75	108.10	105.80
22	23S1	1551	A	C4-C5-N7	-5.75	107.83	110.70
22	23S1	2031	A	C4-C5-C6	5.75	119.87	117.00
23	05S1	52	A	N3-C4-N9	5.75	132.00	127.40
55	PTR1	9	A	N3-C4-N9	5.75	132.00	127.40
1	16S1	1446	A	N9-C4-C5	5.75	108.10	105.80
22	23S1	538	A	C4-C5-C6	5.75	119.87	117.00
22	23S1	1630	A	C5-C6-N1	5.75	120.57	117.70
22	23S1	2094	A	C4-C5-C6	5.75	119.87	117.00
22	23S1	2632	A	N9-C4-C5	5.75	108.10	105.80
1	16S1	437	U	N1-C2-O2	5.75	126.82	122.80
22	23S1	575	A	C4-C5-C6	5.75	119.87	117.00
22	23S1	861	A	C4-C5-C6	5.75	119.87	117.00
1	16S1	411	A	OP1-P-O3'	5.74	117.84	105.20
1	16S1	1035	A	N3-C4-N9	5.74	132.00	127.40
22	23S1	160	A	C4-C5-C6	5.74	119.87	117.00
22	23S1	340	A	C4-C5-C6	5.74	119.87	117.00
22	23S1	1439	A	C4-C5-N7	-5.74	107.83	110.70
22	23S1	1997	C	C6-N1-C2	-5.74	118.00	120.30
22	23S1	2358	A	C4-C5-N7	-5.74	107.83	110.70
1	16S1	560	A	N9-C4-C5	5.74	108.10	105.80
22	23S1	1749	A	C4-C5-N7	-5.74	107.83	110.70
1	16S1	197	A	N3-C4-N9	5.74	131.99	127.40
1	16S1	532	A	C4-C5-C6	5.74	119.87	117.00
1	16S1	996	A	N3-C4-N9	5.74	131.99	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	149	A	C4-C5-N7	-5.74	107.83	110.70
1	16S1	250	A	C8-N9-C4	5.74	108.10	105.80
1	16S1	313	A	C4-C5-N7	-5.74	107.83	110.70
1	16S1	807	A	N3-C4-N9	5.74	131.99	127.40
1	16S1	1280	A	C8-N9-C4	5.74	108.10	105.80
22	23S1	119	A	C4-C5-N7	-5.74	107.83	110.70
22	23S1	126	A	C4-C5-C6	5.74	119.87	117.00
22	23S1	181	A	C4-C5-C6	5.74	119.87	117.00
22	23S1	199	A	C5-C6-N1	5.74	120.57	117.70
22	23S1	272	A	C4-C5-C6	5.74	119.87	117.00
22	23S1	344	A	C4-C5-C6	5.74	119.87	117.00
22	23S1	1194	A	N9-C4-C5	5.74	108.10	105.80
22	23S1	2317	A	N9-C4-C5	5.74	108.09	105.80
22	23S1	2311	A	C5-C6-N1	5.74	120.57	117.70
1	16S1	171	A	C4-C5-N7	-5.74	107.83	110.70
1	16S1	1319	A	N9-C4-C5	5.74	108.09	105.80
22	23S1	323	C	N1-C2-O2	5.74	122.34	118.90
22	23S1	896	A	N3-C4-N9	5.74	131.99	127.40
22	23S1	947	A	C4-C5-C6	5.74	119.87	117.00
22	23S1	1392	A	C5-C6-N1	5.74	120.57	117.70
22	23S1	1672	A	C4-C5-C6	5.74	119.87	117.00
22	23S1	1932	A	N3-C4-N9	5.74	131.99	127.40
22	23S1	2809	A	N9-C4-C5	5.74	108.09	105.80
1	16S1	665	A	C5-C6-N1	5.73	120.57	117.70
1	16S1	1035	A	C4-C5-C6	5.73	119.87	117.00
22	23S1	501	A	C4-C5-C6	5.73	119.87	117.00
22	23S1	2044	C	C6-N1-C2	-5.73	118.01	120.30
22	23S1	311	A	N9-C4-C5	5.73	108.09	105.80
22	23S1	556	A	C8-N9-C4	5.73	108.09	105.80
22	23S1	1427	A	C8-N9-C4	5.73	108.09	105.80
22	23S1	2317	A	C5-C6-N1	5.73	120.57	117.70
1	16S1	1349	A	N3-C4-N9	5.73	131.98	127.40
22	23S1	432	A	N3-C4-N9	5.73	131.99	127.40
22	23S1	1378	A	C4-C5-N7	-5.73	107.83	110.70
22	23S1	1876	A	C4-C5-C6	5.73	119.86	117.00
22	23S1	2497	A	N9-C4-C5	5.73	108.09	105.80
22	23S1	2764	A	C4-C5-N7	-5.73	107.83	110.70
22	23S1	182	A	C5-C6-N1	5.73	120.56	117.70
22	23S1	1690	A	N3-C4-N9	5.73	131.98	127.40
22	23S1	1789	A	N9-C4-C5	5.73	108.09	105.80
1	16S1	282	A	N9-C4-C5	5.73	108.09	105.80
1	16S1	825	A	C8-N9-C4	5.73	108.09	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	352	A	C8-N9-C4	5.73	108.09	105.80
22	23S1	497	A	C4-C5-N7	-5.73	107.84	110.70
22	23S1	670	A	C4-C5-N7	-5.73	107.84	110.70
22	23S1	947	A	C8-N9-C4	5.73	108.09	105.80
22	23S1	2814	A	C8-N9-C4	5.73	108.09	105.80
22	23S1	2900	A	C5-C6-N1	5.73	120.56	117.70
22	23S1	28	A	N3-C4-N9	5.72	131.98	127.40
22	23S1	332	A	C8-N9-C4	5.72	108.09	105.80
22	23S1	1632	A	C4-C5-C6	5.72	119.86	117.00
22	23S1	1668	A	C4-C5-N7	-5.72	107.84	110.70
22	23S1	2117	A	C4-C5-N7	-5.72	107.84	110.70
22	23S1	2459	A	C5-C6-N1	5.72	120.56	117.70
23	05S1	78	A	N3-C4-N9	5.72	131.98	127.40
22	23S1	73	A	N9-C4-C5	5.72	108.09	105.80
22	23S1	111	A	C4-C5-N7	-5.72	107.84	110.70
22	23S1	706	A	N3-C4-N9	5.72	131.98	127.40
22	23S1	1247	A	N9-C4-C5	5.72	108.09	105.80
22	23S1	1365	A	N9-C4-C5	5.72	108.09	105.80
22	23S1	1384	A	N9-C4-C5	5.72	108.09	105.80
22	23S1	1616	A	N3-C4-N9	5.72	131.98	127.40
55	PTR1	59	A	C8-N9-C4	5.72	108.09	105.80
1	16S1	374	A	C4-C5-C6	5.72	119.86	117.00
22	23S1	1525	A	N9-C4-C5	5.72	108.09	105.80
22	23S1	2660	A	C4-C5-C6	5.72	119.86	117.00
1	16S1	364	A	C4-C5-C6	5.72	119.86	117.00
22	23S1	1032	A	C4-C5-N7	-5.72	107.84	110.70
22	23S1	1284	A	N9-C4-C5	5.72	108.09	105.80
22	23S1	1885	A	C8-N9-C4	5.72	108.09	105.80
1	16S1	766	A	C5-C6-N1	5.72	120.56	117.70
22	23S1	352	A	C4-C5-N7	-5.72	107.84	110.70
22	23S1	2013	A	N9-C4-C5	5.72	108.09	105.80
22	23S1	2435	A	C4-C5-N7	-5.72	107.84	110.70
22	23S1	2560	A	C5-C6-N1	5.72	120.56	117.70
22	23S1	2829	A	N9-C4-C5	5.72	108.09	105.80
1	16S1	535	A	C4-C5-C6	5.72	119.86	117.00
1	16S1	535	A	C8-N9-C4	5.72	108.09	105.80
1	16S1	1289	A	C4-C5-C6	5.72	119.86	117.00
1	16S1	1081	A	C5-C6-N1	5.71	120.56	117.70
1	16S1	1465	A	C5-C6-N1	5.71	120.56	117.70
22	23S1	84	A	N9-C4-C5	5.71	108.09	105.80
22	23S1	892	A	C5-C6-N1	5.71	120.56	117.70
22	23S1	1142	A	C4-C5-C6	5.71	119.86	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1876	A	N3-C4-N9	5.71	131.97	127.40
22	23S1	2095	A	C8-N9-C4	5.71	108.09	105.80
22	23S1	2314	A	C4-C5-C6	5.71	119.86	117.00
22	23S1	2378	A	C8-N9-C4	5.71	108.09	105.80
22	23S1	2800	A	C4-C5-C6	5.71	119.86	117.00
1	16S1	131	A	C4-C5-N7	-5.71	107.84	110.70
1	16S1	872	A	N9-C4-C5	5.71	108.08	105.80
22	23S1	1698	A	N3-C4-N9	5.71	131.97	127.40
22	23S1	2386	A	C4-C5-C6	5.71	119.86	117.00
1	16S1	533	A	C4-C5-N7	-5.71	107.84	110.70
22	23S1	515	A	N9-C4-C5	5.71	108.08	105.80
22	23S1	1580	A	C4-C5-N7	-5.71	107.84	110.70
22	23S1	1774	C	N1-C2-O2	5.71	122.33	118.90
22	23S1	2589	A	C8-N9-C4	5.71	108.08	105.80
22	23S1	2900	A	C8-N9-C4	5.71	108.08	105.80
1	16S1	815	A	C4-C5-N7	-5.71	107.84	110.70
1	16S1	1362	A	N3-C4-N9	5.71	131.97	127.40
1	16S1	1	A	C4-C5-C6	5.71	119.85	117.00
1	16S1	19	A	C4-C5-C6	5.71	119.85	117.00
1	16S1	262	A	C4-C5-C6	5.71	119.85	117.00
1	16S1	371	A	C4-C5-C6	5.71	119.85	117.00
1	16S1	1480	A	N3-C4-N9	5.71	131.97	127.40
22	23S1	118	A	C8-N9-C4	5.71	108.08	105.80
22	23S1	222	A	C4-C5-C6	5.71	119.85	117.00
22	23S1	613	A	C5-C6-N1	5.71	120.55	117.70
22	23S1	2381	A	C8-N9-C4	5.71	108.08	105.80
23	05S1	39	A	C8-N9-C4	5.71	108.08	105.80
1	16S1	938	A	N9-C4-C5	5.71	108.08	105.80
22	23S1	1342	A	N3-C4-N9	5.71	131.96	127.40
1	16S1	28	A	C5-C6-N1	5.70	120.55	117.70
22	23S1	172	A	C8-N9-C4	5.70	108.08	105.80
22	23S1	342	A	N3-C4-N9	5.70	131.96	127.40
22	23S1	1754	A	C8-N9-C4	5.70	108.08	105.80
22	23S1	2070	A	N3-C4-N9	5.70	131.96	127.40
22	23S1	2333	A	N3-C4-N9	5.70	131.96	127.40
22	23S1	2435	A	N9-C4-C5	5.70	108.08	105.80
23	05S1	39	A	C4-C5-C6	5.70	119.85	117.00
1	16S1	1080	A	N3-C4-N9	5.70	131.96	127.40
22	23S1	626	A	C4-C5-C6	5.70	119.85	117.00
22	23S1	1359	A	C8-N9-C4	5.70	108.08	105.80
1	16S1	10	A	C5-C6-N1	5.70	120.55	117.70
1	16S1	831	A	N3-C4-N9	5.70	131.96	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1019	A	N9-C4-C5	5.70	108.08	105.80
22	23S1	74	A	C5-C6-N1	5.70	120.55	117.70
22	23S1	311	A	C4-C5-C6	5.70	119.85	117.00
22	23S1	1336	A	C5-C6-N1	5.70	120.55	117.70
23	05S1	39	A	N3-C4-N9	5.70	131.96	127.40
1	16S1	190	A	C6-C5-N7	-5.70	128.31	132.30
1	16S1	1441	A	N3-C4-N9	5.70	131.96	127.40
22	23S1	432	A	C4-C5-N7	-5.70	107.85	110.70
22	23S1	503	A	N9-C4-C5	5.70	108.08	105.80
22	23S1	722	A	C5-C6-N1	5.70	120.55	117.70
22	23S1	1156	A	C8-N9-C4	5.70	108.08	105.80
22	23S1	1505	A	N3-C4-N9	5.70	131.96	127.40
22	23S1	2516	A	C8-N9-C4	5.70	108.08	105.80
1	16S1	608	A	C5-C6-N1	5.70	120.55	117.70
22	23S1	983	A	C8-N9-C4	5.70	108.08	105.80
22	23S1	878	A	N3-C4-N9	5.70	131.96	127.40
22	23S1	1147	A	C4-C5-C6	5.70	119.85	117.00
22	23S1	1287	A	C4-C5-C6	5.70	119.85	117.00
1	16S1	915	A	N9-C4-C5	5.69	108.08	105.80
1	16S1	1157	A	C8-N9-C4	5.69	108.08	105.80
1	16S1	1248	A	C4-C5-N7	-5.69	107.85	110.70
1	16S1	1396	A	C8-N9-C4	5.69	108.08	105.80
22	23S1	6	A	C5-C6-N1	5.69	120.55	117.70
22	23S1	104	A	N3-C4-N9	5.69	131.95	127.40
22	23S1	878	A	C8-N9-C4	5.69	108.08	105.80
22	23S1	1008	A	C8-N9-C4	5.69	108.08	105.80
22	23S1	1205	A	C4-C5-N7	-5.69	107.85	110.70
22	23S1	2003	A	C4-C5-C6	5.69	119.85	117.00
22	23S1	2541	A	N9-C4-C5	5.69	108.08	105.80
1	16S1	65	A	C4-C5-C6	5.69	119.84	117.00
1	16S1	1081	A	C8-N9-C4	5.69	108.08	105.80
1	16S1	1196	A	C4-C5-C6	5.69	119.84	117.00
1	16S1	1534	A	C4-C5-C6	5.69	119.84	117.00
22	23S1	287	G	N1-C6-O6	5.69	123.31	119.90
22	23S1	727	A	C4-C5-C6	5.69	119.84	117.00
22	23S1	1005	C	N3-C2-O2	-5.69	117.92	121.90
22	23S1	1067	A	N3-C4-N9	5.69	131.95	127.40
22	23S1	1762	A	N9-C4-C5	5.69	108.08	105.80
22	23S1	1805	A	C5-C6-N1	5.69	120.55	117.70
1	16S1	19	A	C4-C5-N7	-5.69	107.86	110.70
1	16S1	563	A	C5-C6-N1	5.69	120.55	117.70
22	23S1	449	A	C4-C5-N7	-5.69	107.86	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	548	G	N3-C4-C5	-5.69	125.76	128.60
22	23S1	1700	A	C4-C5-N7	-5.69	107.86	110.70
1	16S1	306	A	N9-C4-C5	5.69	108.08	105.80
1	16S1	618	C	N3-C2-O2	-5.69	117.92	121.90
22	23S1	226	A	C4-C5-C6	5.69	119.84	117.00
22	23S1	592	A	C4-C5-C6	5.69	119.84	117.00
22	23S1	2354	C	N1-C2-O2	5.69	122.31	118.90
22	23S1	2031	A	C8-N9-C4	5.69	108.07	105.80
22	23S1	2119	A	N3-C4-N9	5.69	131.95	127.40
22	23S1	2764	A	C8-N9-C4	5.69	108.07	105.80
1	16S1	58	C	C6-N1-C2	-5.68	118.03	120.30
22	23S1	104	A	C4-C5-N7	-5.68	107.86	110.70
22	23S1	637	A	C8-N9-C4	5.68	108.07	105.80
22	23S1	1069	A	N3-C4-N9	5.68	131.95	127.40
22	23S1	1928	A	C4-C5-N7	-5.68	107.86	110.70
22	23S1	2835	A	N9-C4-C5	5.68	108.07	105.80
1	16S1	120	A	C4-C5-C6	5.68	119.84	117.00
1	16S1	595	A	C8-N9-C4	5.68	108.07	105.80
22	23S1	89	A	C4-C5-C6	5.68	119.84	117.00
22	23S1	590	A	C5-C6-N1	5.68	120.54	117.70
22	23S1	1040	A	C8-N9-C4	5.68	108.07	105.80
22	23S1	1169	A	C8-N9-C4	5.68	108.07	105.80
22	23S1	1253	A	C5-N7-C8	5.68	106.74	103.90
22	23S1	1453	A	C8-N9-C4	5.68	108.07	105.80
22	23S1	2675	A	C4-C5-C6	5.68	119.84	117.00
22	23S1	2675	A	C5-C6-N1	5.68	120.54	117.70
22	23S1	602	A	C4-C5-C6	5.68	119.84	117.00
22	23S1	1677	A	C4-C5-C6	5.68	119.84	117.00
22	23S1	1705	A	C5-C6-N1	5.68	120.54	117.70
22	23S1	2682	A	N3-C4-N9	5.68	131.94	127.40
1	16S1	152	A	C5-C6-N1	5.68	120.54	117.70
22	23S1	897	C	N1-C2-O2	5.68	122.31	118.90
22	23S1	2441	U	N3-C2-O2	-5.68	118.22	122.20
22	23S1	2635	A	C5-C6-N1	5.68	120.54	117.70
22	23S1	2711	A	C4-C5-N7	-5.68	107.86	110.70
22	23S1	2837	A	C5-C6-N1	5.68	120.54	117.70
1	16S1	553	A	N9-C4-C5	5.68	108.07	105.80
22	23S1	877	A	N3-C4-N9	5.68	131.94	127.40
22	23S1	1504	A	C8-N9-C4	5.68	108.07	105.80
1	16S1	4	U	C2-N1-C1'	-5.68	110.89	117.70
1	16S1	336	A	N3-C4-N9	5.68	131.94	127.40
1	16S1	338	A	C4-C5-C6	5.68	119.84	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	958	A	C5-C6-N1	5.68	120.54	117.70
1	16S1	1503	A	C4-C5-N7	-5.68	107.86	110.70
22	23S1	1871	A	C8-N9-C4	5.68	108.07	105.80
22	23S1	2073	C	C6-N1-C2	-5.68	118.03	120.30
22	23S1	2577	A	N3-C4-N9	5.68	131.94	127.40
22	23S1	2778	A	C8-N9-C4	5.68	108.07	105.80
1	16S1	129	A	C4-C5-C6	5.67	119.84	117.00
1	16S1	1428	A	C5-C6-N1	5.67	120.54	117.70
22	23S1	196	A	C4-C5-N7	-5.67	107.86	110.70
22	23S1	909	A	C4-C5-C6	5.67	119.84	117.00
22	23S1	1593	A	C8-N9-C4	5.67	108.07	105.80
22	23S1	1597	A	N3-C4-N9	5.67	131.94	127.40
22	23S1	1254	A	N3-C4-N9	5.67	131.94	127.40
1	16S1	802	A	N3-C4-N9	5.67	131.94	127.40
22	23S1	14	A	N9-C4-C5	5.67	108.07	105.80
22	23S1	103	A	C4-C5-N7	-5.67	107.86	110.70
22	23S1	262	A	C5-C6-N1	5.67	120.54	117.70
22	23S1	2090	A	C5-C6-N1	5.67	120.54	117.70
22	23S1	2288	A	C4-C5-C6	5.67	119.84	117.00
22	23S1	2734	A	C5-C6-N1	5.67	120.54	117.70
1	16S1	98	A	C5-C6-N1	5.67	120.53	117.70
1	16S1	749	A	C8-N9-C4	5.67	108.07	105.80
22	23S1	28	A	C8-N9-C4	5.67	108.07	105.80
22	23S1	1285	A	C4-C5-C6	5.67	119.83	117.00
1	16S1	681	A	C5-C6-N1	5.67	120.53	117.70
22	23S1	632	A	C4-C5-C6	5.67	119.83	117.00
1	16S1	238	A	C8-N9-C4	5.67	108.07	105.80
1	16S1	729	A	N9-C4-C5	5.67	108.07	105.80
22	23S1	626	A	N9-C4-C5	5.67	108.07	105.80
22	23S1	918	A	N3-C4-N9	5.67	131.93	127.40
22	23S1	1151	A	C4-C5-C6	5.67	119.83	117.00
22	23S1	1678	A	C4-C5-C6	5.67	119.83	117.00
22	23S1	1794	A	N9-C4-C5	5.67	108.07	105.80
1	16S1	139	A	C4-C5-C6	5.66	119.83	117.00
1	16S1	553	A	C4-C5-C6	5.66	119.83	117.00
1	16S1	1111	A	N9-C4-C5	5.66	108.06	105.80
1	16S1	1346	A	N9-C4-C5	5.66	108.07	105.80
22	23S1	152	A	C5-C6-N1	5.66	120.53	117.70
22	23S1	226	A	N3-C4-N9	5.66	131.93	127.40
22	23S1	505	A	N3-C4-N9	5.66	131.93	127.40
22	23S1	643	A	N3-C4-N9	5.66	131.93	127.40
22	23S1	743	A	C5-C6-N1	5.66	120.53	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	910	A	N9-C4-C5	5.66	108.06	105.80
22	23S1	1050	A	C4-C5-N7	-5.66	107.87	110.70
22	23S1	1156	A	N3-C4-N9	5.66	131.93	127.40
22	23S1	670	A	N3-C4-N9	5.66	131.93	127.40
1	16S1	169	C	C5-C4-N4	5.66	124.16	120.20
1	16S1	915	A	C8-N9-C4	5.66	108.06	105.80
22	23S1	1328	A	C4-C5-C6	5.66	119.83	117.00
22	23S1	497	A	C4-C5-C6	5.66	119.83	117.00
22	23S1	505	A	N9-C4-C5	5.66	108.06	105.80
22	23S1	2670	A	C5-C6-N1	5.66	120.53	117.70
22	23S1	219	A	C4-C5-C6	5.66	119.83	117.00
1	16S1	949	A	N9-C4-C5	5.66	108.06	105.80
1	16S1	1431	A	C4-C5-C6	5.66	119.83	117.00
22	23S1	19	A	C5-C6-N1	5.66	120.53	117.70
22	23S1	1010	A	N9-C4-C5	5.66	108.06	105.80
22	23S1	1566	A	N3-C4-N9	5.66	131.92	127.40
1	16S1	120	A	N3-C4-N9	5.65	131.92	127.40
1	16S1	143	A	N9-C4-C5	5.65	108.06	105.80
1	16S1	415	A	N9-C4-C5	5.65	108.06	105.80
1	16S1	1150	A	N3-C4-N9	5.65	131.92	127.40
22	23S1	104	A	C8-N9-C4	5.65	108.06	105.80
22	23S1	1260	A	C5-C6-N1	5.65	120.53	117.70
1	16S1	437	U	N3-C2-O2	-5.65	118.24	122.20
1	16S1	468	A	N3-C4-N9	5.65	131.92	127.40
22	23S1	204	A	C4-C5-N7	-5.65	107.87	110.70
22	23S1	262	A	N3-C4-N9	5.65	131.92	127.40
22	23S1	309	A	N9-C4-C5	5.65	108.06	105.80
22	23S1	1057	A	N3-C4-N9	5.65	131.92	127.40
22	23S1	2741	A	C4-C5-C6	5.65	119.83	117.00
22	23S1	227	A	C4-C5-C6	5.65	119.83	117.00
22	23S1	896	A	C4-C5-N7	-5.65	107.88	110.70
22	23S1	1359	A	C5-C6-N1	5.65	120.53	117.70
22	23S1	1544	A	C4-C5-N7	-5.65	107.87	110.70
22	23S1	2268	A	N9-C4-C5	5.65	108.06	105.80
22	23S1	2322	A	C5-C6-N1	5.65	120.53	117.70
22	23S1	2376	A	N3-C4-N9	5.65	131.92	127.40
22	23S1	2750	A	N3-C4-N9	5.65	131.92	127.40
22	23S1	715	A	N3-C4-N9	5.65	131.92	127.40
22	23S1	1264	A	N3-C4-N9	5.65	131.92	127.40
22	23S1	1900	A	C4-C5-C6	5.65	119.83	117.00
1	16S1	687	A	C4-C5-C6	5.65	119.82	117.00
1	16S1	1111	A	N3-C4-N9	5.65	131.92	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	959	A	N9-C4-C5	5.65	108.06	105.80
22	23S1	1413	A	C4-C5-C6	5.65	119.82	117.00
22	23S1	2009	A	N3-C4-N9	5.65	131.92	127.40
23	05S1	94	A	C5-C6-N1	5.65	120.52	117.70
22	23S1	529	A	C5-C6-N1	5.65	120.52	117.70
22	23S1	2297	A	N3-C4-N9	5.65	131.92	127.40
1	16S1	19	A	N9-C4-C5	5.64	108.06	105.80
1	16S1	747	A	N3-C4-N9	5.64	131.91	127.40
22	23S1	42	A	C8-N9-C4	5.64	108.06	105.80
22	23S1	279	A	C8-N9-C4	5.64	108.06	105.80
22	23S1	1096	A	C4-C5-C6	5.64	119.82	117.00
22	23S1	1301	A	C5-C6-N1	5.64	120.52	117.70
22	23S1	1453	A	N3-C4-N9	5.64	131.92	127.40
22	23S1	1889	A	C4-C5-C6	5.64	119.82	117.00
22	23S1	2281	A	C8-N9-C4	5.64	108.06	105.80
22	23S1	2333	A	C4-C5-C6	5.64	119.82	117.00
22	23S1	2333	A	C8-N9-C4	5.64	108.06	105.80
22	23S1	2560	A	N9-C4-C5	5.64	108.06	105.80
1	16S1	223	A	C8-N9-C4	5.64	108.06	105.80
1	16S1	767	A	N9-C4-C5	5.64	108.06	105.80
22	23S1	1593	A	C5-C6-N1	5.64	120.52	117.70
22	23S1	1918	A	C5-C6-N1	5.64	120.52	117.70
22	23S1	2059	A	C8-N9-C4	5.64	108.06	105.80
22	23S1	2632	A	C4-C5-C6	5.64	119.82	117.00
1	16S1	3	A	C8-N9-C4	5.64	108.06	105.80
1	16S1	681	A	N9-C4-C5	5.64	108.06	105.80
1	16S1	787	A	C8-N9-C4	5.64	108.06	105.80
22	23S1	1000	A	C4-C5-N7	-5.64	107.88	110.70
22	23S1	1393	A	N3-C4-N9	5.64	131.91	127.40
22	23S1	1502	A	C5-C6-N1	5.64	120.52	117.70
1	16S1	101	A	C5-C6-N1	5.64	120.52	117.70
22	23S1	1786	A	N9-C4-C5	5.64	108.06	105.80
22	23S1	2534	A	C8-N9-C4	5.64	108.06	105.80
22	23S1	2654	A	N3-C4-N9	5.64	131.91	127.40
22	23S1	2734	A	N3-C4-N9	5.64	131.91	127.40
55	PTR1	38	A	C5-C6-N1	5.64	120.52	117.70
1	16S1	468	A	N9-C4-C5	5.64	108.06	105.80
22	23S1	1237	A	N3-C4-N9	5.64	131.91	127.40
23	05S1	50	A	C8-N9-C4	5.64	108.06	105.80
1	16S1	149	A	N3-C4-N9	5.64	131.91	127.40
1	16S1	374	A	C4-C5-N7	-5.64	107.88	110.70
1	16S1	432	A	N9-C4-C5	5.64	108.06	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2227	A	N9-C4-C5	5.64	108.05	105.80
22	23S1	2781	A	N9-C4-C5	5.64	108.06	105.80
1	16S1	151	A	N3-C4-N9	5.63	131.91	127.40
1	16S1	223	A	C4-C5-N7	-5.63	107.88	110.70
1	16S1	622	A	C5-N7-C8	5.63	106.72	103.90
1	16S1	1036	A	N9-C4-C5	5.63	108.05	105.80
1	16S1	1151	A	C4-C5-N7	-5.63	107.88	110.70
22	23S1	63	A	C4-C5-C6	5.63	119.82	117.00
22	23S1	1067	A	C4-C5-N7	-5.63	107.88	110.70
23	05S1	52	A	C4-C5-C6	5.63	119.82	117.00
55	PTR1	38	A	C8-N9-C4	5.63	108.05	105.80
1	16S1	493	A	N9-C4-C5	5.63	108.05	105.80
22	23S1	1008	A	C4-C5-C6	5.63	119.82	117.00
22	23S1	1342	A	C4-C5-N7	-5.63	107.88	110.70
22	23S1	1791	A	N9-C4-C5	5.63	108.05	105.80
1	16S1	572	A	C4-C5-N7	-5.63	107.89	110.70
1	16S1	1433	A	N3-C4-N9	5.63	131.90	127.40
22	23S1	103	A	N9-C4-C5	5.63	108.05	105.80
22	23S1	152	A	C8-N9-C4	5.63	108.05	105.80
22	23S1	412	A	C4-C5-C6	5.63	119.82	117.00
22	23S1	2009	A	C8-N9-C4	5.63	108.05	105.80
22	23S1	2071	A	C5-C6-N1	5.63	120.52	117.70
1	16S1	389	A	N9-C4-C5	5.63	108.05	105.80
1	16S1	1000	A	C8-N9-C4	5.63	108.05	105.80
22	23S1	223	A	C4-C5-C6	5.63	119.81	117.00
22	23S1	973	A	C5-N7-C8	5.63	106.72	103.90
55	PTR1	69	A	C8-N9-C4	5.63	108.05	105.80
1	16S1	495	A	C4-C5-C6	5.63	119.81	117.00
1	16S1	1480	A	C4-C5-N7	-5.63	107.89	110.70
22	23S1	71	A	C5-C6-N1	5.63	120.51	117.70
22	23S1	1789	A	C4-C5-N7	-5.63	107.89	110.70
22	23S1	2317	A	C4-C5-N7	-5.63	107.89	110.70
55	PTR1	42	A	C5-C6-N1	5.63	120.52	117.70
1	16S1	282	A	C5-C6-N1	5.63	120.51	117.70
1	16S1	825	A	C5-C6-N1	5.63	120.51	117.70
22	23S1	52	A	C8-N9-C4	5.63	108.05	105.80
22	23S1	802	A	C4-C5-C6	5.63	119.81	117.00
22	23S1	1890	A	C4-C5-N7	-5.63	107.89	110.70
22	23S1	2562	U	N3-C2-O2	-5.63	118.26	122.20
22	23S1	415	A	C5-C6-N1	5.62	120.51	117.70
22	23S1	743	A	N9-C4-C5	5.62	108.05	105.80
22	23S1	878	A	C5-C6-N1	5.62	120.51	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	777	A	N9-C4-C5	5.62	108.05	105.80
1	16S1	1082	A	N9-C4-C5	5.62	108.05	105.80
1	16S1	1429	A	C8-N9-C4	5.62	108.05	105.80
22	23S1	925	A	C4-C5-C6	5.62	119.81	117.00
22	23S1	928	A	N9-C4-C5	5.62	108.05	105.80
22	23S1	1596	A	C8-N9-C4	5.62	108.05	105.80
22	23S1	2792	A	C8-N9-C4	5.62	108.05	105.80
1	16S1	781	A	C4-C5-N7	-5.62	107.89	110.70
22	23S1	1509	A	C4-C5-C6	5.62	119.81	117.00
22	23S1	1585	C	C5-C6-N1	5.62	123.81	121.00
1	16S1	59	A	C4-C5-C6	5.62	119.81	117.00
1	16S1	309	A	C4-C5-N7	-5.62	107.89	110.70
22	23S1	721	A	C8-N9-C4	5.62	108.05	105.80
22	23S1	2433	A	N9-C4-C5	5.62	108.05	105.80
22	23S1	2577	A	N9-C4-C5	5.62	108.05	105.80
1	16S1	1362	A	C4-C5-C6	5.62	119.81	117.00
22	23S1	1698	A	C4-C5-C6	5.62	119.81	117.00
1	16S1	3	A	N9-C4-C5	5.62	108.05	105.80
1	16S1	336	A	C4-C5-C6	5.62	119.81	117.00
1	16S1	579	A	C5-C6-N1	5.62	120.51	117.70
1	16S1	790	A	C5-C6-N1	5.62	120.51	117.70
22	23S1	218	A	N9-C4-C5	5.62	108.05	105.80
22	23S1	928	A	C5-C6-N1	5.62	120.51	117.70
22	23S1	1032	A	N9-C4-C5	5.62	108.05	105.80
22	23S1	1431	A	C5-C6-N1	5.62	120.51	117.70
1	16S1	573	A	N9-C4-C5	5.61	108.05	105.80
1	16S1	1476	A	C5-C6-N1	5.61	120.51	117.70
22	23S1	323	C	C2-N1-C1'	5.61	124.97	118.80
22	23S1	2317	A	C8-N9-C4	5.61	108.05	105.80
22	23S1	2590	A	N9-C4-C5	5.61	108.05	105.80
22	23S1	2602	A	C4-C5-C6	5.61	119.81	117.00
1	16S1	1250	A	N3-C4-N9	5.61	131.89	127.40
1	16S1	1398	A	C4-C5-C6	5.61	119.81	117.00
22	23S1	945	A	C4-C5-C6	5.61	119.81	117.00
22	23S1	2721	A	C8-N9-C4	5.61	108.05	105.80
22	23S1	2748	A	N3-C4-N9	5.61	131.89	127.40
22	23S1	2882	A	C8-N9-C4	5.61	108.05	105.80
23	05S1	50	A	C5-C6-N1	5.61	120.51	117.70
1	16S1	1408	A	C8-N9-C4	5.61	108.04	105.80
22	23S1	213	A	C5-C6-N1	5.61	120.50	117.70
22	23S1	715	A	C4-C5-C6	5.61	119.81	117.00
22	23S1	1551	A	N9-C4-C5	5.61	108.04	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1626	A	C8-N9-C4	5.61	108.04	105.80
22	23S1	1772	A	N3-C4-N9	5.61	131.89	127.40
22	23S1	2101	A	N3-C4-N9	5.61	131.89	127.40
22	23S1	2354	C	N3-C2-O2	-5.61	117.97	121.90
1	16S1	974	A	C8-N9-C4	5.61	108.04	105.80
22	23S1	1226	A	N9-C4-C5	5.61	108.04	105.80
1	16S1	509	A	C5-C6-N1	5.61	120.50	117.70
1	16S1	768	A	N9-C4-C5	5.61	108.04	105.80
1	16S1	969	A	C4-C5-C6	5.61	119.80	117.00
1	16S1	1250	A	C4-C5-C6	5.61	119.80	117.00
1	16S1	1408	A	N9-C4-C5	5.61	108.04	105.80
1	16S1	1493	A	C4-C5-C6	5.61	119.80	117.00
22	23S1	1927	A	C4-C5-C6	5.61	119.80	117.00
1	16S1	160	A	N3-C4-N9	5.61	131.88	127.40
1	16S1	459	A	C5-C6-N1	5.61	120.50	117.70
1	16S1	1311	A	C5-C6-N1	5.61	120.50	117.70
22	23S1	199	A	N3-C4-N9	5.61	131.88	127.40
22	23S1	382	A	C8-N9-C4	5.61	108.04	105.80
22	23S1	599	A	C5-C6-N1	5.61	120.50	117.70
22	23S1	1067	A	C4-C5-C6	5.61	119.80	117.00
22	23S1	1655	A	C8-N9-C4	5.61	108.04	105.80
22	23S1	1759	A	C5-C6-N1	5.61	120.50	117.70
1	16S1	996	A	C5-C6-N1	5.60	120.50	117.70
22	23S1	222	A	C5-C6-N1	5.60	120.50	117.70
22	23S1	1640	A	C8-N9-C4	5.60	108.04	105.80
22	23S1	56	A	C5-C6-N1	5.60	120.50	117.70
22	23S1	345	A	C4-C5-N7	-5.60	107.90	110.70
22	23S1	1040	A	C5-C6-N1	5.60	120.50	117.70
22	23S1	1169	A	C5-C6-N1	5.60	120.50	117.70
22	23S1	1545	A	C4-C5-N7	-5.60	107.90	110.70
22	23S1	2700	A	C5-C6-N1	5.60	120.50	117.70
22	23S1	347	A	C4-C5-N7	-5.60	107.90	110.70
22	23S1	497	A	C8-N9-C4	5.60	108.04	105.80
1	16S1	1172	C	N3-C2-O2	-5.60	117.98	121.90
22	23S1	1525	A	N3-C4-N9	5.60	131.88	127.40
22	23S1	1678	A	N3-C4-N9	5.60	131.88	127.40
22	23S1	1805	A	C4-C5-C6	5.60	119.80	117.00
22	23S1	2184	A	N9-C4-C5	5.60	108.04	105.80
1	16S1	1429	A	C5-C6-N1	5.60	120.50	117.70
1	16S1	1437	A	C8-N9-C4	5.60	108.04	105.80
22	23S1	829	A	N3-C4-N9	5.60	131.88	127.40
22	23S1	1247	A	N3-C4-N9	5.60	131.88	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	792	A	C4-C5-N7	-5.60	107.90	110.70
1	16S1	1406	U	C2-N3-C4	-5.60	123.64	127.00
1	16S1	10	A	C4-C5-N7	-5.59	107.90	110.70
1	16S1	195	A	C5-C6-N1	5.59	120.50	117.70
1	16S1	1236	A	C5-C6-N1	5.59	120.50	117.70
22	23S1	91	A	N3-C4-N9	5.59	131.88	127.40
22	23S1	586	A	N9-C4-C5	5.59	108.04	105.80
22	23S1	613	A	N9-C4-C5	5.59	108.04	105.80
22	23S1	706	A	C5-C6-N1	5.59	120.50	117.70
22	23S1	789	A	C5-C6-N1	5.59	120.50	117.70
22	23S1	2412	A	C4-C5-N7	-5.59	107.90	110.70
22	23S1	2837	A	C4-C5-C6	5.59	119.80	117.00
1	16S1	915	A	C4-C5-N7	-5.59	107.90	110.70
22	23S1	2031	A	C5-C6-N1	5.59	120.50	117.70
22	23S1	2880	C	N3-C2-O2	-5.59	117.98	121.90
23	05S1	46	A	N9-C4-C5	5.59	108.04	105.80
1	16S1	869	G	N1-C6-O6	-5.59	116.55	119.90
22	23S1	1134	A	N3-C4-N9	5.59	131.87	127.40
22	23S1	1548	A	C5-C6-N1	5.59	120.50	117.70
22	23S1	1551	A	C5-C6-N1	5.59	120.50	117.70
22	23S1	2837	A	C8-N9-C4	5.59	108.04	105.80
1	16S1	648	A	C5-C6-N1	5.59	120.50	117.70
1	16S1	687	A	N3-C4-N9	5.59	131.87	127.40
1	16S1	706	A	C5-C6-N1	5.59	120.49	117.70
22	23S1	272	A	C5-C6-N1	5.59	120.50	117.70
22	23S1	311	A	N3-C4-N9	5.59	131.87	127.40
22	23S1	1189	A	C8-N9-C4	5.59	108.04	105.80
22	23S1	2860	A	N3-C4-N9	5.59	131.87	127.40
23	05S1	78	A	C4-C5-N7	-5.59	107.91	110.70
50	L341	44	VAL	CA-CB-CG2	5.59	119.28	110.90
1	16S1	1021	A	C8-N9-C4	5.59	108.03	105.80
22	23S1	983	A	N3-C4-N9	5.59	131.87	127.40
22	23S1	2241	A	C4-C5-N7	-5.59	107.91	110.70
1	16S1	263	A	N9-C4-C5	5.59	108.03	105.80
1	16S1	1111	A	C4-C5-C6	5.59	119.79	117.00
22	23S1	1378	A	N9-C4-C5	5.59	108.03	105.80
1	16S1	487	A	N9-C4-C5	5.58	108.03	105.80
1	16S1	918	A	C4-C5-N7	-5.58	107.91	110.70
22	23S1	144	A	C5-C6-N1	5.58	120.49	117.70
22	23S1	984	A	C5-C6-N1	5.58	120.49	117.70
23	05S1	52	A	C8-N9-C4	5.58	108.03	105.80
1	16S1	716	A	C4-C5-C6	5.58	119.79	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	768	A	N3-C4-N9	5.58	131.87	127.40
22	23S1	644	A	C8-N9-C4	5.58	108.03	105.80
22	23S1	734	A	C4-C5-C6	5.58	119.79	117.00
22	23S1	988	A	N9-C4-C5	5.58	108.03	105.80
22	23S1	1165	A	N3-C4-N9	5.58	131.87	127.40
22	23S1	1632	A	C4-C5-N7	-5.58	107.91	110.70
22	23S1	2005	A	N9-C4-C5	5.58	108.03	105.80
22	23S1	2147	A	C4-C5-C6	5.58	119.79	117.00
22	23S1	2654	A	C4-C5-C6	5.58	119.79	117.00
22	23S1	2758	A	C8-N9-C4	5.58	108.03	105.80
23	05S1	99	A	C4-C5-C6	5.58	119.79	117.00
23	05S1	119	A	C4-C5-N7	-5.58	107.91	110.70
1	16S1	1197	A	C8-N9-C4	5.58	108.03	105.80
22	23S1	637	A	N9-C4-C5	5.58	108.03	105.80
22	23S1	2162	G	OP1-P-O3'	5.58	117.48	105.20
22	23S1	2381	A	C4-C5-C6	5.58	119.79	117.00
23	05S1	34	A	C8-N9-C4	5.58	108.03	105.80
1	16S1	1	A	N9-C4-C5	5.58	108.03	105.80
1	16S1	1035	A	N9-C4-C5	5.58	108.03	105.80
22	23S1	348	A	C5-C6-N1	5.58	120.49	117.70
22	23S1	2478	A	C5-C6-N1	5.58	120.49	117.70
1	16S1	72	A	C4-C5-C6	5.58	119.79	117.00
1	16S1	374	A	N9-C4-C5	5.58	108.03	105.80
1	16S1	1410	A	C4-C5-N7	-5.58	107.91	110.70
22	23S1	354	A	C8-N9-C4	5.58	108.03	105.80
22	23S1	432	A	C4-C5-C6	5.58	119.79	117.00
22	23S1	1398	C	N1-C2-O2	5.58	122.25	118.90
22	23S1	1730	C	C6-N1-C1'	-5.58	114.11	120.80
23	05S1	78	A	C4-C5-C6	5.58	119.79	117.00
1	16S1	119	A	C4-C5-C6	5.58	119.79	117.00
1	16S1	338	A	N3-C4-N9	5.58	131.86	127.40
1	16S1	393	A	C8-N9-C4	5.58	108.03	105.80
22	23S1	1853	A	N3-C4-N9	5.58	131.86	127.40
1	16S1	572	A	N3-C4-N9	5.58	131.86	127.40
1	16S1	845	A	N3-C4-N9	5.58	131.86	127.40
22	23S1	936	A	C5-C6-N1	5.58	120.49	117.70
22	23S1	1269	A	C4-C5-N7	-5.58	107.91	110.70
22	23S1	2705	A	N3-C4-N9	5.58	131.86	127.40
22	23S1	2882	A	C4-C5-N7	-5.58	107.91	110.70
1	16S1	574	A	C4-C5-C6	5.57	119.79	117.00
22	23S1	412	A	C5-C6-N1	5.57	120.49	117.70
22	23S1	1744	A	N9-C4-C5	5.57	108.03	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1784	A	N3-C4-N9	5.57	131.86	127.40
22	23S1	2820	A	C5-C6-N1	5.57	120.49	117.70
1	16S1	969	A	C4-C5-N7	-5.57	107.91	110.70
1	16S1	1145	A	N9-C4-C5	5.57	108.03	105.80
22	23S1	104	A	N9-C4-C5	5.57	108.03	105.80
22	23S1	927	A	N9-C4-C5	5.57	108.03	105.80
22	23S1	1590	A	C5-C6-N1	5.57	120.49	117.70
1	16S1	19	A	C8-N9-C4	5.57	108.03	105.80
1	16S1	195	A	C5-N7-C8	5.57	106.69	103.90
1	16S1	1396	A	C5-C6-N1	5.57	120.48	117.70
22	23S1	91	A	C4-C5-C6	5.57	119.78	117.00
22	23S1	111	A	N3-C4-N9	5.57	131.86	127.40
22	23S1	1142	A	C8-N9-C4	5.57	108.03	105.80
22	23S1	1265	A	N9-C4-C5	5.57	108.03	105.80
22	23S1	1453	A	N9-C4-C5	5.57	108.03	105.80
22	23S1	2270	A	N3-C4-N9	5.57	131.86	127.40
22	23S1	2587	A	N3-C4-N9	5.57	131.86	127.40
22	23S1	2654	A	C8-N9-C4	5.57	108.03	105.80
1	16S1	1229	A	C4-C5-N7	-5.57	107.92	110.70
22	23S1	718	A	C8-N9-C4	5.57	108.03	105.80
22	23S1	2070	A	C5-C6-N1	5.57	120.48	117.70
1	16S1	189	A	N9-C4-C5	5.57	108.03	105.80
1	16S1	1251	A	C4-C5-C6	5.57	119.78	117.00
1	16S1	1329	A	C4-C5-C6	5.57	119.78	117.00
1	16S1	1428	A	C4-C5-C6	5.57	119.78	117.00
22	23S1	223	A	N3-C4-N9	5.57	131.85	127.40
22	23S1	502	A	C4-C5-N7	-5.57	107.92	110.70
22	23S1	899	A	N9-C4-C5	5.57	108.03	105.80
22	23S1	1088	A	C4-C5-N7	-5.57	107.92	110.70
22	23S1	1652	A	C4-C5-N7	-5.57	107.92	110.70
22	23S1	1960	A	C5-C6-N1	5.57	120.48	117.70
22	23S1	2577	A	C4-C5-N7	-5.57	107.92	110.70
22	23S1	2776	A	C4-C5-N7	-5.57	107.92	110.70
23	05S1	66	A	N3-C4-N9	5.57	131.85	127.40
1	16S1	1117	A	C8-N9-C4	5.57	108.03	105.80
22	23S1	345	A	C5-C6-N1	5.57	120.48	117.70
22	23S1	480	A	C4-C5-N7	-5.57	107.92	110.70
22	23S1	1966	A	C4-C5-C6	5.57	119.78	117.00
22	23S1	2266	A	C8-N9-C4	5.57	108.03	105.80
22	23S1	2821	A	C8-N9-C4	5.57	108.03	105.80
1	16S1	309	A	C5-C6-N1	5.56	120.48	117.70
1	16S1	325	A	N9-C4-C5	5.56	108.03	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	415	A	C8-N9-C4	5.56	108.03	105.80
22	23S1	928	A	N3-C4-N9	5.56	131.85	127.40
22	23S1	1384	A	N3-C4-N9	5.56	131.85	127.40
22	23S1	2212	A	N3-C4-N9	5.56	131.85	127.40
22	23S1	2882	A	C5-C6-N1	5.56	120.48	117.70
1	16S1	1150	A	C8-N9-C4	5.56	108.02	105.80
22	23S1	2082	A	C5-C6-N1	5.56	120.48	117.70
22	23S1	2314	A	C8-N9-C4	5.56	108.02	105.80
1	16S1	792	A	C4-C5-C6	5.56	119.78	117.00
22	23S1	1039	A	C4-C5-N7	-5.56	107.92	110.70
22	23S1	1046	A	N3-C4-N9	5.56	131.85	127.40
22	23S1	1439	A	N9-C4-C5	5.56	108.02	105.80
22	23S1	1569	A	C5-C6-N1	5.56	120.48	117.70
22	23S1	2189	U	P-O3'-C3'	5.56	126.37	119.70
1	16S1	1261	A	C5-C6-N1	5.56	120.48	117.70
22	23S1	990	A	C4-C5-C6	5.56	119.78	117.00
22	23S1	1133	A	C8-N9-C4	5.56	108.02	105.80
22	23S1	1144	A	C5-C6-N1	5.56	120.48	117.70
22	23S1	1304	A	C4-C5-C6	5.56	119.78	117.00
22	23S1	1347	A	C4-C5-N7	-5.56	107.92	110.70
22	23S1	1384	A	C4-C5-C6	5.56	119.78	117.00
22	23S1	1609	A	C8-N9-C4	5.56	108.02	105.80
22	23S1	2632	A	N3-C4-N9	5.56	131.85	127.40
22	23S1	347	A	N3-C4-N9	5.56	131.84	127.40
23	05S1	108	A	C5-C6-N1	5.56	120.48	117.70
1	16S1	1019	A	C5-C6-N1	5.55	120.48	117.70
1	16S1	1285	A	N3-C4-N9	5.55	131.84	127.40
22	23S1	1080	A	C4-C5-C6	5.55	119.78	117.00
22	23S1	1427	A	N9-C4-C5	5.55	108.02	105.80
22	23S1	2080	A	C5-C6-N1	5.55	120.48	117.70
23	05S1	45	A	C4-C5-C6	5.55	119.78	117.00
1	16S1	468	A	C4-C5-N7	-5.55	107.92	110.70
22	23S1	1477	A	C8-N9-C4	5.55	108.02	105.80
1	16S1	1280	A	N3-C4-N9	5.55	131.84	127.40
22	23S1	76	C	N1-C2-O2	5.55	122.23	118.90
22	23S1	322	A	N3-C4-N9	5.55	131.84	127.40
22	23S1	1641	A	N9-C4-C5	5.55	108.02	105.80
22	23S1	1877	A	N3-C4-N9	5.55	131.84	127.40
1	16S1	320	A	C4-C5-C6	5.55	119.78	117.00
1	16S1	754	C	C6-N1-C2	-5.55	118.08	120.30
22	23S1	42	A	C5-C6-N1	5.55	120.47	117.70
22	23S1	231	A	N9-C4-C5	5.55	108.02	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	311	A	C4-C5-N7	-5.55	107.92	110.70
22	23S1	716	A	C4-C5-N7	-5.55	107.93	110.70
22	23S1	1322	A	C4-C5-C6	5.55	119.78	117.00
22	23S1	1791	A	N3-C4-N9	5.55	131.84	127.40
22	23S1	2336	A	C8-N9-C4	5.55	108.02	105.80
22	23S1	2478	A	N3-C4-N9	5.55	131.84	127.40
23	05S1	31	C	N3-C2-O2	-5.55	118.02	121.90
22	23S1	322	A	N9-C4-C5	5.55	108.02	105.80
22	23S1	2225	A	N9-C4-C5	5.55	108.02	105.80
22	23S1	204	A	N9-C4-C5	5.55	108.02	105.80
22	23S1	1749	A	C4-C5-C6	5.55	119.77	117.00
22	23S1	1829	A	N9-C4-C5	5.55	108.02	105.80
22	23S1	2241	A	C5-C6-N1	5.55	120.47	117.70
22	23S1	2829	A	C4-C5-C6	5.55	119.77	117.00
23	05S1	58	A	N9-C4-C5	5.55	108.02	105.80
1	16S1	50	A	C8-N9-C4	5.54	108.02	105.80
1	16S1	1430	A	C8-N9-C4	5.54	108.02	105.80
1	16S1	1493	A	N3-C4-N9	5.54	131.84	127.40
1	16S1	495	A	N9-C4-C5	5.54	108.02	105.80
1	16S1	583	A	C8-N9-C4	5.54	108.02	105.80
22	23S1	2432	A	N9-C4-C5	5.54	108.02	105.80
22	23S1	2814	A	C4-C5-C6	5.54	119.77	117.00
1	16S1	435	A	C8-N9-C4	5.54	108.02	105.80
1	16S1	914	A	C6-N1-C2	5.54	121.92	118.60
22	23S1	422	A	C5-C6-N1	5.54	120.47	117.70
22	23S1	909	A	N9-C4-C5	5.54	108.02	105.80
22	23S1	1127	A	C4-C5-C6	5.54	119.77	117.00
22	23S1	1427	A	C5-C6-N1	5.54	120.47	117.70
22	23S1	1469	A	C4-C5-N7	-5.54	107.93	110.70
22	23S1	1640	A	C5-C6-N1	5.54	120.47	117.70
22	23S1	1801	A	C8-N9-C4	5.54	108.02	105.80
22	23S1	2126	A	N9-C4-C5	5.54	108.02	105.80
22	23S1	2646	C	N1-C2-O2	5.54	122.22	118.90
22	23S1	1000	A	C4-C5-C6	5.54	119.77	117.00
22	23S1	1635	A	N9-C4-C5	5.54	108.02	105.80
1	16S1	889	A	N3-C4-N9	5.54	131.83	127.40
1	16S1	1150	A	N9-C4-C5	5.54	108.02	105.80
22	23S1	197	A	C5-C6-N1	5.54	120.47	117.70
22	23S1	443	A	N3-C4-N9	5.54	131.83	127.40
22	23S1	866	A	C4-C5-C6	5.54	119.77	117.00
22	23S1	1552	A	N3-C4-N9	5.54	131.83	127.40
22	23S1	1610	A	C8-N9-C4	5.54	108.02	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2411	A	C8-N9-C4	5.54	108.02	105.80
1	16S1	596	A	N3-C4-N9	5.54	131.83	127.40
22	23S1	2726	A	C8-N9-C4	5.54	108.02	105.80
1	16S1	913	A	N3-C4-N9	5.54	131.83	127.40
22	23S1	2227	A	C4-C5-N7	-5.54	107.93	110.70
1	16S1	139	A	C5-C6-N1	5.53	120.47	117.70
1	16S1	1167	A	C4-C5-C6	5.53	119.77	117.00
22	23S1	342	A	N9-C4-C5	5.53	108.01	105.80
22	23S1	439	A	C5-C6-N1	5.53	120.47	117.70
22	23S1	1090	A	N9-C4-C5	5.53	108.01	105.80
22	23S1	1495	A	C4-C5-N7	-5.53	107.93	110.70
22	23S1	1525	A	C4-C5-C6	5.53	119.77	117.00
22	23S1	1665	A	C5-C6-N1	5.53	120.47	117.70
22	23S1	1786	A	C4-C5-N7	-5.53	107.93	110.70
22	23S1	2809	A	C4-C5-N7	-5.53	107.93	110.70
1	16S1	715	A	C4-C5-C6	5.53	119.77	117.00
1	16S1	1447	A	N3-C4-N9	5.53	131.82	127.40
22	23S1	990	A	N3-C4-N9	5.53	131.83	127.40
22	23S1	1272	A	N3-C4-N9	5.53	131.83	127.40
1	16S1	958	A	C4-C5-N7	-5.53	107.93	110.70
22	23S1	322	A	C4-C5-N7	-5.53	107.93	110.70
22	23S1	793	A	C4-C5-N7	-5.53	107.94	110.70
22	23S1	833	A	C5-C6-N1	5.53	120.47	117.70
22	23S1	1634	A	N3-C4-N9	5.53	131.82	127.40
1	16S1	819	A	N9-C4-C5	5.53	108.01	105.80
1	16S1	414	A	C4-C5-C6	5.53	119.76	117.00
1	16S1	1377	A	N3-C4-N9	5.53	131.82	127.40
1	16S1	1394	A	N3-C4-N9	5.53	131.82	127.40
22	23S1	1079	C	N1-C2-O2	5.53	122.22	118.90
22	23S1	1262	A	C4-C5-C6	5.53	119.76	117.00
1	16S1	300	A	C5-C6-N6	5.53	128.12	123.70
1	16S1	374	A	N3-C4-N9	5.53	131.82	127.40
1	16S1	441	A	C5-C6-N1	5.53	120.46	117.70
22	23S1	1509	A	N3-C4-N9	5.53	131.82	127.40
22	23S1	2042	A	C4-C5-C6	5.53	119.76	117.00
22	23S1	2657	A	N9-C4-C5	5.53	108.01	105.80
1	16S1	143	A	N3-C4-N9	5.52	131.82	127.40
1	16S1	192	A	C8-N9-C4	5.52	108.01	105.80
1	16S1	825	A	N9-C4-C5	5.52	108.01	105.80
1	16S1	1188	A	C4-C5-C6	5.52	119.76	117.00
22	23S1	53	A	C5-C6-N1	5.52	120.46	117.70
22	23S1	262	A	C4-C5-N7	-5.52	107.94	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	371	A	C4-C5-N7	-5.52	107.94	110.70
22	23S1	735	A	C4-C5-C6	5.52	119.76	117.00
22	23S1	1285	A	C8-N9-C4	5.52	108.01	105.80
22	23S1	1871	A	C4-C5-N7	-5.52	107.94	110.70
22	23S1	2471	A	C4-C5-C6	5.52	119.76	117.00
22	23S1	2541	A	C5-C6-N1	5.52	120.46	117.70
1	16S1	1289	A	C4-C5-N7	-5.52	107.94	110.70
1	16S1	1493	A	N9-C4-C5	5.52	108.01	105.80
22	23S1	1353	A	C4-C5-C6	5.52	119.76	117.00
22	23S1	2108	A	C4-C5-N7	-5.52	107.94	110.70
10	S101	17	LEU	CA-CB-CG	5.52	128.00	115.30
22	23S1	6	A	N9-C4-C5	5.52	108.01	105.80
22	23S1	1244	A	C8-N9-C4	5.52	108.01	105.80
22	23S1	1877	A	N9-C4-C5	5.52	108.01	105.80
22	23S1	2564	A	N3-C4-N9	5.52	131.81	127.40
1	16S1	465	A	N9-C4-C5	5.52	108.01	105.80
1	16S1	1188	A	N3-C4-N9	5.52	131.81	127.40
22	23S1	510	C	C6-N1-C2	-5.52	118.09	120.30
22	23S1	917	A	C4-C5-N7	-5.52	107.94	110.70
22	23S1	979	A	C4-C5-C6	5.52	119.76	117.00
22	23S1	1981	A	C4-C5-N7	-5.52	107.94	110.70
22	23S1	2225	A	C8-N9-C4	5.52	108.01	105.80
23	05S1	108	A	C4-C5-C6	5.52	119.76	117.00
1	16S1	964	A	N9-C4-C5	5.52	108.01	105.80
22	23S1	1413	A	N9-C4-C5	5.52	108.01	105.80
22	23S1	1640	A	N9-C4-C5	5.52	108.01	105.80
22	23S1	2733	A	C8-N9-C4	5.52	108.01	105.80
22	23S1	19	A	C8-N9-C4	5.51	108.01	105.80
22	23S1	979	A	C8-N9-C4	5.51	108.01	105.80
22	23S1	1155	A	C4-C5-N7	-5.51	107.94	110.70
22	23S1	2020	A	N3-C4-N9	5.51	131.81	127.40
1	16S1	321	A	C8-N9-C4	5.51	108.00	105.80
22	23S1	231	A	C4-C5-C6	5.51	119.76	117.00
22	23S1	144	A	C8-N9-C4	5.51	108.00	105.80
22	23S1	182	A	N9-C4-C5	5.51	108.00	105.80
22	23S1	1067	A	C8-N9-C4	5.51	108.00	105.80
22	23S1	1264	A	C4-C5-C6	5.51	119.76	117.00
1	16S1	181	A	C5-C6-N1	5.51	120.45	117.70
1	16S1	371	A	N9-C4-C5	5.51	108.00	105.80
1	16S1	1246	A	C5-C6-N1	5.51	120.45	117.70
22	23S1	226	A	N9-C4-C5	5.51	108.00	105.80
22	23S1	751	A	N3-C4-N9	5.51	131.81	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	804	A	C4-C5-N7	-5.51	107.94	110.70
22	23S1	979	A	C4-C5-N7	-5.51	107.94	110.70
22	23S1	1073	A	N9-C4-C5	5.51	108.00	105.80
22	23S1	1268	A	N9-C4-C5	5.51	108.00	105.80
22	23S1	1583	A	N3-C4-N9	5.51	131.81	127.40
22	23S1	1816	C	N1-C2-O2	5.51	122.20	118.90
22	23S1	2082	A	C8-N9-C4	5.51	108.00	105.80
1	16S1	909	A	C4-C5-N7	-5.51	107.95	110.70
1	16S1	1288	A	C5-C6-N1	5.51	120.45	117.70
22	23S1	155	A	N9-C4-C5	5.51	108.00	105.80
1	16S1	560	A	C4-C5-N7	-5.51	107.95	110.70
1	16S1	1093	A	C8-N9-C4	5.51	108.00	105.80
22	23S1	165	A	C4-C5-C6	5.51	119.75	117.00
22	23S1	216	A	C4-C5-N7	-5.51	107.95	110.70
22	23S1	216	A	N3-C4-N9	5.51	131.81	127.40
22	23S1	910	A	C4-C5-N7	-5.51	107.95	110.70
22	23S1	1272	A	C4-C5-C6	5.51	119.75	117.00
22	23S1	1395	A	C5-C6-N1	5.51	120.45	117.70
22	23S1	1977	A	C8-N9-C4	5.51	108.00	105.80
1	16S1	211	G	N3-C4-C5	-5.50	125.85	128.60
22	23S1	2266	A	C5-C6-N1	5.50	120.45	117.70
22	23S1	2381	A	C5-C6-N1	5.50	120.45	117.70
22	23S1	21	A	C8-N9-C4	5.50	108.00	105.80
22	23S1	1134	A	C4-C5-C6	5.50	119.75	117.00
22	23S1	2753	A	C4-C5-C6	5.50	119.75	117.00
1	16S1	174	A	C5-C6-N1	5.50	120.45	117.70
1	16S1	262	A	N9-C4-C5	5.50	108.00	105.80
1	16S1	831	A	C5-C6-N1	5.50	120.45	117.70
22	23S1	44	A	C4-C5-N7	-5.50	107.95	110.70
22	23S1	1785	A	C5-N7-C8	5.50	106.65	103.90
22	23S1	1932	A	C4-C5-C6	5.50	119.75	117.00
22	23S1	2287	A	C8-N9-C4	5.50	108.00	105.80
1	16S1	456	A	C5-C6-N1	5.50	120.45	117.70
25	L031	13	ARG	CD-NE-CZ	-5.50	115.90	123.60
1	16S1	228	A	C4-C5-N7	-5.50	107.95	110.70
1	16S1	794	A	C4-C5-N7	-5.50	107.95	110.70
22	23S1	322	A	C4-C5-C6	5.50	119.75	117.00
22	23S1	1133	A	N3-C4-N9	5.50	131.80	127.40
22	23S1	1598	A	N9-C4-C5	5.50	108.00	105.80
22	23S1	2015	A	C4-C5-C6	5.50	119.75	117.00
22	23S1	2432	A	N3-C4-N9	5.50	131.80	127.40
1	16S1	802	A	C8-N9-C4	5.50	108.00	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	609	A	N9-C4-C5	5.50	108.00	105.80
22	23S1	1678	A	C8-N9-C4	5.50	108.00	105.80
22	23S1	2146	C	C6-N1-C2	-5.50	118.10	120.30
22	23S1	2270	A	C8-N9-C4	5.50	108.00	105.80
1	16S1	715	A	N3-C4-N9	5.50	131.80	127.40
1	16S1	1179	A	N9-C4-C5	5.50	108.00	105.80
22	23S1	1070	A	C4-C5-N7	-5.50	107.95	110.70
22	23S1	1378	A	C8-N9-C4	5.50	108.00	105.80
22	23S1	1614	A	C8-N9-C4	5.50	108.00	105.80
22	23S1	1938	A	C4-C5-C6	5.50	119.75	117.00
1	16S1	781	A	N9-C4-C5	5.49	108.00	105.80
1	16S1	1252	A	C5-C6-N1	5.49	120.45	117.70
22	23S1	111	A	C4-C5-C6	5.49	119.75	117.00
22	23S1	348	A	N9-C4-C5	5.49	108.00	105.80
22	23S1	671	C	N3-C2-O2	-5.49	118.05	121.90
22	23S1	945	A	C4-C5-N7	-5.49	107.95	110.70
22	23S1	2530	A	N9-C4-C5	5.49	108.00	105.80
23	05S1	58	A	N3-C4-N9	5.49	131.79	127.40
1	16S1	60	A	C8-N9-C4	5.49	108.00	105.80
22	23S1	2761	A	C4-C5-N7	-5.49	107.95	110.70
22	23S1	479	A	C5-C6-N1	5.49	120.44	117.70
22	23S1	541	A	N9-C4-C5	5.49	108.00	105.80
22	23S1	1928	A	C4-C5-C6	5.49	119.75	117.00
22	23S1	1997	C	N3-C2-O2	-5.49	118.06	121.90
22	23S1	2829	A	C5-C6-N1	5.49	120.44	117.70
55	PTR1	59	A	N3-C4-N9	5.49	131.79	127.40
1	16S1	119	A	C8-N9-C4	5.49	108.00	105.80
22	23S1	920	A	C5-C6-N1	5.49	120.44	117.70
22	23S1	1596	A	C5-C6-N1	5.49	120.44	117.70
1	16S1	648	A	C4-C5-C6	5.49	119.74	117.00
22	23S1	2749	A	N9-C4-C5	5.49	108.00	105.80
22	23S1	2150	C	N1-C2-O2	5.49	122.19	118.90
22	23S1	2758	A	N3-C4-N9	5.49	131.79	127.40
1	16S1	495	A	C4-C5-N7	-5.48	107.96	110.70
1	16S1	1169	A	N9-C4-C5	5.48	107.99	105.80
1	16S1	1374	A	C5-C6-N1	5.48	120.44	117.70
22	23S1	687	C	N3-C2-O2	-5.48	118.06	121.90
22	23S1	1890	A	C4-C5-C6	5.48	119.74	117.00
22	23S1	2377	A	C8-N9-C4	5.48	107.99	105.80
22	23S1	2748	A	C4-C5-C6	5.48	119.74	117.00
1	16S1	119	A	N3-C4-N9	5.48	131.79	127.40
1	16S1	253	A	C8-N9-C4	5.48	107.99	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	583	A	N9-C4-C5	5.48	107.99	105.80
1	16S1	596	A	C4-C5-N7	-5.48	107.96	110.70
1	16S1	1044	A	N9-C4-C5	5.48	107.99	105.80
1	16S1	1204	A	N9-C4-C5	5.48	107.99	105.80
22	23S1	217	A	N9-C4-C5	5.48	107.99	105.80
22	23S1	256	A	C8-N9-C4	5.48	107.99	105.80
22	23S1	804	A	N3-C4-N9	5.48	131.78	127.40
1	16S1	167	A	C4-C5-C6	5.48	119.74	117.00
1	16S1	303	A	C4-C5-N7	-5.48	107.96	110.70
1	16S1	655	A	N9-C4-C5	5.48	107.99	105.80
1	16S1	1333	A	C5-C6-N1	5.48	120.44	117.70
1	16S1	1377	A	C4-C5-C6	5.48	119.74	117.00
22	23S1	239	C	N3-C2-O2	-5.48	118.06	121.90
22	23S1	1522	A	N9-C4-C5	5.48	107.99	105.80
22	23S1	2378	A	N3-C4-N9	5.48	131.78	127.40
1	16S1	1274	A	N3-C4-N9	5.48	131.78	127.40
22	23S1	340	A	C8-N9-C4	5.48	107.99	105.80
1	16S1	878	A	N9-C4-C5	5.48	107.99	105.80
1	16S1	1204	A	N3-C4-N9	5.48	131.78	127.40
22	23S1	443	A	C4-C5-N7	-5.48	107.96	110.70
22	23S1	1803	A	N3-C4-N9	5.48	131.78	127.40
1	16S1	825	A	N3-C4-N9	5.48	131.78	127.40
22	23S1	2700	A	C8-N9-C4	5.48	107.99	105.80
22	23S1	423	A	N9-C4-C5	5.47	107.99	105.80
22	23S1	541	A	C5-C6-N1	5.47	120.44	117.70
22	23S1	1302	A	N3-C4-N9	5.47	131.78	127.40
22	23S1	2298	A	C4-C5-N7	-5.47	107.96	110.70
1	16S1	60	A	N3-C4-N9	5.47	131.78	127.40
1	16S1	456	A	N9-C4-C5	5.47	107.99	105.80
1	16S1	749	A	C5-C6-N1	5.47	120.44	117.70
22	23S1	213	A	C4-C5-N7	-5.47	107.96	110.70
22	23S1	670	A	C4-C5-C6	5.47	119.74	117.00
22	23S1	979	A	N3-C4-N9	5.47	131.78	127.40
22	23S1	1952	A	C5-C6-N1	5.47	120.44	117.70
22	23S1	2425	A	C8-N9-C4	5.47	107.99	105.80
23	05S1	66	A	C8-N9-C4	5.47	107.99	105.80
1	16S1	59	A	C5-C6-N1	5.47	120.44	117.70
1	16S1	728	A	C5-C6-N1	5.47	120.44	117.70
22	23S1	213	A	N9-C4-C5	5.47	107.99	105.80
1	16S1	1274	A	C4-C5-N7	-5.47	107.97	110.70
22	23S1	262	A	N9-C4-C5	5.47	107.99	105.80
22	23S1	2882	A	N3-C4-N9	5.47	131.78	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	152	A	C5-N7-C8	5.47	106.63	103.90
1	16S1	382	A	N9-C4-C5	5.47	107.99	105.80
22	23S1	1789	A	C4-C5-C6	5.47	119.73	117.00
1	16S1	694	A	C8-N9-C4	5.47	107.99	105.80
1	16S1	909	A	C5-C6-N1	5.47	120.43	117.70
1	16S1	1146	A	C8-N9-C4	5.47	107.99	105.80
22	23S1	749	A	N9-C4-C5	5.47	107.99	105.80
22	23S1	792	A	N3-C4-N9	5.47	131.77	127.40
22	23S1	1701	A	N9-C4-C5	5.47	107.99	105.80
22	23S1	2616	C	C6-N1-C2	-5.47	118.11	120.30
22	23S1	241	A	N9-C4-C5	5.46	107.99	105.80
22	23S1	430	A	C4-C5-N7	-5.46	107.97	110.70
22	23S1	633	A	C8-N9-C4	5.46	107.99	105.80
22	23S1	637	A	C5-C6-N1	5.46	120.43	117.70
22	23S1	1342	A	N9-C4-C5	5.46	107.99	105.80
23	05S1	99	A	C5-C6-N1	5.46	120.43	117.70
1	16S1	197	A	C4-C5-C6	5.46	119.73	117.00
1	16S1	1431	A	C4-C5-N7	-5.46	107.97	110.70
22	23S1	207	A	C8-N9-C4	5.46	107.98	105.80
22	23S1	1490	A	C5-C6-N1	5.46	120.43	117.70
1	16S1	1	A	C8-N9-C4	5.46	107.98	105.80
1	16S1	365	U	C2-N3-C4	5.46	130.28	127.00
1	16S1	702	A	C4-C5-C6	5.46	119.73	117.00
1	16S1	807	A	C4-C5-N7	-5.46	107.97	110.70
1	16S1	958	A	C4-C5-C6	5.46	119.73	117.00
22	23S1	1095	A	C4-C5-N7	-5.46	107.97	110.70
22	23S1	2013	A	C5-C6-N1	5.46	120.43	117.70
22	23S1	2060	A	C6-N1-C2	5.46	121.88	118.60
1	16S1	1155	A	C4-C5-C6	5.46	119.73	117.00
22	23S1	2761	A	N9-C4-C5	5.46	107.98	105.80
1	16S1	414	A	N9-C4-C5	5.46	107.98	105.80
1	16S1	1046	A	C4-C5-N7	-5.46	107.97	110.70
22	23S1	196	A	N9-C4-C5	5.46	107.98	105.80
22	23S1	466	A	N3-C4-N9	5.46	131.77	127.40
22	23S1	1453	A	C4-C5-N7	-5.46	107.97	110.70
22	23S1	1637	A	N9-C4-C5	5.46	107.98	105.80
55	PTR1	51	A	C8-N9-C4	5.46	107.98	105.80
1	16S1	238	A	C4-C5-N7	-5.46	107.97	110.70
22	23S1	342	A	C4-C5-C6	5.46	119.73	117.00
22	23S1	590	A	C4-C5-C6	5.46	119.73	117.00
22	23S1	675	A	C4-C5-N7	-5.46	107.97	110.70
22	23S1	1165	A	C4-C5-C6	5.46	119.73	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	120	A	C4-C5-N7	-5.46	107.97	110.70
22	23S1	1194	A	C8-N9-C4	5.46	107.98	105.80
22	23S1	1496	A	N9-C4-C5	5.46	107.98	105.80
1	16S1	600	A	C4-C5-C6	5.45	119.73	117.00
1	16S1	1169	A	N3-C4-N9	5.45	131.76	127.40
1	16S1	1251	A	N3-C4-N9	5.45	131.76	127.40
22	23S1	1073	A	C4-C5-N7	-5.45	107.97	110.70
22	23S1	2513	A	N9-C4-C5	5.45	107.98	105.80
1	16S1	814	A	C5-C6-N1	5.45	120.43	117.70
22	23S1	83	A	C4-C5-C6	5.45	119.73	117.00
22	23S1	706	A	C8-N9-C4	5.45	107.98	105.80
22	23S1	915	C	C6-N1-C2	-5.45	118.12	120.30
22	23S1	2005	A	C8-N9-C4	5.45	107.98	105.80
1	16S1	171	A	N3-C4-N9	5.45	131.76	127.40
1	16S1	329	A	C8-N9-C4	5.45	107.98	105.80
1	16S1	510	A	N3-C4-N9	5.45	131.76	127.40
1	16S1	694	A	N9-C4-C5	5.45	107.98	105.80
1	16S1	1016	A	N9-C4-C5	5.45	107.98	105.80
22	23S1	1640	A	C4-C5-C6	5.45	119.72	117.00
22	23S1	1932	A	C5-C6-N1	5.45	120.42	117.70
22	23S1	2005	A	N3-C4-N9	5.45	131.76	127.40
1	16S1	353	A	C4-C5-C6	5.45	119.72	117.00
1	16S1	1289	A	N3-C4-N9	5.45	131.76	127.40
2	S021	165	ASP	CB-CG-OD2	5.45	123.20	118.30
22	23S1	905	A	C4-C5-C6	5.45	119.72	117.00
22	23S1	1129	A	N3-C4-N9	5.45	131.76	127.40
22	23S1	1392	A	C4-C5-C6	5.45	119.72	117.00
22	23S1	1590	A	C8-N9-C4	5.45	107.98	105.80
1	16S1	98	A	N9-C4-C5	5.45	107.98	105.80
1	16S1	1534	A	C4-C5-N7	-5.45	107.98	110.70
22	23S1	1525	A	C4-C5-N7	-5.45	107.98	110.70
22	23S1	1572	A	C8-N9-C4	5.45	107.98	105.80
1	16S1	1346	A	C4-C5-N7	-5.44	107.98	110.70
22	23S1	996	A	C5-C6-N1	5.44	120.42	117.70
22	23S1	1246	A	N9-C4-C5	5.44	107.98	105.80
22	23S1	2031	A	N9-C4-C5	5.44	107.98	105.80
22	23S1	2225	A	C4-C5-N7	-5.44	107.98	110.70
22	23S1	2530	A	C4-C5-N7	-5.44	107.98	110.70
1	16S1	768	A	C4-C5-N7	-5.44	107.98	110.70
1	16S1	1102	A	C5-C6-N1	5.44	120.42	117.70
22	23S1	829	A	C4-C5-C6	5.44	119.72	117.00
22	23S1	910	A	C5-C6-N1	5.44	120.42	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1264	A	C5-C6-N1	5.44	120.42	117.70
22	23S1	2636	C	N3-C2-O2	-5.44	118.09	121.90
55	PTR1	51	A	C4-C5-C6	5.44	119.72	117.00
1	16S1	729	A	C4-C5-C6	5.44	119.72	117.00
1	16S1	1261	A	C4-C5-C6	5.44	119.72	117.00
1	16S1	1513	A	C8-N9-C4	5.44	107.98	105.80
22	23S1	507	A	N9-C4-C5	5.44	107.98	105.80
22	23S1	730	A	C5-C6-N1	5.44	120.42	117.70
22	23S1	980	A	C4-C5-C6	5.44	119.72	117.00
22	23S1	1494	A	C4-C5-N7	-5.44	107.98	110.70
22	23S1	1759	A	C8-N9-C4	5.44	107.98	105.80
22	23S1	2450	A	N9-C4-C5	5.44	107.98	105.80
1	16S1	298	A	N3-C4-N9	5.44	131.75	127.40
1	16S1	782	A	N9-C4-C5	5.44	107.97	105.80
1	16S1	810	C	N3-C2-O2	-5.44	118.09	121.90
1	16S1	1150	A	C4-C5-C6	5.44	119.72	117.00
1	16S1	1179	A	N3-C4-N9	5.44	131.75	127.40
22	23S1	423	A	C4-C5-C6	5.44	119.72	117.00
22	23S1	1308	A	C4-C5-C6	5.44	119.72	117.00
22	23S1	1757	A	C4-C5-C6	5.44	119.72	117.00
22	23S1	2547	A	C4-C5-N7	-5.44	107.98	110.70
22	23S1	2590	A	C4-C5-N7	-5.44	107.98	110.70
1	16S1	8	A	C4-C5-C6	5.44	119.72	117.00
22	23S1	637	A	C4-C5-N7	-5.44	107.98	110.70
22	23S1	1545	A	C8-N9-C4	5.44	107.97	105.80
55	PTR1	14	A	C8-N9-C4	5.44	107.97	105.80
1	16S1	338	A	N9-C4-C5	5.43	107.97	105.80
1	16S1	983	A	C5-C6-N1	5.43	120.42	117.70
1	16S1	1377	A	N9-C4-C5	5.43	107.97	105.80
4	S041	26	ARG	NE-CZ-NH2	5.43	123.02	120.30
22	23S1	299	A	C4-C5-C6	5.43	119.72	117.00
22	23S1	844	A	C5-C6-N1	5.43	120.42	117.70
1	16S1	466	A	N3-C4-N9	5.43	131.75	127.40
1	16S1	1248	A	C4-C5-C6	5.43	119.72	117.00
22	23S1	563	A	C5-C6-N1	5.43	120.42	117.70
22	23S1	613	A	C4-C5-N7	-5.43	107.98	110.70
22	23S1	637	A	C4-C5-C6	5.43	119.72	117.00
22	23S1	783	A	C5-C6-N1	5.43	120.42	117.70
22	23S1	844	A	C8-N9-C4	5.43	107.97	105.80
22	23S1	1608	A	N9-C4-C5	5.43	107.97	105.80
22	23S1	2119	A	N9-C4-C5	5.43	107.97	105.80
22	23S1	2823	A	N9-C4-C5	5.43	107.97	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	364	A	N9-C4-C5	5.43	107.97	105.80
22	23S1	2733	A	C5-C6-N1	5.43	120.42	117.70
1	16S1	313	A	N3-C4-N9	5.43	131.74	127.40
1	16S1	759	A	C4-C5-N7	-5.43	107.98	110.70
1	16S1	923	A	C5-C6-N1	5.43	120.41	117.70
22	23S1	699	A	N3-C4-N9	5.43	131.74	127.40
22	23S1	1509	A	C4-C5-N7	-5.43	107.99	110.70
22	23S1	2615	U	N3-C2-O2	-5.43	118.40	122.20
55	PTR1	17	U	C4-C5-C6	-5.43	116.44	119.70
1	16S1	7	A	C4-C5-N7	-5.43	107.99	110.70
22	23S1	548	G	C8-N9-C1'	-5.43	119.94	127.00
22	23S1	1214	A	C4-C5-N7	-5.43	107.99	110.70
1	16S1	1157	A	C5-C6-N1	5.43	120.41	117.70
22	23S1	203	A	N9-C4-C5	5.43	107.97	105.80
22	23S1	1090	A	C8-N9-C4	5.43	107.97	105.80
22	23S1	1304	A	C4-C5-N7	-5.43	107.99	110.70
22	23S1	1580	A	N9-C4-C5	5.43	107.97	105.80
22	23S1	2600	A	N9-C4-C5	5.43	107.97	105.80
1	16S1	889	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	1505	A	C4-C5-N7	-5.42	107.99	110.70
22	23S1	1937	A	C4-C5-C6	5.42	119.71	117.00
1	16S1	1398	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	988	A	N3-C4-N9	5.42	131.74	127.40
22	23S1	1383	A	C4-C5-C6	5.42	119.71	117.00
22	23S1	1652	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	1952	A	N9-C4-C5	5.42	107.97	105.80
22	23S1	2005	A	C5-C6-N1	5.42	120.41	117.70
1	16S1	101	A	C8-N9-C4	5.42	107.97	105.80
1	16S1	116	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	213	A	C4-C5-C6	5.42	119.71	117.00
22	23S1	1032	A	N3-C4-N9	5.42	131.74	127.40
22	23S1	1165	A	C4-C5-N7	-5.42	107.99	110.70
22	23S1	2005	A	C4-C5-N7	-5.42	107.99	110.70
22	23S1	2635	A	C4-C5-N7	-5.42	107.99	110.70
23	05S1	104	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	332	A	N9-C4-C5	5.42	107.97	105.80
22	23S1	371	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	1175	A	C5-C6-N1	5.42	120.41	117.70
22	23S1	310	A	N3-C4-N9	5.42	131.74	127.40
22	23S1	423	A	N3-C4-N9	5.42	131.74	127.40
22	23S1	508	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	675	A	C4-C5-C6	5.42	119.71	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1040	A	N9-C4-C5	5.42	107.97	105.80
22	23S1	1967	C	N1-C2-O2	5.42	122.15	118.90
22	23S1	2741	A	N3-C4-N9	5.42	131.74	127.40
1	16S1	10	A	C8-N9-C4	5.42	107.97	105.80
1	16S1	77	A	C5-C6-N1	5.42	120.41	117.70
1	16S1	814	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	453	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	614	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	764	A	N9-C4-C5	5.42	107.97	105.80
22	23S1	996	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	1230	A	C5-C6-N1	5.42	120.41	117.70
22	23S1	1579	A	N9-C4-C5	5.42	107.97	105.80
22	23S1	2054	A	C4-C5-C6	5.42	119.71	117.00
22	23S1	2821	A	N3-C4-N9	5.42	131.73	127.40
23	05S1	109	A	C8-N9-C4	5.42	107.97	105.80
22	23S1	1204	A	N3-C4-N9	5.42	131.73	127.40
1	16S1	349	A	C5-C6-N1	5.41	120.41	117.70
1	16S1	649	A	C4-C5-C6	5.41	119.71	117.00
1	16S1	975	A	N3-C4-N9	5.41	131.73	127.40
22	23S1	371	A	N9-C4-C5	5.41	107.97	105.80
22	23S1	1069	A	C4-C5-N7	-5.41	107.99	110.70
22	23S1	1772	A	C4-C5-C6	5.41	119.71	117.00
22	23S1	2062	A	C5-C6-N1	5.41	120.41	117.70
1	16S1	607	A	C8-N9-C4	5.41	107.97	105.80
1	16S1	574	A	N3-C4-N9	5.41	131.73	127.40
1	16S1	1012	A	C8-N9-C4	5.41	107.97	105.80
22	23S1	501	A	N3-C4-N9	5.41	131.73	127.40
22	23S1	666	A	C4-C5-C6	5.41	119.70	117.00
22	23S1	721	A	C5-C6-N1	5.41	120.41	117.70
22	23S1	1126	A	C5-C6-N1	5.41	120.41	117.70
22	23S1	2480	C	C6-N1-C2	-5.41	118.14	120.30
22	23S1	2660	A	C4-C5-N7	-5.41	108.00	110.70
22	23S1	2765	A	C5-C6-N1	5.41	120.41	117.70
22	23S1	2797	U	N1-C2-O2	5.41	126.59	122.80
23	05S1	15	A	N9-C4-C5	5.41	107.96	105.80
23	05S1	119	A	C5-C6-N1	5.41	120.41	117.70
1	16S1	1098	C	C6-N1-C2	-5.41	118.14	120.30
22	23S1	402	A	C4-C5-C6	5.41	119.70	117.00
22	23S1	429	A	C4-C5-N7	-5.41	108.00	110.70
22	23S1	505	A	C4-C5-N7	-5.41	108.00	110.70
22	23S1	621	A	C8-N9-C4	5.41	107.96	105.80
22	23S1	788	A	C4-C5-C6	5.41	119.70	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1668	A	C5-C6-N1	5.41	120.41	117.70
22	23S1	2328	A	N9-C4-C5	5.41	107.96	105.80
23	05S1	59	A	N9-C4-C5	5.41	107.96	105.80
1	16S1	1	A	C4-C5-N7	-5.41	108.00	110.70
1	16S1	996	A	N9-C4-C5	5.41	107.96	105.80
1	16S1	1035	A	C4-C5-N7	-5.41	108.00	110.70
22	23S1	300	A	N3-C4-N9	5.41	131.73	127.40
22	23S1	1077	A	C4-C5-N7	-5.41	108.00	110.70
22	23S1	2059	A	C5-C6-N1	5.41	120.40	117.70
22	23S1	2328	A	C5-C6-N1	5.41	120.40	117.70
23	05S1	71	C	N1-C2-O2	5.41	122.14	118.90
1	16S1	160	A	C4-C5-C6	5.41	119.70	117.00
1	16S1	1363	A	N9-C4-C5	5.41	107.96	105.80
22	23S1	1635	A	C4-C5-N7	-5.41	108.00	110.70
22	23S1	2023	C	N1-C2-O2	5.41	122.14	118.90
22	23S1	2071	A	C4-C5-N7	-5.41	108.00	110.70
1	16S1	1495	U	C5-C6-N1	5.40	125.40	122.70
22	23S1	781	A	C8-N9-C4	5.40	107.96	105.80
22	23S1	1262	A	C4-C5-N7	-5.40	108.00	110.70
22	23S1	1265	A	C4-C5-N7	-5.40	108.00	110.70
22	23S1	1547	C	N1-C2-O2	5.40	122.14	118.90
22	23S1	933	A	C5-C6-N1	5.40	120.40	117.70
22	23S1	2738	A	N9-C4-C5	5.40	107.96	105.80
22	23S1	547	A	C4-C5-N7	-5.40	108.00	110.70
22	23S1	1522	A	N3-C4-N9	5.40	131.72	127.40
22	23S1	2114	A	C5-N7-C8	5.40	106.60	103.90
22	23S1	2278	A	C8-N9-C4	5.40	107.96	105.80
1	16S1	1092	A	N9-C4-C5	5.40	107.96	105.80
22	23S1	14	A	N3-C4-N9	5.40	131.72	127.40
22	23S1	1046	A	C4-C5-C6	5.40	119.70	117.00
22	23S1	1547	C	N3-C2-O2	-5.40	118.12	121.90
22	23S1	1788	C	C6-N1-C2	-5.40	118.14	120.30
1	16S1	1269	A	N3-C4-N9	5.40	131.72	127.40
22	23S1	1634	A	C4-C5-C6	5.40	119.70	117.00
22	23S1	2063	C	C6-N1-C2	-5.40	118.14	120.30
22	23S1	529	A	C4-C5-N7	-5.39	108.00	110.70
22	23S1	544	C	C6-N1-C1'	-5.39	114.33	120.80
22	23S1	1046	A	C4-C5-N7	-5.39	108.00	110.70
22	23S1	1616	A	C4-C5-C6	5.39	119.70	117.00
22	23S1	2273	A	C4-C5-N7	-5.39	108.00	110.70
22	23S1	2407	A	N9-C4-C5	5.39	107.96	105.80
1	16S1	747	A	C5-C6-N1	5.39	120.40	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	906	A	C8-N9-C4	5.39	107.96	105.80
1	16S1	1357	A	C5-C6-N1	5.39	120.40	117.70
22	23S1	71	A	C4-C5-N7	-5.39	108.00	110.70
22	23S1	216	A	C5-C6-N1	5.39	120.40	117.70
22	23S1	1084	A	C8-N9-C4	5.39	107.96	105.80
55	PTR1	76	A	N3-C4-N9	5.39	131.71	127.40
1	16S1	1035	A	C8-N9-C4	5.39	107.96	105.80
1	16S1	1493	A	C8-N9-C4	5.39	107.96	105.80
22	23S1	439	A	N9-C4-C5	5.39	107.96	105.80
22	23S1	1713	A	C4-C5-C6	5.39	119.70	117.00
23	05S1	36	C	N1-C2-O2	5.39	122.14	118.90
1	16S1	938	A	C4-C5-N7	-5.39	108.00	110.70
22	23S1	590	A	C8-N9-C4	5.39	107.96	105.80
22	23S1	616	A	C4-C5-N7	-5.39	108.00	110.70
22	23S1	905	A	N3-C4-N9	5.39	131.71	127.40
22	23S1	990	A	C4-C5-N7	-5.39	108.00	110.70
22	23S1	1205	A	C4-C5-C6	5.39	119.69	117.00
22	23S1	1503	A	C5-C6-N1	5.39	120.39	117.70
1	16S1	468	A	C5-C6-N1	5.39	120.39	117.70
1	16S1	681	A	C4-C5-N7	-5.39	108.01	110.70
22	23S1	83	A	C8-N9-C4	5.39	107.95	105.80
22	23S1	2117	A	N3-C4-N9	5.39	131.71	127.40
1	16S1	415	A	C4-C5-N7	-5.39	108.01	110.70
1	16S1	996	A	C4-C5-N7	-5.39	108.01	110.70
22	23S1	104	A	C4-C5-C6	5.39	119.69	117.00
22	23S1	1711	A	C8-N9-C4	5.39	107.95	105.80
22	23S1	2015	A	N3-C4-N9	5.39	131.71	127.40
22	23S1	2335	A	N9-C4-C5	5.39	107.95	105.80
22	23S1	2899	A	C5-C6-N1	5.39	120.39	117.70
1	16S1	1248	A	C8-N9-C4	5.38	107.95	105.80
1	16S1	1329	A	C8-N9-C4	5.38	107.95	105.80
1	16S1	1333	A	C4-C5-C6	5.38	119.69	117.00
22	23S1	111	A	C5-C6-N1	5.38	120.39	117.70
22	23S1	262	A	C4-C5-C6	5.38	119.69	117.00
22	23S1	309	A	C5-C6-N1	5.38	120.39	117.70
22	23S1	718	A	N9-C4-C5	5.38	107.95	105.80
22	23S1	1515	A	C4-C5-N7	-5.38	108.01	110.70
23	05S1	34	A	C4-C5-C6	5.38	119.69	117.00
1	16S1	371	A	C8-N9-C4	5.38	107.95	105.80
22	23S1	348	A	C4-C5-N7	-5.38	108.01	110.70
22	23S1	1376	C	N3-C2-O2	-5.38	118.13	121.90
22	23S1	1754	A	N9-C4-C5	5.38	107.95	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1960	A	C4-C5-C6	5.38	119.69	117.00
22	23S1	1304	A	N3-C4-N9	5.38	131.71	127.40
22	23S1	1746	A	N9-C4-C5	5.38	107.95	105.80
22	23S1	2023	C	N3-C2-O2	-5.38	118.13	121.90
22	23S1	2826	A	C5-C6-N1	5.38	120.39	117.70
1	16S1	466	A	C4-C5-N7	-5.38	108.01	110.70
22	23S1	1347	A	N3-C4-N9	5.38	131.70	127.40
1	16S1	460	A	N9-C4-C5	5.38	107.95	105.80
1	16S1	857	C	N1-C2-O2	5.38	122.13	118.90
1	16S1	1032	G	C4-N9-C1'	5.38	133.49	126.50
1	16S1	1288	A	N9-C4-C5	5.38	107.95	105.80
1	16S1	1377	A	C4-C5-N7	-5.38	108.01	110.70
22	23S1	19	A	N9-C4-C5	5.38	107.95	105.80
22	23S1	547	A	N3-C4-N9	5.38	131.70	127.40
22	23S1	655	A	C4-C5-N7	-5.38	108.01	110.70
22	23S1	1670	C	C6-N1-C2	-5.38	118.15	120.30
22	23S1	2090	A	C8-N9-C4	5.38	107.95	105.80
22	23S1	2736	A	C4-C5-N7	-5.38	108.01	110.70
22	23S1	2810	A	N3-C4-N9	5.38	131.70	127.40
1	16S1	635	A	C5-C6-N1	5.38	120.39	117.70
22	23S1	294	A	C4-C5-C6	5.38	119.69	117.00
22	23S1	866	A	C5-C6-N1	5.38	120.39	117.70
22	23S1	1376	C	N1-C2-O2	5.38	122.13	118.90
22	23S1	1494	A	C4-C5-C6	5.38	119.69	117.00
22	23S1	1634	A	C4-C5-N7	-5.38	108.01	110.70
22	23S1	1672	A	C5-C6-N1	5.38	120.39	117.70
22	23S1	2154	A	C8-N9-C4	5.38	107.95	105.80
22	23S1	2376	A	C8-N9-C4	5.38	107.95	105.80
22	23S1	2412	A	C8-N9-C4	5.38	107.95	105.80
55	PTR1	21	A	N9-C4-C5	5.38	107.95	105.80
1	16S1	1499	A	C5-C6-N1	5.37	120.39	117.70
22	23S1	348	A	C8-N9-C4	5.37	107.95	105.80
22	23S1	2070	A	C8-N9-C4	5.37	107.95	105.80
55	PTR1	73	A	N3-C4-N9	5.37	131.70	127.40
1	16S1	4	U	O4'-C1'-N1	5.37	112.50	108.20
1	16S1	288	A	N9-C4-C5	5.37	107.95	105.80
1	16S1	1179	A	C8-N9-C4	5.37	107.95	105.80
22	23S1	222	A	N9-C4-C5	5.37	107.95	105.80
22	23S1	342	A	C8-N9-C4	5.37	107.95	105.80
23	05S1	46	A	C4-C5-C6	5.37	119.69	117.00
1	16S1	781	A	C4-C5-C6	5.37	119.69	117.00
1	16S1	1180	A	N9-C4-C5	5.37	107.95	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1504	A	C5-C6-N1	5.37	120.39	117.70
22	23S1	428	A	C8-N9-C4	5.37	107.95	105.80
22	23S1	632	A	C8-N9-C4	5.37	107.95	105.80
22	23S1	1698	A	C5-C6-N1	5.37	120.38	117.70
22	23S1	2211	A	C4-C5-N7	-5.37	108.02	110.70
23	05S1	75	G	N3-C4-N9	5.37	129.22	126.00
22	23S1	687	C	N1-C2-O2	5.37	122.12	118.90
22	23S1	988	A	C8-N9-C4	5.37	107.95	105.80
22	23S1	1133	A	C4-C5-N7	-5.37	108.02	110.70
1	16S1	51	A	C4-C5-N7	-5.37	108.02	110.70
1	16S1	461	A	C4-C5-C6	5.37	119.68	117.00
1	16S1	815	A	N9-C4-C5	5.37	107.95	105.80
22	23S1	673	C	N3-C4-C5	5.37	124.05	121.90
22	23S1	825	A	C5-C6-N1	5.37	120.38	117.70
22	23S1	972	A	C4-C5-N7	-5.37	108.02	110.70
22	23S1	1366	A	N9-C4-C5	5.37	107.95	105.80
22	23S1	1395	A	C4-C5-N7	-5.37	108.02	110.70
1	16S1	1082	A	C4-C5-N7	-5.36	108.02	110.70
22	23S1	222	A	C4-C5-N7	-5.36	108.02	110.70
22	23S1	2468	A	C5-C6-N1	5.36	120.38	117.70
22	23S1	2639	A	N3-C4-N9	5.36	131.69	127.40
22	23S1	2820	A	C4-C5-N7	-5.36	108.02	110.70
22	23S1	631	A	C5-C6-N1	5.36	120.38	117.70
22	23S1	1610	A	N3-C4-N9	5.36	131.69	127.40
1	16S1	532	A	N9-C4-C5	5.36	107.94	105.80
1	16S1	547	A	N9-C4-C5	5.36	107.94	105.80
1	16S1	1287	A	N3-C4-N9	5.36	131.69	127.40
22	23S1	368	A	C4-C5-C6	5.36	119.68	117.00
22	23S1	1032	A	C5-C6-N1	5.36	120.38	117.70
22	23S1	1347	A	C5-C6-N1	5.36	120.38	117.70
22	23S1	1690	A	C4-C5-N7	-5.36	108.02	110.70
22	23S1	2750	A	C4-C5-C6	5.36	119.68	117.00
1	16S1	336	A	N9-C4-C5	5.36	107.94	105.80
22	23S1	2516	A	C4-C5-C6	5.36	119.68	117.00
1	16S1	1176	A	N9-C4-C5	5.36	107.94	105.80
1	16S1	1324	A	C5-C6-N1	5.36	120.38	117.70
1	16S1	1493	A	C4-C5-N7	-5.36	108.02	110.70
22	23S1	782	A	C4-C5-N7	-5.36	108.02	110.70
22	23S1	1284	A	C5-C6-N1	5.36	120.38	117.70
22	23S1	1774	C	N3-C2-O2	-5.36	118.15	121.90
22	23S1	2314	A	N9-C4-C5	5.36	107.94	105.80
22	23S1	2560	A	C4-C5-N7	-5.36	108.02	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1194	A	C4-C5-N7	-5.36	108.02	110.70
55	PTR1	59	A	C4-C5-C6	5.36	119.68	117.00
1	16S1	59	A	C8-N9-C4	5.35	107.94	105.80
1	16S1	729	A	N3-C4-N9	5.35	131.68	127.40
1	16S1	1395	C	C6-N1-C2	-5.35	118.16	120.30
22	23S1	74	A	C4-C5-N7	-5.35	108.02	110.70
22	23S1	173	A	C8-N9-C4	5.35	107.94	105.80
22	23S1	1755	A	C5-C6-N1	5.35	120.38	117.70
22	23S1	1901	A	C5-C6-N1	5.35	120.38	117.70
1	16S1	1150	A	C5-C6-N1	5.35	120.38	117.70
22	23S1	53	A	N3-C4-N9	5.35	131.68	127.40
22	23S1	94	A	C5-C6-N1	5.35	120.38	117.70
22	23S1	199	A	C4-C5-C6	5.35	119.68	117.00
22	23S1	833	A	N9-C4-C5	5.35	107.94	105.80
22	23S1	1328	A	C5-C6-N1	5.35	120.38	117.70
22	23S1	1508	A	C5-C6-N1	5.35	120.38	117.70
22	23S1	2033	A	C4-C5-C6	5.35	119.68	117.00
22	23S1	2837	A	N9-C4-C5	5.35	107.94	105.80
1	16S1	8	A	C4-C5-N7	-5.35	108.02	110.70
1	16S1	10	A	N9-C4-C5	5.35	107.94	105.80
1	16S1	753	A	C4-C5-C6	5.35	119.68	117.00
22	23S1	5	A	C5-C6-N1	5.35	120.38	117.70
22	23S1	165	A	N3-C4-N9	5.35	131.68	127.40
22	23S1	2600	A	C4-C5-N7	-5.35	108.03	110.70
1	16S1	831	A	C4-C5-C6	5.35	119.67	117.00
1	16S1	1318	A	N9-C4-C5	5.35	107.94	105.80
1	16S1	1413	A	C4-C5-C6	5.35	119.67	117.00
22	23S1	428	A	C5-C6-N1	5.35	120.38	117.70
22	23S1	514	A	N9-C4-C5	5.35	107.94	105.80
22	23S1	685	A	C5-C6-N1	5.35	120.38	117.70
22	23S1	727	A	C8-N9-C4	5.35	107.94	105.80
22	23S1	1090	A	C4-C5-N7	-5.35	108.03	110.70
22	23S1	2107	G	N1-C6-O6	-5.35	116.69	119.90
1	16S1	782	A	C5-C6-N1	5.35	120.37	117.70
1	16S1	1168	U	N3-C2-O2	-5.35	118.46	122.20
1	16S1	1441	A	C4-C5-C6	5.35	119.67	117.00
22	23S1	917	A	N9-C4-C5	5.35	107.94	105.80
22	23S1	1367	A	N9-C4-C5	5.35	107.94	105.80
22	23S1	2335	A	C4-C5-N7	-5.35	108.03	110.70
23	05S1	15	A	C8-N9-C4	5.35	107.94	105.80
1	16S1	171	A	C8-N9-C4	5.35	107.94	105.80
1	16S1	831	A	C4-C5-N7	-5.35	108.03	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1141	C	C5-C6-N1	5.35	123.67	121.00
1	16S1	1280	A	C4-C5-C6	5.35	119.67	117.00
22	23S1	2311	A	N3-C4-N9	5.35	131.68	127.40
22	23S1	2856	A	C8-N9-C4	5.35	107.94	105.80
1	16S1	498	A	C4-C5-N7	-5.34	108.03	110.70
1	16S1	675	A	C4-C5-C6	5.34	119.67	117.00
22	23S1	300	A	C4-C5-C6	5.34	119.67	117.00
22	23S1	1532	A	C5-C6-N1	5.34	120.37	117.70
22	23S1	1566	A	C4-C5-N7	-5.34	108.03	110.70
22	23S1	2369	A	C5-C6-N1	5.34	120.37	117.70
22	23S1	2741	A	N9-C4-C5	5.34	107.94	105.80
1	16S1	560	A	C5-C6-N1	5.34	120.37	117.70
4	S041	9	LEU	CB-CG-CD2	-5.34	101.92	111.00
22	23S1	1342	A	C4-C5-C6	5.34	119.67	117.00
22	23S1	1689	A	N9-C4-C5	5.34	107.94	105.80
22	23S1	2266	A	C4-C5-C6	5.34	119.67	117.00
22	23S1	2432	A	C4-C5-N7	-5.34	108.03	110.70
22	23S1	2733	A	C4-C5-N7	-5.34	108.03	110.70
1	16S1	320	A	C8-N9-C4	5.34	107.94	105.80
1	16S1	382	A	C5-C6-N1	5.34	120.37	117.70
1	16S1	1430	A	C5-C6-N1	5.34	120.37	117.70
22	23S1	402	A	N3-C4-N9	5.34	131.67	127.40
22	23S1	1580	A	C8-N9-C4	5.34	107.94	105.80
1	16S1	131	A	C8-N9-C4	5.34	107.94	105.80
1	16S1	857	C	C6-N1-C2	-5.34	118.17	120.30
1	16S1	975	A	C4-C5-C6	5.34	119.67	117.00
22	23S1	2060	A	N9-C4-C5	5.34	107.94	105.80
1	16S1	325	A	C4-C5-N7	-5.34	108.03	110.70
1	16S1	364	A	C4-C5-N7	-5.34	108.03	110.70
1	16S1	573	A	C5-C6-N1	5.34	120.37	117.70
22	23S1	118	A	N3-C4-N9	5.34	131.67	127.40
22	23S1	156	A	C8-N9-C4	5.34	107.94	105.80
22	23S1	715	A	C4-C5-N7	-5.34	108.03	110.70
22	23S1	1147	A	N9-C4-C5	5.34	107.94	105.80
22	23S1	1156	A	C4-C5-C6	5.34	119.67	117.00
22	23S1	2060	A	C4-C5-N7	-5.34	108.03	110.70
22	23S1	2837	A	C4-C5-N7	-5.34	108.03	110.70
1	16S1	1499	A	N9-C4-C5	5.33	107.93	105.80
22	23S1	671	C	N1-C2-O2	5.33	122.10	118.90
1	16S1	573	A	C4-C5-N7	-5.33	108.03	110.70
1	16S1	1145	A	C4-C5-N7	-5.33	108.03	110.70
1	16S1	1287	A	N9-C4-C5	5.33	107.93	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1368	A	C5-C6-N1	5.33	120.37	117.70
22	23S1	685	A	C4-C5-C6	5.33	119.67	117.00
22	23S1	2461	A	C4-C5-N7	-5.33	108.03	110.70
23	05S1	78	A	C5-C6-N1	5.33	120.37	117.70
1	16S1	313	A	C4-C5-C6	5.33	119.67	117.00
1	16S1	1398	A	N9-C4-C5	5.33	107.93	105.80
22	23S1	592	A	C5-C6-N1	5.33	120.36	117.70
22	23S1	941	A	C8-N9-C4	5.33	107.93	105.80
22	23S1	1420	A	C4-C5-N7	-5.33	108.03	110.70
22	23S1	2660	A	N3-C4-N9	5.33	131.66	127.40
23	05S1	39	A	N9-C4-C5	5.33	107.93	105.80
1	16S1	937	A	C5-C6-N1	5.33	120.36	117.70
1	16S1	1433	A	C4-C5-N7	-5.33	108.03	110.70
22	23S1	2376	A	N9-C4-C5	5.33	107.93	105.80
22	23S1	2378	A	N9-C4-C5	5.33	107.93	105.80
1	16S1	969	A	N3-C4-N9	5.33	131.66	127.40
22	23S1	19	A	C4-C5-N7	-5.33	108.04	110.70
22	23S1	103	A	N3-C4-N9	5.33	131.66	127.40
22	23S1	233	A	C5-C6-N1	5.33	120.36	117.70
22	23S1	973	A	N3-C4-N9	5.33	131.66	127.40
22	23S1	1069	A	C4-C5-C6	5.33	119.66	117.00
22	23S1	1084	A	C4-C5-N7	-5.33	108.04	110.70
22	23S1	1096	A	N3-C4-N9	5.33	131.66	127.40
22	23S1	1544	A	C4-C5-C6	5.33	119.66	117.00
22	23S1	1548	A	C8-N9-C4	5.33	107.93	105.80
22	23S1	1566	A	C5-C6-N1	5.33	120.36	117.70
22	23S1	2314	A	C4-C5-N7	-5.33	108.04	110.70
22	23S1	2814	A	N3-C4-N9	5.33	131.66	127.40
1	16S1	1110	A	N9-C4-C5	5.33	107.93	105.80
22	23S1	1383	A	C4-C5-N7	-5.33	108.04	110.70
22	23S1	1494	A	C8-N9-C4	5.33	107.93	105.80
22	23S1	1735	A	C5-C6-N1	5.33	120.36	117.70
1	16S1	130	A	C4-C5-C6	5.33	119.66	117.00
1	16S1	702	A	N9-C4-C5	5.33	107.93	105.80
22	23S1	761	A	C5-N7-C8	5.33	106.56	103.90
22	23S1	1009	A	C4-C5-N7	-5.33	108.04	110.70
22	23S1	1276	A	C4-C5-N7	-5.33	108.04	110.70
22	23S1	2205	A	C4-C5-N7	-5.33	108.04	110.70
23	05S1	39	A	C4-C5-N7	-5.33	108.04	110.70
1	16S1	435	A	N9-C4-C5	5.32	107.93	105.80
22	23S1	753	A	N9-C4-C5	5.32	107.93	105.80
22	23S1	927	A	C4-C5-N7	-5.32	108.04	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1048	A	C8-N9-C4	5.32	107.93	105.80
22	23S1	1650	A	C5-C6-N1	5.32	120.36	117.70
22	23S1	2776	A	N3-C4-N9	5.32	131.66	127.40
1	16S1	572	A	C4-C5-C6	5.32	119.66	117.00
1	16S1	1362	A	N9-C4-C5	5.32	107.93	105.80
1	16S1	1408	A	C5-C6-N1	5.32	120.36	117.70
22	23S1	2043	C	N3-C2-O2	-5.32	118.17	121.90
1	16S1	182	A	N3-C4-N9	5.32	131.66	127.40
22	23S1	310	A	C4-C5-C6	5.32	119.66	117.00
22	23S1	751	A	C4-C5-C6	5.32	119.66	117.00
22	23S1	1237	A	C5-C6-N1	5.32	120.36	117.70
22	23S1	1637	A	C4-C5-N7	-5.32	108.04	110.70
1	16S1	353	A	N3-C4-N9	5.32	131.66	127.40
1	16S1	1513	A	C4-C5-N7	-5.32	108.04	110.70
22	23S1	572	A	N9-C4-C5	5.32	107.93	105.80
22	23S1	1367	A	C4-C5-N7	-5.32	108.04	110.70
22	23S1	1678	A	N9-C4-C5	5.32	107.93	105.80
1	16S1	44	A	C8-N9-C4	5.32	107.93	105.80
1	16S1	675	A	N3-C4-N9	5.32	131.65	127.40
1	16S1	996	A	C4-C5-C6	5.32	119.66	117.00
1	16S1	1465	A	C8-N9-C4	5.32	107.93	105.80
22	23S1	191	A	C4-C5-N7	-5.32	108.04	110.70
22	23S1	310	A	C4-C5-N7	-5.32	108.04	110.70
22	23S1	1772	A	N9-C4-C5	5.32	107.93	105.80
22	23S1	1885	A	C5-C6-N1	5.32	120.36	117.70
22	23S1	2243	U	N3-C2-O2	-5.32	118.48	122.20
23	05S1	46	A	C4-C5-N7	-5.32	108.04	110.70
22	23S1	1608	A	C5-C6-N1	5.32	120.36	117.70
22	23S1	2358	A	C4-C5-C6	5.32	119.66	117.00
23	05S1	58	A	C4-C5-N7	-5.32	108.04	110.70
55	PTR1	58	A	C5-C6-N1	5.32	120.36	117.70
1	16S1	87	C	N3-C2-O2	-5.31	118.18	121.90
1	16S1	539	A	C5-C6-N1	5.31	120.36	117.70
22	23S1	182	A	C4-C5-N7	-5.31	108.04	110.70
22	23S1	44	A	C5-C6-N1	5.31	120.36	117.70
22	23S1	190	A	C4-C5-N7	-5.31	108.04	110.70
22	23S1	282	A	C4-C5-C6	5.31	119.66	117.00
22	23S1	340	A	N9-C4-C5	5.31	107.92	105.80
22	23S1	1433	A	C5-C6-N1	5.31	120.36	117.70
22	23S1	2267	A	C4-C5-C6	5.31	119.66	117.00
22	23S1	2386	A	C8-N9-C4	5.31	107.92	105.80
22	23S1	2749	A	C8-N9-C4	5.31	107.92	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	238	A	N9-C4-C5	5.31	107.92	105.80
1	16S1	718	A	C5-C6-N1	5.31	120.36	117.70
22	23S1	1398	C	C6-N1-C2	-5.31	118.18	120.30
22	23S1	2540	C	N3-C2-O2	-5.31	118.18	121.90
1	16S1	16	A	N3-C4-N9	5.31	131.65	127.40
22	23S1	936	A	C8-N9-C4	5.31	107.92	105.80
22	23S1	1698	A	C4-C5-N7	-5.31	108.05	110.70
22	23S1	2183	A	N9-C4-C5	5.31	107.92	105.80
1	16S1	236	A	C5-C6-N1	5.31	120.35	117.70
1	16S1	1433	A	C5-C6-N1	5.31	120.35	117.70
1	16S1	1447	A	C4-C5-C6	5.31	119.65	117.00
22	23S1	515	A	C8-N9-C4	5.31	107.92	105.80
22	23S1	1504	A	N9-C4-C5	5.31	107.92	105.80
22	23S1	2883	A	C4-C5-N7	-5.31	108.05	110.70
22	23S1	631	A	N9-C4-C5	5.31	107.92	105.80
22	23S1	1147	A	C8-N9-C4	5.31	107.92	105.80
22	23S1	2886	A	C5-C6-N1	5.31	120.35	117.70
1	16S1	1257	A	C4-C5-N7	-5.30	108.05	110.70
1	16S1	1362	A	C5-C6-N1	5.30	120.35	117.70
1	16S1	1468	A	C8-N9-C4	5.30	107.92	105.80
22	23S1	83	A	N9-C4-C5	5.30	107.92	105.80
22	23S1	1502	A	C8-N9-C4	5.30	107.92	105.80
22	23S1	2119	A	C4-C5-C6	5.30	119.65	117.00
55	PTR1	59	A	C5-C6-N1	5.30	120.35	117.70
22	23S1	127	A	N9-C4-C5	5.30	107.92	105.80
22	23S1	2126	A	C4-C5-N7	-5.30	108.05	110.70
22	23S1	2814	A	N9-C4-C5	5.30	107.92	105.80
1	16S1	716	A	C4-C5-N7	-5.30	108.05	110.70
1	16S1	1016	A	C8-N9-C4	5.30	107.92	105.80
22	23S1	443	A	C4-C5-C6	5.30	119.65	117.00
22	23S1	603	A	N3-C4-N9	5.30	131.64	127.40
22	23S1	643	A	C6-N1-C2	5.30	121.78	118.60
22	23S1	654	A	C5-C6-N1	5.30	120.35	117.70
22	23S1	1549	A	C5-C6-N1	5.30	120.35	117.70
22	23S1	1787	A	C5-C6-N1	5.30	120.35	117.70
22	23S1	1876	A	C4-C5-N7	-5.30	108.05	110.70
22	23S1	2736	A	N9-C4-C5	5.30	107.92	105.80
1	16S1	729	A	C4-C5-N7	-5.30	108.05	110.70
1	16S1	913	A	C4-C5-C6	5.30	119.65	117.00
22	23S1	14	A	C5-C6-N1	5.30	120.35	117.70
22	23S1	71	A	N9-C4-C5	5.30	107.92	105.80
22	23S1	526	A	C4-C5-N7	-5.30	108.05	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1322	A	N3-C4-N9	5.30	131.64	127.40
22	23S1	1746	A	C5-C6-N1	5.30	120.35	117.70
22	23S1	2434	A	N3-C4-N9	5.30	131.64	127.40
7	S071	13	LEU	CB-CG-CD1	-5.30	101.99	111.00
22	23S1	2434	A	C4-C5-N7	-5.30	108.05	110.70
1	16S1	909	A	C4-C5-C6	5.30	119.65	117.00
1	16S1	1275	A	C4-C5-N7	-5.30	108.05	110.70
22	23S1	789	A	C4-C5-N7	-5.30	108.05	110.70
1	16S1	547	A	N3-C4-N9	5.29	131.64	127.40
22	23S1	1960	A	N9-C4-C5	5.29	107.92	105.80
22	23S1	2080	A	N9-C4-C5	5.29	107.92	105.80
23	05S1	34	A	N3-C4-N9	5.29	131.64	127.40
1	16S1	435	A	C5-C6-N1	5.29	120.35	117.70
1	16S1	729	A	C8-N9-C4	5.29	107.92	105.80
1	16S1	1046	A	N9-C4-C5	5.29	107.92	105.80
1	16S1	1350	A	N9-C4-C5	5.29	107.92	105.80
22	23S1	218	A	C4-C5-N7	-5.29	108.05	110.70
22	23S1	368	A	C4-C5-N7	-5.29	108.05	110.70
22	23S1	1579	A	C8-N9-C4	5.29	107.92	105.80
22	23S1	1815	A	C8-N9-C4	5.29	107.92	105.80
22	23S1	1876	A	N9-C4-C5	5.29	107.92	105.80
22	23S1	2184	A	C5-C6-N1	5.29	120.35	117.70
54	MRN1	5	G	P-O3'-C3'	5.29	126.05	119.70
1	16S1	642	A	C4-C5-N7	-5.29	108.05	110.70
1	16S1	864	A	C5-C6-N1	5.29	120.35	117.70
22	23S1	979	A	C5-C6-N1	5.29	120.35	117.70
22	23S1	1786	A	C4-C5-C6	5.29	119.65	117.00
22	23S1	1794	A	C4-C5-N7	-5.29	108.06	110.70
22	23S1	2336	A	N9-C4-C5	5.29	107.92	105.80
22	23S1	702	U	N1-C2-O2	5.29	126.50	122.80
22	23S1	1254	A	C5-C6-N1	5.29	120.34	117.70
1	16S1	238	A	C5-C6-N1	5.29	120.34	117.70
1	16S1	279	A	N9-C4-C5	5.29	107.92	105.80
1	16S1	787	A	C4-C5-C6	5.29	119.64	117.00
1	16S1	831	A	N9-C4-C5	5.29	107.92	105.80
1	16S1	1408	A	C4-C5-N7	-5.29	108.06	110.70
22	23S1	195	A	C5-C6-N1	5.29	120.34	117.70
22	23S1	599	A	C4-C5-C6	5.29	119.64	117.00
1	16S1	1082	A	C5-C6-N1	5.29	120.34	117.70
22	23S1	2826	A	C4-C5-N7	-5.29	108.06	110.70
55	PTR1	58	A	C4-C5-N7	-5.29	108.06	110.70
1	16S1	602	A	N9-C4-C5	5.29	107.91	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	10	A	N3-C4-N9	5.29	131.63	127.40
22	23S1	1077	A	C4-C5-C6	5.29	119.64	117.00
22	23S1	1247	A	C4-C5-C6	5.29	119.64	117.00
1	16S1	179	A	N3-C4-N9	5.28	131.63	127.40
22	23S1	1772	A	C8-N9-C4	5.28	107.91	105.80
22	23S1	2176	A	N3-C4-N9	5.28	131.63	127.40
22	23S1	2761	A	C8-N9-C4	5.28	107.91	105.80
1	16S1	1168	U	N1-C2-O2	5.28	126.50	122.80
22	23S1	223	A	C8-N9-C4	5.28	107.91	105.80
22	23S1	1302	A	C4-C5-C6	5.28	119.64	117.00
1	16S1	7	A	C4-C5-C6	5.28	119.64	117.00
22	23S1	239	C	N1-C2-O2	5.28	122.07	118.90
22	23S1	423	A	C8-N9-C4	5.28	107.91	105.80
22	23S1	541	A	C8-N9-C4	5.28	107.91	105.80
22	23S1	1053	C	N1-C2-O2	5.28	122.07	118.90
22	23S1	1268	A	C4-C5-N7	-5.28	108.06	110.70
22	23S1	1927	A	C5-C6-N1	5.28	120.34	117.70
22	23S1	2376	A	C4-C5-C6	5.28	119.64	117.00
1	16S1	131	A	C4-C5-C6	5.28	119.64	117.00
22	23S1	497	A	N3-C4-N9	5.28	131.62	127.40
22	23S1	526	A	C8-N9-C4	5.28	107.91	105.80
22	23S1	1204	A	N9-C4-C5	5.28	107.91	105.80
22	23S1	1591	A	C4-C5-C6	5.28	119.64	117.00
22	23S1	2448	A	C4-C5-N7	-5.28	108.06	110.70
1	16S1	143	A	C4-C5-N7	-5.28	108.06	110.70
1	16S1	635	A	C4-C5-N7	-5.28	108.06	110.70
1	16S1	916	U	N3-C2-O2	-5.28	118.51	122.20
1	16S1	949	A	C8-N9-C4	5.28	107.91	105.80
1	16S1	1151	A	N9-C4-C5	5.28	107.91	105.80
1	16S1	1248	A	N3-C4-N9	5.28	131.62	127.40
1	16S1	1346	A	C5-C6-N1	5.28	120.34	117.70
1	16S1	1408	A	N3-C4-N9	5.28	131.62	127.40
22	23S1	103	A	C4-C5-C6	5.28	119.64	117.00
22	23S1	382	A	C4-C5-N7	-5.28	108.06	110.70
22	23S1	1284	A	C4-C5-C6	5.28	119.64	117.00
22	23S1	2352	A	N9-C4-C5	5.28	107.91	105.80
23	05S1	109	A	N9-C4-C5	5.28	107.91	105.80
1	16S1	825	A	C4-C5-N7	-5.28	108.06	110.70
1	16S1	974	A	C5-C6-N1	5.28	120.34	117.70
22	23S1	149	A	C5-C6-N1	5.28	120.34	117.70
22	23S1	1328	A	N3-C4-N9	5.28	131.62	127.40
22	23S1	1347	A	C8-N9-C4	5.28	107.91	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1579	A	C4-C5-N7	-5.28	108.06	110.70
22	23S1	2020	A	C4-C5-C6	5.28	119.64	117.00
1	16S1	262	A	C5-C6-N1	5.27	120.34	117.70
1	16S1	1004	A	C5-C6-N1	5.27	120.34	117.70
22	23S1	1155	A	C5-C6-N1	5.27	120.34	117.70
22	23S1	1566	A	C4-C5-C6	5.27	119.64	117.00
22	23S1	1668	A	C8-N9-C4	5.27	107.91	105.80
22	23S1	1794	A	C5-C6-N1	5.27	120.34	117.70
22	23S1	2020	A	C8-N9-C4	5.27	107.91	105.80
22	23S1	2497	A	C5-C6-N1	5.27	120.34	117.70
1	16S1	547	A	C4-C5-N7	-5.27	108.06	110.70
1	16S1	792	A	C5-C6-N1	5.27	120.34	117.70
22	23S1	104	A	C5-C6-N1	5.27	120.34	117.70
22	23S1	197	A	N9-C4-C5	5.27	107.91	105.80
22	23S1	1665	A	C8-N9-C4	5.27	107.91	105.80
22	23S1	2727	A	C8-N9-C4	5.27	107.91	105.80
1	16S1	495	A	N3-C4-N9	5.27	131.62	127.40
22	23S1	592	A	C8-N9-C4	5.27	107.91	105.80
22	23S1	626	A	N3-C4-N9	5.27	131.62	127.40
22	23S1	2154	A	C5-C6-N1	5.27	120.33	117.70
1	16S1	915	A	C4-C5-C6	5.27	119.63	117.00
22	23S1	149	A	N9-C4-C5	5.27	107.91	105.80
22	23S1	374	A	C5-C6-N1	5.27	120.33	117.70
22	23S1	502	A	C5-C6-N1	5.27	120.33	117.70
22	23S1	621	A	C4-C5-N7	-5.27	108.07	110.70
22	23S1	900	A	C5-C6-N1	5.27	120.33	117.70
22	23S1	1566	A	N9-C4-C5	5.27	107.91	105.80
22	23S1	1829	A	C8-N9-C4	5.27	107.91	105.80
22	23S1	1889	A	C8-N9-C4	5.27	107.91	105.80
22	23S1	2449	U	C6-N1-C2	5.27	124.16	121.00
23	05S1	104	A	C4-C5-N7	-5.27	108.07	110.70
1	16S1	946	A	C5-C6-N1	5.27	120.33	117.70
1	16S1	1111	A	C4-C5-N7	-5.27	108.07	110.70
1	16S1	1180	A	C4-C5-N7	-5.27	108.07	110.70
1	16S1	1508	A	C5-C6-N1	5.27	120.33	117.70
22	23S1	1632	A	C5-C6-N1	5.27	120.33	117.70
22	23S1	2813	A	N9-C4-C5	5.27	107.91	105.80
1	16S1	223	A	N9-C4-C5	5.26	107.91	105.80
1	16S1	648	A	C4-C5-N7	-5.26	108.07	110.70
22	23S1	300	A	C5-C6-N1	5.26	120.33	117.70
22	23S1	1304	A	C5-C6-N1	5.26	120.33	117.70
22	23S1	1403	A	C8-N9-C4	5.26	107.91	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1596	A	N9-C4-C5	5.26	107.91	105.80
22	23S1	2274	A	N9-C4-C5	5.26	107.91	105.80
22	23S1	2381	A	N9-C4-C5	5.26	107.91	105.80
22	23S1	927	A	C5-C6-N1	5.26	120.33	117.70
22	23S1	2736	A	C5-C6-N1	5.26	120.33	117.70
55	PTR1	42	A	C8-N9-C4	5.26	107.91	105.80
1	16S1	478	A	C4-C5-N7	-5.26	108.07	110.70
22	23S1	661	A	C4-C5-C6	5.26	119.63	117.00
22	23S1	675	A	C5-C6-N1	5.26	120.33	117.70
22	23S1	781	A	C4-C5-N7	-5.26	108.07	110.70
22	23S1	1308	A	N3-C4-N9	5.26	131.61	127.40
22	23S1	2850	A	C4-C5-N7	-5.26	108.07	110.70
1	16S1	889	A	C4-C5-N7	-5.26	108.07	110.70
22	23S1	1669	A	C4-C5-N7	-5.26	108.07	110.70
22	23S1	2278	A	C5-C6-N1	5.26	120.33	117.70
22	23S1	2634	A	C5-C6-N1	5.26	120.33	117.70
1	16S1	205	A	N9-C4-C5	5.26	107.90	105.80
1	16S1	978	A	C8-N9-C4	5.26	107.90	105.80
22	23S1	592	A	N9-C4-C5	5.26	107.90	105.80
22	23S1	2682	A	C4-C5-C6	5.26	119.63	117.00
1	16S1	807	A	C5-C6-N1	5.26	120.33	117.70
1	16S1	1507	A	C5-C6-N1	5.26	120.33	117.70
22	23S1	125	A	C4-C5-N7	-5.26	108.07	110.70
22	23S1	1960	A	C4-C5-N7	-5.26	108.07	110.70
22	23S1	2198	A	N3-C4-N9	5.26	131.61	127.40
1	16S1	288	A	C4-C5-N7	-5.25	108.07	110.70
1	16S1	802	A	C4-C5-N7	-5.25	108.07	110.70
1	16S1	802	A	N9-C4-C5	5.25	107.90	105.80
22	23S1	2740	A	C4-C5-C6	5.25	119.63	117.00
22	23S1	2835	A	C4-C5-N7	-5.25	108.07	110.70
1	16S1	336	A	C5-C6-N1	5.25	120.33	117.70
1	16S1	371	A	C4-C5-N7	-5.25	108.07	110.70
1	16S1	767	A	C4-C5-N7	-5.25	108.07	110.70
1	16S1	900	A	C5-C6-N1	5.25	120.33	117.70
1	16S1	1430	A	C4-C5-C6	5.25	119.63	117.00
22	23S1	878	A	C4-C5-C6	5.25	119.63	117.00
1	16S1	130	A	C8-N9-C4	5.25	107.90	105.80
1	16S1	1201	A	C4-C5-N7	-5.25	108.07	110.70
22	23S1	173	A	C5-C6-N1	5.25	120.33	117.70
22	23S1	1080	A	C5-C6-N1	5.25	120.33	117.70
22	23S1	1257	C	C6-N1-C2	-5.25	118.20	120.30
22	23S1	1569	A	N3-C4-N9	5.25	131.60	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2052	A	C8-N9-C4	5.25	107.90	105.80
22	23S1	2711	A	C5-C6-N1	5.25	120.33	117.70
22	23S1	2810	A	C4-C5-N7	-5.25	108.07	110.70
22	23S1	155	A	C4-C5-C6	5.25	119.62	117.00
22	23S1	287	G	C5-C6-O6	-5.25	125.45	128.60
22	23S1	906	U	O4'-C1'-N1	5.25	112.40	108.20
22	23S1	1378	A	N3-C4-N9	5.25	131.60	127.40
1	16S1	1329	A	N3-C4-N9	5.25	131.60	127.40
1	16S1	1434	A	C5-C6-N1	5.25	120.32	117.70
22	23S1	621	A	C5-C6-N1	5.25	120.33	117.70
22	23S1	789	A	C4-C5-C6	5.25	119.62	117.00
22	23S1	866	A	C4-C5-N7	-5.25	108.08	110.70
22	23S1	1084	A	N9-C4-C5	5.25	107.90	105.80
23	05S1	15	A	C4-C5-N7	-5.25	108.08	110.70
22	23S1	1342	A	C5-C6-N1	5.25	120.32	117.70
22	23S1	1354	A	N9-C4-C5	5.25	107.90	105.80
22	23S1	1365	A	C4-C5-N7	-5.25	108.08	110.70
22	23S1	2572	A	C4-C5-C6	5.25	119.62	117.00
23	05S1	104	A	N9-C4-C5	5.25	107.90	105.80
1	16S1	872	A	C5-N7-C8	5.25	106.52	103.90
22	23S1	739	A	C5-C6-N1	5.25	120.32	117.70
22	23S1	2412	A	N9-C4-C5	5.25	107.90	105.80
1	16S1	621	A	N9-C4-C5	5.24	107.90	105.80
22	23S1	1039	A	C8-N9-C4	5.24	107.90	105.80
22	23S1	1321	A	C8-N9-C4	5.24	107.90	105.80
22	23S1	1885	A	C4-C5-N7	-5.24	108.08	110.70
1	16S1	553	A	C8-N9-C4	5.24	107.90	105.80
22	23S1	631	A	C4-C5-C6	5.24	119.62	117.00
22	23S1	2639	A	N9-C4-C5	5.24	107.90	105.80
1	16S1	607	A	C4-C5-C6	5.24	119.62	117.00
1	16S1	1022	A	C4-C5-N7	-5.24	108.08	110.70
22	23S1	362	A	C5-C6-N6	5.24	127.89	123.70
22	23S1	505	A	C8-N9-C4	5.24	107.90	105.80
22	23S1	1050	A	N9-C4-C5	5.24	107.90	105.80
22	23S1	1652	A	C5-C6-N1	5.24	120.32	117.70
22	23S1	2378	A	C4-C5-N7	-5.24	108.08	110.70
22	23S1	2443	C	N3-C2-O2	-5.24	118.23	121.90
1	16S1	655	A	C4-C5-N7	-5.24	108.08	110.70
22	23S1	310	A	N9-C4-C5	5.24	107.89	105.80
22	23S1	689	A	C8-N9-C4	5.24	107.90	105.80
22	23S1	1366	A	N3-C4-N9	5.24	131.59	127.40
22	23S1	1553	A	C8-N9-C4	5.24	107.89	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2587	A	N9-C4-C5	5.24	107.90	105.80
1	16S1	1067	A	C4-C5-N7	-5.24	108.08	110.70
1	16S1	1141	C	C6-N1-C2	-5.24	118.20	120.30
22	23S1	1286	A	C5-C6-N1	5.24	120.32	117.70
22	23S1	1783	A	C4-C5-C6	5.24	119.62	117.00
23	05S1	53	A	C8-N9-C4	5.24	107.89	105.80
23	05S1	58	A	C8-N9-C4	5.24	107.89	105.80
1	16S1	143	A	C8-N9-C4	5.24	107.89	105.80
1	16S1	192	A	C5-C6-N1	5.24	120.32	117.70
1	16S1	532	A	C8-N9-C4	5.24	107.89	105.80
1	16S1	937	A	N9-C4-C5	5.24	107.89	105.80
1	16S1	969	A	C8-N9-C4	5.24	107.89	105.80
22	23S1	541	A	C4-C5-N7	-5.24	108.08	110.70
22	23S1	899	A	C5-C6-N1	5.24	120.32	117.70
22	23S1	941	A	C5-C6-N1	5.24	120.32	117.70
22	23S1	1701	A	C4-C5-C6	5.24	119.62	117.00
22	23S1	2247	A	C8-N9-C4	5.24	107.89	105.80
22	23S1	899	A	C4-C5-N7	-5.23	108.08	110.70
22	23S1	1133	A	N9-C4-C5	5.23	107.89	105.80
22	23S1	1722	A	C8-N9-C4	5.23	107.89	105.80
22	23S1	1918	A	N9-C4-C5	5.23	107.89	105.80
22	23S1	2015	A	N9-C4-C5	5.23	107.89	105.80
1	16S1	309	A	N9-C4-C5	5.23	107.89	105.80
1	16S1	1150	A	C4-C5-N7	-5.23	108.08	110.70
1	16S1	1216	A	C4-C5-C6	5.23	119.62	117.00
1	16S1	1483	A	C4-C5-N7	-5.23	108.08	110.70
22	23S1	646	U	C4-C5-C6	5.23	122.84	119.70
22	23S1	693	A	C4-C5-N7	-5.23	108.08	110.70
22	23S1	2392	A	C8-N9-C4	5.23	107.89	105.80
22	23S1	792	A	N9-C4-C5	5.23	107.89	105.80
22	23S1	2013	A	C8-N9-C4	5.23	107.89	105.80
22	23S1	2366	A	C8-N9-C4	5.23	107.89	105.80
55	PTR1	26	A	C4-C5-N7	-5.23	108.08	110.70
22	23S1	5	A	N9-C4-C5	5.23	107.89	105.80
1	16S1	192	A	C4-C5-N7	-5.23	108.09	110.70
1	16S1	1171	A	C5-C6-N1	5.23	120.31	117.70
22	23S1	346	A	C8-N9-C4	5.23	107.89	105.80
22	23S1	849	A	N9-C4-C5	5.23	107.89	105.80
22	23S1	1437	C	N1-C2-O2	5.23	122.04	118.90
22	23S1	1597	A	C5-C6-N1	5.23	120.31	117.70
22	23S1	2020	A	N9-C4-C5	5.23	107.89	105.80
1	16S1	363	A	C5-C6-N1	5.23	120.31	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	878	A	C5-C6-N1	5.23	120.31	117.70
1	16S1	1188	A	N9-C4-C5	5.23	107.89	105.80
22	23S1	1644	C	C6-N1-C2	-5.23	118.21	120.30
22	23S1	1757	A	C5-C6-N1	5.23	120.31	117.70
1	16S1	629	A	N9-C4-C5	5.22	107.89	105.80
22	23S1	676	A	N9-C4-C5	5.22	107.89	105.80
22	23S1	959	A	C4-C5-N7	-5.22	108.09	110.70
22	23S1	2471	A	C4-C5-N7	-5.22	108.09	110.70
22	23S1	2734	A	C4-C5-C6	5.22	119.61	117.00
22	23S1	95	A	C4-C5-N7	-5.22	108.09	110.70
22	23S1	126	A	N9-C4-C5	5.22	107.89	105.80
22	23S1	1241	A	C8-N9-C4	5.22	107.89	105.80
22	23S1	1496	A	C5-C6-N1	5.22	120.31	117.70
22	23S1	1919	A	C4-C5-C6	5.22	119.61	117.00
22	23S1	2748	A	N9-C4-C5	5.22	107.89	105.80
23	05S1	73	A	C5-C6-N1	5.22	120.31	117.70
55	PTR1	65	C	N1-C2-O2	5.22	122.03	118.90
1	16S1	857	C	N3-C2-O2	-5.22	118.25	121.90
1	16S1	949	A	C5-C6-N1	5.22	120.31	117.70
1	16S1	1306	A	C5-C6-N1	5.22	120.31	117.70
22	23S1	143	C	N3-C2-O2	-5.22	118.25	121.90
22	23S1	483	A	C4-C5-N7	-5.22	108.09	110.70
22	23S1	1246	A	C4-C5-N7	-5.22	108.09	110.70
22	23S1	1596	A	C4-C5-N7	-5.22	108.09	110.70
22	23S1	1656	C	C6-N1-C2	-5.22	118.21	120.30
22	23S1	1779	U	C2-N1-C1'	5.22	123.96	117.70
22	23S1	2461	A	N9-C4-C5	5.22	107.89	105.80
22	23S1	2639	A	C8-N9-C4	5.22	107.89	105.80
23	05S1	109	A	C5-C6-N1	5.22	120.31	117.70
1	16S1	695	A	N9-C4-C5	5.22	107.89	105.80
1	16S1	1035	A	C5-C6-N1	5.22	120.31	117.70
22	23S1	5	A	C4-C5-N7	-5.22	108.09	110.70
22	23S1	945	A	N3-C4-N9	5.22	131.57	127.40
22	23S1	706	A	C4-C5-C6	5.22	119.61	117.00
22	23S1	722	A	C8-N9-C4	5.22	107.89	105.80
22	23S1	784	G	C3'-C2'-C1'	5.22	105.67	101.50
22	23S1	1014	A	N9-C4-C5	5.22	107.89	105.80
22	23S1	1525	A	C8-N9-C4	5.22	107.89	105.80
22	23S1	2602	A	C4-C5-N7	-5.22	108.09	110.70
1	16S1	1340	A	C4-C5-N7	-5.21	108.09	110.70
22	23S1	526	A	C5-C6-N1	5.21	120.31	117.70
22	23S1	575	A	C8-N9-C4	5.21	107.89	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	676	A	C5-C6-N1	5.21	120.31	117.70
22	23S1	1336	A	C8-N9-C4	5.21	107.89	105.80
23	05S1	34	A	C5-C6-N1	5.21	120.31	117.70
22	23S1	1086	A	C5-C6-N1	5.21	120.31	117.70
22	23S1	1755	A	C4-C5-C6	5.21	119.61	117.00
1	16S1	600	A	C4-C5-N7	-5.21	108.09	110.70
1	16S1	665	A	C8-N9-C4	5.21	107.89	105.80
1	16S1	784	A	C4-C5-N7	-5.21	108.09	110.70
1	16S1	1239	A	N9-C4-C5	5.21	107.89	105.80
22	23S1	265	A	N3-C4-N9	5.21	131.57	127.40
22	23S1	340	A	C4-C5-N7	-5.21	108.09	110.70
22	23S1	655	A	N3-C4-N9	5.21	131.57	127.40
22	23S1	1027	A	C8-N9-C4	5.21	107.89	105.80
22	23S1	1847	A	C5-C6-N1	5.21	120.31	117.70
22	23S1	2097	A	N9-C4-C5	5.21	107.89	105.80
22	23S1	2273	A	N9-C4-C5	5.21	107.89	105.80
1	16S1	781	A	C8-N9-C4	5.21	107.88	105.80
22	23S1	1819	A	C5-C6-N1	5.21	120.31	117.70
22	23S1	2052	A	C4-C5-C6	5.21	119.61	117.00
22	23S1	2450	A	N3-C4-N9	5.21	131.57	127.40
22	23S1	800	A	C4-C5-C6	5.21	119.60	117.00
22	23S1	1626	A	C5-C6-N1	5.21	120.30	117.70
22	23S1	2572	A	N9-C4-C5	5.21	107.88	105.80
1	16S1	119	A	N9-C4-C5	5.21	107.88	105.80
1	16S1	572	A	N9-C4-C5	5.21	107.88	105.80
1	16S1	1055	A	N9-C4-C5	5.21	107.88	105.80
22	23S1	217	A	C4-C5-N7	-5.21	108.10	110.70
22	23S1	1630	A	N3-C4-N9	5.21	131.56	127.40
22	23S1	1755	A	N3-C4-N9	5.21	131.57	127.40
1	16S1	907	A	C8-N9-C4	5.21	107.88	105.80
1	16S1	1225	A	N9-C4-C5	5.21	107.88	105.80
1	16S1	1319	A	N3-C4-N9	5.21	131.56	127.40
22	23S1	1127	A	N3-C4-N9	5.21	131.56	127.40
22	23S1	1285	A	N3-C4-N9	5.21	131.56	127.40
22	23S1	685	A	C8-N9-C4	5.20	107.88	105.80
22	23S1	1354	A	C5-C6-N1	5.20	120.30	117.70
22	23S1	2829	A	C4-C5-N7	-5.20	108.10	110.70
1	16S1	199	A	C4-C5-N7	-5.20	108.10	110.70
1	16S1	1287	A	C4-C5-C6	5.20	119.60	117.00
22	23S1	1286	A	C4-C5-N7	-5.20	108.10	110.70
22	23S1	2682	A	C4-C5-N7	-5.20	108.10	110.70
22	23S1	2835	A	C5-C6-N1	5.20	120.30	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	167	A	N9-C4-C5	5.20	107.88	105.80
1	16S1	993	G	C4-N9-C1'	5.20	133.26	126.50
22	23S1	877	A	N9-C4-C5	5.20	107.88	105.80
22	23S1	1276	A	C8-N9-C4	5.20	107.88	105.80
22	23S1	2273	A	C5-C6-N1	5.20	120.30	117.70
22	23S1	2321	U	C2-N1-C1'	5.20	123.94	117.70
1	16S1	182	A	C4-C5-C6	5.20	119.60	117.00
1	16S1	553	A	C4-C5-N7	-5.20	108.10	110.70
1	16S1	878	A	C4-C5-N7	-5.20	108.10	110.70
22	23S1	861	A	C5-C6-N1	5.20	120.30	117.70
22	23S1	988	A	C4-C5-C6	5.20	119.60	117.00
22	23S1	1321	A	C5-C6-N1	5.20	120.30	117.70
22	23S1	1366	A	C4-C5-N7	-5.20	108.10	110.70
22	23S1	1815	A	C5-C6-N1	5.20	120.30	117.70
1	16S1	696	A	N9-C4-C5	5.20	107.88	105.80
1	16S1	906	A	N9-C4-C5	5.20	107.88	105.80
22	23S1	603	A	N9-C4-C5	5.20	107.88	105.80
22	23S1	1230	A	C8-N9-C4	5.20	107.88	105.80
1	16S1	915	A	C5-C6-N1	5.20	120.30	117.70
1	16S1	958	A	C8-N9-C4	5.20	107.88	105.80
22	23S1	111	A	C8-N9-C4	5.20	107.88	105.80
22	23S1	201	C	N3-C2-O2	-5.20	118.26	121.90
22	23S1	634	C	C6-N1-C2	-5.20	118.22	120.30
22	23S1	792	A	C5-C6-N1	5.20	120.30	117.70
22	23S1	1987	A	C5-C6-N1	5.20	120.30	117.70
22	23S1	198	C	C5-C6-N1	5.19	123.60	121.00
22	23S1	279	A	C4-C5-N7	-5.19	108.10	110.70
1	16S1	676	A	C4-C5-N7	-5.19	108.10	110.70
22	23S1	63	A	C5-C6-N1	5.19	120.30	117.70
22	23S1	453	A	C5-C6-N1	5.19	120.30	117.70
22	23S1	528	A	C4-C5-N7	-5.19	108.10	110.70
22	23S1	1040	A	C4-C5-N7	-5.19	108.10	110.70
22	23S1	1469	A	N9-C4-C5	5.19	107.88	105.80
22	23S1	1535	A	C8-N9-C4	5.19	107.88	105.80
22	23S1	2781	A	N3-C4-N9	5.19	131.55	127.40
1	16S1	243	A	C4-C5-C6	5.19	119.59	117.00
1	16S1	510	A	N9-C4-C5	5.19	107.88	105.80
22	23S1	332	A	N3-C4-N9	5.19	131.55	127.40
22	23S1	590	A	N9-C4-C5	5.19	107.88	105.80
22	23S1	706	A	N9-C4-C5	5.19	107.88	105.80
22	23S1	794	A	N9-C4-C5	5.19	107.88	105.80
22	23S1	1010	A	N3-C4-N9	5.19	131.55	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1366	A	C4-C5-C6	5.19	119.60	117.00
1	16S1	282	A	C4-C5-C6	5.19	119.59	117.00
1	16S1	306	A	C5-C6-N1	5.19	120.30	117.70
22	23S1	368	A	C8-N9-C4	5.19	107.88	105.80
22	23S1	603	A	C4-C5-C6	5.19	119.59	117.00
22	23S1	2020	A	C5-C6-N1	5.19	120.29	117.70
22	23S1	2471	A	N9-C4-C5	5.19	107.88	105.80
1	16S1	196	A	C4-C5-C6	5.19	119.59	117.00
1	16S1	547	A	C4-C5-C6	5.19	119.59	117.00
1	16S1	596	A	C8-N9-C4	5.19	107.88	105.80
22	23S1	1188	U	N1-C2-O2	5.19	126.43	122.80
22	23S1	1419	A	N9-C4-C5	5.19	107.88	105.80
22	23S1	2434	A	C5-C6-N1	5.19	120.29	117.70
22	23S1	2820	A	C8-N9-C4	5.19	107.88	105.80
1	16S1	1080	A	N9-C4-C5	5.18	107.87	105.80
22	23S1	472	A	N9-C4-C5	5.18	107.87	105.80
22	23S1	702	U	N3-C2-O2	-5.18	118.57	122.20
22	23S1	981	A	C8-N9-C4	5.18	107.87	105.80
22	23S1	2267	A	C8-N9-C4	5.18	107.87	105.80
22	23S1	2577	A	C8-N9-C4	5.18	107.87	105.80
22	23S1	471	A	C5-C6-N1	5.18	120.29	117.70
22	23S1	1260	A	C4-C5-C6	5.18	119.59	117.00
22	23S1	2327	A	C4-C5-N7	-5.18	108.11	110.70
22	23S1	2778	A	C4-C5-N7	-5.18	108.11	110.70
22	23S1	749	A	C4-C5-N7	-5.18	108.11	110.70
22	23S1	988	A	C4-C5-N7	-5.18	108.11	110.70
1	16S1	7	A	C8-N9-C4	5.18	107.87	105.80
1	16S1	88	U	N1-C2-O2	5.18	126.43	122.80
1	16S1	192	A	N9-C4-C5	5.18	107.87	105.80
1	16S1	1311	A	C4-C5-N7	-5.18	108.11	110.70
22	23S1	460	A	C4-C5-N7	-5.18	108.11	110.70
22	23S1	753	A	C4-C5-N7	-5.18	108.11	110.70
22	23S1	1786	A	C8-N9-C4	5.18	107.87	105.80
1	16S1	298	A	C4-C5-C6	5.18	119.59	117.00
1	16S1	600	A	N9-C4-C5	5.18	107.87	105.80
22	23S1	83	A	C5-C6-N1	5.18	120.29	117.70
22	23S1	515	A	C4-C5-N7	-5.18	108.11	110.70
22	23S1	1640	A	C4-C5-N7	-5.18	108.11	110.70
22	23S1	42	A	C4-C5-N7	-5.18	108.11	110.70
22	23S1	311	A	C5-C6-N1	5.18	120.29	117.70
22	23S1	529	A	N3-C4-N9	5.18	131.54	127.40
22	23S1	608	A	C5-C6-N1	5.18	120.29	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2800	A	C5-C6-N1	5.18	120.29	117.70
1	16S1	523	A	C5-C6-N1	5.17	120.29	117.70
1	16S1	1468	A	C5-C6-N1	5.17	120.29	117.70
22	23S1	547	A	C4-C5-C6	5.17	119.59	117.00
22	23S1	928	A	C4-C5-C6	5.17	119.59	117.00
22	23S1	1853	A	C4-C5-C6	5.17	119.59	117.00
22	23S1	2274	A	N3-C4-N9	5.17	131.54	127.40
1	16S1	753	A	C4-C5-N7	-5.17	108.11	110.70
1	16S1	1375	A	C8-N9-C4	5.17	107.87	105.80
22	23S1	10	A	N9-C4-C5	5.17	107.87	105.80
22	23S1	478	A	C5-C6-N1	5.17	120.29	117.70
22	23S1	1054	A	N9-C4-C5	5.17	107.87	105.80
22	23S1	1913	A	C5-C6-N1	5.17	120.29	117.70
1	16S1	364	A	C8-N9-C4	5.17	107.87	105.80
1	16S1	539	A	C8-N9-C4	5.17	107.87	105.80
1	16S1	1197	A	C4-C5-N7	-5.17	108.11	110.70
22	23S1	64	A	C5-C6-N1	5.17	120.29	117.70
22	23S1	528	A	C8-N9-C4	5.17	107.87	105.80
22	23S1	918	A	C5-C6-N1	5.17	120.29	117.70
22	23S1	1213	A	C4-C5-N7	-5.17	108.11	110.70
22	23S1	1803	A	N9-C4-C5	5.17	107.87	105.80
1	16S1	167	A	C4-C5-N7	-5.17	108.11	110.70
1	16S1	382	A	C4-C5-N7	-5.17	108.11	110.70
22	23S1	532	A	C4-C5-N7	-5.17	108.11	110.70
22	23S1	2654	A	N9-C4-C5	5.17	107.87	105.80
23	05S1	52	A	N9-C4-C5	5.17	107.87	105.80
22	23S1	346	A	C4-C5-C6	5.17	119.58	117.00
22	23S1	666	A	C5-C6-N1	5.17	120.28	117.70
22	23S1	789	A	N9-C4-C5	5.17	107.87	105.80
22	23S1	821	A	C5-C6-N1	5.17	120.28	117.70
55	PTR1	20	U	C6-N1-C2	5.17	124.10	121.00
1	16S1	130	A	N9-C4-C5	5.17	107.87	105.80
1	16S1	199	A	C8-N9-C4	5.17	107.87	105.80
22	23S1	342	A	C4-C5-N7	-5.17	108.12	110.70
22	23S1	1214	A	N3-C4-N9	5.17	131.53	127.40
22	23S1	1713	A	C5-C6-N1	5.17	120.28	117.70
22	23S1	2531	A	C5-C6-N1	5.17	120.28	117.70
22	23S1	2572	A	N3-C4-N9	5.17	131.53	127.40
1	16S1	174	A	N9-C4-C5	5.17	107.87	105.80
1	16S1	298	A	N9-C4-C5	5.17	107.87	105.80
1	16S1	819	A	C5-C6-N1	5.17	120.28	117.70
55	PTR1	73	A	C4-C5-N7	-5.17	108.12	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	246	A	C4-C5-N7	-5.16	108.12	110.70
1	16S1	1513	A	C5-C6-N1	5.16	120.28	117.70
22	23S1	802	A	C4-C5-N7	-5.16	108.12	110.70
22	23S1	1001	A	C4-C5-N7	-5.16	108.12	110.70
22	23S1	1194	A	N3-C4-N9	5.16	131.53	127.40
22	23S1	1495	A	C8-N9-C4	5.16	107.86	105.80
22	23S1	2336	A	N3-C4-N9	5.16	131.53	127.40
1	16S1	1016	A	C4-C5-N7	-5.16	108.12	110.70
1	16S1	1197	A	C5-C6-N1	5.16	120.28	117.70
1	16S1	1446	A	C5-C6-N1	5.16	120.28	117.70
22	23S1	973	A	C5-C6-N1	5.16	120.28	117.70
1	16S1	454	G	N3-C4-C5	-5.16	126.02	128.60
1	16S1	908	A	N9-C4-C5	5.16	107.86	105.80
1	16S1	932	C	N1-C2-O2	5.16	122.00	118.90
1	16S1	1213	A	C4-C5-C6	5.16	119.58	117.00
22	23S1	42	A	N9-C4-C5	5.16	107.86	105.80
22	23S1	430	A	C5-C6-N1	5.16	120.28	117.70
22	23S1	1032	A	C4-C5-C6	5.16	119.58	117.00
22	23S1	2565	A	C4-C5-N7	-5.16	108.12	110.70
1	16S1	622	A	C5-C6-N1	5.16	120.28	117.70
1	16S1	892	A	N9-C4-C5	5.16	107.86	105.80
22	23S1	2147	A	N3-C4-N9	5.16	131.53	127.40
22	23S1	2513	A	C4-C5-N7	-5.16	108.12	110.70
22	23S1	84	A	C4-C5-N7	-5.16	108.12	110.70
22	23S1	1039	A	N3-C4-N9	5.16	131.53	127.40
22	23S1	1088	A	N9-C4-C5	5.16	107.86	105.80
22	23S1	2750	A	C5-C6-N1	5.16	120.28	117.70
1	16S1	768	A	C4-C5-C6	5.16	119.58	117.00
1	16S1	937	A	C8-N9-C4	5.16	107.86	105.80
1	16S1	1500	A	C4-C5-N7	-5.16	108.12	110.70
22	23S1	181	A	C4-C5-N7	-5.16	108.12	110.70
22	23S1	347	A	C8-N9-C4	5.16	107.86	105.80
22	23S1	918	A	N9-C4-C5	5.16	107.86	105.80
22	23S1	1156	A	C4-C5-N7	-5.16	108.12	110.70
22	23S1	1853	A	C8-N9-C4	5.16	107.86	105.80
1	16S1	1204	A	C8-N9-C4	5.15	107.86	105.80
22	23S1	1664	A	C5-C6-N1	5.15	120.28	117.70
22	23S1	1819	A	C4-C5-N7	-5.15	108.12	110.70
22	23S1	2009	A	C4-C5-C6	5.15	119.58	117.00
22	23S1	2134	A	C5-C6-N1	5.15	120.28	117.70
23	05S1	78	A	C8-N9-C4	5.15	107.86	105.80
1	16S1	802	A	C4-C5-C6	5.15	119.58	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	244	A	N9-C4-C5	5.15	107.86	105.80
22	23S1	990	A	C5-C6-N1	5.15	120.28	117.70
22	23S1	1077	A	N3-C4-N9	5.15	131.52	127.40
22	23S1	1762	A	C5-C6-N1	5.15	120.28	117.70
22	23S1	1815	A	N3-C4-N9	5.15	131.52	127.40
22	23S1	2820	A	C4-C5-C6	5.15	119.58	117.00
1	16S1	1441	A	C4-C5-N7	-5.15	108.12	110.70
22	23S1	1048	A	C4-C5-N7	-5.15	108.12	110.70
22	23S1	2090	A	N9-C4-C5	5.15	107.86	105.80
1	16S1	1476	A	C4-C5-N7	-5.15	108.12	110.70
22	23S1	1054	A	C5-C6-N1	5.15	120.27	117.70
22	23S1	1226	A	N3-C4-N9	5.15	131.52	127.40
22	23S1	1749	A	C8-N9-C4	5.15	107.86	105.80
22	23S1	2205	A	C5-C6-N1	5.15	120.27	117.70
1	16S1	1055	A	C4-C5-N7	-5.15	108.13	110.70
1	16S1	1534	A	N3-C4-N9	5.15	131.52	127.40
22	23S1	457	A	C4-C5-N7	-5.15	108.13	110.70
22	23S1	676	A	N3-C4-N9	5.15	131.52	127.40
22	23S1	752	A	C4-C5-C6	5.15	119.57	117.00
22	23S1	1213	A	N9-C4-C5	5.15	107.86	105.80
22	23S1	1469	A	C8-N9-C4	5.15	107.86	105.80
22	23S1	1928	A	C8-N9-C4	5.15	107.86	105.80
22	23S1	2565	A	C8-N9-C4	5.15	107.86	105.80
22	23S1	2665	A	C4-C5-N7	-5.15	108.13	110.70
1	16S1	1005	A	C4-C5-N7	-5.15	108.13	110.70
1	16S1	1012	A	N9-C4-C5	5.15	107.86	105.80
22	23S1	95	A	C5-C6-N1	5.15	120.27	117.70
22	23S1	2051	A	N9-C4-C5	5.15	107.86	105.80
1	16S1	546	A	C5-C6-N1	5.14	120.27	117.70
1	16S1	722	G	C4-N9-C1'	5.14	133.19	126.50
1	16S1	1456	A	N9-C4-C5	5.14	107.86	105.80
22	23S1	83	A	C4-C5-N7	-5.14	108.13	110.70
22	23S1	920	A	C8-N9-C4	5.14	107.86	105.80
22	23S1	1772	A	C5-C6-N1	5.14	120.27	117.70
22	23S1	1866	A	C5-C6-N1	5.14	120.27	117.70
22	23S1	2284	A	C4-C5-N7	-5.14	108.13	110.70
23	05S1	29	A	C5-C6-N1	5.14	120.27	117.70
1	16S1	759	A	N9-C4-C5	5.14	107.86	105.80
22	23S1	231	A	C8-N9-C4	5.14	107.86	105.80
22	23S1	479	A	C4-C5-C6	5.14	119.57	117.00
22	23S1	1583	A	C4-C5-N7	-5.14	108.13	110.70
22	23S1	2154	A	N9-C4-C5	5.14	107.86	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2268	A	C4-C5-N7	-5.14	108.13	110.70
23	05S1	26	C	N1-C2-O2	5.14	121.98	118.90
22	23S1	1308	A	C5-C6-N1	5.14	120.27	117.70
1	16S1	753	A	N9-C4-C5	5.14	107.86	105.80
22	23S1	342	A	C5-C6-N1	5.14	120.27	117.70
22	23S1	655	A	N9-C4-C5	5.14	107.86	105.80
22	23S1	2733	A	N9-C4-C5	5.14	107.86	105.80
23	05S1	50	A	C4-C5-N7	-5.14	108.13	110.70
1	16S1	819	A	C4-C5-N7	-5.14	108.13	110.70
22	23S1	401	A	N9-C4-C5	5.14	107.86	105.80
22	23S1	1289	C	N1-C2-O2	5.14	121.98	118.90
22	23S1	2530	A	C5-C6-N1	5.14	120.27	117.70
22	23S1	2634	A	N9-C4-C5	5.14	107.86	105.80
22	23S1	2657	A	C4-C5-N7	-5.14	108.13	110.70
1	16S1	243	A	C8-N9-C4	5.14	107.85	105.80
22	23S1	457	A	N9-C4-C5	5.14	107.85	105.80
22	23S1	460	A	N9-C4-C5	5.14	107.86	105.80
22	23S1	782	A	N9-C4-C5	5.14	107.85	105.80
22	23S1	2146	C	P-O3'-C3'	5.14	125.86	119.70
22	23S1	2311	A	C4-C5-C6	5.14	119.57	117.00
23	05S1	94	A	C8-N9-C4	5.14	107.85	105.80
1	16S1	116	A	C5-C6-N1	5.13	120.27	117.70
1	16S1	120	A	N9-C4-C5	5.13	107.85	105.80
1	16S1	642	A	N9-C4-C5	5.13	107.85	105.80
1	16S1	1287	A	C4-C5-N7	-5.13	108.13	110.70
1	16S1	1324	A	N9-C4-C5	5.13	107.85	105.80
22	23S1	1717	A	C5-C6-N1	5.13	120.27	117.70
22	23S1	2165	C	C6-N1-C2	-5.13	118.25	120.30
55	PTR1	20	U	C4-C5-C6	-5.13	116.62	119.70
1	16S1	327	A	C8-N9-C4	5.13	107.85	105.80
1	16S1	411	A	C4-C5-C6	5.13	119.57	117.00
22	23S1	1652	A	N3-C4-N9	5.13	131.51	127.40
22	23S1	2377	A	C5-C6-N1	5.13	120.27	117.70
1	16S1	253	A	C5-C6-N1	5.13	120.27	117.70
1	16S1	274	A	C4-C5-C6	5.13	119.56	117.00
1	16S1	1274	A	C5-C6-N1	5.13	120.27	117.70
22	23S1	391	A	C5-C6-N1	5.13	120.27	117.70
22	23S1	920	A	N9-C4-C5	5.13	107.85	105.80
22	23S1	975	A	C8-N9-C4	5.13	107.85	105.80
22	23S1	1689	A	C4-C5-N7	-5.13	108.13	110.70
22	23S1	2776	A	C4-C5-C6	5.13	119.57	117.00
22	23S1	330	A	C8-N9-C4	5.13	107.85	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	129	A	C8-N9-C4	5.13	107.85	105.80
1	16S1	825	A	C4-C5-C6	5.13	119.56	117.00
1	16S1	1179	A	C4-C5-N7	-5.13	108.14	110.70
22	23S1	988	A	C5-C6-N1	5.13	120.26	117.70
22	23S1	2033	A	N3-C4-N9	5.13	131.50	127.40
22	23S1	2534	A	C5-C6-N1	5.13	120.27	117.70
22	23S1	2541	A	C4-C5-N7	-5.13	108.14	110.70
55	PTR1	6	C	C2-N1-C1'	5.13	124.44	118.80
1	16S1	915	A	N3-C4-N9	5.13	131.50	127.40
22	23S1	833	A	C4-C5-C6	5.13	119.56	117.00
22	23S1	1786	A	C5-C6-N1	5.13	120.26	117.70
22	23S1	2196	C	N3-C2-O2	-5.13	118.31	121.90
22	23S1	2346	A	C8-N9-C4	5.13	107.85	105.80
22	23S1	2461	A	C8-N9-C4	5.13	107.85	105.80
1	16S1	72	A	C8-N9-C4	5.12	107.85	105.80
1	16S1	1092	A	C4-C5-N7	-5.12	108.14	110.70
22	23S1	299	A	C5-C6-N1	5.12	120.26	117.70
22	23S1	2227	A	C8-N9-C4	5.12	107.85	105.80
22	23S1	2734	A	N9-C4-C5	5.12	107.85	105.80
1	16S1	1105	A	N9-C4-C5	5.12	107.85	105.80
1	16S1	1196	A	C5-C6-N1	5.12	120.26	117.70
1	16S1	74	A	C4-C5-C6	5.12	119.56	117.00
1	16S1	79	G	N3-C4-N9	5.12	129.07	126.00
1	16S1	303	A	C8-N9-C4	5.12	107.85	105.80
1	16S1	321	A	C4-C5-N7	-5.12	108.14	110.70
1	16S1	702	A	N3-C4-N9	5.12	131.50	127.40
1	16S1	901	A	C6-C5-N7	-5.12	128.72	132.30
22	23S1	28	A	C5-C6-N1	5.12	120.26	117.70
22	23S1	71	A	C8-N9-C4	5.12	107.85	105.80
22	23S1	114	U	C2-N1-C1'	5.12	123.85	117.70
22	23S1	158	U	N1-C2-O2	5.12	126.39	122.80
22	23S1	1126	A	N9-C4-C5	5.12	107.85	105.80
22	23S1	1757	A	N9-C4-C5	5.12	107.85	105.80
22	23S1	1848	A	C5-C6-N1	5.12	120.26	117.70
22	23S1	2882	A	C4-C5-C6	5.12	119.56	117.00
30	L311	56	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	16S1	1280	A	N9-C4-C5	5.12	107.85	105.80
22	23S1	501	A	C5-C6-N1	5.12	120.26	117.70
22	23S1	1931	U	N1-C2-O2	5.12	126.38	122.80
1	16S1	279	A	N3-C4-N9	5.12	131.50	127.40
1	16S1	747	A	C4-C5-N7	-5.12	108.14	110.70
1	16S1	1204	A	C4-C5-C6	5.12	119.56	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	310	A	C5-C6-N1	5.12	120.26	117.70
22	23S1	1504	A	C4-C5-N7	-5.12	108.14	110.70
22	23S1	1509	A	N9-C4-C5	5.12	107.85	105.80
22	23S1	1810	A	C5-N7-C8	5.12	106.46	103.90
22	23S1	2322	A	C4-C5-N7	-5.12	108.14	110.70
22	23S1	900	A	C8-N9-C4	5.12	107.85	105.80
22	23S1	1230	A	N9-C4-C5	5.12	107.85	105.80
22	23S1	2003	A	C4-C5-N7	-5.12	108.14	110.70
22	23S1	2534	A	N9-C4-C5	5.12	107.85	105.80
22	23S1	2711	A	N9-C4-C5	5.12	107.85	105.80
1	16S1	353	A	N9-C4-C5	5.12	107.85	105.80
1	16S1	790	A	C8-N9-C4	5.12	107.85	105.80
22	23S1	538	A	C4-C5-N7	-5.12	108.14	110.70
22	23S1	655	A	C4-C5-C6	5.12	119.56	117.00
22	23S1	1495	A	C4-C5-C6	5.12	119.56	117.00
22	23S1	1634	A	N9-C4-C5	5.12	107.85	105.80
22	23S1	2171	A	C5-C6-N1	5.12	120.26	117.70
22	23S1	2211	A	C5-C6-N1	5.12	120.26	117.70
22	23S1	677	A	C8-N9-C4	5.11	107.85	105.80
22	23S1	802	A	N9-C4-C5	5.11	107.85	105.80
22	23S1	1603	A	C8-N9-C4	5.11	107.85	105.80
22	23S1	1610	A	C4-C5-C6	5.11	119.56	117.00
22	23S1	1754	A	C6-N1-C2	5.11	121.67	118.60
22	23S1	1916	A	N9-C4-C5	5.11	107.84	105.80
22	23S1	2307	G	C5-C6-O6	-5.11	125.53	128.60
22	23S1	2321	U	N1-C2-O2	5.11	126.38	122.80
22	23S1	2432	A	C8-N9-C4	5.11	107.84	105.80
1	16S1	160	A	C4-C5-N7	-5.11	108.14	110.70
1	16S1	439	U	C5-C4-O4	-5.11	122.83	125.90
22	23S1	1084	A	C5-C6-N1	5.11	120.26	117.70
22	23S1	1637	A	C5-C6-N1	5.11	120.26	117.70
1	16S1	274	A	C4-C5-N7	-5.11	108.14	110.70
1	16S1	129	A	C5-C6-N1	5.11	120.25	117.70
22	23S1	56	A	N9-C4-C5	5.11	107.84	105.80
22	23S1	756	A	N9-C4-C5	5.11	107.84	105.80
22	23S1	2682	A	N9-C4-C5	5.11	107.84	105.80
55	PTR1	73	A	C4-C5-C6	5.11	119.56	117.00
1	16S1	630	A	N9-C4-C5	5.11	107.84	105.80
22	23S1	155	A	C8-N9-C4	5.11	107.84	105.80
22	23S1	550	C	N1-C2-O2	5.11	121.97	118.90
22	23S1	1001	A	C4-C5-C6	5.11	119.55	117.00
22	23S1	1156	A	N9-C4-C5	5.11	107.84	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1885	A	N9-C4-C5	5.11	107.84	105.80
1	16S1	162	A	C6-C5-N7	-5.11	128.72	132.30
1	16S1	435	A	C4-C5-N7	-5.11	108.15	110.70
22	23S1	265	A	C4-C5-C6	5.11	119.55	117.00
22	23S1	1175	A	C8-N9-C4	5.11	107.84	105.80
22	23S1	1189	A	C5-C6-N1	5.11	120.25	117.70
22	23S1	1322	A	N9-C4-C5	5.11	107.84	105.80
22	23S1	1641	A	C4-C5-N7	-5.11	108.15	110.70
22	23S1	2058	A	C5-C6-N1	5.11	120.25	117.70
1	16S1	1513	A	N9-C4-C5	5.10	107.84	105.80
22	23S1	574	A	C5-C6-N1	5.10	120.25	117.70
22	23S1	752	A	N3-C4-N9	5.10	131.48	127.40
22	23S1	1274	A	C4-C5-N7	-5.10	108.15	110.70
1	16S1	1059	C	C6-N1-C2	-5.10	118.26	120.30
1	16S1	607	A	N3-C4-N9	5.10	131.48	127.40
1	16S1	994	A	C5-C6-N1	5.10	120.25	117.70
22	23S1	231	A	C4-C5-N7	-5.10	108.15	110.70
22	23S1	734	A	C5-C6-N1	5.10	120.25	117.70
22	23S1	1020	A	N9-C4-C5	5.10	107.84	105.80
1	16S1	3	A	C4-C5-N7	-5.10	108.15	110.70
22	23S1	126	A	C8-N9-C4	5.10	107.84	105.80
1	16S1	3	A	C4-C5-C6	5.10	119.55	117.00
1	16S1	160	A	N9-C4-C5	5.10	107.84	105.80
1	16S1	695	A	C4-C5-N7	-5.10	108.15	110.70
1	16S1	1339	A	N9-C4-C5	5.10	107.84	105.80
22	23S1	1829	A	C5-C6-N1	5.10	120.25	117.70
22	23S1	2749	A	C5-C6-N1	5.10	120.25	117.70
23	05S1	115	A	C5-C6-N1	5.10	120.25	117.70
22	23S1	2098	U	N3-C2-O2	-5.10	118.63	122.20
22	23S1	2797	U	N3-C2-O2	-5.10	118.63	122.20
1	16S1	205	A	C5-C6-N1	5.09	120.25	117.70
1	16S1	978	A	C4-C5-C6	5.09	119.55	117.00
1	16S1	1225	A	C4-C5-N7	-5.09	108.15	110.70
22	23S1	89	A	C4-C5-N7	-5.09	108.15	110.70
22	23S1	127	A	N3-C4-N9	5.09	131.47	127.40
22	23S1	1384	A	C5-C6-N1	5.09	120.25	117.70
22	23S1	1772	A	C4-C5-N7	-5.09	108.15	110.70
22	23S1	1889	A	C5-C6-N1	5.09	120.25	117.70
1	16S1	609	A	N9-C4-C5	5.09	107.84	105.80
1	16S1	924	C	C6-N1-C2	-5.09	118.26	120.30
1	16S1	1507	A	C8-N9-C4	5.09	107.84	105.80
22	23S1	344	A	C5-C6-N1	5.09	120.25	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	927	A	C8-N9-C4	5.09	107.84	105.80
22	23S1	1260	A	N9-C4-C5	5.09	107.84	105.80
1	16S1	236	A	C8-N9-C4	5.09	107.84	105.80
1	16S1	532	A	C4-C5-N7	-5.09	108.15	110.70
1	16S1	780	A	N9-C4-C5	5.09	107.84	105.80
22	23S1	141	G	C4-N9-C1'	5.09	133.12	126.50
22	23S1	332	A	C5-C6-N1	5.09	120.25	117.70
22	23S1	1262	A	C5-C6-N1	5.09	120.25	117.70
22	23S1	1815	A	N9-C4-C5	5.09	107.84	105.80
23	05S1	119	A	C8-N9-C4	5.09	107.84	105.80
22	23S1	1134	A	N9-C4-C5	5.09	107.84	105.80
22	23S1	1383	A	N3-C4-N9	5.09	131.47	127.40
22	23S1	1505	A	C5-C6-N1	5.09	120.25	117.70
22	23S1	1583	A	C5-C6-N1	5.09	120.25	117.70
22	23S1	2158	A	C5-C6-N1	5.09	120.24	117.70
22	23S1	2298	A	N9-C4-C5	5.09	107.83	105.80
1	16S1	428	G	C4-N9-C1'	-5.09	119.89	126.50
1	16S1	1319	A	C4-C5-N7	-5.09	108.16	110.70
1	16S1	1480	A	C8-N9-C4	5.09	107.83	105.80
22	23S1	947	A	C5-C6-N1	5.09	120.24	117.70
22	23S1	1477	A	C5-C6-N1	5.09	120.24	117.70
22	23S1	2119	A	C5-C6-N1	5.09	120.24	117.70
1	16S1	16	A	C6-N1-C2	5.08	121.65	118.60
22	23S1	507	A	C5-C6-N1	5.08	120.24	117.70
22	23S1	2406	A	C5-C6-N1	5.08	120.24	117.70
55	PTR1	26	A	N9-C4-C5	5.08	107.83	105.80
1	16S1	306	A	C4-C5-N7	-5.08	108.16	110.70
1	16S1	704	A	C6-N1-C2	5.08	121.65	118.60
1	16S1	1067	A	C6-N1-C2	5.08	121.65	118.60
1	16S1	1132	C	C5-C6-N1	5.08	123.54	121.00
1	16S1	1510	C	N3-C2-O2	-5.08	118.34	121.90
22	23S1	781	A	N9-C4-C5	5.08	107.83	105.80
22	23S1	804	A	C4-C5-C6	5.08	119.54	117.00
22	23S1	1153	C	N3-C2-O2	-5.08	118.34	121.90
22	23S1	1276	A	C5-C6-N1	5.08	120.24	117.70
22	23S1	1413	A	C4-C5-N7	-5.08	108.16	110.70
22	23S1	2748	A	C5-C6-N1	5.08	120.24	117.70
1	16S1	2	A	C4-C5-N7	-5.08	108.16	110.70
1	16S1	602	A	C8-N9-C4	5.08	107.83	105.80
1	16S1	681	A	C8-N9-C4	5.08	107.83	105.80
1	16S1	1339	A	C5-C6-N1	5.08	120.24	117.70
22	23S1	1098	A	C4-C5-N7	-5.08	108.16	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2333	A	N9-C4-C5	5.08	107.83	105.80
22	23S1	2453	A	C5-C6-N1	5.08	120.24	117.70
1	16S1	313	A	C5-C6-N1	5.08	120.24	117.70
1	16S1	574	A	N9-C4-C5	5.08	107.83	105.80
1	16S1	1413	A	N3-C4-N9	5.08	131.46	127.40
22	23S1	279	A	N9-C4-C5	5.08	107.83	105.80
22	23S1	443	A	N9-C4-C5	5.08	107.83	105.80
22	23S1	804	A	C8-N9-C4	5.08	107.83	105.80
22	23S1	981	A	N9-C4-C5	5.08	107.83	105.80
22	23S1	1966	A	C5-C6-N1	5.08	120.24	117.70
1	16S1	349	A	C4-C5-N7	-5.08	108.16	110.70
1	16S1	845	A	C4-C5-C6	5.08	119.54	117.00
1	16S1	1019	A	C4-C5-N7	-5.08	108.16	110.70
22	23S1	142	A	C8-N9-C4	5.08	107.83	105.80
22	23S1	1433	A	N9-C4-C5	5.08	107.83	105.80
22	23S1	1515	A	C8-N9-C4	5.08	107.83	105.80
22	23S1	1650	A	N9-C4-C5	5.08	107.83	105.80
22	23S1	1664	A	C4-C5-N7	-5.08	108.16	110.70
22	23S1	2212	A	C5-C6-N1	5.08	120.24	117.70
22	23S1	1086	A	C8-N9-C4	5.08	107.83	105.80
22	23S1	2850	A	C5-C6-N1	5.08	120.24	117.70
51	L351	32	ILE	CG1-CB-CG2	-5.08	100.23	111.40
1	16S1	7	A	N3-C4-N9	5.08	131.46	127.40
1	16S1	1254	A	C5-C6-N1	5.08	120.24	117.70
22	23S1	748	G	O4'-C1'-N9	5.08	112.26	108.20
22	23S1	1194	A	C4-C5-C6	5.08	119.54	117.00
22	23S1	1359	A	C4-C5-N7	-5.08	108.16	110.70
22	23S1	1547	C	C6-N1-C2	-5.08	118.27	120.30
22	23S1	2225	A	C5-C6-N1	5.08	120.24	117.70
29	L091	117	LEU	CA-CB-CG	5.08	126.98	115.30
1	16S1	488	C	N1-C2-O2	5.07	121.94	118.90
22	23S1	715	A	C8-N9-C4	5.07	107.83	105.80
22	23S1	758	C	N1-C2-O2	5.07	121.94	118.90
22	23S1	1095	A	N9-C4-C5	5.07	107.83	105.80
23	05S1	52	A	C5-C6-N1	5.07	120.24	117.70
1	16S1	1375	A	C4-C5-N7	-5.07	108.16	110.70
1	16S1	1500	A	N3-C4-N9	5.07	131.46	127.40
22	23S1	2051	A	C5-C6-N1	5.07	120.24	117.70
22	23S1	2094	A	C4-C5-N7	-5.07	108.16	110.70
22	23S1	2764	A	C4-C5-C6	5.07	119.54	117.00
1	16S1	787	A	C5-C6-N1	5.07	120.23	117.70
1	16S1	1098	C	N1-C2-O2	5.07	121.94	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	644	A	N9-C4-C5	5.07	107.83	105.80
22	23S1	1783	A	C8-N9-C4	5.07	107.83	105.80
22	23S1	2750	A	C4-C5-N7	-5.07	108.17	110.70
1	16S1	1480	A	C5-C6-N1	5.07	120.23	117.70
22	23S1	1147	A	C4-C5-N7	-5.07	108.17	110.70
22	23S1	1630	A	C8-N9-C4	5.07	107.83	105.80
22	23S1	1700	A	C5-C6-N1	5.07	120.23	117.70
1	16S1	676	A	C8-N9-C4	5.07	107.83	105.80
1	16S1	906	A	C5-C6-N1	5.07	120.23	117.70
1	16S1	960	U	C2-N1-C1'	5.07	123.78	117.70
22	23S1	668	A	C4-C5-C6	5.07	119.53	117.00
22	23S1	1920	C	N1-C2-O2	5.07	121.94	118.90
22	23S1	2376	A	C5-C6-N1	5.07	120.23	117.70
22	23S1	2388	A	C4-C5-N7	-5.07	108.17	110.70
1	16S1	32	A	C8-N9-C4	5.07	107.83	105.80
1	16S1	338	A	C5-C6-N1	5.07	120.23	117.70
1	16S1	608	A	N9-C4-C5	5.07	107.83	105.80
1	16S1	1204	A	C4-C5-N7	-5.07	108.17	110.70
1	16S1	1256	A	C5-C6-N1	5.07	120.23	117.70
1	16S1	1465	A	N9-C4-C5	5.07	107.83	105.80
22	23S1	282	A	C5-C6-N1	5.07	120.23	117.70
22	23S1	454	A	N3-C4-N9	5.07	131.45	127.40
22	23S1	460	A	C8-N9-C4	5.07	107.83	105.80
22	23S1	609	A	C4-C5-N7	-5.07	108.17	110.70
22	23S1	632	A	C5-C6-N1	5.07	120.23	117.70
22	23S1	735	A	C4-C5-N7	-5.07	108.17	110.70
22	23S1	1494	A	N3-C4-N9	5.07	131.45	127.40
22	23S1	2497	A	C4-C5-N7	-5.07	108.17	110.70
1	16S1	1167	A	C5-C6-N1	5.06	120.23	117.70
1	16S1	1332	A	N9-C4-C5	5.06	107.83	105.80
1	16S1	1408	A	C4-C5-C6	5.06	119.53	117.00
1	16S1	649	A	N3-C4-N9	5.06	131.45	127.40
1	16S1	865	A	C5-C6-N1	5.06	120.23	117.70
22	23S1	1427	A	C4-C5-N7	-5.06	108.17	110.70
22	23S1	156	A	N9-C4-C5	5.06	107.82	105.80
22	23S1	616	A	C5-C6-N1	5.06	120.23	117.70
1	16S1	579	A	N9-C4-C5	5.06	107.82	105.80
22	23S1	5	A	C8-N9-C4	5.06	107.82	105.80
22	23S1	572	A	C5-C6-N1	5.06	120.23	117.70
22	23S1	936	A	C4-C5-N7	-5.06	108.17	110.70
22	23S1	1275	A	C6-N1-C2	5.06	121.64	118.60
22	23S1	2033	A	C5-C6-N1	5.06	120.23	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1	A	C5-C6-N1	5.06	120.23	117.70
1	16S1	502	A	N9-C4-C5	5.06	107.82	105.80
1	16S1	1374	A	C8-N9-C4	5.06	107.82	105.80
22	23S1	366	C	C6-N1-C2	-5.06	118.28	120.30
22	23S1	401	A	C4-C5-N7	-5.06	108.17	110.70
22	23S1	2183	A	C5-C6-N1	5.06	120.23	117.70
22	23S1	654	A	N9-C4-C5	5.06	107.82	105.80
22	23S1	1057	A	C4-C5-C6	5.06	119.53	117.00
22	23S1	1690	A	C5-C6-N1	5.06	120.23	117.70
22	23S1	2077	A	C8-N9-C4	5.06	107.82	105.80
1	16S1	1155	A	N9-C4-C5	5.05	107.82	105.80
1	16S1	1377	A	C5-C6-N1	5.05	120.23	117.70
22	23S1	821	A	C8-N9-C4	5.05	107.82	105.80
1	16S1	321	A	N9-C4-C5	5.05	107.82	105.80
1	16S1	676	A	N9-C4-C5	5.05	107.82	105.80
1	16S1	1246	A	C4-C5-N7	-5.05	108.17	110.70
22	23S1	219	A	C4-C5-N7	-5.05	108.17	110.70
22	23S1	508	A	C4-C5-N7	-5.05	108.17	110.70
22	23S1	1503	A	C8-N9-C4	5.05	107.82	105.80
1	16S1	816	A	N9-C4-C5	5.05	107.82	105.80
22	23S1	484	C	C5-C6-N1	5.05	123.53	121.00
22	23S1	1652	A	C4-C5-C6	5.05	119.53	117.00
22	23S1	2478	A	N9-C4-C5	5.05	107.82	105.80
1	16S1	1238	A	C4-C5-C6	5.05	119.53	117.00
22	23S1	502	A	N3-C4-N9	5.05	131.44	127.40
22	23S1	522	A	C4-C5-N7	-5.05	108.17	110.70
22	23S1	670	A	C5-C6-N1	5.05	120.22	117.70
22	23S1	959	A	C5-C6-N1	5.05	120.22	117.70
22	23S1	1678	A	C4-C5-N7	-5.05	108.17	110.70
22	23S1	2009	A	C4-C5-N7	-5.05	108.17	110.70
22	23S1	2095	A	C4-C5-C6	5.05	119.53	117.00
22	23S1	756	A	C4-C5-N7	-5.05	108.18	110.70
22	23S1	2646	C	N3-C2-O2	-5.05	118.37	121.90
22	23S1	2726	A	C5-C6-N1	5.05	120.22	117.70
1	16S1	298	A	C4-C5-N7	-5.05	108.18	110.70
1	16S1	487	A	C8-N9-C4	5.05	107.82	105.80
1	16S1	908	A	C4-C5-N7	-5.05	108.18	110.70
22	23S1	715	A	C5-C6-N1	5.05	120.22	117.70
22	23S1	2566	A	C4-C5-N7	-5.05	108.18	110.70
22	23S1	2748	A	C8-N9-C4	5.05	107.82	105.80
22	23S1	1365	A	C5-C6-N1	5.04	120.22	117.70
22	23S1	1668	A	N3-C4-N9	5.04	131.44	127.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2288	A	C6-N1-C2	5.04	121.63	118.60
1	16S1	53	A	N9-C4-C5	5.04	107.82	105.80
1	16S1	496	A	C8-N9-C4	5.04	107.82	105.80
1	16S1	777	A	C4-C5-N7	-5.04	108.18	110.70
1	16S1	1456	A	C4-C5-N7	-5.04	108.18	110.70
22	23S1	515	A	N3-C4-N9	5.04	131.44	127.40
22	23S1	616	A	N9-C4-C5	5.04	107.82	105.80
22	23S1	1253	A	C8-N9-C4	5.04	107.82	105.80
1	16S1	263	A	C4-C5-N7	-5.04	108.18	110.70
1	16S1	364	A	C5-C6-N1	5.04	120.22	117.70
1	16S1	753	A	C5-C6-N1	5.04	120.22	117.70
1	16S1	1093	A	C4-C5-N7	-5.04	108.18	110.70
22	23S1	716	A	N9-C4-C5	5.04	107.82	105.80
22	23S1	735	A	C5-C6-N1	5.04	120.22	117.70
22	23S1	2336	A	C4-C5-C6	5.04	119.52	117.00
22	23S1	2534	A	C4-C5-N7	-5.04	108.18	110.70
22	23S1	2776	A	N9-C4-C5	5.04	107.82	105.80
1	16S1	759	A	C5-C6-N1	5.04	120.22	117.70
1	16S1	196	A	N3-C4-N9	5.04	131.43	127.40
1	16S1	288	A	C8-N9-C4	5.04	107.81	105.80
22	23S1	2575	C	N3-C2-O2	-5.04	118.37	121.90
23	05S1	53	A	N9-C4-C5	5.04	107.81	105.80
1	16S1	535	A	C5-C6-N1	5.04	120.22	117.70
22	23S1	127	A	C4-C5-C6	5.04	119.52	117.00
22	23S1	503	A	C4-C5-N7	-5.04	108.18	110.70
22	23S1	1307	A	C5-C6-N1	5.04	120.22	117.70
1	16S1	389	A	C4-C5-N7	-5.04	108.18	110.70
22	23S1	241	A	C8-N9-C4	5.04	107.81	105.80
22	23S1	522	A	N9-C4-C5	5.04	107.81	105.80
22	23S1	644	A	C5-C6-N1	5.04	120.22	117.70
22	23S1	781	A	C5-C6-N1	5.04	120.22	117.70
22	23S1	1635	A	C8-N9-C4	5.04	107.81	105.80
22	23S1	1913	A	C4-C5-N7	-5.04	108.18	110.70
22	23S1	2285	C	C2-N1-C1'	5.04	124.34	118.80
1	16S1	432	A	C8-N9-C4	5.03	107.81	105.80
22	23S1	1230	A	C4-C5-N7	-5.03	108.18	110.70
22	23S1	1977	A	C4-C5-N7	-5.03	108.18	110.70
22	23S1	2600	A	C5-C6-N1	5.03	120.22	117.70
1	16S1	629	A	C5-C6-N1	5.03	120.22	117.70
1	16S1	1465	A	C4-C5-N7	-5.03	108.18	110.70
22	23S1	347	A	C5-C6-N1	5.03	120.22	117.70
22	23S1	1144	A	N9-C4-C5	5.03	107.81	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1204	A	C4-C5-N7	-5.03	108.18	110.70
1	16S1	270	A	N9-C4-C5	5.03	107.81	105.80
1	16S1	1251	A	C5-C6-N1	5.03	120.22	117.70
22	23S1	311	A	C8-N9-C4	5.03	107.81	105.80
22	23S1	782	A	C5-C6-N1	5.03	120.22	117.70
22	23S1	1276	A	N9-C4-C5	5.03	107.81	105.80
22	23S1	2270	A	C5-C6-N1	5.03	120.22	117.70
22	23S1	2411	A	N9-C4-C5	5.03	107.81	105.80
22	23S1	2639	A	C4-C5-C6	5.03	119.52	117.00
22	23S1	2749	A	N3-C4-N9	5.03	131.43	127.40
1	16S1	448	A	C8-N9-C4	5.03	107.81	105.80
1	16S1	1311	A	N9-C4-C5	5.03	107.81	105.80
22	23S1	753	A	C8-N9-C4	5.03	107.81	105.80
22	23S1	980	A	C8-N9-C4	5.03	107.81	105.80
22	23S1	1775	U	N3-C2-O2	-5.03	118.68	122.20
1	16S1	409	U	N3-C2-O2	-5.03	118.68	122.20
22	23S1	764	A	N3-C4-N9	5.03	131.42	127.40
1	16S1	430	A	C4-C5-N7	-5.03	108.19	110.70
22	23S1	241	A	N3-C4-N9	5.03	131.42	127.40
22	23S1	401	A	C8-N9-C4	5.03	107.81	105.80
22	23S1	592	A	C4-C5-N7	-5.03	108.19	110.70
22	23S1	792	A	C4-C5-C6	5.03	119.51	117.00
22	23S1	849	A	C4-C5-N7	-5.03	108.19	110.70
22	23S1	1583	A	C4-C5-C6	5.03	119.51	117.00
22	23S1	1654	A	N9-C4-C5	5.03	107.81	105.80
22	23S1	1665	A	N9-C4-C5	5.03	107.81	105.80
22	23S1	2090	A	C4-C5-N7	-5.03	108.19	110.70
22	23S1	2376	A	C4-C5-N7	-5.03	108.19	110.70
22	23S1	1021	A	N9-C4-C5	5.02	107.81	105.80
22	23S1	1918	A	C4-C5-N7	-5.02	108.19	110.70
1	16S1	532	A	C5-C6-N1	5.02	120.21	117.70
22	23S1	2014	A	C4-C5-N7	-5.02	108.19	110.70
22	23S1	2476	A	C5-C6-N1	5.02	120.21	117.70
1	16S1	53	A	C4-C5-N7	-5.02	108.19	110.70
1	16S1	706	A	C4-C5-N7	-5.02	108.19	110.70
22	23S1	2821	A	C4-C5-N7	-5.02	108.19	110.70
1	16S1	131	A	N3-C4-N9	5.02	131.41	127.40
1	16S1	493	A	N3-C4-N9	5.02	131.41	127.40
22	23S1	432	A	C8-N9-C4	5.02	107.81	105.80
22	23S1	439	A	C4-C5-N7	-5.02	108.19	110.70
22	23S1	972	A	C5-C6-N1	5.02	120.21	117.70
22	23S1	1745	A	C8-N9-C4	5.02	107.81	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2117	A	N9-C4-C5	5.02	107.81	105.80
22	23S1	270	A	C5-C6-N1	5.02	120.21	117.70
22	23S1	1330	C	N1-C2-O2	5.02	121.91	118.90
22	23S1	1802	A	C4-C5-N7	-5.02	108.19	110.70
22	23S1	2439	A	C4-C5-N7	-5.02	108.19	110.70
1	16S1	325	A	C8-N9-C4	5.02	107.81	105.80
1	16S1	468	A	C4-C5-C6	5.02	119.51	117.00
1	16S1	1447	A	N9-C4-C5	5.02	107.81	105.80
22	23S1	2100	G	N3-C4-N9	5.02	129.01	126.00
1	16S1	315	A	C4-C5-C6	5.01	119.51	117.00
1	16S1	356	A	N9-C4-C5	5.01	107.81	105.80
1	16S1	408	A	C5-C6-N1	5.01	120.21	117.70
22	23S1	1669	A	C5-C6-N1	5.01	120.21	117.70
22	23S1	2247	A	C5-C6-N1	5.01	120.21	117.70
22	23S1	2682	A	C5-C6-N1	5.01	120.21	117.70
1	16S1	865	A	C4-C5-N7	-5.01	108.19	110.70
1	16S1	1499	A	C8-N9-C4	5.01	107.81	105.80
22	23S1	53	A	N9-C4-C5	5.01	107.81	105.80
22	23S1	2009	A	C5-C6-N1	5.01	120.21	117.70
22	23S1	2482	A	N9-C4-C5	5.01	107.81	105.80
1	16S1	766	A	C8-N9-C4	5.01	107.81	105.80
1	16S1	1130	A	C4-C5-N7	-5.01	108.19	110.70
1	16S1	1176	A	C8-N9-C4	5.01	107.81	105.80
1	16S1	1350	A	C4-C5-N7	-5.01	108.19	110.70
22	23S1	218	A	C5-C6-N1	5.01	120.21	117.70
22	23S1	255	A	C8-N9-C4	5.01	107.81	105.80
22	23S1	1155	A	N3-C4-N9	5.01	131.41	127.40
22	23S1	1385	A	N3-C4-N9	5.01	131.41	127.40
22	23S1	1785	A	N3-C4-N9	5.01	131.41	127.40
22	23S1	2564	A	C4-C5-C6	5.01	119.50	117.00
23	05S1	50	A	N9-C4-C5	5.01	107.80	105.80
1	16S1	1398	A	N3-C4-N9	5.01	131.41	127.40
22	23S1	332	A	C4-C5-C6	5.01	119.50	117.00
22	23S1	794	A	C4-C5-N7	-5.01	108.20	110.70
22	23S1	1073	A	C8-N9-C4	5.01	107.80	105.80
22	23S1	1322	A	C4-C5-N7	-5.01	108.19	110.70
22	23S1	1367	A	C8-N9-C4	5.01	107.80	105.80
22	23S1	2820	A	N3-C4-N9	5.01	131.41	127.40
22	23S1	727	A	C5-C6-N1	5.01	120.20	117.70
22	23S1	1535	A	C4-C5-N7	-5.01	108.20	110.70
1	16S1	44	A	C5-C6-N1	5.01	120.20	117.70
22	23S1	76	C	N3-C2-O2	-5.01	118.40	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	1144	A	C4-C5-N7	-5.01	108.20	110.70
22	23S1	1586	A	C4-C5-N7	-5.01	108.20	110.70
1	16S1	1092	A	C4-C5-C6	5.00	119.50	117.00
22	23S1	204	A	C5-C6-N1	5.00	120.20	117.70
22	23S1	1918	A	C8-N9-C4	5.00	107.80	105.80
1	16S1	129	A	N9-C4-C5	5.00	107.80	105.80
1	16S1	1196	A	N9-C4-C5	5.00	107.80	105.80
1	16S1	1492	A	C4-C5-N7	-5.00	108.20	110.70
22	23S1	1603	A	C5-C6-N1	5.00	120.20	117.70
22	23S1	2077	A	C5-C6-N1	5.00	120.20	117.70
1	16S1	583	A	N3-C4-N9	5.00	131.40	127.40
22	23S1	2542	A	C4-C5-C6	5.00	119.50	117.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	L091	114	GLU	Peptide
29	L091	70	GLU	Peptide
33	L151	35	HIS	Peptide
47	L301	3	LYS	Peptide
51	L351	31	HIS	Peptide
2	S021	123	ASP	Peptide
2	S021	126	PHE	Sidechain
2	S021	5	SER	Peptide
9	S091	24	GLY	Peptide
10	S101	56	HIS	Peptide
10	S101	57	VAL	Mainchain
13	S131	45	ILE	Peptide
13	S131	65	VAL	Peptide
13	S131	7	ILE	Peptide
19	S191	81	ARG	Mainchain
21	S211	54	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16S1	32930	0	0	0	0
2	S021	1753	0	0	0	0
3	S031	1624	0	0	0	0
4	S041	1643	0	0	0	0
5	S051	1144	0	0	0	0
6	S061	862	0	0	0	0
7	S071	1181	0	0	0	0
8	S081	979	0	0	0	0
9	S091	1022	0	0	0	0
10	S101	795	0	0	0	0
11	S111	877	0	0	0	0
12	S121	957	0	0	0	0
13	S131	883	0	0	0	0
14	S141	799	0	0	0	0
15	S151	714	0	0	0	0
16	S161	649	0	0	0	0
17	S171	648	0	0	0	0
18	S181	455	0	0	0	0
19	S191	656	0	0	0	0
20	S201	670	0	0	0	0
21	S211	465	0	0	0	0
22	23S1	62209	0	0	0	0
23	05S1	2569	0	0	0	0
24	L021	2082	0	0	0	0
25	L031	1566	0	0	0	0
26	L041	1552	0	0	0	0
27	L051	1410	0	0	0	0
28	L061	1323	0	0	0	0
29	L091	1110	0	0	0	0
30	L311	522	0	0	0	0
31	L131	1129	0	0	0	0
32	L141	946	0	0	0	0
33	L151	1053	0	0	0	0
34	L161	1075	0	0	0	0
35	L171	945	0	0	0	0
36	L181	900	0	0	0	0
37	L191	917	0	0	0	0
38	L201	947	0	0	0	0
39	L211	816	0	0	0	0
40	L221	857	0	0	0	0
41	L231	738	0	0	0	0
42	L241	779	0	0	0	0
43	L251	753	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	L271	580	0	0	0	0
45	L281	625	0	0	0	0
46	L291	501	0	0	0	0
47	L301	449	0	0	0	0
48	L321	444	0	0	0	0
49	L331	414	0	0	0	0
50	L341	377	0	0	0	0
51	L351	504	0	0	0	0
52	L361	302	0	0	0	0
53	SPE1	300	0	0	0	0
54	MRN1	146	0	0	0	0
55	PTR1	1627	0	0	0	0
56	16S1	87	0	0	0	0
56	23S1	250	0	0	0	0
56	L231	1	0	0	0	0
56	PTR1	1	0	0	0	0
57	05S1	1	0	0	0	0
57	16S1	39	0	0	0	0
57	23S1	105	0	0	0	0
57	L031	1	0	0	0	0
57	L161	1	0	0	0	0
58	05S1	9	0	0	0	0
58	16S1	148	0	0	0	0
58	23S1	919	0	0	0	0
58	L021	20	0	0	0	0
58	L031	14	0	0	0	0
58	L041	10	0	0	0	0
58	L131	5	0	0	0	0
58	L141	7	0	0	0	0
58	L151	4	0	0	0	0
58	L161	3	0	0	0	0
58	L171	5	0	0	0	0
58	L181	1	0	0	0	0
58	L191	4	0	0	0	0
58	L201	7	0	0	0	0
58	L211	1	0	0	0	0
58	L221	8	0	0	0	0
58	L231	1	0	0	0	0
58	L241	2	0	0	0	0
58	L251	1	0	0	0	0
58	L271	1	0	0	0	0
58	L281	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	L321	2	0	0	0	0
58	L331	1	0	0	0	0
58	L341	7	0	0	0	0
58	L351	4	0	0	0	0
58	MRN1	1	0	0	0	0
58	PTR1	3	0	0	0	0
58	S021	1	0	0	0	0
58	S031	1	0	0	0	0
58	S111	2	0	0	0	0
58	S131	1	0	0	0	0
58	S171	1	0	0	0	0
58	SPE1	6	0	0	0	0
59	L311	1	0	0	0	0
59	L361	1	0	0	0	0
59	S021	1	0	0	0	0
60	23S1	9	0	0	0	0
61	16S1	165	0	0	0	0
61	23S1	616	0	0	0	0
61	L021	6	0	0	0	0
61	L031	2	0	0	0	0
61	L151	2	0	0	0	0
61	L171	2	0	0	0	0
61	S111	1	0	0	0	0
61	S131	2	0	0	0	0
61	S141	3	0	0	0	0
61	S171	1	0	0	0	0
All	All	146672	0	0	0	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 2.

There are no clashes within the asymmetric unit.

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	S021	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	S031	204/233 (88%)	194 (95%)	10 (5%)	0	100	100
4	S041	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	S051	153/167 (92%)	146 (95%)	7 (5%)	0	100	100
6	S061	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	S071	149/179 (83%)	140 (94%)	9 (6%)	0	100	100
8	S081	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
9	S091	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
10	S101	97/103 (94%)	92 (95%)	4 (4%)	1 (1%)	13	33
11	S111	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
12	S121	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
13	S131	112/118 (95%)	101 (90%)	10 (9%)	1 (1%)	14	35
14	S141	99/102 (97%)	87 (88%)	11 (11%)	1 (1%)	13	33
15	S151	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	S161	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	S171	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
18	S181	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
19	S191	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
20	S201	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
21	S211	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
24	L021	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
25	L031	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	25	49
26	L041	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
27	L051	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
28	L061	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
29	L091	147/149 (99%)	129 (88%)	18 (12%)	0	100	100
30	L311	64/70 (91%)	59 (92%)	5 (8%)	0	100	100
31	L131	140/142 (99%)	140 (100%)	0	0	100	100
32	L141	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	L151	142/144 (99%)	137 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	L161	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
35	L171	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
36	L181	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
37	L191	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
38	L201	115/118 (98%)	115 (100%)	0	0	100	100
39	L211	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
40	L221	108/110 (98%)	108 (100%)	0	0	100	100
41	L231	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
42	L241	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
43	L251	92/94 (98%)	92 (100%)	0	0	100	100
44	L271	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
45	L281	75/78 (96%)	75 (100%)	0	0	100	100
46	L291	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
47	L301	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	L321	54/57 (95%)	54 (100%)	0	0	100	100
49	L331	49/55 (89%)	49 (100%)	0	0	100	100
50	L341	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
51	L351	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	8	21
52	L361	36/38 (95%)	36 (100%)	0	0	100	100
53	SPE1	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5607/5948 (94%)	5397 (96%)	205 (4%)	5 (0%)	50	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	S101	57	VAL
25	L031	149	ASN
51	L351	32	ILE
13	S131	66	GLU
14	S141	54	ASP

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S021	186/199 (94%)	185 (100%)	1 (0%)	86	95
3	S031	170/190 (90%)	170 (100%)	0	100	100
4	S041	172/173 (99%)	168 (98%)	4 (2%)	45	74
5	S051	118/126 (94%)	117 (99%)	1 (1%)	79	91
6	S061	92/116 (79%)	92 (100%)	0	100	100
7	S071	124/147 (84%)	121 (98%)	3 (2%)	44	73
8	S081	104/105 (99%)	104 (100%)	0	100	100
9	S091	105/107 (98%)	103 (98%)	2 (2%)	52	79
10	S101	87/90 (97%)	87 (100%)	0	100	100
11	S111	90/99 (91%)	90 (100%)	0	100	100
12	S121	102/103 (99%)	101 (99%)	1 (1%)	73	89
13	S131	92/96 (96%)	91 (99%)	1 (1%)	70	87
14	S141	79/84 (94%)	79 (100%)	0	100	100
15	S151	76/77 (99%)	75 (99%)	1 (1%)	65	85
16	S161	65/65 (100%)	62 (95%)	3 (5%)	23	49
17	S171	74/78 (95%)	74 (100%)	0	100	100
18	S181	48/65 (74%)	47 (98%)	1 (2%)	48	76
19	S191	71/79 (90%)	70 (99%)	1 (1%)	62	84
20	S201	65/66 (98%)	64 (98%)	1 (2%)	60	83
21	S211	48/61 (79%)	47 (98%)	1 (2%)	48	76
24	L021	216/218 (99%)	215 (100%)	1 (0%)	86	95
25	L031	163/163 (100%)	162 (99%)	1 (1%)	84	94
26	L041	165/165 (100%)	163 (99%)	2 (1%)	67	86
27	L051	148/150 (99%)	148 (100%)	0	100	100
28	L061	137/138 (99%)	137 (100%)	0	100	100
29	L091	114/114 (100%)	113 (99%)	1 (1%)	75	90
30	L311	59/62 (95%)	57 (97%)	2 (3%)	32	61
31	L131	116/116 (100%)	116 (100%)	0	100	100
32	L141	104/104 (100%)	104 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	L151	103/103 (100%)	102 (99%)	1 (1%)	73	89
34	L161	108/108 (100%)	108 (100%)	0	100	100
35	L171	98/103 (95%)	97 (99%)	1 (1%)	73	89
36	L181	87/87 (100%)	87 (100%)	0	100	100
37	L191	99/100 (99%)	99 (100%)	0	100	100
38	L201	89/90 (99%)	88 (99%)	1 (1%)	70	87
39	L211	84/84 (100%)	84 (100%)	0	100	100
40	L221	93/93 (100%)	92 (99%)	1 (1%)	70	87
41	L231	80/84 (95%)	79 (99%)	1 (1%)	65	85
42	L241	83/85 (98%)	83 (100%)	0	100	100
43	L251	78/78 (100%)	78 (100%)	0	100	100
44	L271	57/63 (90%)	57 (100%)	0	100	100
45	L281	67/68 (98%)	65 (97%)	2 (3%)	36	65
46	L291	54/55 (98%)	54 (100%)	0	100	100
47	L301	48/49 (98%)	48 (100%)	0	100	100
48	L321	47/48 (98%)	46 (98%)	1 (2%)	48	76
49	L331	45/49 (92%)	45 (100%)	0	100	100
50	L341	38/38 (100%)	38 (100%)	0	100	100
51	L351	51/52 (98%)	51 (100%)	0	100	100
52	L361	34/34 (100%)	33 (97%)	1 (3%)	37	67
53	SPE1	31/31 (100%)	28 (90%)	3 (10%)	6	17
All	All	4664/4858 (96%)	4624 (99%)	40 (1%)	74	90

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S021	128	LYS
4	S041	26	ARG
4	S041	56	ARG
4	S041	63	ARG
4	S041	188	ARG
5	S051	69	ARG
7	S071	3	ARG
7	S071	5	ARG
7	S071	79	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	S091	11	ARG
9	S091	113	ARG
12	S121	86	ARG
13	S131	3	ARG
15	S151	89	ARG
16	S161	1	MET
16	S161	5	ARG
16	S161	80	LYS
18	S181	73	ARG
19	S191	81	ARG
20	S201	10	ARG
21	S211	7	ARG
24	L021	80	ARG
25	L031	33	ARG
26	L041	21	ARG
26	L041	44	ARG
29	L091	41	LYS
30	L311	40	CYS
30	L311	59	ARG
33	L151	78	ARG
35	L171	2	ARG
38	L201	51	ARG
40	L221	92	ARG
41	L231	3	ARG
45	L281	27	ARG
45	L281	72	ARG
48	L321	40	ARG
52	L361	12	ARG
53	SPE1	4	ASN
53	SPE1	12	ARG
53	SPE1	32	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16S1	1530/1534 (99%)	173 (11%)	1 (0%)
22	23S1	2890/2897 (99%)	296 (10%)	18 (0%)
23	05S1	119/120 (99%)	7 (5%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	MRN1	6/7 (85%)	3 (50%)	1 (16%)
55	PTR1	73/76 (96%)	11 (15%)	1 (1%)
All	All	4618/4634 (99%)	490 (10%)	21 (0%)

All (490) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16S1	7	A
1	16S1	9	G
1	16S1	22	G
1	16S1	32	A
1	16S1	39	G
1	16S1	47	C
1	16S1	48	C
1	16S1	51	A
1	16S1	69	G
1	16S1	71	A
1	16S1	72	A
1	16S1	76	G
1	16S1	78	A
1	16S1	83	C
1	16S1	84	U
1	16S1	85	U
1	16S1	86	G
1	16S1	87	C
1	16S1	88	U
1	16S1	89	U
1	16S1	95	C
1	16S1	98	A
1	16S1	116	A
1	16S1	130	A
1	16S1	131	A
1	16S1	144	G
1	16S1	163	C
1	16S1	164	G
1	16S1	181	A
1	16S1	197	A
1	16S1	210	C
1	16S1	226	G
1	16S1	245	U
1	16S1	247	G
1	16S1	251	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16S1	266	G
1	16S1	267	C
1	16S1	289	G
1	16S1	306	A
1	16S1	321	A
1	16S1	328	C
1	16S1	329	A
1	16S1	352	C
1	16S1	354	G
1	16S1	367	U
1	16S1	372	C
1	16S1	373	A
1	16S1	384	G
1	16S1	392	C
1	16S1	397	A
1	16S1	398	U
1	16S1	406	G
1	16S1	413	G
1	16S1	429	U
1	16S1	467	U
1	16S1	468	A
1	16S1	478	A
1	16S1	479	U
1	16S1	481	G
1	16S1	484	G
1	16S1	486	U
1	16S1	497	G
1	16S1	509	A
1	16S1	511	C
1	16S1	513	C
1	16S1	516	PSU
1	16S1	518	C
1	16S1	527	G7M
1	16S1	529	G
1	16S1	532	A
1	16S1	547	A
1	16S1	559	A
1	16S1	572	A
1	16S1	573	A
1	16S1	576	C
1	16S1	577	G
1	16S1	579	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16S1	633	G
1	16S1	650	G
1	16S1	653	U
1	16S1	665	A
1	16S1	718	A
1	16S1	721	G
1	16S1	722	G
1	16S1	734	G
1	16S1	755	G
1	16S1	777	A
1	16S1	793	U
1	16S1	794	A
1	16S1	815	A
1	16S1	817	C
1	16S1	821	G
1	16S1	828	U
1	16S1	832	G
1	16S1	841	C
1	16S1	842	U
1	16S1	843	U
1	16S1	846	G
1	16S1	914	A
1	16S1	926	G
1	16S1	934	C
1	16S1	935	A
1	16S1	942	G
1	16S1	960	U
1	16S1	966	2MG
1	16S1	969	A
1	16S1	975	A
1	16S1	976	G
1	16S1	977	A
1	16S1	993	G
1	16S1	1004	A
1	16S1	1005	A
1	16S1	1019	A
1	16S1	1020	G
1	16S1	1026	G
1	16S1	1028	C
1	16S1	1029	U
1	16S1	1030	U
1	16S1	1032	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16S1	1045	C
1	16S1	1053	G
1	16S1	1065	U
1	16S1	1094	G
1	16S1	1095	U
1	16S1	1101	A
1	16S1	1132	C
1	16S1	1139	G
1	16S1	1140	C
1	16S1	1141	C
1	16S1	1157	A
1	16S1	1159	U
1	16S1	1168	U
1	16S1	1169	A
1	16S1	1172	C
1	16S1	1184	G
1	16S1	1196	A
1	16S1	1197	A
1	16S1	1212	U
1	16S1	1213	A
1	16S1	1225	A
1	16S1	1226	C
1	16S1	1227	A
1	16S1	1238	A
1	16S1	1256	A
1	16S1	1257	A
1	16S1	1258	G
1	16S1	1280	A
1	16S1	1285	A
1	16S1	1299	A
1	16S1	1300	G
1	16S1	1302	C
1	16S1	1317	C
1	16S1	1320	C
1	16S1	1340	A
1	16S1	1353	G
1	16S1	1363	A
1	16S1	1364	U
1	16S1	1370	G
1	16S1	1419	G
1	16S1	1429	A
1	16S1	1441	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16S1	1455	G
1	16S1	1487	G
1	16S1	1492	A
1	16S1	1493	A
1	16S1	1497	G
1	16S1	1499	A
1	16S1	1502	A
1	16S1	1503	A
1	16S1	1506	U
1	16S1	1517	G
1	16S1	1529	G
1	16S1	1530	G
22	23S1	23	G
22	23S1	34	U
22	23S1	71	A
22	23S1	74	A
22	23S1	75	G
22	23S1	84	A
22	23S1	101	A
22	23S1	118	A
22	23S1	119	A
22	23S1	120	U
22	23S1	125	A
22	23S1	163	C
22	23S1	165	A
22	23S1	181	A
22	23S1	196	A
22	23S1	215	G
22	23S1	216	A
22	23S1	221	A
22	23S1	222	A
22	23S1	233	A
22	23S1	248	G
22	23S1	265	A
22	23S1	276	U
22	23S1	278	A
22	23S1	302	C
22	23S1	303	G
22	23S1	311	A
22	23S1	324	A
22	23S1	330	A
22	23S1	386	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23S1	396	G
22	23S1	411	G
22	23S1	481	G
22	23S1	491	G
22	23S1	505	A
22	23S1	509	C
22	23S1	529	A
22	23S1	530	G
22	23S1	531	C
22	23S1	532	A
22	23S1	544	C
22	23S1	546	U
22	23S1	547	A
22	23S1	548	G
22	23S1	549	G
22	23S1	563	A
22	23S1	573	U
22	23S1	575	A
22	23S1	586	A
22	23S1	603	A
22	23S1	613	A
22	23S1	614	A
22	23S1	637	A
22	23S1	645	C
22	23S1	647	G
22	23S1	653	U
22	23S1	654	A
22	23S1	655	A
22	23S1	685	A
22	23S1	686	U
22	23S1	717	C
22	23S1	730	A
22	23S1	738	G
22	23S1	747	5MU
22	23S1	764	A
22	23S1	765	C
22	23S1	775	G
22	23S1	776	G
22	23S1	782	A
22	23S1	784	G
22	23S1	789	A
22	23S1	805	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23S1	812	C
22	23S1	827	U
22	23S1	828	U
22	23S1	846	U
22	23S1	847	U
22	23S1	858	G
22	23S1	859	G
22	23S1	866	A
22	23S1	884	U
22	23S1	896	A
22	23S1	910	A
22	23S1	931	U
22	23S1	946	C
22	23S1	961	C
22	23S1	974	G
22	23S1	983	A
22	23S1	996	A
22	23S1	1009	A
22	23S1	1012	U
22	23S1	1013	C
22	23S1	1022	G
22	23S1	1026	G
22	23S1	1033	U
22	23S1	1054	A
22	23S1	1070	A
22	23S1	1088	A
22	23S1	1107	G
22	23S1	1112	G
22	23S1	1130	U
22	23S1	1132	U
22	23S1	1133	A
22	23S1	1135	C
22	23S1	1142	A
22	23S1	1173	U
22	23S1	1174	U
22	23S1	1175	A
22	23S1	1176	U
22	23S1	1250	G
22	23S1	1253	A
22	23S1	1256	G
22	23S1	1271	G
22	23S1	1272	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23S1	1273	U
22	23S1	1300	G
22	23S1	1301	A
22	23S1	1329	U
22	23S1	1352	U
22	23S1	1365	A
22	23S1	1379	U
22	23S1	1383	A
22	23S1	1403	A
22	23S1	1416	G
22	23S1	1420	A
22	23S1	1428	C
22	23S1	1452	G
22	23S1	1453	A
22	23S1	1482	G
22	23S1	1508	A
22	23S1	1509	A
22	23S1	1515	A
22	23S1	1566	A
22	23S1	1569	A
22	23S1	1578	U
22	23S1	1606	C
22	23S1	1608	A
22	23S1	1617	C
22	23S1	1647	U
22	23S1	1648	U
22	23S1	1649	G
22	23S1	1674	G
22	23S1	1729	U
22	23S1	1730	C
22	23S1	1738	G
22	23S1	1744	A
22	23S1	1757	A
22	23S1	1758	U
22	23S1	1764	C
22	23S1	1773	A
22	23S1	1782	U
22	23S1	1800	C
22	23S1	1801	A
22	23S1	1802	A
22	23S1	1808	A
22	23S1	1811	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23S1	1816	C
22	23S1	1829	A
22	23S1	1871	A
22	23S1	1872	A
22	23S1	1873	G
22	23S1	1906	G
22	23S1	1914	C
22	23S1	1929	G
22	23S1	1930	G
22	23S1	1937	A
22	23S1	1938	A
22	23S1	1939	5MU
22	23S1	1955	U
22	23S1	1967	C
22	23S1	1970	A
22	23S1	1971	U
22	23S1	1972	G
22	23S1	1991	U
22	23S1	1993	U
22	23S1	2020	A
22	23S1	2023	C
22	23S1	2027	G
22	23S1	2031	A
22	23S1	2033	A
22	23S1	2043	C
22	23S1	2055	C
22	23S1	2056	G
22	23S1	2060	A
22	23S1	2061	G
22	23S1	2069	G7M
22	23S1	2093	G
22	23S1	2108	A
22	23S1	2110	G
22	23S1	2111	U
22	23S1	2112	G
22	23S1	2113	U
22	23S1	2115	G
22	23S1	2116	G
22	23S1	2117	A
22	23S1	2118	U
22	23S1	2119	A
22	23S1	2121	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23S1	2123	G
22	23S1	2124	G
22	23S1	2125	G
22	23S1	2126	A
22	23S1	2127	G
22	23S1	2128	G
22	23S1	2131	U
22	23S1	2132	U
22	23S1	2133	G
22	23S1	2137	U
22	23S1	2142	A
22	23S1	2146	C
22	23S1	2147	A
22	23S1	2157	G
22	23S1	2158	A
22	23S1	2163	A
22	23S1	2164	C
22	23S1	2169	A
22	23S1	2171	A
22	23S1	2172	U
22	23S1	2173	A
22	23S1	2182	U
22	23S1	2183	A
22	23S1	2188	U
22	23S1	2189	U
22	23S1	2190	G
22	23S1	2195	U
22	23S1	2198	A
22	23S1	2204	G
22	23S1	2211	A
22	23S1	2225	A
22	23S1	2238	G
22	23S1	2252	G
22	23S1	2278	A
22	23S1	2283	C
22	23S1	2287	A
22	23S1	2288	A
22	23S1	2305	U
22	23S1	2308	G
22	23S1	2322	A
22	23S1	2325	G
22	23S1	2333	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23S1	2336	A
22	23S1	2345	G
22	23S1	2347	C
22	23S1	2350	C
22	23S1	2368	C
22	23S1	2383	G
22	23S1	2385	C
22	23S1	2402	U
22	23S1	2406	A
22	23S1	2425	A
22	23S1	2429	G
22	23S1	2435	A
22	23S1	2441	U
22	23S1	2448	A
22	23S1	2476	A
22	23S1	2491	U
22	23S1	2502	G
22	23S1	2504	PSU
22	23S1	2505	G
22	23S1	2518	A
22	23S1	2529	G
22	23S1	2547	A
22	23S1	2566	A
22	23S1	2567	G
22	23S1	2573	C
22	23S1	2602	A
22	23S1	2609	U
22	23S1	2613	U
22	23S1	2615	U
22	23S1	2629	U
22	23S1	2646	C
22	23S1	2663	G
22	23S1	2682	A
22	23S1	2689	U
22	23S1	2690	U
22	23S1	2714	G
22	23S1	2726	A
22	23S1	2733	A
22	23S1	2744	G
22	23S1	2748	A
22	23S1	2757	A
22	23S1	2765	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23S1	2778	A
22	23S1	2791	G
22	23S1	2820	A
22	23S1	2821	A
22	23S1	2835	A
22	23S1	2836	U
22	23S1	2849	U
22	23S1	2861	U
22	23S1	2873	A
22	23S1	2880	C
22	23S1	2883	A
22	23S1	2884	U
22	23S1	2885	G
22	23S1	2891	U
23	05S1	35	C
23	05S1	44	G
23	05S1	56	G
23	05S1	89	U
23	05S1	90	C
23	05S1	105	G
23	05S1	109	A
54	MRN1	4	C
54	MRN1	6	U
54	MRN1	7	U
55	PTR1	14	A
55	PTR1	16	C
55	PTR1	17	U
55	PTR1	17(A)	G
55	PTR1	19	A
55	PTR1	20	U
55	PTR1	46	G7M
55	PTR1	54	5MU
55	PTR1	57	G
55	PTR1	59	A
55	PTR1	76	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16S1	1225	A
22	23S1	125	A
22	23S1	199	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23S1	685	A
22	23S1	764	A
22	23S1	784	G
22	23S1	984	A
22	23S1	1142	A
22	23S1	1508	A
22	23S1	1608	A
22	23S1	1970	A
22	23S1	2146	C
22	23S1	2162	G
22	23S1	2188	U
22	23S1	2189	U
22	23S1	2251	OMG
22	23S1	2518	A
22	23S1	2756	U
22	23S1	2873	A
54	MRN1	5	G
55	PTR1	19	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	23S1	955	22	18,21,22	4.02	7 (38%)	22,30,33	1.94	5 (22%)
22	G7M	23S1	2069	57,22	20,26,27	2.25	6 (30%)	17,39,42	1.27	3 (17%)
55	5MU	PTR1	54	55	19,22,23	1.01	2 (10%)	28,32,35	1.21	4 (14%)
1	MA6	16S1	1519	1	18,26,27	1.25	1 (5%)	19,38,41	3.34	2 (10%)
34	4D4	L161	81	34	9,11,12	2.55	3 (33%)	8,13,15	1.21	1 (12%)
12	D2T	S121	89	12	7,9,10	1.02	0	6,11,13	2.29	2 (33%)
1	2MG	16S1	1516	1	18,26,27	2.33	7 (38%)	16,38,41	1.51	4 (25%)
55	PSU	PTR1	55	55	18,21,22	4.27	7 (38%)	22,30,33	1.76	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	16S1	1207	57,1	18,26,27	2.40	7 (38%)	16,38,41	1.45	3 (18%)
1	G7M	16S1	527	57,1	20,26,27	2.40	6 (30%)	17,39,42	1.18	2 (11%)
22	5MU	23S1	1939	57,22	19,22,23	0.73	0	28,32,35	1.25	3 (10%)
22	PSU	23S1	2580	57,22	18,21,22	4.10	7 (38%)	22,30,33	2.04	6 (27%)
22	PSU	23S1	2605	22	18,21,22	4.04	7 (38%)	22,30,33	1.87	5 (22%)
55	4SU	PTR1	8	55	18,21,22	3.47	8 (44%)	26,30,33	1.65	4 (15%)
1	4OC	16S1	1402	56,1	20,23,24	2.93	8 (40%)	26,32,35	1.09	2 (7%)
1	2MG	16S1	966	1	18,26,27	2.41	7 (38%)	16,38,41	1.49	4 (25%)
1	PSU	16S1	516	56,1	18,21,22	4.07	8 (44%)	22,30,33	1.70	4 (18%)
22	PSU	23S1	2457	22	18,21,22	4.07	7 (38%)	22,30,33	2.05	5 (22%)
25	MEQ	L031	150	25	8,9,10	1.49	2 (25%)	5,10,12	1.81	2 (40%)
22	1MG	23S1	745	22	18,26,27	2.50	5 (27%)	19,39,42	1.52	4 (21%)
22	PSU	23S1	1917	22	18,21,22	4.13	7 (38%)	22,30,33	1.67	4 (18%)
22	PSU	23S1	1911	22	18,21,22	4.18	7 (38%)	22,30,33	1.89	5 (22%)
22	6MZ	23S1	2030	22	18,25,26	2.88	5 (27%)	16,36,39	2.80	4 (25%)
22	OMC	23S1	2498	56,22	19,22,23	2.73	7 (36%)	26,31,34	1.01	1 (3%)
22	5MU	23S1	747	22	19,22,23	0.78	0	28,32,35	1.21	2 (7%)
22	PSU	23S1	2604	22	18,21,22	4.00	7 (38%)	22,30,33	1.78	5 (22%)
22	2MG	23S1	1835	22	18,26,27	2.29	7 (38%)	16,38,41	1.47	4 (25%)
1	MA6	16S1	1518	1	18,26,27	1.22	1 (5%)	19,38,41	3.13	2 (10%)
55	G7M	PTR1	46	55	20,26,27	2.56	6 (30%)	17,39,42	1.23	3 (17%)
22	3TD	23S1	1915	22	18,22,23	4.10	8 (44%)	22,32,35	1.63	2 (9%)
22	2MG	23S1	2445	22	18,26,27	2.29	7 (38%)	16,38,41	1.49	3 (18%)
22	2MA	23S1	2503	56,22,57	19,25,26	3.25	6 (31%)	21,37,40	1.75	2 (9%)
1	UR3	16S1	1498	1	19,22,23	2.98	8 (42%)	26,32,35	1.39	2 (7%)
53	FME	SPE1	1	53	8,9,10	0.98	0	7,9,11	1.14	1 (14%)
22	6MZ	23S1	1618	22	18,25,26	2.96	4 (22%)	16,36,39	2.10	3 (18%)
22	PSU	23S1	746	56,22	18,21,22	4.04	7 (38%)	22,30,33	1.91	5 (22%)
55	RSP	PTR1	32	55	17,21,22	3.90	6 (35%)	22,30,33	1.15	2 (9%)
55	2MG	PTR1	37	55	18,26,27	2.40	7 (38%)	16,38,41	1.41	4 (25%)
22	OMG	23S1	2251	57,22,55	18,26,27	2.46	8 (44%)	19,38,41	1.99	7 (36%)
22	5MC	23S1	1962	57,22	18,22,23	3.29	7 (38%)	26,32,35	1.03	2 (7%)
22	PSU	23S1	2504	57,22	18,21,22	4.16	7 (38%)	22,30,33	1.74	4 (18%)
22	OMU	23S1	2552	56,22	19,22,23	2.80	7 (36%)	26,31,34	1.83	5 (19%)
1	5MC	16S1	967	1	18,22,23	3.42	7 (38%)	26,32,35	1.04	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	16S1	1407	1	18,22,23	3.38	7 (38%)	26,32,35	1.03	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	23S1	955	22	-	0/7/25/26	0/2/2/2
22	G7M	23S1	2069	57,22	-	2/3/25/26	0/3/3/3
55	5MU	PTR1	54	55	-	2/7/25/26	0/2/2/2
1	MA6	16S1	1519	1	-	2/7/29/30	0/3/3/3
34	4D4	L161	81	34	-	3/11/12/14	-
12	D2T	S121	89	12	-	1/7/12/14	-
1	2MG	16S1	1516	1	-	0/5/27/28	0/3/3/3
55	PSU	PTR1	55	55	-	0/7/25/26	0/2/2/2
1	2MG	16S1	1207	57,1	-	0/5/27/28	0/3/3/3
1	G7M	16S1	527	57,1	-	2/3/25/26	0/3/3/3
22	5MU	23S1	1939	57,22	-	2/7/25/26	0/2/2/2
22	PSU	23S1	2580	57,22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2605	22	-	0/7/25/26	0/2/2/2
55	4SU	PTR1	8	55	-	0/7/25/26	0/2/2/2
1	4OC	16S1	1402	56,1	-	2/9/29/30	0/2/2/2
1	2MG	16S1	966	1	-	2/5/27/28	0/3/3/3
1	PSU	16S1	516	56,1	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2457	22	-	0/7/25/26	0/2/2/2
25	MEQ	L031	150	25	-	2/8/9/11	-
22	1MG	23S1	745	22	-	0/3/25/26	0/3/3/3
22	PSU	23S1	1917	22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	1911	22	-	0/7/25/26	0/2/2/2
22	6MZ	23S1	2030	22	-	2/5/27/28	0/3/3/3
22	OMC	23S1	2498	56,22	-	0/9/27/28	0/2/2/2
22	5MU	23S1	747	22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2604	22	-	0/7/25/26	0/2/2/2
22	2MG	23S1	1835	22	-	0/5/27/28	0/3/3/3
1	MA6	16S1	1518	1	-	0/7/29/30	0/3/3/3
55	G7M	PTR1	46	55	-	1/3/25/26	0/3/3/3
22	3TD	23S1	1915	22	-	0/7/25/26	0/2/2/2
22	2MG	23S1	2445	22	-	2/5/27/28	0/3/3/3
22	2MA	23S1	2503	56,22,57	-	2/3/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	16S1	1498	1	-	0/7/25/26	0/2/2/2
53	FME	SPE1	1	53	-	6/7/9/11	-
22	6MZ	23S1	1618	22	-	0/5/27/28	0/3/3/3
22	PSU	23S1	746	56,22	-	1/7/25/26	0/2/2/2
55	RSP	PTR1	32	55	-	2/7/25/26	0/2/2/2
55	2MG	PTR1	37	55	-	1/5/27/28	0/3/3/3
22	OMG	23S1	2251	57,22,55	-	0/5/27/28	0/3/3/3
22	5MC	23S1	1962	57,22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2504	57,22	-	2/7/25/26	0/2/2/2
22	OMU	23S1	2552	56,22	-	1/9/27/28	0/2/2/2
1	5MC	16S1	967	1	-	0/7/25/26	0/2/2/2
1	5MC	16S1	1407	1	-	0/7/25/26	0/2/2/2

All (248) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	32	RSP	C2-N3	11.95	1.49	1.36
22	23S1	1915	3TD	C6-C5	11.82	1.49	1.35
22	23S1	2504	PSU	C6-C5	11.47	1.48	1.35
22	23S1	1911	PSU	C6-C5	11.22	1.48	1.35
55	PTR1	55	PSU	C6-C5	11.21	1.48	1.35
22	23S1	1618	6MZ	C6-N6	11.16	1.53	1.35
22	23S1	1917	PSU	C6-C5	11.15	1.48	1.35
22	23S1	2457	PSU	C6-C5	11.15	1.48	1.35
22	23S1	2580	PSU	C6-C5	11.07	1.48	1.35
22	23S1	2605	PSU	C6-C5	11.00	1.48	1.35
22	23S1	746	PSU	C6-C5	10.88	1.48	1.35
22	23S1	955	PSU	C6-C5	10.83	1.47	1.35
22	23S1	2604	PSU	C6-C5	10.75	1.47	1.35
22	23S1	2030	6MZ	C6-N6	10.71	1.52	1.35
1	16S1	516	PSU	C6-C5	10.71	1.47	1.35
55	PTR1	55	PSU	C2-N1	9.66	1.49	1.36
22	23S1	1911	PSU	C2-N1	9.47	1.49	1.36
22	23S1	1917	PSU	C2-N1	9.25	1.49	1.36
22	23S1	2580	PSU	C2-N1	9.15	1.49	1.36
1	16S1	516	PSU	C2-N1	9.14	1.49	1.36
22	23S1	2605	PSU	C2-N1	9.11	1.49	1.36
22	23S1	2604	PSU	C2-N1	9.03	1.49	1.36
1	16S1	1407	5MC	C6-C5	9.01	1.49	1.34
22	23S1	2504	PSU	C2-N1	8.98	1.48	1.36
22	23S1	746	PSU	C2-N1	8.92	1.48	1.36
22	23S1	2457	PSU	C2-N1	8.84	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	955	PSU	C2-N1	8.70	1.48	1.36
1	16S1	967	5MC	C6-C5	8.67	1.48	1.34
22	23S1	1962	5MC	C6-C5	8.58	1.48	1.34
22	23S1	1915	3TD	C2-N1	8.46	1.48	1.37
22	23S1	2503	2MA	C4-N3	8.15	1.48	1.35
1	16S1	1498	UR3	C2-N1	7.98	1.50	1.38
55	PTR1	55	PSU	C2-N3	7.20	1.49	1.37
22	23S1	2503	2MA	C2-N3	7.08	1.46	1.34
22	23S1	1911	PSU	C2-N3	6.84	1.49	1.37
55	PTR1	8	4SU	C4-N3	6.79	1.44	1.37
1	16S1	516	PSU	C2-N3	6.76	1.49	1.37
22	23S1	2504	PSU	C2-N3	6.75	1.49	1.37
22	23S1	1917	PSU	C2-N3	6.75	1.49	1.37
22	23S1	955	PSU	C2-N3	6.74	1.49	1.37
22	23S1	2457	PSU	C2-N3	6.64	1.48	1.37
22	23S1	746	PSU	C2-N3	6.61	1.48	1.37
22	23S1	2580	PSU	C2-N3	6.57	1.48	1.37
55	PTR1	8	4SU	C2-N1	6.47	1.48	1.38
22	23S1	2604	PSU	C2-N3	6.44	1.48	1.37
22	23S1	745	1MG	C2-N3	6.40	1.46	1.34
22	23S1	2605	PSU	C2-N3	6.37	1.48	1.37
55	PTR1	8	4SU	C2-N3	6.36	1.49	1.38
1	16S1	967	5MC	C4-N3	6.30	1.44	1.34
22	23S1	2552	OMU	C2-N1	6.27	1.48	1.38
1	16S1	1402	4OC	C4-N3	6.21	1.43	1.32
22	23S1	2552	OMU	C2-N3	6.17	1.49	1.38
34	L161	81	4D4	CZ-NE	6.12	1.45	1.33
22	23S1	2503	2MA	C2-N1	6.04	1.44	1.34
1	16S1	1402	4OC	C6-C5	6.01	1.49	1.35
1	16S1	967	5MC	C2-N3	5.87	1.48	1.36
55	PTR1	32	RSP	C6-C5	5.86	1.48	1.35
22	23S1	1962	5MC	C4-N3	5.84	1.44	1.34
55	PTR1	8	4SU	C6-C5	5.74	1.48	1.35
22	23S1	1962	5MC	C2-N3	5.66	1.47	1.36
1	16S1	1498	UR3	C6-C5	5.63	1.48	1.35
1	16S1	1407	5MC	C4-N3	5.50	1.43	1.34
22	23S1	2498	OMC	C6-C5	5.50	1.47	1.35
1	16S1	1407	5MC	C2-N3	5.47	1.47	1.36
55	PTR1	46	G7M	C2-N3	5.47	1.46	1.33
1	16S1	527	G7M	C2-N3	5.40	1.46	1.33
22	23S1	2498	OMC	C2-N3	5.39	1.47	1.36
1	16S1	1402	4OC	C2-N3	5.34	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	37	2MG	C2-N2	5.19	1.44	1.33
1	16S1	966	2MG	C2-N2	5.18	1.44	1.33
55	PTR1	32	RSP	C4-N4	5.17	1.46	1.33
55	PTR1	46	G7M	C6-N1	5.15	1.45	1.37
22	23S1	2552	OMU	C6-C5	5.14	1.47	1.35
22	23S1	745	1MG	C4-N3	5.10	1.49	1.37
1	16S1	1207	2MG	C2-N2	5.07	1.44	1.33
55	PTR1	55	PSU	C6-N1	5.03	1.44	1.36
22	23S1	1915	3TD	C6-N1	5.03	1.44	1.36
22	23S1	2251	OMG	C2-N3	4.99	1.45	1.33
1	16S1	1516	2MG	C2-N2	4.99	1.44	1.33
22	23S1	2503	2MA	C6-N1	4.96	1.42	1.33
1	16S1	527	G7M	C4-N3	4.93	1.49	1.37
55	PTR1	46	G7M	C4-N3	4.87	1.49	1.37
22	23S1	2445	2MG	C2-N2	4.85	1.44	1.33
22	23S1	1915	3TD	C1'-C5	-4.84	1.39	1.50
1	16S1	1498	UR3	C2-N3	4.82	1.48	1.39
55	PTR1	32	RSP	C4-N3	4.82	1.44	1.34
22	23S1	1835	2MG	C2-N2	4.81	1.44	1.33
22	23S1	1917	PSU	C6-N1	4.78	1.44	1.36
1	16S1	516	PSU	C6-N1	4.78	1.44	1.36
1	16S1	966	2MG	C4-N3	4.77	1.48	1.37
22	23S1	2069	G7M	C2-N3	4.68	1.44	1.33
22	23S1	1911	PSU	C6-N1	4.66	1.44	1.36
22	23S1	2605	PSU	C6-N1	4.64	1.43	1.36
1	16S1	1207	2MG	C4-N3	4.64	1.48	1.37
55	PTR1	37	2MG	C2-N1	4.60	1.44	1.36
1	16S1	1207	2MG	C2-N1	4.58	1.44	1.36
1	16S1	527	G7M	C6-N1	4.57	1.44	1.37
22	23S1	2251	OMG	C4-N3	4.56	1.48	1.37
22	23S1	1915	3TD	C2-N3	4.55	1.48	1.38
1	16S1	1407	5MC	C6-N1	4.55	1.45	1.38
22	23S1	2457	PSU	C6-N1	4.55	1.43	1.36
1	16S1	1516	2MG	C4-N3	4.53	1.48	1.37
1	16S1	966	2MG	C2-N1	4.52	1.43	1.36
22	23S1	2504	PSU	C6-N1	4.49	1.43	1.36
22	23S1	2069	G7M	C4-N3	4.49	1.48	1.37
55	PTR1	37	2MG	C4-N3	4.48	1.48	1.37
22	23S1	745	1MG	C2-N2	4.46	1.42	1.34
22	23S1	2069	G7M	C6-N1	4.46	1.44	1.37
22	23S1	2251	OMG	C2-N2	4.44	1.44	1.34
22	23S1	746	PSU	C6-N1	4.44	1.43	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2604	PSU	C6-N1	4.43	1.43	1.36
22	23S1	955	PSU	C6-N1	4.41	1.43	1.36
22	23S1	1835	2MG	C4-N3	4.39	1.48	1.37
55	PTR1	8	4SU	C5-C4	4.39	1.48	1.42
55	PTR1	8	4SU	C4-S4	-4.37	1.60	1.68
22	23S1	2498	OMC	C2-N1	4.37	1.49	1.40
22	23S1	2498	OMC	C4-N4	4.32	1.44	1.33
22	23S1	2498	OMC	C4-N3	4.31	1.43	1.34
1	16S1	967	5MC	C4-N4	4.27	1.45	1.34
22	23S1	2580	PSU	C6-N1	4.26	1.43	1.36
22	23S1	2445	2MG	C4-N3	4.26	1.47	1.37
1	16S1	1498	UR3	O4-C4	-4.22	1.14	1.23
22	23S1	1835	2MG	C2-N1	4.22	1.43	1.36
1	16S1	967	5MC	C6-N1	4.20	1.45	1.38
1	16S1	1516	2MG	C2-N1	4.18	1.43	1.36
1	16S1	1407	5MC	C4-N4	4.16	1.44	1.34
55	PTR1	46	G7M	C2-N2	4.10	1.43	1.34
22	23S1	1962	5MC	C4-N4	4.05	1.44	1.34
1	16S1	1402	4OC	C4-N4	4.01	1.44	1.35
22	23S1	2445	2MG	C2-N1	3.98	1.43	1.36
1	16S1	527	G7M	C2-N2	3.97	1.43	1.34
22	23S1	1962	5MC	C6-N1	3.93	1.44	1.38
1	16S1	1402	4OC	C2-N1	3.92	1.48	1.40
55	PTR1	55	PSU	C4-N3	3.92	1.46	1.38
1	16S1	967	5MC	C2-N1	3.82	1.48	1.40
1	16S1	1407	5MC	C2-N1	3.80	1.48	1.40
22	23S1	2069	G7M	C2-N2	3.74	1.43	1.34
1	16S1	1402	4OC	O2-C2	-3.70	1.16	1.23
22	23S1	2552	OMU	O4-C4	-3.65	1.17	1.24
55	PTR1	46	G7M	C5-C6	3.63	1.54	1.45
22	23S1	2504	PSU	C4-N3	3.58	1.45	1.38
22	23S1	1911	PSU	C4-N3	3.55	1.45	1.38
55	PTR1	32	RSP	C6-N1	3.54	1.46	1.38
22	23S1	1917	PSU	C4-N3	3.54	1.45	1.38
1	16S1	516	PSU	C4-N3	3.50	1.45	1.38
22	23S1	955	PSU	C4-N3	3.48	1.45	1.38
1	16S1	1402	4OC	C5-C4	3.47	1.48	1.40
1	16S1	527	G7M	C5-C6	3.44	1.54	1.45
22	23S1	746	PSU	C4-N3	3.39	1.45	1.38
22	23S1	1962	5MC	C2-N1	3.38	1.47	1.40
22	23S1	2552	OMU	C4-N3	3.34	1.44	1.38
55	PTR1	37	2MG	C6-N1	3.34	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	2604	PSU	C4-N3	3.28	1.44	1.38
22	23S1	2580	PSU	C4-N3	3.27	1.44	1.38
22	23S1	2457	PSU	C4-N3	3.25	1.44	1.38
22	23S1	2445	2MG	C5-C4	-3.25	1.34	1.43
22	23S1	2498	OMC	O2-C2	-3.24	1.17	1.23
22	23S1	2605	PSU	C4-N3	3.23	1.44	1.38
1	16S1	966	2MG	C6-N1	3.23	1.42	1.37
34	L161	81	4D4	CZ-NH2	3.18	1.45	1.32
22	23S1	2069	G7M	C5-C6	3.15	1.53	1.45
1	16S1	1519	MA6	C5-C4	-3.15	1.32	1.40
55	PTR1	32	RSP	C2-S2	-3.15	1.59	1.67
1	16S1	1207	2MG	C6-N1	3.14	1.42	1.37
1	16S1	1516	2MG	C5-C4	-3.11	1.35	1.43
22	23S1	2251	OMG	C5-C4	-3.10	1.35	1.43
22	23S1	1618	6MZ	C2-N3	3.10	1.37	1.32
1	16S1	1407	5MC	O2-C2	-3.08	1.18	1.23
22	23S1	1962	5MC	O2-C2	-3.07	1.18	1.23
22	23S1	1835	2MG	C5-C4	-3.06	1.35	1.43
1	16S1	1516	2MG	C6-N1	3.04	1.42	1.37
22	23S1	745	1MG	C5-C4	-3.04	1.35	1.43
1	16S1	1207	2MG	C5-C6	3.04	1.53	1.47
1	16S1	1518	MA6	C5-C4	-3.04	1.32	1.40
1	16S1	1402	4OC	C6-N1	3.02	1.45	1.38
22	23S1	2030	6MZ	C2-N3	3.02	1.37	1.32
22	23S1	1835	2MG	C6-N1	3.01	1.42	1.37
22	23S1	2498	OMC	C6-N1	2.98	1.45	1.38
22	23S1	2552	OMU	O2-C2	-2.95	1.17	1.23
55	PTR1	37	2MG	C5-C4	-2.93	1.35	1.43
1	16S1	1498	UR3	O2-C2	-2.92	1.17	1.22
25	L031	150	MEQ	OE1-CD	-2.91	1.17	1.23
22	23S1	2251	OMG	C6-N1	2.91	1.42	1.37
55	PTR1	54	5MU	C2-N1	2.89	1.43	1.38
1	16S1	1498	UR3	C5-C4	2.88	1.51	1.43
55	PTR1	8	4SU	C6-N1	2.87	1.44	1.38
1	16S1	966	2MG	C5-C4	-2.87	1.35	1.43
22	23S1	2445	2MG	O6-C6	-2.86	1.17	1.23
22	23S1	2503	2MA	C6-C5	2.84	1.53	1.43
1	16S1	967	5MC	O2-C2	-2.82	1.18	1.23
1	16S1	1207	2MG	C5-C4	-2.82	1.35	1.43
55	PTR1	46	G7M	C2-N1	2.80	1.44	1.37
22	23S1	2251	OMG	O6-C6	-2.76	1.17	1.23
22	23S1	1835	2MG	O6-C6	-2.76	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	37	2MG	C5-C6	2.74	1.53	1.47
22	23S1	2251	OMG	C5-C6	2.73	1.53	1.47
22	23S1	2445	2MG	C5-C6	2.71	1.52	1.47
22	23S1	2445	2MG	C6-N1	2.70	1.41	1.37
22	23S1	2580	PSU	O4-C4	-2.66	1.18	1.23
22	23S1	2580	PSU	O4'-C1'	-2.64	1.40	1.43
22	23S1	745	1MG	O6-C6	-2.63	1.17	1.22
1	16S1	1516	2MG	O6-C6	-2.62	1.18	1.23
1	16S1	966	2MG	C5-C6	2.61	1.52	1.47
22	23S1	1618	6MZ	C5-C4	-2.61	1.34	1.40
22	23S1	2457	PSU	O4-C4	-2.61	1.18	1.23
1	16S1	966	2MG	O6-C6	-2.59	1.18	1.23
55	PTR1	8	4SU	O2-C2	-2.58	1.18	1.23
22	23S1	2030	6MZ	C5-C4	-2.58	1.34	1.40
1	16S1	1516	2MG	C5-C6	2.58	1.52	1.47
22	23S1	1618	6MZ	C9-N6	2.54	1.49	1.45
22	23S1	2604	PSU	O4-C4	-2.54	1.18	1.23
1	16S1	1207	2MG	O6-C6	-2.50	1.18	1.23
22	23S1	955	PSU	O4-C4	-2.50	1.18	1.23
1	16S1	527	G7M	C2-N1	2.49	1.43	1.37
1	16S1	1498	UR3	C6-N1	2.48	1.44	1.38
22	23S1	2030	6MZ	C9-N6	2.47	1.49	1.45
22	23S1	1835	2MG	C5-C6	2.47	1.52	1.47
22	23S1	1915	3TD	O2-C2	-2.47	1.18	1.23
22	23S1	2552	OMU	C6-N1	2.46	1.43	1.38
22	23S1	746	PSU	O4-C4	-2.44	1.18	1.23
22	23S1	2504	PSU	C1'-C5	2.43	1.55	1.50
22	23S1	2605	PSU	O4-C4	-2.43	1.19	1.23
22	23S1	2069	G7M	C2-N1	2.43	1.43	1.37
22	23S1	2503	2MA	C6-N6	-2.41	1.25	1.34
22	23S1	1911	PSU	O4-C4	-2.39	1.19	1.23
34	L161	81	4D4	CZ-NH1	-2.38	1.25	1.34
22	23S1	1915	3TD	C4-N3	2.37	1.45	1.40
22	23S1	2251	OMG	C2-N1	2.36	1.43	1.37
22	23S1	2504	PSU	O4-C4	-2.35	1.19	1.23
55	PTR1	55	PSU	C1'-C5	2.33	1.55	1.50
25	L031	150	MEQ	CD-NE2	2.29	1.45	1.34
1	16S1	516	PSU	O4-C4	-2.28	1.19	1.23
55	PTR1	37	2MG	O6-C6	-2.27	1.18	1.23
22	23S1	746	PSU	O4'-C1'	-2.24	1.40	1.43
1	16S1	1498	UR3	C3U-N3	-2.22	1.43	1.47
55	PTR1	54	5MU	C2-N3	2.22	1.41	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1915	3TD	O4-C4	-2.21	1.18	1.23
22	23S1	1917	PSU	C1'-C5	2.18	1.55	1.50
1	16S1	516	PSU	O4'-C1'	-2.17	1.40	1.43
1	16S1	516	PSU	C1'-C5	2.14	1.55	1.50
22	23S1	955	PSU	C1'-C5	2.12	1.55	1.50
55	PTR1	55	PSU	O4-C4	-2.11	1.19	1.23
22	23S1	2457	PSU	C1'-C5	2.09	1.55	1.50
22	23S1	2030	6MZ	C5-N7	-2.08	1.32	1.39
22	23S1	1911	PSU	C1'-C5	2.08	1.55	1.50
22	23S1	1917	PSU	O4-C4	-2.05	1.19	1.23
22	23S1	2605	PSU	C1'-C5	2.01	1.54	1.50
22	23S1	2604	PSU	C1'-C5	2.01	1.54	1.50

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1519	MA6	N1-C6-N6	-12.83	103.56	117.06
1	16S1	1518	MA6	N1-C6-N6	-11.96	104.47	117.06
22	23S1	2030	6MZ	C9-N6-C6	-7.25	116.63	122.87
22	23S1	2503	2MA	C2-N3-C4	6.28	120.62	115.52
1	16S1	1518	MA6	N3-C2-N1	-6.07	119.19	128.68
1	16S1	1519	MA6	N3-C2-N1	-6.07	119.20	128.68
22	23S1	1618	6MZ	N3-C2-N1	-5.98	119.33	128.68
22	23S1	2552	OMU	C4-N3-C2	-5.81	118.92	126.58
22	23S1	2030	6MZ	N3-C2-N1	-5.78	119.64	128.68
55	PTR1	8	4SU	C4-N3-C2	-5.33	122.17	127.34
22	23S1	1915	3TD	N1-C2-N3	5.26	120.29	116.14
1	16S1	1498	UR3	C4-N3-C2	-5.22	119.65	124.56
22	23S1	2457	PSU	N1-C2-N3	4.97	120.76	115.13
22	23S1	2457	PSU	C4-N3-C2	-4.93	119.24	126.34
22	23S1	2030	6MZ	C2-N1-C6	4.89	120.79	116.59
22	23S1	955	PSU	C4-N3-C2	-4.87	119.32	126.34
22	23S1	1911	PSU	C4-N3-C2	-4.79	119.44	126.34
22	23S1	746	PSU	C4-N3-C2	-4.78	119.45	126.34
22	23S1	2580	PSU	N1-C2-N3	4.78	120.54	115.13
22	23S1	955	PSU	N1-C2-N3	4.68	120.43	115.13
55	PTR1	55	PSU	C4-N3-C2	-4.61	119.70	126.34
22	23S1	2605	PSU	C4-N3-C2	-4.58	119.75	126.34
22	23S1	746	PSU	N1-C2-N3	4.57	120.31	115.13
22	23S1	2580	PSU	C4-N3-C2	-4.57	119.75	126.34
22	23S1	2504	PSU	C4-N3-C2	-4.47	119.90	126.34
22	23S1	1911	PSU	N1-C2-N3	4.46	120.18	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2605	PSU	N1-C2-N3	4.44	120.16	115.13
22	23S1	745	1MG	C5-C6-N1	4.38	120.48	113.90
22	23S1	2604	PSU	C4-N3-C2	-4.36	120.06	126.34
22	23S1	2604	PSU	N1-C2-N3	4.23	119.92	115.13
22	23S1	2504	PSU	N1-C2-N3	4.22	119.91	115.13
1	16S1	516	PSU	C4-N3-C2	-4.16	120.35	126.34
55	PTR1	8	4SU	C5-C4-N3	4.07	118.47	114.69
22	23S1	1915	3TD	C4-N3-C2	-3.98	120.29	124.61
22	23S1	2552	OMU	N3-C2-N1	3.98	120.17	114.89
22	23S1	1618	6MZ	C2-N1-C6	3.96	119.99	116.59
12	S121	89	D2T	CB1-SB-CB	3.95	109.58	102.44
22	23S1	1917	PSU	C4-N3-C2	-3.93	120.68	126.34
55	PTR1	55	PSU	N1-C2-N3	3.93	119.58	115.13
22	23S1	2251	OMG	C5-C6-N1	3.83	120.72	113.95
22	23S1	1917	PSU	N1-C2-N3	3.81	119.45	115.13
22	23S1	2552	OMU	C5-C4-N3	3.80	120.53	114.84
1	16S1	516	PSU	N1-C2-N3	3.74	119.36	115.13
1	16S1	1516	2MG	C5-C6-N1	3.72	120.53	113.95
22	23S1	2445	2MG	C5-C6-N1	3.66	120.42	113.95
1	16S1	966	2MG	C5-C6-N1	3.60	120.32	113.95
1	16S1	1207	2MG	C5-C6-N1	3.54	120.21	113.95
22	23S1	2580	PSU	C6-N1-C2	-3.50	119.11	122.68
25	L031	150	MEQ	CG-CD-NE2	3.48	121.12	116.29
22	23S1	2580	PSU	C6-C5-C4	3.48	120.63	118.20
22	23S1	2251	OMG	O3'-C3'-C2'	3.46	120.98	111.17
22	23S1	1835	2MG	C5-C6-N1	3.44	120.02	113.95
22	23S1	1618	6MZ	C9-N6-C6	-3.43	119.92	122.87
1	16S1	967	5MC	C5-C6-N1	-3.39	119.86	123.34
22	23S1	2251	OMG	C2-N1-C6	-3.32	118.99	125.10
55	PTR1	37	2MG	C5-C6-N1	3.26	119.71	113.95
22	23S1	2457	PSU	C6-C5-C4	3.26	120.48	118.20
22	23S1	2457	PSU	C6-N1-C2	-3.25	119.36	122.68
55	PTR1	32	RSP	S2-C2-N3	-3.14	116.04	121.49
55	PTR1	8	4SU	N3-C2-N1	3.13	119.04	114.89
22	23S1	747	5MU	C6-C5-C4	3.11	120.63	118.03
22	23S1	1917	PSU	C6-N1-C2	-3.11	119.51	122.68
22	23S1	746	PSU	C6-N1-C2	-3.11	119.51	122.68
22	23S1	2503	2MA	N3-C2-N1	-3.10	120.06	125.73
55	PTR1	54	5MU	C4-N3-C2	-3.09	123.35	127.35
22	23S1	955	PSU	C6-N1-C2	-3.09	119.53	122.68
22	23S1	1939	5MU	C4-N3-C2	-3.08	123.36	127.35
22	23S1	1939	5MU	C6-C5-C4	3.04	120.57	118.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2605	PSU	C6-N1-C2	-3.02	119.59	122.68
1	16S1	1402	4OC	O2-C2-N3	-3.02	117.41	122.33
22	23S1	2030	6MZ	C1'-N9-C4	-3.02	121.33	126.64
22	23S1	955	PSU	O2-C2-N1	-3.01	119.47	122.79
22	23S1	746	PSU	C6-C5-C4	3.00	120.30	118.20
22	23S1	2552	OMU	O4-C4-C5	-3.00	119.89	125.16
22	23S1	1911	PSU	C6-N1-C2	-2.97	119.64	122.68
22	23S1	1962	5MC	C5-C6-N1	-2.96	120.30	123.34
1	16S1	516	PSU	C6-N1-C2	-2.94	119.68	122.68
22	23S1	747	5MU	C4-N3-C2	-2.92	123.57	127.35
22	23S1	1962	5MC	CM5-C5-C6	-2.91	118.97	122.85
22	23S1	2069	G7M	N2-C2-N1	2.90	122.88	116.71
22	23S1	2604	PSU	C6-N1-C2	-2.89	119.73	122.68
22	23S1	2498	OMC	O2-C2-N3	-2.88	117.65	122.33
12	S121	89	D2T	OD2-CG-CB	2.85	119.30	113.15
22	23S1	2504	PSU	C6-N1-C2	-2.84	119.78	122.68
22	23S1	2457	PSU	O2-C2-N1	-2.82	119.68	122.79
22	23S1	2251	OMG	C8-N7-C5	2.81	108.35	102.99
22	23S1	1835	2MG	CM2-N2-C2	-2.81	117.66	123.86
22	23S1	746	PSU	O2-C2-N1	-2.81	119.70	122.79
22	23S1	745	1MG	C8-N7-C5	2.80	108.33	102.99
22	23S1	2605	PSU	C6-C5-C4	2.77	120.14	118.20
55	PTR1	37	2MG	CM2-N2-C2	-2.77	117.75	123.86
22	23S1	2445	2MG	CM2-N2-C2	-2.75	117.80	123.86
22	23S1	1911	PSU	C6-C5-C4	2.72	120.10	118.20
1	16S1	527	G7M	C2-N1-C6	-2.72	120.09	125.10
22	23S1	2251	OMG	O3'-C3'-C4'	2.72	118.91	111.05
55	PTR1	46	G7M	C2-N1-C6	-2.69	120.15	125.10
22	23S1	2580	PSU	O2-C2-N1	-2.64	119.88	122.79
22	23S1	2445	2MG	C8-N7-C5	2.64	108.01	102.99
1	16S1	1207	2MG	C8-N7-C5	2.60	107.94	102.99
55	PTR1	55	PSU	C6-N1-C2	-2.59	120.03	122.68
22	23S1	1917	PSU	C6-C5-C4	2.58	120.00	118.20
1	16S1	1516	2MG	C8-N7-C5	2.58	107.90	102.99
1	16S1	966	2MG	C8-N7-C5	2.57	107.88	102.99
55	PTR1	32	RSP	C1'-N1-C2	2.56	124.11	118.44
22	23S1	2069	G7M	C2-N1-C6	-2.56	120.38	125.10
1	16S1	966	2MG	CM2-N2-C2	-2.55	118.22	123.86
22	23S1	1835	2MG	C8-N7-C5	2.54	107.83	102.99
1	16S1	1407	5MC	C5-C6-N1	-2.53	120.74	123.34
22	23S1	2604	PSU	C6-C5-C4	2.52	119.96	118.20
55	PTR1	37	2MG	C8-N7-C5	2.50	107.76	102.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	516	PSU	C6-C5-C4	2.49	119.94	118.20
22	23S1	1911	PSU	O2-C2-N1	-2.45	120.09	122.79
55	PTR1	55	PSU	O2-C2-N1	-2.44	120.11	122.79
22	23S1	1939	5MU	C5-C6-N1	-2.43	120.84	123.34
1	16S1	966	2MG	O6-C6-C5	-2.41	119.67	124.37
55	PTR1	46	G7M	N2-C2-N1	2.40	121.82	116.71
1	16S1	1516	2MG	O6-C6-C5	-2.39	119.70	124.37
22	23S1	955	PSU	C6-C5-C4	2.39	119.87	118.20
53	SPE1	1	FME	C-CA-N	2.39	114.04	109.73
22	23S1	2251	OMG	O6-C6-C5	-2.38	119.71	124.37
22	23S1	2580	PSU	O4'-C1'-C2'	2.38	108.50	105.14
22	23S1	2504	PSU	O2-C2-N1	-2.37	120.19	122.79
55	PTR1	54	5MU	C6-C5-C4	2.35	120.00	118.03
22	23S1	2251	OMG	C3'-C2'-C1'	-2.35	98.47	102.89
22	23S1	1835	2MG	O6-C6-C5	-2.33	119.83	124.37
1	16S1	1498	UR3	C6-N1-C2	-2.29	119.73	121.79
1	16S1	967	5MC	CM5-C5-C6	-2.29	119.78	122.85
1	16S1	1207	2MG	CM2-N2-C2	-2.27	118.84	123.86
1	16S1	1516	2MG	CM2-N2-C2	-2.26	118.87	123.86
22	23S1	745	1MG	O6-C6-C5	-2.26	120.20	124.19
55	PTR1	55	PSU	C6-C5-C4	2.22	119.75	118.20
1	16S1	1407	5MC	O2-C2-N3	-2.21	118.74	122.33
55	PTR1	37	2MG	O6-C6-C5	-2.20	120.07	124.37
1	16S1	1402	4OC	C6-C5-C4	2.19	119.64	116.96
55	PTR1	54	5MU	C5M-C5-C6	-2.16	119.96	122.85
55	PTR1	54	5MU	C5-C4-N3	2.14	117.14	115.31
1	16S1	1407	5MC	C5-C4-N3	-2.14	119.37	121.67
22	23S1	2604	PSU	O2-C2-N1	-2.14	120.44	122.79
22	23S1	2069	G7M	N1-C2-N3	-2.13	119.34	123.32
34	L161	81	4D4	CG-CD-NE	-2.13	105.73	111.87
1	16S1	527	G7M	N2-C2-N1	2.11	121.21	116.71
22	23S1	745	1MG	CM1-N1-C6	2.09	120.41	117.55
22	23S1	2552	OMU	O2-C2-N1	-2.07	120.04	122.79
55	PTR1	46	G7M	N1-C2-N3	-2.05	119.48	123.32
55	PTR1	8	4SU	C5-C4-S4	-2.02	121.87	124.47
25	L031	150	MEQ	OE1-CD-CG	-2.01	118.33	122.02
22	23S1	2605	PSU	O2-C2-N1	-2.00	120.58	122.79

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16S1	527	G7M	O4'-C4'-C5'-O5'
1	16S1	527	G7M	C3'-C4'-C5'-O5'
1	16S1	966	2MG	O4'-C4'-C5'-O5'
1	16S1	1519	MA6	O4'-C4'-C5'-O5'
25	L031	150	MEQ	N-CA-CB-CG
25	L031	150	MEQ	C-CA-CB-CG
53	SPE1	1	FME	CB-CA-N-CN
53	SPE1	1	FME	C-CA-CB-CG
53	SPE1	1	FME	O-C-CA-CB
22	23S1	2030	6MZ	O4'-C4'-C5'-O5'
55	PTR1	32	RSP	C3'-C4'-C5'-O5'
55	PTR1	54	5MU	C3'-C4'-C5'-O5'
53	SPE1	1	FME	CA-CB-CG-SD
1	16S1	966	2MG	C3'-C4'-C5'-O5'
22	23S1	2030	6MZ	C3'-C4'-C5'-O5'
22	23S1	2504	PSU	O4'-C4'-C5'-O5'
1	16S1	1402	4OC	O4'-C4'-C5'-O5'
1	16S1	1519	MA6	C3'-C4'-C5'-O5'
22	23S1	2504	PSU	C3'-C4'-C5'-O5'
53	SPE1	1	FME	CB-CG-SD-CE
53	SPE1	1	FME	N-CA-CB-CG
55	PTR1	32	RSP	O4'-C4'-C5'-O5'
55	PTR1	54	5MU	O4'-C4'-C5'-O5'
22	23S1	2445	2MG	C3'-C4'-C5'-O5'
34	L161	81	4D4	OB-CB-CG-CD
22	23S1	1939	5MU	O4'-C4'-C5'-O5'
12	S121	89	D2T	CG-CB-SB-CB1
55	PTR1	46	G7M	C4'-C5'-O5'-P
1	16S1	1402	4OC	C3'-C4'-C5'-O5'
22	23S1	1939	5MU	C3'-C4'-C5'-O5'
34	L161	81	4D4	CA-CB-CG-CD
22	23S1	2069	G7M	C4'-C5'-O5'-P
22	23S1	2503	2MA	O4'-C4'-C5'-O5'
22	23S1	2445	2MG	O4'-C4'-C5'-O5'
22	23S1	2552	OMU	C3'-C2'-O2'-CM2
34	L161	81	4D4	CG-CD-NE-CZ
22	23S1	2503	2MA	C4'-C5'-O5'-P
22	23S1	2069	G7M	O4'-C4'-C5'-O5'
22	23S1	746	PSU	O4'-C1'-C5'-C6
55	PTR1	37	2MG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1691 ligands modelled in this entry, 489 are monoatomic and 1201 are unknown - 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	$\# Z > 2$
60	ORN	23S1	3001	-	7,8,8	0.78	0	8,9,9	0.71	0

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
60	ORN	23S1	3001	-	-	2/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	23S1	3001	ORN	N-CA-CB-CG
60	23S1	3001	ORN	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	23S1	2
55	PTR1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	23S1	885:C	O3'	892:A	P	13.18
1	PTR1	46:G7M	O3'	48:C	P	5.16
1	23S1	2099:U	O3'	2100:G	P	4.33